



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 08:49 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

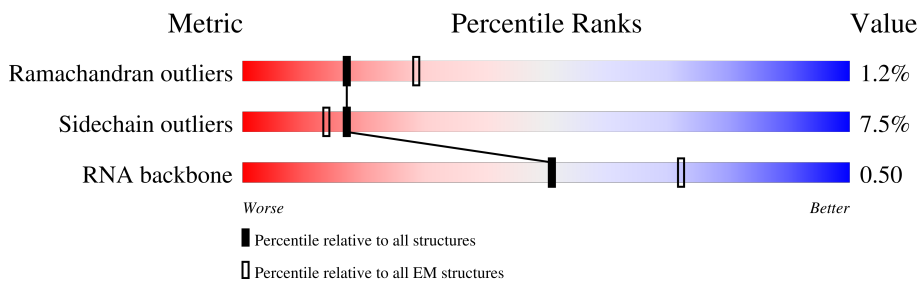
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	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	69% 54% 33% 10%
10	A	76	41% 58% 38%
10	B	76	43% 46% 49% 5%
11	AA	1342	100% 99%
12	AB	181	77% 67% 18% 10%
13	AC	329	91% 90% 9%
13	AD	329	91% 91% 9%
14	AE	1407	95% 89% 5% 5%
15	AF	91	90% 90% 10%
16	AG	495	74% 69% 27%
17	C	75	8% 85% 12%
18	D	1542	78% 20%
19	E	87	7% 93% 6%
20	F	71	17% 94%
21	G	241	6% 90% 7%
22	H	557	46% 41% 54%
23	I	233	5% 86% 11%
24	J	206	96%
25	K	167	88% 5% 7%
26	L	135	6% 72% 23%
27	M	179	9% 80% 16%
28	N	130	97%
29	O	130	5% 93% 5%
30	P	103	17% 87% 9%
31	Q	129	87% 9%

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Mol	Chain	Length	Quality of chain
32	R	124	5% 92% 6%
33	S	101	95%
34	T	89	85% 13%
35	U	82	93% 7%
36	V	84	93% 5%
37	W	92	53% 86% 10%
38	X	118	67% 88% 10%
39	Y	142	87% 68% 27%
40	Z	121	25% 12% 12% 75%
41	a	2904	29% 81% 18%
42	b	85	52% 88% 11%
43	c	78	77% 94% 5%
44	d	120	12% 86% 14%
45	e	63	59% 97%
46	f	59	64% 95%
47	g	70	63% 86% 9% 6%
48	h	273	66% 93% 7%
49	i	57	61% 88% 11%
50	j	209	69% 97%
51	k	55	53% 89% 5% 5%
52	l	201	67% 93% 7%
53	m	46	72% 93% 7%
54	n	179	51% 89% 10%
55	o	65	66% 91% 8%
56	p	177	55% 97%

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Mol	Chain	Length	Quality of chain
57	q	38	<p>66% 95% 5%</p>
58	r	149	<p>72% 93% 7%</p>
59	s	142	<p>68% 96% .</p>
60	t	123	<p>71% 95% 5%</p>
61	u	144	<p>72% 96% .</p>
62	v	136	<p>61% 96% .</p>
63	w	127	<p>65% 87% 6% 6%</p>
64	x	117	<p>52% 94% 5% .</p>
65	y	115	<p>64% 95% . .</p>
66	z	118	<p>70% 97% . .</p>

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	
			Total	C	H	N	O			S
1	0	103	1655	516	839	153	145	2	0	0

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

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

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

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

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

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

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

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

- Molecule 6 is a DNA chain called NT DNA.

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

- Molecule 7 is a DNA chain called T DNA.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	7	33	784	307	97	96	251	33	0	0

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	deletion	GB 1837817527
B	?	-	U	deletion	GB 1837817527

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AA	1340	10567	6631	1841	2052	43	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AC	301	Total	C	N	O	S	0	0
			2094	1296	379	413	6		
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
			Total	C	H	N	O	S		
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	variant	UNP A0A4S1NBU2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AF	82	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
			Total	C	N	O	S		
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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	P		
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	
			Total	C	H	N	O			S
19	E	86	1388	414	719	138	114	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

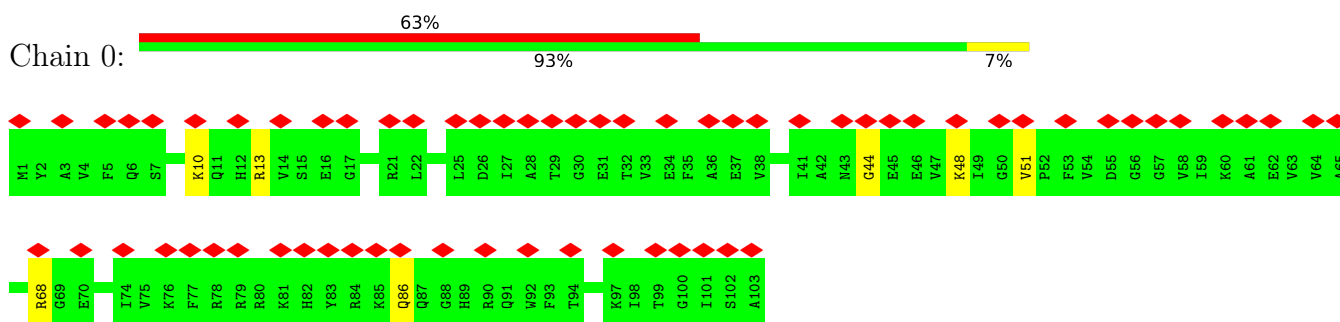
- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

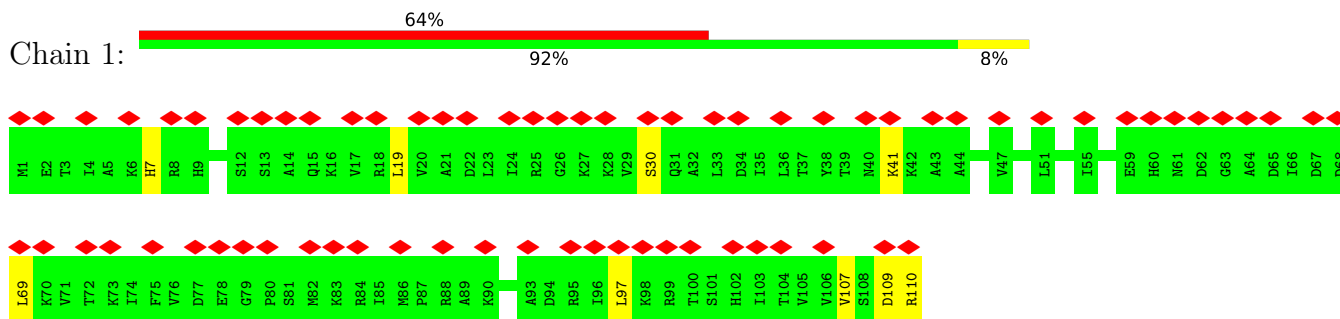
3 Residue-property plots [i](#)

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

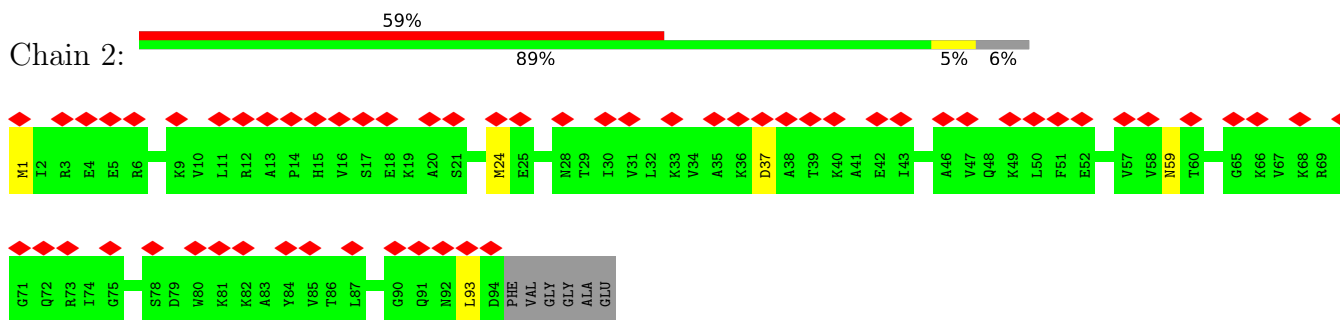
- Molecule 1: 50S ribosomal protein L21



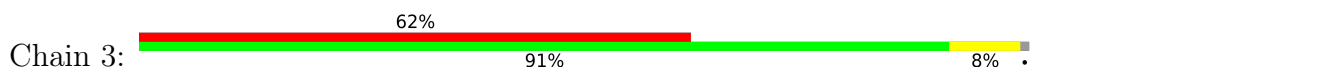
- Molecule 2: 50S ribosomal protein L22

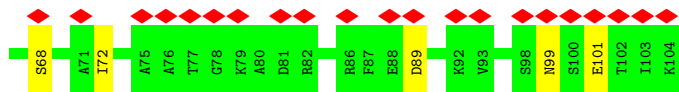
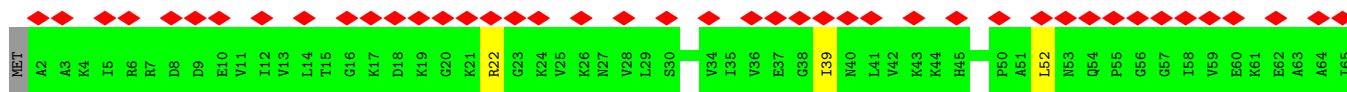


- Molecule 3: 50S ribosomal protein L23

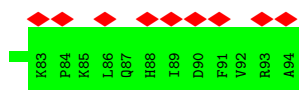
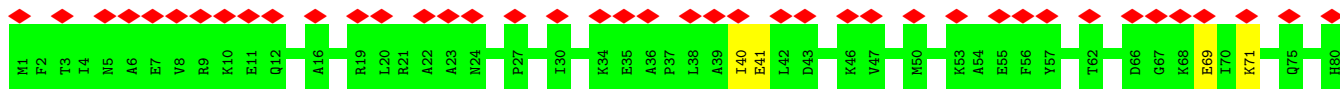


- Molecule 4: 50S ribosomal protein L24

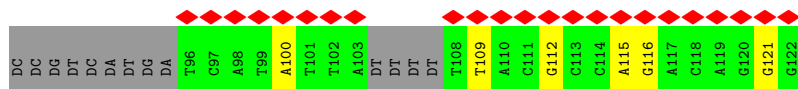




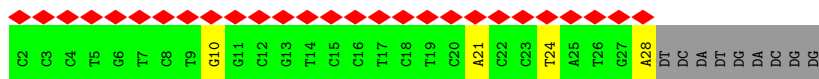
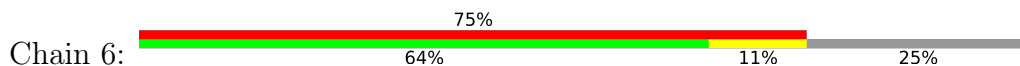
• Molecule 5: 50S ribosomal protein L25



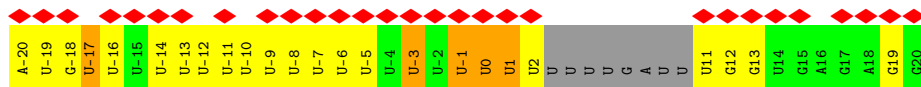
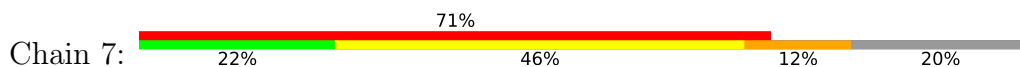
• Molecule 6: NT DNA



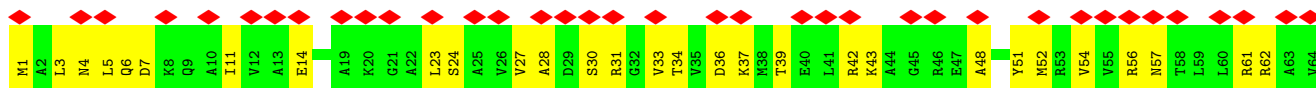
• Molecule 7: T DNA

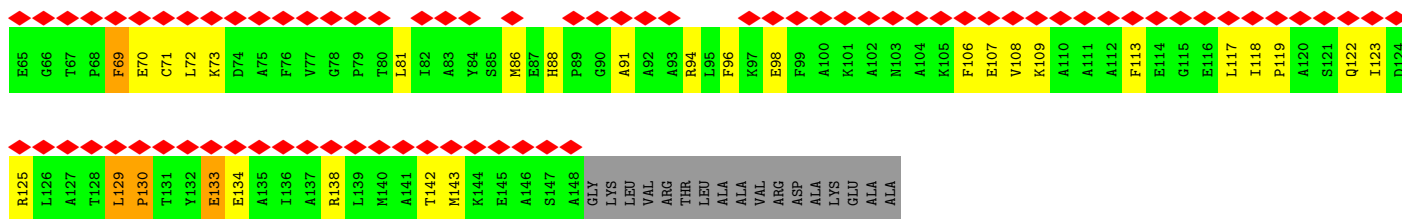


• Molecule 8: mRNA with 24 nt long spacer

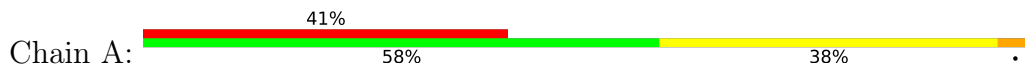


• Molecule 9: 50S ribosomal protein L10

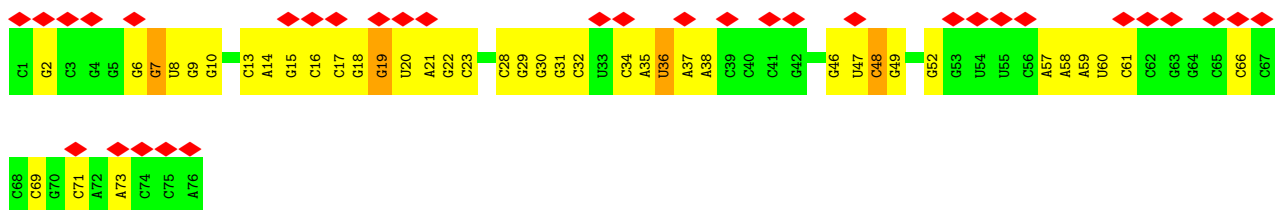
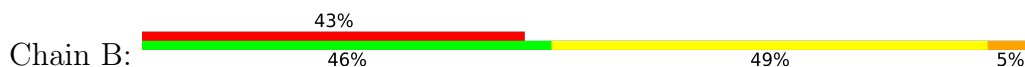




• Molecule 10: E-site and P-site tRNA (fMet)



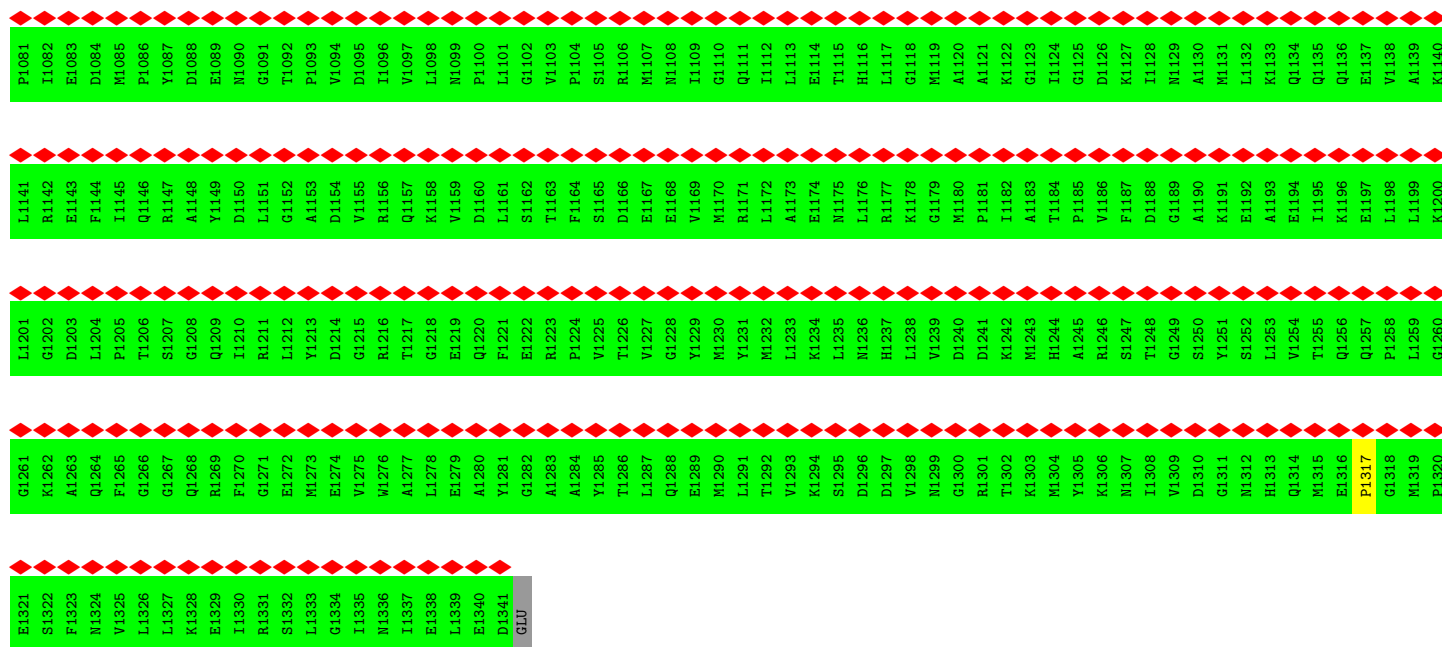
• Molecule 10: E-site and P-site tRNA (fMet)



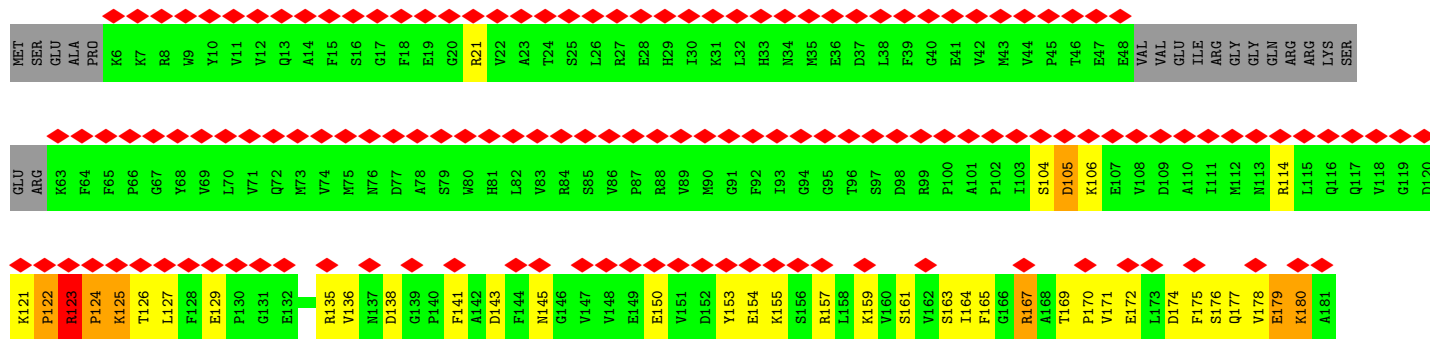
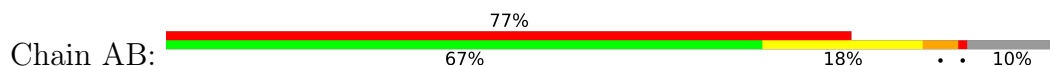
• Molecule 11: DNA-directed RNA polymerase subunit beta



