Full wwPDB EM Validation Report (i)

Nov 14, 2022 – 08:49 PM EST

PDB ID	:	6X6T
EMDB ID	:	EMD-22082
Title	:	Cryo-EM structure of an Escherichia coli coupled transcription-translation 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 (i) 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 (i)) were used in the production of this report:

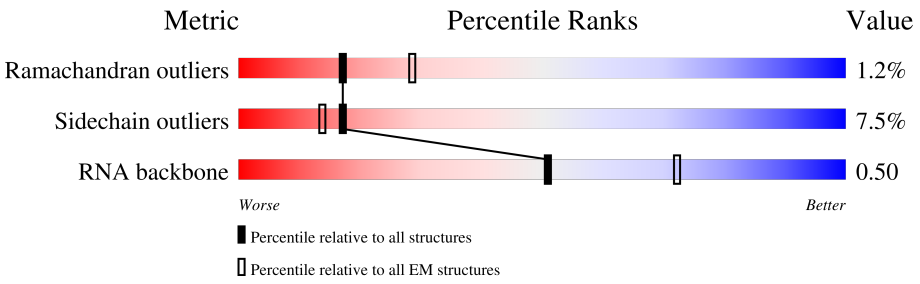
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	63%; 93%; 7%
2	1	110	64%; 92%; 8%
3	2	100	59%; 89%; 5%; 6%
4	3	104	62%; 91%; 8%; •
5	4	94	53%; 96%; •
6	5	36	64%; 47%; 17%; 36%
7	6	36	75%; 64%; 11%; 25%
8	7	41	71%; 22%; 46%; 12%; 20%

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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	66% 95% 5%
58	r	149	72% 93% 7%
59	s	142	68% 96%
60	t	123	71% 95% 5%
61	u	144	72% 96%
62	v	136	61% 96%
63	w	127	65% 87% 6% 6%
64	x	117	52% 94% 5%
65	y	115	64% 95%
66	z	118	70% 97%

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	2094	1296	379	413	6	0	0
13	AD	299	2078	1287	378	407	6	0	0

- 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	21000	6526	10612	1854	1958	50	0	0

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	650	396	122	131	1	0	0

- 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	3852	2396	669	774	13	0	0

- 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	1103	344	559	102	97	1	0	0

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

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

- 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
			Total	Mg	
67	7	1	1	1	0

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

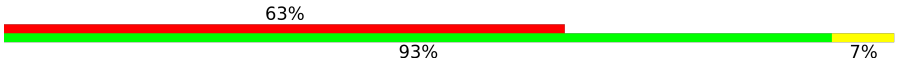
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
68	AA	2	2	2	0

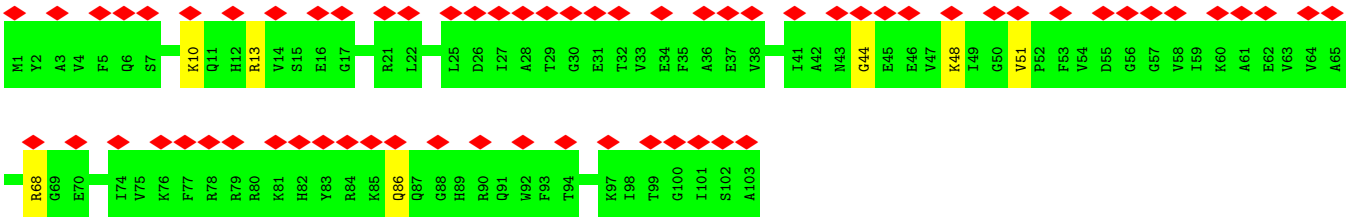
3 Residue-property plots (i)

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

- Molecule 1: 50S ribosomal protein L21

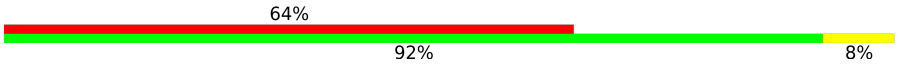
Chain 0:

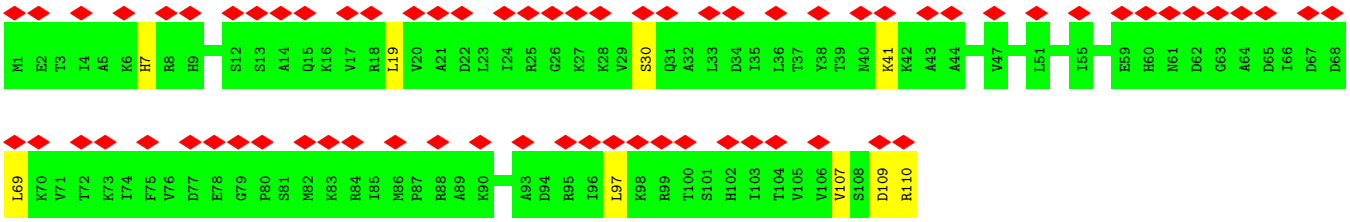




- Molecule 2: 50S ribosomal protein L22

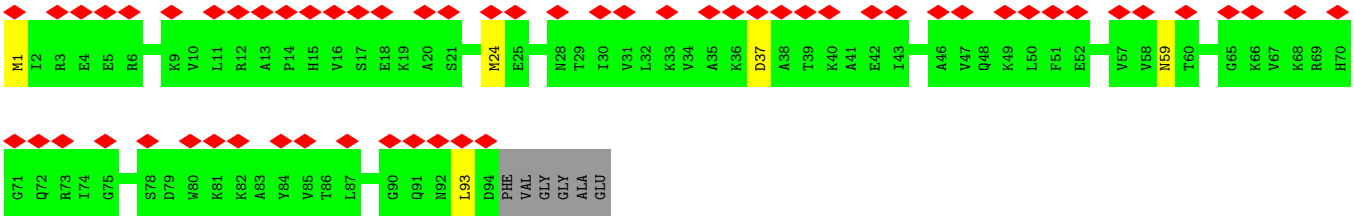
Chain 1:





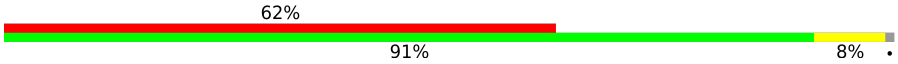
- Molecule 3: 50S ribosomal protein L23

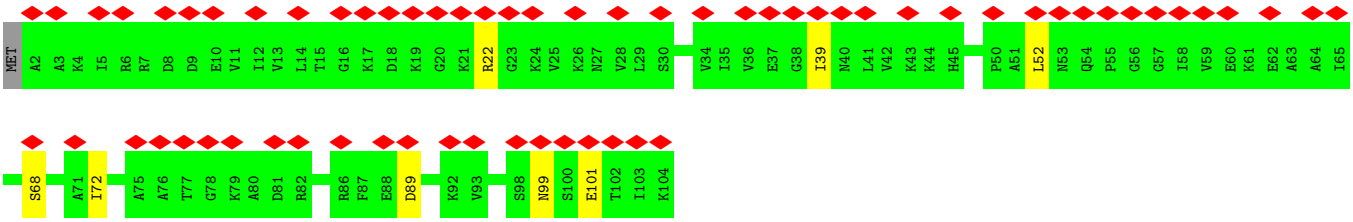
Chain 2:



- Molecule 4: 50S ribosomal protein L24

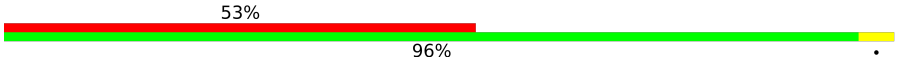
Chain 3:

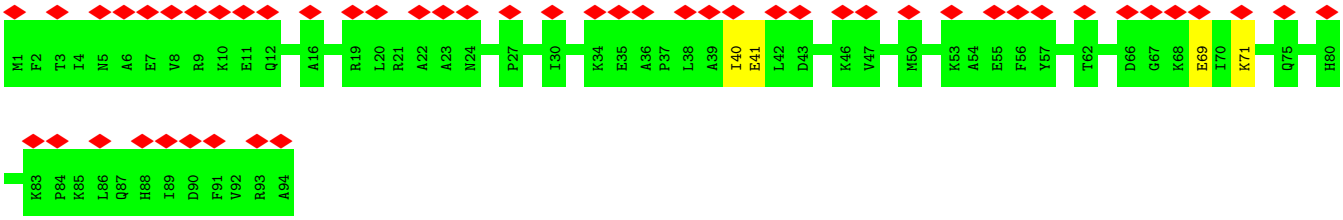




- Molecule 5: 50S ribosomal protein L25

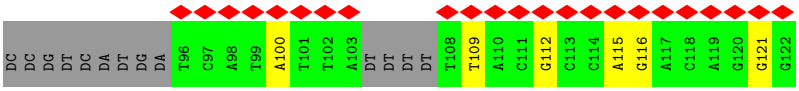
Chain 4:





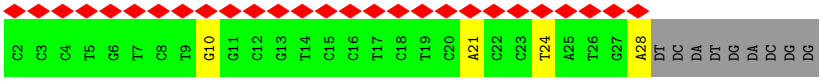
- Molecule 6: NT DNA

Chain 5:



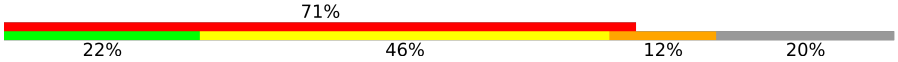
- Molecule 7: T DNA

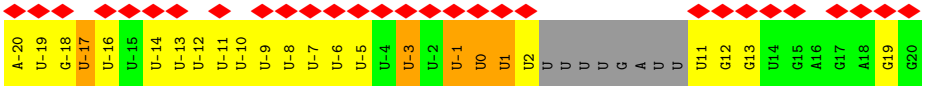
Chain 6:



- Molecule 8: mRNA with 24 nt long spacer

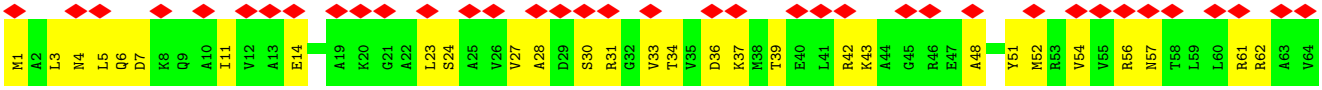
Chain 7:

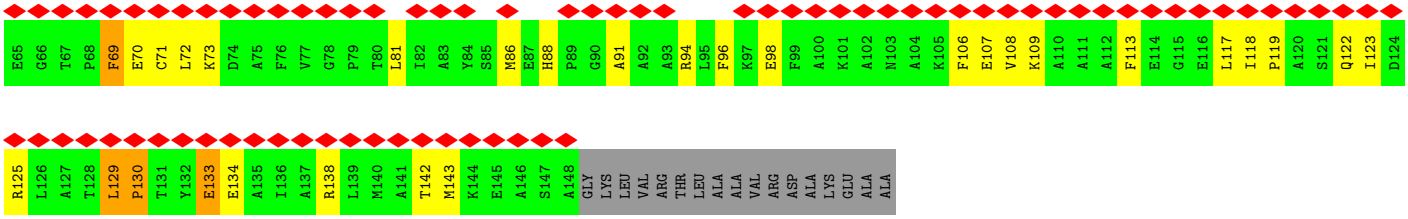




- Molecule 9: 50S ribosomal protein L10

Chain 9:



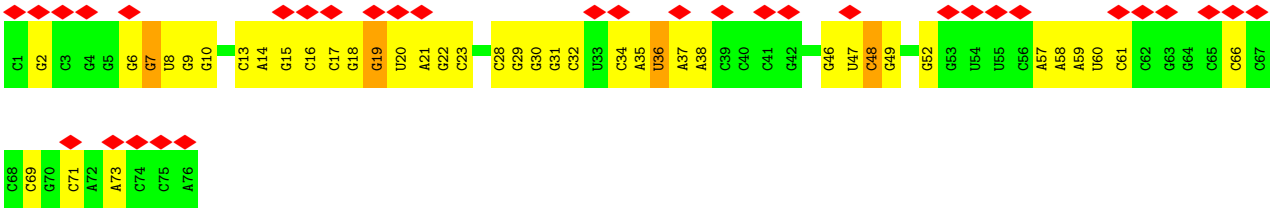


- Molecule 10: E-site and P-site tRNA (fMet)

Chain A:

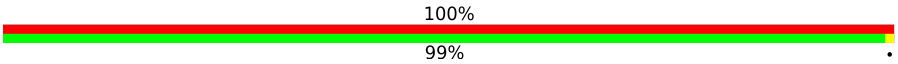
- Molecule 10: E-site and P-site tRNA (fMet)

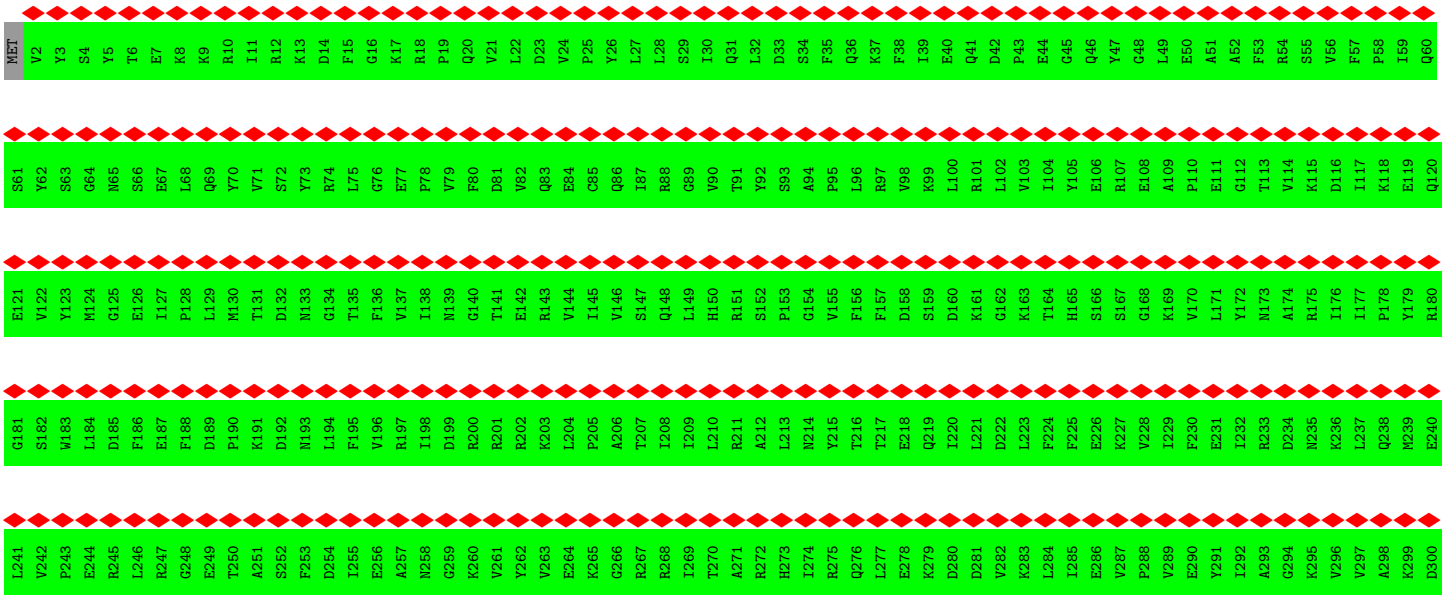
Chain B:



- Molecule 11: DNA-directed RNA polymerase subunit beta

Chain AA:





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S361 A362 L363 V364 E365 I366 Y367 R368 M369 M370 R371 P372 G373 E374 P375 P376 T377 R378 E379 A380 A381 E382 S383 L384 F385 E386 N387 L388 F389 F390 S391 E392 D393 R394 Y395 D396 L397 S398 A399 V400 G401 R402 M403 K404 F405 N406 R407 S408 L409 L410 R411 E412 E413 I414 E415 G416 S417 G418 I419 L420

