Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 12:26 pm GMT

PDB ID	:	5LZX
EMDB ID	:	EMD-4135
Title	:	Structure of the mammalian rescue complex with Pelota and Hbs1l assembled on a UGA stop codon.
Authors	:	Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on	:	2016-10-02
Resolution	:	3.67 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 (1)) were used in the production of this report:

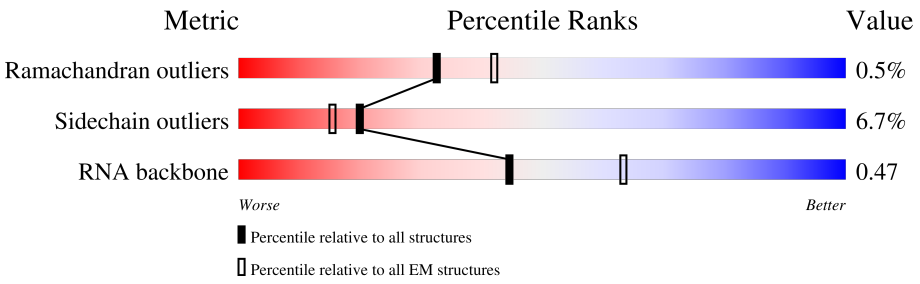
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.67 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	A	257	56% 89% 7% •
2	B	403	53% 93% 5% •
3	C	425	48% 80% 5% 15%
4	D	297	61% 94% • •
5	E	291	48% 70% • 26%
6	F	247	48% 85% 6% 9%
7	G	319	53% 69% • 27%
8	H	192	65% 93% 6% •

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Mol	Chain	Length	Quality of chain
9	I	214	57% 91% 5%
10	J	178	76% 92%
11	L	211	67% 95%
12	M	218	30% 60% 37%
13	N	204	57% 95% 5%
14	O	203	45% 92% 6%
15	P	184	33% 78% 5% 17%
16	Q	188	60% 93% 7%
17	R	196	66% 86% 6% 8%
18	S	176	48% 93% 7%
19	T	160	59% 92% 7%
20	U	128	66% 75% 23%
21	V	140	66% 86% 7% 6%
22	W	157	57% 66% 32%
23	X	156	59% 72% 24%
24	Y	145	52% 88% 8%
25	Z	136	63% 96%
26	a	148	45% 98%
27	b	245	36% 41% 58%
28	c	115	60% 83% 15%
29	d	125	44% 77% 9% 14%
30	e	135	54% 88% 7% 5%
31	f	110	41% 94% 5%
32	g	117	65% 92% 5%
33	h	123	76% 95%

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Mol	Chain	Length	Quality of chain
34	i	105	74% 95%
35	j	97	64% 84% 5% 11%
36	k	70	91% 96%
37	l	51	75% 96%
38	m	102	31% 49% 49%
39	n	25	100% 92% 8%
40	o	106	64% 92% 6%
41	p	92	64% 97%
42	r	137	44% 82% 8% 9%
43	s	318	62% 59% 38%
44	t	165	93% 90% 7%
45	1	7	100% 100%
46	2	76	99% 83% 17%
47	3	75	100% 64% 36%
48	5	3543	38% 74% 25%
49	7	120	13% 88% 12%
50	8	156	38% 74% 23%
51	9	1869	57% 67% 23% 9%
52	AA	295	62% 67% 6% 26%
53	BB	264	72% 75% 5% 19%
54	CC	293	61% 70% 5% 25%
55	DD	243	86% 86% 8% 6%
56	EE	263	82% 94% 5%
57	FF	204	81% 86% 5% 9%
58	GG	249	93% 87% 8% 5%

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Mol	Chain	Length	Quality of chain
59	HH	194	91% 88% 8% 5%
60	II	208	84% 93% 6%
61	JJ	194	81% 89% 6% 5%
62	KK	165	58% 53% 5% 42%
63	LL	158	69% 81% 9% 9%
64	MM	132	89% 79% 10% 11%
65	NN	151	85% 88% 11%
66	OO	168	67% 73% 8% 19%
67	PP	145	83% 74% 8% 17%
68	QQ	146	90% 92% 5%
69	RR	135	84% 87% 10%
70	SS	152	93% 86% 9% 5%
71	TT	145	91% 90% 7%
72	UU	119	76% 77% 7% 16%
73	VV	83	89% 96%
74	WW	130	76% 95% 5%
75	XX	143	82% 92% 6%
76	YY	130	85% 87% 8% 5%
77	ZZ	125	58% 56% 40%
78	aa	115	70% 80% 7% 12%
79	bb	84	89% 89% 8%
80	cc	69	83% 83% 7% 10%
81	dd	56	86% 89% 9%
82	ee	133	41% 40% 59%
83	ff	156	44% 40% 56%

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Mol	Chain	Length	Quality of chain
84	gg	317	98% / 95%
85	hh	8	100% / 50% / 50%
86	ii	403	92% / 88% / 8%
87	jj	710	59% / 55% / 40%

2 Entry composition (i)

There are 90 unique types of molecules in this entry. The entry contains 222005 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	248	1898	1189	389	314	6	0	0

- Molecule 2 is a protein called Ul3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	394	3172	2020	597	542	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	362	2883	1812	577	480	14	0	0

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	293	2391	1512	438	427	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	216	1729	1115	329	282	3	0	0

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	225	1875	1205	358	303	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	233	1879	1199	361	315	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	190	1516	954	284	272	6	0	0

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	205	1664	1056	321	274	13	0	0

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	170	1362	861	254	241	6	0	0

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	210	1702	1065	354	279	4	0	0

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	138	1137	727	221	182	7	0	0

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	203	1701	1072	359	266	4	0	0

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	199	1630	1051	319	255	5	0	0

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	153	1242	777	241	215	9	0	0

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	187	1515	946	315	250	4	0	0

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	180	1508	933	328	238	9	0	0

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	176	1462	930	285	236	11	0	0

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	159	1298	823	252	217	6	0	0

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	99	809	519	141	147	2	0	0

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	131	979	618	184	172	5	0	0

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	106	860	538	174	144	4	0	0

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	118	967	618	181	167	1	0	0

- Molecule 24 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	134	1115	700	226	186	3	0	0

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	135	1107	714	208	182	3	0	0

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	147	1162	734	239	185	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	104	848	527	189	129	3	0	0

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	98	761	481	134	140	6	0	0

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	107	888	560	171	155	2	0	0

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	128	1053	667	216	165	5	0	0

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	109	876	555	174	143	4	0	0

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	114	906	566	187	147	6	0	0

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	122	1013	640	204	168	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	102	830	520	176	129	5	0	0

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	86	705	434	155	111	5	0	0

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	69	569	366	103	99	1	0	0

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	50	447	286	96	64	1	0	0

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	52	429	266	90	67	6	0	0

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	25	239	145	64	27	3	0	0

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	104	851	533	174	138	6	0	0

- Molecule 41 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	91	708	445	136	120	7	0	0

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	r	124	994	616	205	167	6	0	0

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	s	196	1507	959	263	276	9	0	0

- Molecule 44 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	t	153	1160	722	218	217	3	0	0

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	1	7	49	31	8	10	0	0

- Molecule 46 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	2	76	1616	723	291	527	75	0	0

- Molecule 47 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	3	75	1593	712	281	526	74	0	0

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	5	3543	75972	33833	13910	24686	3543	0	0

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	7	120	2558	1141	456	842	119	0	0

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	8	151	3208	1432	564	1062	150	0	0

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	9	1698	36249	16180	6508	11864	1697	0	0

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	AA	217	1710	1086	300	316	8	0	0

- Molecule 53 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	BB	213	1729	1098	309	308	14	0	0

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	CC	221	1716	1111	295	301	9	0	0

- Molecule 55 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	DD	228	1768	1126	318	316	8	0	0

- Molecule 56 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	EE	262	2076	1324	386	358	8	0	0

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	FF	185	1471	921	277	266	7	0	0

- Molecule 58 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	GG	237	1923	1200	387	329	7	0	0

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	HH	185	1488	952	271	264	1	0	0

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	II	206	1686	1058	332	291	5	0	0

- Molecule 61 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	JJ	185	1525	969	306	248	2	0	0

- Molecule 62 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	KK	96	810	530	143	131	6	0	0

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	LL	143	1175	749	222	198	6	0	0

- Molecule 64 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	MM	117	908	570	161	169	8	0	0

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	NN	149	1202	770	228	203	1	0	0

- Molecule 66 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	OO	136	1016	621	199	190	6	0	0

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	PP	120	997	635	187	168	7	0	0

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	QQ	142	1128	717	213	195	3	0	0

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	RR	132	1068	670	199	195	4	0	0

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	SS	144	1190	746	241	202	1	0	0

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	TT	141	1097	688	211	195	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	UU	100	795	498	152	141	4	0	0

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	VV	83	636	393	117	121	5	0	0

- Molecule 74 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	WW	129	1034	659	193	176	6	0	0

- Molecule 75 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	XX	141	1098	693	219	183	3	0	0

- Molecule 76 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	YY	124	1011	640	198	168	5	0	0

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	ZZ	75	598	382	111	104	1	0	0

- Molecule 78 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	aa	101	814	507	170	132	5	0	0

- Molecule 79 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	bb	83	651	408	121	115	7	0	0

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	cc	62	488	297	97	92	2	0	0

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	dd	55	459	286	94	74	5	0	0

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	ee	55	443	274	97	71	1	0	0

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	ff	68	555	351	103	94	7	0	0

- Molecule 84 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	gg	313	2436	1535	424	465	12	0	0

- Molecule 85 is a RNA chain called mRNA (UGA stop codon).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
85	hh	8	169	76	29	56	8	0	0

- Molecule 86 is a protein called Protein pelota homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	ii	372	2947	1844	528	559	16	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	221	MET	LEU	variant	UNP Q9BRX2
ii	386	GLY	-	expression tag	UNP Q9BRX2
ii	387	SER	-	expression tag	UNP Q9BRX2
ii	388	GLU	-	expression tag	UNP Q9BRX2
ii	389	ASN	-	expression tag	UNP Q9BRX2
ii	390	LEU	-	expression tag	UNP Q9BRX2
ii	391	TYR	-	expression tag	UNP Q9BRX2
ii	392	PHE	-	expression tag	UNP Q9BRX2
ii	393	GLN	-	expression tag	UNP Q9BRX2
ii	394	GLY	-	expression tag	UNP Q9BRX2
ii	395	ALA	-	expression tag	UNP Q9BRX2
ii	396	HIS	-	expression tag	UNP Q9BRX2
ii	397	HIS	-	expression tag	UNP Q9BRX2
ii	398	HIS	-	expression tag	UNP Q9BRX2
ii	399	HIS	-	expression tag	UNP Q9BRX2
ii	400	HIS	-	expression tag	UNP Q9BRX2
ii	401	HIS	-	expression tag	UNP Q9BRX2
ii	402	SER	-	expression tag	UNP Q9BRX2
ii	403	THR	-	expression tag	UNP Q9BRX2

- Molecule 87 is a protein called HBS1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	jj	425	3292	2100	565	609	18	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	-25	MET	-	initiating methionine	UNP Q9Y450
jj	-24	ASP	-	expression tag	UNP Q9Y450

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Chain	Residue	Modelled	Actual	Comment	Reference
jj	-23	TYR	-	expression tag	UNP Q9Y450
jj	-22	LYS	-	expression tag	UNP Q9Y450
jj	-21	ASP	-	expression tag	UNP Q9Y450
jj	-20	HIS	-	expression tag	UNP Q9Y450
jj	-19	ASP	-	expression tag	UNP Q9Y450
jj	-18	GLY	-	expression tag	UNP Q9Y450
jj	-17	ASP	-	expression tag	UNP Q9Y450
jj	-16	TYR	-	expression tag	UNP Q9Y450
jj	-15	LYS	-	expression tag	UNP Q9Y450
jj	-14	ASP	-	expression tag	UNP Q9Y450
jj	-13	HIS	-	expression tag	UNP Q9Y450
jj	-12	ASP	-	expression tag	UNP Q9Y450
jj	-11	ILE	-	expression tag	UNP Q9Y450
jj	-10	ASP	-	expression tag	UNP Q9Y450
jj	-9	TYR	-	expression tag	UNP Q9Y450
jj	-8	LYS	-	expression tag	UNP Q9Y450
jj	-7	ASP	-	expression tag	UNP Q9Y450
jj	-6	ASP	-	expression tag	UNP Q9Y450
jj	-5	ASP	-	expression tag	UNP Q9Y450
jj	-4	ASP	-	expression tag	UNP Q9Y450
jj	-3	LYS	-	expression tag	UNP Q9Y450
jj	-2	ALA	-	expression tag	UNP Q9Y450
jj	-1	GLY	-	expression tag	UNP Q9Y450
jj	0	SER	-	expression tag	UNP Q9Y450

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
88	B	1	1	1	0
88	I	1	1	1	0
88	L	1	1	1	0
88	P	2	2	2	0
88	V	1	1	1	0
88	a	1	1	1	0
88	e	1	1	1	0

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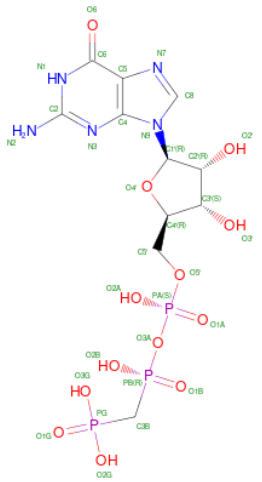
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
88	g	1	1	1	0
88	j	1	1	1	0
88	5	176	176	176	0
88	7	5	5	5	0
88	8	6	6	6	0
88	9	66	66	66	0
88	jj	1	1	1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
89	g	1	1	1	0
89	j	1	1	1	0
89	m	1	1	1	0
89	o	1	1	1	0
89	p	1	1	1	0
89	aa	1	1	1	0
89	dd	1	1	1	0
89	ff	1	1	1	0

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

GCP



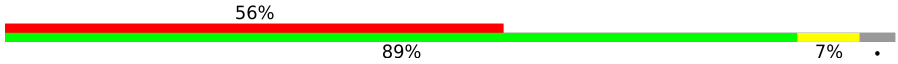
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
90	jj	1	32	11	5	13	3	0

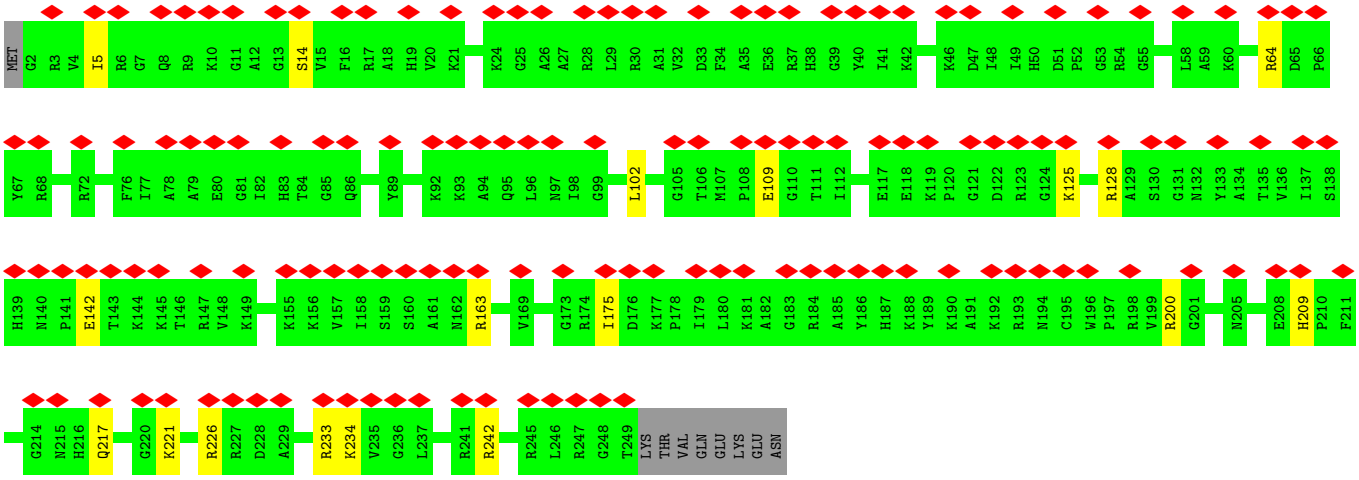
3 Residue-property plots (i)

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: uL2

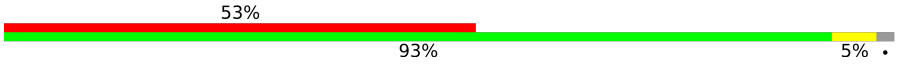
Chain A:

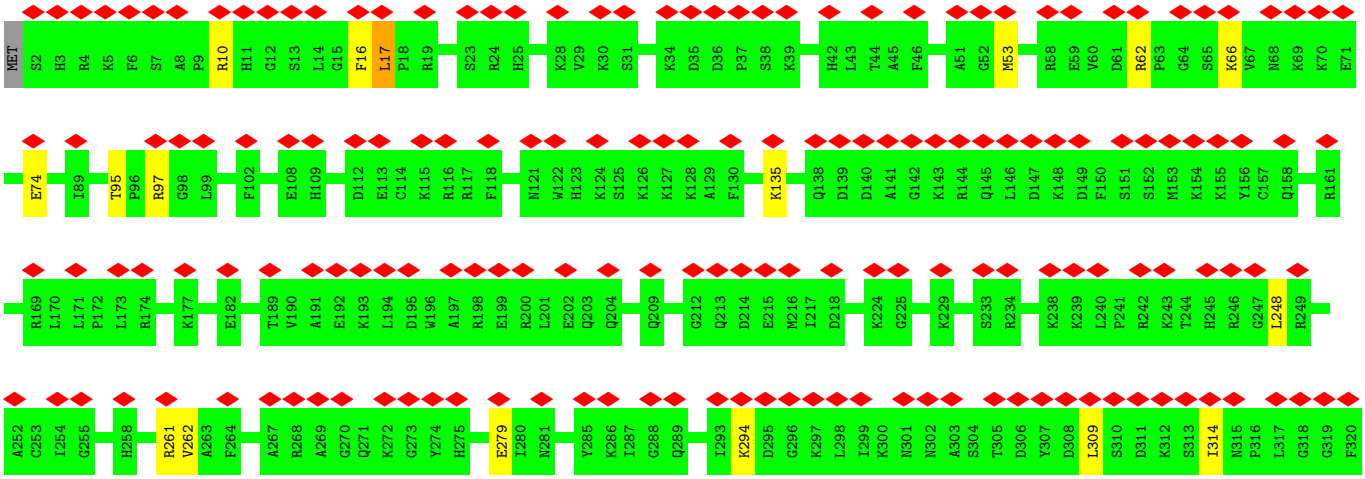


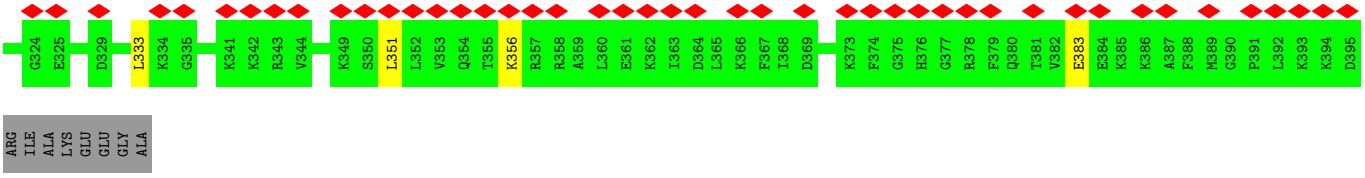


- Molecule 2: Ul3

Chain B:

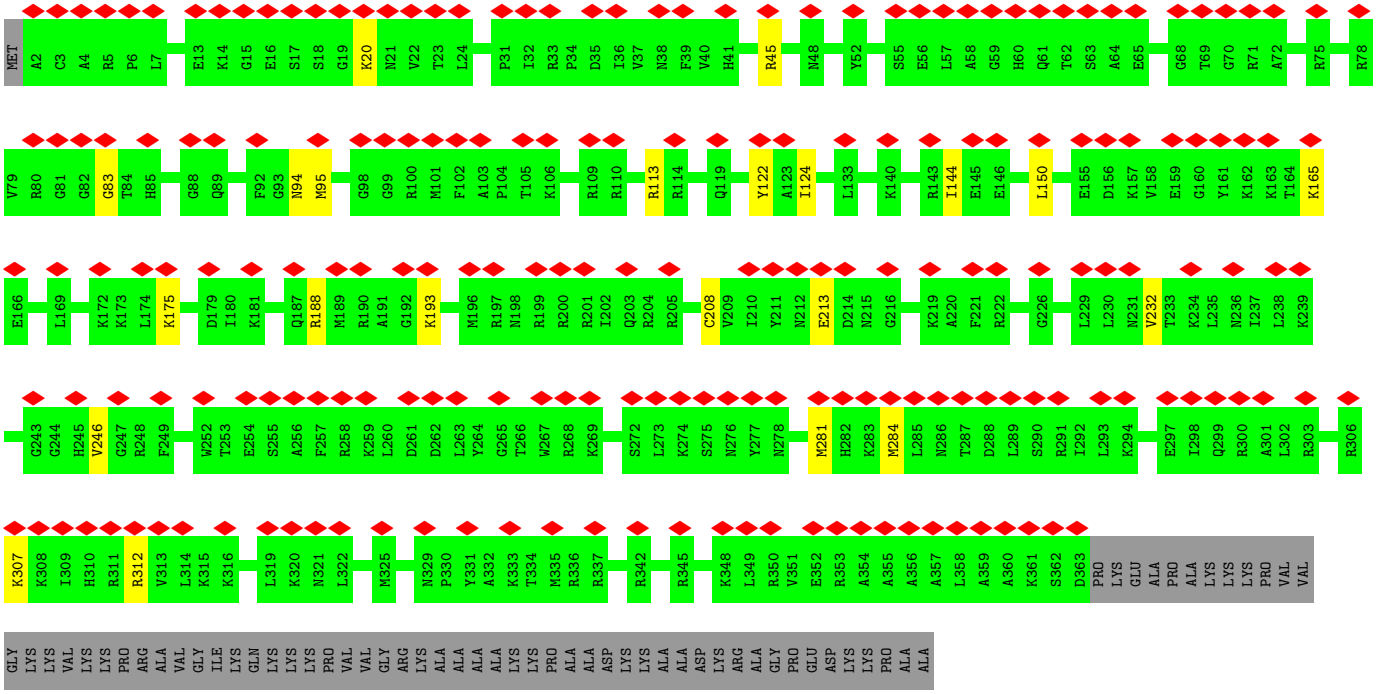






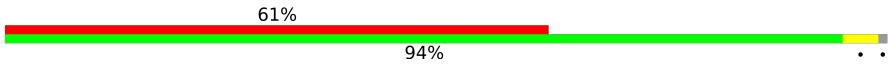
• Molecule 3: uL4

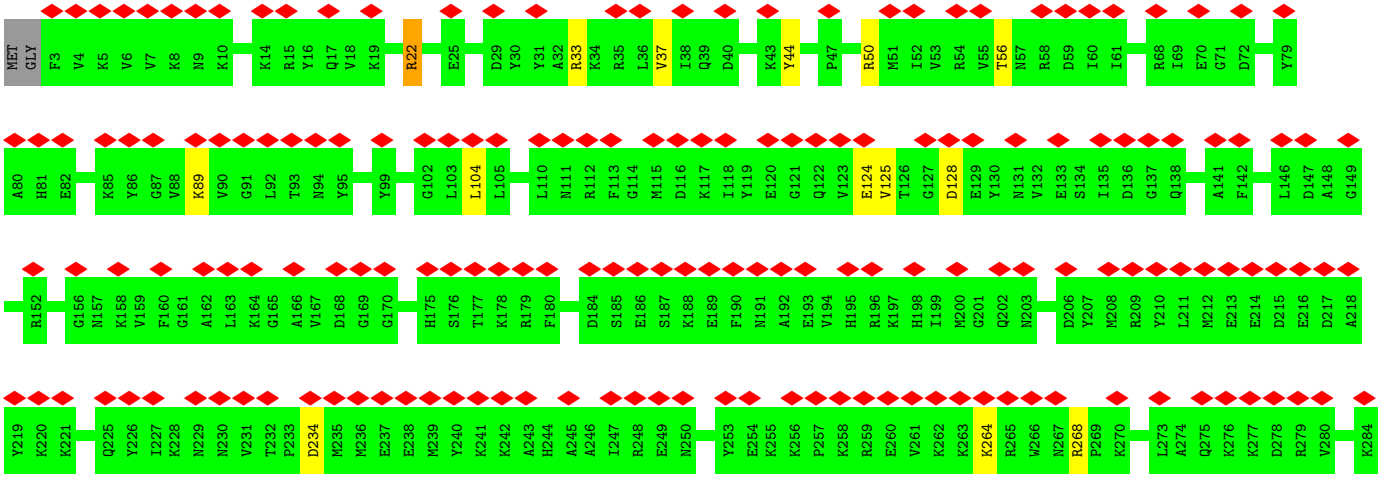
Chain C:

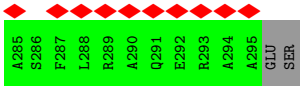


• Molecule 4: 60S ribosomal protein L5

Chain D:

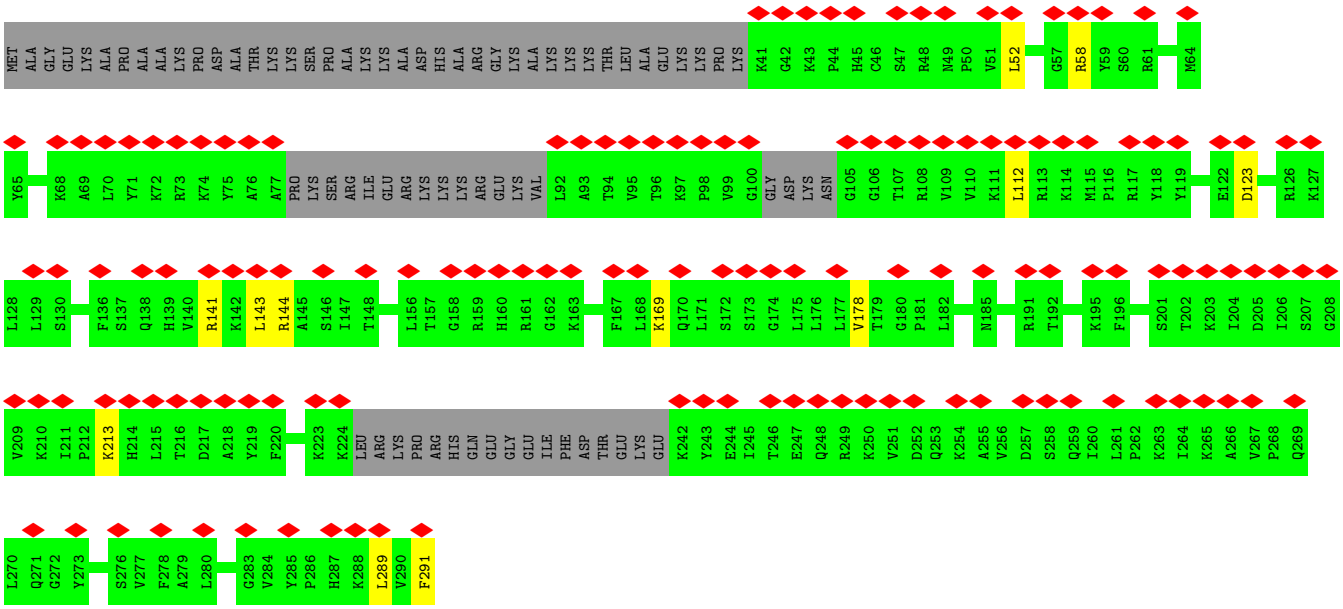






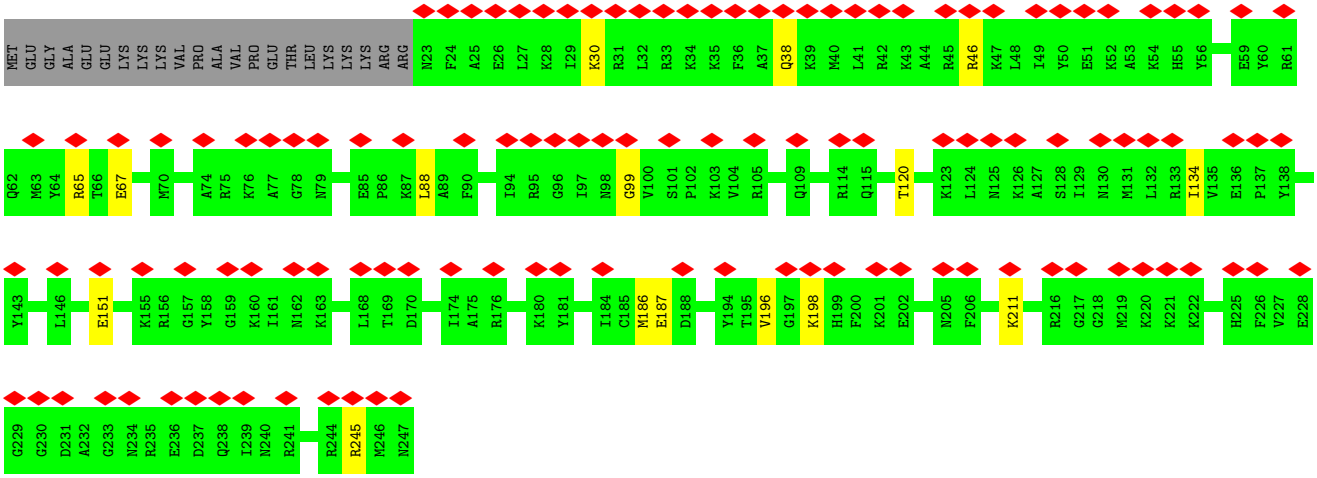
- Molecule 5: 60S ribosomal protein L6

Chain E:



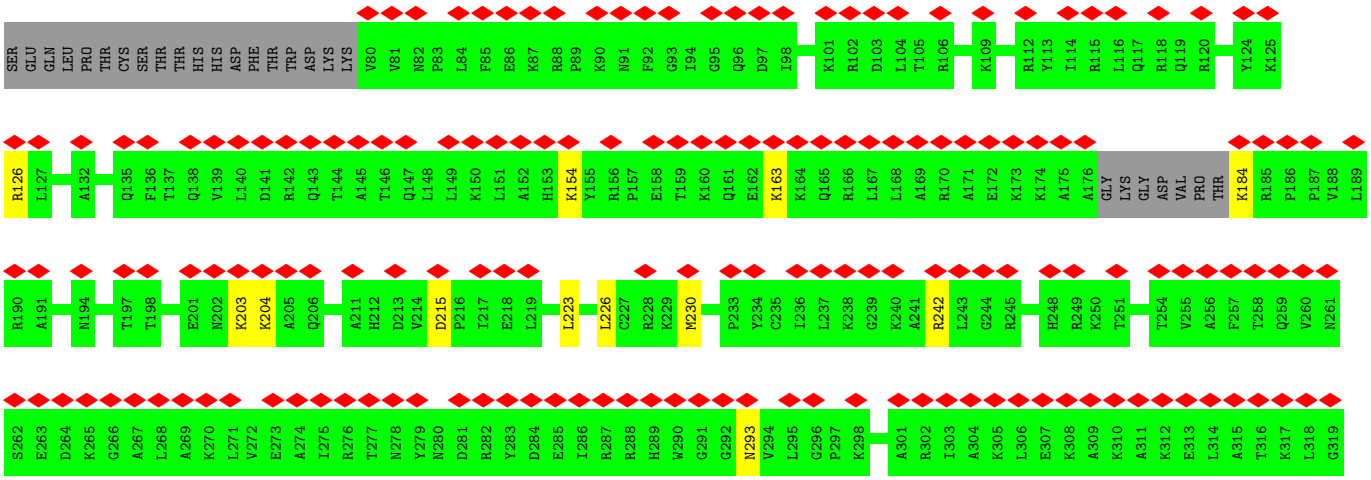
- Molecule 6: uL30

Chain F:



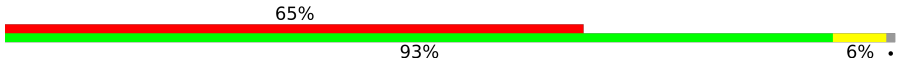
- Molecule 7: eL8

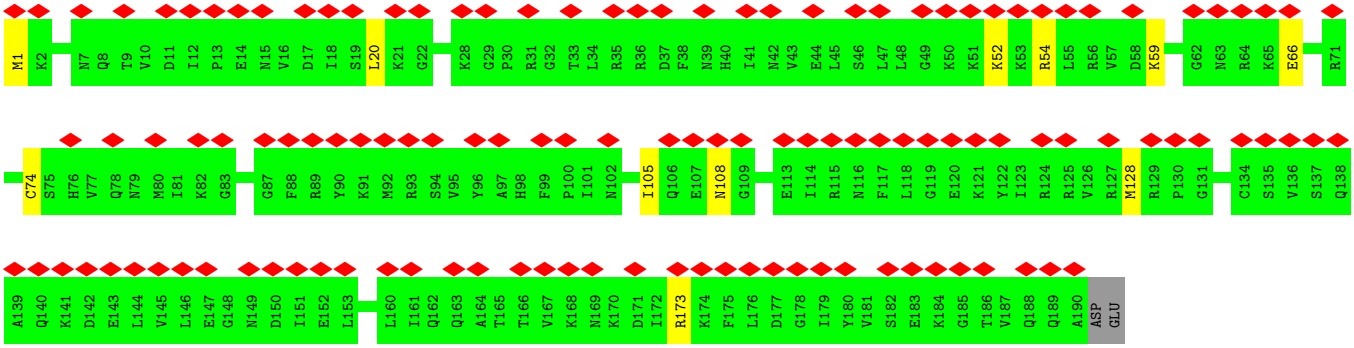
Chain G:



- Molecule 8: uL6

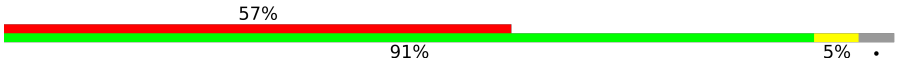
Chain H:

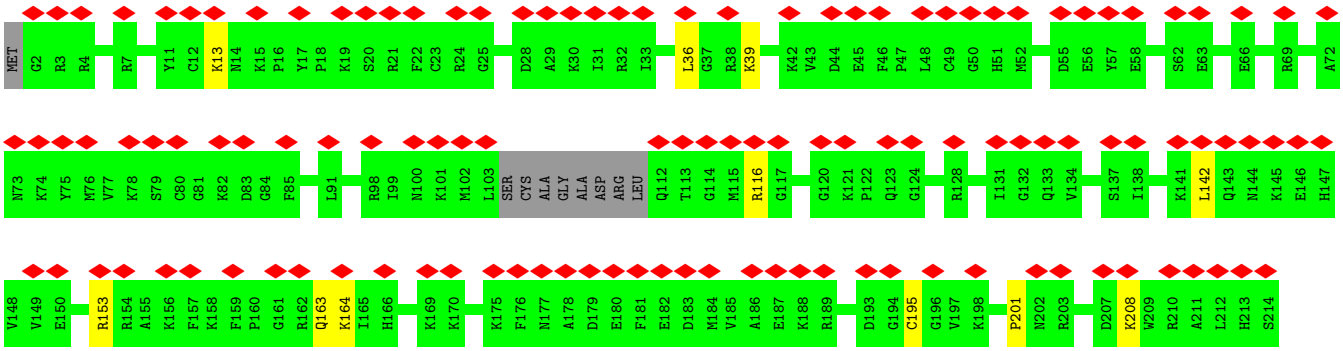




- Molecule 9: Ribosomal protein L10 (Predicted)

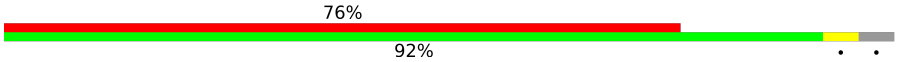
Chain I:

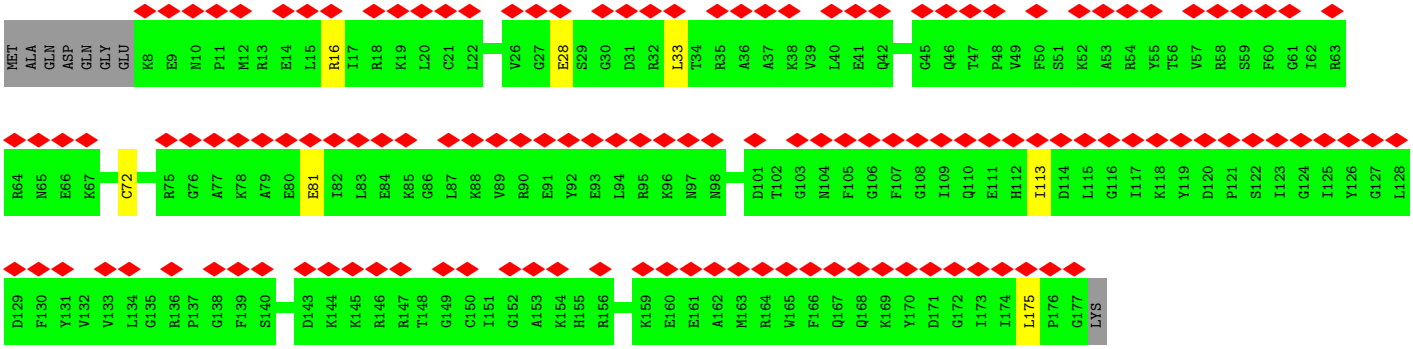




- Molecule 10: uL5

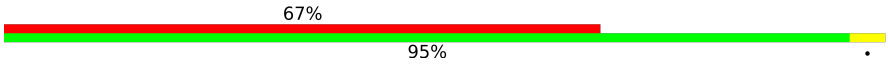
Chain J:

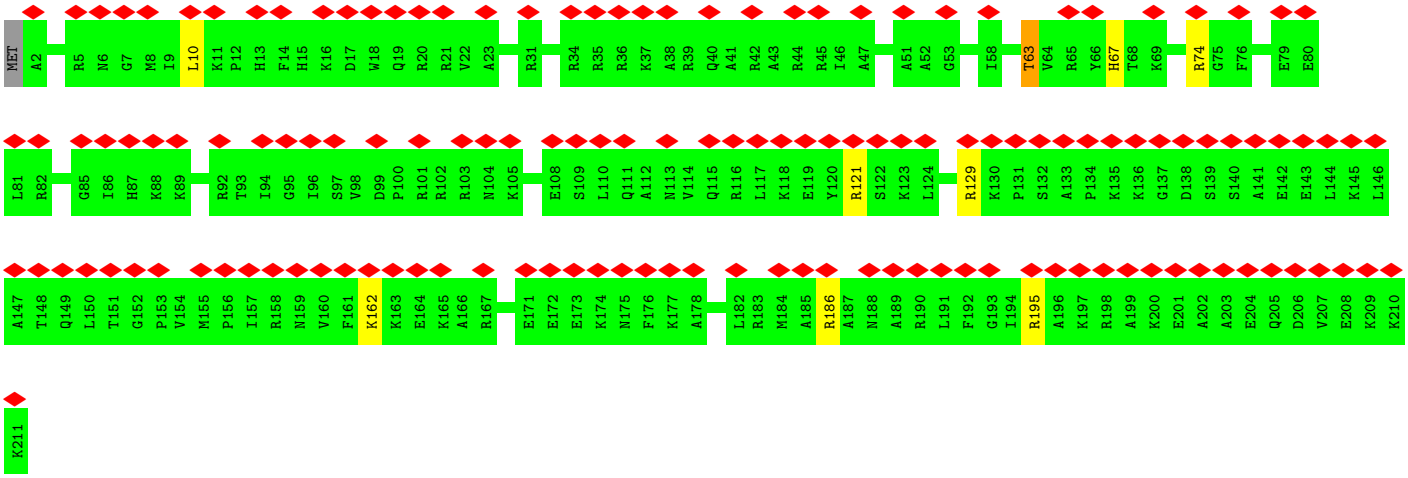




• Molecule 11: eL13

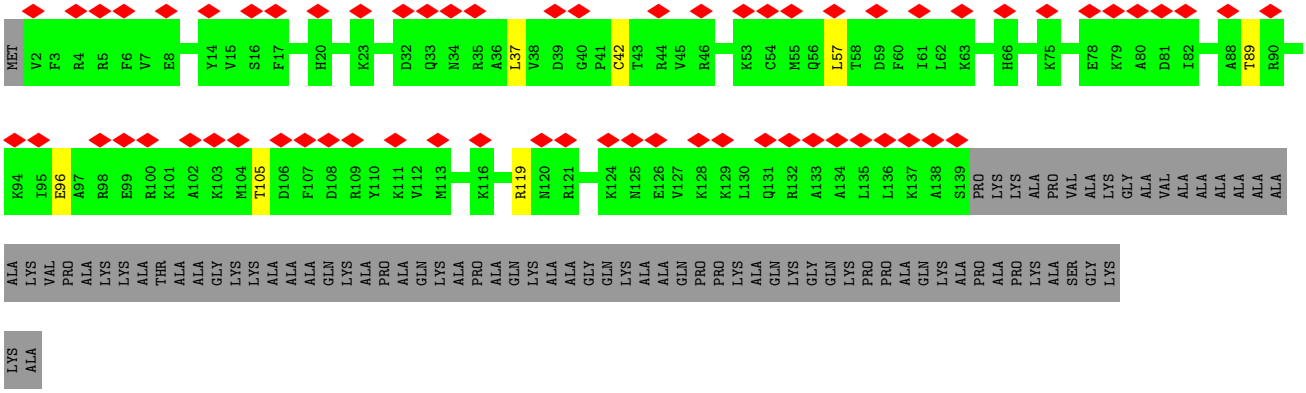
Chain L:





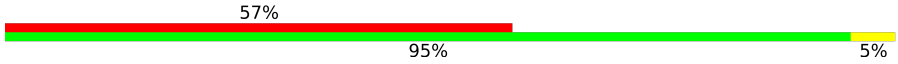
• Molecule 12: eL14

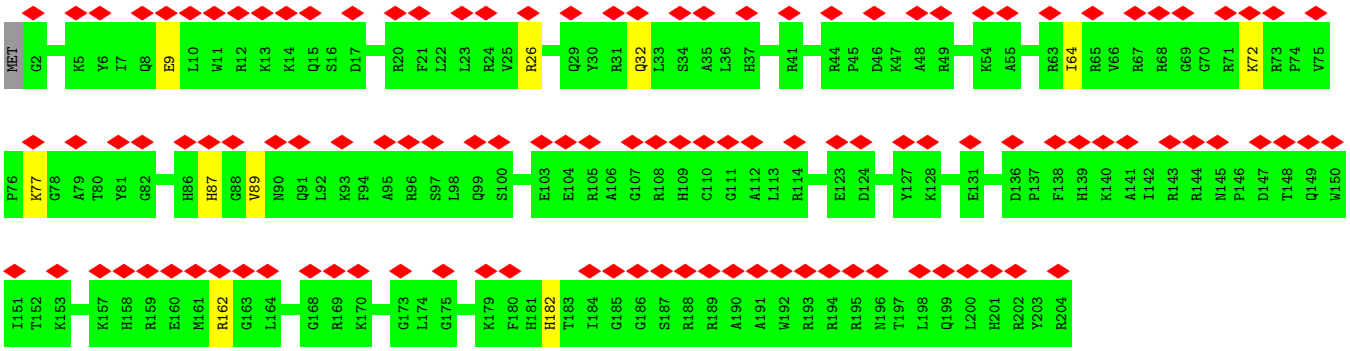
Chain M:



• Molecule 13: Ribosomal protein L15

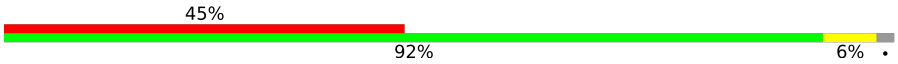
Chain N:

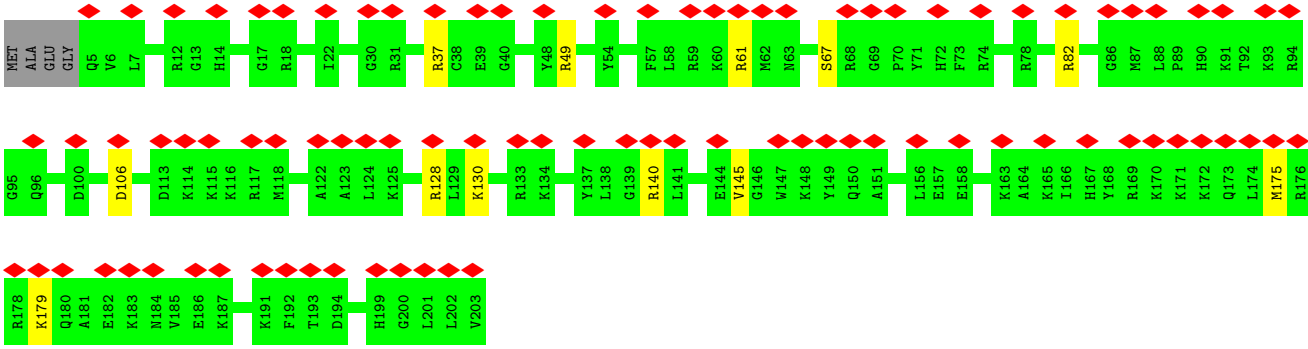




- Molecule 14: uL13

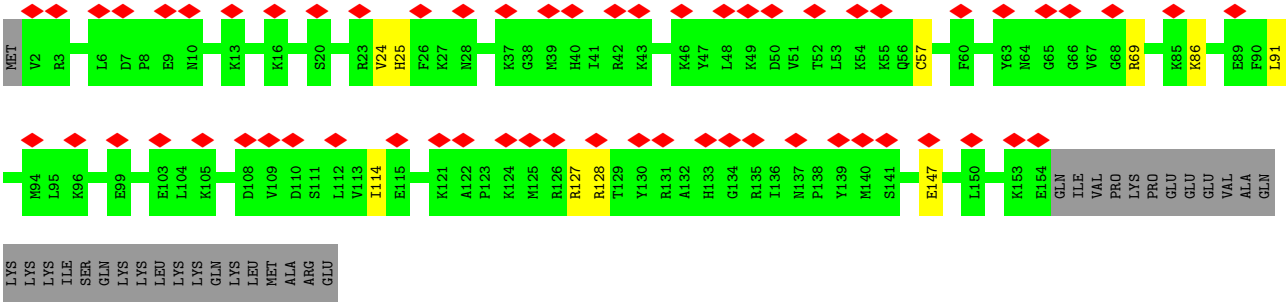
Chain O:





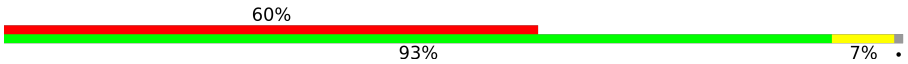
- Molecule 15: uL22

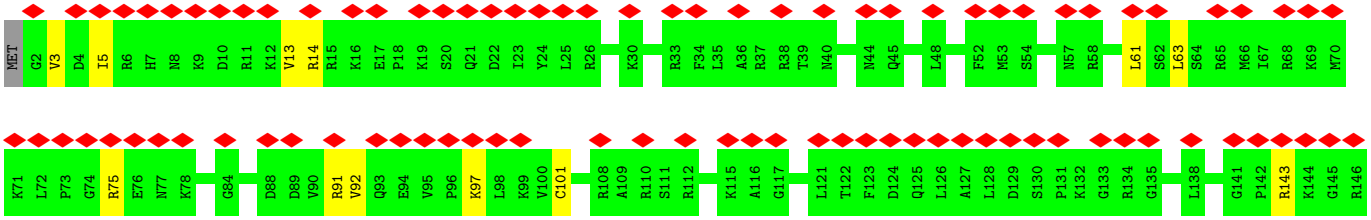
Chain P:

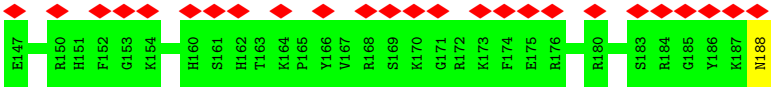


- Molecule 16: eL18

Chain Q:

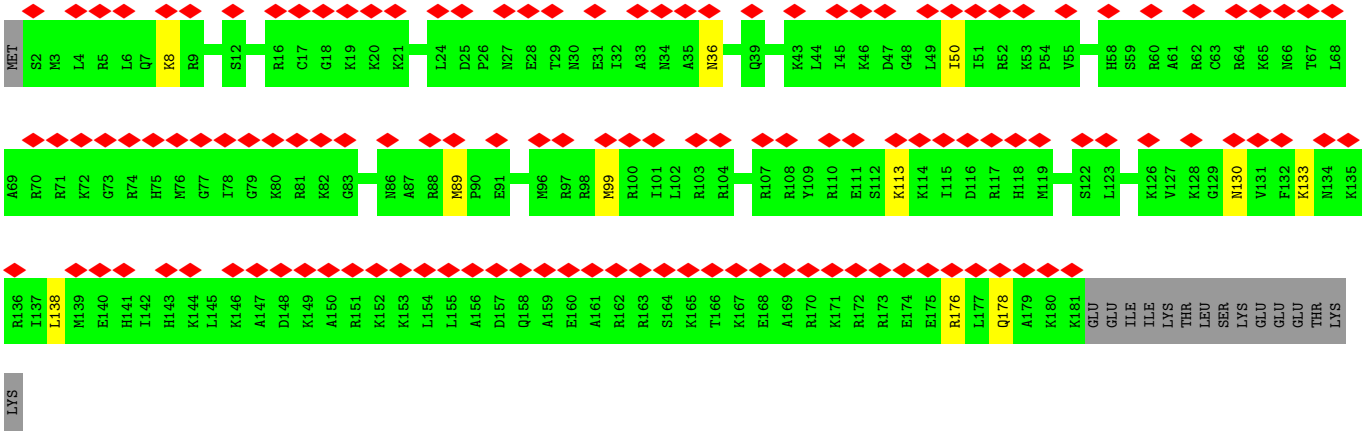






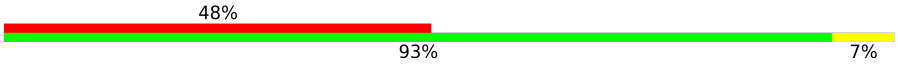
- Molecule 17: eL19

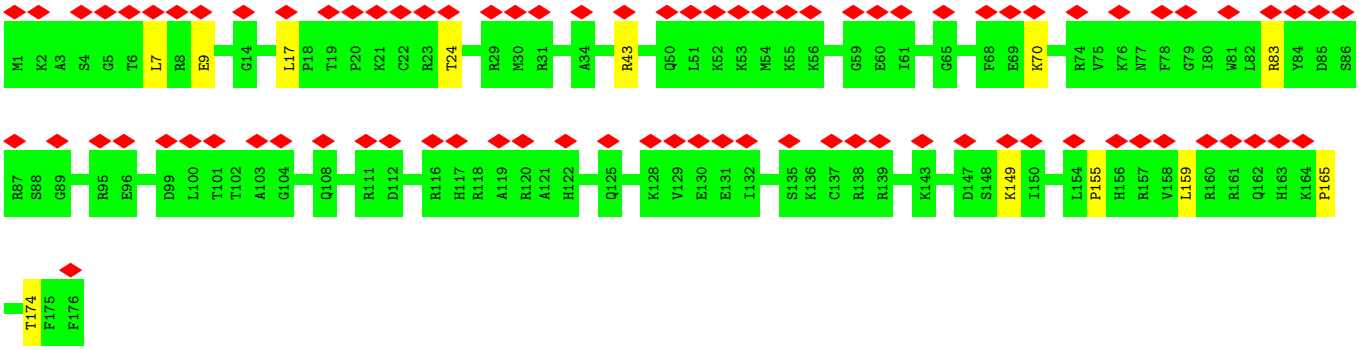
Chain R:



- Molecule 18: eL20

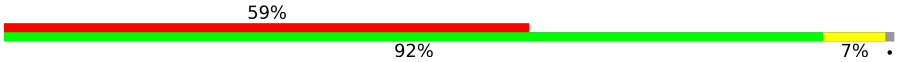
Chain S:

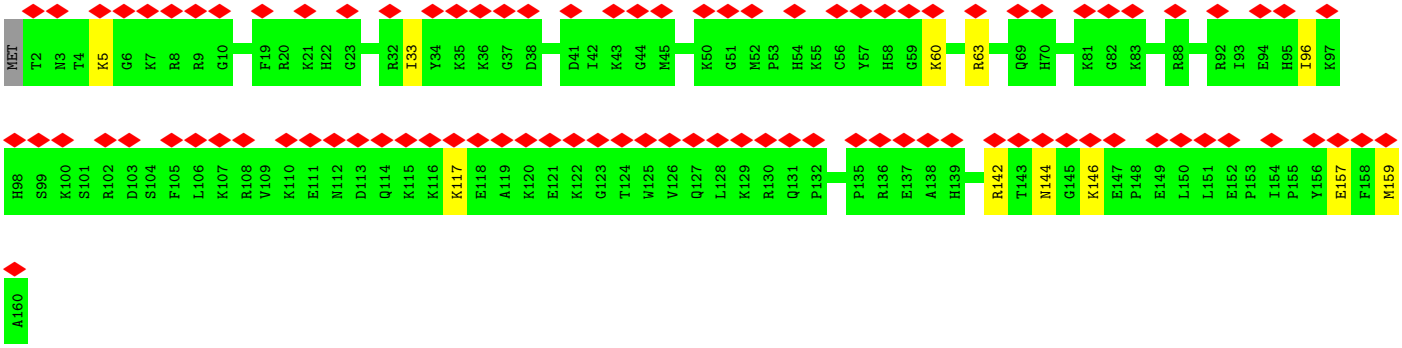




- Molecule 19: eL21

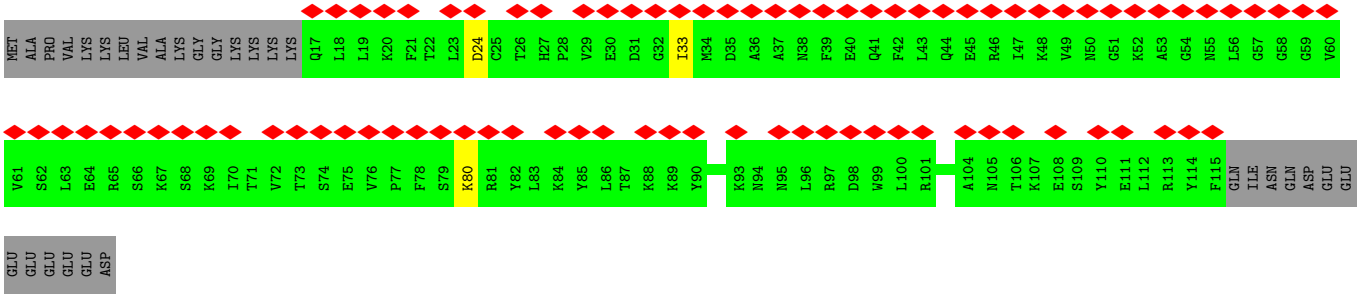
Chain T:





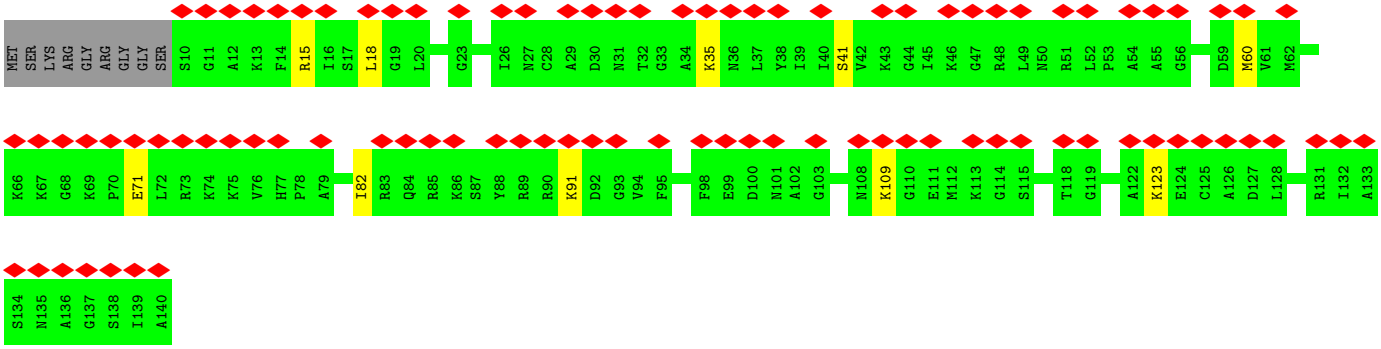
- Molecule 20: eL22

Chain U:



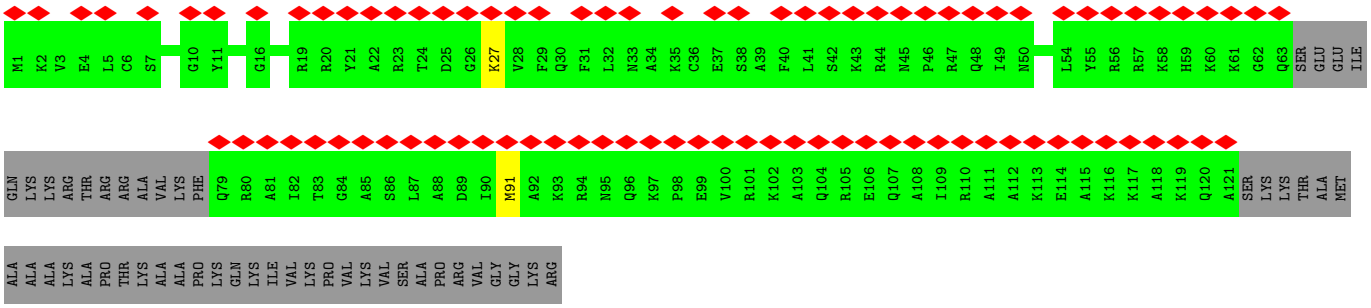
- Molecule 21: uL14

Chain V:



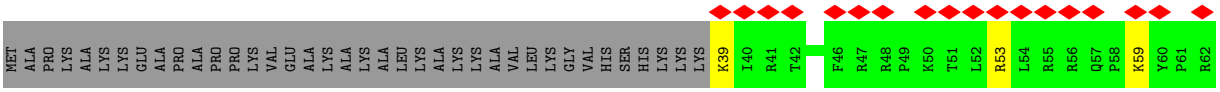
- Molecule 22: eL24

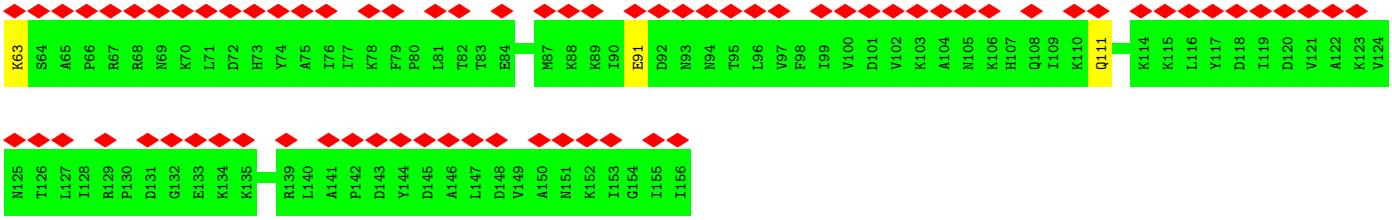
Chain W:



- Molecule 23: uL23

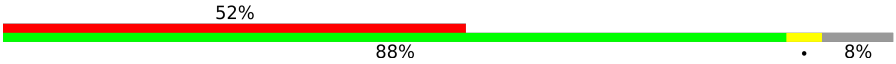
Chain X:

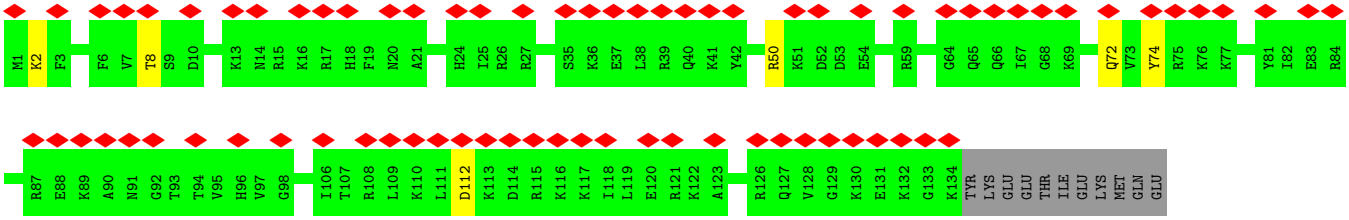




- Molecule 24: uL24

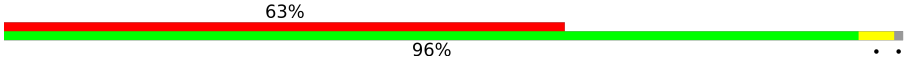
Chain Y:

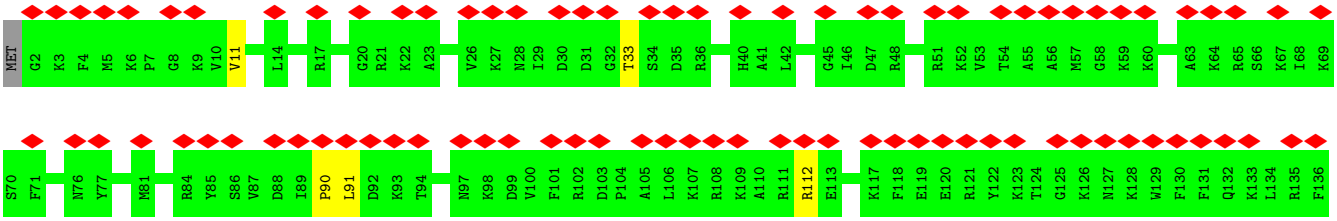




- Molecule 25: 60S ribosomal protein L27

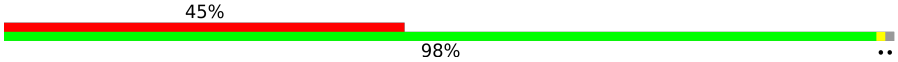
Chain Z:

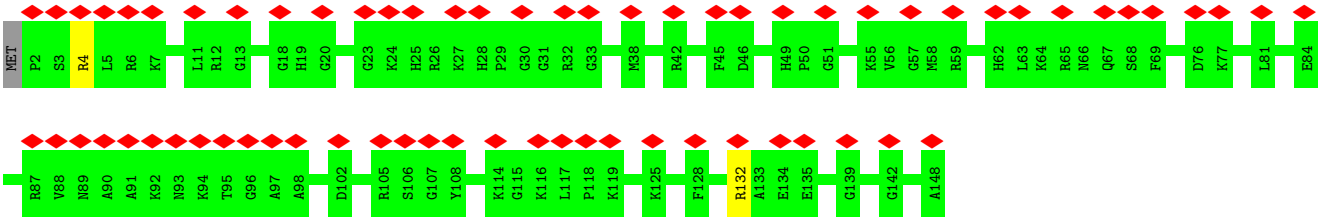




- Molecule 26: uL15

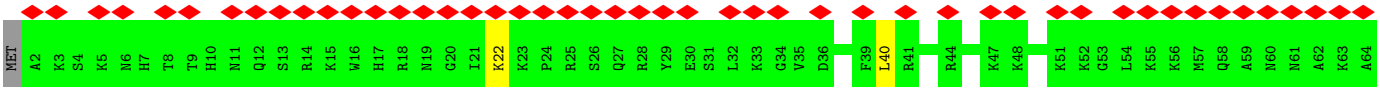
Chain a:

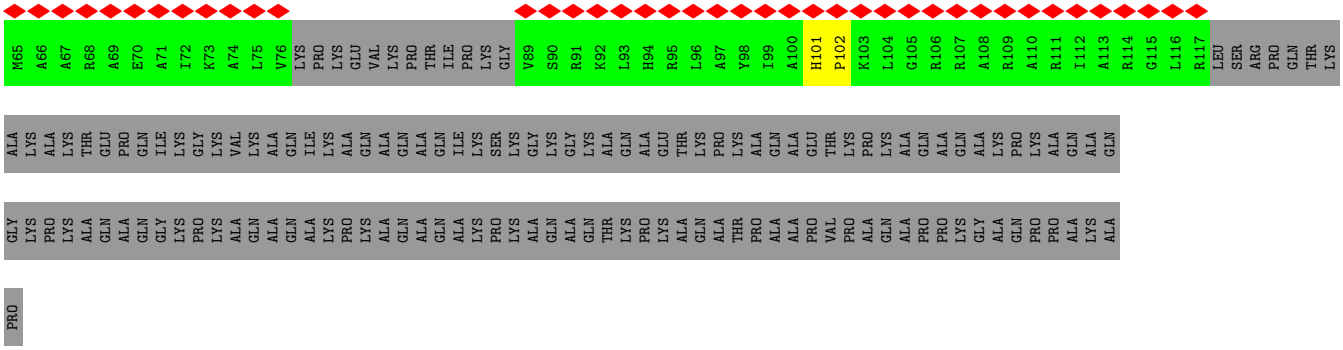




- Molecule 27: eL29

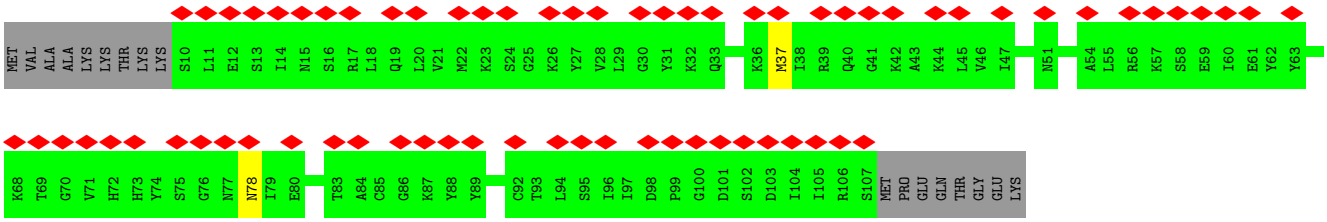
Chain b:





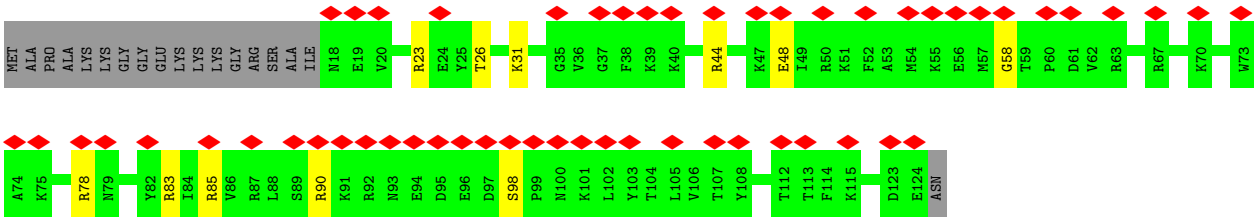
- Molecule 28: eL30

Chain c:



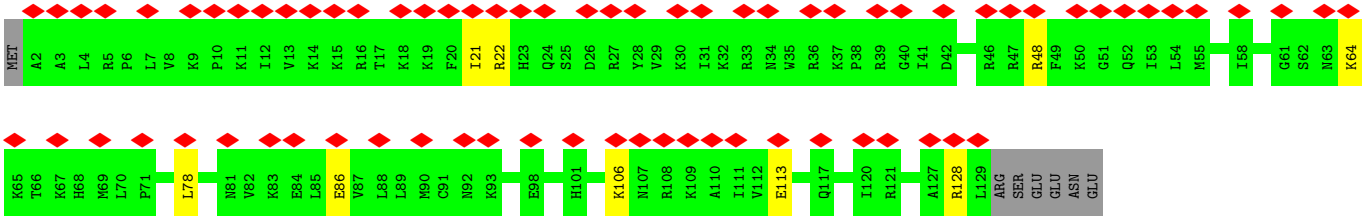
- Molecule 29: eL31

Chain d:



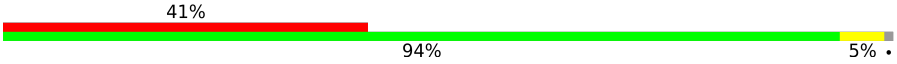
- Molecule 30: eL32

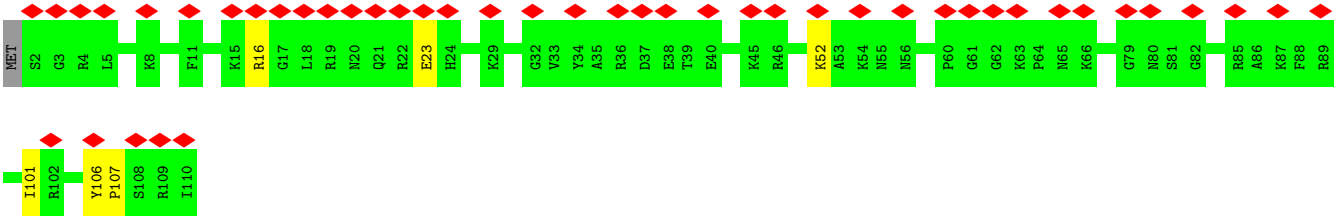
Chain e:



- Molecule 31: eL33

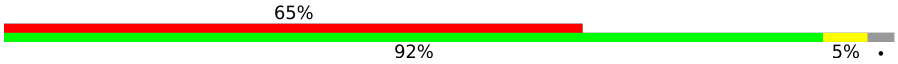
Chain f:

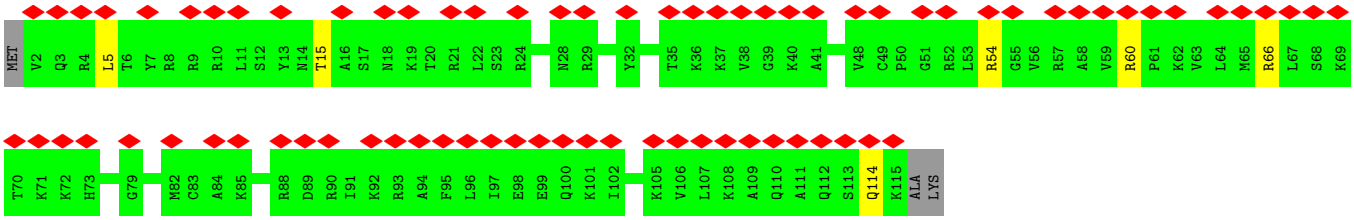




- Molecule 32: eL34

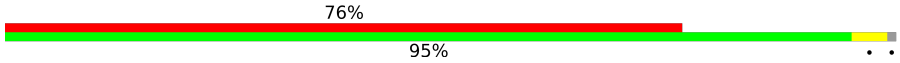
Chain g:

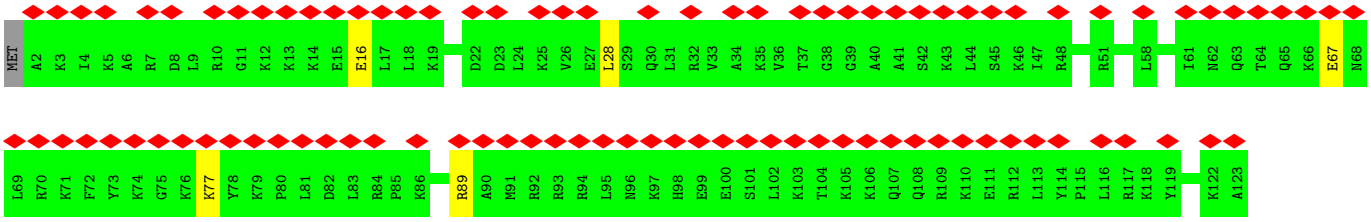




- Molecule 33: uL29

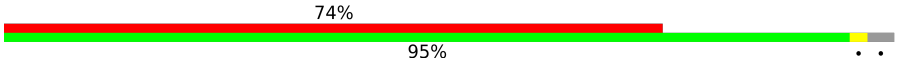
Chain h:

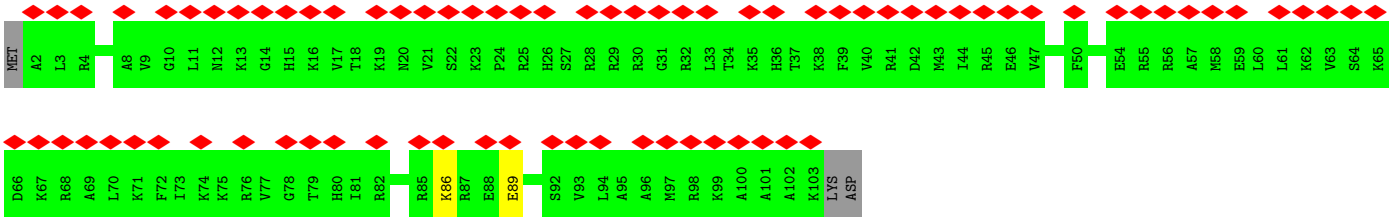




- Molecule 34: 60S ribosomal protein L36

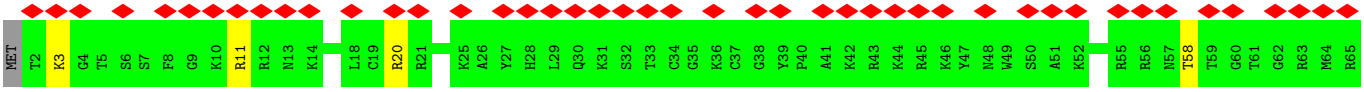
Chain i:

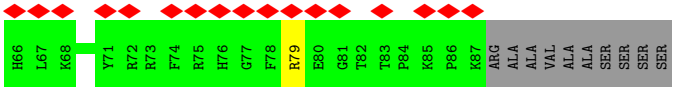




- Molecule 35: Ribosomal protein L37

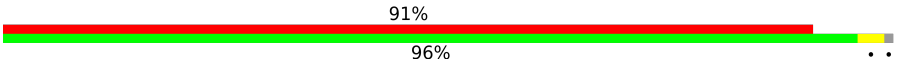
Chain j:

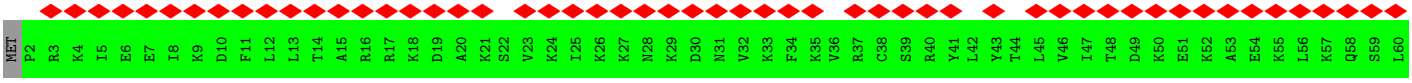


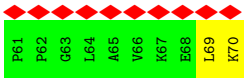


- Molecule 36: eL38

Chain k:

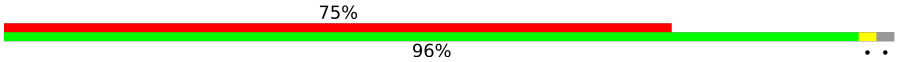


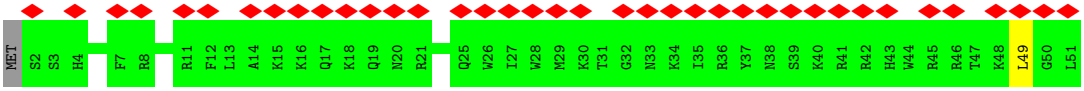




- Molecule 37: eL39

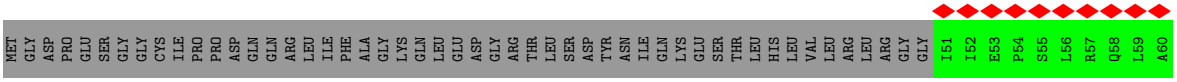
Chain l:

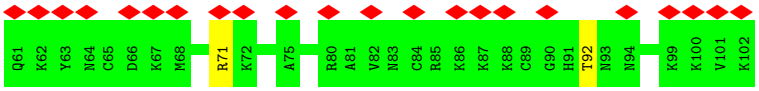




- Molecule 38: eL40

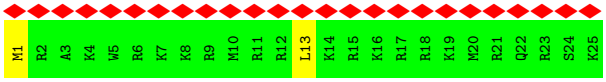
Chain m:





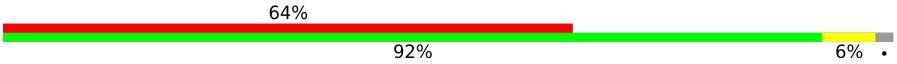
- Molecule 39: eL41

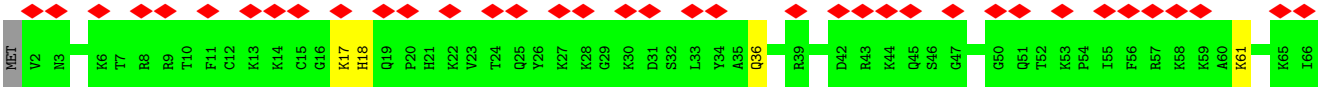
Chain n:

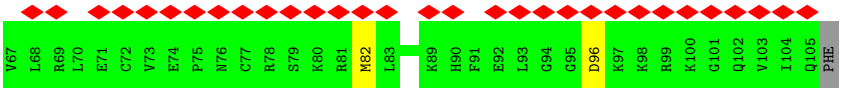


- Molecule 40: eL42

Chain o:







- Molecule 41: eL43

Chain p: 64% 97%

MET A2 K3 R4 T5 K6 K7 V8 G9 I10 V11 G12 R17 Y18 G19 L22 R23 K24 M25 V26 K27 K28 I29 E30 Q33 H34 A35 K36 Y37 T38 F41 T45 K46 M47 K48 R49 R50 A51 V52 G53 H56 C57 G58 S59 C60 M61 W69 N72 T73 T74 S75 A76

V77 T78 V79 K80 S81 A82 I83 R84 R85 L86 K87 E88 L89 K90 D91 Q92

- Molecule 42: eL28

Chain r: 44% 82% 8% 9%

MET S2 A3 H4 L5 Q6 W7 M8 R11 N12 C13 F16 R20 E28 P29 N30 N31 L32 K33 A34 R35 N36 S37 F38 R39 Y40 N41 G42 L43 R46 K47 E52 P53 A54 A55 D56 G57 K58 G59 M64 K65 R66 R67 S68 G69 Q70 R71 T75 R79 T80 T81

I82 N83 K84 N85 A86 R87 A88 S91 I97 R98 K99 N100 K101 Y102 H103 P104 D105 L106 R107 M108 A109 A110 T117 L118 R119 S120 Q121 K122 P123 V124 M125 VAL LYS ARG LYS ARG THR ARG PRO THR LYS SER SER

- Molecule 43: uL10

Chain s: 62% 59% 38%

MET PRO ARG GLU D5 R6 A7 T8 W9 K10 S11 N12 Y13 F14 L15 K16 I17 I18 Q19 L20 L21 D22 D23 Y24 P25 K26 C27 F28 I29 V30 G31 A32 D33 N34 V35 G36 S37 K38 Q39 M40 Q41 Q42 I43 R44 M45 S46 L47 R48 G49 K50 A51 V52 V53 L54 M55 G56 K57 N58 T59 M60

M61 R62 K63 A64 I65 R66 G67 H68 L69 E70 N71 N72 P73 A74 L75 E76 K77 L78 L79 P80 H81 I82 R83 G84 N85 V86 G87 F88 V89 F90 T91 K92 E93 D94 L95 T96 E97 I98 R99 D100 M101 L102 L103 A104 N105 K106 V107 P108 A109 A110 A111 R112 A113 G114 A115 I116 A117 P118 C119 E120

V121 T122 V123 P124 A125 Q126 N127 T128 G129 L130 G131 P132 E133 K134 T135 S136 F137 F138 Q139 A140 L141 G142 I143 T144 T145 K146 I147 S148 R149 G150 T151 I152 E153 I154 L155 S156 D157 V158 Q159 L160 I161 K162 T163 G164 D165 K166 V167 G168 A169 S170 E171 A172 T173 G174 L175 N176 M177 L178 N179 I180

S181 P182 F183 S184 F185 G186 L187 I188 I189 Q190 Q191 V192 F193 D194 N195 G196 S197 I198 Y199 N200 PRO GLU VAL LEU ASP ILE THR GLU ASP THR LEU HIS SER ARG PHE LEU GLU GLY VAL ARG ASN VAL ALA SER VAL CYS LEU GLN ILE GLY TYR PRO THR VAL ALA SER VAL PRO HIS SER

ILE ILE ASN GLY TYR LYS ARG VAL LEU ALA LEU SER VAL GLU THR GLU TYR THR PHE PRO LEU ALA GLU LYS VAL LYS ALA PHE LEU ALA ASP PRO SER ALA PHE VAL ALA ALA ALA PRO VAL ALA ALA ALA SER THR ALA ALA PRO ALA ALA ALA ALA ALA ALA PRO ALA LYS VAL GLU

ALA LYS GLU GLU SER GLU GLU SER ASP GLU ASP MET GLY PHE GLY LEU PHE ASP

- Molecule 44: uL11

Chain t: 93% 90% 7%

MET PRO PRO LYS PHE ASP PRO ASN E9 I10 K11 V12 V13 Y14 L15 R16 C17 T18 G19 G20 E21 V22 G23 A24 T25 S26 A27 L28 A29 P30 K31 I32 G33 P34 L35 G36 L37 S38 P39 K40 K41 V42 G43 D44 D45 I46 A47 K48 A49 T50 G51 D52 W53 K54 G55 L56 R57 I58 T59 V60

K61 L62 T63 I64 Q65 N66 R67 Q68 A69 Q70 I71 E72 V73 V74 P75 S76 A77 S78 A79 L80 I81 I82 K83 A84 L85 K86 E87 P88 P89 R90 D91 R92 K93 K94 Q95 K96 N97 I98 K99 H100 S101 G102 N103 I104 T105 F106 D107 E108 I109 V110 N111 I112 A113 R114 Q115 M116 R117 H118 R119 S120

L121 A122 R123 E124 L125 S126 G127 T128 I129 K130 E131 I132 L133 G134 T135 A136 Q137 S138 V139 G140 C141 N142 V143 D144 G145 R146 H147 P148 H149 D150 I151 I152 D153 D154 I155 N156 S157 G158 A159 V160 E161 CYS PRO ALA SER

- Molecule 45: Nascent chain

Chain 1: 100% / 100%

D62 S63 P64 G65 L66 K67 V68

- Molecule 46: P-site tRNA

Chain 2: 99% / 83% / 17%

G1 U2 C3 U4 C5 C6 G7 U8 A9 G10 U11 G12 U13 A14 G15 C16 G18 G19 U20 U20A A21 U22 C23 A24 C25 G26 U27 U28 C29 G30 C31 C32 U33 A34 A35 C36 A37 C38 G39 C40 G41 A42 A43 A44 G45 G46 U47 C48 C49 U50 C51 G52 G53 U54 U55 C56 G57 A58 A59 A60

C61 C62 G63 G64 G65 C66 G67 G68 A69 A70 A71 C72 A73 C74 C75 A76

- Molecule 47: E-site tRNA

Chain 3: 100% / 64% / 36%

G1 C2 C3 C4 G5 G6 A7 U8 A9 G10 C11 U12 C13 A14 G15 C16 U18 G19 U20 A21 G22 A23 G24 C25 A26 U27 C28 A29 G30 A31 C32 U33 U34 U35 U36 A37 A38 U39 C40 U41 G42 A43 G44 G45 G46 U47 C48 C49 A50 G51 G52 G53 U54 U55 C56 A57 A58 G59 U60 C61

C62 C63 U64 G65 U66 U67 C68 G69 G70 G71 C72 G73 C74 C75 A76

- Molecule 48: 28S ribosomal RNA

Chain 5: 38% / 74% / 25%

C1 G2 C3 A12 U13 C14 A15 G16 A17 U20 C23 G24 A25 C26 G29 C30 U35 A39 A42 U43 A44 A47 G48 U49 A56 G57 G58 A59 A64 A65 C72 A73 G90 G91 C92 G93 C100 G103 A108 G109 C110 C115 G116 C117

C118 G119 A120 C124 C125 C126 G127 C128 C129 C130 C131 G132 C133 G134 G135 C136 G137 G138 G139 G140 C141 G142 C143 G144 U157 A158 C159 G160 A163 G164 A165 C166 C167 C168 A169 C170 U171 C172 C173 C174 C175 G176 G177 C178 G179 C180 C181 G182 G189 G190 G191 G192 G193 C194 U200 C201

C202 U203 U204 C205 U206 U209 C216 C217 A218 G219 C220 C221 U224 G225 G226 A227 U233 G234 C245 G246 G247 C248 C249 C250 C251 C252 G253 G254 C255 G256 C257 G258 C259 C260 G261 G262 G263 C264 C265 C266 G267 G268 G269 U270 C271 U272 U273 C274 C275 C276 G277 G278 A279 G280 U281

A296 U297 A306 C309 G310 G315 U316 C320 U321 C322 A334 C340 G341 G342 G343 A344 C345 G346 A347 C350 U357 C358 C361 A362 A363 C367 A378 A385 A386 G387 A398 G399 C406 A407 A408 G409 A410 G411 G412 G413 G417 A427

G430 G431 U432 A433 A434 A435 U445 C446 C447 G448 C449 G450 C451 A452 G453 U454 C455 C456 G457 C458 C459 C460 G461 G462 A463 G464 G465 A466 U467 U468 C469 A470 A471 C472 C473 C474 G475 G476 G481 C481A G482 G483 U484 C485 C486 G487 G488 C489 C490 G491 U492 G493 C494 C495 G496 G497 C498 G499

G500 G504 G505 C506 G507 G508 A509 U510 C511 U512 C515 C516 C517 G518 C519 U520 C521 C522 C523 G638 U639 C640 G641 G642 C643 G644 G645 G646 G647 G648 A649 C650 C651 G652 C653 C654 C655 C656 C657 C658 G659 G660 C661 C662 G663 C664 C665 G666 A667 C668 C669 G670 G671 C672 C673 G674 C675 G682 C683

G684 C685 A686 U687 U688 A692 C693 C694 G695 C696 G697 G698 C699 G700 G701 U702 G703 C704 G705 G708 C719 G729 G730 G731 C738 C738A G739 G740 C741 G742 G743 G744 G745 A746 A747 G748 G749 U750 G751 G752 C753 C754 C755 G756 G757 G758 G759 G760 C904 C905 C906 C907 G908 G909 G910

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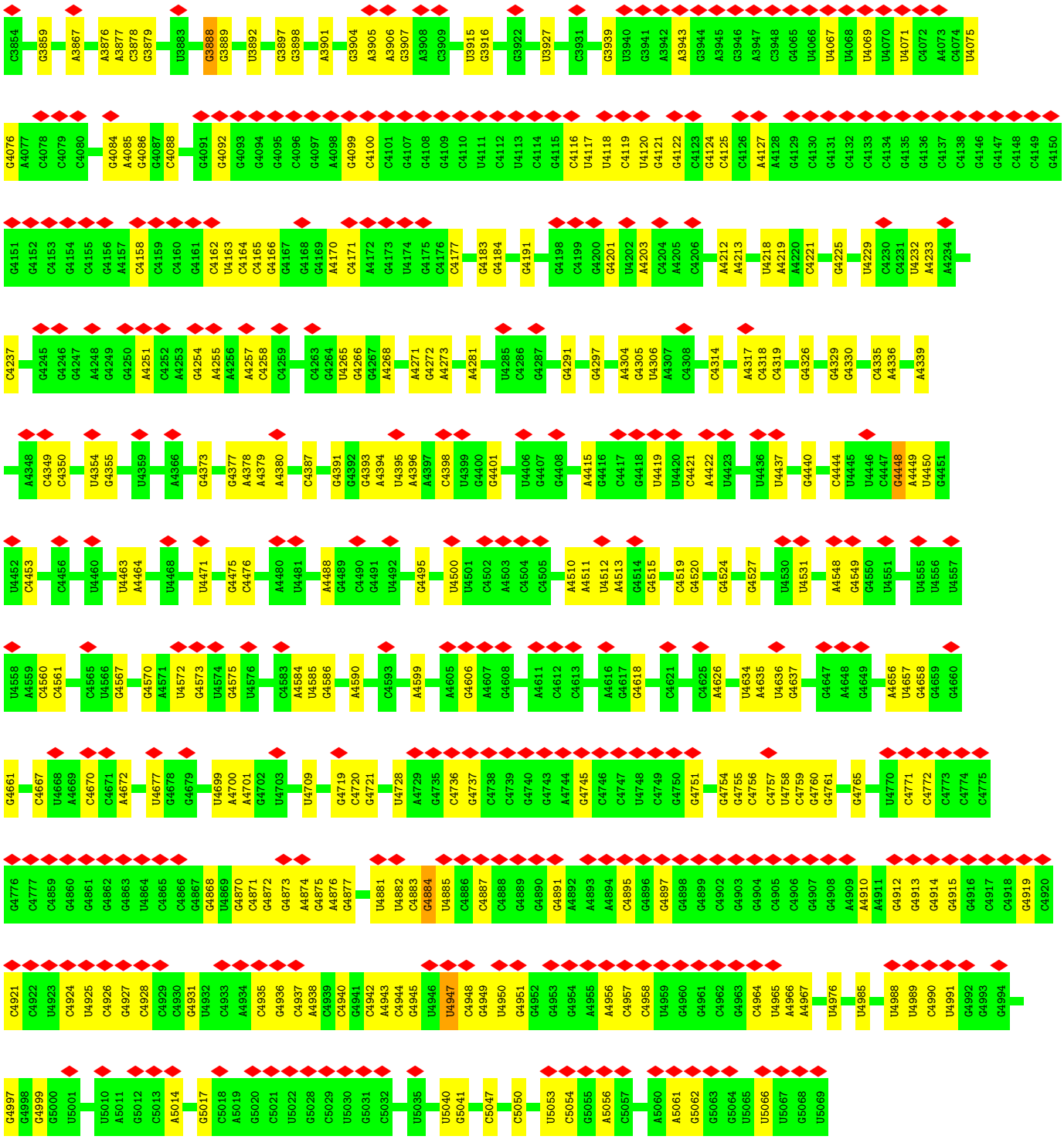
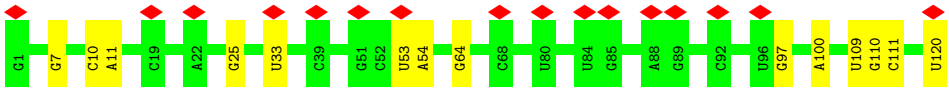