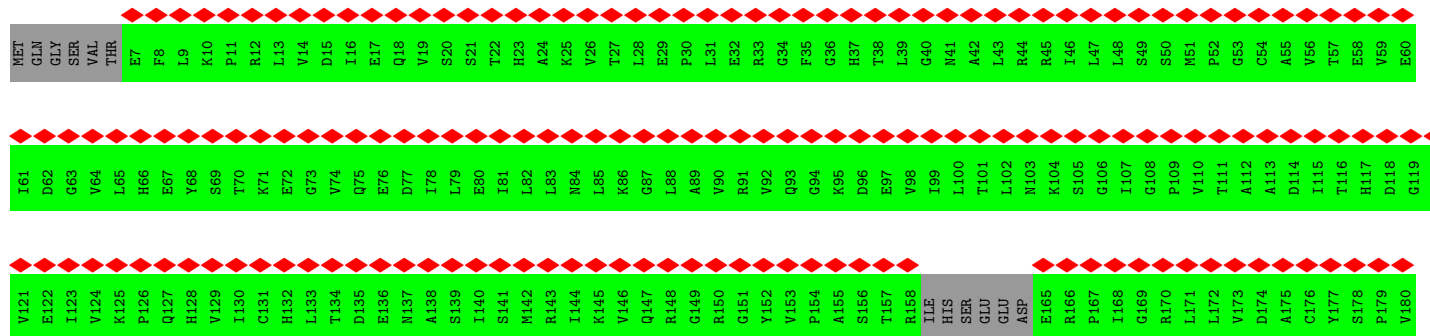
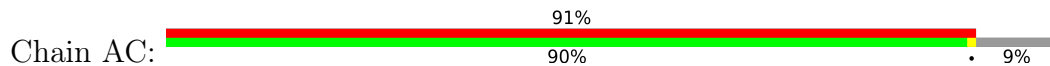
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E1024	L964	K844	A784	V724	G664	H604	G544	L484	D424	V364	E304
F1025	Q965	L845	D785	V725	A665	Y605	F545	D485	I425	E365	S305
E1026	F906	G846	G786	Q726	S666	L606	E546	T486	I426	I366	T306
K1027	G907	P847	P787	V727	L667	S607	V547	L487	D427	Y367	G307
K1028	E908	E848	S788	D728	1668	A608	R548	M488	V428	R368	E308
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E1030	A910	T850	D790	S730	F670	E610	V550	Q490	K430	M370	I310
A1031	S911	T851	L791	R731	L671	E611	H551	D491	K431	R371	C311
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T1037	S917	V857	G797	M737	N677	A617	R557	P497	R437	T377	L317
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G1039	R919	E859	M799	D739	A679	A619	C559	S499	K439	E379	L319
D1040	V920	A860	H800	E740	L680	N620	P560	A500	G440	A380	D320
D1041	A921	A861	R801	M741	M681	S621	I561	A501	E441	A381	L321
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E985	S925	L865	M805	E745	M685	E625	E565	F505	I445	F385	L325
G1046	G926	D866	P806	A746	Q686	E626	G566	F506	D446	E386	S326
V1047	T927	E867	M807	G747	R687	G627	P567	F507	H447	N387	Q327
K1048	V928	S868	N808	I748	Q688	H628	N568	S508	L448	L388	S328
I1049	R929	G869	G809	D749	A689	F629	I569	S509	G449	F389	G329
V1050	D930	L870	Y810	I750	V690	V630	G570	Q510	N450	F390	H330
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Y1053	R933	E873	E813	L753	L693	L633	N573	Q513	I453	D393	I333
L1054	F934	G874	D814	T754	R694	V634	S574	F514	R454	R394	E334
A1055	T935	A875	S815	K755	A695	T635	L575	S455	S455	Y395	T335
V1056	R936	E876	L816	Y756	D696	G636	S576	V456	V456	D396	L336
K1057	D937	V877	L817	T757	K697	R637	V577	G457	G457	L397	F337
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R1059	V939	G879	S819	S759	L699	K639	A579	N519	M459	A399	N339
I1060	E940	G880	E820	N760	V700	G640	Q580	P520	A460	V400	D340
Q1061	D941	D881	R821	Q761	G701	E641	T581	L521	E461	G401	L341
L1062	D942	L882	V822	N762	T702	S642	N582	S522	R402	R402	D342
G1063	K943	L883	W823	T763	G703	S643	E583	E523	Q463	M403	H343
D1064	R944	H884	Q824	C764	M704	L644	Y584	I524	F464	K404	G344
E1065	A945	G885	E825	I765	E705	F645	G585	T525	R465	F405	P345
M1066	L946	K886	D826	N766	R706	S646	G586	H526	V466	N406	P346
A1067	E947	V887	R827	Q767	A707	R647	L587	K527	G467	R407	I347
Q1068	I948	T888	F828	M768	V708	D648	E588	R528	L468	S408	S348
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G1071	M951	G891	L831	V771	D711	D651	Y591	S531	V471	R411	L351
K1072	Q952	E892	H832	S772	S712	Y652	R592	A532	E472	E412	R352
L1073	L953	T893	L833	L773	G713	M653	K593	L533	R473	E413	V353
G1074	K954	D894	Q834	G774	V714	D654	Y594	G534	A474	I414	D354
V1075	Q955	L895	E835	E775	T715	V655	T595	P535	V475	E415	P355
I1076	A956	T896	L836	P776	A716	S656	D596	G536	K476	G416	T356
S1077	K957	P897	A837	V777	V717	T657	G597	G537	E477	S417	N357
K1078	I958	E898	C838	E778	A718	Q658	V598	L538	R478	G418	D358
I1079	D959	E899	W839	R779	K719	Q659	V599	T539	L479	I419	R359
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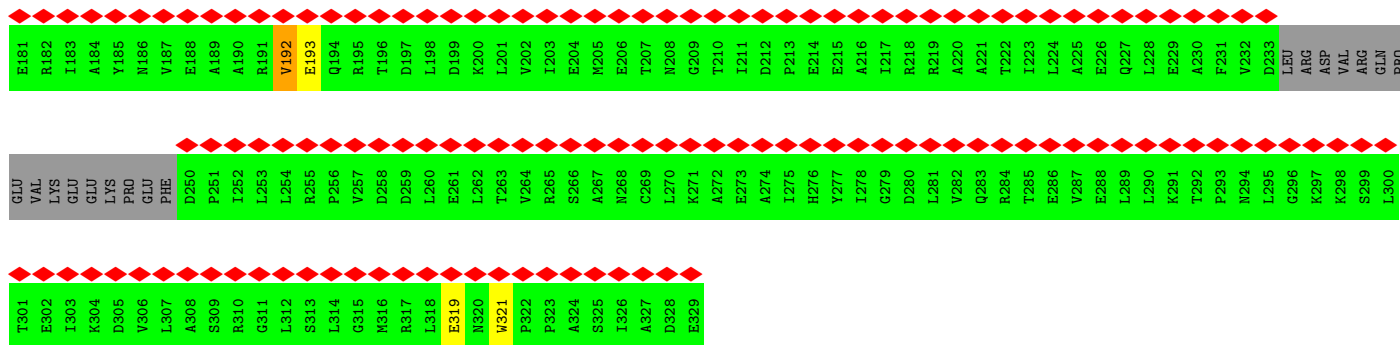


● Molecule 12: Transcription termination/antitermination protein NusG

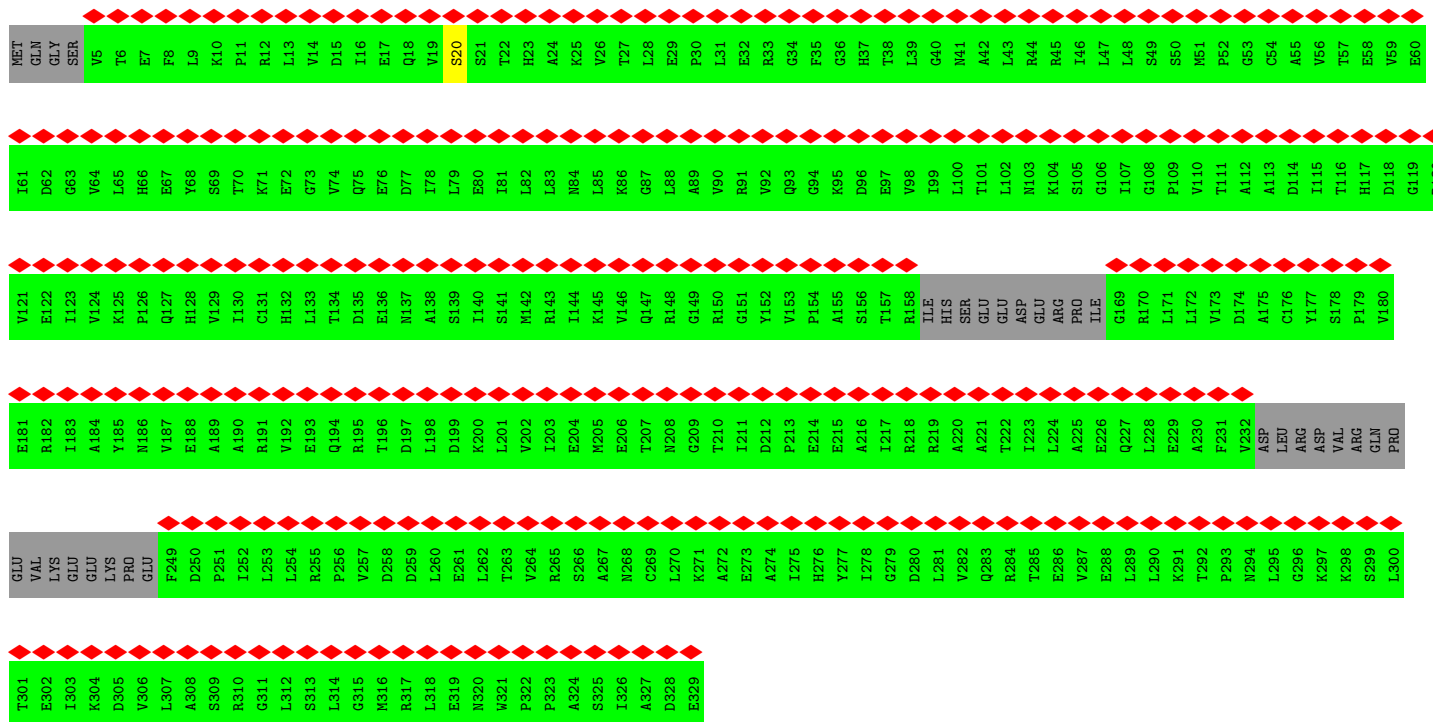


● Molecule 13: DNA-directed RNA polymerase subunit alpha

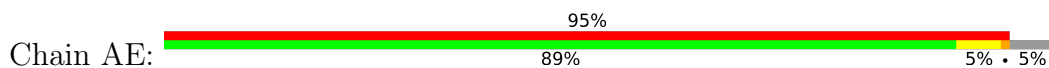




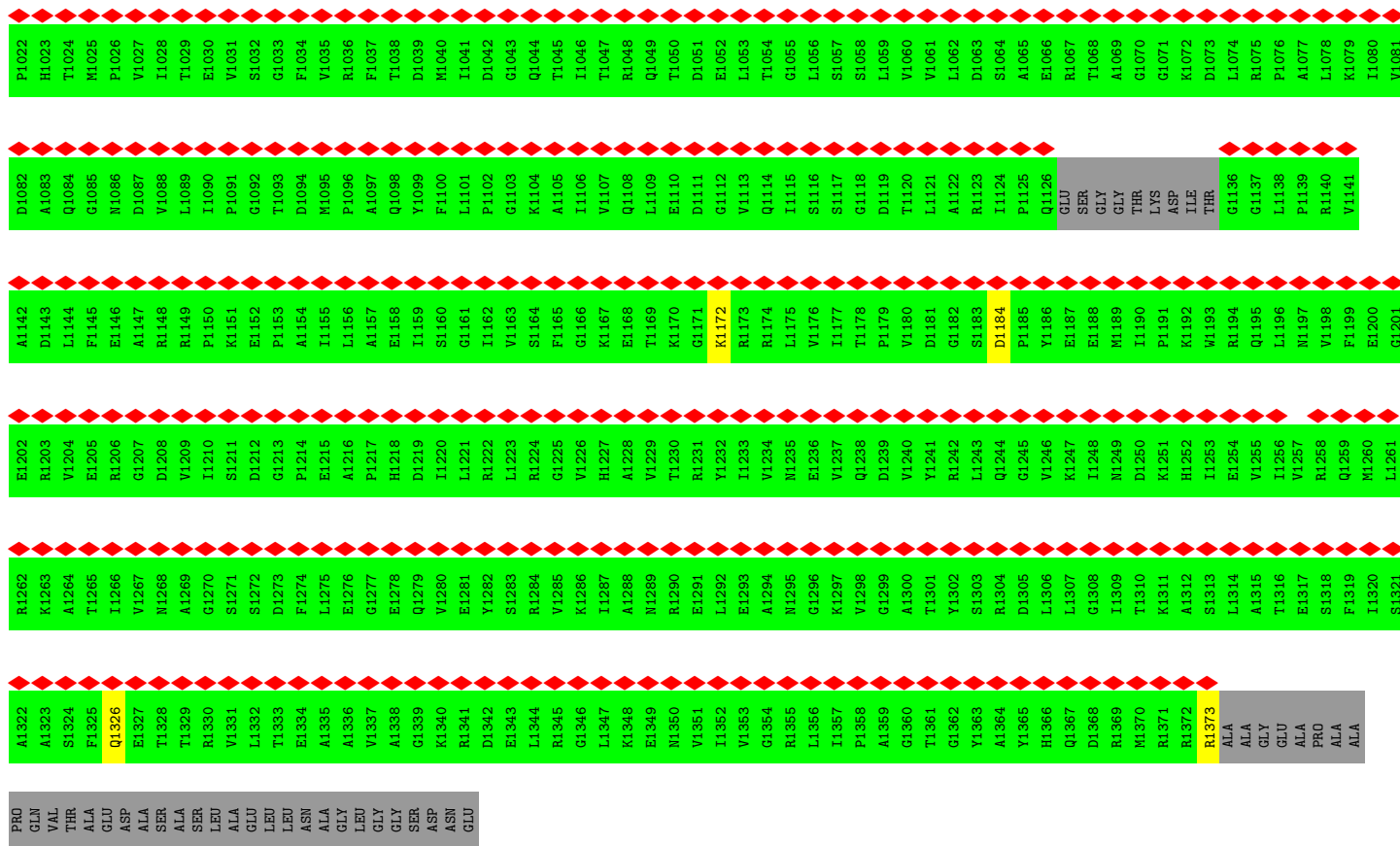
• Molecule 13: DNA-directed RNA polymerase subunit alpha



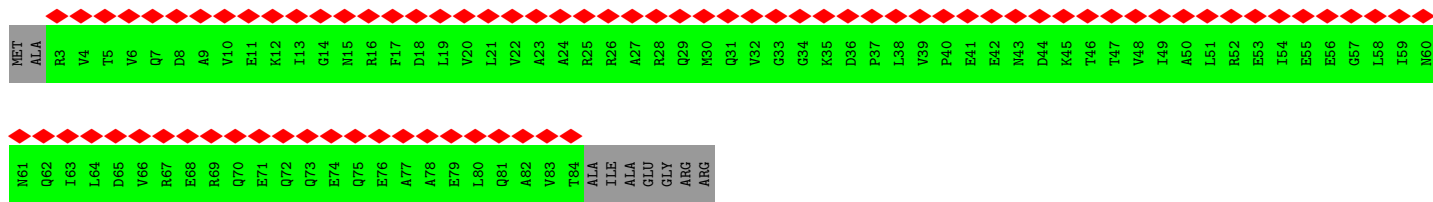
• Molecule 14: DNA-directed RNA polymerase subunit beta'



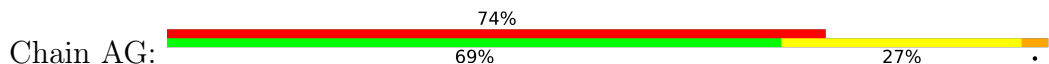
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R842	V843	T844	A845	E846	D847	V848	L849	K850	G852	T853	A854	D855	L856	L857	V858	P859	R860	H861	T862	L863	L864	H865	E866	Q867	M868	C869	D870	L871	L872	E873	E874	H875	S876	H877	D878	A879	W880	K881	W882	R883	S884	V885	V886	C888	D889	T890	D891	F892	G893	H894	C895	A896	H897	C898	Y899	G900	R901			
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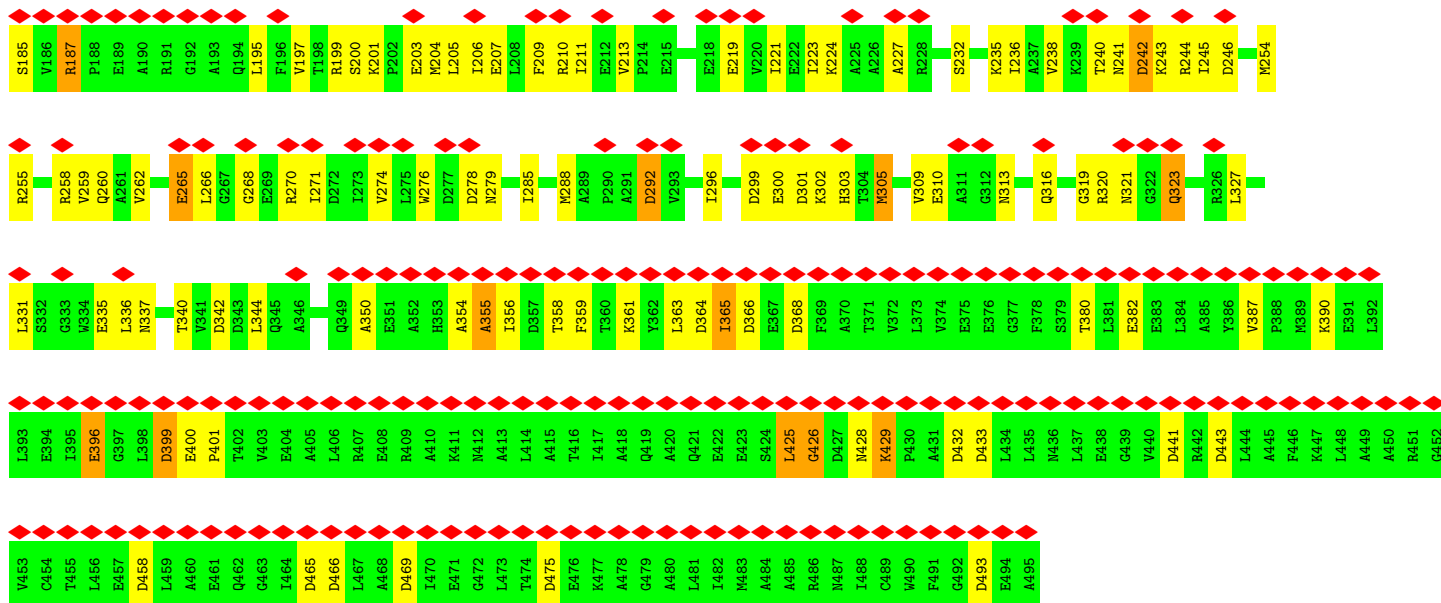


• Molecule 15: DNA-directed RNA polymerase subunit omega

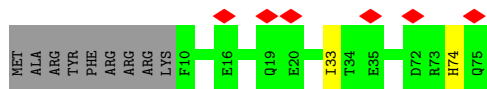
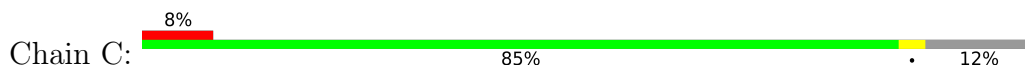


• Molecule 16: Transcription termination/antitermination protein NusA

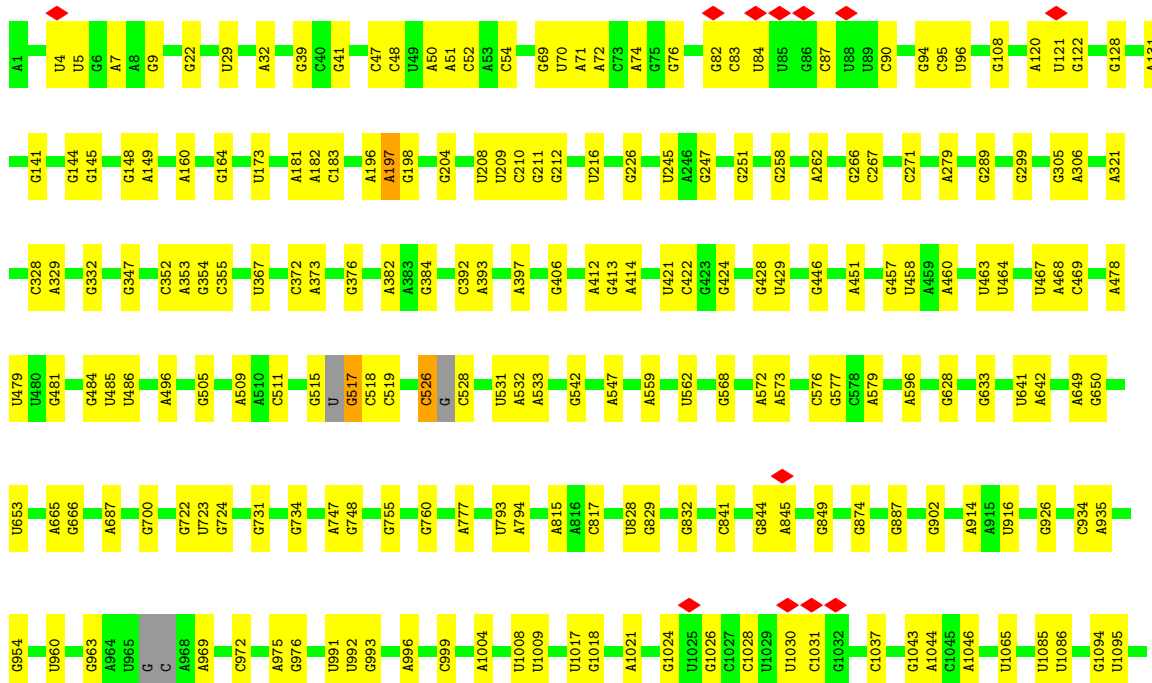
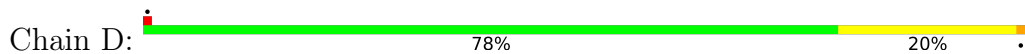


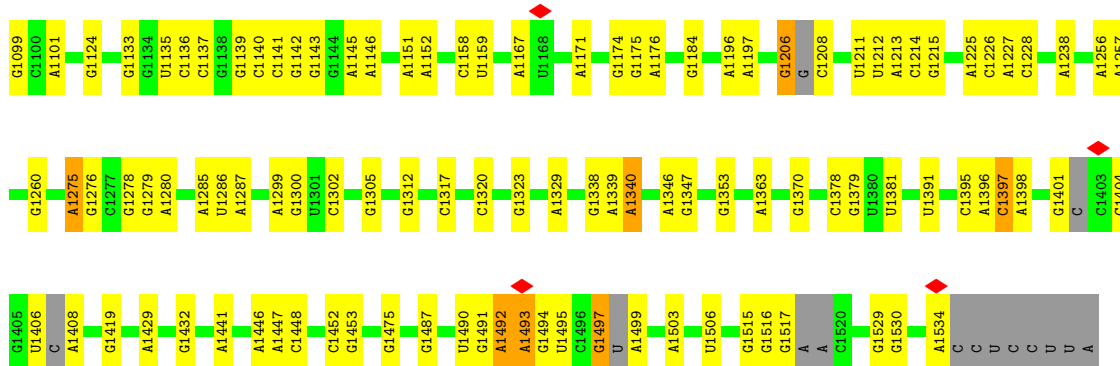


- Molecule 17: 30S ribosomal protein S18

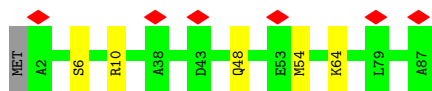


- Molecule 18: 16S rRNA

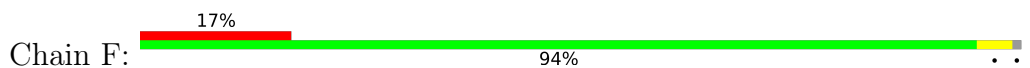




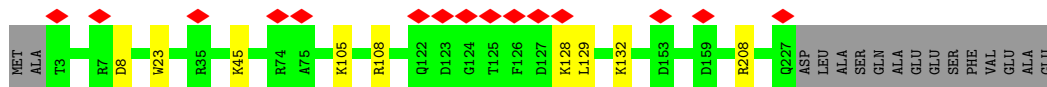
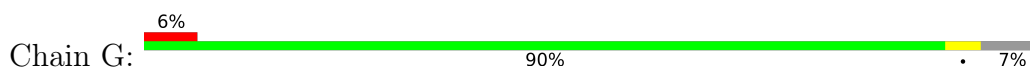
• Molecule 19: 30S ribosomal protein S20