S421 K422 D423 D424 I425 I426 D427 V428 M429 K430 K431 L432 I433 D434 I435 R436 M437 G438 K439 G440 E441 V442 D443 D444 I445 D446 H447 L448 G449 N450 R451 R452 I453 R454 S455 V456 G457 E458 M459 A460 E461 N462 Q463 F464 R465 V466 G467 L468 V469 R470 V471 E472 R473 A474 V475 K476 E477 R478 L479 S480

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- Molecule 12: Transcription termination/antitermination protein NusG

Chain AB: 77% 67% 18% 10%

MET SER GLU ALA PRO K6 K7 R8 W9 Y10 V11 V12 Q13 A14 F15 S16 G17 F18 E19 G20 R21 V22 A23 T24 S25 L26 R27 E28 H29 I30 K31 L32 H33 M34 M35 E36 D37 L38 F39 G40 E41 V42 M43 V44 P45 T46 E47 E48 VAL VAL GLU ILE ARG GLY GLY GLN ARG ARG LYS SER

GLU ARG K63 F64 F65 P66 G67 Y68 V69 L70 V71 Q72 M73 V74 M75 N76 D77 A78 S79 W80 H81 L82 V83 R84 S85 V86 P87 R88 V89 M90 G91 F92 I93 G94 G95 T96 S97 D98 R99 P100 A101 P102 I103 S104 D105 K106 E107 V108 D109 A110 I111 M112 N113 R114 L115 Q116 Q117 V118 G119 D120

K121 P122 R123 P124 K125 T126 L127 F128 E129 P130 G131 E132 R135 V136 N137 D138 G139 P140 F141 A142 D143 F144 N145 G146 V147 V148 E149 E150 V151 D152 Y153 E154 K155 S156 R157 L158 K159 V160 S161 V162 S163 I164 F165 G166 R167 A168 T169 P170 V171 E172 L173 D174 F175 S176 Q177 V178 E179 K180 A181

- Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AC: 91% 90% 9%

MET GLN GLY SER VAL THR E7 F8 L9 K10 P11 R12 L13 V14 D15 I16 E17 Q18 V19 S20 S21 T22 H23 A24 K25 V26 T27 L28 E29 P30 L31 E32 R33 G34 F35 G36 H37 T38 L39 G40 N41 A42 L43 R44 R45 I46 L47 L48 S49 S50 M51 P52 G53 C54 A55 V56 T57 E58 V59 E60

I61 D62 G63 V64 L65 H66 E67 Y68 S69 T70 K71 E72 G73 V74 Q75 E76 D77 I78 L79 E80 I81 L82 L83 N84 L85 K86 G87 L88 A89 V90 R91 V92 Q93 G94 K95 D96 E97 V98 I99 L100 T101 L102 N103 K104 S105 G106 I107 G108 P109 V110 T111 A112 A113 D114 I115 T116 H117 D118 G119 D120

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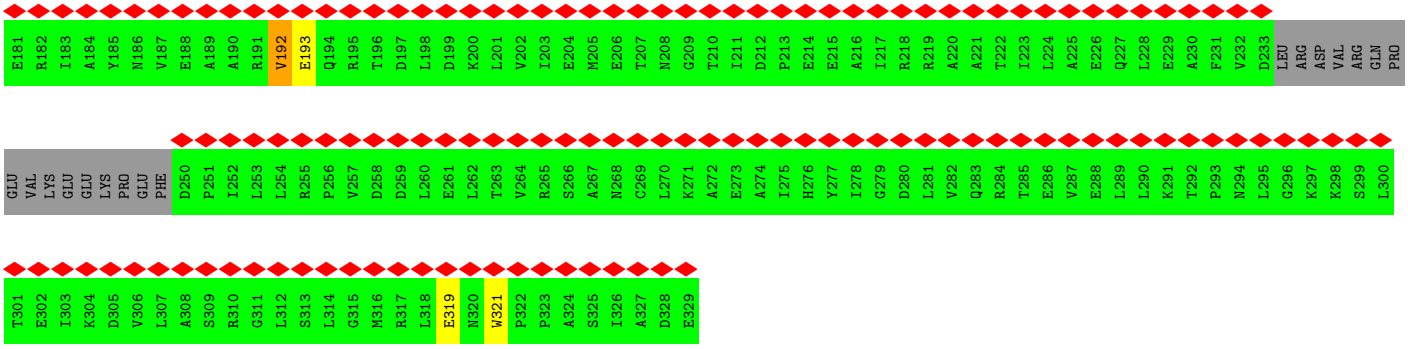
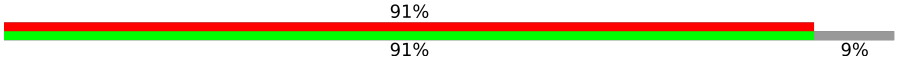
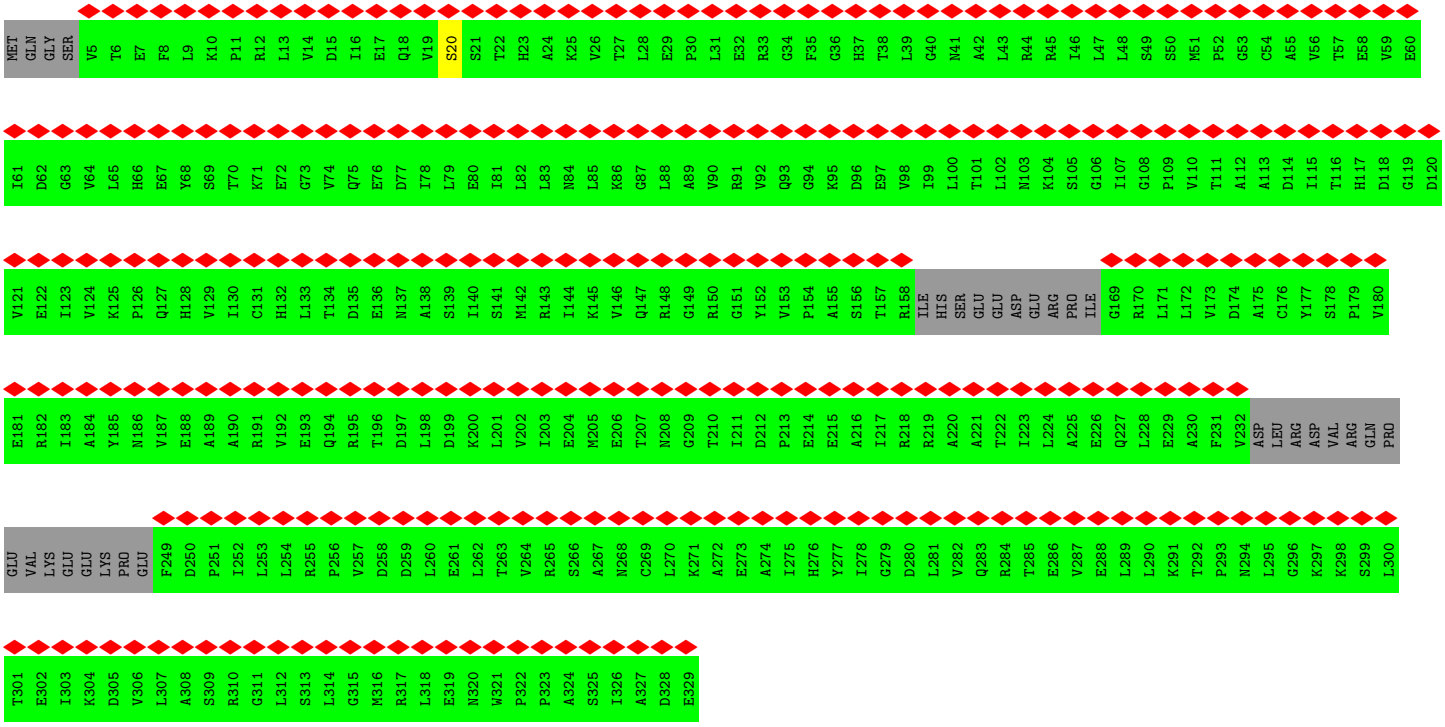


• Molecule 13: DNA-directed RNA polymerase subunit alpha

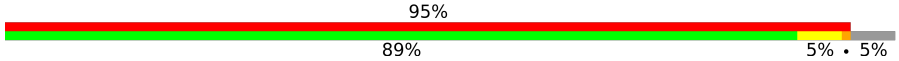
Chain AD:

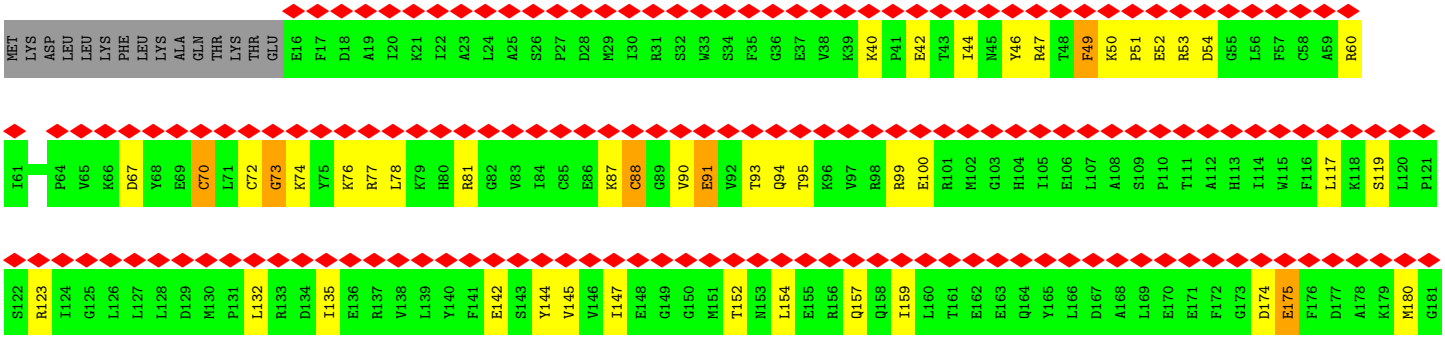


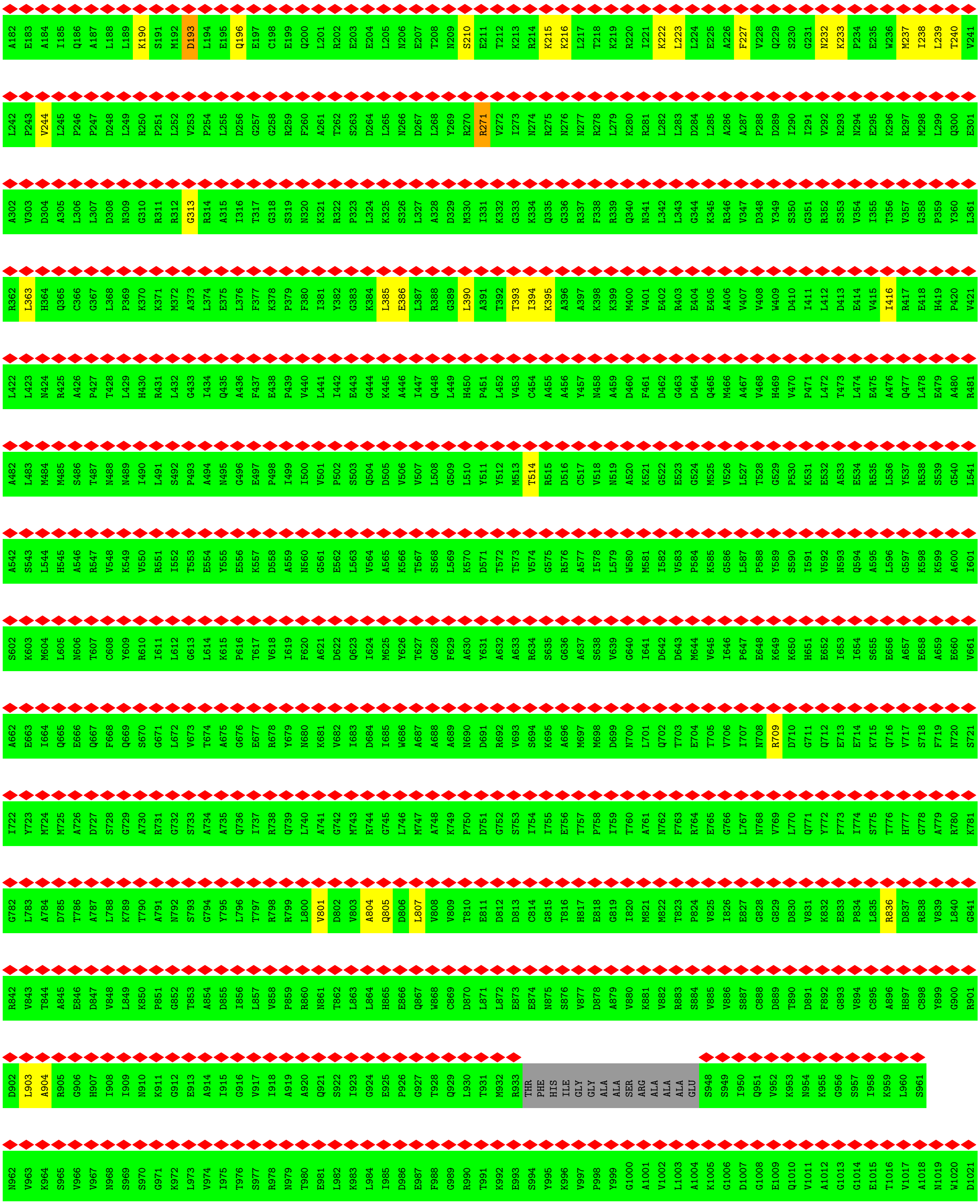


• Molecule 14: DNA-directed RNA polymerase subunit beta'

Chain AE:



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L242 P243 V244 L245 P246 P247 D248 L249 R250 P251 L252 V253 P254 L255 D256 G257 G258 R259 F260 A261 T262 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 N276 N277 R278 L279 K280 R281 L282 L283 D284 L285 A286 A287 P288 D289 I290 I291 V292 R293 N294 E295 K296 R297 M298 L299 Q300 E301
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R842 V843 T844 A845 E846 D847 V848 L849 K850 P851 G852 T853 A854 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 Q867 W868 C869 D870 L871 L872 E873 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 V886 S887 C888 D889 T890 D891 F892 G893 V894 C895 A896 H897 C898 Y899 G900 R901
D902 L903 A904 R905 G906 H907 I908 I909 N910 K911 G912 E913 A914 I915 G916 V917 I918 A919 A920 Q921 S922 I923 G924 E925 P926 G927 T928 Q929 L930 T931 M932 R933 THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU S948 S949 I950 Q951 V952 K953 N954 K955 G956 S957 I958 K959 L960 S961
N962 V963 K964 S965 V966 V967 N968 S969 S970 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 K992 E993 S994 Y995 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021

P1022 H1023 T1024 M1025 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081

D1082 A1083 Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 GLU SER GLY GLY THR LYS ASP ILE THR G1136 G1137 L1138 P1139 R1140 V1141

A1142 D1143 L1144 F1145 E1146 A1147 R1148 R1149 P1150 K1151 E1152 P1153 A1154 I1155 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 K1192 W1193 R1194 Q1195 L1196 N1197 V1198 F1199 E1200 G1201

E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209 I1210 S1211 D1212 G1213 P1214 E1215 A1216 P1217 H1218 D1219 I1220 L1221 R1222 L1223 R1224 G1225 V1226 H1227 A1228 V1229 T1230 R1231 Y1232 I1233 V1234 N1235 E1236 V1237 Q1238 D1239 V1240 Y1241 R1242 L1243 Q1244 G1245 V1246 K1247 I1248 N1249 D1250 K1251 H1252 I1253 E1254 V1255 I1256 V1257 R1258 Q1259 M1260 L1261