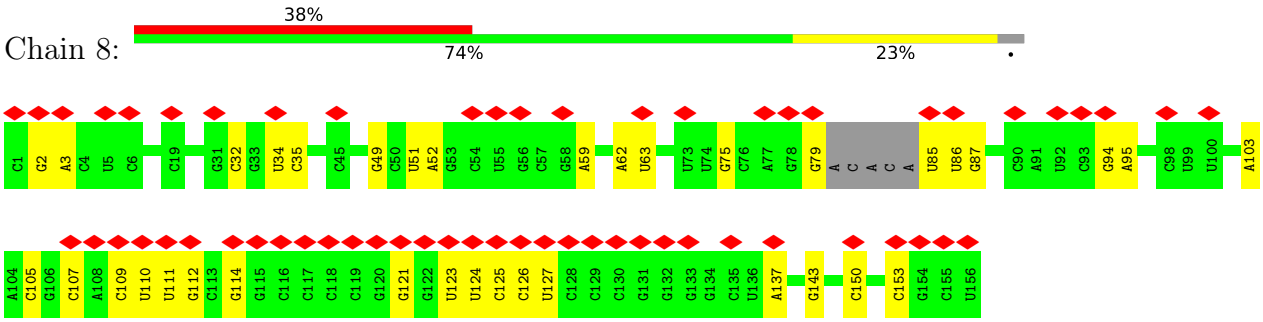
- Molecule 49: 5S ribosomal RNA

Chain 7:



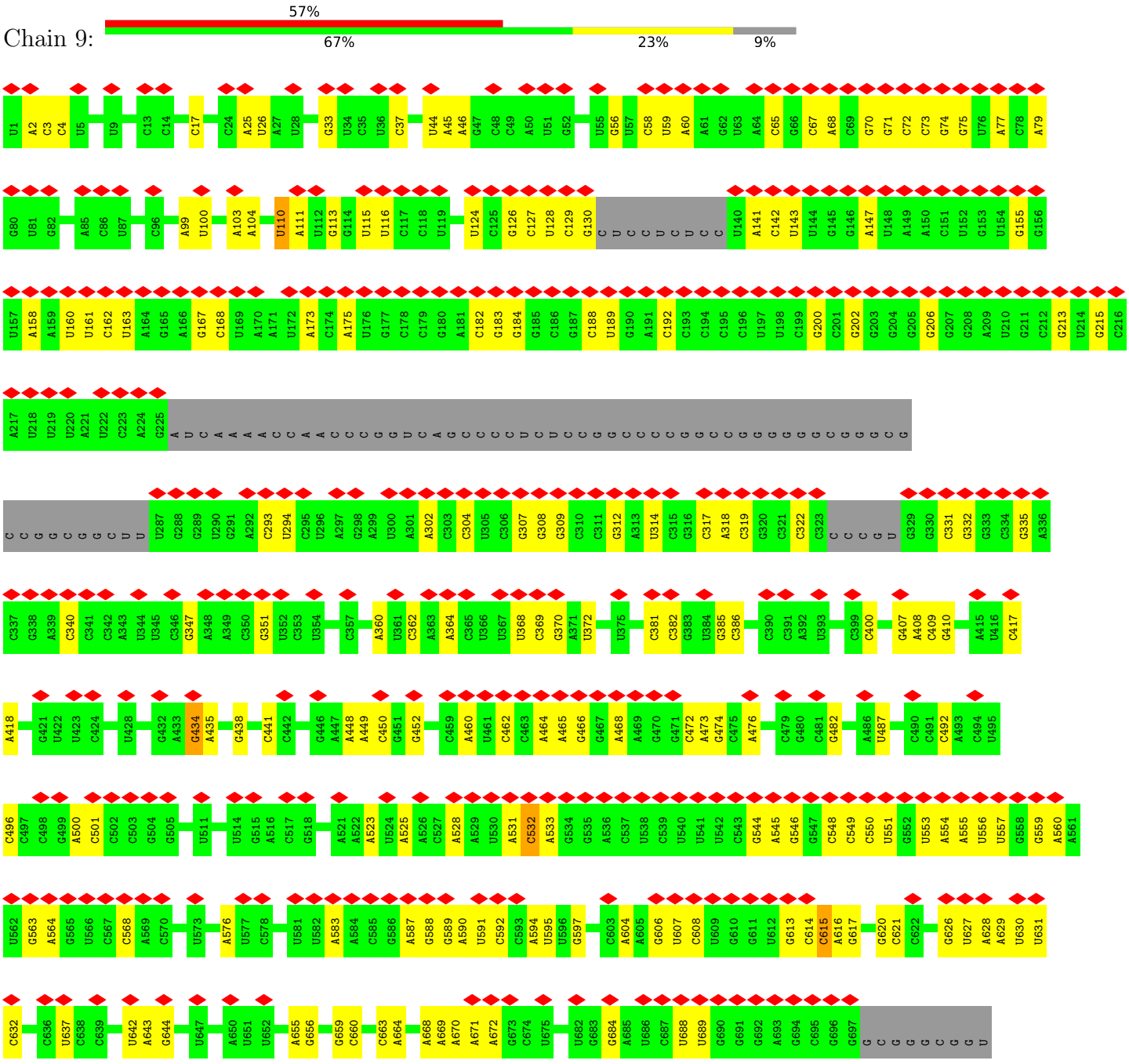
- Molecule 50: 5.8S ribosomal RNA

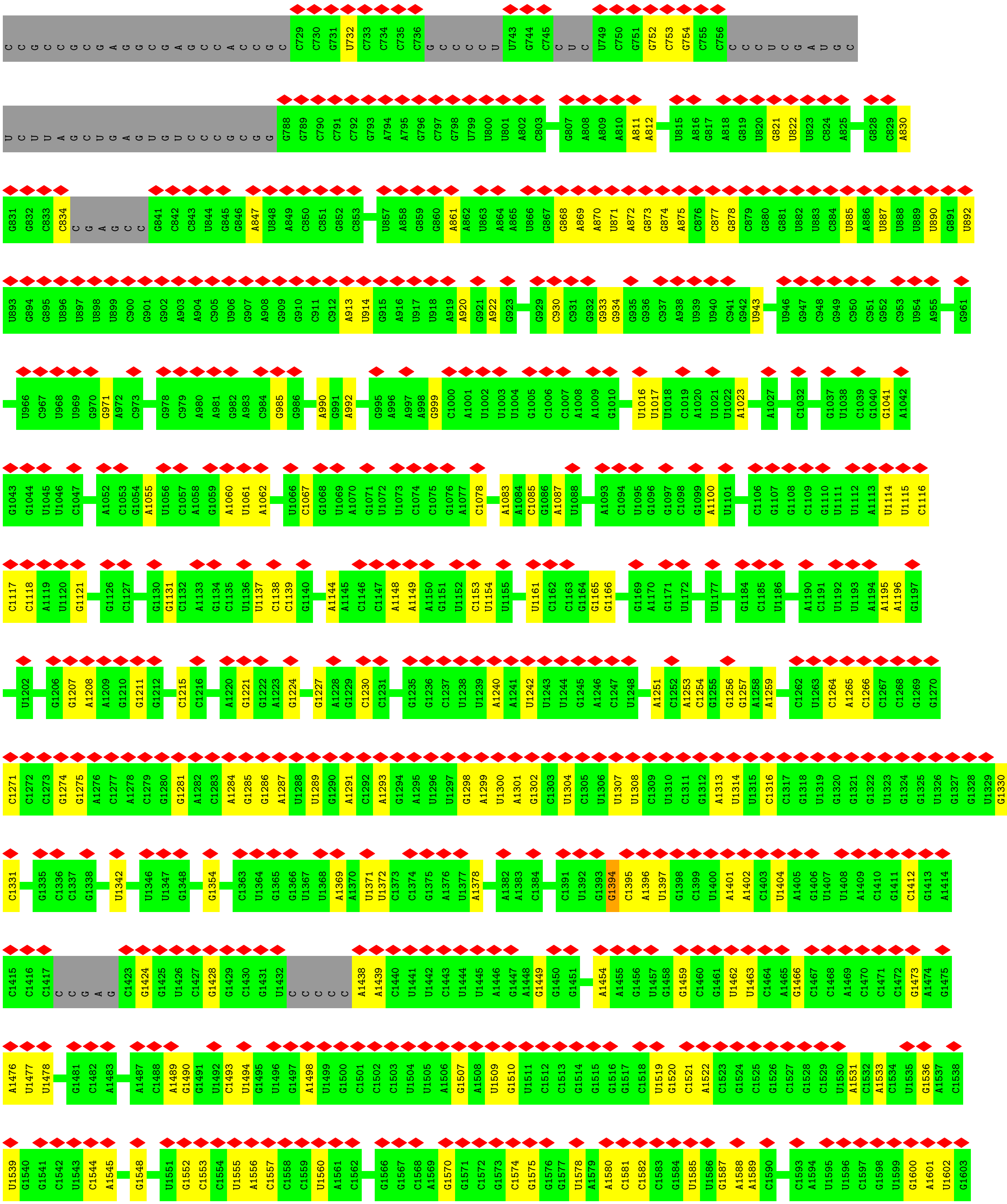
Chain 8:



- Molecule 51: 18S ribosomal RNA

Chain 9:

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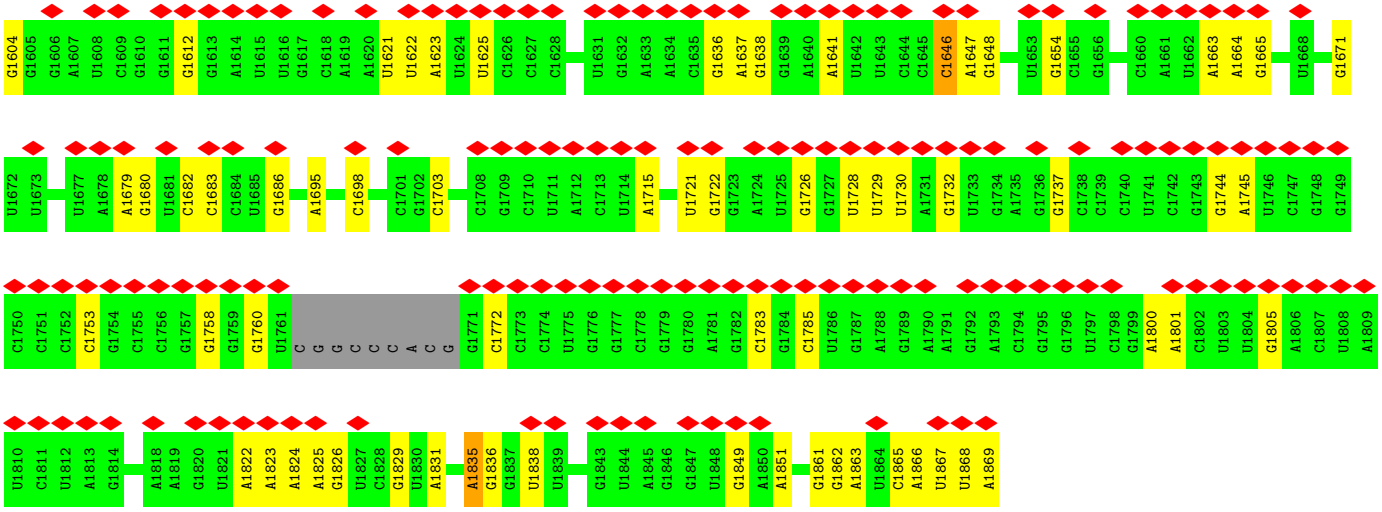
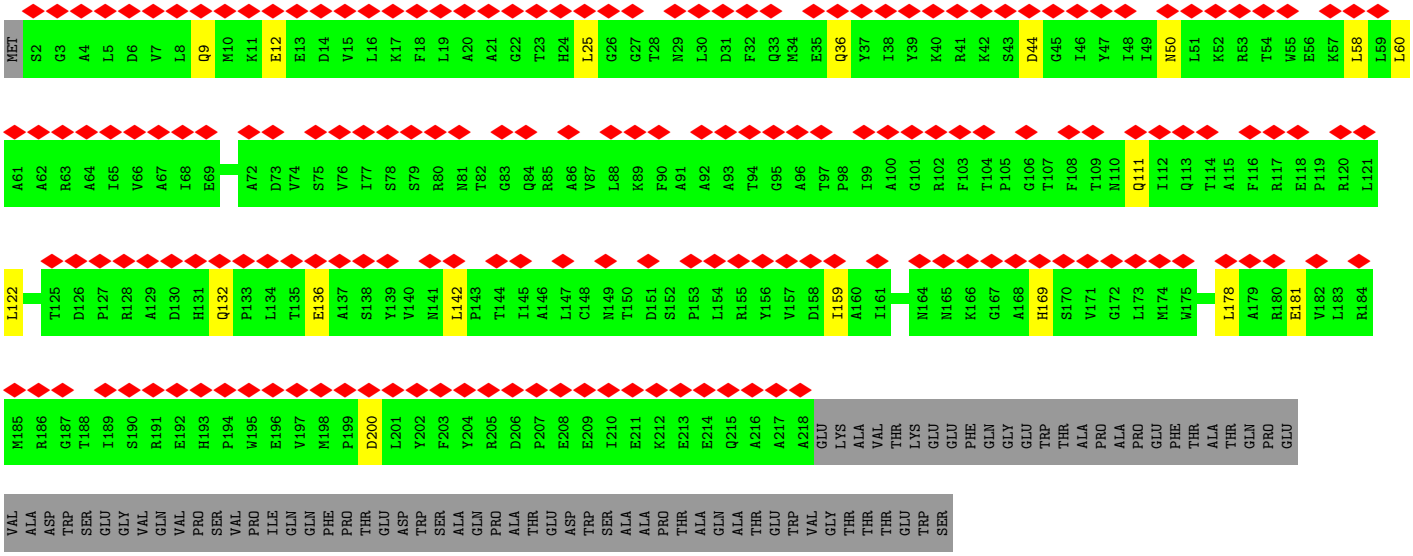


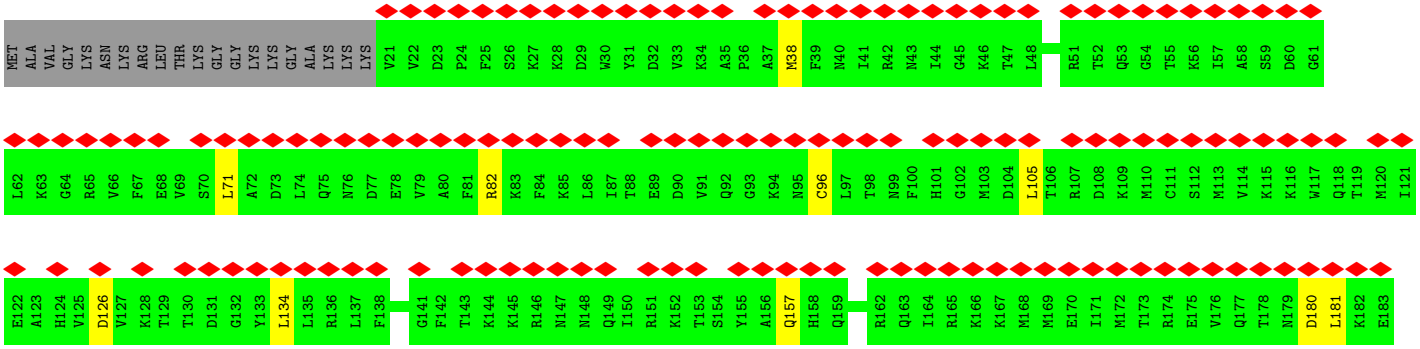
- Molecule 52: uS2

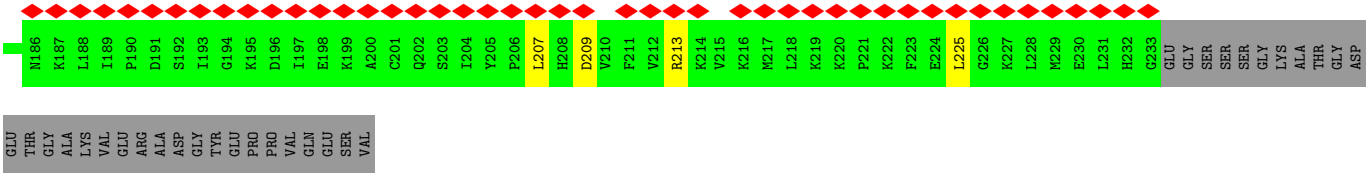
Chain AA:



- Molecule 53: 40S ribosomal protein S3a

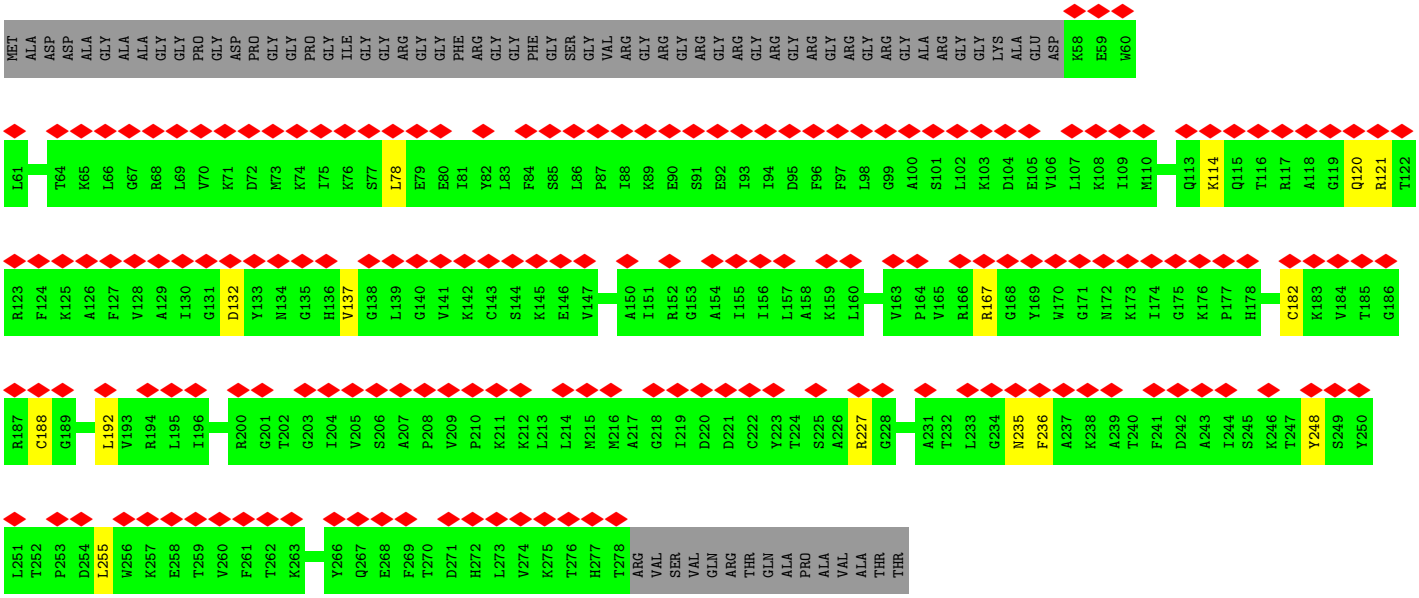
Chain BB:





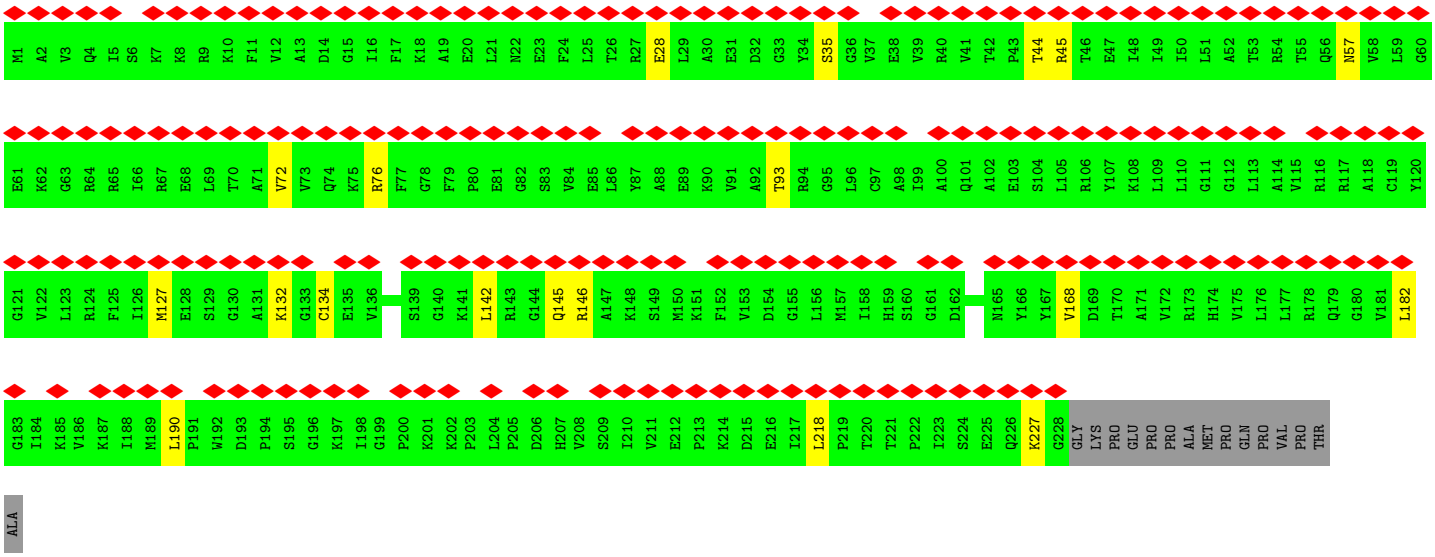
- Molecule 54: uS5

Chain CC:



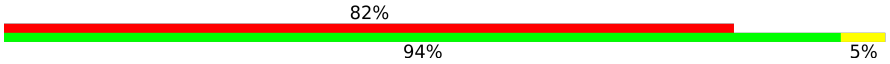
- Molecule 55: uS3

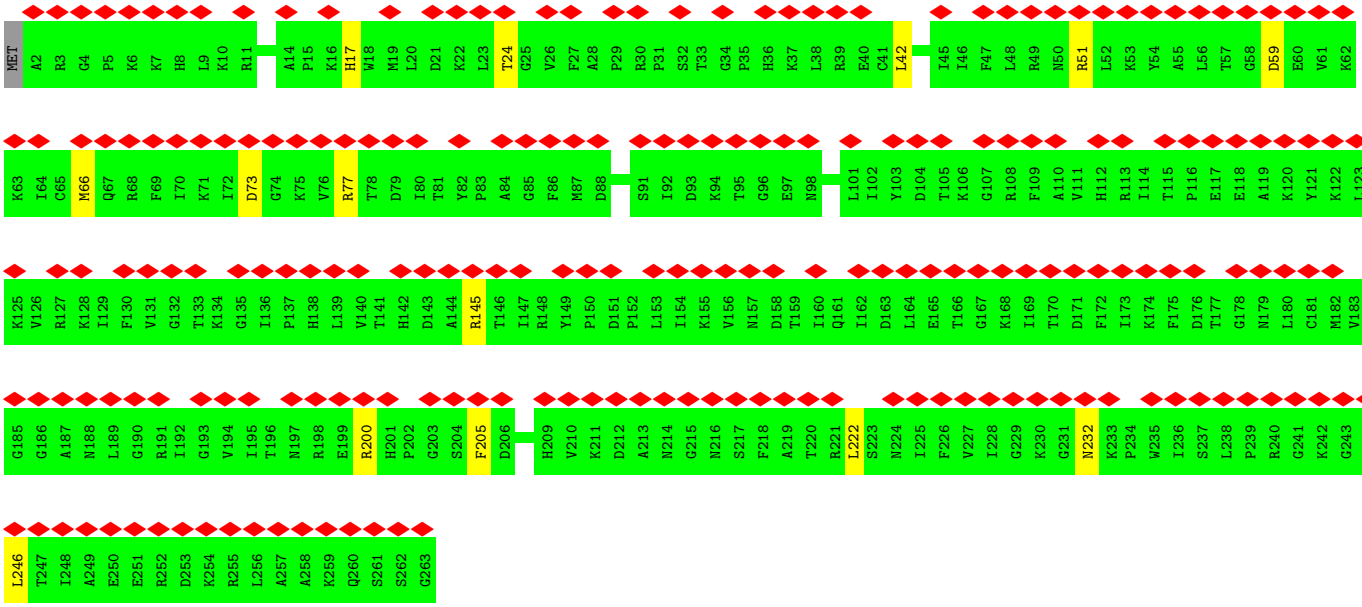
Chain DD:



- Molecule 56: eS4

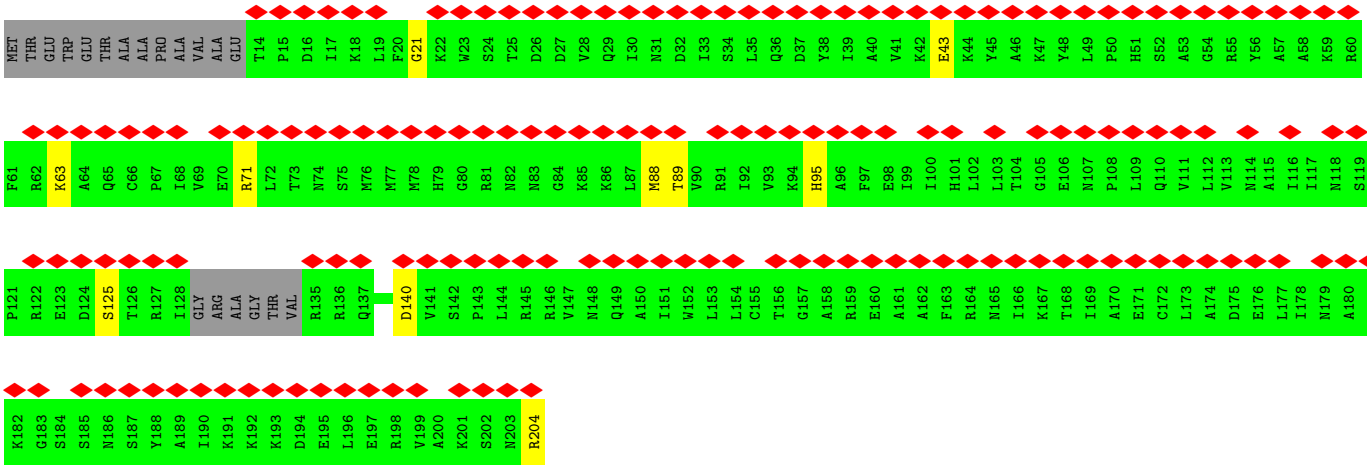
Chain EE:





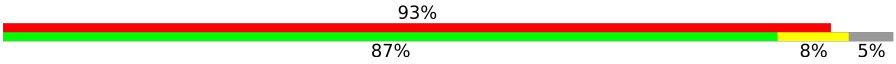
- Molecule 57: uS7

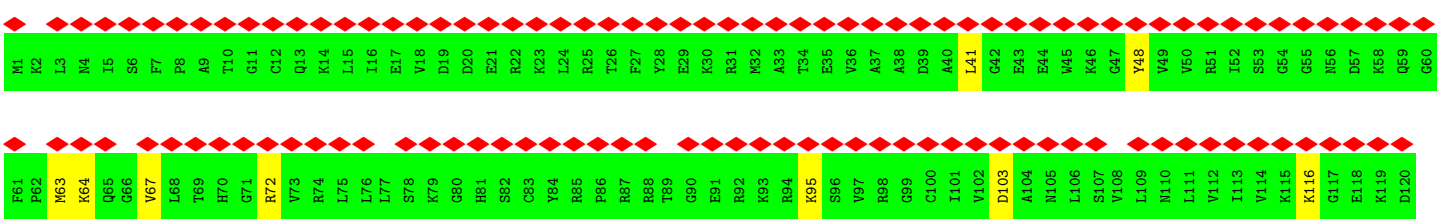
Chain FF:

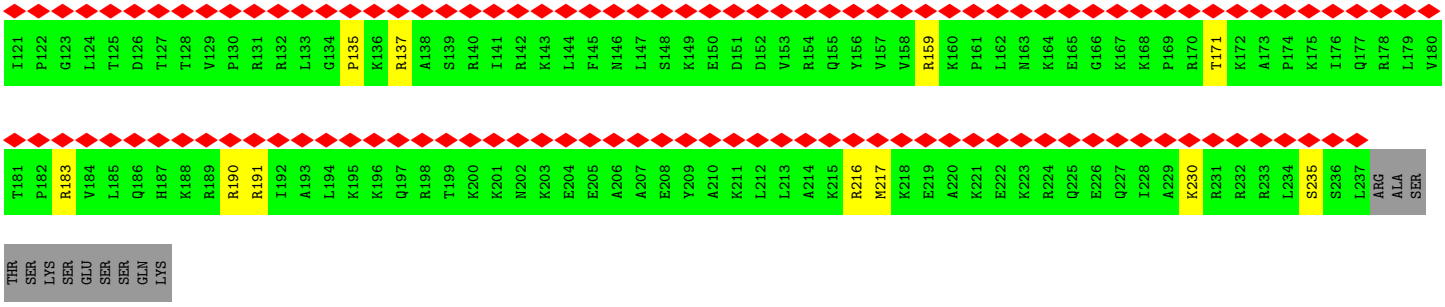


- Molecule 58: 40S ribosomal protein S6

Chain GG:

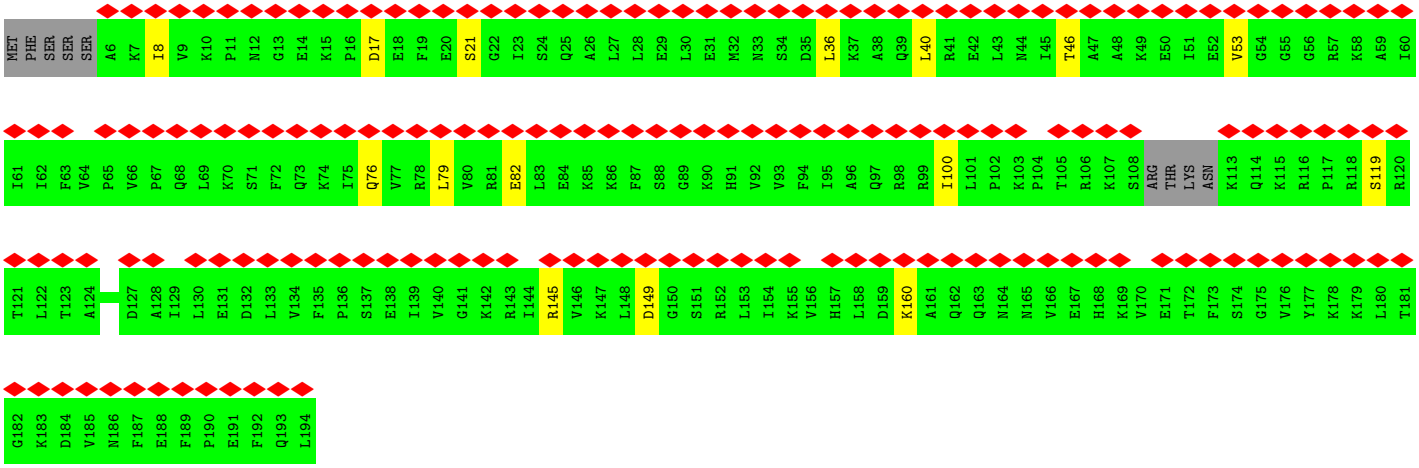






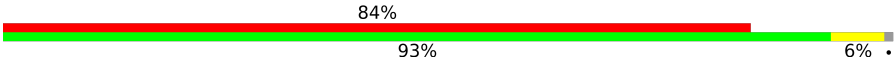
- Molecule 59: eS7

Chain HH:



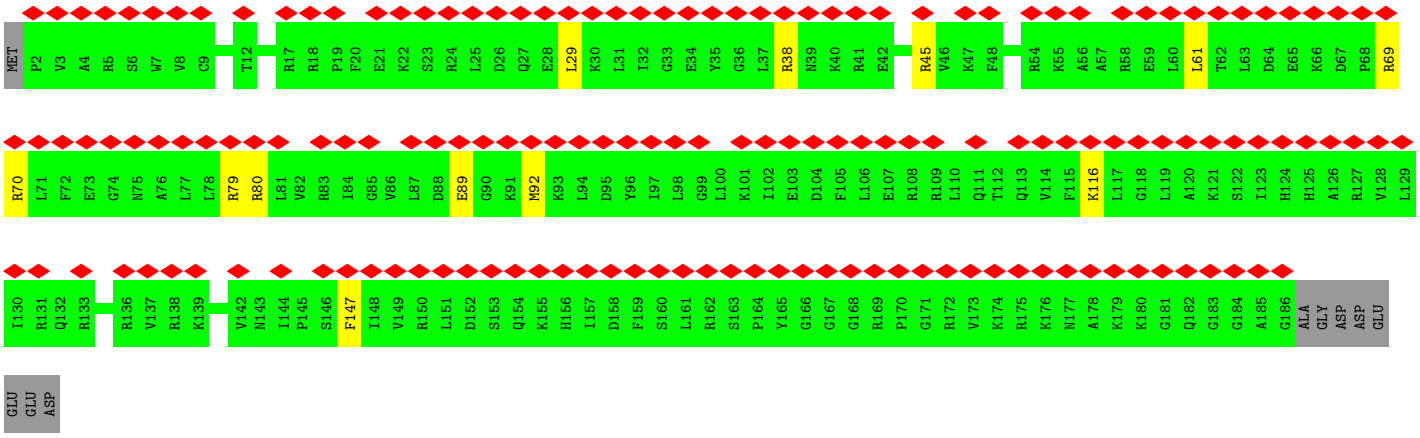
- Molecule 60: eS8

Chain II:



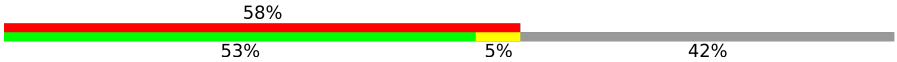
- Molecule 61: Ribosomal protein S9 (Predicted)

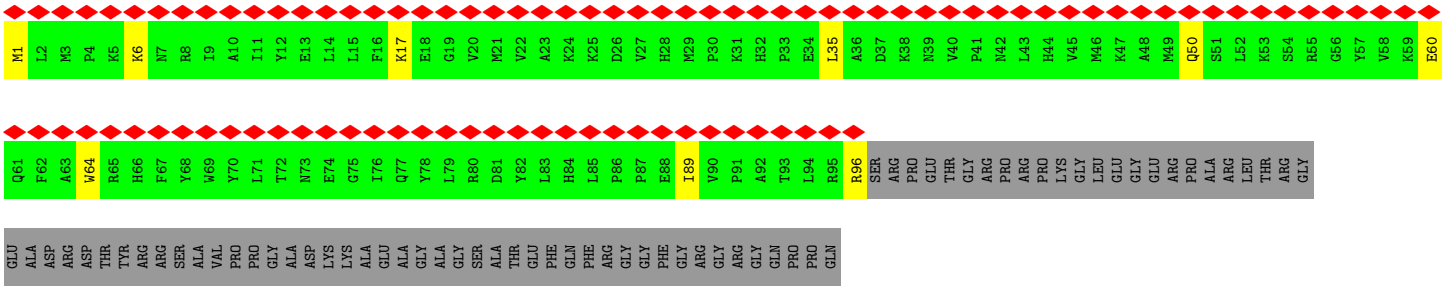
Chain JJ:



- Molecule 62: eS10

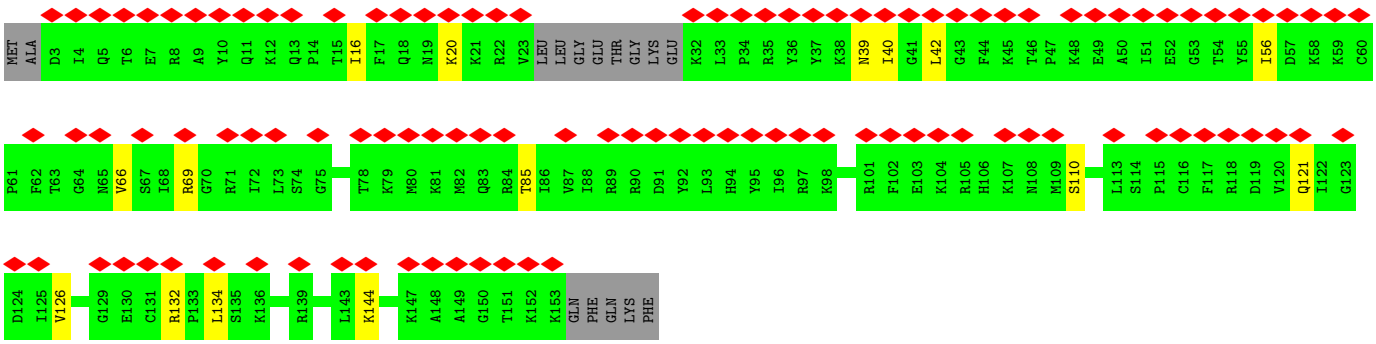
Chain KK:





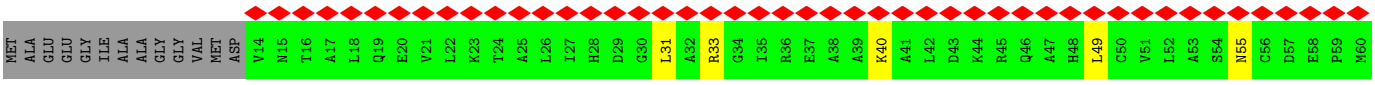
- Molecule 63: uS17

Chain LL:



- Molecule 64: 40S ribosomal protein S12

Chain MM:



Y61 V62 K63 L64 V65 E66 A67 L68 C69 A70 E71 H72 Q73 I74 N75 L76 I77 K78 V79 D80 D81 N82 K83 K84 L85 G86 E87 W88 V89 G90 L91 C92 K93 I94 D95 R96 E97 G98 K99 P100 R101 K102 V103 V104 G105 C106 S107 C108 V109 V110 V111 K112 D113 Y114 G115 K116 E117 S118 Q119 A120

K121 D122 V123 I124 E125 E126 Y127 F128 K129 C130 LYS LYS

- Molecule 65: uS15

Chain NN: 85% 88% 11%

MET G2 R3 M4 H5 A6 P7 G8 K9 G10 L11 S12 Q13 S14 A15 L16 P17 Y18 R19 R20 S21 V22 P23 T24 W25 L26 K27 L28 T29 S30 D31 D32 V33 K34 E35 Q36 I37 Y38 K39 L40 A41 K42 K43 G44 L45 T46 P47 S48 Q49 I50 G51 V52 I53 L54 R55 D56 S57 H58 G59 V60

A61 Q62 V63 R64 F65 V66 T67 G68 M69 K70 I71 L72 R73 I74 L75 K76 S77 K78 G79 L80 A81 P82 D83 L84 P85 E86 D87 L88 Y89 H90 L91 I92 K93 K94 A95 V96 A97 V98 R99 K100 H101 L102 E103 R104 N105 R106 K107 D108 K109 D110 A111 K112 F113 R114 L115 I116 L117 I118 E119 S120

R121 I122 H123 R124 L125 A126 R127 Y128 Y129 K130 T131 K132 R133 V134 L135 P136 P137 N138 W139 K140 Y141 E142 S143 S144 T145 A146 L149 V150 ALA

- Molecule 66: uS11

Chain OO: 67% 73% 8% 19%

MET LYS ALA ARG ALA LEU SER GLY SER GLY VAL ARG ARG ARG ARG ALA ALA MET ALA PRO ARG LYS GLY LYS GLU LYS LYS GLU GLU GLN VAL ILE S16 L17 G18 P19 Q20 V21 A22 E23 G24 E25 N26 V27 F28 G29 V30 C31 H32 I33 F34 A35 S36 F37 N38 D39 T40 F41 V42 H43

D46 L47 S48 G49 K50 E51 T52 I53 C54 R55 V56 T57 G58 G59 M60 K61 V62 K63 A64 D65 R66 D67 E68 S69 S70 P71 Y72 A73 A74 M75 L76 A77 A78 Q79 D80 V81 A82 Q83 R84 C85 K86 E87 L88 G89 I90 T91 A92 I95 K96 L97 R98 A99 T100 G101 G102 N103 R104 T105

K106 T107 P108 G109 P110 G111 A112 Q113 S114 A115 L116 R117 A118 L119 A120 R121 S122 G123 M124 K125 I126 G127 R128 I129 E130 D131 V132 T133 P134 I135 P136 S137 D138 S139 T140 R141 R142 K143 R146 R147 G148 R149 R150 L151

- Molecule 67: uS19

Chain PP: 83% 74% 8% 17%

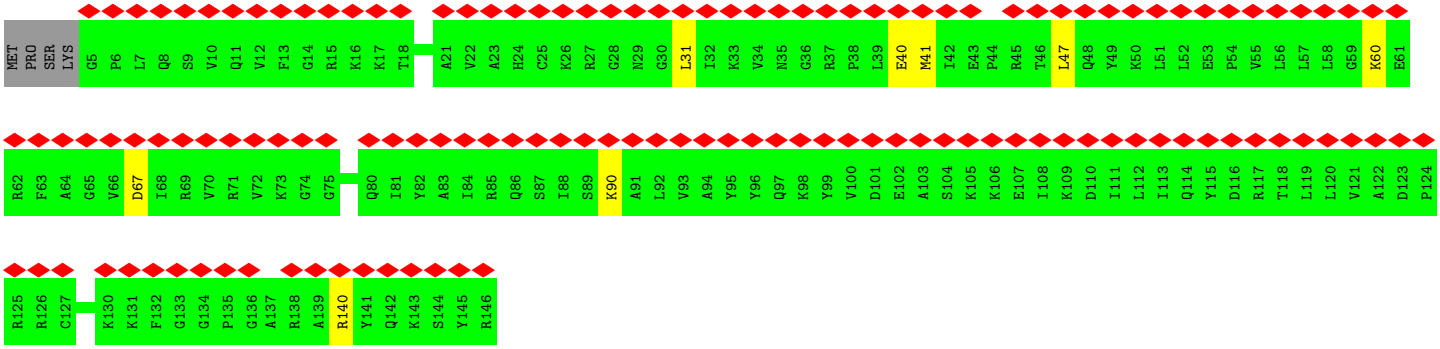
MET ALA GLU VAL GLU GLN LYS LYS LYS ARG THR F12 R13 K14 F15 T16 Y17 R18 G19 V20 D21 L22 D23 Q24 L25 L26 D27 M28 S29 Y30 E31 Q32 L33 M34 Q35 L36 Y37 S38 A39 R40 Q41 R42 R43 R44 L45 S46 R47 G48 L49 R50 R51 K52 Q53 H54 S55 L56 L57 K58 R59 L60

R61 K62 A63 K64 K65 E66 A67 P68 P69 M70 E71 K72 P73 E74 V75 V76 K77 T78 H79 L80 R81 D82 M83 I84 I85 L86 P87 E88 M89 V90 G91 S92 M93 V94 G95 V96 Y97 N98 G99 K100 T101 F102 N103 Q104 V105 E106 I107 K108 P109 E110 M111 I112 G113 H114 Y115 L116 G117 E118 F119 S120

I121 T122 Y123 K124 P125 V126 K127 H128 G129 R130 P131 GLY ILE GLY ALA THR HIS SER SER ARG PHE ILE PRO LEU LYS

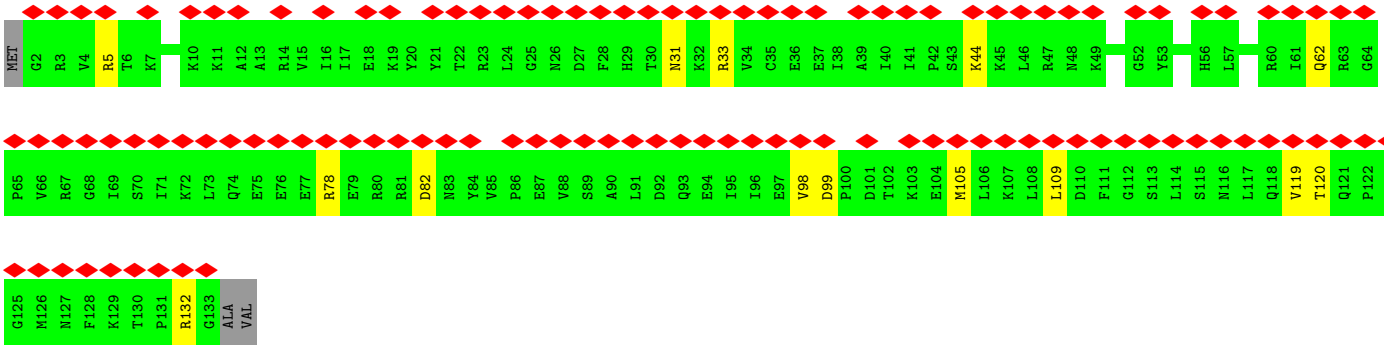
- Molecule 68: uS9

Chain QQ: 90% 92% 5%



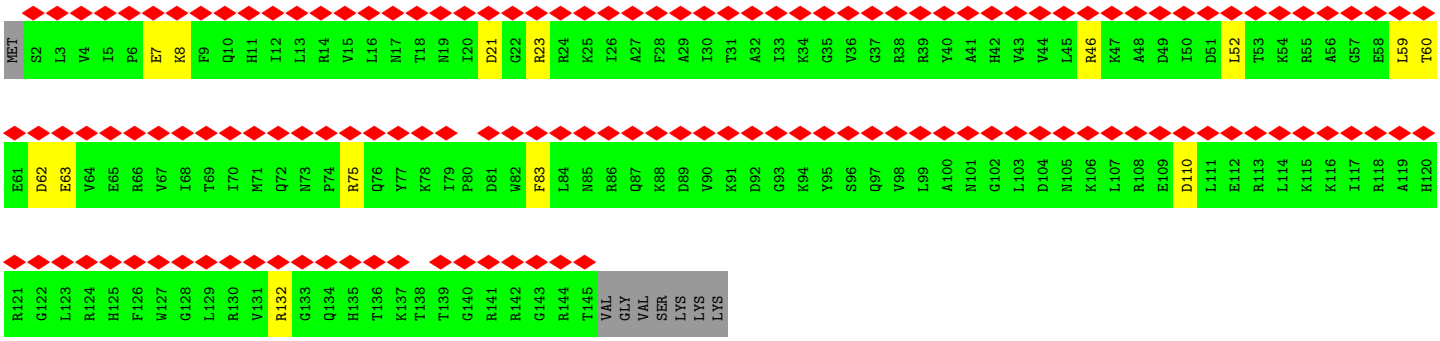
- Molecule 69: eS17

Chain RR: 84% 87% 10%



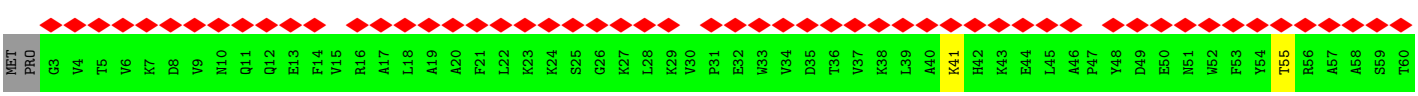
- Molecule 70: uS13

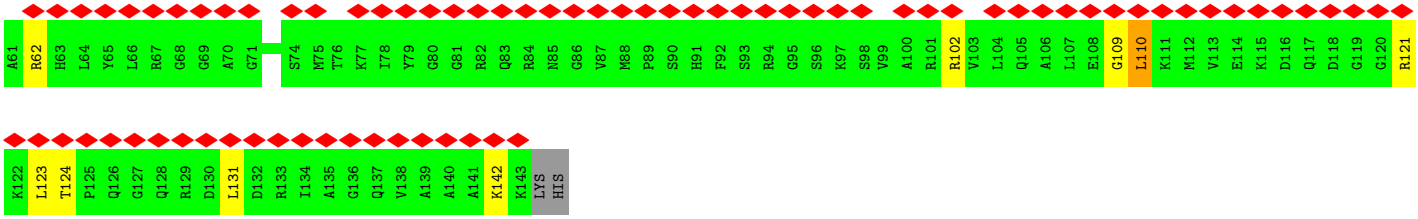
Chain SS: 93% 86% 9% 5%



- Molecule 71: eS19

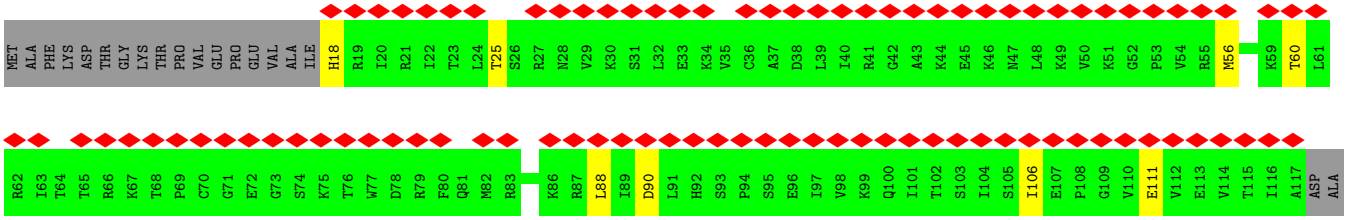
Chain TT: 91% 90% 7%





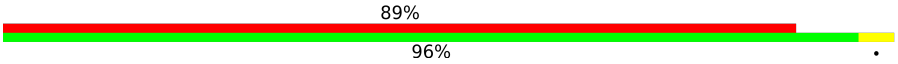
- Molecule 72: uS10

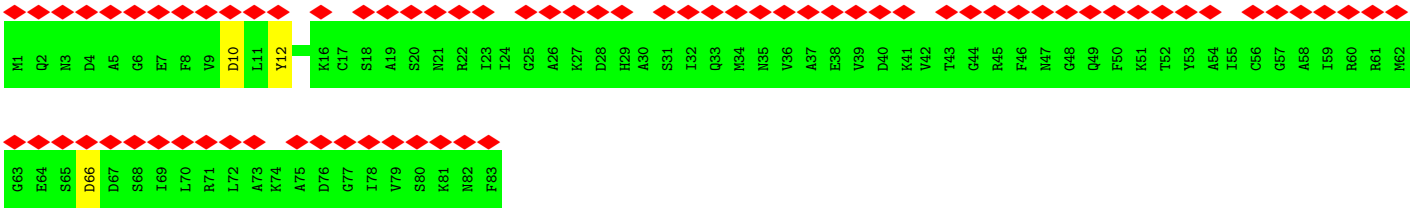
Chain UU:



- Molecule 73: eS21

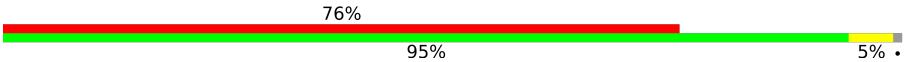
Chain VV:

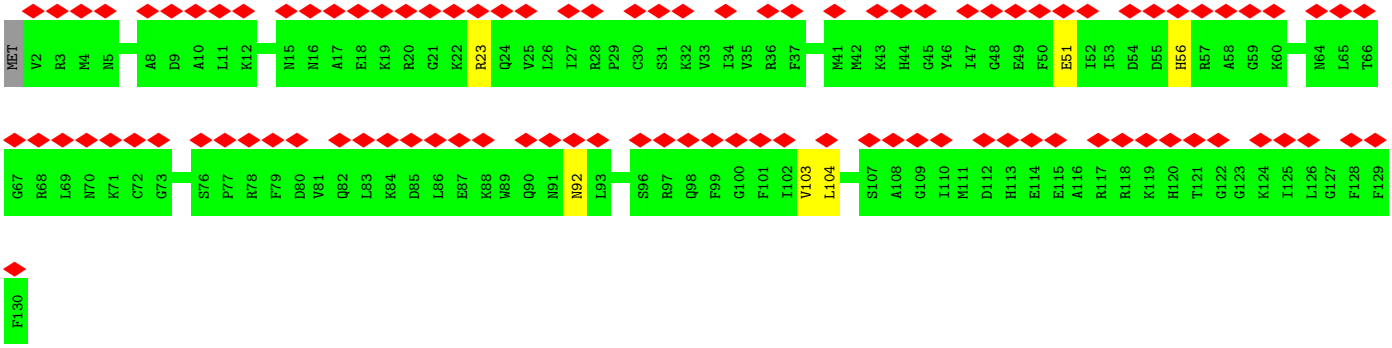




- Molecule 74: uS8

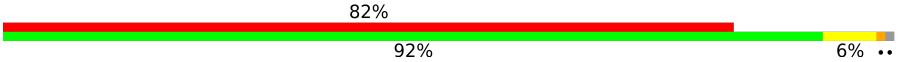
Chain WW:

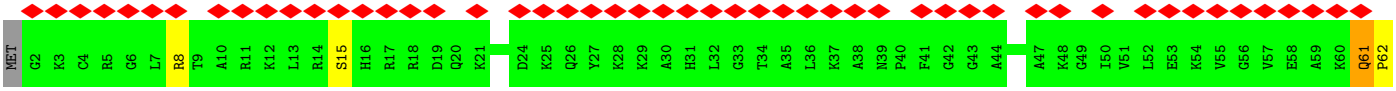




- Molecule 75: uS12

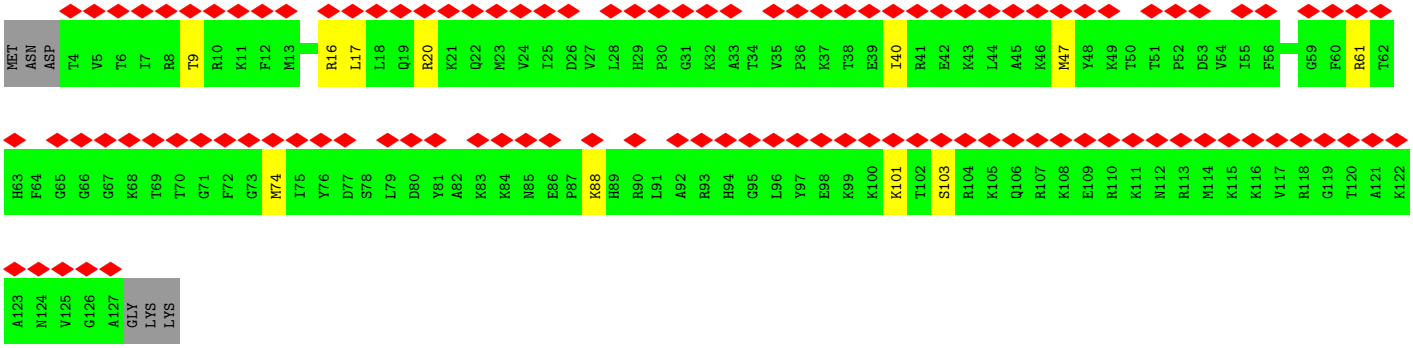
Chain XX:





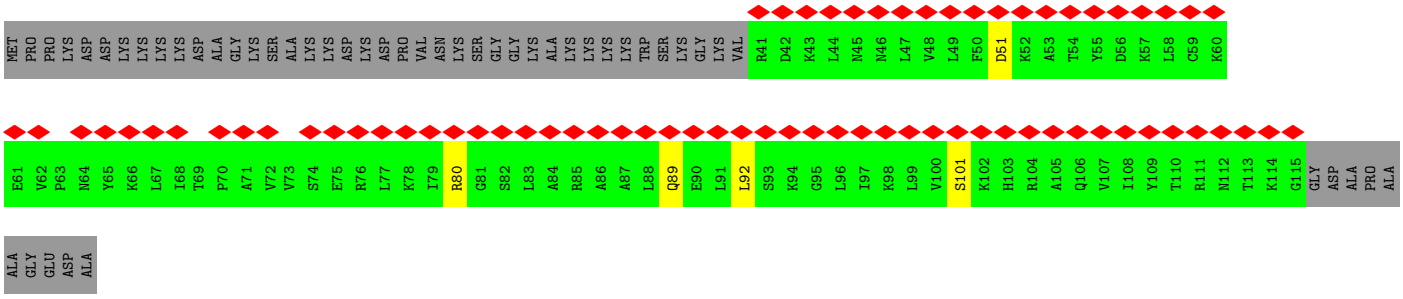
- Molecule 76: eS24

Chain YY:



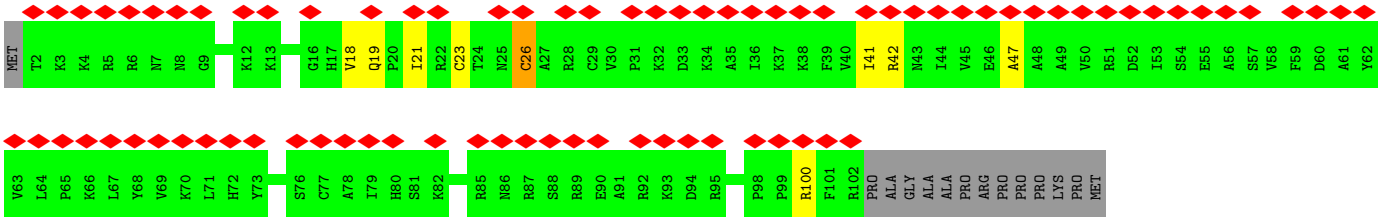
- Molecule 77: eS25

Chain ZZ:



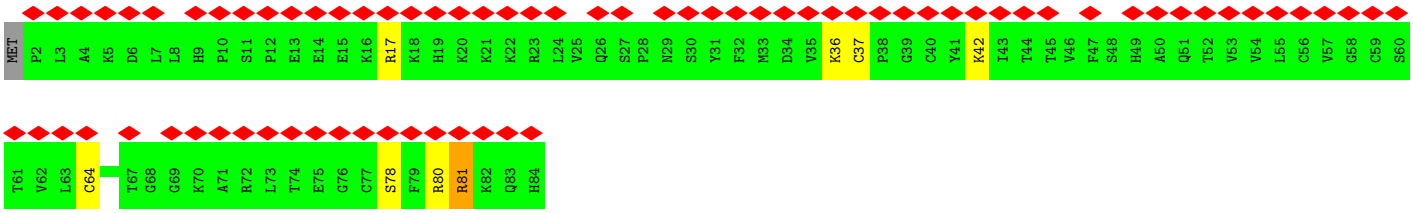
- Molecule 78: eS26

Chain aa:



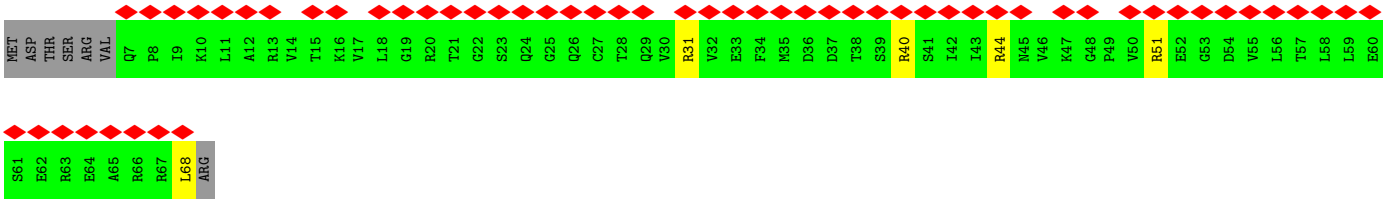
- Molecule 79: 40S ribosomal protein S27

Chain bb:



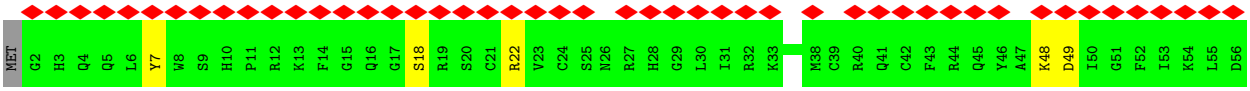
- Molecule 80: eS28

Chain cc:



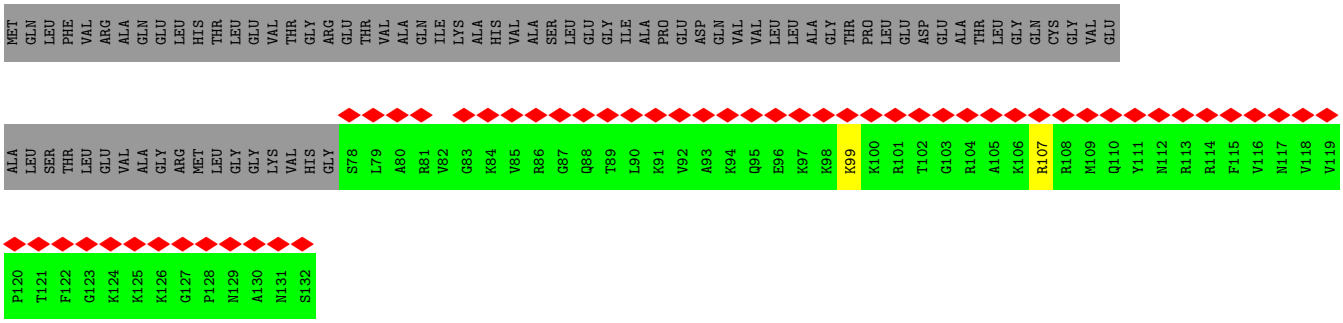
- Molecule 81: uS14

Chain dd:



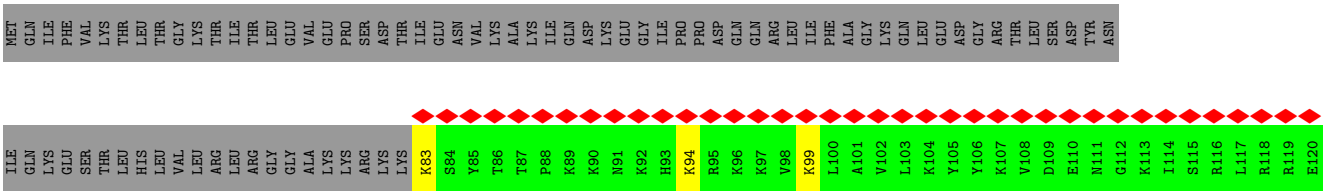
- Molecule 82: eS30

Chain ee:



- Molecule 83: eS31

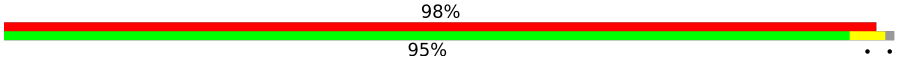
Chain ff:



C121 P122 S123 D124 E125 C126 G127 A128 G129 V130 F131 M132 A133 S134 H135 F136 D137 R138 H139 Y140 C141 G142 K143 C144 C145 L146 T147 Y148 C149 F150 ASN LYS PRO GLU ASP LYS

- Molecule 84: RACK1

Chain gg:



MET T2 E3 Q4 M5 T6 L7 R8 G9 T10 L11 K12 G13 H14 N15 G16 W17 V18 T19 Q20 I21 A22 T23 T24 P25 Q26 F27 P28 D29 M30 I31 L32 S33 A34 S35 R36 D37 K38 T39 I40 I41 M42 W43 K44 L45 T46 R47 D48 E49 T50 N51 Y52 G53 I54 P55 Q56 R57 A58 L59 R60

G61 H62 S63 H64 F65 V66 S67 D68 V69 V70 I71 S72 S73 D74 G75 Q76 F77 A78 L79 S80 G81 S82 W83 D84 G85 T86 L87 R88 L89 W90 D91 L92 T93 T94 G95 T96 T97 T98 R99 R100 F101 V102 G103 H104 T105 K106 D107 V108 L109 S110 V111 A112 F113 S114 S115 D116 N117 R118 Q119 I120

V121 S122 G123 S124 R125 D126 K127 T128 I129 K130 L131 W132 N133 T134 L135 G136 V137 C138 K139 Y140 T141 V142 Q143 D144 E145 S146 H147 S148 E149 W150 V151 S152 C153 V154 R155 F156 S157 P158 N159 S160 S161 N162 P163 I164 I165 V166 S167 C168 G169 W170 D171 K172 L173 V174 K175 V176 W177 N178 L179 A180

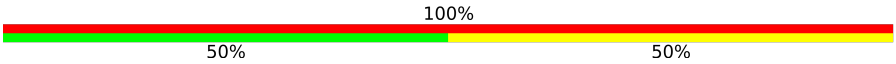
N181 C182 K183 L184 K185 T186 N187 H188 I189 G190 H191 T192 G193 Y194 L195 N196 T197 V198 T199 V200 S201 P202 D203 G204 S205 L206 C207 A208 S209 G210 G211 K212 D213 G214 Q215 A216 M217 L218 W219 D220 L221 N222 E223 G224 K225 H226 L227 Y228 T229 L230 D231 G232 G233 D234 I235 I236 N237 A238 L239 C240

F241 S242 P243 N244 R245 Y246 W247 L248 C249 A250 A251 T252 G253 P254 S255 I256 K257 I258 W259 D260 L261 E262 G263 K264 I265 I266 V267 D268 E269 L270 K271 Q272 E273 V274 I275 S276 T277 S278 S279 K280 A281 E282 P283 P284 Q285 C286 T287 S288 L289 A290 W291 S292 A293 D294 G295 Q296 T297 L298 F299 A300

G301 Y302 T303 D304 N305 L306 V307 R308 V309 W310 Q311 V312 T313 I314 GLY THR ARG

- Molecule 85: mRNA (UGA stop codon)

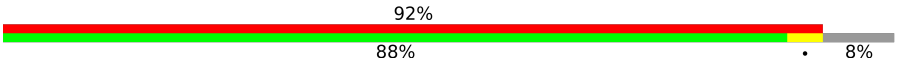
Chain hh:



U41 C42 A43 A44 A45 G46 U47 U48

- Molecule 86: Protein pelota homolog

Chain ii:



M1 K2 L3 V4 R5 K6 N7 I8 E9 K10 D11 N12 A13 G14 Q15 V16 T17 L18 V19 P20 E21 E22 P23 E24 D25 M26 W27 H28 T29 Y30 N31 L32 V33 Q34 V35 G36 D37 S38 L39 R40 A41 S42 T43 I44 R45 K46 V47 Q48 T49 E50 S51 S52 T53 G54 S55 V56 G57 S58 N59 R60

V61 R62 T63 T64 L65 T66 L67 C68 V69 E70 A71 I72 D73 F74 D75 S76 Q77 A78 C79 Q80 L81 R82 V83 K84 G85 T86 N87 I88 Q89 E90 N91 E92 Y93 V94 K95 M96 G97 A98 Y99 H100 T101 I102 E103 L104 E105 P106 N107 R108 Q109 F110 T111 L112 A113 K114 K115 Q116 W117 D118 S119 V120

V121 L122 E123 R124 I125 E126 Q127 A128 C129 D130 P131 A132 W133 S134 A135 D136 V137 A138 A139 V140 V141 M142 Q143 E144 G145 L146 A147 H148 I149 C150 L151 V152 T153 P154 S155 M156 T157 L158 T159 R160 A161 K162 V163 E164 V165 N166 I167 P168 R169 K170 R171 K172 G173 N174 C175 S176 Q177 H178 D179 R180

A181 L182 E183 R184 F185 Y186 E187 Q188 V189 V190 Q191 A192 I193 Q194 R195 H196 I197 H198 F199 D200 V201 V202 K203 C204 I205 L206 V207 A208 S209 P210 G211 F212 V213 R214 E215 Q216 F217 C218 D219 Y220 M221 F222 Q223 Q224 A225 V226 K227 T228 D229 N230 K231 L232 L233 L234 E235 N236 R237 S238 K239 F240

L241 Q242 V243 H244 A245 S246 S247 G248 H249 K250 Y251 S252 L253 K254 E255 A256 L257 C258 D259 P260 T261 V262 A263 S264 R265 L266 S267 D268 T269 K270 A271 A272 G273 E274 V275 K276 A277 L278 D279 D280 F281 Y282 K283 M284 L285 Q286 H287 E288 P289 D290 R291 A292 F293 Y294 G295 L296 K297 Q298 V299 E300

K301 A302 N303 E304 A305 M306 A307 I308 D309 T310 L311 L312 I313 S314 D315 E316 L317 F318 R319 H320 Q321 D322 V323 A324 T325 R326 S327 R328 Y329 V330 R331 L332 V333 D334 S335 V336 K337 E338 N339 A340 G341 T342 V343 R344 I345 F346 S347 S348 L349 H350 V351 S352 G353 E354 Q355 L356 S357 Q358 L359 T360

G361 V362 A363 A364 I365 L366 R367 F368 P369 V370 P371 E372 LEU SER ASP GLN GLU GLY ASP SER SER SER GLU GLU ASP GLY SER GLU ASN LEU TYR PHE GLN GLY ALA HIS HIS HIS HIS HIS HIS SER THR

- Molecule 87: HBS1-like protein

Chain jj: 59% | 55% • 40%

MET ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP ASP LYS ALA GLY SER MET ALA ARG HIS ARG ASN VAL ARG GLY TYR ASN TYR ASP GLU ASP PHE GLU ASP ASP ASP LEU TYR GLY GLN SER VAL GLU ASP ASP TYR CYS ILE SER PRO

SER THR ALA ALA GLN PHE ILE TYR SER ARG ARG ASP LYS PRO SER VAL GLU PRO VAL GLU GLU TYR ASP TYR GLU ASP LEU LYS GLU SER SER ASN SER VAL SER ASN HIS GLN LEU SER GLY PHE ASP GLN ALA ARG LEU TYR SER CYS LEU ASP HIS MET ARG GLU VAL LEU GLY ASP

ALA VAL PRO ASP GLU ILE LEU ILE GLU ALA VAL LEU LYS ASN LYS PHE ASP VAL GLN LYS ALA LEU SER GLY VAL LEU GLU GLN ASP ARG VAL GLN SER LEU LYS ASP LYS ASN GLU ALA THR VAL SER THR GLY LYS ILE ALA LYS GLY LYS PRO VAL ASP SER GLN THR SER ARG SER

GLU SER GLU ILE VAL PRO LYS VAL ALA LYS MET THR VAL SER GLY LYS LYS GLN THR MET GLY PHE GLU VAL PRO GLY VAL SER SER GLU GLU ASN GLY HIS SER PHE HIS THR PRO GLN LYS GLY PRO PRO ILE GLU ASP ALA ILE ALA SER SER ASP VAL LEU GLU THR ALA SER LYS

SER ALA ASN PRO PRO HIS THR ILE GLN ALA SER GLU GLU GLN SER SER THR PRO ALA PRO VAL LYS LYS SER GLY LYS LEU ARG GLN GLN ILE ASP VAL LYS ALA GLU LEU GLU LYS ARG GLN GLY GLY LYS GLN L260 L261 N262 L263 V264 V265 I266 G267 H268 V269 D270 A271 G272 K273 S274

T275 L276 M277 G278 H279 M280 L281 Y282 L283 L284 G285 N286 I287 N288 K289 R290 T291 M292 H293 K294 Y295 E296 Q297 E298 S299 K300 K301 A302 G303 K304 A305 S306 F307 A308 Y309 A310 W311 V312 L313 D314 E315 T316 G317 E318 E319 R320 E321 R322 G323 V324 T325 M326 D327 V328 G329 M330 T331 K332 F333 E334

T335 T336 T337 K338 V339 I340 T341 L342 M343 D344 A345 P346 G347 H348 K349 D350 F351 I352 P353 N354 M355 I356 T357 G358 A359 A360 Q361 A362 D363 V364 A365 V366 L367 V368 V369 D370 A371 S372 R373 G374 E375 F376 E377 A378 G379 F380 E381 T382 G383 G384 Q385 T386 R387 E388 H389 G390 L391 L392 V393 R394

S395 L396 G397 V398 T399 Q400 L401 A402 V403 A404 V405 N406 K407 M408 D409 Q410 V411 N412 W413 Q414 Q415 E416 R417 F418 Q419 E420 I421 T422 G423 K424 L425 G426 H427 F428 L429 K430 Q431 A432 G433 F434 K435 E436 S437 D438 V439 G440 F441 I442 P443 T444 S445 G446 L447 S448 G449 E450 N451 L452 I453 T454

R455 S456 Q457 S458 S459 E460 L461 T462 K463 W464 Y465 K466 G467 L468 C469 L470 L471 E472 Q473 I474 D475 S476 F477 K478 P479 P480 Q481 R482 S483 I484 D485 K486 P487 F488 R489 L490 C491 V492 S493 D494 V495 F496 K497 D498 Q499 G500 S501 G502 F503 C504 I505 T506 G507 K508 I509 E510 A511 G512 Y513 I514

Q515 T516 G517 D518 R519 L520 L521 A522 M523 P524 P525 N526 E527 T528 C529 T530 V531 K532 G533 I534 T535 L536 H537 D538 E539 P540 V541 D542 W543 A544 A545 A546 G547 D548 H549 V550 S551 L552 T553 L554 V555 G556 M557 D558 I559 I560 K561 I562 N563 V564 G565 C566 I567 F568 C569 G570 P571 K572 V573 P574

I575 K576 A577 C578 T579 R580 F581 R582 A583 R584 I585 L586 I587 F588 N589 I590 E591 I592 P593 I594 T595 K596 G597 F598 P599 V600 L601 L602 H603 Y604 Q605 T606 V607 S608 E609 P610 A611 V612 I613 K614 R615 L616 I617 S618 V619 L620 N621 K622 S623 T624 G625 E626 V627 T628 K629 K630 K631 P632 K633 F634

L635 T636 K637 G638 Q639 N640 A641 L642 V643 E644 L645 Q646 T647 Q648 R649 P650 I651 A652 L653 E654 L655 Y656 K657 D658 F659 K660 E661 L662 G663 R664 F665 M666 L667 R668 Y669 G670 G671 S672 T673 I674 A675 A676 G677 V678 V679 T680 E681 I682 K683 E684

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37432	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: ZN, GCP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.35	0/1936	0.70	0/2596
2	B	0.36	0/3240	0.65	0/4339
3	C	0.34	0/2937	0.67	0/3946
4	D	0.34	0/2437	0.62	2/3264 (0.1%)
5	E	0.33	0/1762	0.62	0/2362
6	F	0.36	0/1911	0.65	0/2549
7	G	0.34	0/1910	0.62	0/2569
8	H	0.33	0/1535	0.61	0/2063
9	I	0.34	0/1702	0.63	0/2272
10	J	0.34	0/1385	0.61	0/1852
11	L	0.34	0/1733	0.68	0/2316
12	M	0.36	0/1158	0.68	0/1547
13	N	0.35	0/1746	0.67	0/2338
14	O	0.36	0/1662	0.66	0/2222
15	P	0.36	0/1268	0.64	0/1700
16	Q	0.35	0/1539	0.73	0/2054
17	R	0.34	0/1524	0.66	0/2013
18	S	0.35	0/1501	0.65	0/2012
19	T	0.34	0/1326	0.62	0/1770
20	U	0.35	0/823	0.56	0/1104
21	V	0.34	0/993	0.63	0/1332
22	W	0.35	0/873	0.57	0/1158
23	X	0.31	0/984	0.60	0/1323
24	Y	0.32	0/1132	0.62	0/1504
25	Z	0.36	0/1130	0.63	0/1507
26	a	0.33	0/1191	0.63	0/1590
27	b	0.33	0/861	0.58	0/1138
28	c	0.31	0/771	0.54	0/1034
29	d	0.35	0/903	0.66	0/1216
30	e	0.34	0/1071	0.64	0/1429
31	f	0.38	0/895	0.70	0/1198
32	g	0.34	0/916	0.69	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.31	0/1021	0.61	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.35	0/720	0.70	0/952
36	k	0.31	0/575	0.54	0/761
37	l	0.35	0/459	0.63	0/608
38	m	0.31	0/435	0.60	0/575
39	n	0.36	0/240	0.67	0/305
40	o	0.34	0/864	0.62	0/1140
41	p	0.34	0/718	0.59	0/953
42	r	0.34	0/1010	0.65	0/1354
43	s	0.37	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.53	0/1582
45	1	0.44	0/49	0.61	0/65
46	2	0.21	0/1805	0.66	0/2809
47	3	0.21	0/1777	0.65	0/2763
48	5	0.31	14/84961 (0.0%)	0.76	62/132460 (0.0%)
49	7	0.28	0/2858	0.67	0/4455
50	8	0.27	0/3581	0.67	0/5577
51	9	0.27	1/40523 (0.0%)	0.70	8/63130 (0.0%)
52	AA	0.35	0/1747	0.61	0/2374
53	BB	0.33	0/1756	0.58	0/2350
54	CC	0.34	0/1753	0.63	0/2369
55	DD	0.35	0/1796	0.62	0/2417
56	EE	0.35	0/2118	0.64	0/2849
57	FF	0.34	0/1492	0.61	0/2005
58	GG	0.35	0/1946	0.66	0/2590
59	HH	0.35	0/1510	0.58	0/2022
60	II	0.34	0/1715	0.66	0/2287
61	JJ	0.34	0/1550	0.70	0/2069
62	KK	0.35	0/834	0.57	0/1125
63	LL	0.34	0/1195	0.69	0/1597
64	MM	0.36	0/918	0.59	0/1233
65	NN	0.33	0/1226	0.64	0/1649
66	OO	0.34	0/1029	0.72	0/1380
67	PP	0.37	0/1017	0.65	0/1358
68	QQ	0.34	0/1146	0.60	0/1534
69	RR	0.35	0/1082	0.61	0/1452
70	SS	0.35	0/1208	0.66	0/1618
71	TT	0.37	0/1115	0.63	1/1493 (0.1%)
72	UU	0.33	0/805	0.64	0/1081
73	VV	0.36	0/643	0.65	0/860
74	WW	0.34	0/1051	0.68	0/1406
75	XX	0.34	0/1116	0.65	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	YY	0.37	0/1028	0.64	0/1366
77	ZZ	0.35	0/604	0.61	0/810
78	aa	0.35	0/828	0.73	0/1109
79	bb	0.35	0/665	0.62	0/891
80	cc	0.33	0/490	0.68	0/656
81	dd	0.38	0/470	0.65	0/623
82	ee	0.35	0/447	0.65	0/587
83	ff	0.37	0/567	0.57	0/753
84	gg	0.33	0/2493	0.55	0/3394
85	hh	0.28	0/188	0.81	0/290
86	ii	0.34	0/2996	0.57	0/4050
87	jj	0.34	0/3352	0.55	0/4523
All	All	0.32	15/237792 (0.0%)	0.70	73/348210 (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
2	B	0	1
48	5	0	2
75	XX	0	1
78	aa	0	1
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C5-C6	-17.76	1.25	1.41
48	5	922(A)	G	O3'-P	13.89	1.77	1.61
48	5	935	A	C6-N1	-12.33	1.26	1.35
48	5	935	A	C2-N3	10.66	1.43	1.33
48	5	1411(B)	C	O3'-P	9.43	1.72	1.61
48	5	481	G	N1-C2	-9.42	1.30	1.37
48	5	481	G	C5-C6	8.11	1.50	1.42
48	5	935	A	N3-C4	7.71	1.39	1.34
48	5	1411(C)	C	O5'-C5'	7.46	1.56	1.44
48	5	922	C	O3'-P	6.70	1.69	1.61
48	5	481	G	C2-N3	-6.37	1.27	1.32
48	5	1411(C)	C	C5'-C4'	6.12	1.58	1.51
48	5	481	G	C2-N2	-5.86	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	922(A)	G	C3'-O3'	5.82	1.50	1.42
51	9	615	C	O3'-P	5.12	1.67	1.61

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	481	G	N1-C2-N2	-51.75	69.62	116.20
48	5	481	G	C8-N9-C1'	-51.47	60.09	127.00
48	5	935	A	C5-C6-N6	-47.28	85.88	123.70
48	5	935	A	C6-N1-C2	-34.46	97.92	118.60
48	5	935	A	N1-C6-N6	-34.37	97.98	118.60
48	5	481	G	N3-C2-N2	-31.28	98.00	119.90
48	5	935	A	C4-C5-C6	-29.50	102.25	117.00
48	5	481	G	C6-N1-C2	-22.06	111.86	125.10
48	5	481	G	C2-N3-C4	-20.13	101.84	111.90
48	5	481	G	N9-C1'-C2'	14.58	132.96	114.00
48	5	922	C	C2'-C3'-O3'	13.20	138.53	109.50
48	5	935	A	N3-C4-C5	-13.06	117.66	126.80
48	5	935	A	N1-C2-N3	-11.86	123.37	129.30
48	5	481	G	C4-N9-C1'	-10.14	113.32	126.50
48	5	922	C	N1-C1'-C2'	-10.06	100.92	114.00
48	5	922	C	C4'-C3'-C2'	-8.81	93.78	102.60
48	5	922	C	C5'-C4'-O4'	8.80	119.66	109.10
48	5	1411	C	C4'-C3'-O3'	8.55	130.10	113.00
48	5	922	C	O4'-C4'-C3'	-8.35	95.65	104.00
48	5	1411(C)	C	P-O5'-C5'	8.29	134.17	120.90
51	9	1835	A	C2'-C3'-O3'	8.10	127.32	109.50
48	5	922(B)	C	C1'-C2'-O2'	-7.69	87.54	110.60
51	9	1394	G	C2'-C3'-O3'	7.62	126.26	109.50
48	5	481	G	N3-C4-C5	-7.41	124.90	128.60
4	D	22	ARG	NE-CZ-NH1	7.17	123.88	120.30
48	5	922(A)	G	P-O3'-C3'	7.17	128.30	119.70
48	5	3888	G	C2'-C3'-O3'	7.02	124.95	109.50
48	5	922(A)	G	N9-C1'-C2'	6.92	123.00	114.00
48	5	1411	C	C5'-C4'-C3'	6.92	127.07	116.00
48	5	1477	C	C2'-C3'-O3'	6.88	124.70	113.70
48	5	1411(C)	C	C5'-C4'-O4'	6.87	117.34	109.10
51	9	615	C	N1-C1'-C2'	-6.86	104.45	112.00
48	5	481	G	C5-C6-N1	-6.75	108.12	111.50
51	9	434	G	C2'-C3'-O3'	6.73	124.47	113.70
48	5	922	C	O4'-C1'-N1	6.35	113.28	108.20
51	9	1646	C	C2'-C3'-O3'	6.28	123.74	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	4947	U	C2'-C3'-O3'	6.24	123.69	113.70
48	5	2046	G	C2'-C3'-O3'	6.16	123.55	113.70
51	9	615	C	C3'-C2'-C1'	6.00	106.30	101.50
48	5	3697	U	C2'-C3'-O3'	6.00	123.30	113.70
48	5	1411	C	O4'-C4'-C3'	-6.00	98.00	104.00
48	5	406	C	C2'-C3'-O3'	5.99	123.28	113.70
48	5	90	G	C2'-C3'-O3'	5.99	123.28	113.70
48	5	1211	G	C2'-C3'-O3'	5.97	123.25	113.70
48	5	275	C	C2'-C3'-O3'	5.96	123.23	113.70
48	5	125	C	C2'-C3'-O3'	5.93	123.19	113.70
51	9	110	U	C2'-C3'-O3'	5.87	123.10	113.70
48	5	1455	G	C2'-C3'-O3'	5.84	123.04	113.70
48	5	47	A	C4'-C3'-O3'	5.71	124.42	113.00
48	5	1563	A	N9-C1'-C2'	-5.63	105.81	112.00
48	5	1818	G	C2'-C3'-O3'	5.62	122.70	113.70
48	5	2695	A	C2'-C3'-O3'	5.58	122.63	113.70
48	5	385	A	C4'-C3'-O3'	5.56	124.13	113.00
48	5	481	G	N3-C4-N9	5.56	129.34	126.00
48	5	1329	G	C2'-C3'-O3'	5.55	122.58	113.70
48	5	922(B)	C	C5'-C4'-O4'	5.41	115.59	109.10
48	5	922(A)	G	C2'-C3'-O3'	5.40	122.33	113.70
48	5	4884	G	C2'-C3'-O3'	5.39	122.33	113.70
48	5	245	C	C2'-C3'-O3'	5.32	122.21	113.70
48	5	922(B)	C	P-O5'-C5'	5.29	129.36	120.90
48	5	1445	U	C2'-C3'-O3'	5.29	122.16	113.70
4	D	22	ARG	CG-CD-NE	5.22	122.76	111.80
48	5	1291	G	C2'-C3'-O3'	5.18	121.99	113.70
48	5	2474	G	C2'-C3'-O3'	5.16	121.96	113.70
48	5	1411	C	O4'-C1'-N1	5.14	112.31	108.20
51	9	532	C	C2'-C3'-O3'	5.12	121.89	113.70
71	TT	110	LEU	CA-CB-CG	5.11	127.06	115.30
48	5	4448	G	C4'-C3'-O3'	5.08	123.16	113.00
48	5	971(A)	G	C4'-C3'-O3'	5.08	123.15	113.00
48	5	930	G	C2'-C3'-O3'	5.07	121.81	113.70
48	5	1411	C	C2'-C3'-O3'	-5.06	98.37	109.50
48	5	1834	U	C2'-C3'-O3'	5.03	121.75	113.70
48	5	1411(B)	C	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
2	B	16	PHE	Peptide
75	XX	61	GLN	Peptide
78	aa	26	CYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	224 (91%)	19 (8%)	3 (1%)	13	49
2	B	392/403 (97%)	367 (94%)	24 (6%)	1 (0%)	41	74
3	C	360/425 (85%)	338 (94%)	20 (6%)	2 (1%)	25	62
4	D	291/297 (98%)	279 (96%)	10 (3%)	2 (1%)	22	59
5	E	208/291 (72%)	190 (91%)	18 (9%)	0	100	100
6	F	223/247 (90%)	210 (94%)	11 (5%)	2 (1%)	17	54
7	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	183 (91%)	17 (8%)	1 (0%)	29	66
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	29	66
12	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
13	N	201/204 (98%)	186 (92%)	14 (7%)	1 (0%)	29	66
14	O	197/203 (97%)	183 (93%)	14 (7%)	0	100	100
15	P	151/184 (82%)	142 (94%)	8 (5%)	1 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	185/188 (98%)	168 (91%)	15 (8%)	2 (1%)	14	50
17	R	178/196 (91%)	170 (96%)	8 (4%)	0	100	100
18	S	174/176 (99%)	163 (94%)	9 (5%)	2 (1%)	14	50
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	10 (10%)	1 (1%)	15	51
21	V	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	15	51
23	X	116/156 (74%)	111 (96%)	5 (4%)	0	100	100
24	Y	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	10	44
26	a	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
27	b	100/245 (41%)	92 (92%)	7 (7%)	1 (1%)	15	51
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	90 (86%)	14 (13%)	1 (1%)	15	51
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	8	40
32	g	112/117 (96%)	104 (93%)	8 (7%)	0	100	100
33	h	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
34	i	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
35	j	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
36	k	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
37	l	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
38	m	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	96 (94%)	5 (5%)	1 (1%)	15	51
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	14	50
42	r	122/137 (89%)	109 (89%)	11 (9%)	2 (2%)	9	43
43	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	15	51
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	12	47
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	198 (92%)	16 (7%)	1 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BB	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
54	CC	219/293 (75%)	204 (93%)	15 (7%)	0	100	100
55	DD	226/243 (93%)	207 (92%)	17 (8%)	2 (1%)	17	54
56	EE	260/263 (99%)	248 (95%)	11 (4%)	1 (0%)	34	69
57	FF	181/204 (89%)	169 (93%)	10 (6%)	2 (1%)	14	50
58	GG	235/249 (94%)	226 (96%)	8 (3%)	1 (0%)	34	69
59	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
60	II	204/208 (98%)	190 (93%)	13 (6%)	1 (0%)	29	66
61	JJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	29	66
62	KK	94/165 (57%)	87 (93%)	6 (6%)	1 (1%)	14	50
63	LL	139/158 (88%)	127 (91%)	11 (8%)	1 (1%)	22	59
64	MM	115/132 (87%)	100 (87%)	15 (13%)	0	100	100
65	NN	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
66	OO	134/168 (80%)	124 (92%)	9 (7%)	1 (1%)	22	59
67	PP	118/145 (81%)	104 (88%)	14 (12%)	0	100	100
68	QQ	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
69	RR	130/135 (96%)	117 (90%)	12 (9%)	1 (1%)	19	56
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	22	59
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	19	56
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	6	37
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/115 (86%)	90 (91%)	7 (7%)	2 (2%)	7	39
79	bb	81/84 (96%)	70 (86%)	10 (12%)	1 (1%)	13	49
80	cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	4 (8%)	1 (2%)	8	40
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	gg	311/317 (98%)	282 (91%)	26 (8%)	3 (1%)	15	51
86	ii	370/403 (92%)	342 (92%)	27 (7%)	1 (0%)	41	74
87	jj	423/710 (60%)	388 (92%)	31 (7%)	4 (1%)	17	54
All	All	12317/14495 (85%)	11449 (93%)	804 (6%)	64 (0%)	32	66

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	S	155	PRO
75	XX	62	PRO
75	XX	86	PRO
1	A	217	GLN
3	C	83	GLY
3	C	94	ASN
6	F	99	GLY
13	N	89	VAL
43	s	142	GLY
44	t	125	LEU
1	A	14	SER
11	L	63	THR
22	W	27	LYS
25	Z	91	LEU
27	b	102	PRO
31	f	107	PRO
42	r	68	SER
62	KK	64	TRP
66	OO	20	GLN
74	WW	56	HIS
78	aa	47	ALA
79	bb	81	ARG
87	jj	605	GLN
87	jj	618	SER
1	A	234	LYS
2	B	17	LEU
4	D	44	TYR
16	Q	14	ARG
25	Z	90	PRO
31	f	106	TYR
52	AA	159	ILE
56	EE	73	ASP
81	dd	7	TYR