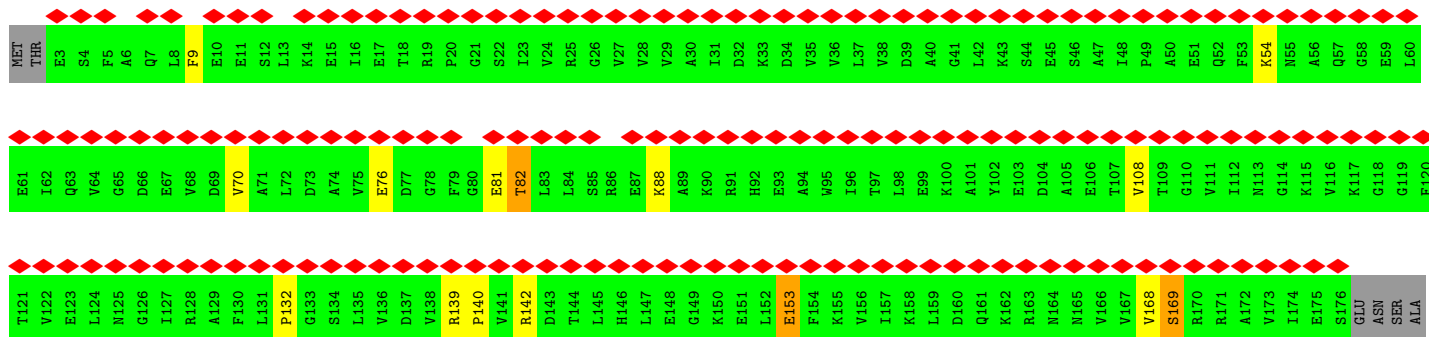
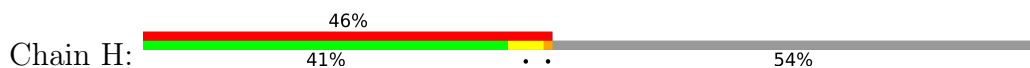
• Molecule 20: 30S ribosomal protein S21

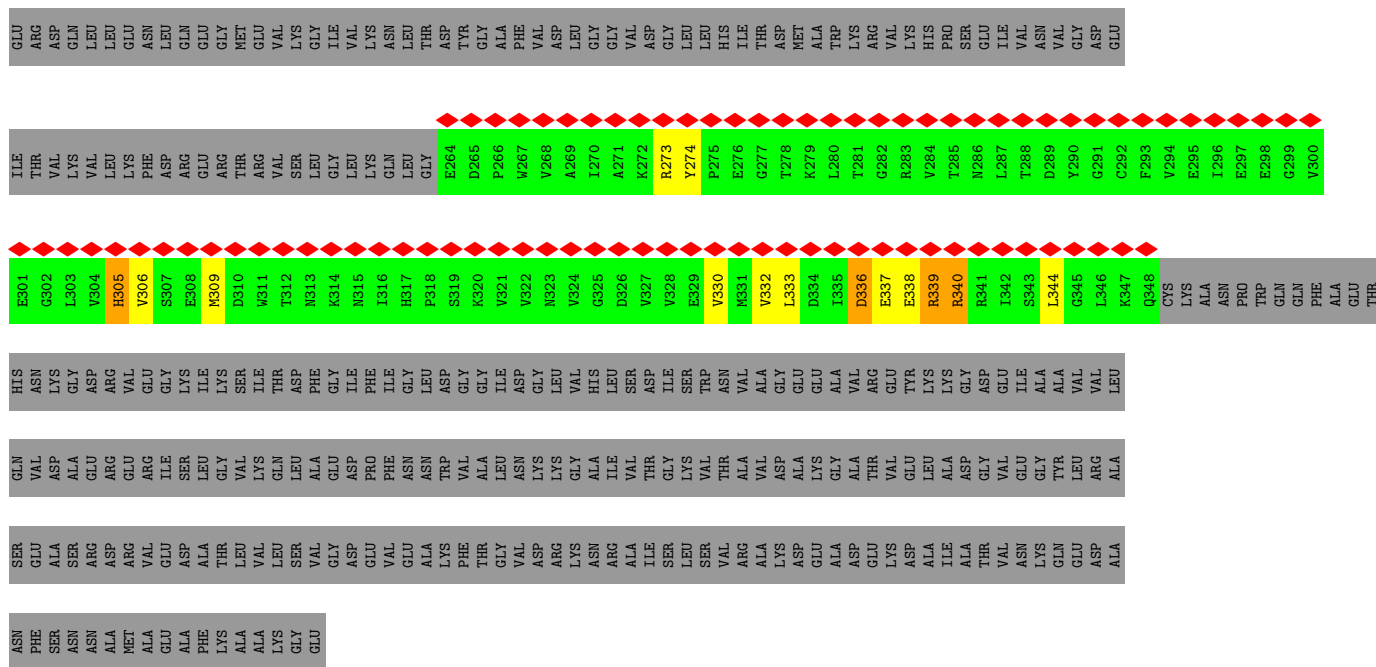


• Molecule 21: 30S ribosomal protein S2

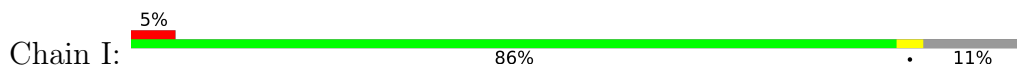


• Molecule 22: 30S ribosomal protein S1





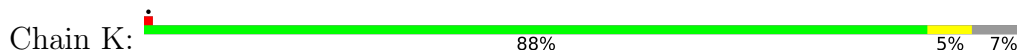
• Molecule 23: 30S ribosomal protein S3



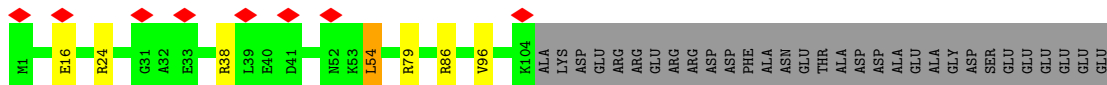
• Molecule 24: 30S ribosomal protein S4



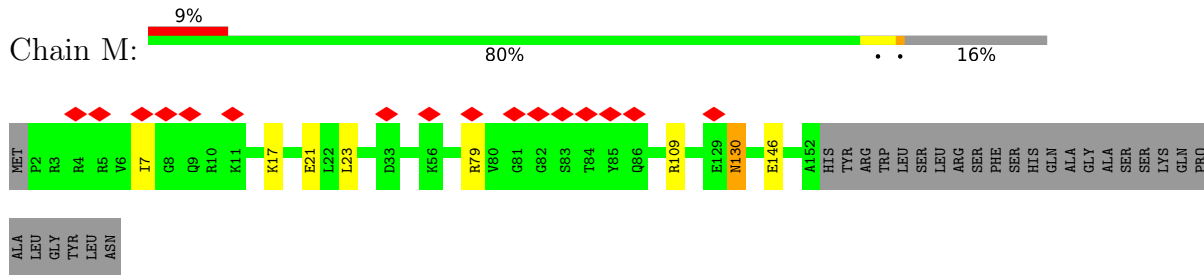
• Molecule 25: 30S ribosomal protein S5



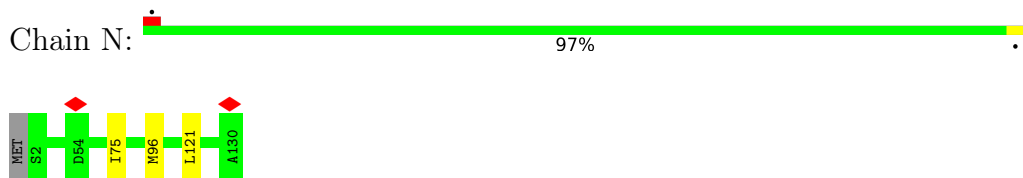
• Molecule 26: 30S ribosomal protein S6



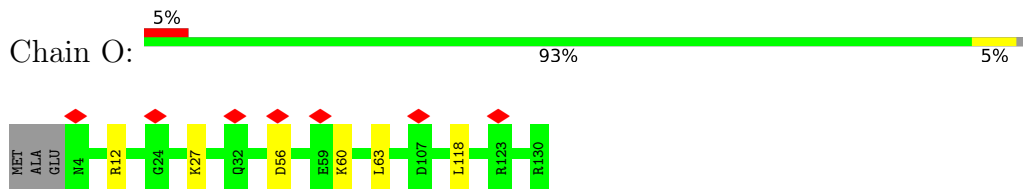
- Molecule 27: 30S ribosomal protein S7



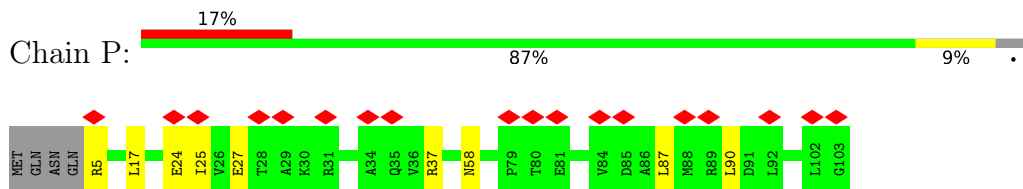
- Molecule 28: 30S ribosomal protein S8



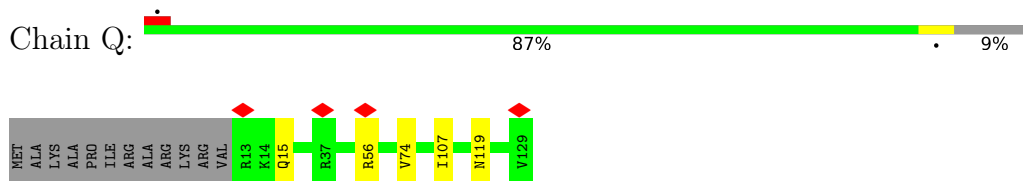
- Molecule 29: 30S ribosomal protein S9



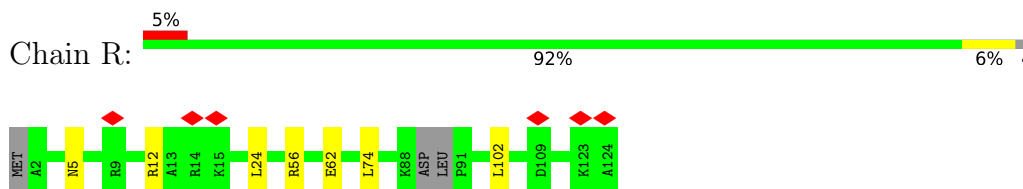
- Molecule 30: 30S ribosomal protein S10



- Molecule 31: 30S ribosomal protein S11



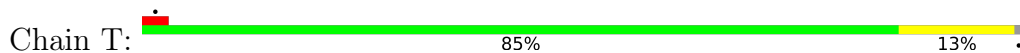
- Molecule 32: 30S ribosomal protein S12



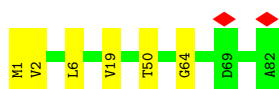
- Molecule 33: 30S ribosomal protein S14



• Molecule 34: 30S ribosomal protein S15



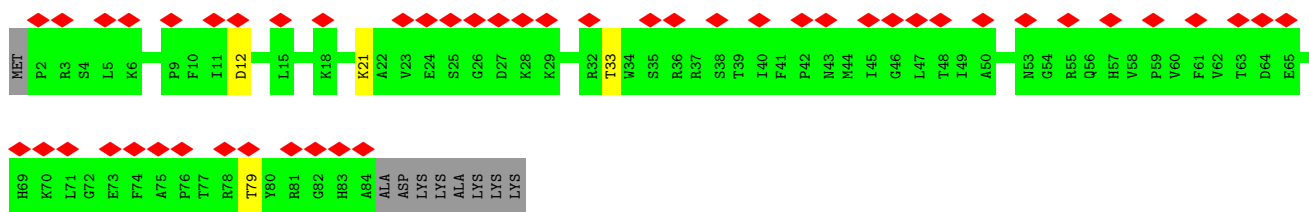
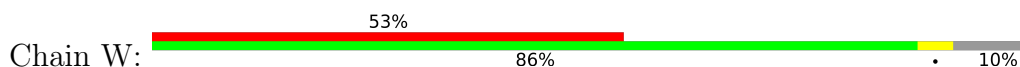
• Molecule 35: 30S ribosomal protein S16



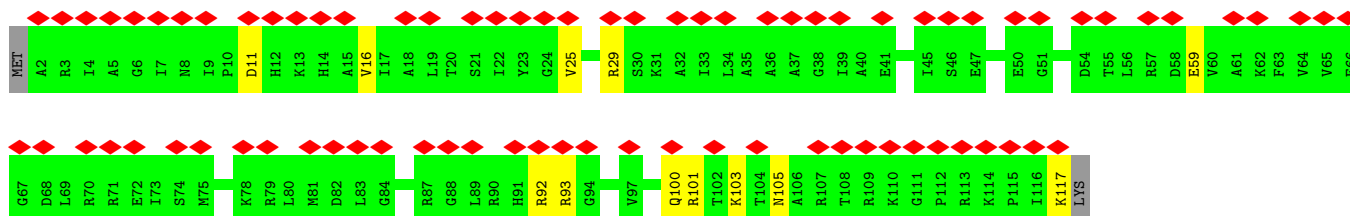
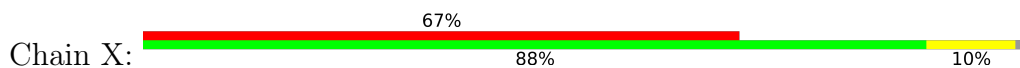
• Molecule 36: 30S ribosomal protein S17



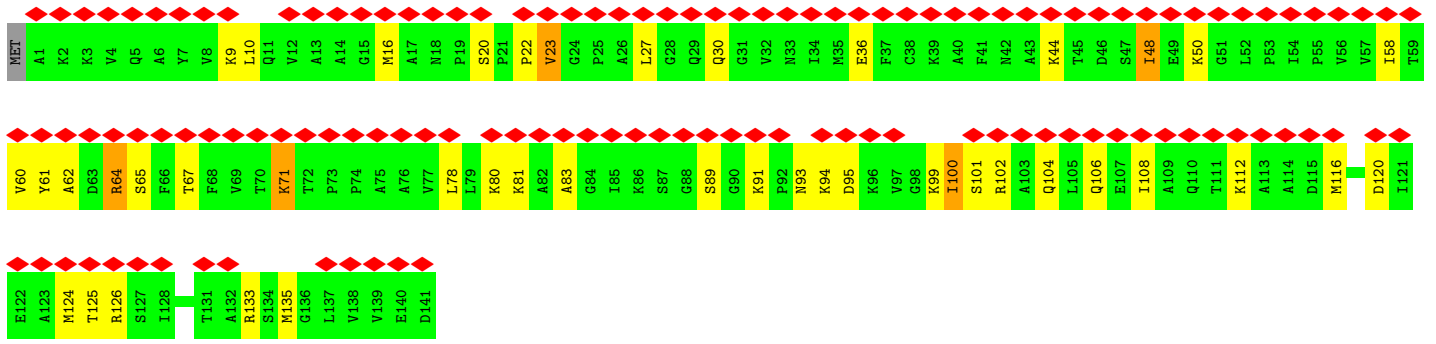
• Molecule 37: 30S ribosomal protein S19



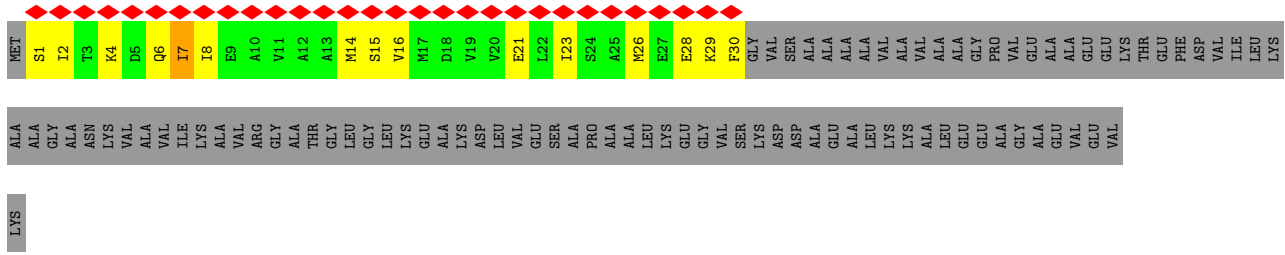
• Molecule 38: 30S ribosomal protein S13



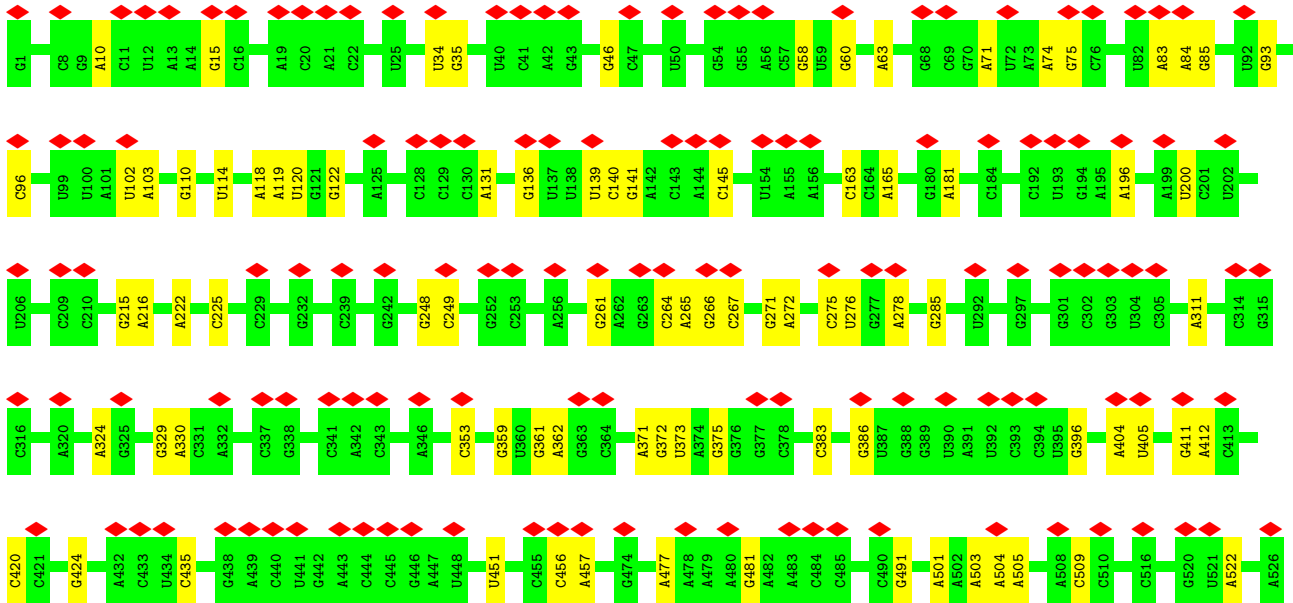
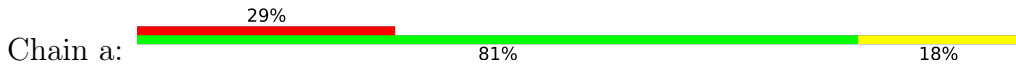
• Molecule 39: 50S ribosomal protein L11