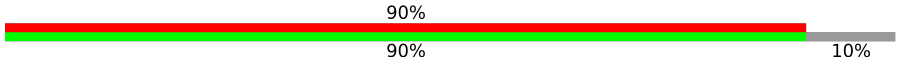
R1262 K1263 A1264 T1265 I1266 V1267 N1268 A1269 G1270 S1271 S1272 D1273 F1274 L1275 E1276 G1277 E1278 Q1279 V1280 E1281 Y1282 S1283 R1284 V1285 K1286 I1287 A1288 N1289 R1290 E1291 L1292 E1293 A1294 N1295 G1296 K1297 V1298 G1299 A1300 T1301 Y1302 S1303 R1304 D1305 L1306 L1307 G1308 I1309 T1310 K1311 A1312 S1313 L1314 A1315 T1316 E1317 S1318 F1319 I1320 S1321

A1322 A1323 S1324 F1325 Q1326 E1327 T1328 T1329 R1330 V1331 L1332 T1333 E1334 A1335 A1336 V1337 A1338 G1339 K1340 R1341 D1342 E1343 L1344 R1345 G1346 L1347 K1348 E1349 N1350 V1351 I1352 V1353 G1354 R1355 L1356 I1357 P1358 A1359 G1360 T1361 G1362 Y1363 A1364 Y1365 H1366 Q1367 D1368 R1369 M1370 R1371 R1372 R1373 ALA ALA GLY GLU ALA PRO ALA ALA

PRO GLN VAL THR ALA GLU ASP ALA SER ALA SER LEU ALA GLU LEU LEU ASN ALA GLY LEU GLY GLY SER ASP ASN GLU

- Molecule 15: DNA-directed RNA polymerase subunit omega

Chain AF:



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N61 Q62 I63 L64 D65 V66 R67 E68 R69 Q70 E71 Q72 Q73 E74 Q75 E76 A77 A78 E79 L80 Q81 A82 V83 T84 ALA ILE ALA GLU GLY ARG ARG

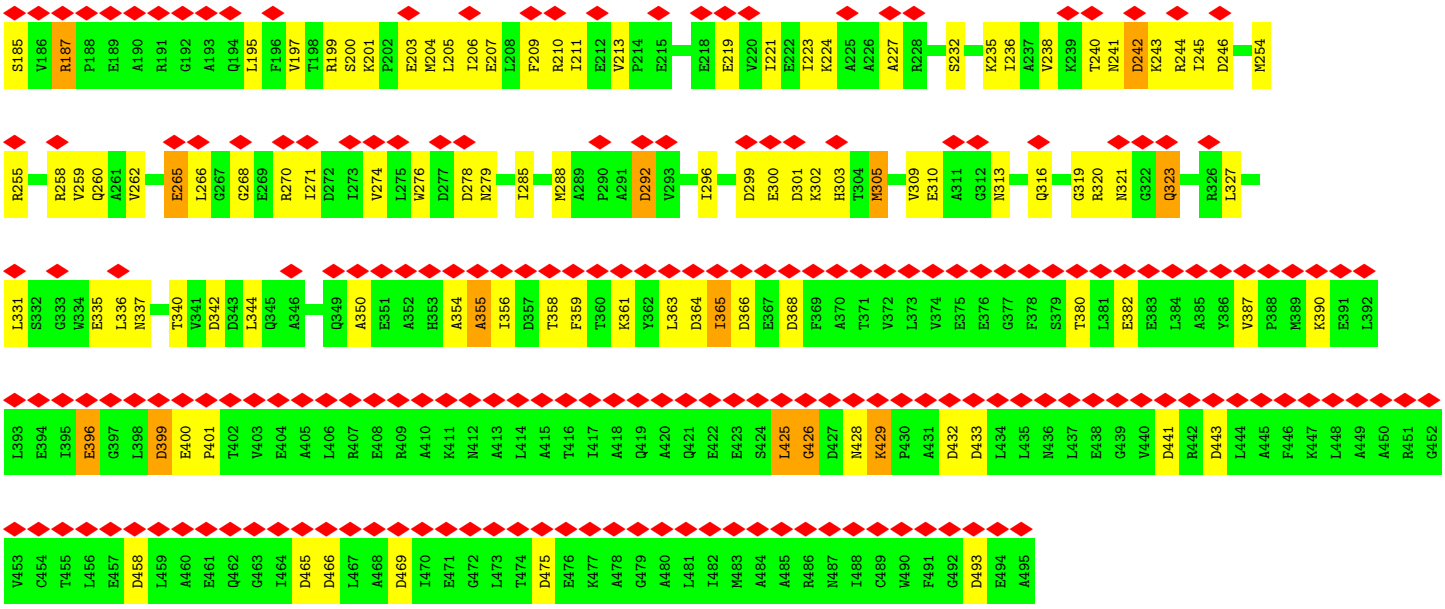
- Molecule 16: Transcription termination/antitermination protein NusA

Chain AG:

M1 N2 K3 E4 I5 L6 A7 V8 V9 E10 A11 V12 S13 N14 E15 K16 A17 L18 P19 R20 E21 K22 I23 F24 E25 A26 L27 E28 S29 A30 L31 A32 T33 A34 T35 K36 K37 K38 Y39 E40 Q41 E42 I43 D44 V45 R46 V47 Q48 I49 D50 R51 K52 S53 G54 D55 F56 D57 T58 F59 R60

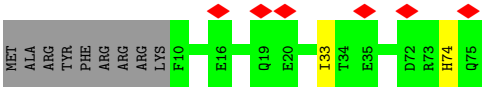
R61 W62 L63 V64 V65 D66 E67 V68 T69 Q70 P71 T72 K73 E74 I75 T76 L77 E78 A79 A80 R81 Y82 E83 D84 E85 S86 L87 N88 L89 G90 D91 Y92 V93 E94 D95 Q96 I97 E98 S99 V100 T101 F102 D103 R104 I105 T106 T107 Q108 T109 A110 K111 Q112 V113 I114 V115 Q116 K117 V118 R119 E120

A121 E122 R123 A124 M125 V126 V127 D128 Q129 F130 R131 E132 H133 E134 I138 T139 G140 V141 V142 K143 K144 V145 N146 R147 D148 N149 I150 D153 L154 G155 N156 N157 A158 E159 I162 L163 R164 E165 D166 M167 L168 P169 R170 E171 N172 F173 R174 P175 G176 D177 R178 V179 R180 G181 V182 L183 Y184



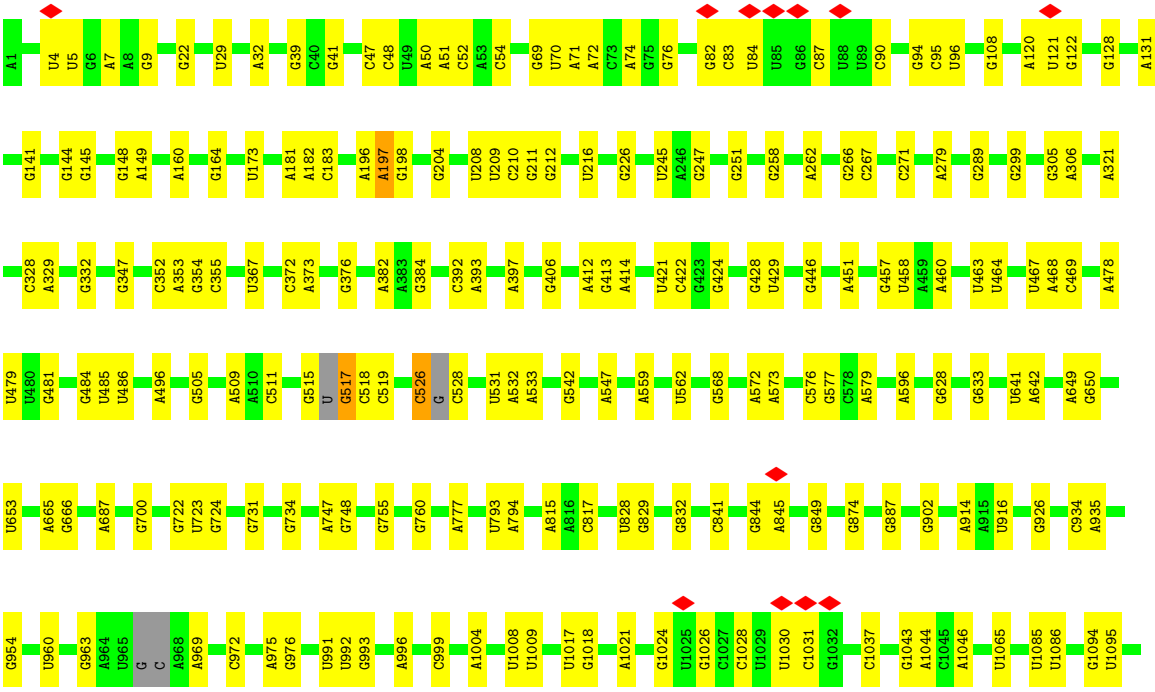
- Molecule 17: 30S ribosomal protein S18

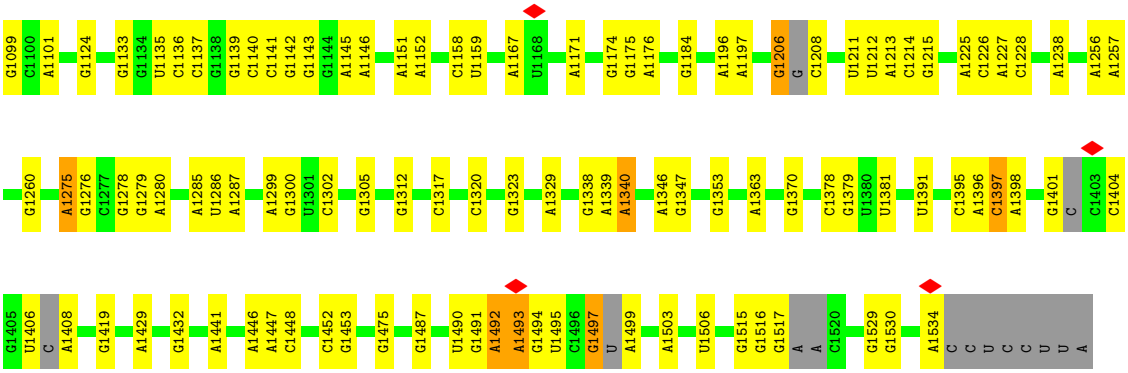
Chain C:



- Molecule 18: 16S rRNA

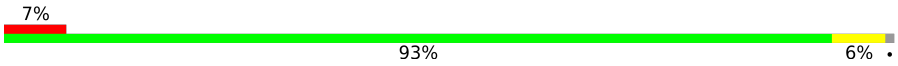
Chain D:

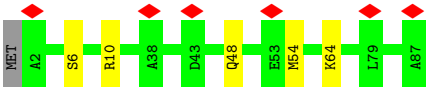




- Molecule 19: 30S ribosomal protein S20

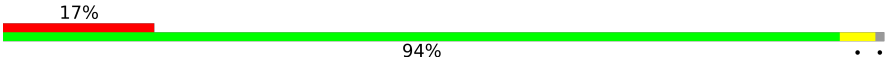
Chain E:

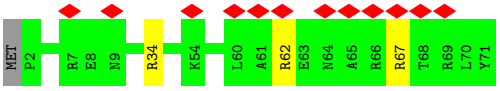




- Molecule 20: 30S ribosomal protein S21

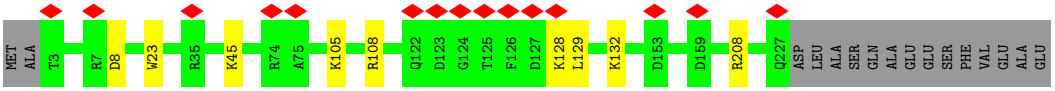
Chain F:





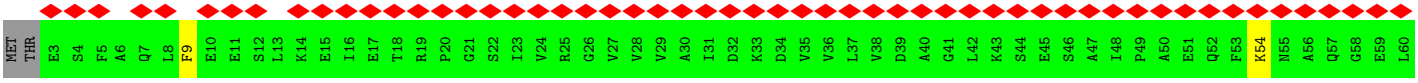
- Molecule 21: 30S ribosomal protein S2

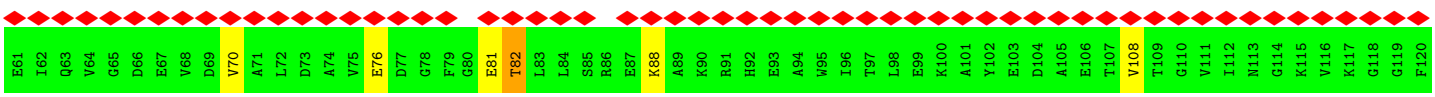
Chain G:

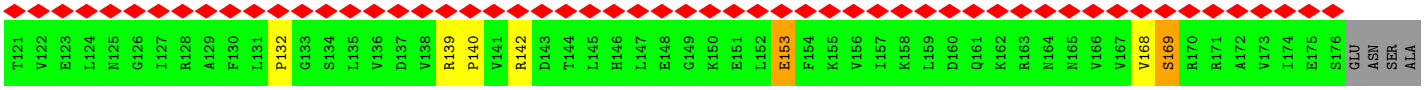


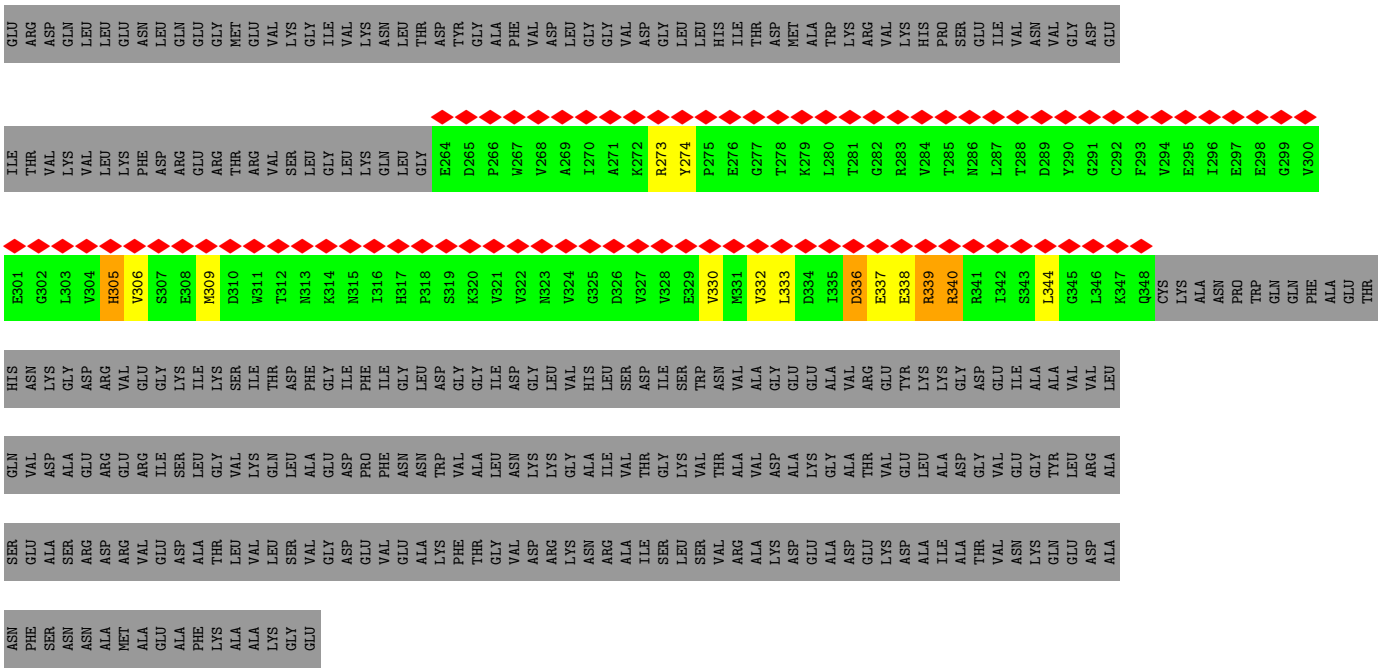
- Molecule 22: 30S ribosomal protein S1

Chain H:



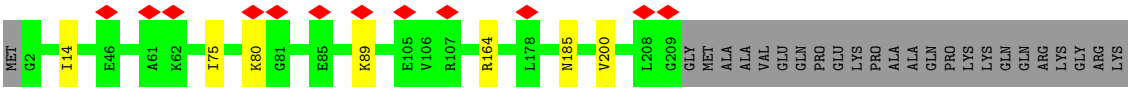






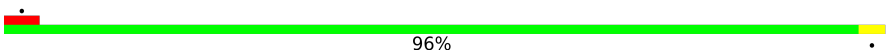
- Molecule 23: 30S ribosomal protein S3

Chain I:



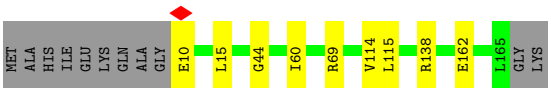
- Molecule 24: 30S ribosomal protein S4

Chain J:



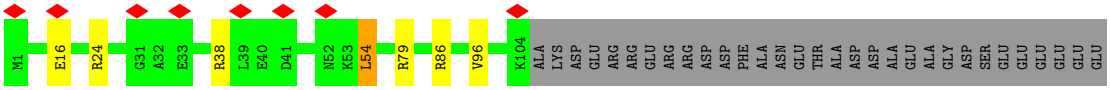
- Molecule 25: 30S ribosomal protein S5

Chain K:



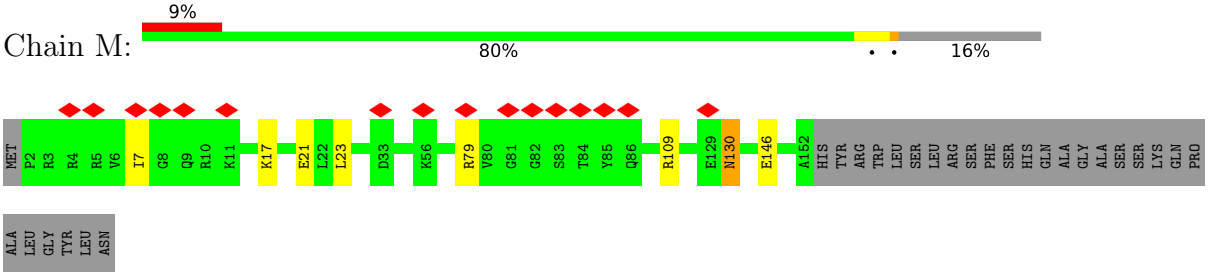
- Molecule 26: 30S ribosomal protein S6

Chain L:



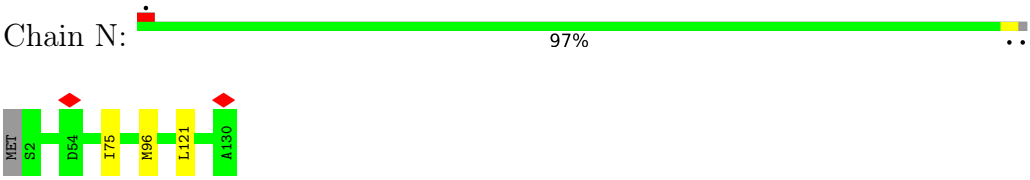
• Molecule 27: 30S ribosomal protein S7

Chain M:



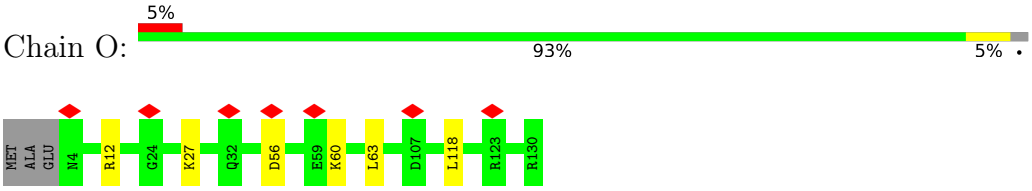
• Molecule 28: 30S ribosomal protein S8

Chain N:



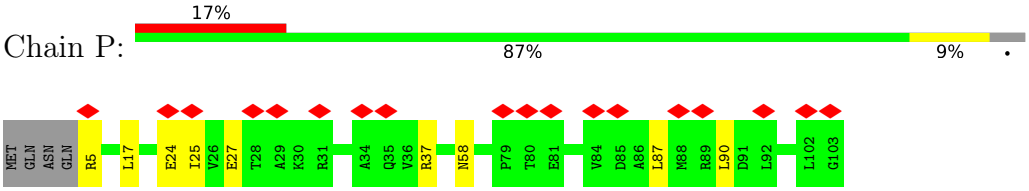
• Molecule 29: 30S ribosomal protein S9

Chain O:



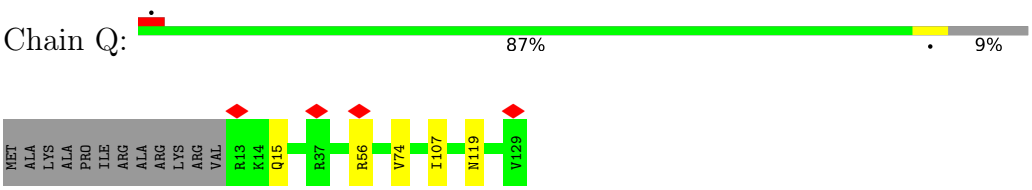
• Molecule 30: 30S ribosomal protein S10

Chain P:



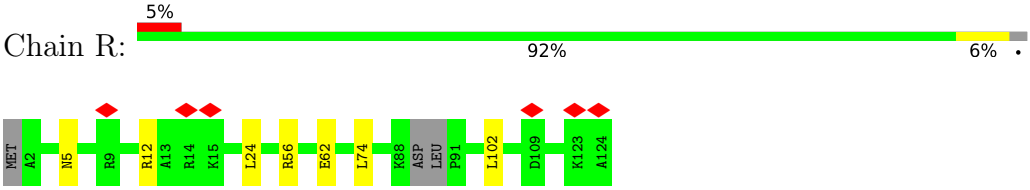
• Molecule 31: 30S ribosomal protein S11

Chain Q:



• Molecule 32: 30S ribosomal protein S12

Chain R:



• Molecule 33: 30S ribosomal protein S14

Chain S: 95%

MET A2 D18 M35 V45 L46 M89 E92 W101

• Molecule 34: 30S ribosomal protein S15

Chain T: 85% 13%

MET S2 K10 R17 T22 L39 Q40 R64 K65 L66 L67 L70 K73 E83 R84 L85 R89

• Molecule 35: 30S ribosomal protein S16

Chain U: 93% 7%

M1 V2 L6 V19 T50 G64 D69 A82

• Molecule 36: 30S ribosomal protein S17

Chain V: 93% 5%

MET THR ASP K4 N50 L75 K81 A82 V83 LEU

• Molecule 37: 30S ribosomal protein S19

Chain W: 53% 86% 10%

MET P2 R3 S4 L5 K6 P9 F10 I11 D12 L15 K18 K21 A22 V23 E24 S25 G26 D27 K28 K29 R32 T33 W34 S35 R36 R37 S38 T39 I40 F41 P42 N43 M44 I45 G46 L47 T48 I49 A50 N53 G54 R55 Q56 H57 V58 P59 V60 F61 V62 T63 D64 E65

H69 K70 L71 G72 E73 F74 A75 P76 T77 R78 T79 Y80 R81 G82 H83 A84 ALA ASP LYS LYS ALA LYS LYS LYS

• Molecule 38: 30S ribosomal protein S13

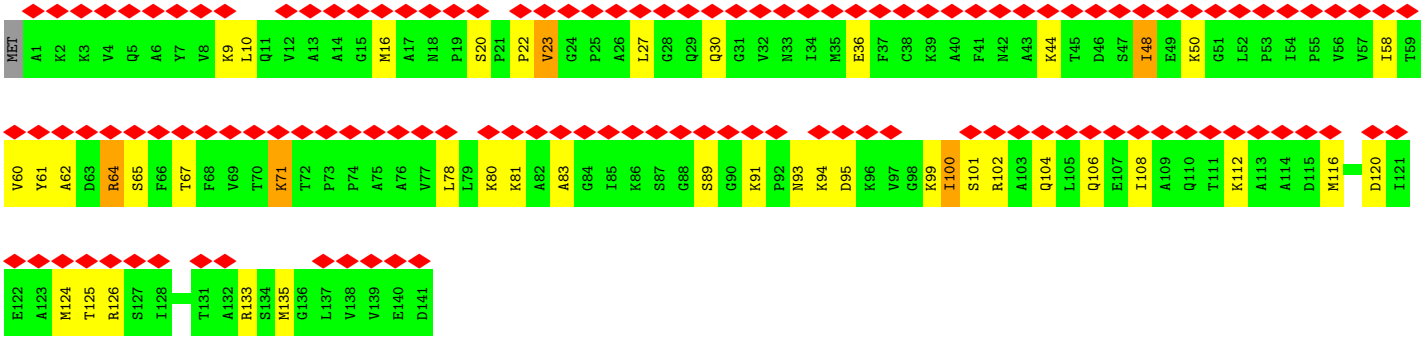
Chain X: 67% 88% 10%

MET A2 R3 I4 A5 G6 I7 N8 I9 P10 D11 H12 K13 H14 A15 V16 I17 A18 L19 T20 S21 I22 Y23 G24 V25 R29 S30 K31 A32 I33 L34 A35 A36 A37 G38 I39 A40 E41 I45 S46 E47 E50 G51 D54 T55 L56 R57 D58 E59 V60 A61 K62 F63 V64 V65 E66

G67 D68 L69 R70 R71 E72 I73 S74 M75 K78 R79 L80 M81 D82 L83 G84 R87 G88 L89 R90 H91 R92 R93 G94 V97 Q100 R101 T102 K103 T104 N105 A106 R107 T108 R109 K110 G111 P112 R113 K114 P115 I116 K117 LYS

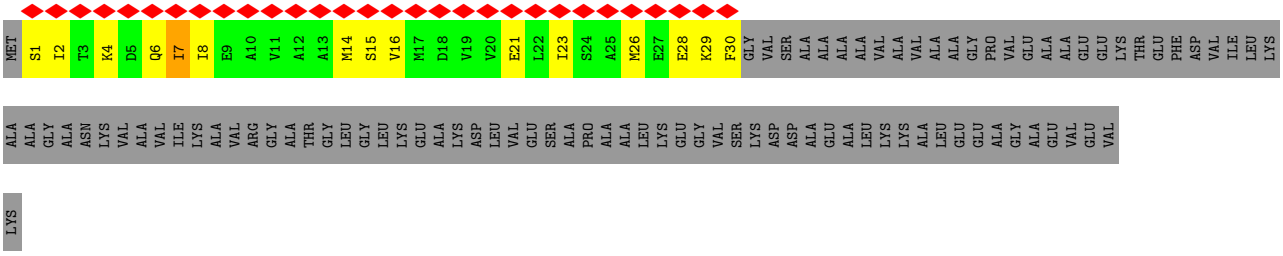
- Molecule 39: 50S ribosomal protein L11

Chain Y:



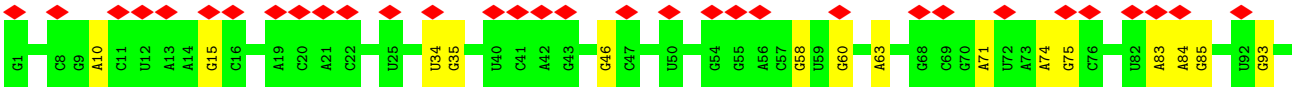
- Molecule 40: 50S ribosomal protein L7/L12

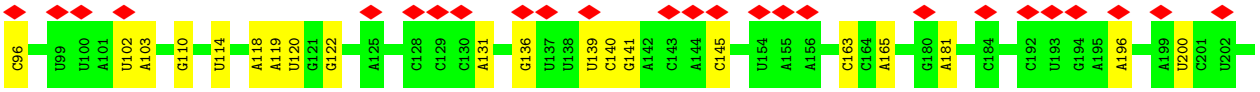
Chain Z:

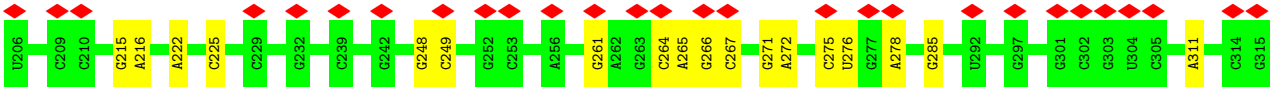


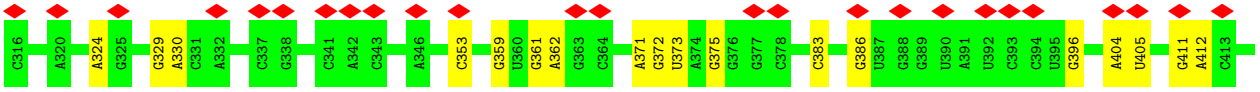
- Molecule 41: 23S rRNA

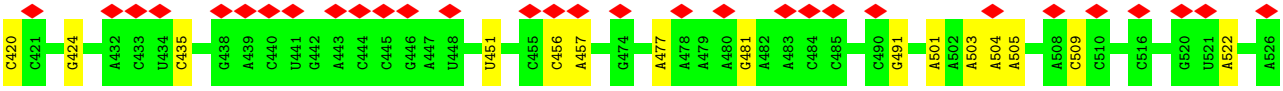
Chain a:

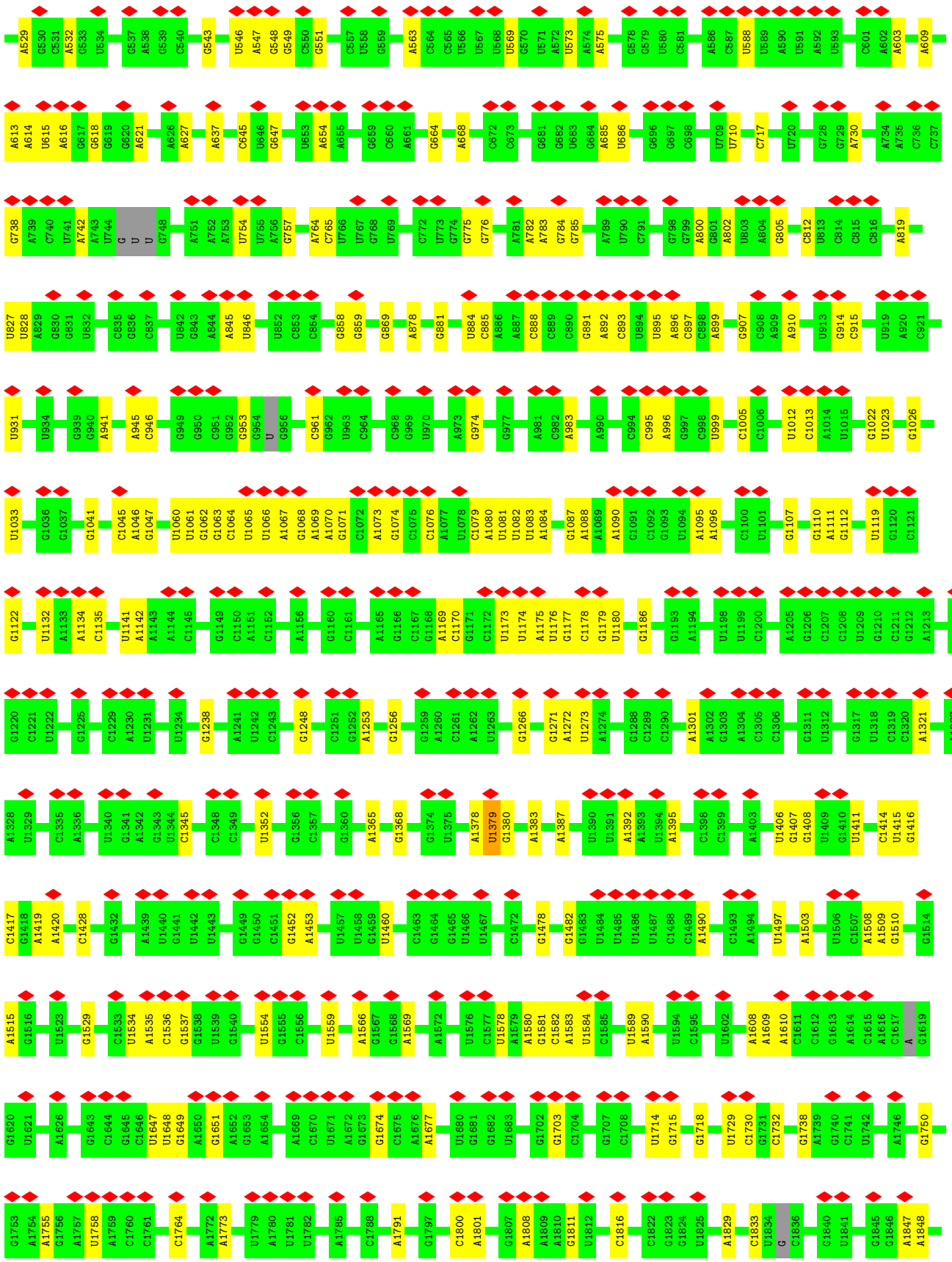








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A613 A614 U615 A616 G617 G618 G619 G620 A621 A626 A627 A637 C645 U646 G647 U653 A654 A655 G659 C660 A661 G664 A668 C672 C673 G681 G682 U683 G684 A685 U686 G696 G697 C698 U709 U710 C717 U720 G728 G729 A730 A734 A735 C736 C737
G738 A739 C740 U741 A742 A743 U744 G U U G748 A751 A752 A753 U754 U755 A756 G757 A764 C765 U766 U767 G768 U769 C772 U773 G774 G775 G776 A781 A782 A783 G784 G785 A789 U790 C791 G798 G799 A800 G801 A802 U803 A804 G805 C812 U813 C814 C815 C816 A819
U827 U828 A829 G830 G831 U832 C835 G836 C837 U842 G843 A844 A845 U846 U852 C853 C854 G858 G859 G869 A878 G881 U884 C885 A886 A887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 G907 C908 A909 A910 U913 G914 C915 U919 A920 C921
U931 U934 G939 G940 A941 A945 C946 G949 G950 C951 G952 G953 G954 U U G956 C961 G962 U963 C964 G968 G969 U970 A973 G974 G977 A981 C982 A983 A990 C994 C995 A996 G997 C998 U999 C1005 C1006 U1012 C1013 A1014 U1015 G1022 U1023 G1026
U1033 G1036 G1037 G1041 C1045 A1046 G1047 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 C1100 U1101 G1107 G1110 A1111 G1112 U1119 G1120 C1121
G1122 U1132 A1133 A1134 C1135 U1141 A1142 A1143 A1144 C1145 G1149 C1150 A1151 C1152 A1156 G1160 C1161 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 G1186 G1193 A1194 U1198 U1199 C1200 A1205 G1206 C1207 C1208 U1209 G1210 C1211 G1212 A1213 U1219
G1220 C1221 U1222 G1225 C1229 A1230 U1231 U1234 G1238 A1241 U1242 C1243 G1248 C1251 G1252 A1253 G1256 G1259 A1260 C1261 A1262 U1263 G1266 G1271 A1272 U1273 A1274 G1288 C1289 C1290 A1301 A1302 G1303 A1304 C1305 C1306 G1311 U1312 G1317 U1318 C1319 C1320 A1321 A1327
A1328 U1329 C1335 A1336 U1340 G1341 A1342 G1343 U1344 C1345 C1348 C1349 U1352 G1356 C1357 G1360 A1365 G1368 G1374 U1375 A1378 U1379 G1380 A1383 A1387 U1390 U1391 A1392 A1393 U1394 A1395 C1398 C1399 A1403 U1406 G1407 G1408 U1409 G1410 U1411 C1414 U1415 G1416
C1417 G1418 A1419 A1420 C1428 G1432 A1439 U1440 G1441 U1442 U1443 G1449 G1450 C1451 G1452 A1453 U1457 U1458 G1459 U1460 C1463 G1464 G1465 U1466 U1467 C1472 G1478 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 A1490 C1493 A1494 U1497 A1503 U1506 C1507 A1508 A1509 G1510 G1514
A1515 G1516 U1523 G1529 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 U1554 G1555 C1556 U1559 A1566 G1567 G1568 A1569 A1572 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 U1589 A1590 U1594 C1595 U1602 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A G1619
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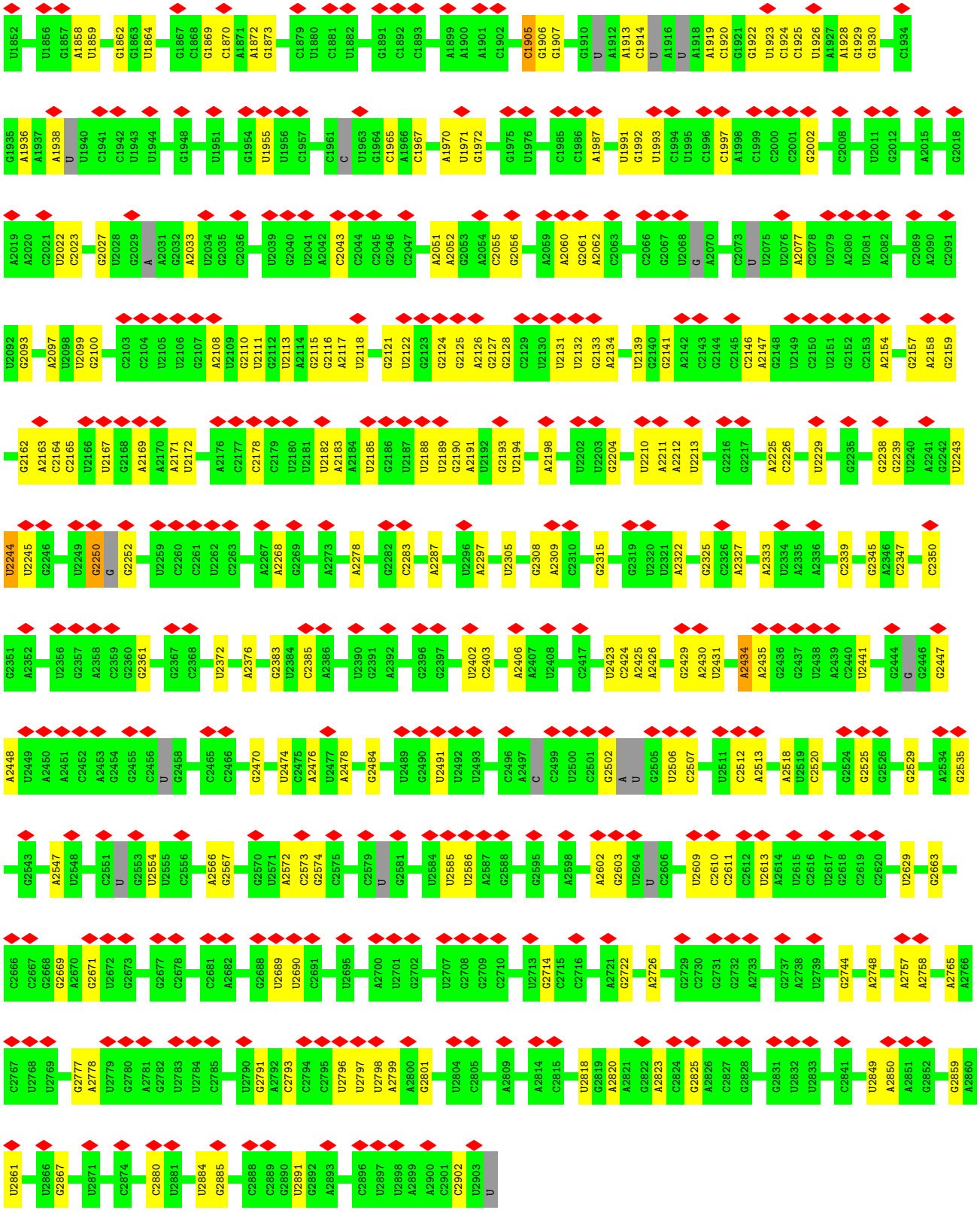
G1753 A1754 A1755 G1756 A1757 U1758 A1759 C1760 C1761 C1764 A1772 A1773 U1779 A1780 U1781 U1782 A1785 C1788 A1791 G1797 C1800 A1801 G1807 A1808 A1809 A1810 G1811 U1812 C1816 C1822 G1823 G1824 U1825 A1829 C1833 U1834 G C1836 G1840 U1841 G1845 G1846 A1847 A1848

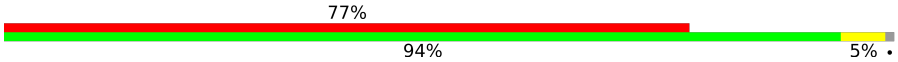


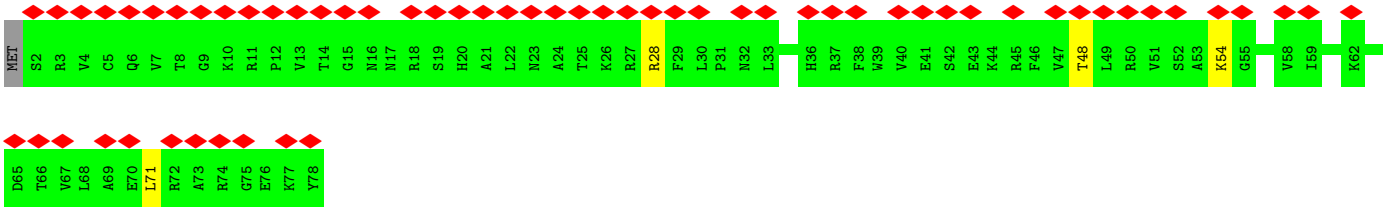
- Molecule 42: 50S ribosomal protein L27

Chain b: 52% 88% 11%

• Molecule 43: 50S ribosomal protein L28

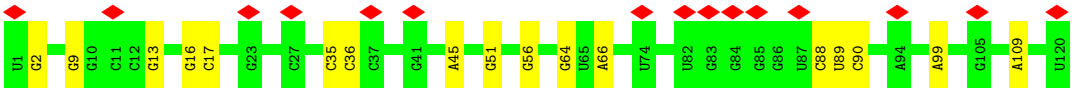
Chain c:





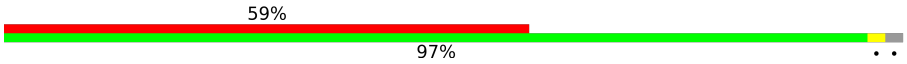
• Molecule 44: 5S rRNA

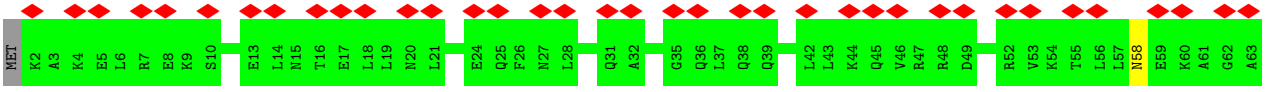
Chain d:



• Molecule 45: 50S ribosomal protein L29

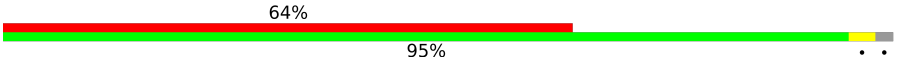
Chain e:

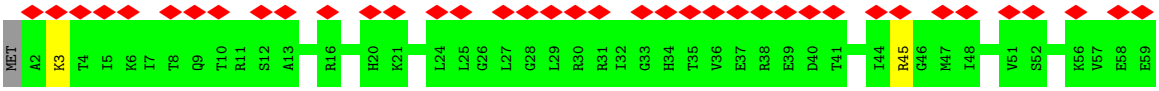




• Molecule 46: 50S ribosomal protein L30

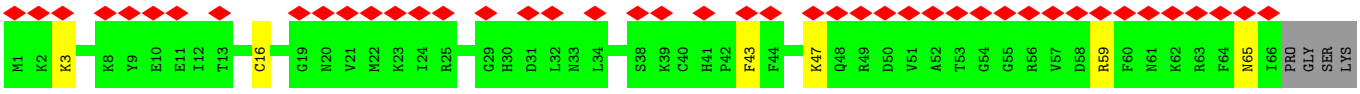
Chain f:





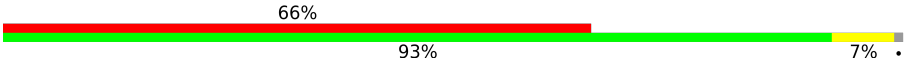
• Molecule 47: 50S ribosomal protein L31

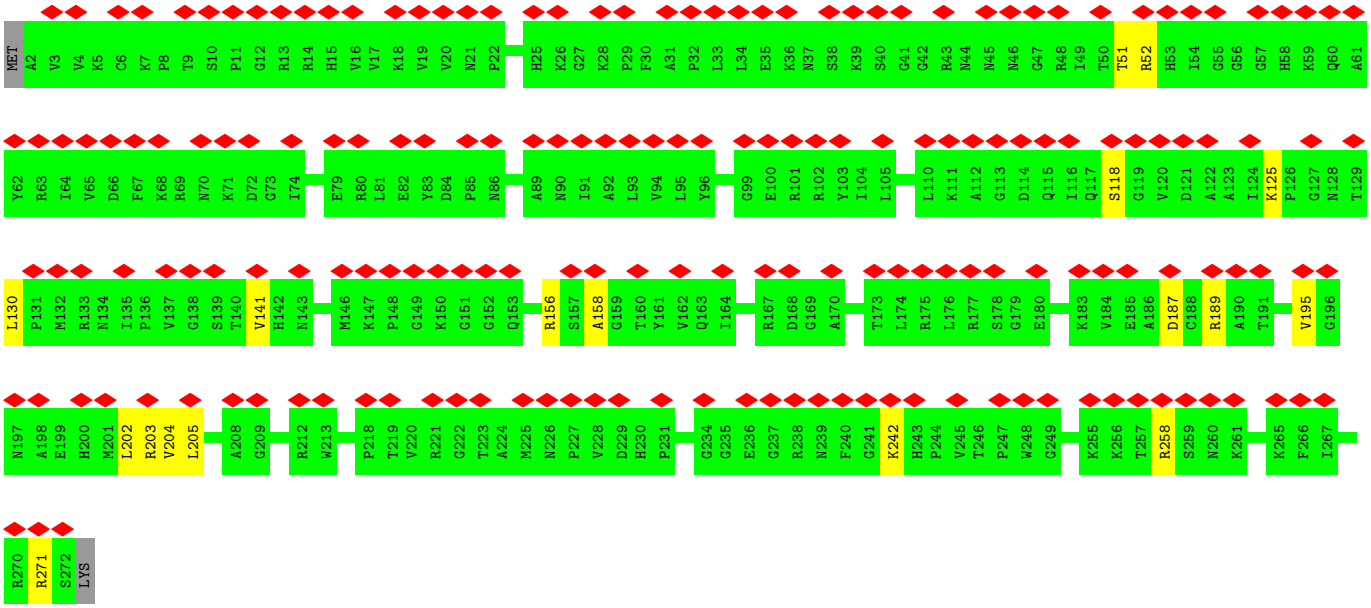
Chain g:



• Molecule 48: 50S ribosomal protein L2

Chain h:



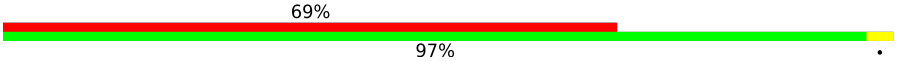


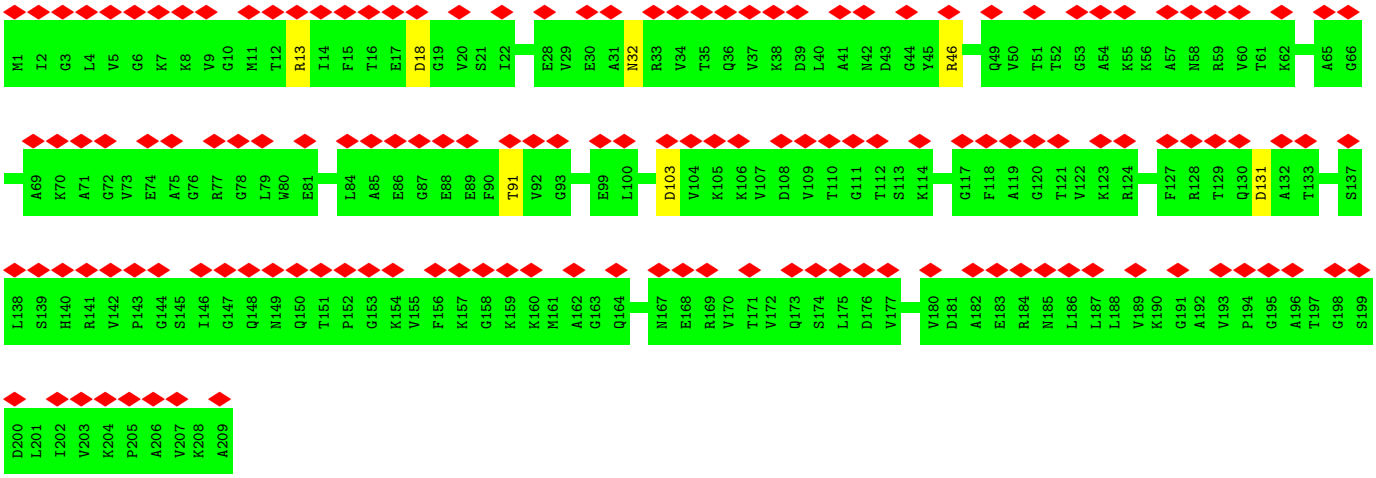
- Molecule 49: 50S ribosomal protein L32

Chain i:

- Molecule 50: 50S ribosomal protein L3

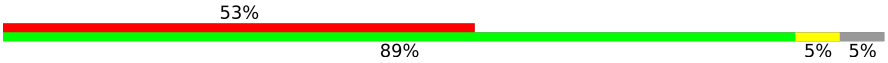
Chain j:

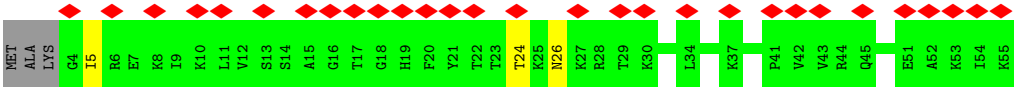




- Molecule 51: 50S ribosomal protein L33

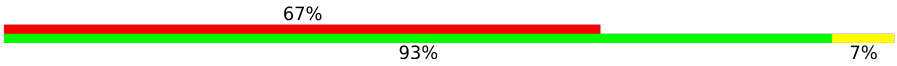
Chain k:

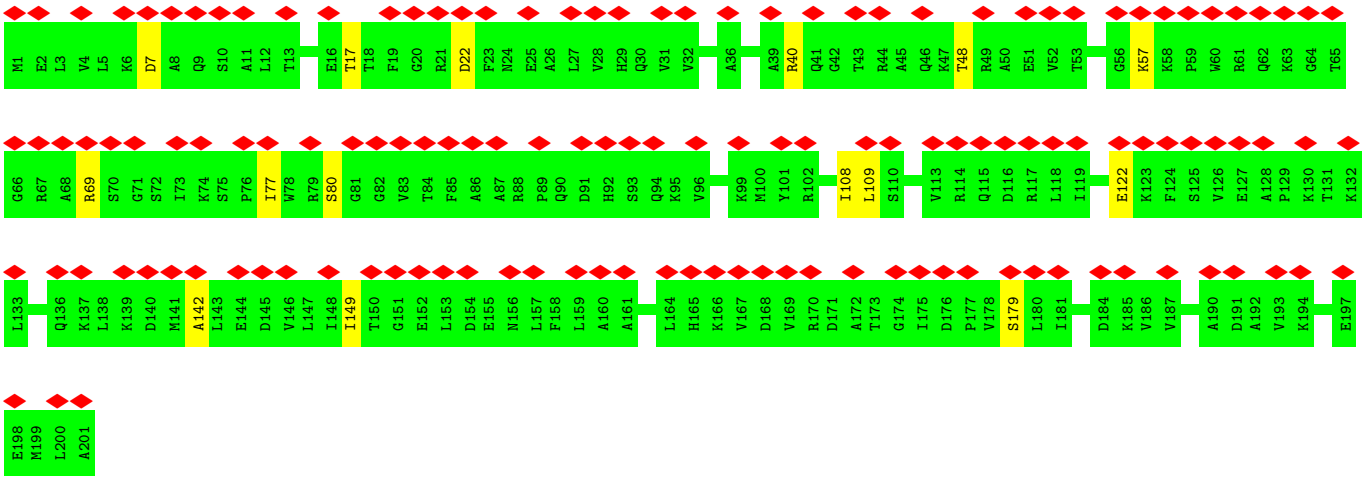




- Molecule 52: 50S ribosomal protein L4

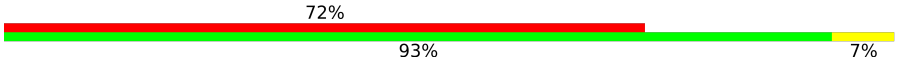
Chain l:

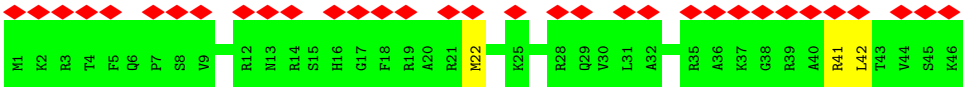




- Molecule 53: 50S ribosomal protein L34

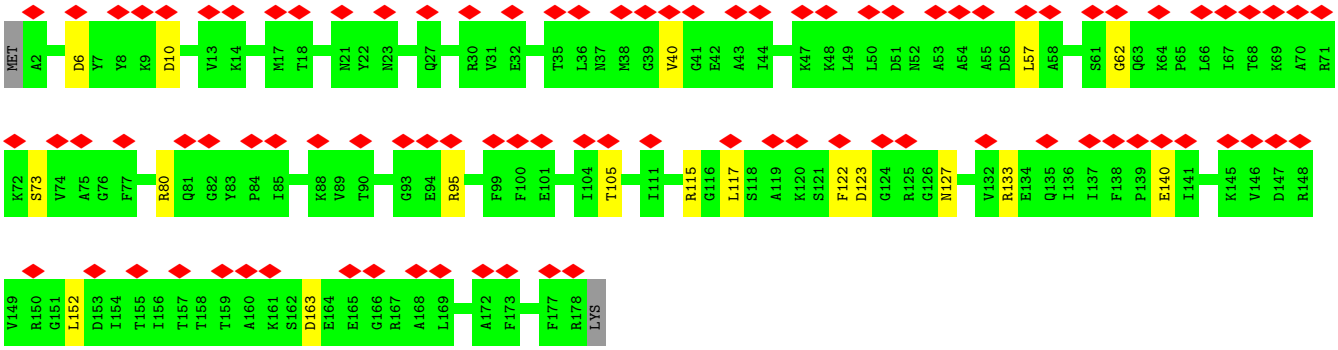
Chain m:





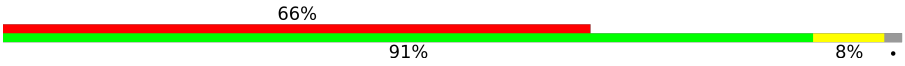
- Molecule 54: 50S ribosomal protein L5

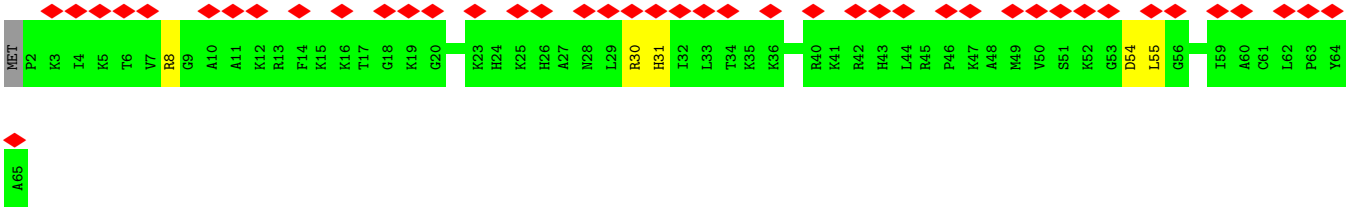
Chain n:



- Molecule 55: 50S ribosomal protein L35

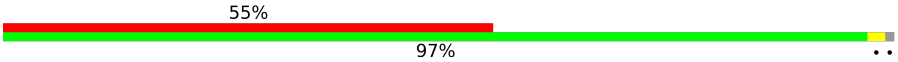
Chain o:

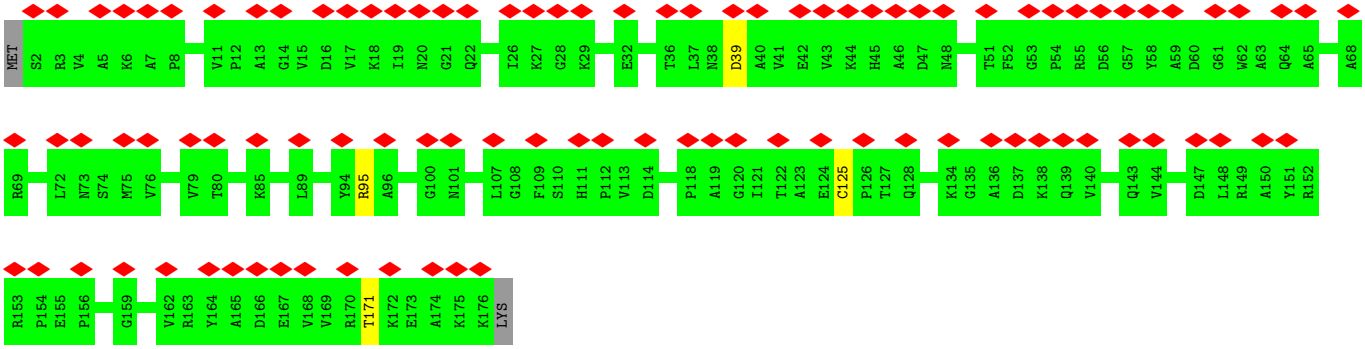




• Molecule 56: 50S ribosomal protein L6

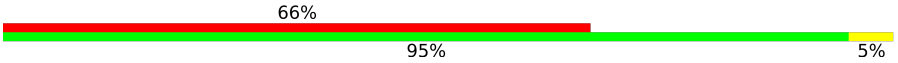
Chain p:

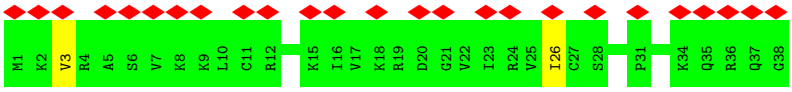




• Molecule 57: 50S ribosomal protein L36

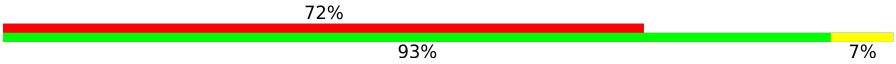
Chain q:

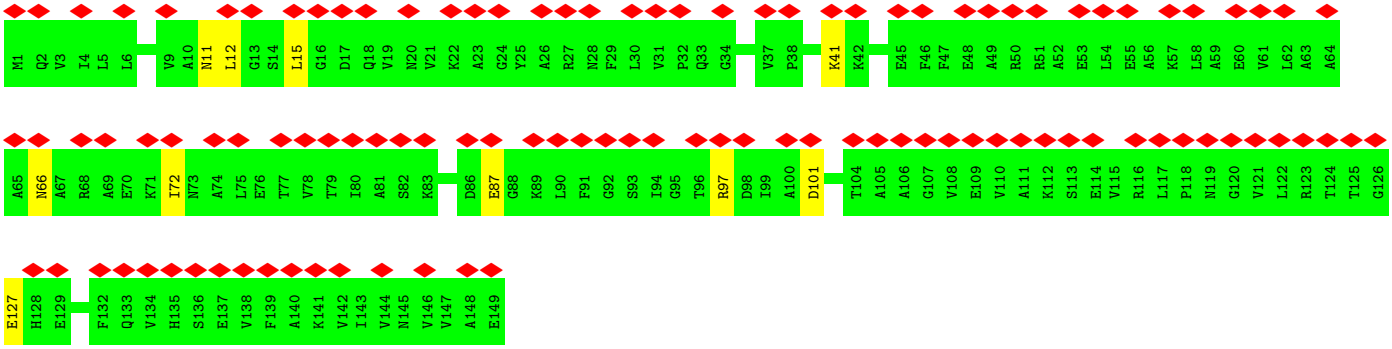




• Molecule 58: 50S ribosomal protein L9

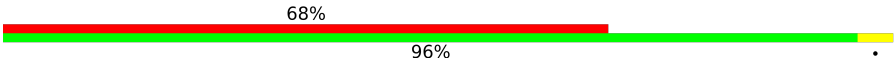
Chain r:





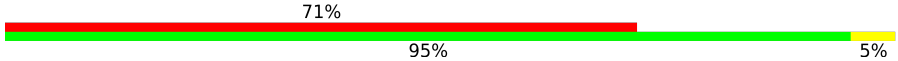
• Molecule 59: 50S ribosomal protein L13

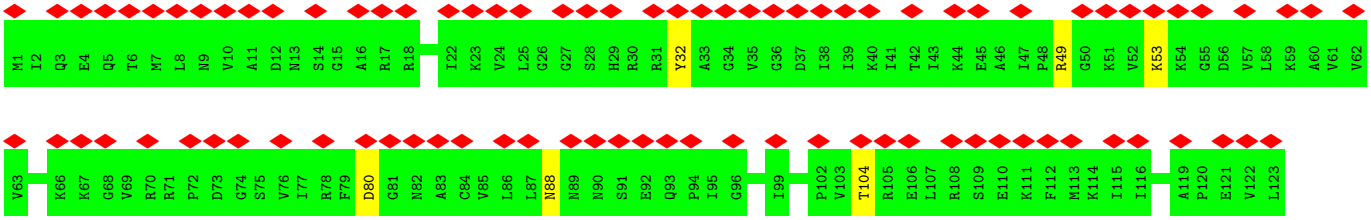
Chain s:



- Molecule 60: 50S ribosomal protein L14

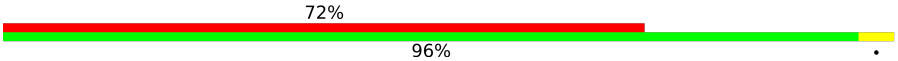
Chain t:

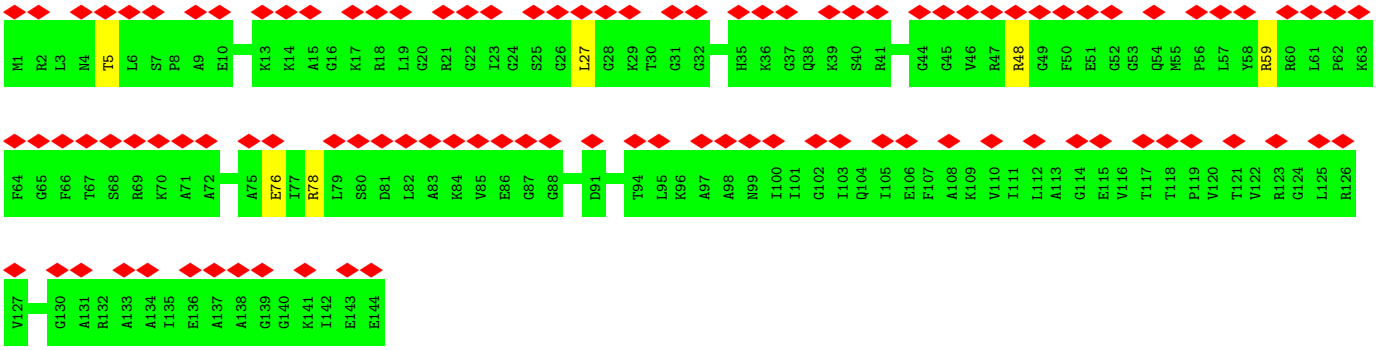




- Molecule 61: 50S ribosomal protein L15

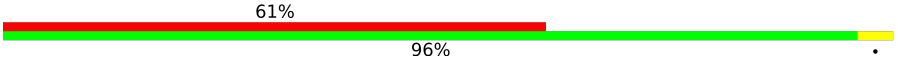
Chain u:

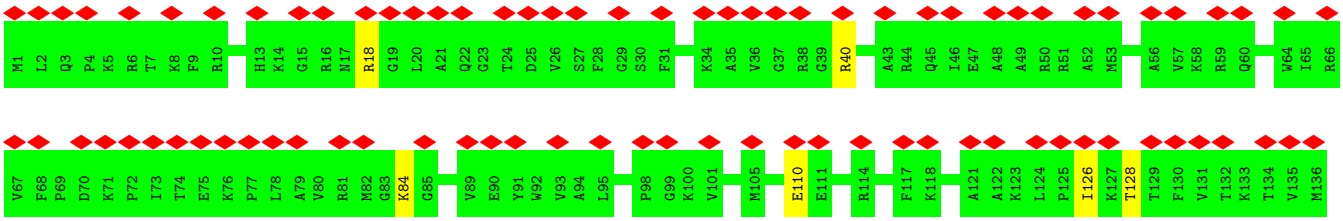




- Molecule 62: 50S ribosomal protein L16

Chain v:



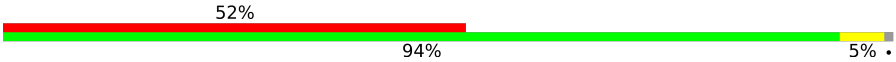


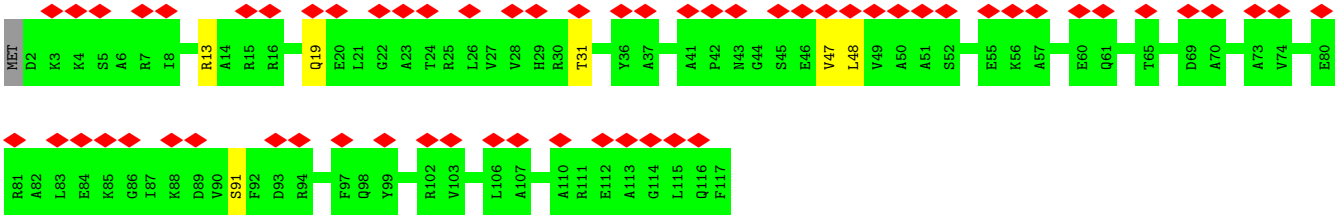
- Molecule 63: 50S ribosomal protein L17

Chain w:

- Molecule 64: 50S ribosomal protein L18

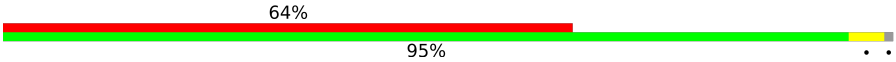
Chain x:

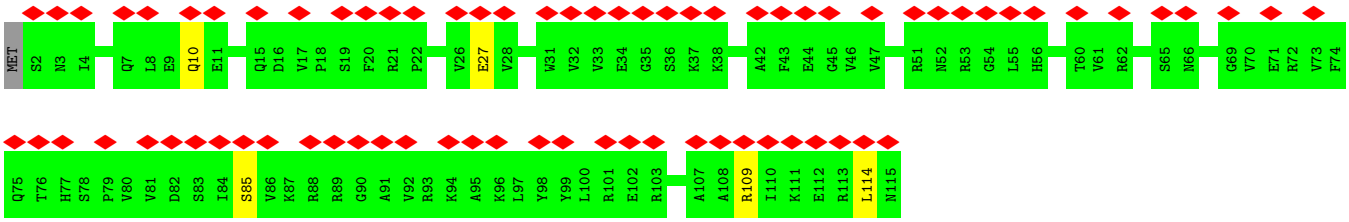




- Molecule 65: 50S ribosomal protein L19

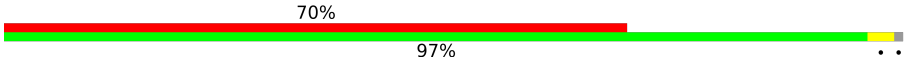
Chain y:

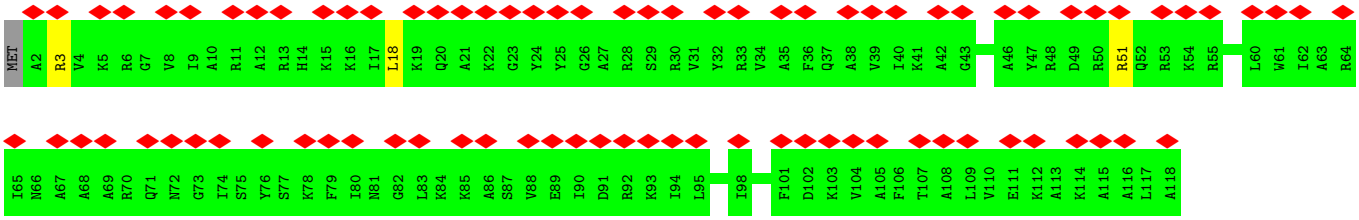




- Molecule 66: 50S ribosomal protein L20

Chain z:





4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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

Continued on next page...

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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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

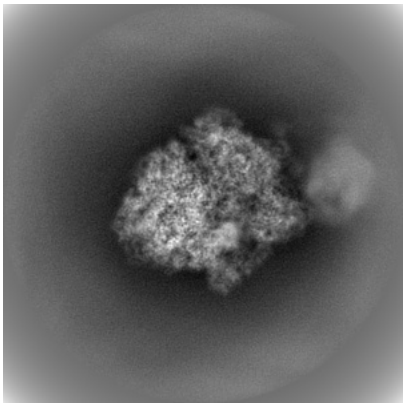
6 Map visualisation (i)

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

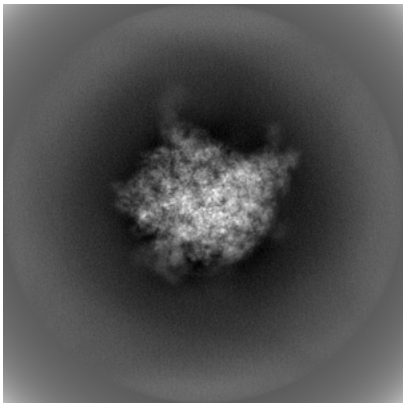
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

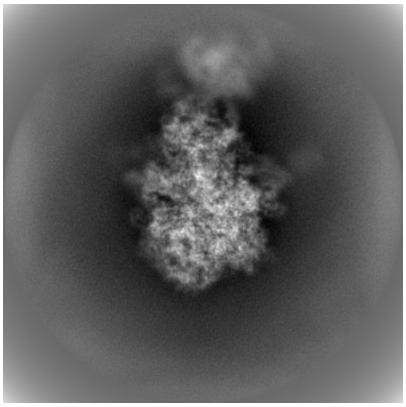
6.1.1 Primary map



X



Y

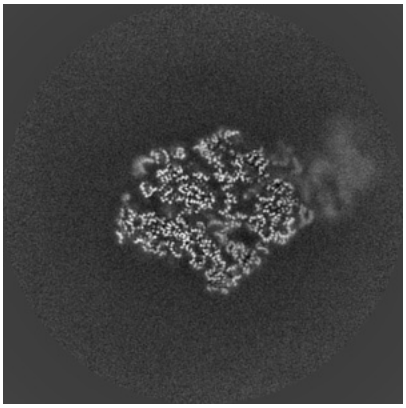


Z

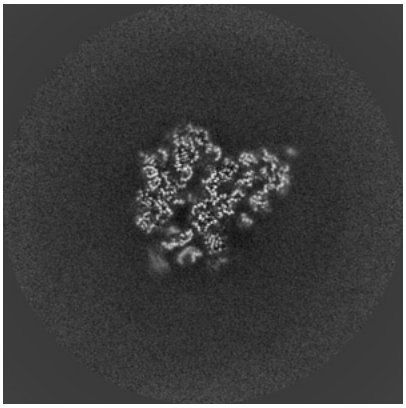
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

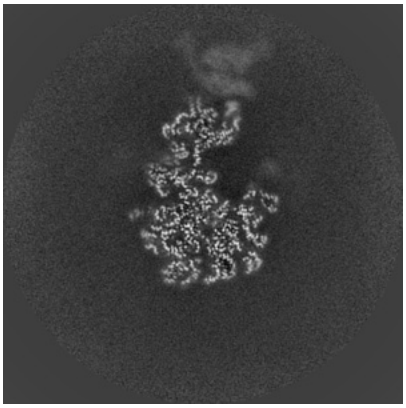
6.2.1 Primary map



X Index: 256



Y Index: 256

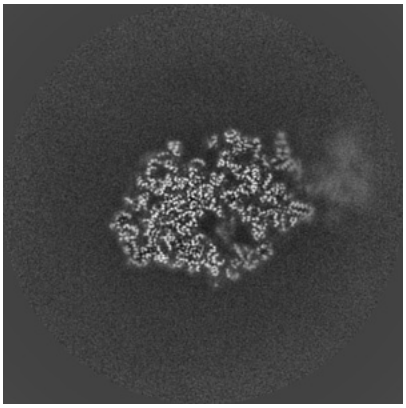


Z Index: 256

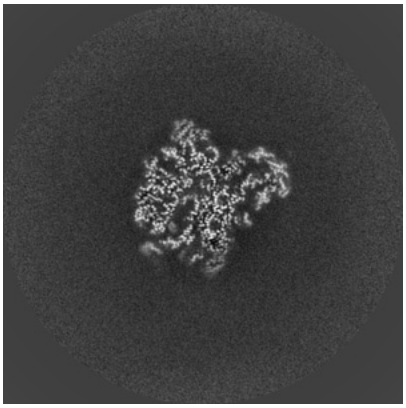
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

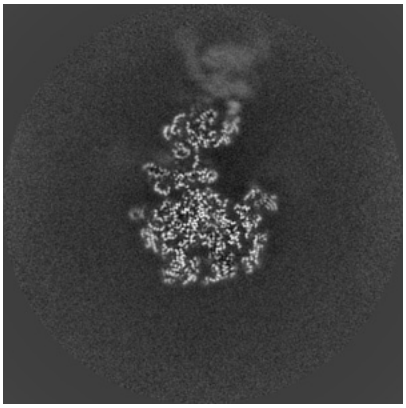
6.3.1 Primary map



X Index: 242



Y Index: 250



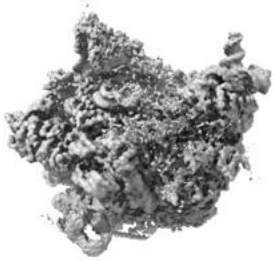
Z Index: 259

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

6.4 Orthogonal 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.

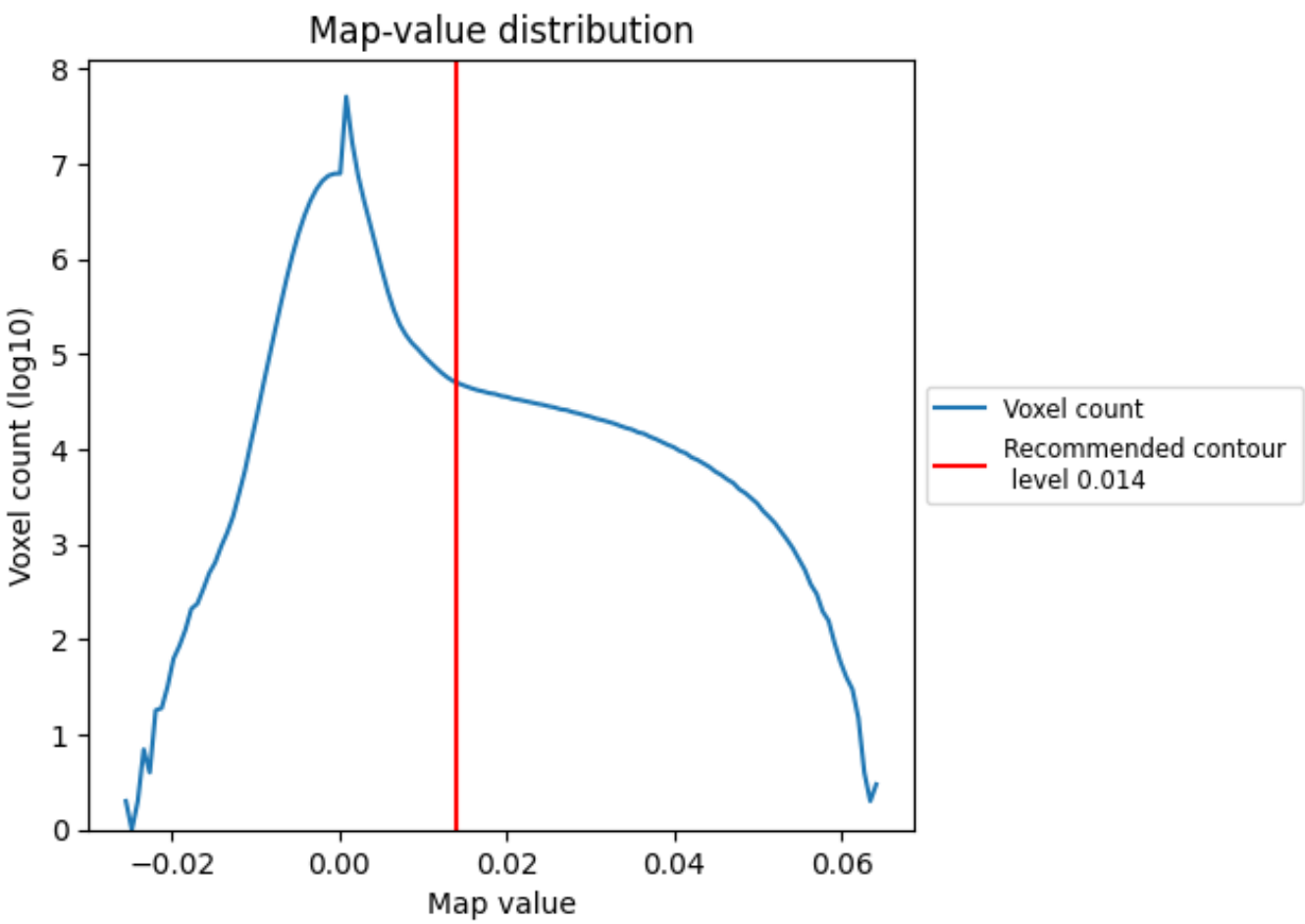
6.5 Mask visualisation (i)