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Mol	Chain	Res	Type
86	ii	12	ASN
87	jj	269	VAL
87	jj	596	LYS
20	U	24	ASP
42	r	33	LYS
44	t	54	LYS
55	DD	44	THR
55	DD	93	THR
61	JJ	147	PHE
75	XX	61	GLN
78	aa	26	CYS
15	P	114	ILE
29	d	58	GLY
40	o	96	ASP
43	s	25	PRO
57	FF	43	GLU
63	LL	66	VAL
16	Q	92	VAL
58	GG	135	PRO
9	I	201	PRO
18	S	165	PRO
60	II	3	ILE
84	gg	224	GLY
4	D	125	VAL
69	RR	119	VAL
71	TT	109	GLY
84	gg	61	GLY
6	F	196	VAL
41	p	9	GLY
57	FF	21	GLY
84	gg	13	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	175 (92%)	15 (8%)	12	42
2	B	342/348 (98%)	322 (94%)	20 (6%)	20	52
3	C	302/347 (87%)	282 (93%)	20 (7%)	16	48
4	D	247/250 (99%)	235 (95%)	12 (5%)	25	56
5	E	190/251 (76%)	178 (94%)	12 (6%)	18	49
6	F	196/215 (91%)	182 (93%)	14 (7%)	14	45
7	G	200/272 (74%)	188 (94%)	12 (6%)	19	50
8	H	169/171 (99%)	158 (94%)	11 (6%)	17	48
9	I	175/181 (97%)	165 (94%)	10 (6%)	20	52
10	J	143/149 (96%)	136 (95%)	7 (5%)	25	56
11	L	175/176 (99%)	166 (95%)	9 (5%)	24	55
12	M	117/161 (73%)	110 (94%)	7 (6%)	19	50
13	N	171/172 (99%)	162 (95%)	9 (5%)	22	54
14	O	171/173 (99%)	159 (93%)	12 (7%)	15	45
15	P	134/163 (82%)	125 (93%)	9 (7%)	16	47
16	Q	164/165 (99%)	153 (93%)	11 (7%)	16	47
17	R	159/175 (91%)	148 (93%)	11 (7%)	15	46
18	S	157/157 (100%)	147 (94%)	10 (6%)	17	48
19	T	139/140 (99%)	128 (92%)	11 (8%)	12	42
20	U	89/114 (78%)	87 (98%)	2 (2%)	52	72
21	V	101/107 (94%)	91 (90%)	10 (10%)	8	32
22	W	86/126 (68%)	85 (99%)	1 (1%)	71	84
23	X	106/134 (79%)	100 (94%)	6 (6%)	20	52
24	Y	124/135 (92%)	118 (95%)	6 (5%)	25	56
25	Z	117/118 (99%)	114 (97%)	3 (3%)	46	69
26	a	119/120 (99%)	117 (98%)	2 (2%)	60	79
27	b	84/184 (46%)	81 (96%)	3 (4%)	35	62
28	c	84/98 (86%)	82 (98%)	2 (2%)	49	70
29	d	98/110 (89%)	88 (90%)	10 (10%)	7	31
30	e	114/121 (94%)	105 (92%)	9 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	f	88/89 (99%)	84 (96%)	4 (4%)	27	57
32	g	98/100 (98%)	92 (94%)	6 (6%)	18	50
33	h	109/110 (99%)	104 (95%)	5 (5%)	27	57
34	i	86/89 (97%)	84 (98%)	2 (2%)	50	71
35	j	73/80 (91%)	68 (93%)	5 (7%)	16	47
36	k	64/65 (98%)	62 (97%)	2 (3%)	40	65
37	l	47/48 (98%)	46 (98%)	1 (2%)	53	73
38	m	48/90 (53%)	46 (96%)	2 (4%)	30	59
39	n	24/24 (100%)	22 (92%)	2 (8%)	11	40
40	o	92/94 (98%)	87 (95%)	5 (5%)	22	54
41	p	74/75 (99%)	73 (99%)	1 (1%)	67	82
42	r	108/121 (89%)	99 (92%)	9 (8%)	11	40
43	s	164/258 (64%)	158 (96%)	6 (4%)	34	61
44	t	126/137 (92%)	123 (98%)	3 (2%)	49	70
45	1	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	163 (91%)	17 (9%)	8	35
53	BB	194/231 (84%)	180 (93%)	14 (7%)	14	45
54	CC	187/225 (83%)	172 (92%)	15 (8%)	12	42
55	DD	190/202 (94%)	173 (91%)	17 (9%)	9	37
56	EE	224/225 (100%)	211 (94%)	13 (6%)	20	52
57	FF	158/170 (93%)	150 (95%)	8 (5%)	24	55
58	GG	207/218 (95%)	188 (91%)	19 (9%)	9	36
59	HH	165/174 (95%)	150 (91%)	15 (9%)	9	36
60	II	178/180 (99%)	166 (93%)	12 (7%)	16	47
61	JJ	161/168 (96%)	150 (93%)	11 (7%)	16	47
62	KK	87/136 (64%)	79 (91%)	8 (9%)	9	36
63	LL	130/142 (92%)	116 (89%)	14 (11%)	6	29
64	MM	99/108 (92%)	86 (87%)	13 (13%)	4	22
65	NN	130/131 (99%)	114 (88%)	16 (12%)	4	24
66	OO	106/130 (82%)	94 (89%)	12 (11%)	6	28
67	PP	109/130 (84%)	97 (89%)	12 (11%)	6	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	QQ	117/121 (97%)	109 (93%)	8 (7%)	16	47
69	RR	119/121 (98%)	106 (89%)	13 (11%)	6	29
70	SS	125/132 (95%)	111 (89%)	14 (11%)	6	28
71	TT	111/115 (96%)	101 (91%)	10 (9%)	9	37
72	UU	92/107 (86%)	84 (91%)	8 (9%)	10	39
73	VV	67/67 (100%)	64 (96%)	3 (4%)	27	57
74	WW	112/113 (99%)	107 (96%)	5 (4%)	27	57
75	XX	113/115 (98%)	106 (94%)	7 (6%)	18	49
76	YY	107/112 (96%)	96 (90%)	11 (10%)	7	31
77	ZZ	66/103 (64%)	61 (92%)	5 (8%)	13	43
78	aa	88/98 (90%)	81 (92%)	7 (8%)	12	42
79	bb	75/76 (99%)	67 (89%)	8 (11%)	6	30
80	cc	55/62 (89%)	50 (91%)	5 (9%)	9	36
81	dd	48/49 (98%)	44 (92%)	4 (8%)	11	40
82	ee	46/106 (43%)	44 (96%)	2 (4%)	29	58
83	ff	61/140 (44%)	55 (90%)	6 (10%)	8	33
84	gg	272/275 (99%)	262 (96%)	10 (4%)	34	61
86	ii	326/353 (92%)	309 (95%)	17 (5%)	23	55
87	jj	358/608 (59%)	330 (92%)	28 (8%)	12	42
All	All	10733/12306 (87%)	10017 (93%)	716 (7%)	20	47

All (716) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	109	GLU
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	163	ARG
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS

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Mol	Chain	Res	Type
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	62	ARG
2	B	66	LYS
2	B	74	GLU
2	B	95	THR
2	B	97	ARG
2	B	135	LYS
2	B	248	LEU
2	B	261	ARG
2	B	262	VAL
2	B	279	GLU
2	B	294	LYS
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	383	GLU
3	C	20	LYS
3	C	45	ARG
3	C	95	MET
3	C	113	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	208	CYS
3	C	213	GLU
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET

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Mol	Chain	Res	Type
3	C	307	LYS
3	C	312	ARG
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	128	ASP
4	D	234	ASP
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	123	ASP
5	E	141	ARG
5	E	143	LEU
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	289	LEU
5	E	291	PHE
6	F	30	LYS
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU
6	F	88	LEU
6	F	120	THR
6	F	134	ILE
6	F	151	GLU
6	F	186	MET
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	245	ARG
7	G	126	ARG
7	G	154	LYS

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Mol	Chain	Res	Type
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	215	ASP
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	293	ASN
8	H	1	MET
8	H	20	LEU
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	105	ILE
8	H	108	ASN
8	H	128	MET
8	H	173	ARG
9	I	13	LYS
9	I	36	LEU
9	I	39	LYS
9	I	116	ARG
9	I	142	LEU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	195	CYS
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	72	CYS
10	J	81	GLU
10	J	113	ILE
10	J	175	LEU
11	L	10	LEU
11	L	63	THR
11	L	67	HIS
11	L	74	ARG

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Mol	Chain	Res	Type
11	L	121	ARG
11	L	129	ARG
11	L	162	LYS
11	L	186	ARG
11	L	195	ARG
12	M	37	LEU
12	M	42	CYS
12	M	57	LEU
12	M	89	THR
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	32	GLN
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	162	ARG
13	N	182	HIS
14	O	37	ARG
14	O	49	ARG
14	O	61	ARG
14	O	67	SER
14	O	82	ARG
14	O	106	ASP
14	O	128	ARG
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	175	MET
14	O	179	LYS
15	P	24	VAL
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU

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Mol	Chain	Res	Type
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	97	LYS
16	Q	101	CYS
16	Q	143	ARG
16	Q	188	ASN
17	R	8	LYS
17	R	36	ASN
17	R	50	ILE
17	R	89	MET
17	R	99	MET
17	R	113	LYS
17	R	130	ASN
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	83	ARG
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	63	ARG
19	T	96	ILE
19	T	117	LYS
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	157	GLU

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Mol	Chain	Res	Type
19	T	159	MET
20	U	33	ILE
20	U	80	LYS
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	41	SER
21	V	60	MET
21	V	71	GLU
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
22	W	91	MET
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	91	GLU
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	72	GLN
24	Y	74	TYR
24	Y	112	ASP
25	Z	11	VAL
25	Z	33	THR
25	Z	112	ARG
26	a	4	ARG
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	78	ASN
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	78	ARG

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Mol	Chain	Res	Type
29	d	83	ARG
29	d	85	ARG
29	d	90	ARG
29	d	98	SER
30	e	21	ILE
30	e	22	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	113	GLU
30	e	128	ARG
31	f	16	ARG
31	f	23	GLU
31	f	52	LYS
31	f	101	ILE
32	g	5	LEU
32	g	15	THR
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	16	GLU
33	h	28	LEU
33	h	67	GLU
33	h	77	LYS
33	h	89	ARG
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
35	j	79	ARG
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	92	THR
39	n	1	MET
39	n	13	LEU

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Mol	Chain	Res	Type
40	o	17	LYS
40	o	18	HIS
40	o	36	GLN
40	o	61	LYS
40	o	82	MET
41	p	8	VAL
42	r	8	MET
42	r	20	ARG
42	r	32	LEU
42	r	35	ARG
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	103	HIS
42	r	118	LEU
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	98	ILE
44	t	133	LEU
52	AA	9	GLN
52	AA	12	GLU
52	AA	25	LEU
52	AA	36	GLN
52	AA	44	ASP
52	AA	50	ASN
52	AA	58	LEU
52	AA	60	LEU
52	AA	111	GLN
52	AA	122	LEU
52	AA	132	GLN
52	AA	136	GLU
52	AA	142	LEU
52	AA	169	HIS
52	AA	178	LEU
52	AA	181	GLU
52	AA	200	ASP
53	BB	38	MET

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Mol	Chain	Res	Type
53	BB	71	LEU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	126	ASP
53	BB	134	LEU
53	BB	157	GLN
53	BB	180	ASP
53	BB	181	LEU
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
54	CC	78	LEU
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	132	ASP
54	CC	137	VAL
54	CC	167	ARG
54	CC	182	CYS
54	CC	188	CYS
54	CC	192	LEU
54	CC	227	ARG
54	CC	235	ASN
54	CC	236	PHE
54	CC	248	TYR
54	CC	255	LEU
55	DD	28	GLU
55	DD	35	SER
55	DD	45	ARG
55	DD	57	ASN
55	DD	72	VAL
55	DD	76	ARG
55	DD	127	MET
55	DD	132	LYS
55	DD	134	CYS
55	DD	142	LEU
55	DD	145	GLN
55	DD	146	ARG
55	DD	168	VAL
55	DD	182	LEU

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Mol	Chain	Res	Type
55	DD	190	LEU
55	DD	218	LEU
55	DD	227	LYS
56	EE	17	HIS
56	EE	24	THR
56	EE	42	LEU
56	EE	51	ARG
56	EE	59	ASP
56	EE	66	MET
56	EE	77	ARG
56	EE	145	ARG
56	EE	200	ARG
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	246	LEU
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	95	HIS
57	FF	125	SER
57	FF	140	ASP
57	FF	204	ARG
58	GG	41	LEU
58	GG	48	TYR
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	72	ARG
58	GG	95	LYS
58	GG	103	ASP
58	GG	116	LYS
58	GG	137	ARG
58	GG	159	ARG
58	GG	171	THR
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	216	ARG
58	GG	217	MET
58	GG	230	LYS

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Mol	Chain	Res	Type
58	GG	235	SER
59	HH	8	ILE
59	HH	17	ASP
59	HH	21	SER
59	HH	36	LEU
59	HH	40	LEU
59	HH	46	THR
59	HH	53	VAL
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	119	SER
59	HH	145	ARG
59	HH	149	ASP
59	HH	160	LYS
60	II	6	ASP
60	II	12	ARG
60	II	23	LYS
60	II	26	LYS
60	II	49	ARG
60	II	92	ARG
60	II	99	ASN
60	II	121	LEU
60	II	128	LYS
60	II	130	THR
60	II	168	GLN
60	II	178	ARG
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	80	ARG
61	JJ	89	GLU
61	JJ	92	MET
61	JJ	116	LYS
62	KK	1	MET
62	KK	6	LYS
62	KK	17	LYS

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Mol	Chain	Res	Type
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	56	ILE
63	LL	69	ARG
63	LL	85	THR
63	LL	110	SER
63	LL	121	GLN
63	LL	126	VAL
63	LL	132	ARG
63	LL	134	LEU
63	LL	144	LYS
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	49	LEU
64	MM	55	ASN
64	MM	76	LEU
64	MM	83	LYS
64	MM	85	LEU
64	MM	96	ARG
64	MM	99	LYS
64	MM	101	ARG
64	MM	112	LYS
64	MM	122	ASP
65	NN	3	ARG
65	NN	20	ARG
65	NN	27	LYS
65	NN	29	THR
65	NN	36	GLN
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU

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Mol	Chain	Res	Type
65	NN	86	GLU
65	NN	107	LYS
65	NN	110	ASP
65	NN	120	SER
65	NN	125	LEU
65	NN	132	LYS
66	OO	25	GLU
66	OO	31	CYS
66	OO	34	PHE
66	OO	38	ASN
66	OO	46	ASP
66	OO	51	GLU
66	OO	56	VAL
66	OO	104	ARG
66	OO	128	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	44	ARG
67	PP	51	ARG
67	PP	58	LYS
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	108	LYS
67	PP	130	ARG
68	QQ	31	LEU
68	QQ	40	GLU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	60	LYS
68	QQ	67	ASP
68	QQ	90	LYS
68	QQ	140	ARG
69	RR	5	ARG
69	RR	31	ASN
69	RR	33	ARG
69	RR	44	LYS

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Mol	Chain	Res	Type
69	RR	62	GLN
69	RR	78	ARG
69	RR	82	ASP
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	109	LEU
69	RR	120	THR
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	21	ASP
70	SS	23	ARG
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	62	ASP
70	SS	63	GLU
70	SS	75	ARG
70	SS	83	PHE
70	SS	110	ASP
70	SS	132	ARG
71	TT	41	LYS
71	TT	55	THR
71	TT	62	ARG
71	TT	102	ARG
71	TT	110	LEU
71	TT	121	ARG
71	TT	123	LEU
71	TT	124	THR
71	TT	131	LEU
71	TT	142	LYS
72	UU	18	HIS
72	UU	25	THR
72	UU	56	MET
72	UU	60	THR
72	UU	88	LEU
72	UU	90	ASP
72	UU	106	ILE
72	UU	111	GLU
73	VV	10	ASP

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Mol	Chain	Res	Type
73	VV	12	TYR
73	VV	66	ASP
74	WW	23	ARG
74	WW	51	GLU
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
75	XX	8	ARG
75	XX	15	SER
75	XX	67	ARG
75	XX	105	PHE
75	XX	115	ILE
75	XX	119	ARG
75	XX	135	LYS
76	YY	9	THR
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	40	ILE
76	YY	47	MET
76	YY	61	ARG
76	YY	74	MET
76	YY	88	LYS
76	YY	101	LYS
76	YY	103	SER
77	ZZ	51	ASP
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	101	SER
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	41	ILE
78	aa	42	ARG
78	aa	100	ARG
79	bb	17	ARG
79	bb	36	LYS
79	bb	37	CYS
79	bb	42	LYS
79	bb	64	CYS

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Mol	Chain	Res	Type
79	bb	78	SER
79	bb	80	ARG
79	bb	81	ARG
80	cc	31	ARG
80	cc	40	ARG
80	cc	44	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	18	SER
81	dd	22	ARG
81	dd	48	LYS
81	dd	49	ASP
82	ee	99	LYS
82	ee	107	ARG
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	138	ARG
83	ff	140	TYR
83	ff	149	CYS
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	38	LYS
84	gg	119	GLN
84	gg	198	VAL
84	gg	207	CYS
84	gg	273	GLU
84	gg	289	LEU
84	gg	306	LEU
86	ii	40	ARG
86	ii	68	CYS
86	ii	81	LEU
86	ii	107	ASN
86	ii	148	HIS
86	ii	149	ILE
86	ii	156	MET
86	ii	170	LYS
86	ii	183	GLU
86	ii	198	HIS
86	ii	243	VAL
86	ii	258	CYS

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Mol	Chain	Res	Type
86	ii	297	LYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG
86	ii	349	LEU
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU
87	jj	304	LYS
87	jj	313	LEU
87	jj	325	THR
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	389	HIS
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	482	ARG
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	524	PRO
87	jj	548	ASP
87	jj	557	MET
87	jj	590	ILE
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
7	G	135	GLN
12	M	48	GLN
14	O	65	ASN
17	R	130	ASN

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Mol	Chain	Res	Type
22	W	48	GLN
23	X	93	ASN
23	X	105	ASN
28	c	78	ASN
42	r	70	GLN
42	r	103	HIS
42	r	121	GLN
43	s	34	ASN
52	AA	132	GLN
54	CC	235	ASN
56	EE	260	GLN
59	HH	114	GLN
61	JJ	111	GLN
66	OO	20	GLN
67	PP	41	GLN
67	PP	79	HIS
68	QQ	35	ASN
68	QQ	142	GLN
70	SS	10	GLN
70	SS	97	GLN
74	WW	92	ASN
75	XX	77	ASN
79	bb	49	HIS
82	ee	117	ASN
86	ii	109	GLN
87	jj	385	GLN
87	jj	389	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	27 (37%)	1 (1%)
48	5	3506/3543 (98%)	849 (24%)	165 (4%)
49	7	119/120 (99%)	12 (10%)	2 (1%)
50	8	150/156 (96%)	35 (23%)	7 (4%)
51	9	1680/1869 (89%)	425 (25%)	84 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5608/5847 (95%)	1365 (24%)	259 (4%)

All (1365) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	21	A
46	2	43	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	61	C
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	51	G
47	3	53	G
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	71	G
47	3	72	C
47	3	74	C
47	3	75	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A

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Mol	Chain	Res	Type
48	5	25	A
48	5	30	C
48	5	35	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	157	U
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C

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Mol	Chain	Res	Type
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	246	G
48	5	253	G
48	5	262	G
48	5	263	G
48	5	265	C
48	5	266	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	386	A
48	5	387	G
48	5	399	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G

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Mol	Chain	Res	Type
48	5	413	G
48	5	431	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	649	A
48	5	654	C
48	5	658	C
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G

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Mol	Chain	Res	Type
48	5	708	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	739	G
48	5	742	G
48	5	744	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	915	A
48	5	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	957	G
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C

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Mol	Chain	Res	Type
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1070	G
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1184	A
48	5	1185	G
48	5	1195	G
48	5	1211	G
48	5	1212	G
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1291	G

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Mol	Chain	Res	Type
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1328	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1416	G
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	1433	A
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1441	C
48	5	1442	C

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Mol	Chain	Res	Type
48	5	1445	U
48	5	1446	C
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1475	G
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G

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Mol	Chain	Res	Type
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1724	G
48	5	1726	U
48	5	1729	A
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1787	A
48	5	1797	G
48	5	1799	G
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G
48	5	1822	U

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Mol	Chain	Res	Type
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1933	G
48	5	1941	A
48	5	1948	G
48	5	1952	G
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G

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Mol	Chain	Res	Type
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2017	A
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2033	A
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2109	A
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G

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Mol	Chain	Res	Type
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2279	A
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2316	G
48	5	2332	A
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2352	U
48	5	2360	A
48	5	2364	G
48	5	2370	A
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2416	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2483	G
48	5	2485	U
48	5	2488	C
48	5	2489	C

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Mol	Chain	Res	Type
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2572	C
48	5	2575	U
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2639	U
48	5	2640	G
48	5	2647	A
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2689	C
48	5	2695	A
48	5	2696	A

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Mol	Chain	Res	Type
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2754	G
48	5	2755	A
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2789	A
48	5	2790	U
48	5	2794	C
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2835	A
48	5	2838	G
48	5	2842	G
48	5	2855	G
48	5	2875	C
48	5	2884	G

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Mol	Chain	Res	Type
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3722	G
48	5	3729	U
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3759	A
48	5	3760	A
48	5	3761	C
48	5	3763	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3810	C

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Mol	Chain	Res	Type
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3916	G
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C

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Mol	Chain	Res	Type
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4158	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4171	C
48	5	4177	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A
48	5	4213	A
48	5	4218	U
48	5	4219	A
48	5	4225	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4237	C
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A

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Mol	Chain	Res	Type
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4326	G
48	5	4329	G
48	5	4330	G
48	5	4335	C
48	5	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4437	U
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4471	U

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Mol	Chain	Res	Type
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4606	G
48	5	4618	G
48	5	4635	A
48	5	4636	U
48	5	4637	G
48	5	4656	A
48	5	4657	U
48	5	4658	G
48	5	4661	G
48	5	4667	C
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4700	A
48	5	4701	A

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Mol	Chain	Res	Type
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G
48	5	4756	C
48	5	4757	C
48	5	4758	U
48	5	4759	C
48	5	4760	G
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4881	U
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G

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Mol	Chain	Res	Type
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4925	U
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4945	G
48	5	4947	U
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4997	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C

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Mol	Chain	Res	Type
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	11	A
49	7	25	G
49	7	33	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	97	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	103	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G

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Mol	Chain	Res	Type
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	150	C
50	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A

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Mol	Chain	Res	Type
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	173	A
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U

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Mol	Chain	Res	Type
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	372	U
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	408	A
51	9	409	C
51	9	410	G
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	452	G
51	9	460	A
51	9	462	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C

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Mol	Chain	Res	Type
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	523	A
51	9	525	A
51	9	528	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G

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Mol	Chain	Res	Type
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	620	G
51	9	621	C
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	630	U
51	9	631	U
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	732	U
51	9	752	G
51	9	753	C
51	9	754	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C

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Mol	Chain	Res	Type
51	9	847	A
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	885	U
51	9	887	U
51	9	890	U
51	9	892	U
51	9	913	A
51	9	914	U
51	9	920	A
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1100	A
51	9	1114	U

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Mol	Chain	Res	Type
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1265	A
51	9	1266	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1284	A
51	9	1285	G

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Mol	Chain	Res	Type
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1291	A
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1354	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A

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Mol	Chain	Res	Type
51	9	1477	U
51	9	1478	U
51	9	1489	A
51	9	1490	G
51	9	1493	C
51	9	1494	U
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1612	G
51	9	1621	U
51	9	1622	U

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Mol	Chain	Res	Type
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1695	A
51	9	1698	C
51	9	1703	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1728	U
51	9	1729	U
51	9	1730	U
51	9	1732	G
51	9	1737	G
51	9	1744	G
51	9	1745	A
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1822	A
51	9	1823	A
51	9	1824	A
51	9	1825	A

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Mol	Chain	Res	Type
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G

All (259) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G

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Mol	Chain	Res	Type
48	5	315	G
48	5	385	A
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	466	A
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	963	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U

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Mol	Chain	Res	Type
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1378	C
48	5	1380	G
48	5	1420	A
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1534	A
48	5	1563	A
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1892	A
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G

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Mol	Chain	Res	Type
48	5	2313	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2529	A
48	5	2546	G
48	5	2553	A
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2754	G
48	5	2794	C
48	5	2806	A
48	5	3603	G
48	5	3625	G
48	5	3648	A
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3759	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4266	G

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Mol	Chain	Res	Type
48	5	4272	G
48	5	4291	G
48	5	4378	A
48	5	4395	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4510	A
48	5	4527	G
48	5	4572	U
48	5	4626	A
48	5	4634	U
48	5	4699	U
48	5	4719	G
48	5	4872	G
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4947	U
48	5	4965	U
48	5	4966	A
49	7	10	C
49	7	109	U
50	8	2	G
50	8	51	U
50	8	85	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	128	U
51	9	142	C
51	9	160	U
51	9	182	C
51	9	293	C
51	9	312	G

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Mol	Chain	Res	Type
51	9	369	C
51	9	434	G
51	9	465	A
51	9	500	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	591	U
51	9	594	A
51	9	606	G
51	9	607	U
51	9	613	G
51	9	614	C
51	9	620	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	752	G
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	875	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1115	U
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1284	A

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Mol	Chain	Res	Type
51	9	1285	G
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1578	U
51	9	1581	C
51	9	1621	U
51	9	1622	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1665	G
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

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 273 ligands modelled in this entry, 272 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
90	GCP	jj	700	88	27,34,34	1.59	6 (22%)	34,54,54	1.86	8 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GCP	jj	700	88	-	4/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C5-C6	4.46	1.49	1.41
90	jj	700	GCP	PG-O3G	2.86	1.61	1.54
90	jj	700	GCP	PG-O2G	2.85	1.61	1.54
90	jj	700	GCP	PB-O3A	2.80	1.61	1.58
90	jj	700	GCP	C5-C4	2.60	1.47	1.40
90	jj	700	GCP	PB-O2B	2.19	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	jj	700	GCP	C2-N3-C4	5.05	121.13	115.36
90	jj	700	GCP	C2-N1-C6	3.90	122.13	115.93
90	jj	700	GCP	C4-C5-C6	-3.83	117.14	120.80
90	jj	700	GCP	C5-C6-N1	-3.80	118.23	123.43
90	jj	700	GCP	N3-C2-N1	-3.43	122.65	127.22
90	jj	700	GCP	C4-C5-N7	-2.73	106.55	109.40
90	jj	700	GCP	C3'-C2'-C1'	2.68	105.01	100.98
90	jj	700	GCP	PB-O3A-PA	-2.38	125.02	132.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

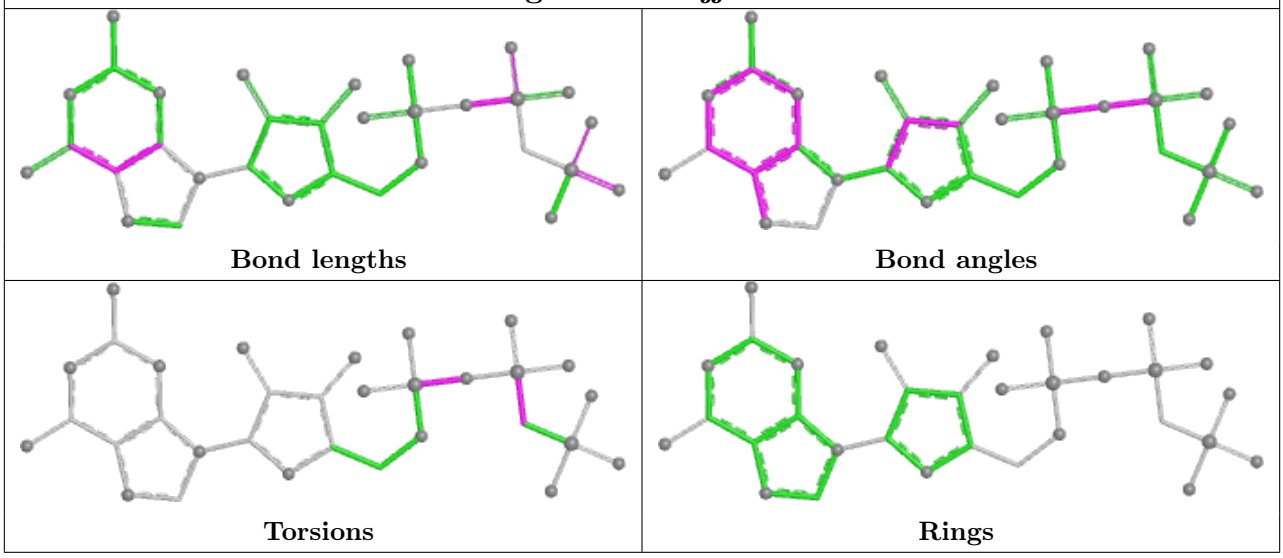
Mol	Chain	Res	Type	Atoms
90	jj	700	GCP	PG-C3B-PB-O1B
90	jj	700	GCP	PG-C3B-PB-O2B
90	jj	700	GCP	PG-C3B-PB-O3A
90	jj	700	GCP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GCP jj 700



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	43
51	9	8
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.91
1	5	1252:C	O3'	1271:G	P	35.78
1	5	1405:C	O3'	1406:G	P	23.41
1	5	1219:G	O3'	1233:G	P	22.71
1	5	1406:G	O3'	1406(A):G	P	20.12
1	5	3948:C	O3'	4065:G	P	19.81
1	5	4138:C	O3'	4146:G	P	18.04
1	5	990:C	O3'	1064:G	P	18.02
1	5	523:C	O3'	638:G	P	18.01
1	5	4101:C	O3'	4107:G	P	17.41
1	5	4777:C	O3'	4859:C	P	16.47
1	5	1406(C):G	O3'	1411:C	P	15.34
1	5	760:G	O3'	904:C	P	14.93
1	5	5022:U	O3'	5028:G	P	14.86
1	5	1696:C	O3'	1720:C	P	14.79
1	5	1364:U	O3'	1368:A	P	14.36
1	5	182:G	O3'	189:G	P	13.89
1	5	1411:C	O3'	1411(A):G	P	13.71
1	5	2901:G	O3'	3597:G	P	13.37
1	5	921:C	O3'	922:C	P	13.07
1	5	970:G	O3'	971:U	P	10.72
1	5	481:G	O3'	481(A):C	P	10.70
1	5	934:C	O3'	935:A	P	10.36
1	5	512:U	O3'	515:C	P	9.76
1	5	4729:A	O3'	4735:G	P	9.75
1	5	737:C	O3'	738:C	P	9.61
1	5	971:U	O3'	971(A):G	P	9.59
1	5	1180:C	O3'	1183:C	P	9.18
1	5	500:G	O3'	504:G	P	6.68
1	5	1100:U	O3'	1168:G	P	5.83
1	3	19:G	O3'	20:U	P	5.67
1	5	1239:C	O3'	1244:G	P	5.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	322:C	O3'	323:C	P	5.12
1	5	4740:G	O3'	4743:G	P	5.00
1	3	16:C	O3'	18:U	P	4.98
1	5	480:C	O3'	481:G	P	4.96
1	9	798:G	O3'	799:U	P	4.62
1	9	309:G	O3'	310:C	P	4.59
1	9	304:C	O3'	305:U	P	4.45
1	2	16:C	O3'	18:G	P	4.28
1	5	935:A	O3'	935(A):G	P	4.20
1	5	738:C	O3'	738(A):C	P	3.96
1	5	170:C	O3'	171:U	P	3.88
1	5	1438:U	O3'	1440:U	P	3.39
1	5	4899:G	O3'	4902:C	P	3.38
1	9	902:G	O3'	903:A	P	3.37
1	9	903:A	O3'	904:A	P	3.33
1	9	1295:A	O3'	1296:U	P	3.27
1	5	267:G	O3'	268:G	P	3.19
1	9	593:C	O3'	594:A	P	3.16
1	5	5020:G	O3'	5021:C	P	3.14
1	5	751:G	O3'	752:G	P	2.96
1	5	2031:C	O3'	2032:U	P	2.78
1	5	922(A):G	O3'	922(B):C	P	1.77