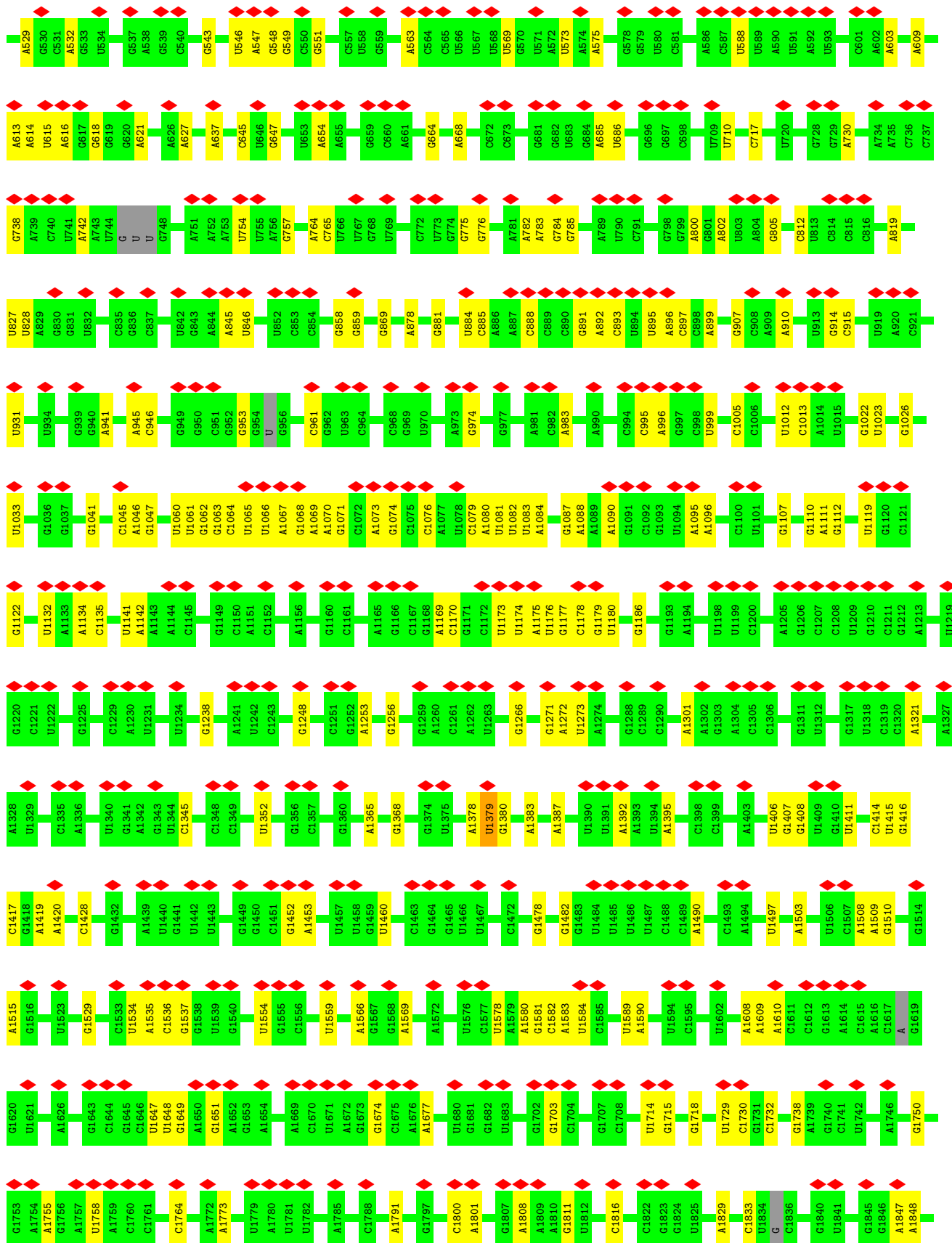


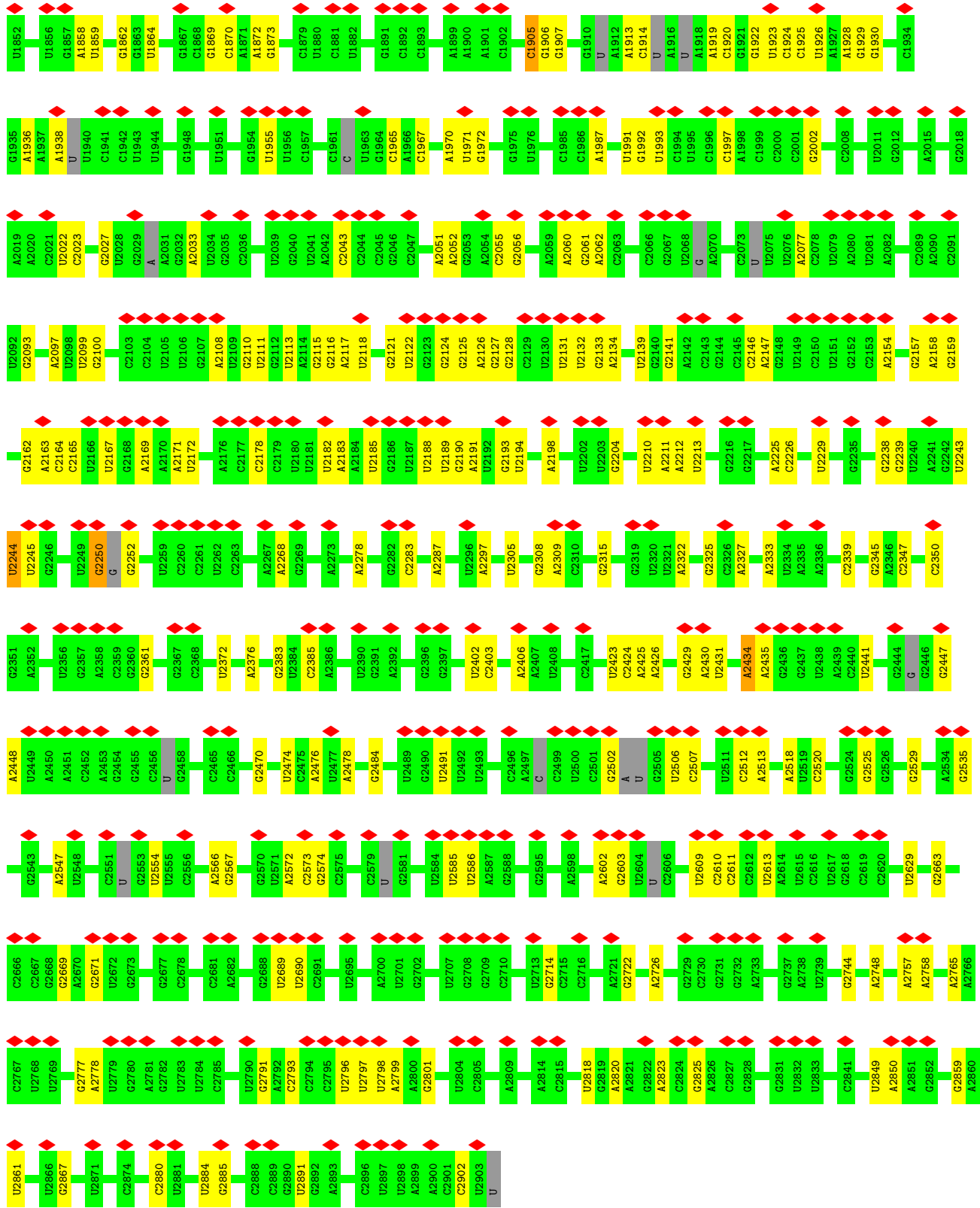
• Molecule 40: 50S ribosomal protein L7/L12



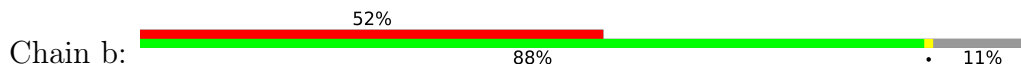
• Molecule 41: 23S rRNA





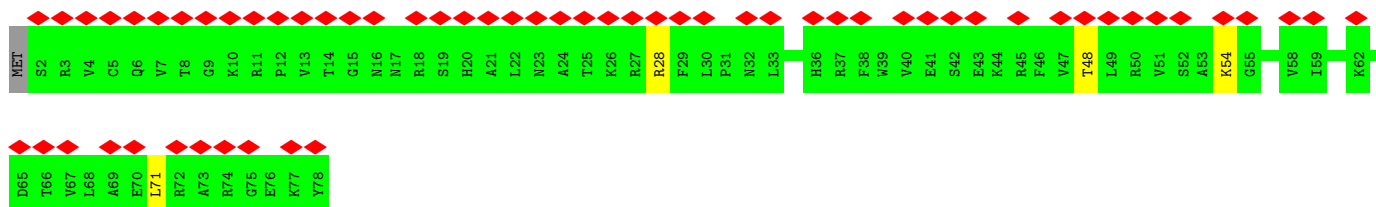
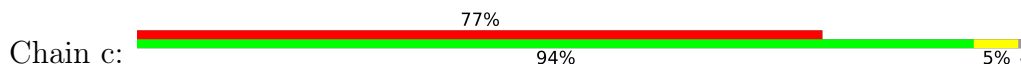


• Molecule 42: 50S ribosomal protein L27

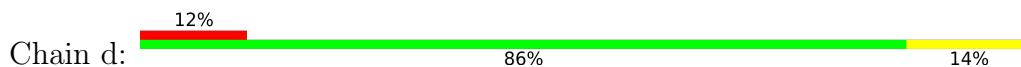




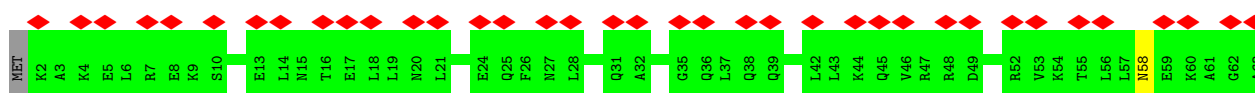
• Molecule 43: 50S ribosomal protein L28



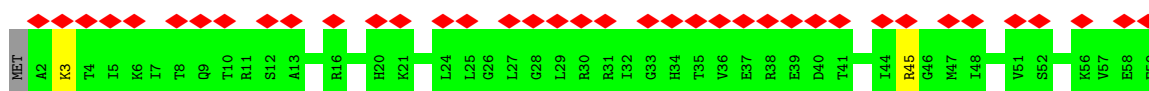
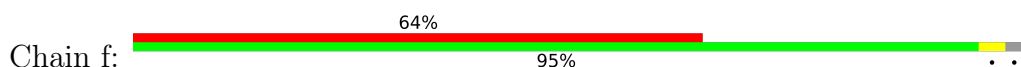
• Molecule 44: 5S rRNA



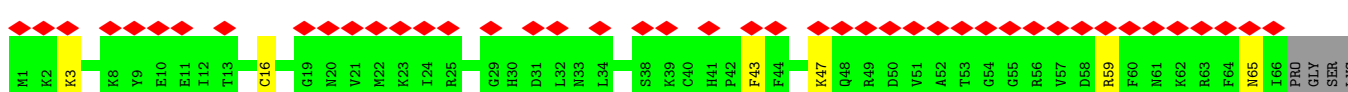
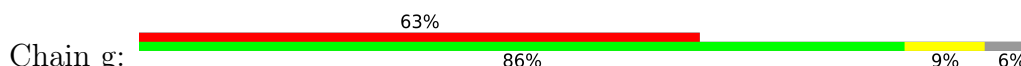
• Molecule 45: 50S ribosomal protein L29



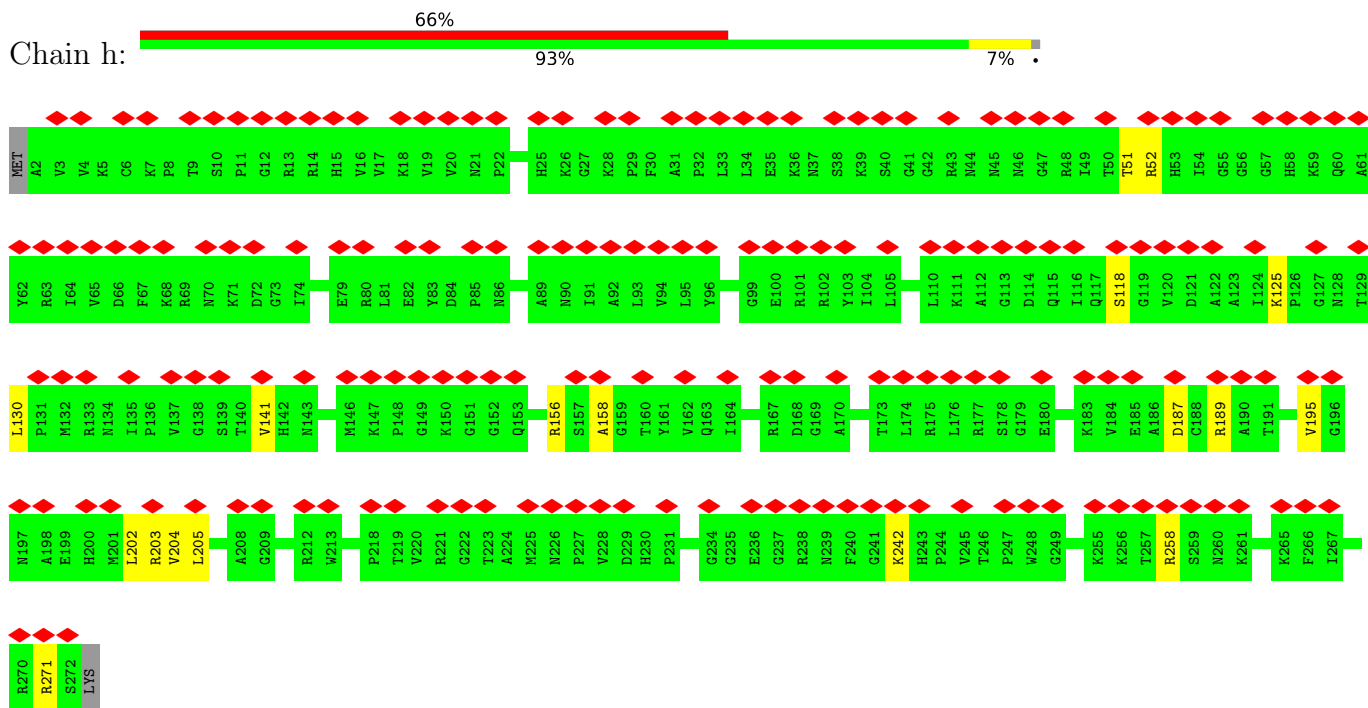
• Molecule 46: 50S ribosomal protein L30



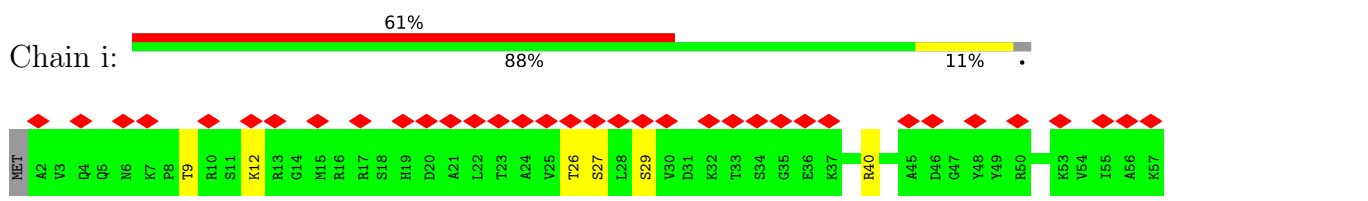
• Molecule 47: 50S ribosomal protein L31



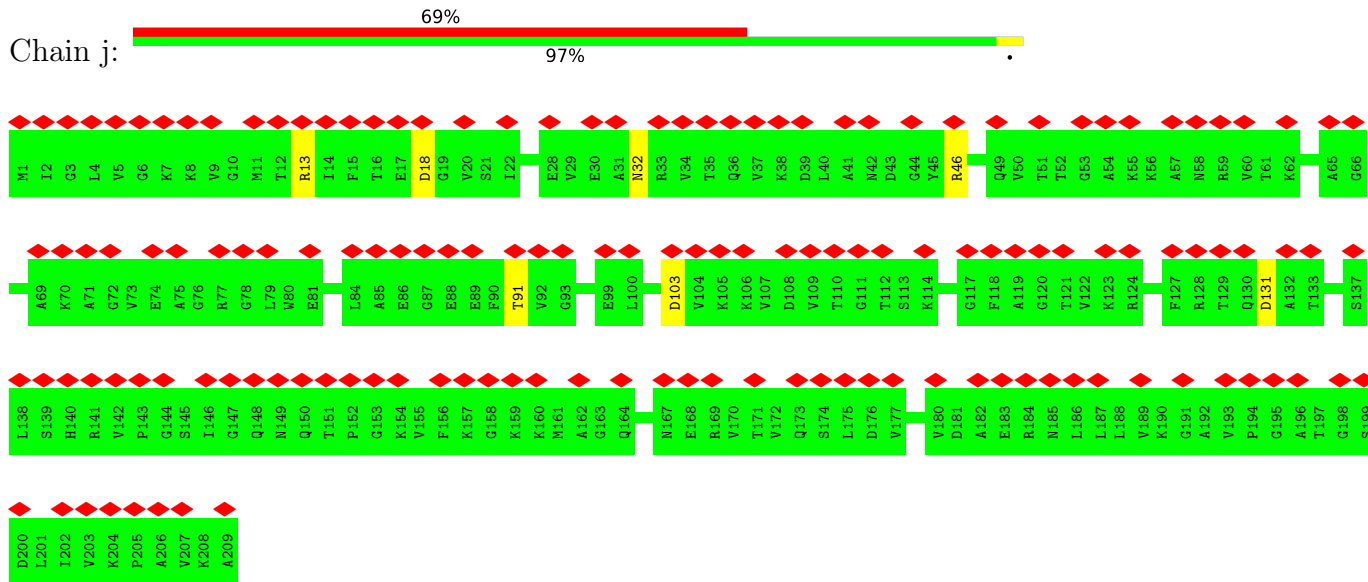
• Molecule 48: 50S ribosomal protein L2



• Molecule 49: 50S ribosomal protein L32

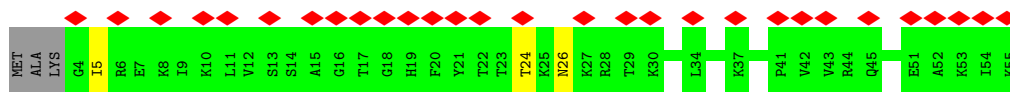


• Molecule 50: 50S ribosomal protein L3

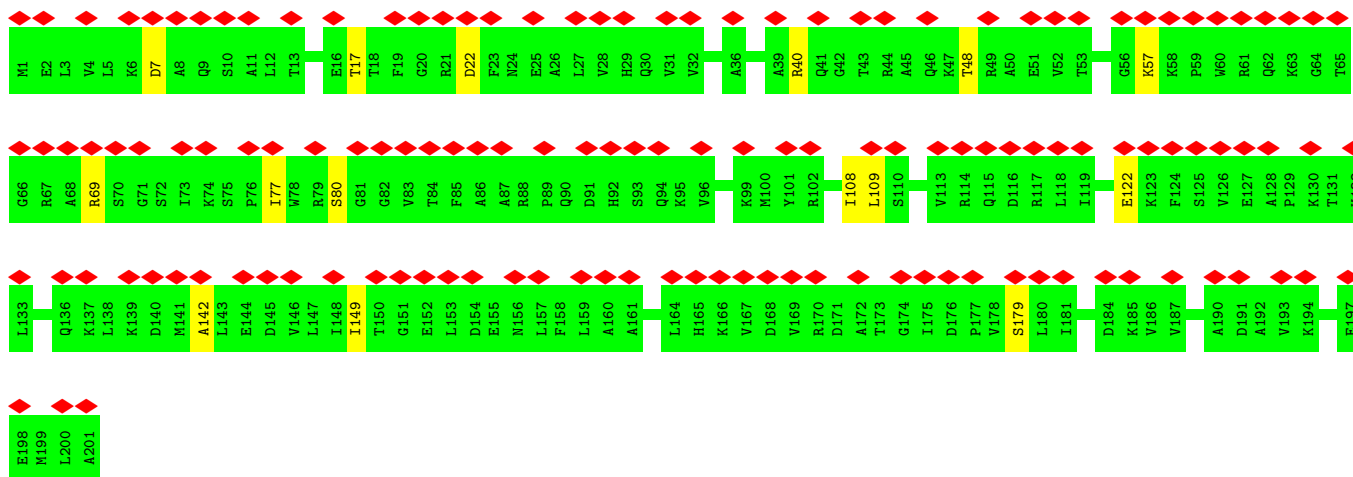
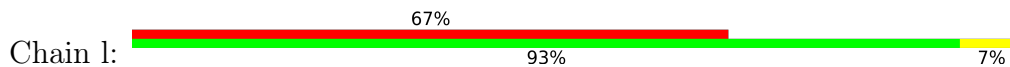


• Molecule 51: 50S ribosomal protein L33

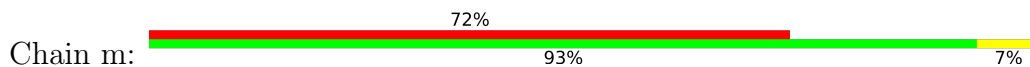




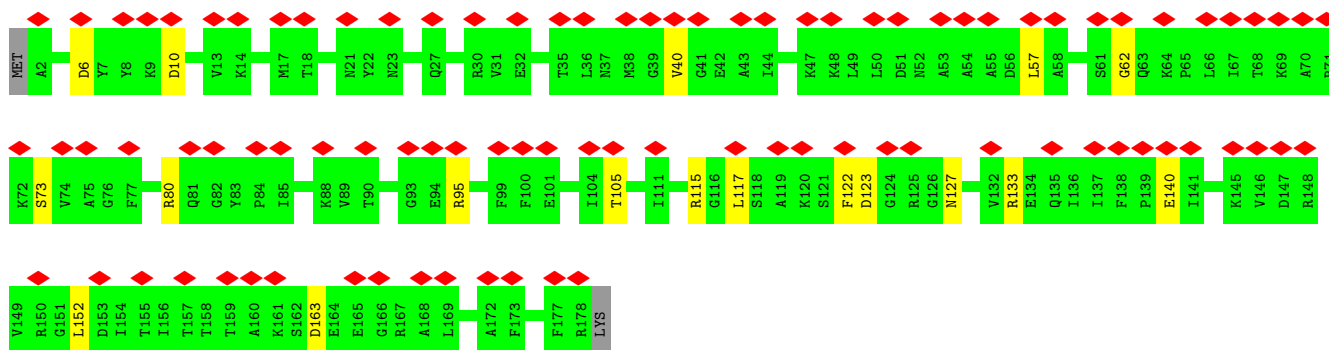
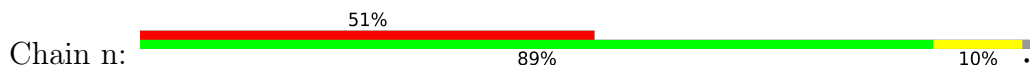
• Molecule 52: 50S ribosomal protein L4



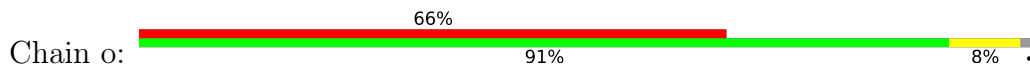
• Molecule 53: 50S ribosomal protein L34

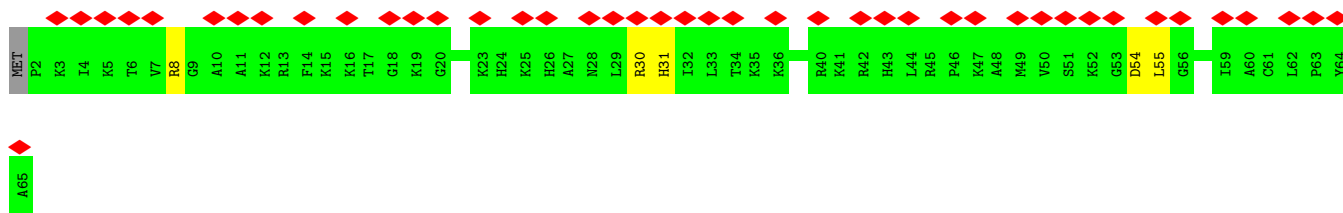


• Molecule 54: 50S ribosomal protein L5

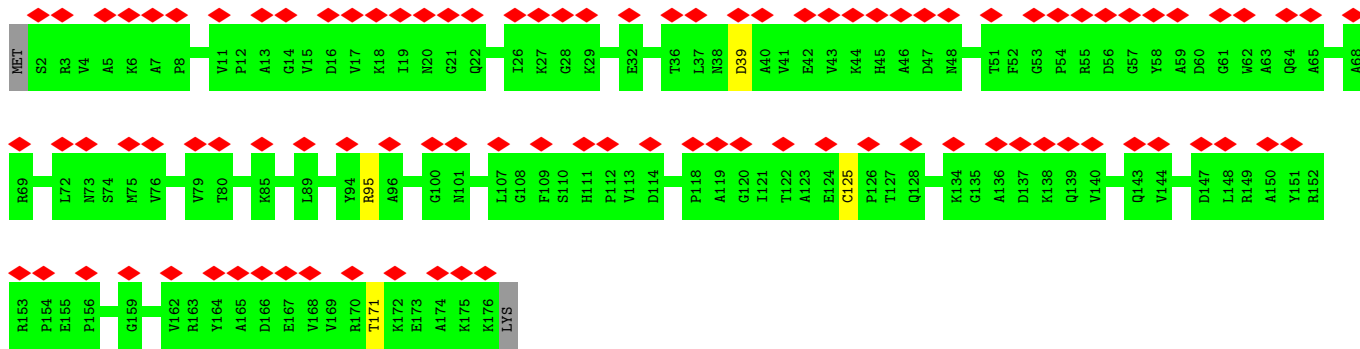


• Molecule 55: 50S ribosomal protein L35

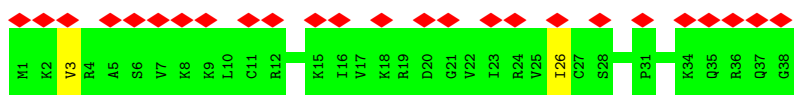
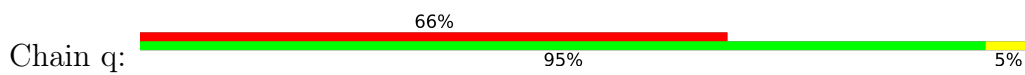