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

7 Map analysis (i)

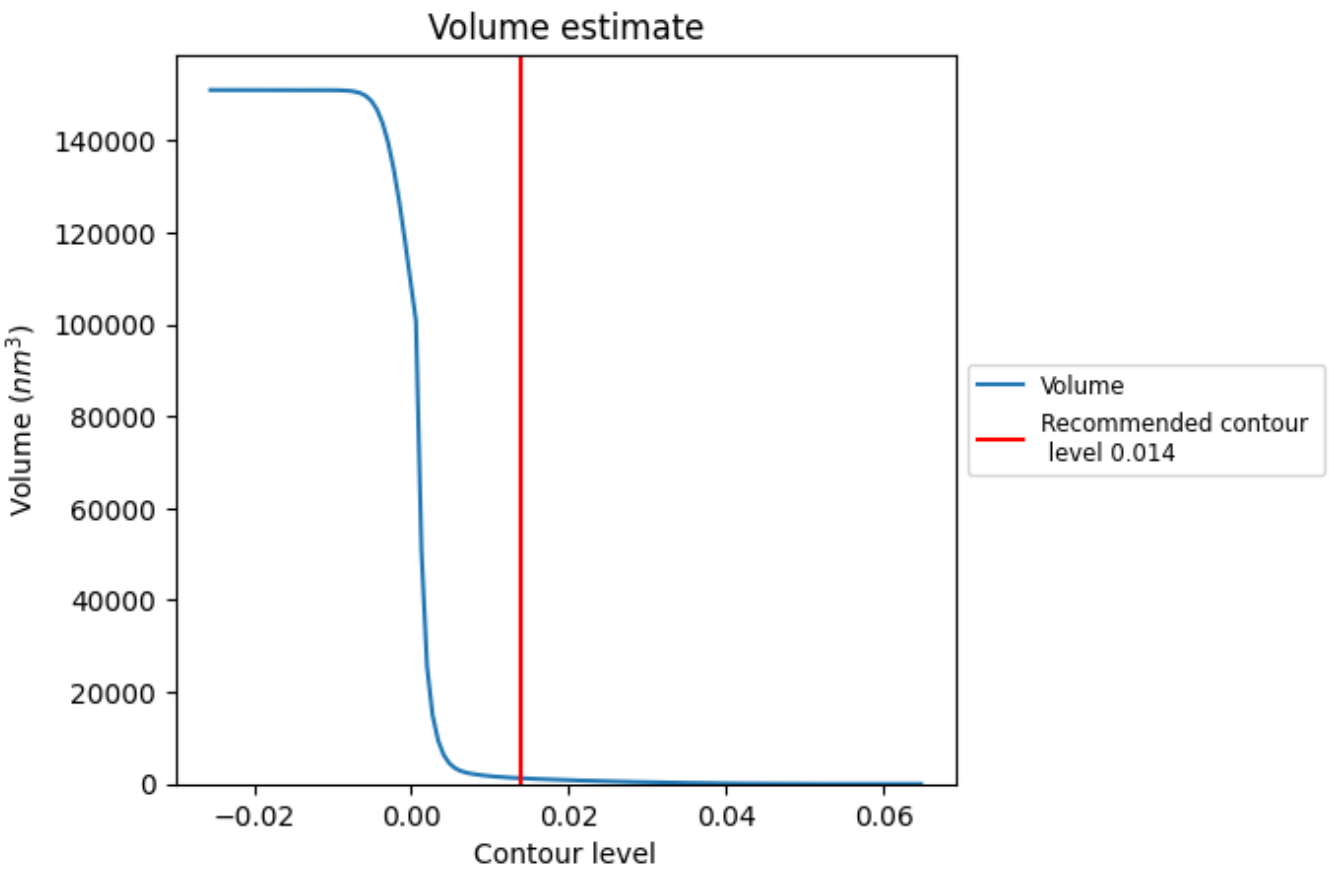
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

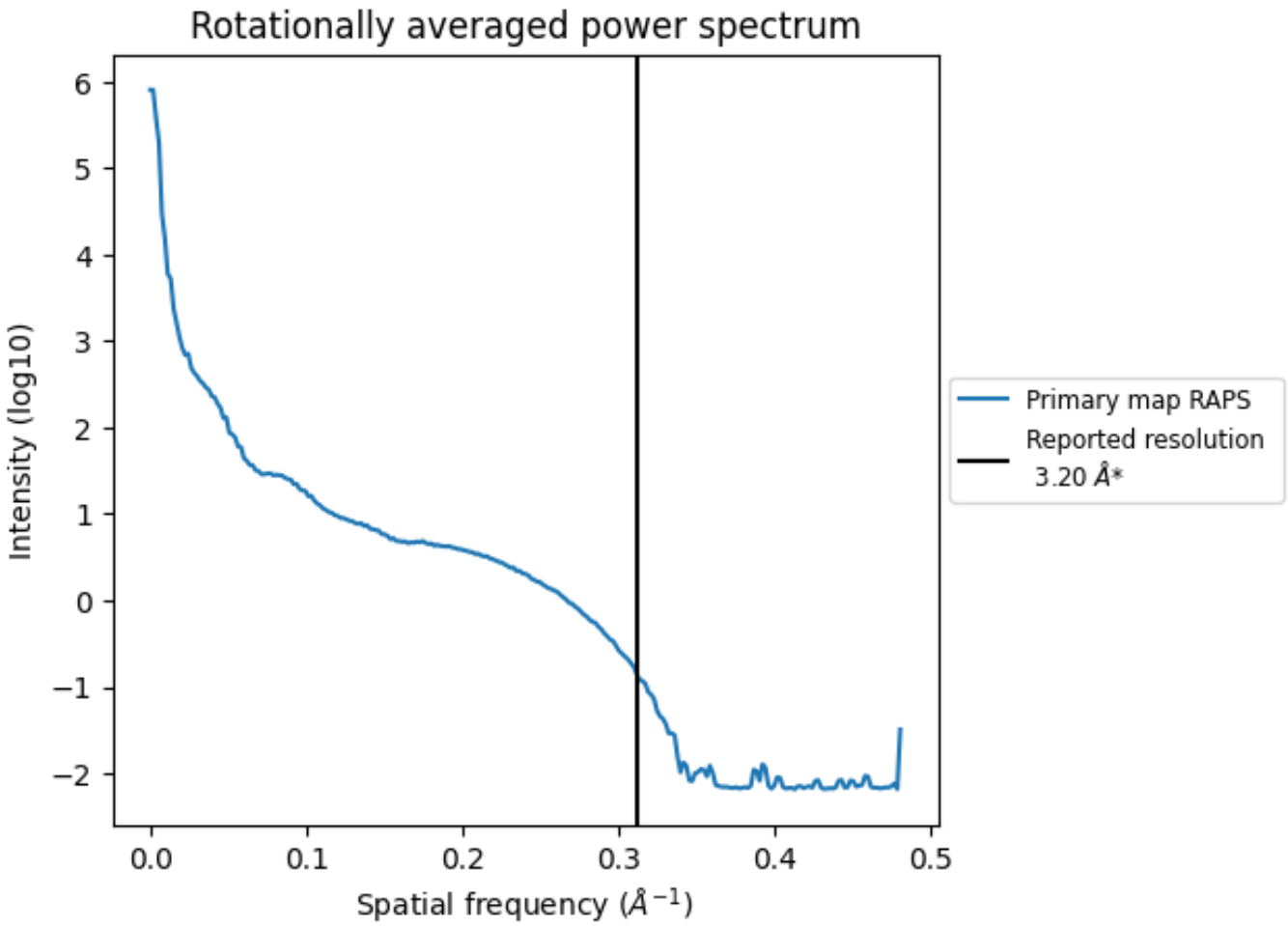
7.2 Volume estimate (i)



The volume at the recommended contour level is 1238 nm^3; this corresponds to an approximate mass of 1118 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

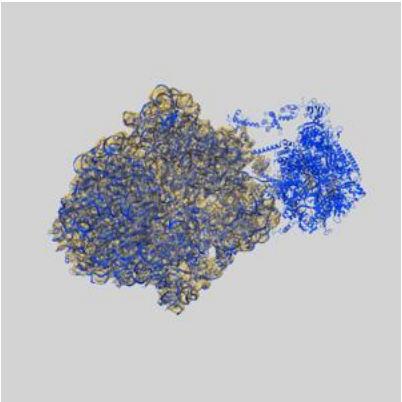
8 Fourier-Shell correlation (i)

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

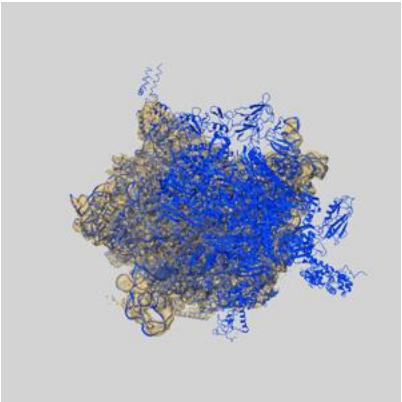
9 Map-model fit (i)

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

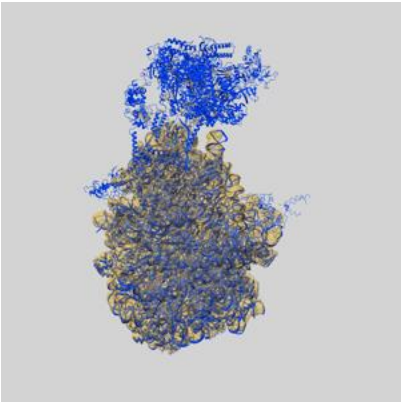
9.1 Map-model overlay (i)



X



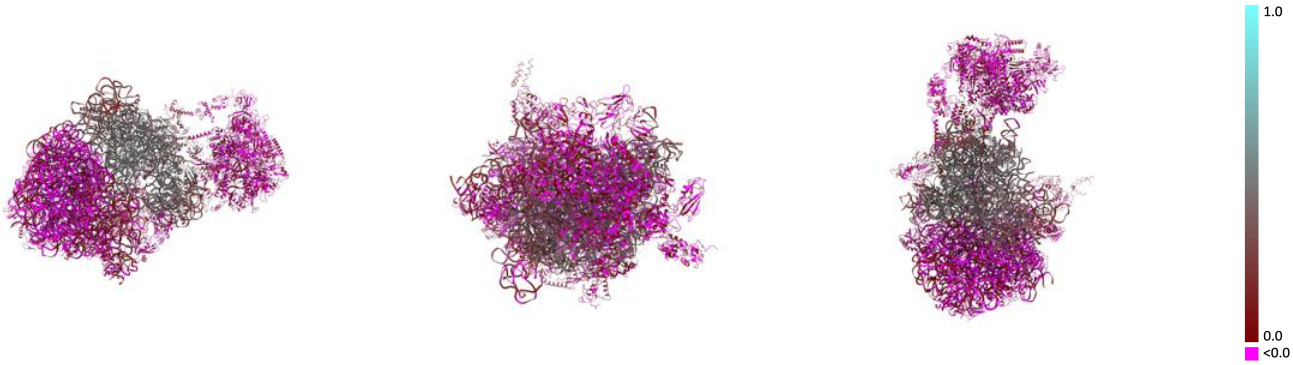
Y



Z

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

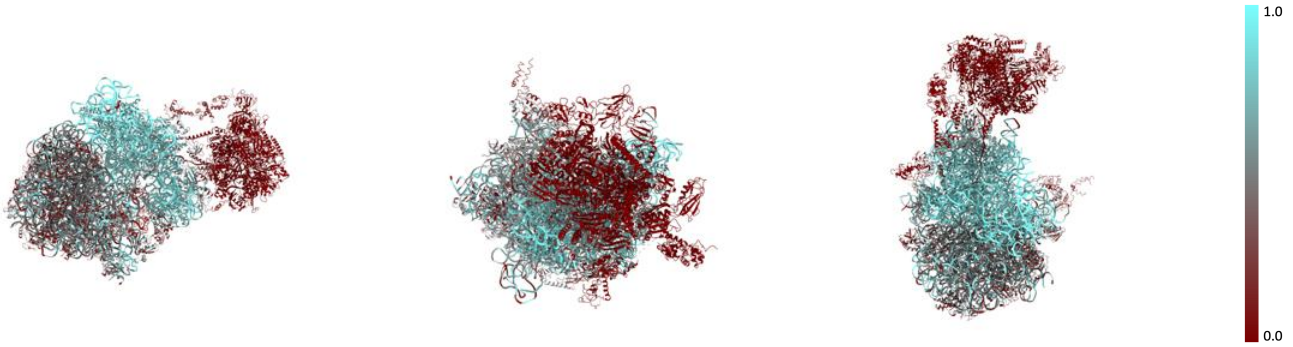
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

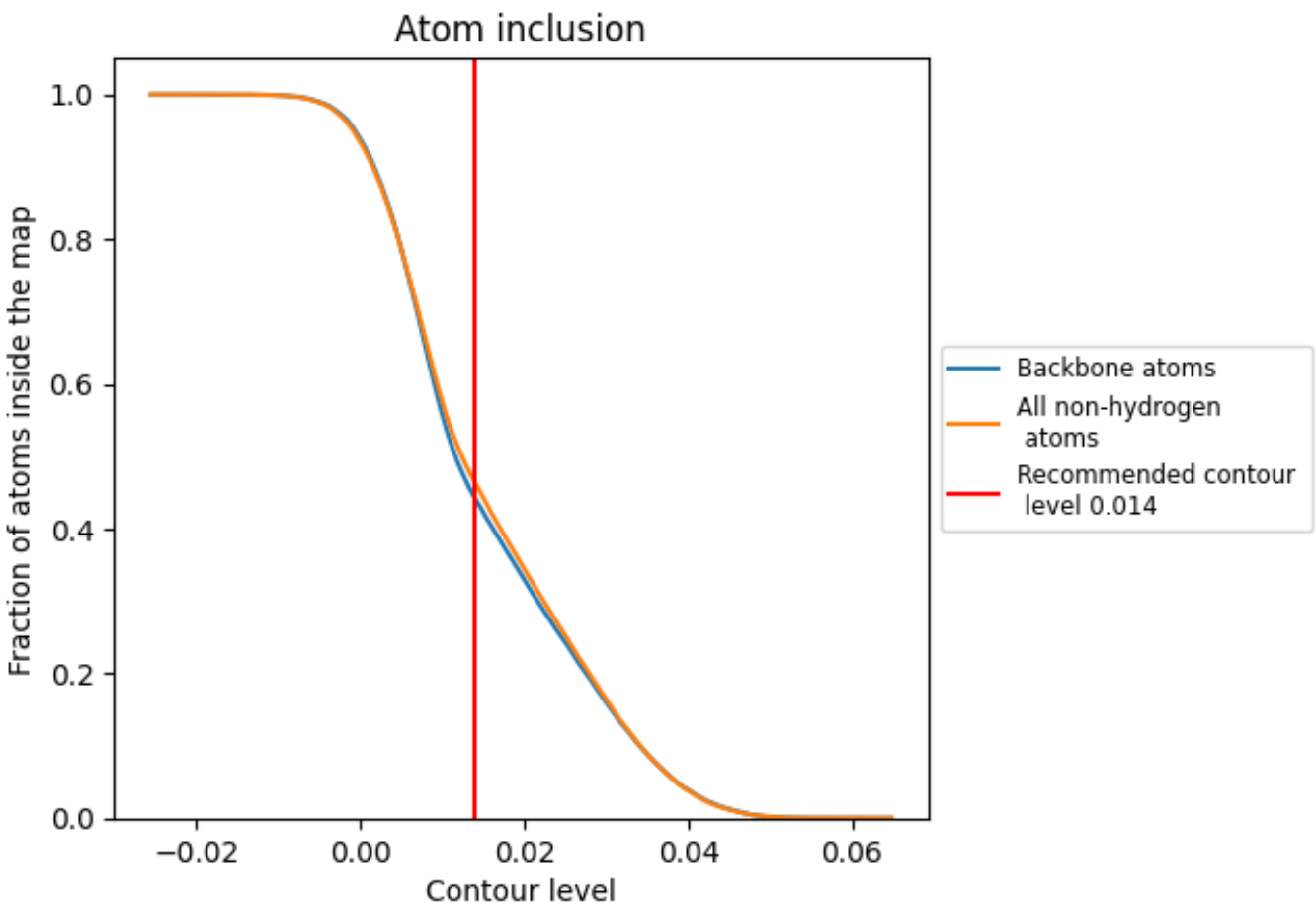
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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