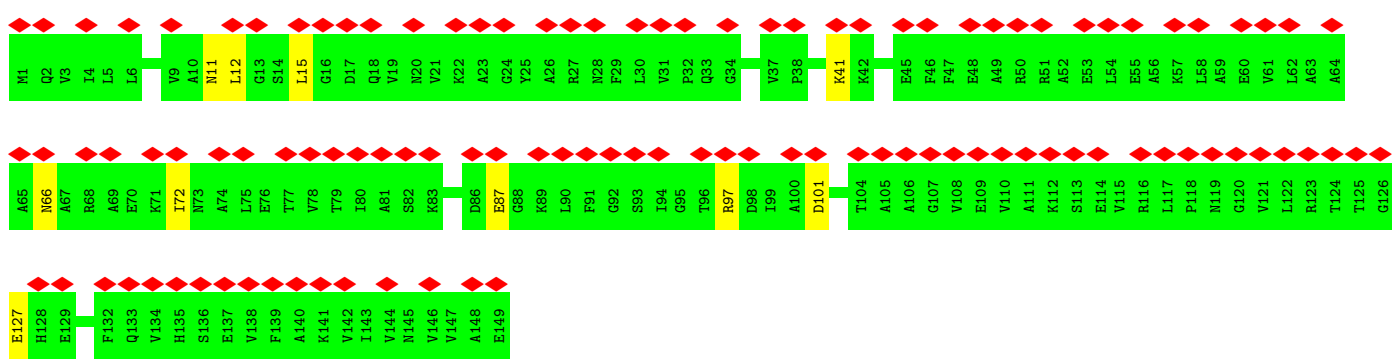
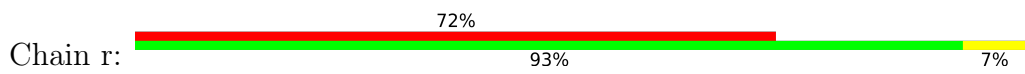
• Molecule 56: 50S ribosomal protein L6



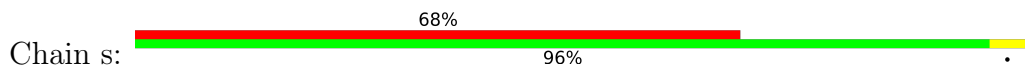
• Molecule 57: 50S ribosomal protein L36

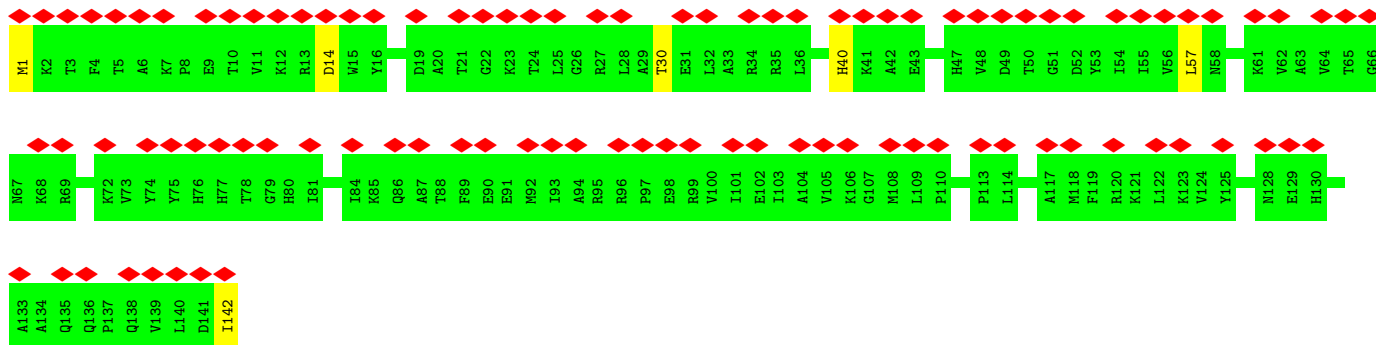


• Molecule 58: 50S ribosomal protein L9

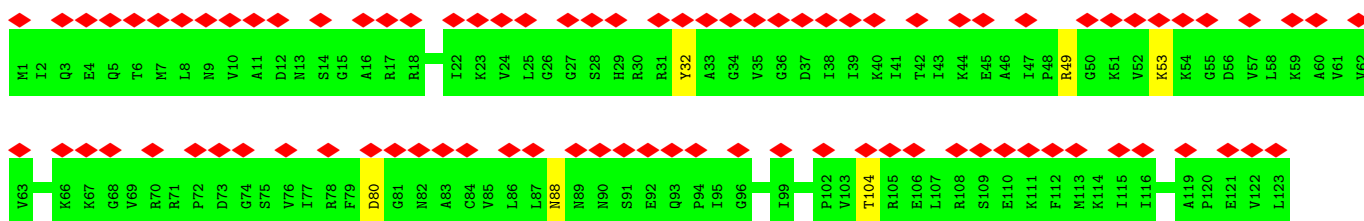


• Molecule 59: 50S ribosomal protein L13

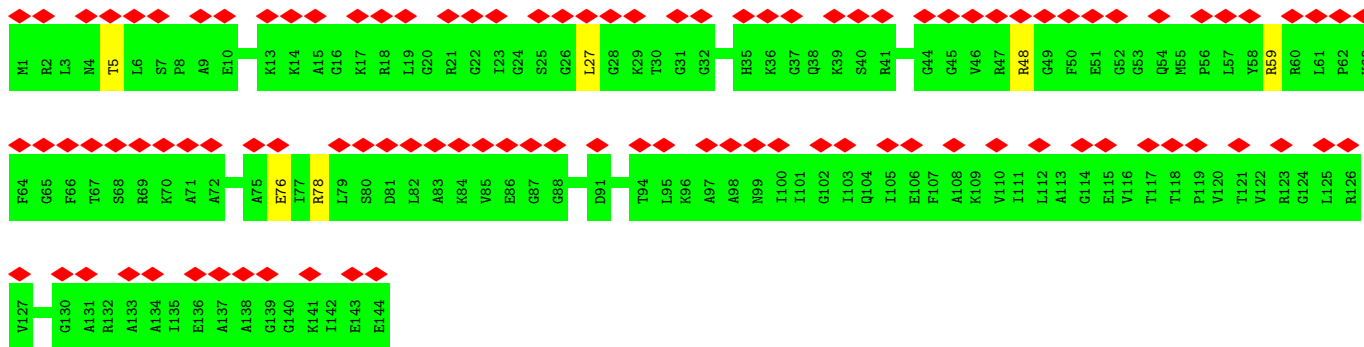




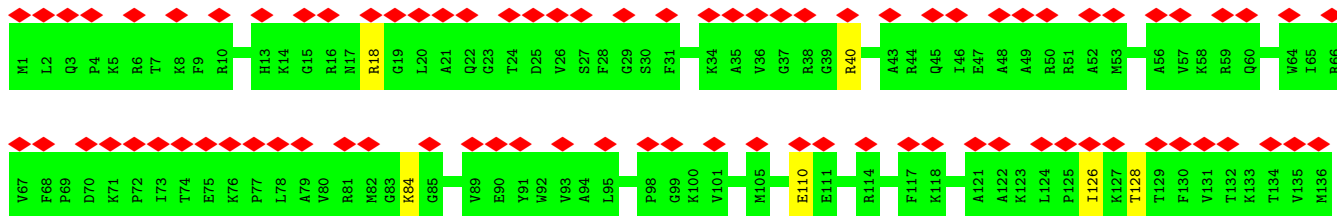
• Molecule 60: 50S ribosomal protein L14



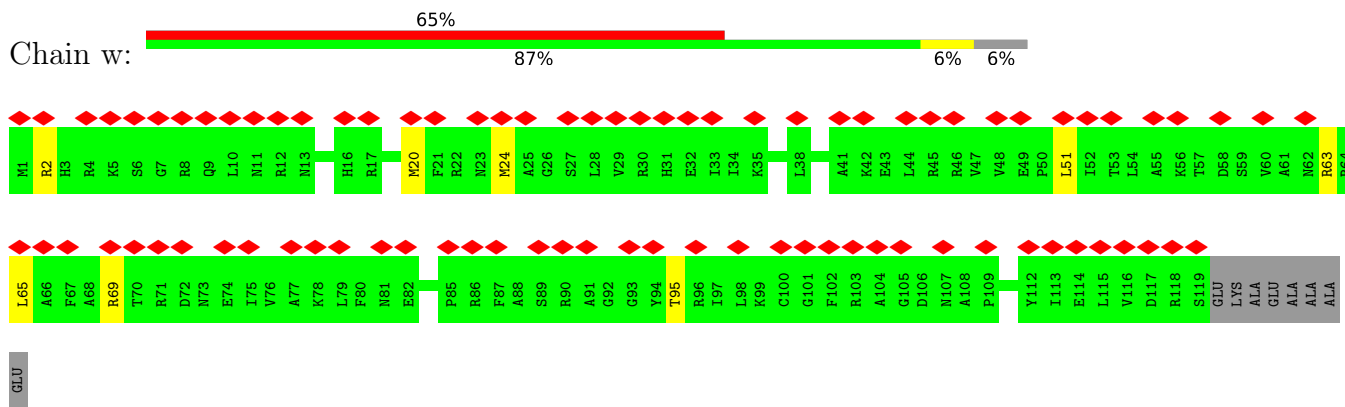
• Molecule 61: 50S ribosomal protein L15



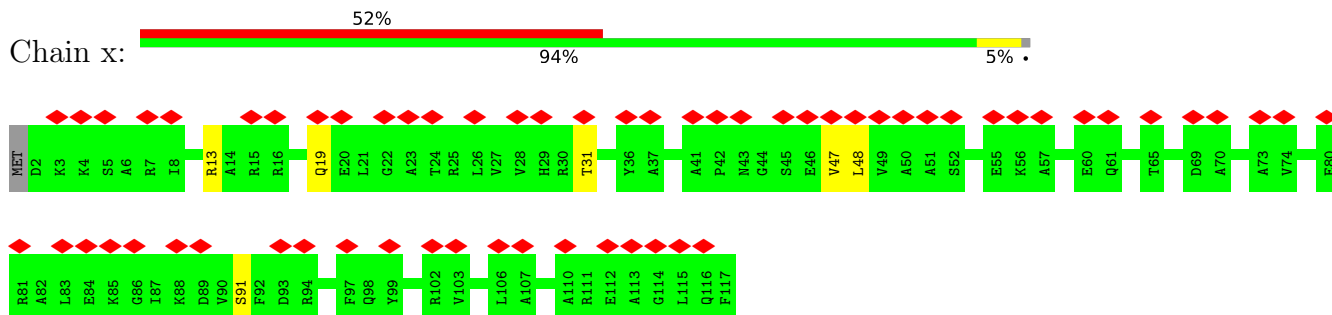
• Molecule 62: 50S ribosomal protein L16



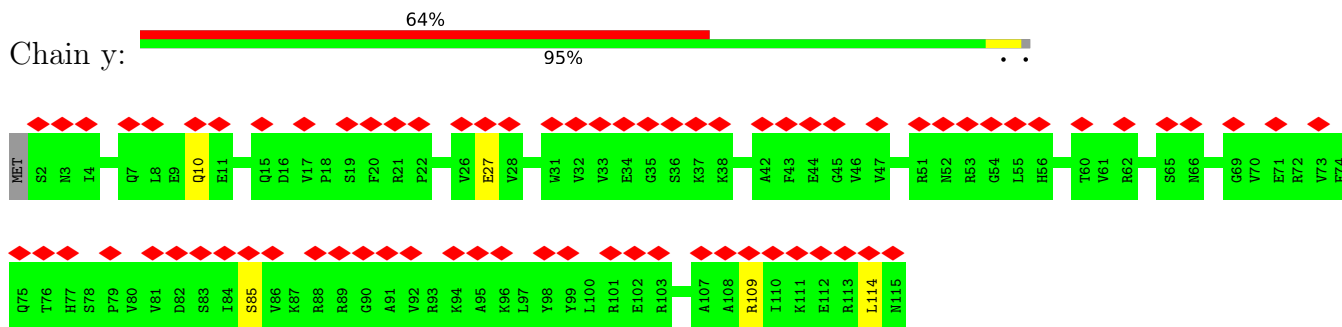
• Molecule 63: 50S ribosomal protein L17



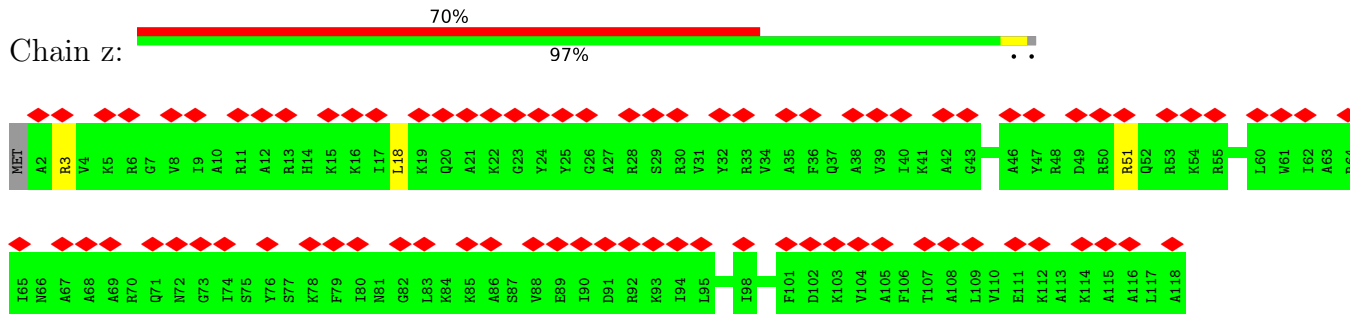
• Molecule 64: 50S ribosomal protein L18



• 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 (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/829	0.67	0/1107
2	1	0.49	0/864	0.82	0/1156
3	2	0.41	0/752	0.71	0/1005
4	3	0.35	0/796	0.66	2/1062 (0.2%)
5	4	0.40	0/766	0.68	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.96	0/926
8	7	0.74	7/761 (0.9%)	0.99	3/1178 (0.3%)
9	9	0.79	2/1131 (0.2%)	0.64	1/1524 (0.1%)
10	A	0.38	0/1810	0.75	1/2821 (0.0%)
10	B	0.46	2/1810 (0.1%)	0.85	7/2821 (0.2%)
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	0.65	2/3897 (0.1%)	0.89	31/5273 (0.6%)
17	C	0.48	0/553	0.83	0/743
18	D	0.33	10/36610 (0.0%)	0.73	30/57091 (0.1%)
19	E	0.57	0/675	0.85	0/895
20	F	0.56	0/597	0.87	0/792
21	G	0.48	0/1791	0.71	0/2413
22	H	0.54	1/1746 (0.1%)	1.03	13/2382 (0.5%)
23	I	0.43	0/1663	0.71	0/2241
24	J	0.47	0/1665	0.73	0/2227
25	K	0.45	0/1165	0.75	0/1568
26	L	0.43	0/867	0.76	1/1171 (0.1%)
27	M	0.50	0/1195	0.81	0/1602
28	N	0.41	0/989	0.69	0/1326
29	O	0.43	0/1034	0.75	0/1375
30	P	0.43	0/800	0.75	0/1082

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Q	0.40	0/893	0.70	0/1205
32	R	0.35	0/952	0.74	0/1274
33	S	0.49	0/817	0.79	0/1088
34	T	0.53	0/722	0.86	0/964
35	U	0.44	0/659	0.78	0/884
36	V	0.34	0/657	0.61	0/881
37	W	0.38	0/680	0.62	0/915
38	X	0.49	0/909	0.86	0/1215
39	Y	0.66	0/1046	0.58	0/1410
40	Z	0.69	0/227	0.57	0/304
41	a	0.38	3/69247 (0.0%)	0.72	18/107985 (0.0%)
42	b	0.39	0/589	0.71	0/779
43	c	0.48	0/635	0.81	2/848 (0.2%)
44	d	0.29	0/2872	0.69	0/4478
45	e	0.54	0/502	0.82	0/667
46	f	0.45	0/452	0.78	0/605
47	g	0.43	0/531	0.68	0/709
48	h	0.39	0/2121	0.78	0/2852
49	i	0.40	0/450	0.79	0/599
50	j	0.43	0/1586	0.69	0/2134
51	k	0.35	0/433	0.65	0/576
52	l	0.46	0/1571	0.77	0/2113
53	m	0.53	0/380	0.99	0/498
54	n	0.49	0/1434	0.88	3/1926 (0.2%)
55	o	0.45	0/513	0.83	0/676
56	p	0.39	0/1333	0.67	0/1805
57	q	0.37	0/303	0.77	0/397
58	r	0.43	0/1122	0.69	0/1515
59	s	0.50	0/1152	0.75	0/1551
60	t	0.41	0/955	0.78	0/1279
61	u	0.40	0/1062	0.76	0/1413
62	v	0.46	0/1093	0.81	0/1460
63	w	0.52	0/964	0.87	0/1289
64	x	0.46	0/902	0.81	0/1209
65	y	0.41	0/929	0.72	1/1242 (0.1%)
66	z	0.60	0/960	0.91	0/1278
All	All	0.43	44/195002 (0.0%)	0.73	124/286738 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	A	0	2
10	B	0	2
13	AC	0	3
13	AD	0	1
14	AE	0	5
16	AG	0	6
22	H	0	3
38	X	0	1
All	All	0	23

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	13.75	1.70	1.47
18	D	1516	G	O3'-P	-13.40	1.45	1.61
12	AB	124	PRO	N-CA	13.13	1.69	1.47
18	D	1339	A	O3'-P	10.58	1.73	1.61
14	AE	88	CYS	CB-SG	-10.21	1.64	1.82
16	AG	429	LYS	C-N	8.82	1.51	1.34
6	5	109	DT	O3'-P	8.67	1.71	1.61
16	AG	246	ASP	C-N	8.47	1.50	1.34
18	D	145	G	O3'-P	8.42	1.71	1.61
11	AA	920	VAL	C-N	8.39	1.50	1.34
18	D	196	A	O3'-P	8.27	1.71	1.61
7	6	10	DG	C1'-N9	-8.20	1.35	1.47
18	D	1275	A	O3'-P	7.84	1.70	1.61
41	a	2434	A	O3'-P	7.56	1.70	1.61
22	H	169	SER	N-CA	7.53	1.61	1.46
18	D	1515	G	O3'-P	-7.29	1.52	1.61
6	5	121	DG	C1'-N9	-7.26	1.37	1.47
18	D	1395	C	O3'-P	7.21	1.69	1.61
8	7	19	G	C1'-N9	-7.19	1.36	1.46
8	7	-19	U	C1'-N1	6.86	1.59	1.48
18	D	1490	U	O3'-P	6.85	1.69	1.61
6	5	112	DG	C1'-N9	-6.69	1.37	1.47
18	D	1492	A	O3'-P	6.63	1.69	1.61
41	a	1905	C	O3'-P	6.59	1.69	1.61
41	a	2167	U	O3'-P	6.51	1.69	1.61
6	5	100	DA	C1'-N9	-6.51	1.38	1.47
7	6	21	DA	C1'-N9	-6.46	1.38	1.47
14	AE	93	THR	CA-C	6.23	1.69	1.52
6	5	116	DG	C1'-N9	-6.13	1.38	1.47
9	9	129	LEU	C-N	6.09	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AB	123	ARG	C-N	6.03	1.45	1.34
6	5	115	DA	C1'-N9	-5.97	1.38	1.47
14	AE	70	CYS	CA-CB	-5.83	1.41	1.53
10	B	36	U	O3'-P	5.81	1.68	1.61
7	6	28	DA	C1'-N9	-5.73	1.39	1.47
18	D	1397	C	O3'-P	5.71	1.68	1.61
7	6	24	DT	C1'-N1	5.31	1.56	1.49
8	7	-1	U	C1'-N1	5.25	1.56	1.48
8	7	0	U	C1'-N1	5.18	1.56	1.48
8	7	1	U	C1'-N1	5.14	1.56	1.48
8	7	2	U	C1'-N1	5.10	1.56	1.48
8	7	-3	U	C1'-N1	5.08	1.56	1.48
14	AE	801	VAL	CB-CG2	-5.04	1.42	1.52
10	B	35	A	O3'-P	5.00	1.67	1.61

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	1516	G	P-O3'-C3'	-19.01	96.89	119.70
18	D	1516	G	O3'-P-O5'	13.81	130.24	104.00
16	AG	104	ARG	C-N-CA	13.00	154.21	121.70
41	a	2252	G	N9-C1'-C2'	-10.96	99.75	114.00
12	AB	124	PRO	CA-N-CD	-10.70	96.53	111.50
18	D	1401	G	N9-C1'-C2'	-10.68	100.11	114.00
54	n	73	SER	N-CA-CB	-10.61	94.58	110.50
18	D	1499	A	N9-C1'-C2'	-10.31	100.60	114.00
18	D	528	C	N1-C1'-C2'	-10.20	100.75	114.00
22	H	169	SER	N-CA-C	9.99	137.98	111.00
18	D	1339	A	P-O3'-C3'	9.90	131.59	119.70
10	B	29	G	N9-C1'-C2'	-9.79	101.23	112.00
10	B	28	C	P-O3'-C3'	9.63	131.25	119.70
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
18	D	196	A	P-O3'-C3'	9.37	130.94	119.70
14	AE	271	ARG	NE-CZ-NH2	-9.27	115.67	120.30
18	D	526	C	N1-C1'-C2'	-8.83	102.29	112.00
22	H	88	LYS	C-N-CA	8.75	143.58	121.70
16	AG	355	ALA	CB-CA-C	8.70	123.16	110.10
18	D	1208	C	N1-C1'-C2'	-8.59	102.56	112.00
41	a	2167	U	P-O3'-C3'	8.57	129.99	119.70
18	D	1206	G	N9-C1'-C2'	-8.39	102.77	112.00
9	9	130	PRO	CA-N-CD	-8.26	99.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	2434	A	P-O3'-C3'	8.26	129.61	119.70
18	D	1406	U	N1-C1'-C2'	-7.83	103.39	112.00
18	D	1275	A	P-O3'-C3'	7.65	128.88	119.70
41	a	1905	C	P-O3'-C3'	7.65	128.88	119.70
18	D	1492	A	P-O3'-C3'	7.57	128.79	119.70
18	D	1490	U	P-O3'-C3'	7.56	128.77	119.70
22	H	305	HIS	N-CA-C	7.44	131.09	111.00
10	B	29	G	C3'-C2'-O2'	7.37	134.66	113.30
8	7	-20	A	OP2-P-O3'	7.19	121.02	105.20
18	D	1206	G	C4'-C3'-O3'	7.17	127.34	113.00
18	D	1493	A	C2'-C3'-O3'	7.13	125.18	109.50
16	AG	108	GLN	N-CA-CB	7.12	123.42	110.60
10	B	35	A	P-O3'-C3'	7.08	128.20	119.70
41	a	2245	U	N1-C1'-C2'	-7.05	104.24	112.00
18	D	145	G	P-O3'-C3'	7.02	128.12	119.70
18	D	1395	C	P-O3'-C3'	6.99	128.09	119.70
18	D	1516	G	OP1-P-O3'	-6.99	89.83	105.20
8	7	-20	A	O3'-P-O5'	-6.79	91.10	104.00
16	AG	355	ALA	N-CA-CB	6.78	119.59	110.10
54	n	73	SER	CB-CA-C	6.72	122.88	110.10
18	D	1515	G	O3'-P-O5'	-6.68	91.31	104.00
18	D	1401	G	C4'-C3'-O3'	6.62	126.24	113.00
16	AG	108	GLN	CB-CA-C	-6.61	97.19	110.40
41	a	2250	G	C4'-C3'-O3'	-6.60	95.53	109.40
16	AG	354	ALA	CA-C-N	6.58	131.68	117.20
41	a	2243	U	N1-C1'-C2'	-6.56	104.79	112.00
41	a	1379	U	C2'-C3'-O3'	6.54	124.17	113.70
18	D	1515	G	P-O3'-C3'	6.50	127.50	119.70
22	H	339	ARG	C-N-CA	6.47	137.88	121.70
18	D	515	G	N9-C1'-C2'	-6.45	104.90	112.00
18	D	1497	G	N9-C1'-C2'	-6.39	104.97	112.00
6	5	109	DT	P-O3'-C3'	6.37	127.35	119.70
18	D	1408	A	N9-C1'-C2'	-6.37	104.99	112.00
10	B	34	C	P-O3'-C3'	6.35	127.32	119.70
16	AG	105	ILE	C-N-CA	6.09	136.93	121.70
22	H	140	PRO	N-CA-CB	5.96	110.45	103.30
10	B	29	G	P-O3'-C3'	5.96	126.85	119.70
16	AG	33	THR	CA-CB-CG2	5.95	120.73	112.40
16	AG	106	THR	OG1-CB-CG2	-5.93	96.36	110.00
22	H	330	VAL	N-CA-C	5.90	126.93	111.00
16	AG	426	GLY	O-C-N	-5.89	113.28	122.70
22	H	336	ASP	CB-CA-C	-5.87	98.65	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	754	U	N1-C1'-C2'	5.87	121.64	114.00
12	AB	122	PRO	N-CA-CB	5.83	110.29	103.30
22	H	132	PRO	N-CA-CB	5.79	110.25	103.30
22	H	168	VAL	C-N-CA	5.78	136.14	121.70
14	AE	903	LEU	C-N-CA	5.77	136.12	121.70
18	D	517	G	C5'-C4'-C3'	5.75	125.19	116.00
22	H	344	LEU	CA-CB-CG	5.67	128.35	115.30
54	n	127	ASN	CB-CA-C	5.64	121.69	110.40
16	AG	102	PHE	C-N-CA	5.64	135.80	121.70
16	AG	33	THR	C-N-CA	5.63	135.78	121.70
41	a	2244	U	C1'-C2'-O2'	-5.63	93.71	110.60
16	AG	35	THR	CA-CB-OG1	-5.60	97.24	109.00
14	AE	363	LEU	CA-CB-CG	5.59	128.15	115.30
26	L	54	LEU	CA-CB-CG	5.57	128.12	115.30
11	AA	920	VAL	C-N-CD	-5.54	108.42	120.60
41	a	783	A	C4'-C3'-O3'	5.47	123.94	113.00
16	AG	104	ARG	O-C-N	5.42	131.37	122.70
16	AG	104	ARG	CA-C-N	-5.39	105.34	117.20
4	3	22	ARG	NE-CZ-NH1	5.38	122.99	120.30
65	y	109	ARG	NE-CZ-NH2	5.37	122.98	120.30
18	D	1397	C	P-O3'-C3'	5.36	126.14	119.70
16	AG	458	ASP	CB-CG-OD2	5.33	123.10	118.30
43	c	28	ARG	NE-CZ-NH2	-5.33	117.64	120.30
18	D	1340	A	C5'-C4'-C3'	5.30	124.48	116.00
16	AG	469	ASP	CB-CG-OD2	5.26	123.04	118.30
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
18	D	1340	A	C5'-C4'-O4'	5.25	115.40	109.10
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
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	742	A	C8-N9-C1'	-5.22	118.30	127.70
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
22	H	169	SER	N-CA-CB	-5.21	102.68	110.50
16	AG	366	ASP	CB-CG-OD2	5.21	122.99	118.30
41	a	404	A	C2'-C3'-O3'	5.18	122.00	113.70
41	a	2244	U	C4'-C3'-O3'	5.18	123.35	113.00
8	7	-17	U	C2'-C3'-O3'	5.16	121.95	113.70
16	AG	493	ASP	CB-CG-OD2	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AG	441	ASP	CB-CG-OD2	5.15	122.93	118.30
4	3	22	ARG	NE-CZ-NH2	-5.11	117.75	120.30
41	a	2252	G	C4'-C3'-O3'	5.10	123.21	113.00
10	A	48	C	N1-C1'-C2'	5.10	120.63	114.00
16	AG	246	ASP	C-N-CD	-5.09	109.40	120.60
43	c	28	ARG	NE-CZ-NH1	5.08	122.84	120.30
10	B	48	C	N1-C1'-C2'	5.07	120.60	114.00
41	a	742	A	C4-N9-C1'	5.07	135.43	126.30
14	AE	807	LEU	CB-CG-CD2	-5.06	102.40	111.00
18	D	197	A	C2'-C3'-O3'	5.05	121.78	113.70
41	a	2243	U	C4'-C3'-O3'	5.03	123.06	113.00
14	AE	73	GLY	N-CA-C	5.03	125.67	113.10
22	H	332	VAL	N-CA-C	5.02	124.55	111.00
41	a	1141	U	N1-C1'-C2'	5.01	120.52	114.00
22	H	153	GLU	N-CA-C	-5.01	97.47	111.00
14	AE	90	VAL	CA-C-N	5.01	128.22	117.20

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
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	Mainchain,Peptide
16	AG	11	ALA	Peptide
16	AG	292	ASP	Mainchain
16	AG	426	GLY	Mainchain
10	B	19	G	Sidechain
10	B	7	G	Sidechain
22	H	274	TYR	Peptide
22	H	81	GLU	Peptide
22	H	82	THR	Peptide

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Mol	Chain	Res	Type	Group
38	X	100	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	54
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	54
5	4	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	3
11	AA	1338/1342 (100%)	1206 (90%)	126 (9%)	6 (0%)	34	69
12	AB	158/181 (87%)	119 (75%)	26 (16%)	13 (8%)	1	5
13	AC	295/329 (90%)	274 (93%)	19 (6%)	2 (1%)	22	61
13	AD	293/329 (89%)	269 (92%)	24 (8%)	0	100	100
14	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	22	61
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	AG	493/495 (100%)	376 (76%)	86 (17%)	31 (6%)	1	10
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
20	F	68/71 (96%)	68 (100%)	0	0	100	100
21	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	17
23	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	29	67
24	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
25	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	64
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15	54
27	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	22	61
28	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19	58
29	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	19	58
30	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	15	54
31	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	9	42
32	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
33	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
34	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
35	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12	47
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
37	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
38	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	8	41
39	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	1	4
40	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	8
42	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
45	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
48	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	34	69
49	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
51	k	50/55 (91%)	50 (100%)	0	0	100	100
52	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29	67
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
56	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
57	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
58	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
59	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
60	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
61	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
62	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
63	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
64	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
65	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
66	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	56
All	All	10159/11072 (92%)	9261 (91%)	778 (8%)	120 (1%)	17	49

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
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	227	ALA
22	H	139	ARG
22	H	153	GLU
22	H	169	SER
22	H	306	VAL
22	H	340	ARG
29	O	56	ASP
38	X	103	LYS
39	Y	48	ILE
9	9	33	VAL
9	9	119	PRO
11	AA	905	ILE

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Mol	Chain	Res	Type
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	242	ASP
16	AG	268	GLY
16	AG	279	ASN
16	AG	350	ALA
16	AG	365	ILE
22	H	108	VAL
22	H	309	MET
22	H	333	LEU
39	Y	93	ASN
48	h	158	ALA
52	l	142	ALA
66	z	3	ARG
9	9	48	ALA
9	9	91	ALA
9	9	118	ILE
9	9	130	PRO
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	76	GLU
22	H	142	ARG
27	M	130	ASN
30	P	58	ASN
31	Q	119	ASN
38	X	105	ASN
39	Y	20	SER
39	Y	64	ARG

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Mol	Chain	Res	Type
39	Y	106	GLN
9	9	69	PHE
9	9	73	LYS
9	9	108	VAL
9	9	129	LEU
9	9	133	GLU
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	82	THR
23	I	80	LYS
39	Y	83	ALA
40	Z	21	GLU
54	n	40	VAL
12	AB	167	ARG
12	AB	178	VAL
12	AB	179	GLU
14	AE	91	GLU
16	AG	224	LYS
16	AG	399	ASP
22	H	70	VAL
39	Y	22	PRO
39	Y	71	LYS
39	Y	89	SER
40	Z	7	ILE
4	3	39	ILE
9	9	28	ALA
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

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Mol	Chain	Res	Type
16	AG	364	ASP
16	AG	382	GLU
39	Y	62	ALA
12	AB	170	PRO
26	L	96	VAL
39	Y	23	VAL
39	Y	100	ILE
1	0	44	GLY
31	Q	74	VAL
35	U	64	GLY
9	9	54	VAL
11	AA	1317	PRO
25	K	44	GLY
54	n	62	GLY
28	N	75	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	78 (93%)	6 (7%)	14	47
2	1	93/93 (100%)	84 (90%)	9 (10%)	8	31
3	2	81/84 (96%)	76 (94%)	5 (6%)	18	53
4	3	84/85 (99%)	78 (93%)	6 (7%)	14	47
5	4	78/78 (100%)	74 (95%)	4 (5%)	24	60
9	9	112/123 (91%)	65 (58%)	47 (42%)	0	0
11	AA	1155/1157 (100%)	1142 (99%)	13 (1%)	73	88
12	AB	138/158 (87%)	104 (75%)	34 (25%)	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%)	18	53
15	AF	70/75 (93%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AG	409/409 (100%)	297 (73%)	112 (27%)	0	1
17	C	57/65 (88%)	55 (96%)	2 (4%)	36	69
19	E	65/66 (98%)	60 (92%)	5 (8%)	13	44
20	F	60/61 (98%)	57 (95%)	3 (5%)	24	60
21	G	187/199 (94%)	178 (95%)	9 (5%)	25	61
22	H	137/461 (30%)	128 (93%)	9 (7%)	16	51
23	I	171/190 (90%)	165 (96%)	6 (4%)	36	69
24	J	172/173 (99%)	165 (96%)	7 (4%)	30	66
25	K	119/126 (94%)	111 (93%)	8 (7%)	16	50
26	L	91/116 (78%)	85 (93%)	6 (7%)	16	51
27	M	124/147 (84%)	116 (94%)	8 (6%)	17	51
28	N	104/105 (99%)	102 (98%)	2 (2%)	57	81
29	O	105/107 (98%)	100 (95%)	5 (5%)	25	61
30	P	86/90 (96%)	78 (91%)	8 (9%)	9	33
31	Q	90/99 (91%)	87 (97%)	3 (3%)	38	71
32	R	101/104 (97%)	94 (93%)	7 (7%)	15	49
33	S	83/84 (99%)	79 (95%)	4 (5%)	25	61
34	T	76/77 (99%)	64 (84%)	12 (16%)	2	12
35	U	65/65 (100%)	60 (92%)	5 (8%)	13	44
36	V	74/78 (95%)	72 (97%)	2 (3%)	44	75
37	W	72/79 (91%)	68 (94%)	4 (6%)	21	57
38	X	94/96 (98%)	85 (90%)	9 (10%)	8	32
39	Y	109/110 (99%)	72 (66%)	37 (34%)	0	0
40	Z	26/85 (31%)	12 (46%)	14 (54%)	0	0
42	b	58/63 (92%)	57 (98%)	1 (2%)	60	83
43	c	67/68 (98%)	64 (96%)	3 (4%)	27	63
45	e	54/55 (98%)	53 (98%)	1 (2%)	57	81
46	f	48/49 (98%)	46 (96%)	2 (4%)	30	65
47	g	59/62 (95%)	53 (90%)	6 (10%)	7	29
48	h	216/218 (99%)	199 (92%)	17 (8%)	12	43
49	i	47/48 (98%)	41 (87%)	6 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	j	164/164 (100%)	157 (96%)	7 (4%)	29	64
51	k	47/49 (96%)	44 (94%)	3 (6%)	17	52
52	l	165/165 (100%)	151 (92%)	14 (8%)	10	38
53	m	38/38 (100%)	35 (92%)	3 (8%)	12	43
54	n	148/150 (99%)	134 (90%)	14 (10%)	8	32
55	o	51/52 (98%)	46 (90%)	5 (10%)	8	31
56	p	136/138 (99%)	132 (97%)	4 (3%)	42	74
57	q	34/34 (100%)	32 (94%)	2 (6%)	19	54
58	r	114/114 (100%)	104 (91%)	10 (9%)	10	36
59	s	116/116 (100%)	110 (95%)	6 (5%)	23	59
60	t	104/104 (100%)	98 (94%)	6 (6%)	20	55
61	u	103/103 (100%)	97 (94%)	6 (6%)	20	55
62	v	109/109 (100%)	103 (94%)	6 (6%)	21	57
63	w	99/103 (96%)	91 (92%)	8 (8%)	11	42
64	x	86/87 (99%)	80 (93%)	6 (7%)	15	48
65	y	99/100 (99%)	95 (96%)	4 (4%)	31	66
66	z	89/90 (99%)	87 (98%)	2 (2%)	52	79
All	All	8314/9148 (91%)	7692 (92%)	622 (8%)	17	45

All (622) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	13	ARG
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
2	1	7	HIS
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	109	ASP

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Mol	Chain	Res	Type
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	59	ASN
3	2	93	LEU
4	3	52	LEU
4	3	68	SER
4	3	72	ILE
4	3	89	ASP
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	41	GLU
5	4	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	11	ILE
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	27	VAL
9	9	30	SER
9	9	31	ARG
9	9	34	THR
9	9	36	ASP
9	9	37	LYS
9	9	39	THR
9	9	42	ARG
9	9	43	LYS
9	9	51	TYR
9	9	52	MET
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	62	ARG
9	9	69	PHE

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Mol	Chain	Res	Type
9	9	70	GLU
9	9	71	CYS
9	9	72	LEU
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	142	THR
9	9	143	MET
11	AA	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
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

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Mol	Chain	Res	Type
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	165	PHE
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	213	VAL
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	240	THR
16	AG	241	ASN
16	AG	242	ASP
16	AG	243	LYS
16	AG	244	ARG
16	AG	245	ILE
16	AG	254	MET
16	AG	255	ARG
16	AG	258	ARG
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

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Mol	Chain	Res	Type
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
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	33	ILE
17	C	74	HIS
19	E	6	SER

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Mol	Chain	Res	Type
19	E	10	ARG
19	E	48	GLN
19	E	54	MET
19	E	64	LYS
20	F	34	ARG
20	F	62	ARG
20	F	67	ARG
21	G	8	ASP
21	G	23	TRP
21	G	45	LYS
21	G	105	LYS
21	G	108	ARG
21	G	128	LYS
21	G	129	LEU
21	G	132	LYS
21	G	208	ARG
22	H	9	PHE
22	H	54	LYS
22	H	273	ARG
22	H	305	HIS
22	H	336	ASP
22	H	337	GLU
22	H	338	GLU
22	H	339	ARG
22	H	340	ARG
23	I	14	ILE
23	I	75	ILE
23	I	89	LYS
23	I	164	ARG
23	I	185	ASN
23	I	200	VAL
24	J	47	ARG
24	J	48	LEU
24	J	95	GLU
24	J	104	ARG
24	J	116	GLN
24	J	138	SER
24	J	143	VAL
25	K	10	GLU
25	K	15	LEU
25	K	60	ILE
25	K	69	ARG

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Mol	Chain	Res	Type
25	K	114	VAL
25	K	115	LEU
25	K	138	ARG
25	K	162	GLU
26	L	16	GLU
26	L	24	ARG
26	L	38	ARG
26	L	54	LEU
26	L	79	ARG
26	L	86	ARG
27	M	7	ILE
27	M	17	LYS
27	M	21	GLU
27	M	23	LEU
27	M	79	ARG
27	M	109	ARG
27	M	130	ASN
27	M	146	GLU
28	N	96	MET
28	N	121	LEU
29	O	12	ARG
29	O	27	LYS
29	O	60	LYS
29	O	63	LEU
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	87	LEU
30	P	90	LEU
31	Q	15	GLN
31	Q	56	ARG
31	Q	107	ILE
32	R	5	ASN
32	R	12	ARG
32	R	24	LEU
32	R	56	ARG
32	R	62	GLU
32	R	74	LEU

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Mol	Chain	Res	Type
32	R	102	LEU
33	S	45	VAL
33	S	46	LEU
33	S	89	MET
33	S	92	GLU
34	T	10	LYS
34	T	17	ARG
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	84	ARG
34	T	85	LEU
35	U	1	MET
35	U	2	VAL
35	U	6	LEU
35	U	19	VAL
35	U	50	THR
36	V	75	LEU
36	V	81	LYS
37	W	12	ASP
37	W	21	LYS
37	W	33	THR
37	W	79	THR
38	X	11	ASP
38	X	16	VAL
38	X	25	VAL
38	X	29	ARG
38	X	59	GLU
38	X	92	ARG
38	X	93	ARG
38	X	101	ARG
38	X	117	LYS
39	Y	9	LYS
39	Y	10	LEU
39	Y	16	MET
39	Y	23	VAL
39	Y	27	LEU

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Mol	Chain	Res	Type
39	Y	30	GLN
39	Y	36	GLU
39	Y	44	LYS
39	Y	48	ILE
39	Y	50	LYS
39	Y	58	ILE
39	Y	60	VAL
39	Y	61	TYR
39	Y	64	ARG
39	Y	65	SER
39	Y	67	THR
39	Y	71	LYS
39	Y	78	LEU
39	Y	80	LYS
39	Y	81	LYS
39	Y	91	LYS
39	Y	94	LYS
39	Y	95	ASP
39	Y	99	LYS
39	Y	100	ILE
39	Y	101	SER
39	Y	102	ARG
39	Y	104	GLN
39	Y	108	ILE
39	Y	112	LYS
39	Y	116	MET
39	Y	120	ASP
39	Y	124	MET
39	Y	125	THR
39	Y	126	ARG
39	Y	133	ARG
39	Y	135	MET
40	Z	1	SER
40	Z	2	ILE
40	Z	4	LYS
40	Z	6	GLN
40	Z	7	ILE
40	Z	8	ILE
40	Z	14	MET
40	Z	15	SER
40	Z	16	VAL
40	Z	23	ILE

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Mol	Chain	Res	Type
40	Z	26	MET
40	Z	28	GLU
40	Z	29	LYS
40	Z	30	PHE
42	b	70	GLU
43	c	48	THR
43	c	54	LYS
43	c	71	LEU
45	e	58	ASN
46	f	3	LYS
46	f	45	ARG
47	g	3	LYS
47	g	16	CYS
47	g	43	PHE
47	g	47	LYS
47	g	59	ARG
47	g	65	ASN
48	h	51	THR
48	h	52	ARG
48	h	118	SER
48	h	125	LYS
48	h	130	LEU
48	h	141	VAL
48	h	156	ARG
48	h	187	ASP
48	h	189	ARG
48	h	195	VAL
48	h	202	LEU
48	h	203	ARG
48	h	204	VAL
48	h	205	LEU
48	h	242	LYS
48	h	258	ARG
48	h	271	ARG
49	i	9	THR
49	i	12	LYS
49	i	26	THR
49	i	27	SER
49	i	29	SER
49	i	40	ARG
50	j	13	ARG
50	j	18	ASP

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Mol	Chain	Res	Type
50	j	32	ASN
50	j	46	ARG
50	j	91	THR
50	j	103	ASP
50	j	131	ASP
51	k	5	ILE
51	k	24	THR
51	k	26	ASN
52	l	7	ASP
52	l	17	THR
52	l	22	ASP
52	l	40	ARG
52	l	48	THR
52	l	57	LYS
52	l	69	ARG
52	l	77	ILE
52	l	80	SER
52	l	108	ILE
52	l	109	LEU
52	l	122	GLU
52	l	149	ILE
52	l	179	SER
53	m	22	MET
53	m	41	ARG
53	m	42	LEU
54	n	6	ASP
54	n	10	ASP
54	n	57	LEU
54	n	80	ARG
54	n	95	ARG
54	n	105	THR
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	152	LEU
54	n	163	ASP
55	o	8	ARG
55	o	30	ARG
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	95	ARG
56	p	125	CYS
56	p	171	THR
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	87	GLU
58	r	97	ARG
58	r	101	ASP
58	r	127	GLU
59	s	1	MET
59	s	14	ASP
59	s	30	THR
59	s	40	HIS
59	s	57	LEU
59	s	142	ILE
60	t	32	TYR
60	t	49	ARG
60	t	53	LYS
60	t	80	ASP
60	t	88	ASN
60	t	104	THR
61	u	5	THR
61	u	27	LEU
61	u	48	ARG
61	u	59	ARG
61	u	76	GLU
61	u	78	ARG
62	v	18	ARG
62	v	40	ARG
62	v	84	LYS
62	v	110	GLU
62	v	126	ILE
62	v	128	THR

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Mol	Chain	Res	Type
63	w	2	ARG
63	w	20	MET
63	w	24	MET
63	w	51	LEU
63	w	63	ARG
63	w	65	LEU
63	w	69	ARG
63	w	95	THR
64	x	13	ARG
64	x	19	GLN
64	x	31	THR
64	x	47	VAL
64	x	48	LEU
64	x	91	SER
65	y	10	GLN
65	y	27	GLU
65	y	85	SER
65	y	114	LEU
66	z	18	LEU
66	z	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
9	9	103	ASN
11	AA	69	GLN
11	AA	150	HIS
11	AA	314	ASN
11	AA	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

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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
21	G	18	HIS
25	K	70	ASN
38	X	105	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
18	D	1514/1542 (98%)	288 (19%)	34 (2%)
41	a	2859/2904 (98%)	533 (18%)	0
44	d	119/120 (99%)	17 (14%)	0
8	7	32/41 (78%)	19 (59%)	4 (12%)
All	All	4674/4759 (98%)	921 (19%)	50 (1%)

All (921) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-18	G
8	7	-17	U
8	7	-16	U
8	7	-14	U
8	7	-13	U
8	7	-12	U
8	7	-11	U
8	7	-10	U
8	7	-9	U
8	7	-8	U
8	7	-7	U
8	7	-6	U
8	7	-5	U
8	7	-3	U
8	7	-1	U
8	7	0	U

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Mol	Chain	Res	Type
8	7	1	U
8	7	12	G
8	7	13	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C

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Mol	Chain	Res	Type
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	31	G
10	B	32	C
10	B	36	U
10	B	37	A
10	B	38	A
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
18	D	4	U
18	D	5	U
18	D	9	G
18	D	22	G
18	D	29	U
18	D	32	A
18	D	39	G
18	D	41	G
18	D	47	C
18	D	48	C
18	D	50	A
18	D	51	A
18	D	52	C
18	D	54	C
18	D	69	G
18	D	70	U
18	D	71	A

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Mol	Chain	Res	Type
18	D	72	A
18	D	74	A
18	D	76	G
18	D	82	G
18	D	83	C
18	D	84	U
18	D	87	C
18	D	90	C
18	D	94	G
18	D	95	C
18	D	96	U
18	D	108	G
18	D	120	A
18	D	122	G
18	D	128	G
18	D	131	A
18	D	141	G
18	D	144	G
18	D	148	G
18	D	149	A
18	D	160	A
18	D	164	G
18	D	173	U
18	D	181	A
18	D	182	A
18	D	197	A
18	D	198	G
18	D	204	G
18	D	208	U
18	D	209	U
18	D	210	C
18	D	211	G
18	D	212	G
18	D	216	U
18	D	226	G
18	D	245	U
18	D	247	G
18	D	251	G
18	D	258	G
18	D	262	A
18	D	266	G
18	D	267	C

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Mol	Chain	Res	Type
18	D	271	C
18	D	279	A
18	D	289	G
18	D	299	G
18	D	306	A
18	D	321	A
18	D	328	C
18	D	329	A
18	D	332	G
18	D	347	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
18	D	376	G
18	D	382	A
18	D	384	G
18	D	392	C
18	D	393	A
18	D	397	A
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	424	G
18	D	429	U
18	D	446	G
18	D	451	A
18	D	457	G
18	D	458	U
18	D	460	A
18	D	463	U
18	D	464	U
18	D	467	U
18	D	468	A
18	D	469	C
18	D	478	A

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Mol	Chain	Res	Type
18	D	479	U
18	D	481	G
18	D	484	G
18	D	485	U
18	D	486	U
18	D	505	G
18	D	509	A
18	D	511	C
18	D	518	C
18	D	519	C
18	D	526	C
18	D	531	U
18	D	532	A
18	D	533	A
18	D	542	G
18	D	547	A
18	D	559	A
18	D	562	U
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	628	G
18	D	633	G
18	D	642	A
18	D	649	A
18	D	650	G
18	D	653	U
18	D	665	A
18	D	666	G
18	D	687	A
18	D	700	G
18	D	723	U
18	D	724	G
18	D	731	G
18	D	734	G
18	D	747	A
18	D	748	G
18	D	755	G

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Mol	Chain	Res	Type
18	D	760	G
18	D	777	A
18	D	793	U
18	D	794	A
18	D	815	A
18	D	817	C
18	D	828	U
18	D	829	G
18	D	832	G
18	D	841	C
18	D	844	G
18	D	845	A
18	D	849	G
18	D	874	G
18	D	887	G
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	954	G
18	D	960	U
18	D	963	G
18	D	969	A
18	D	972	C
18	D	975	A
18	D	976	G
18	D	991	U
18	D	992	U
18	D	993	G
18	D	996	A
18	D	999	C
18	D	1004	A
18	D	1008	U
18	D	1009	U
18	D	1017	U
18	D	1018	G
18	D	1021	A
18	D	1024	G
18	D	1026	G
18	D	1028	C

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Mol	Chain	Res	Type
18	D	1030	U
18	D	1031	C
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	1086	U
18	D	1094	G
18	D	1095	U
18	D	1099	G
18	D	1101	A
18	D	1124	G
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	1143	G
18	D	1145	A
18	D	1146	A
18	D	1151	A
18	D	1152	A
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	1206	G
18	D	1211	U
18	D	1212	U
18	D	1213	A
18	D	1214	C

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Mol	Chain	Res	Type
18	D	1215	G
18	D	1226	C
18	D	1227	A
18	D	1228	C
18	D	1238	A
18	D	1256	A
18	D	1257	A
18	D	1260	G
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
18	D	1299	A
18	D	1300	G
18	D	1302	C
18	D	1305	G
18	D	1312	G
18	D	1317	C
18	D	1320	C
18	D	1323	G
18	D	1329	A
18	D	1338	G
18	D	1340	A
18	D	1346	A
18	D	1347	G
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	1396	A
18	D	1397	C
18	D	1398	A
18	D	1404	C
18	D	1419	G
18	D	1429	A

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Mol	Chain	Res	Type
18	D	1441	A
18	D	1446	A
18	D	1447	A
18	D	1448	C
18	D	1452	C
18	D	1453	G
18	D	1475	G
18	D	1487	G
18	D	1492	A
18	D	1493	A
18	D	1494	G
18	D	1495	U
18	D	1497	G
18	D	1503	A
18	D	1506	U
18	D	1517	G
18	D	1529	G
18	D	1530	G
18	D	1534	A
41	a	10	A
41	a	15	G
41	a	34	U
41	a	35	G
41	a	46	G
41	a	58	G
41	a	60	G
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	93	G
41	a	96	C
41	a	102	U
41	a	103	A
41	a	110	G
41	a	114	U
41	a	118	A
41	a	119	A
41	a	120	U

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Mol	Chain	Res	Type
41	a	122	G
41	a	131	A
41	a	136	G
41	a	139	U
41	a	140	C
41	a	141	G
41	a	145	C
41	a	163	C
41	a	165	A
41	a	181	A
41	a	196	A
41	a	200	U
41	a	215	G
41	a	216	A
41	a	222	A
41	a	225	C
41	a	248	G
41	a	249	C
41	a	261	G
41	a	264	C
41	a	265	A
41	a	266	G
41	a	267	C
41	a	271	G
41	a	272	A
41	a	275	C
41	a	276	U
41	a	278	A
41	a	285	G
41	a	311	A
41	a	324	A
41	a	329	G
41	a	330	A
41	a	353	C
41	a	359	G
41	a	361	G
41	a	362	A
41	a	371	A
41	a	372	G
41	a	373	U
41	a	375	G
41	a	383	C

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Mol	Chain	Res	Type
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	435	C
41	a	451	U
41	a	456	C
41	a	457	A
41	a	477	A
41	a	481	G
41	a	491	G
41	a	501	A
41	a	503	A
41	a	504	A
41	a	505	A
41	a	509	C
41	a	522	A
41	a	529	A
41	a	532	A
41	a	543	G
41	a	546	U
41	a	547	A
41	a	548	G
41	a	549	G
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	618	G
41	a	621	A
41	a	627	A

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Mol	Chain	Res	Type
41	a	637	A
41	a	645	C
41	a	647	G
41	a	654	A
41	a	664	G
41	a	668	A
41	a	685	A
41	a	686	U
41	a	710	U
41	a	717	C
41	a	730	A
41	a	738	G
41	a	757	G
41	a	764	A
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	800	A
41	a	802	A
41	a	805	G
41	a	812	C
41	a	819	A
41	a	827	U
41	a	828	U
41	a	845	A
41	a	846	U
41	a	858	G
41	a	859	G
41	a	869	G
41	a	878	A
41	a	881	G
41	a	884	U
41	a	885	C
41	a	888	C
41	a	891	G
41	a	892	A
41	a	893	C
41	a	895	U
41	a	896	A

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Mol	Chain	Res	Type
41	a	897	C
41	a	899	A
41	a	907	G
41	a	910	A
41	a	914	G
41	a	915	C
41	a	931	U
41	a	941	A
41	a	945	A
41	a	946	C
41	a	953	G
41	a	961	C
41	a	974	G
41	a	983	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	1022	G
41	a	1023	U
41	a	1026	G
41	a	1033	U
41	a	1041	G
41	a	1045	C
41	a	1046	A
41	a	1047	G
41	a	1060	U
41	a	1061	U
41	a	1062	G
41	a	1063	G
41	a	1064	C
41	a	1065	U
41	a	1066	U
41	a	1067	A
41	a	1068	G
41	a	1069	A
41	a	1070	A
41	a	1071	G
41	a	1073	A
41	a	1074	G

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Mol	Chain	Res	Type
41	a	1076	C
41	a	1079	C
41	a	1080	A
41	a	1081	U
41	a	1082	U
41	a	1083	U
41	a	1084	A
41	a	1087	G
41	a	1088	A
41	a	1090	A
41	a	1095	A
41	a	1096	A
41	a	1107	G
41	a	1110	G
41	a	1111	A
41	a	1112	G
41	a	1119	U
41	a	1122	G
41	a	1132	U
41	a	1134	A
41	a	1135	C
41	a	1142	A
41	a	1169	A
41	a	1170	C
41	a	1173	U
41	a	1174	U
41	a	1175	A
41	a	1176	U
41	a	1177	G
41	a	1178	C
41	a	1179	G
41	a	1180	U
41	a	1186	G
41	a	1238	G
41	a	1248	G
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	1301	A

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Mol	Chain	Res	Type
41	a	1321	A
41	a	1345	C
41	a	1352	U
41	a	1365	A
41	a	1368	G
41	a	1378	A
41	a	1379	U
41	a	1380	G
41	a	1383	A
41	a	1387	A
41	a	1392	A
41	a	1395	A
41	a	1406	U
41	a	1407	G
41	a	1408	G
41	a	1411	U
41	a	1414	C
41	a	1415	U
41	a	1416	G
41	a	1417	C
41	a	1419	A
41	a	1420	A
41	a	1428	C
41	a	1452	G
41	a	1453	A
41	a	1460	U
41	a	1478	G
41	a	1482	G
41	a	1490	A
41	a	1497	U
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	1534	U
41	a	1535	A
41	a	1536	C
41	a	1537	G
41	a	1554	U
41	a	1559	U

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Mol	Chain	Res	Type
41	a	1566	A
41	a	1569	A
41	a	1578	U
41	a	1580	A
41	a	1581	G
41	a	1582	C
41	a	1583	A
41	a	1584	U
41	a	1589	U
41	a	1590	A
41	a	1608	A
41	a	1609	A
41	a	1610	A
41	a	1647	U
41	a	1648	U
41	a	1649	G
41	a	1651	G
41	a	1674	G
41	a	1677	A
41	a	1703	G
41	a	1714	U
41	a	1715	G
41	a	1718	G
41	a	1729	U
41	a	1730	C
41	a	1732	C
41	a	1738	G
41	a	1750	G
41	a	1755	A
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

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Mol	Chain	Res	Type
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	1872	A
41	a	1873	G
41	a	1905	C
41	a	1906	G
41	a	1907	G
41	a	1913	A
41	a	1914	C
41	a	1919	A
41	a	1920	C
41	a	1922	G
41	a	1923	U
41	a	1924	C
41	a	1925	C
41	a	1926	U
41	a	1928	A
41	a	1929	G
41	a	1930	G
41	a	1936	A
41	a	1938	A
41	a	1955	U
41	a	1965	C
41	a	1967	C
41	a	1970	A
41	a	1971	U
41	a	1972	G
41	a	1987	A
41	a	1991	U
41	a	1992	G
41	a	1993	U
41	a	1997	C
41	a	2002	G
41	a	2022	U
41	a	2023	C
41	a	2027	G
41	a	2033	A
41	a	2043	C

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Mol	Chain	Res	Type
41	a	2051	A
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	2077	A
41	a	2093	G
41	a	2097	A
41	a	2099	U
41	a	2100	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	2121	G
41	a	2122	U
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	2141	G
41	a	2146	C
41	a	2147	A
41	a	2154	A
41	a	2157	G
41	a	2158	A
41	a	2159	G
41	a	2162	G
41	a	2163	A
41	a	2164	C

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Mol	Chain	Res	Type
41	a	2165	C
41	a	2169	A
41	a	2171	A
41	a	2172	U
41	a	2178	C
41	a	2182	U
41	a	2183	A
41	a	2185	U
41	a	2188	U
41	a	2189	U
41	a	2190	G
41	a	2191	A
41	a	2193	G
41	a	2194	U
41	a	2198	A
41	a	2204	G
41	a	2210	U
41	a	2211	A
41	a	2212	A
41	a	2213	U
41	a	2225	A
41	a	2226	C
41	a	2229	U
41	a	2238	G
41	a	2239	G
41	a	2244	U
41	a	2250	G
41	a	2268	A
41	a	2278	A
41	a	2283	C
41	a	2287	A
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	2339	C
41	a	2345	G

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Mol	Chain	Res	Type
41	a	2347	C
41	a	2350	C
41	a	2361	G
41	a	2372	U
41	a	2376	A
41	a	2383	G
41	a	2385	C
41	a	2402	U
41	a	2403	C
41	a	2406	A
41	a	2423	U
41	a	2424	C
41	a	2425	A
41	a	2426	A
41	a	2429	G
41	a	2430	A
41	a	2431	U
41	a	2434	A
41	a	2435	A
41	a	2441	U
41	a	2447	G
41	a	2448	A
41	a	2470	G
41	a	2474	U
41	a	2476	A
41	a	2478	A
41	a	2484	G
41	a	2491	U
41	a	2502	G
41	a	2506	U
41	a	2507	C
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	2547	A
41	a	2554	U
41	a	2566	A
41	a	2567	G

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

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Mol	Chain	Res	Type
41	a	2867	G
41	a	2880	C
41	a	2884	U
41	a	2885	G
41	a	2891	U
41	a	2902	C
44	d	2	G
44	d	9	G
44	d	13	G
44	d	16	G
44	d	17	C
44	d	35	C
44	d	36	C
44	d	45	A
44	d	51	G
44	d	56	G
44	d	64	G
44	d	66	A
44	d	88	C
44	d	89	U
44	d	90	C
44	d	99	A
44	d	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-17	U
8	7	-14	U
8	7	-11	U
8	7	11	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	22	G
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G
10	B	9	G
10	B	22	G
10	B	37	A

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Mol	Chain	Res	Type
10	B	60	U
18	D	7	A
18	D	70	U
18	D	121	U
18	D	181	A
18	D	183	C
18	D	197	A
18	D	209	U
18	D	305	G
18	D	328	C
18	D	428	G
18	D	496	A
18	D	517	G
18	D	531	U
18	D	532	A
18	D	562	U
18	D	641	U
18	D	722	G
18	D	793	U
18	D	991	U
18	D	992	U
18	D	1145	A
18	D	1196	A
18	D	1211	U
18	D	1212	U
18	D	1213	A
18	D	1214	C
18	D	1225	A
18	D	1299	A
18	D	1396	A
18	D	1432	G
18	D	1447	A
18	D	1491	G
18	D	1492	A
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

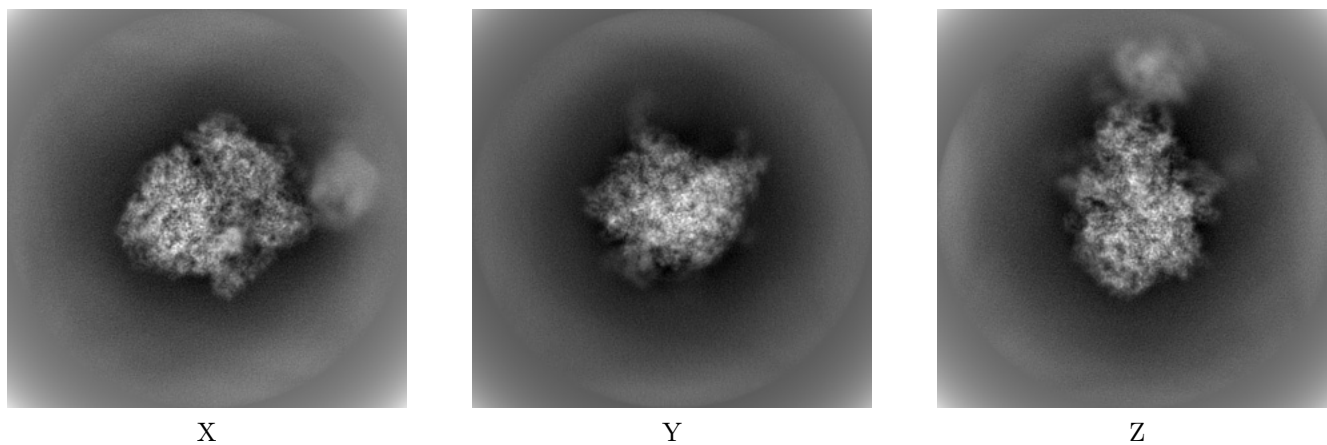
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-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](#)

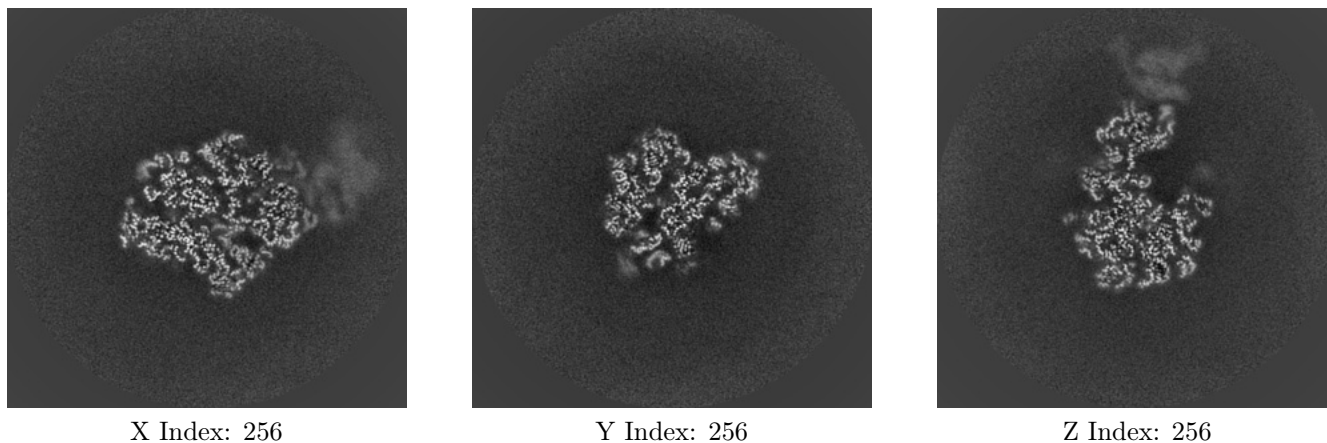
6.1.1 Primary map



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

6.2 Central slices [i](#)

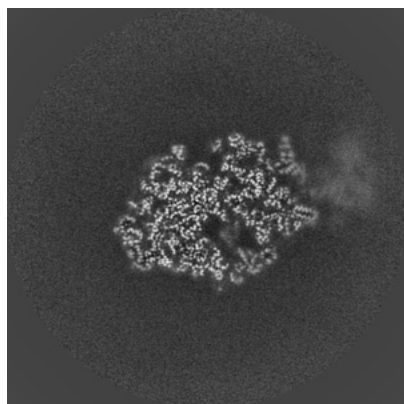
6.2.1 Primary map



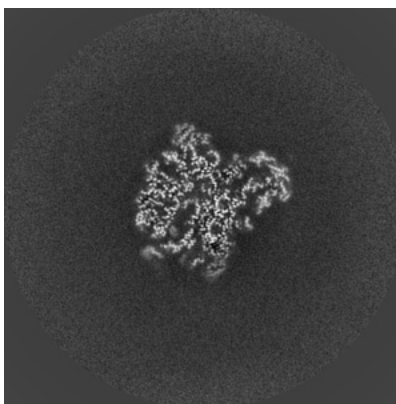
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

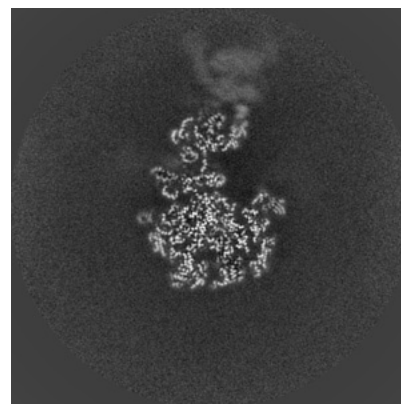
6.3.1 Primary map



X Index: 242



Y Index: 250



Z Index: 259

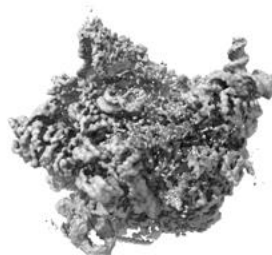
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

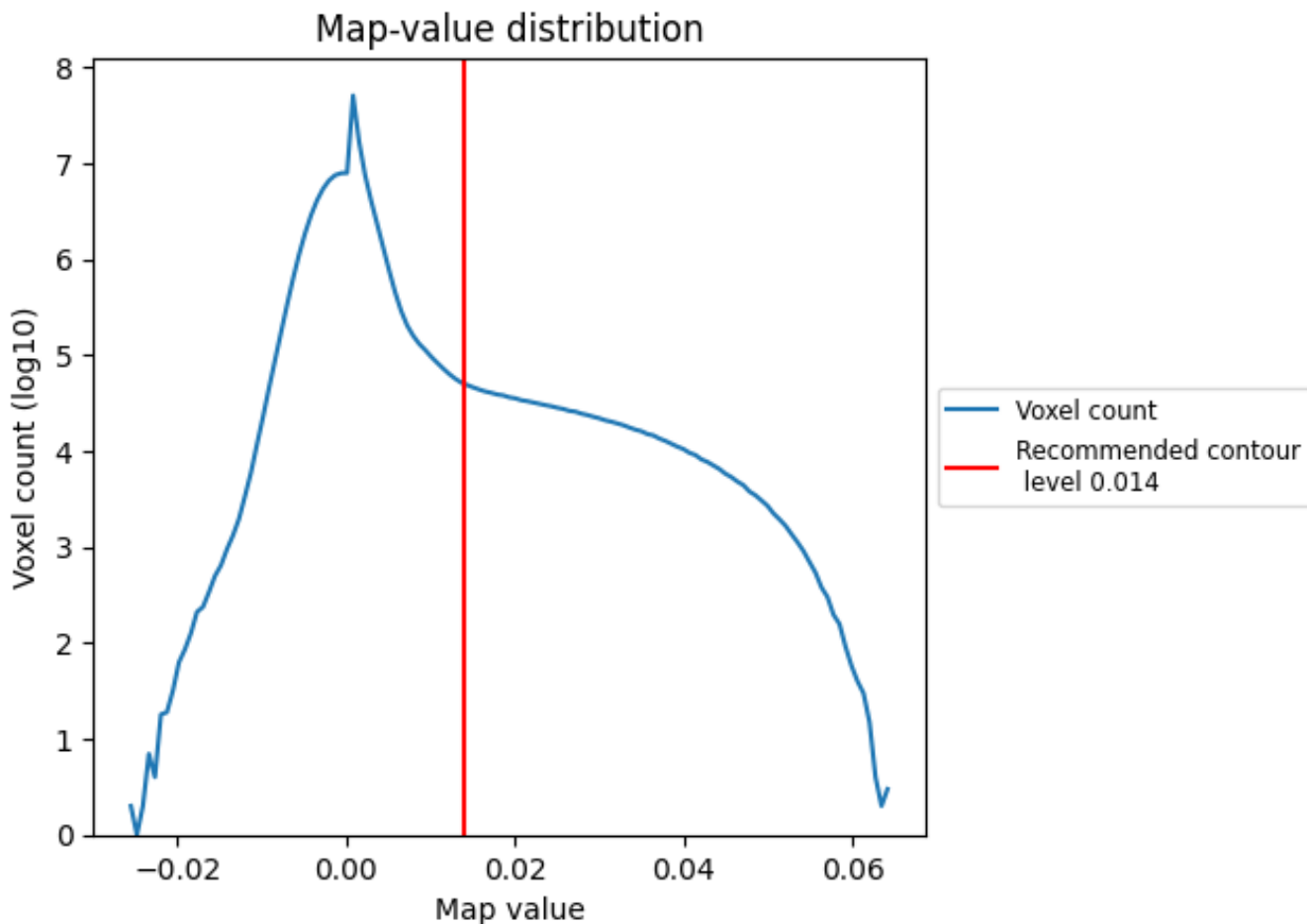
6.5 Mask visualisation

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

7 Map analysis [i](#)

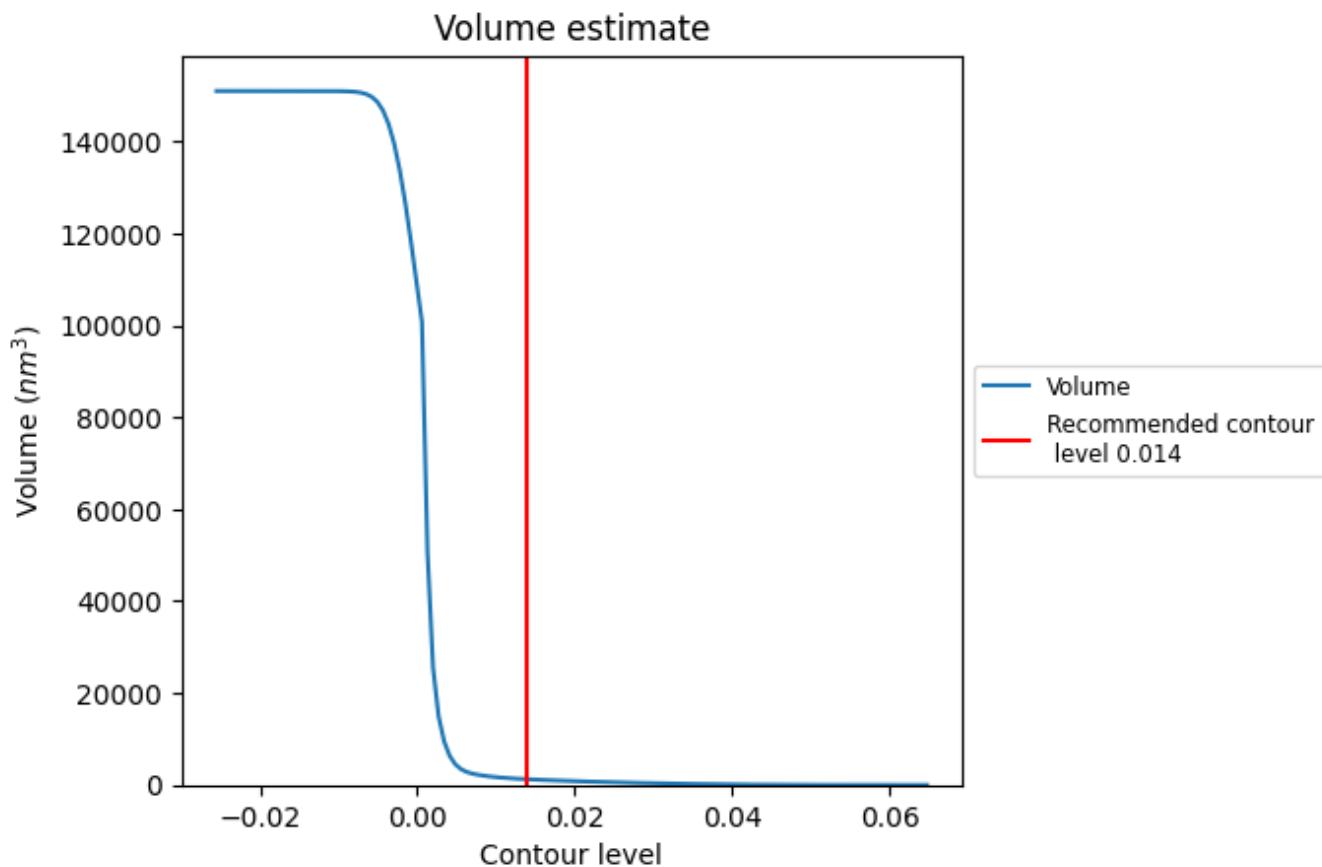
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

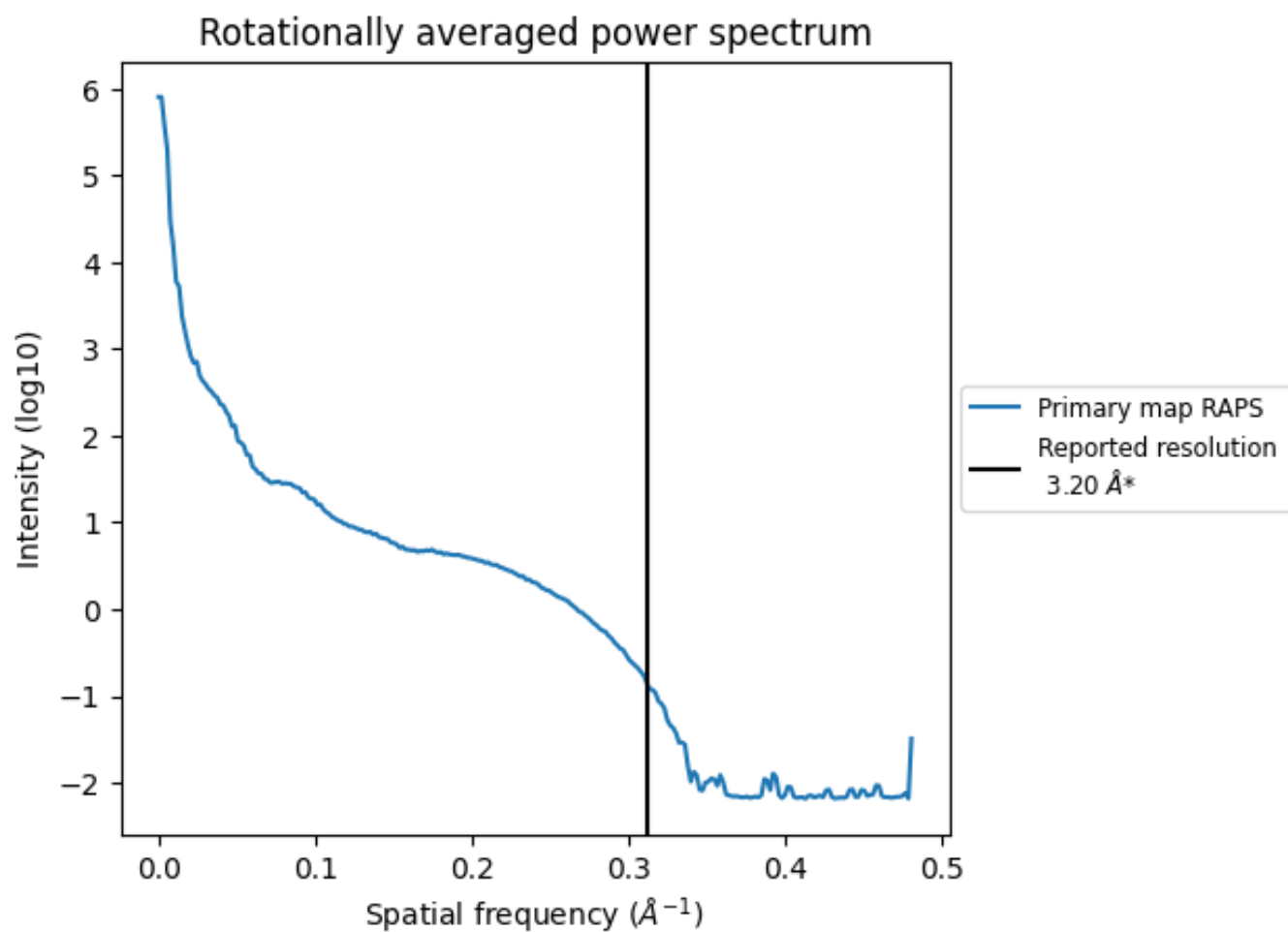
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 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 i



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

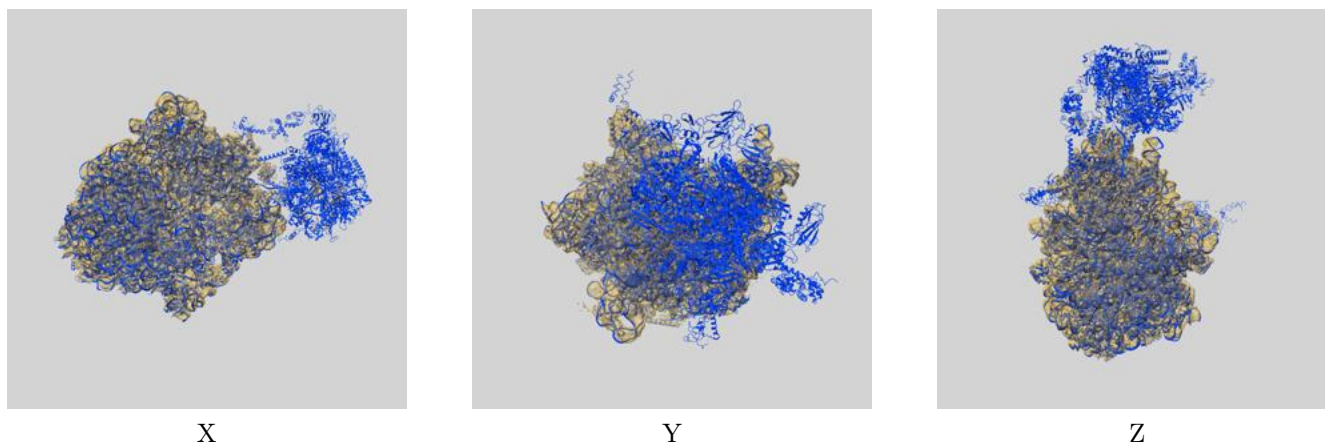
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

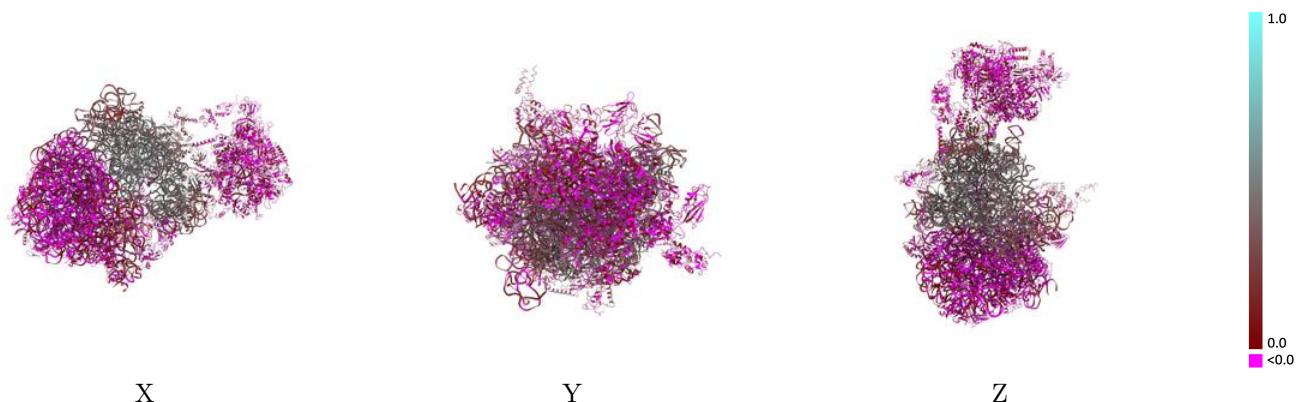
This section contains information regarding the fit between EMDB map EMD-22082 and PDB model 6X6T. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



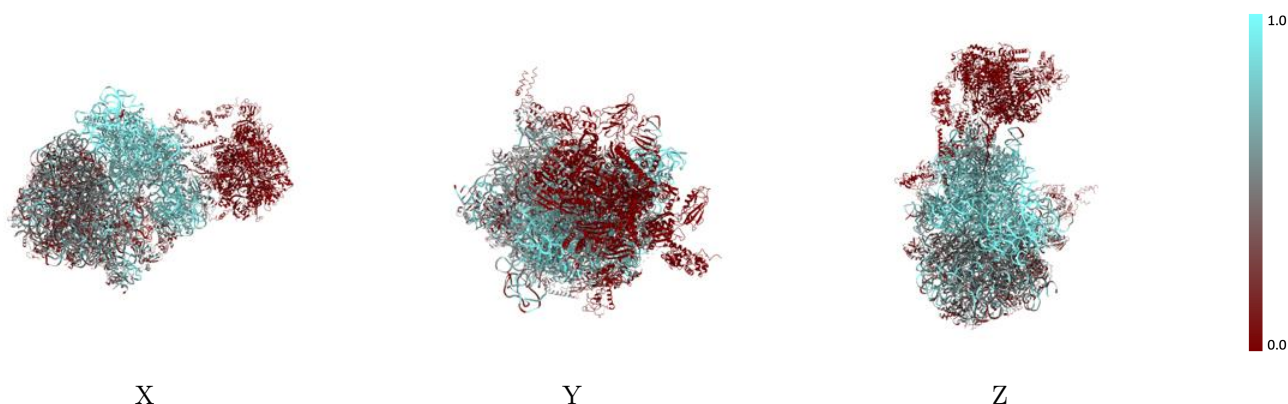
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



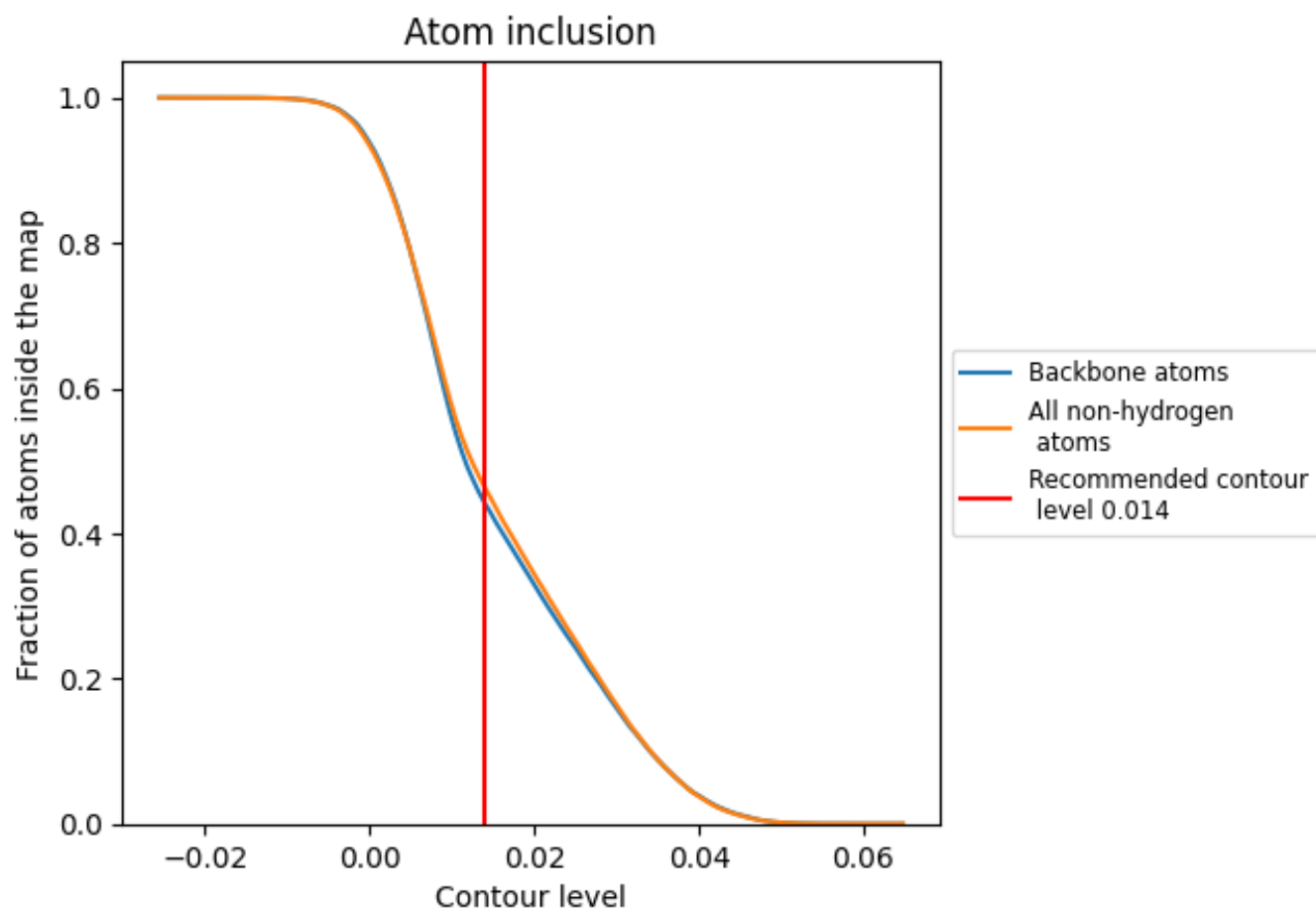
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 46% 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	 0.4633	 0.1180
0	 0.3501	 -0.0380
1	 0.3385	 -0.0430
2	 0.3192	 -0.0530
3	 0.3235	 -0.0190
4	 0.3957	 0.0260
5	 0.0254	 0.0380
6	 0.0756	 0.0390
7	 0.1206	 0.0400
9	 0.2258	 0.1050
A	 0.5154	 0.1640
AA	 0.0073	 0.0250
AB	 0.1219	 0.1120
AC	 0.0005	 0.0090
AD	 0.0005	 0.0120
AE	 0.0032	 0.0160
AF	 0.0000	 0.0220
AG	 0.1944	 0.1360
B	 0.4617	 0.0880
C	 0.6750	 0.3960
D	 0.9082	 0.4050
E	 0.7049	 0.3360
F	 0.5653	 0.3510
G	 0.6721	 0.3610
H	 0.0275	 0.0640
I	 0.6629	 0.3950
J	 0.7057	 0.4110
K	 0.7257	 0.4400
L	 0.6602	 0.3570
M	 0.6337	 0.3240
N	 0.7438	 0.4290
O	 0.6813	 0.3310
P	 0.5974	 0.3090
Q	 0.7128	 0.4160
R	 0.7238	 0.4650



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Chain	Atom inclusion	Q-score
S	 0.7028	 0.3650
T	 0.7188	 0.3920
U	 0.7241	 0.3890
V	 0.6915	 0.4010
W	 0.3617	 0.0050
X	 0.3295	 0.0050
Y	 0.0959	 0.1150
Z	 0.0000	 0.1320
a	 0.5290	 -0.0020
b	 0.3728	 0.0030
c	 0.2729	 -0.0660
d	 0.6353	 0.0670
e	 0.3620	 -0.0030
f	 0.3211	 -0.0570
g	 0.3092	 0.0450
h	 0.3105	 -0.0520
i	 0.3084	 -0.0780
j	 0.2978	 -0.0760
k	 0.3445	 -0.0350
l	 0.3079	 -0.0270
m	 0.2761	 -0.0740
n	 0.4151	 0.0490
o	 0.2933	 -0.0540
p	 0.3831	 0.0470
q	 0.2979	 -0.0410
r	 0.2555	 0.0580
s	 0.2936	 -0.0600
t	 0.2834	 -0.0500
u	 0.2832	 -0.0420
v	 0.3570	 0.0050
w	 0.3133	 -0.0780
x	 0.4148	 0.0240
y	 0.3232	 -0.0430
z	 0.3249	 -0.0520