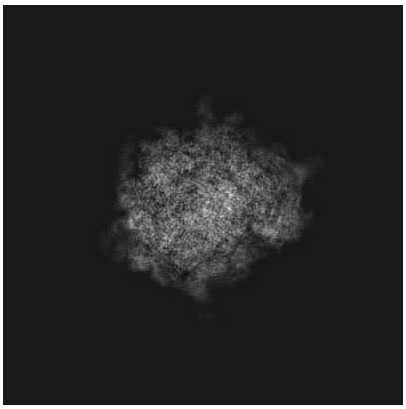
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4135. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



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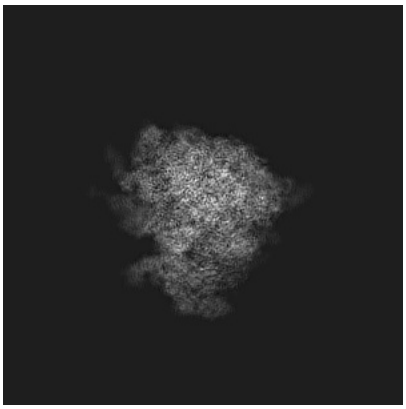
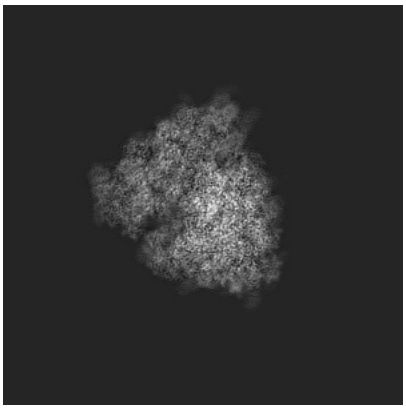
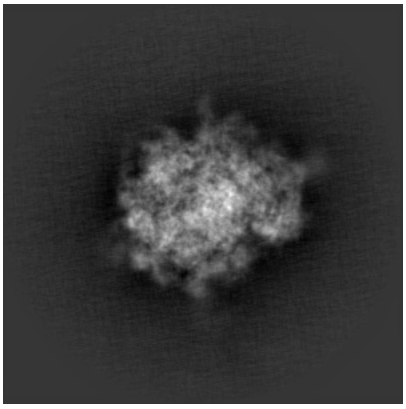


Y

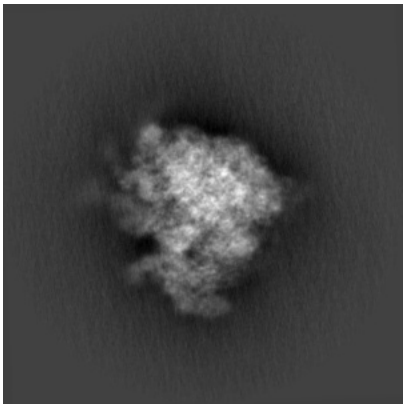


Z

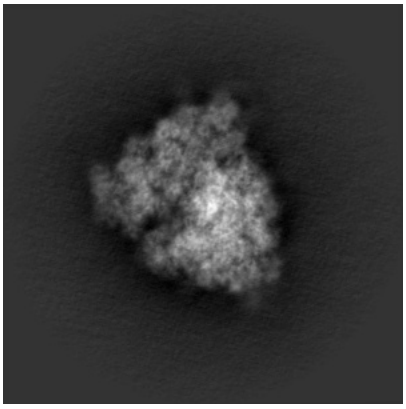
6.1.2 Raw map



X



Y

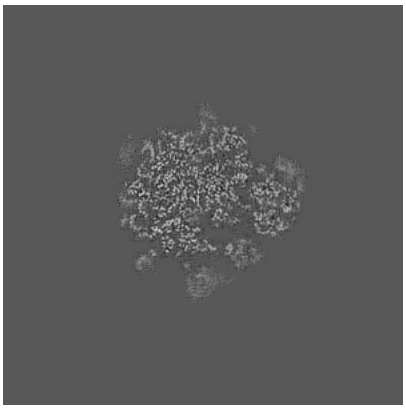


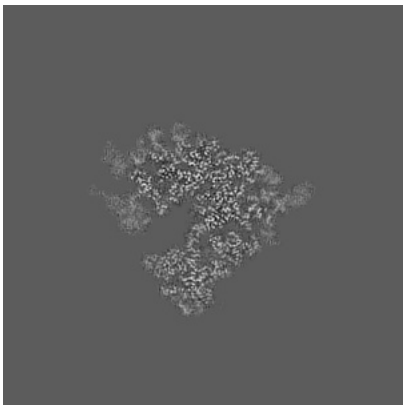
Z

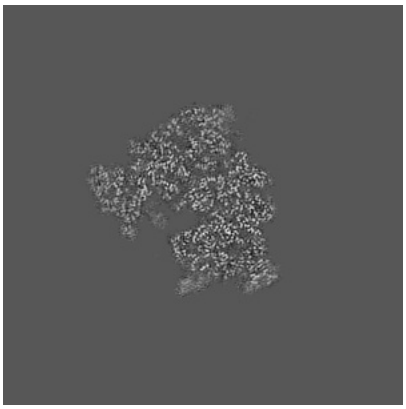
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

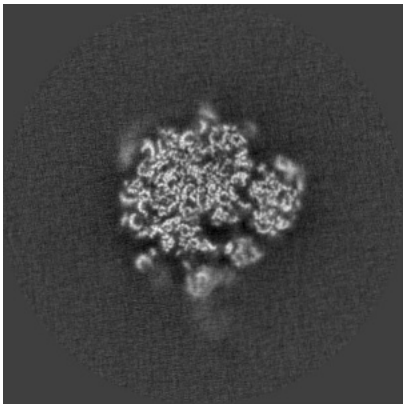
6.2.1 Primary map

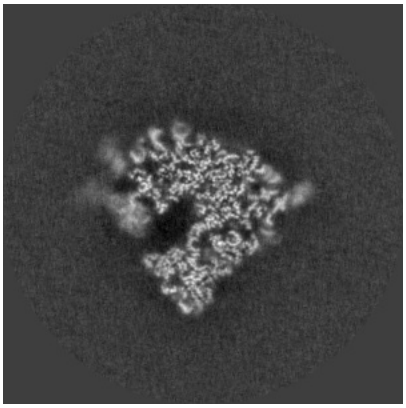

X Index: 210

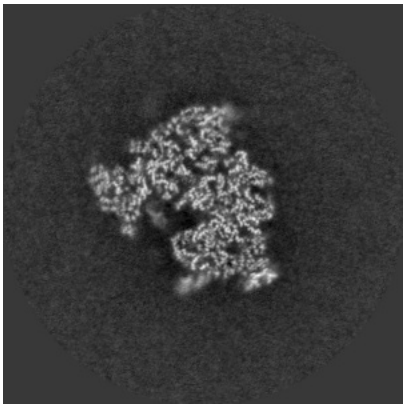

Y Index: 210


Z Index: 210

6.2.2 Raw map


X Index: 210

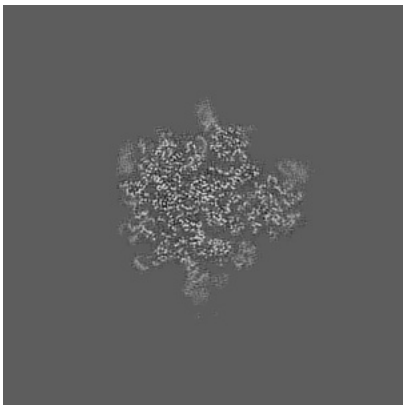

Y Index: 210


Z Index: 210

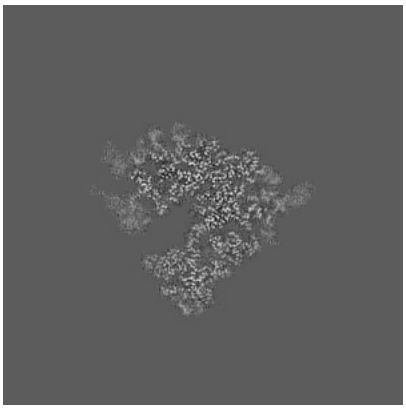
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

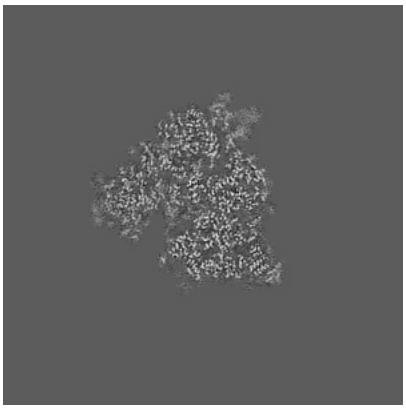
6.3.1 Primary map



X Index: 216

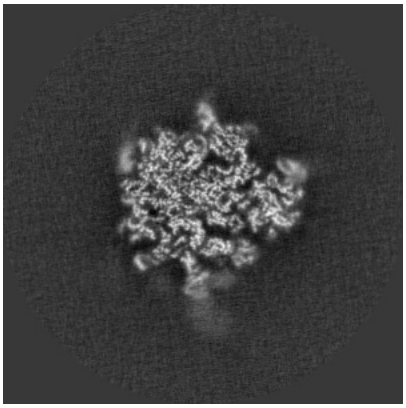


Y Index: 210

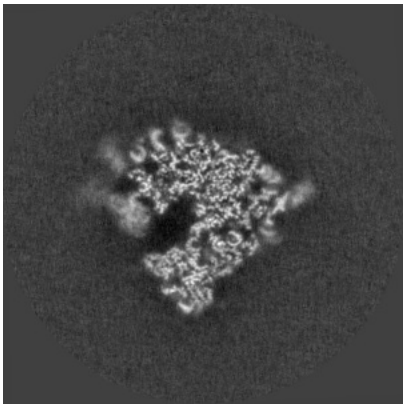


Z Index: 202

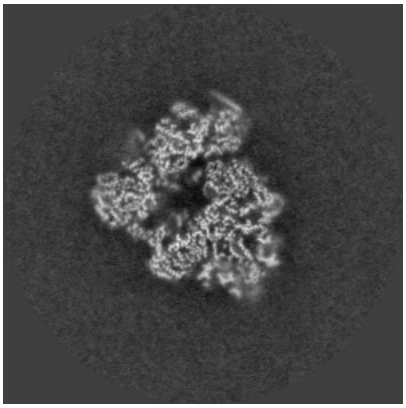
6.3.2 Raw map



X Index: 215



Y Index: 211



Z Index: 187

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

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

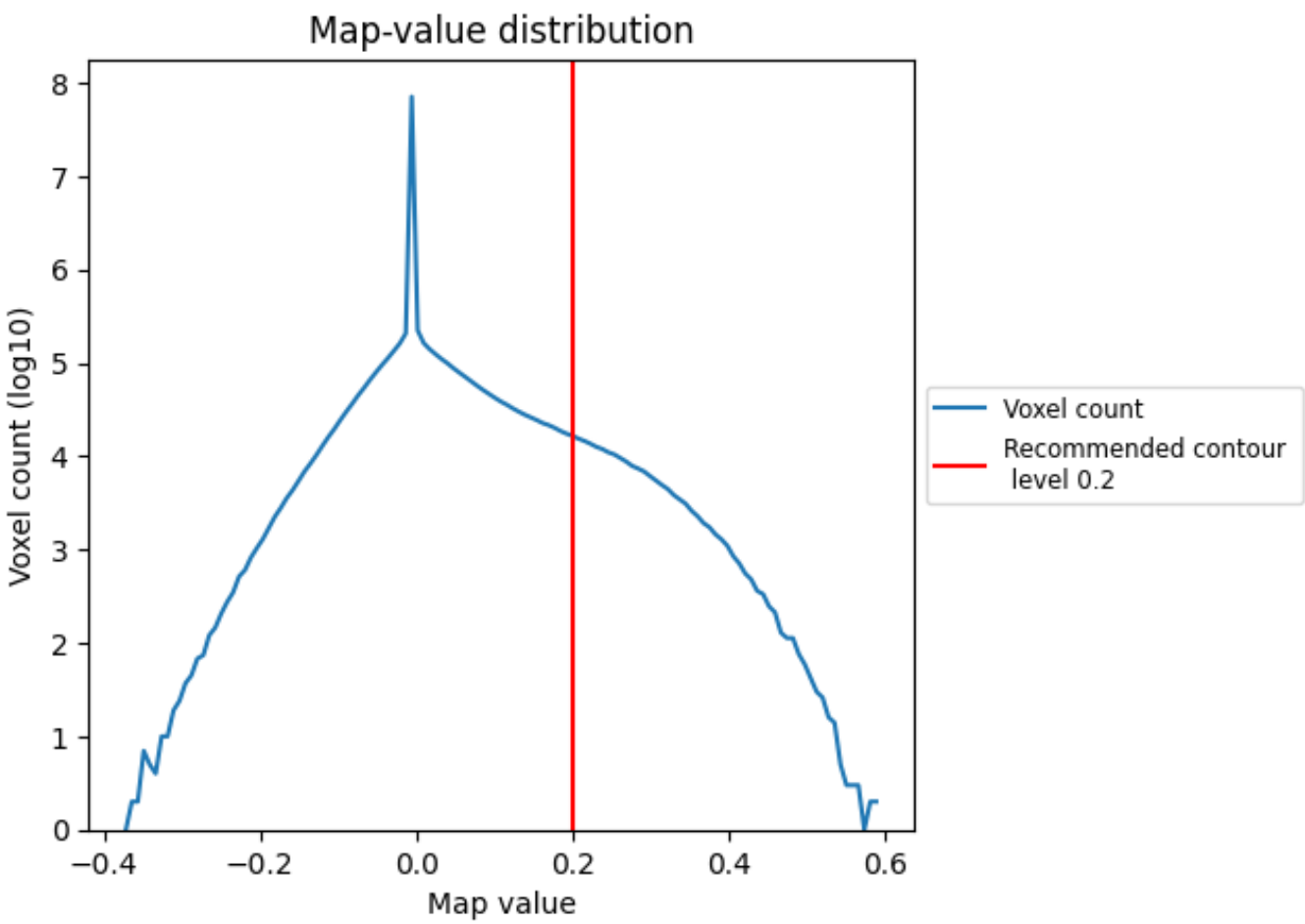
6.5 Mask visualisation (i)

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

7 Map analysis (i)

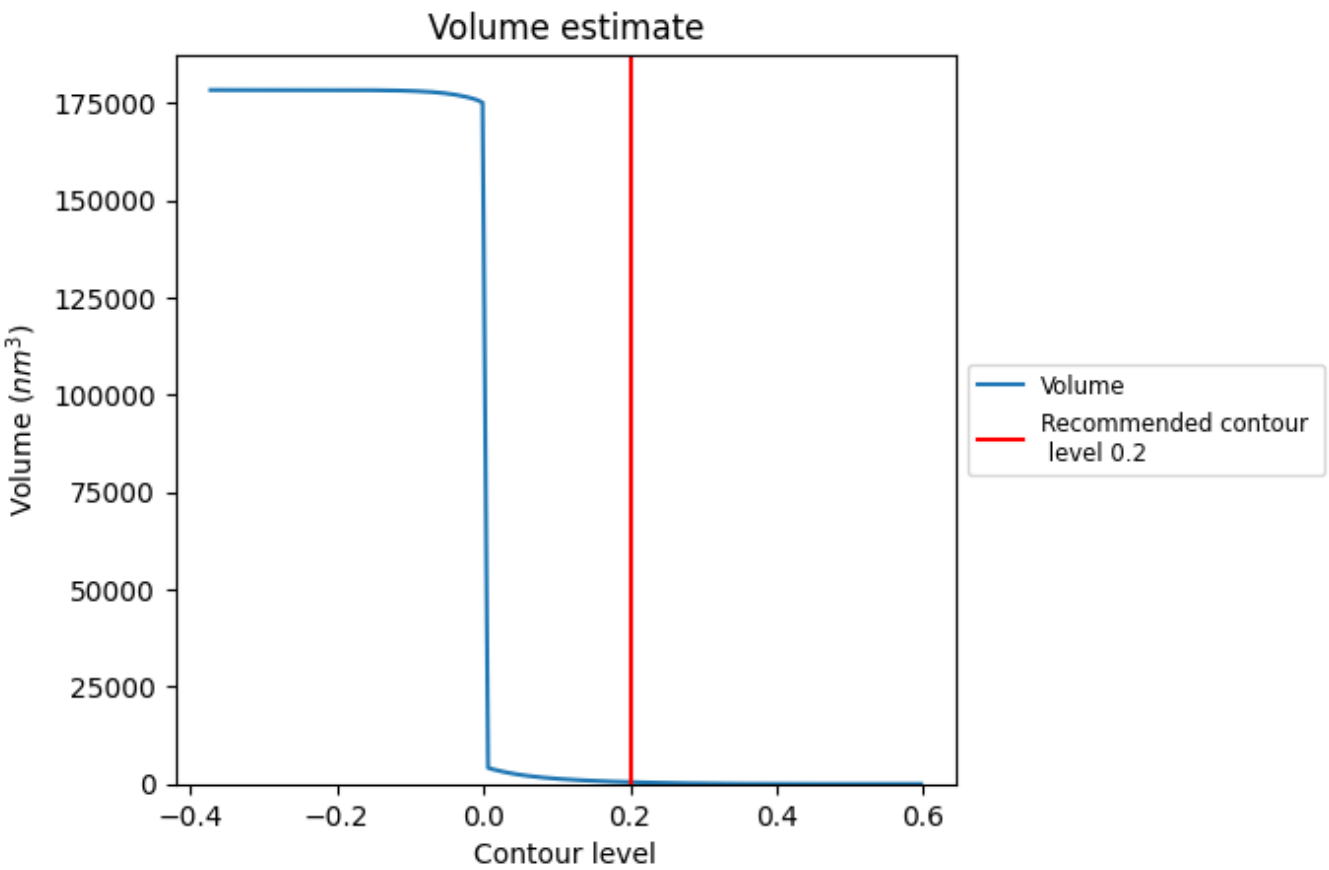
This section contains the results of statistical analysis of the map.

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.

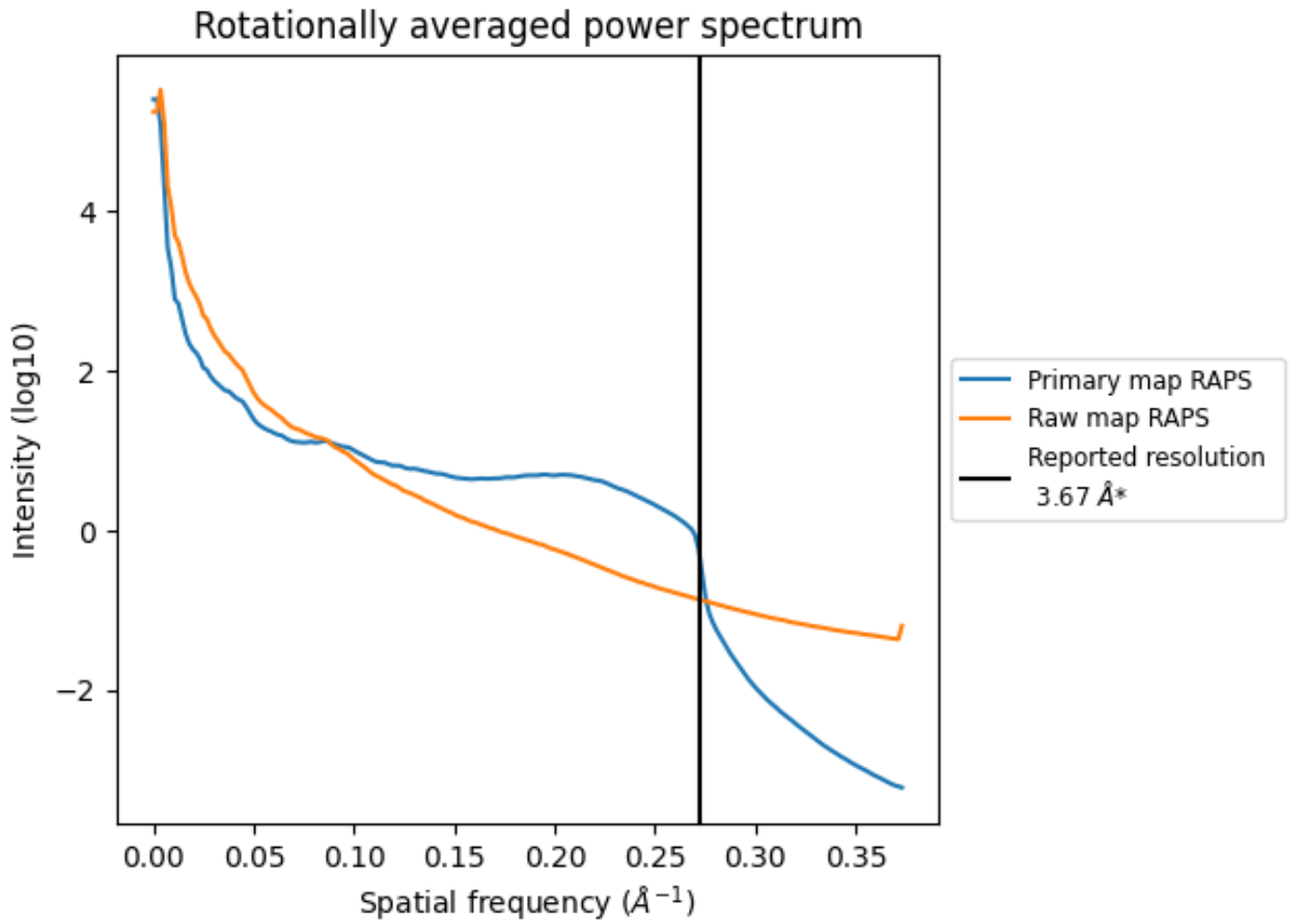
7.2 Volume estimate (i)



The volume at the recommended contour level is 470 nm^3; this corresponds to an approximate mass of 425 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)

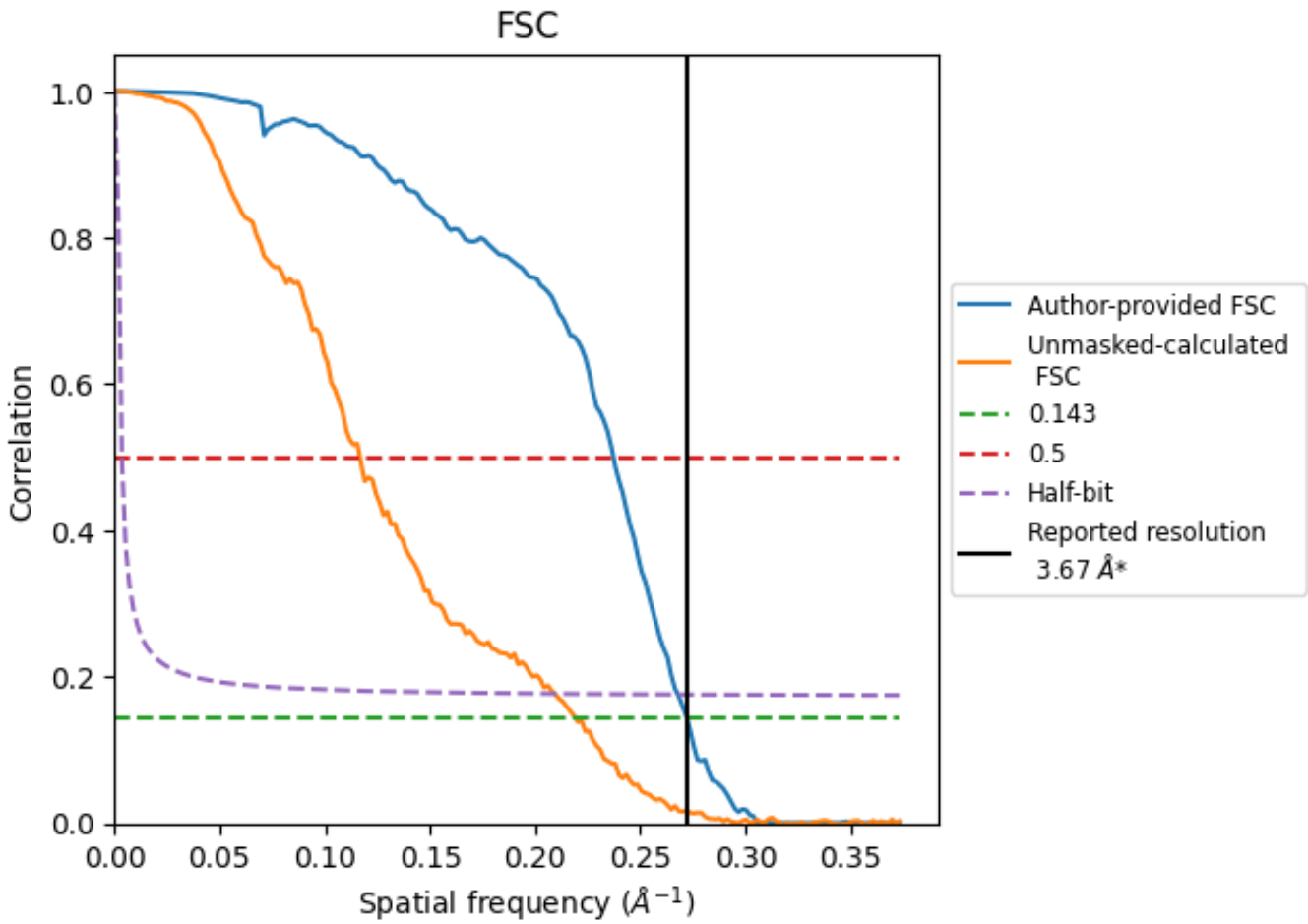


*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8.2 Resolution estimates (i)

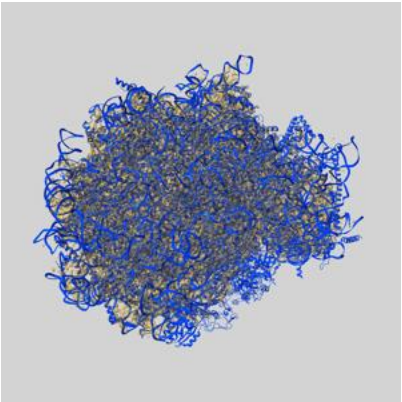
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.68	4.22	3.73
Unmasked-calculated*	4.56	8.57	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.56 differs from the reported value 3.67 by more than 10 %

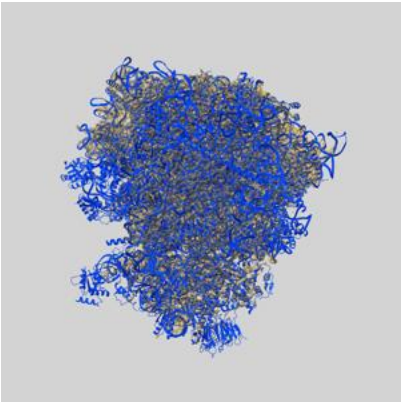
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4135 and PDB model 5LZX. Per-residue inclusion information can be found in section 3 on page 24.

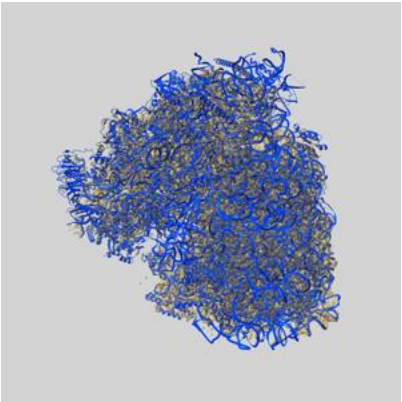
9.1 Map-model overlay (i)



X



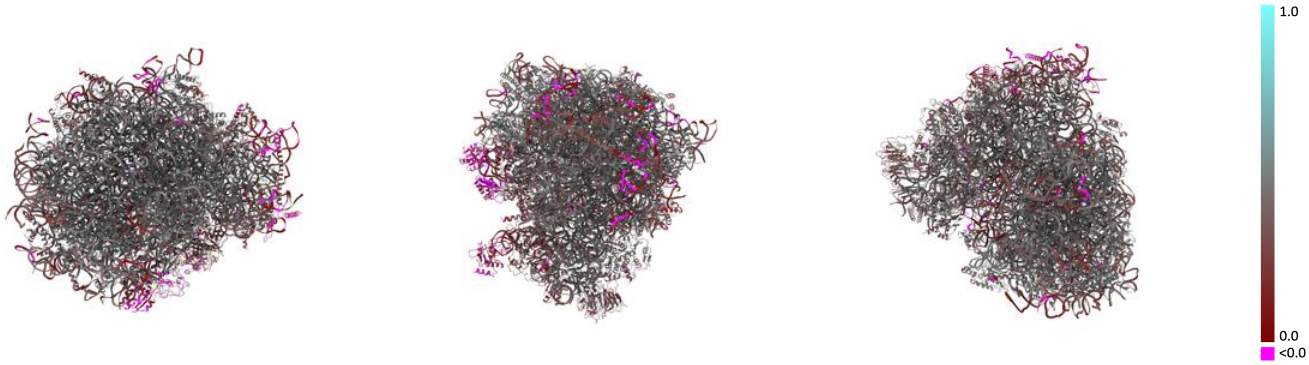
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

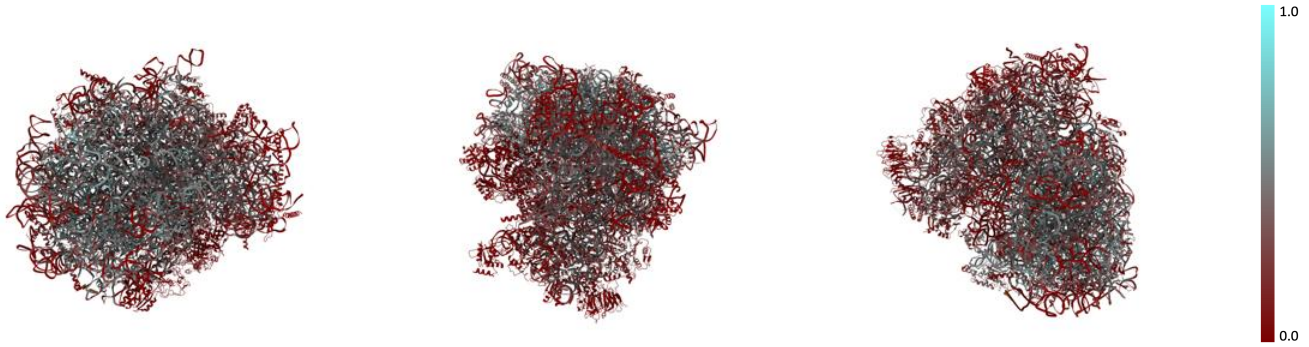
9.2 Q-score mapped to coordinate model (i)



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.

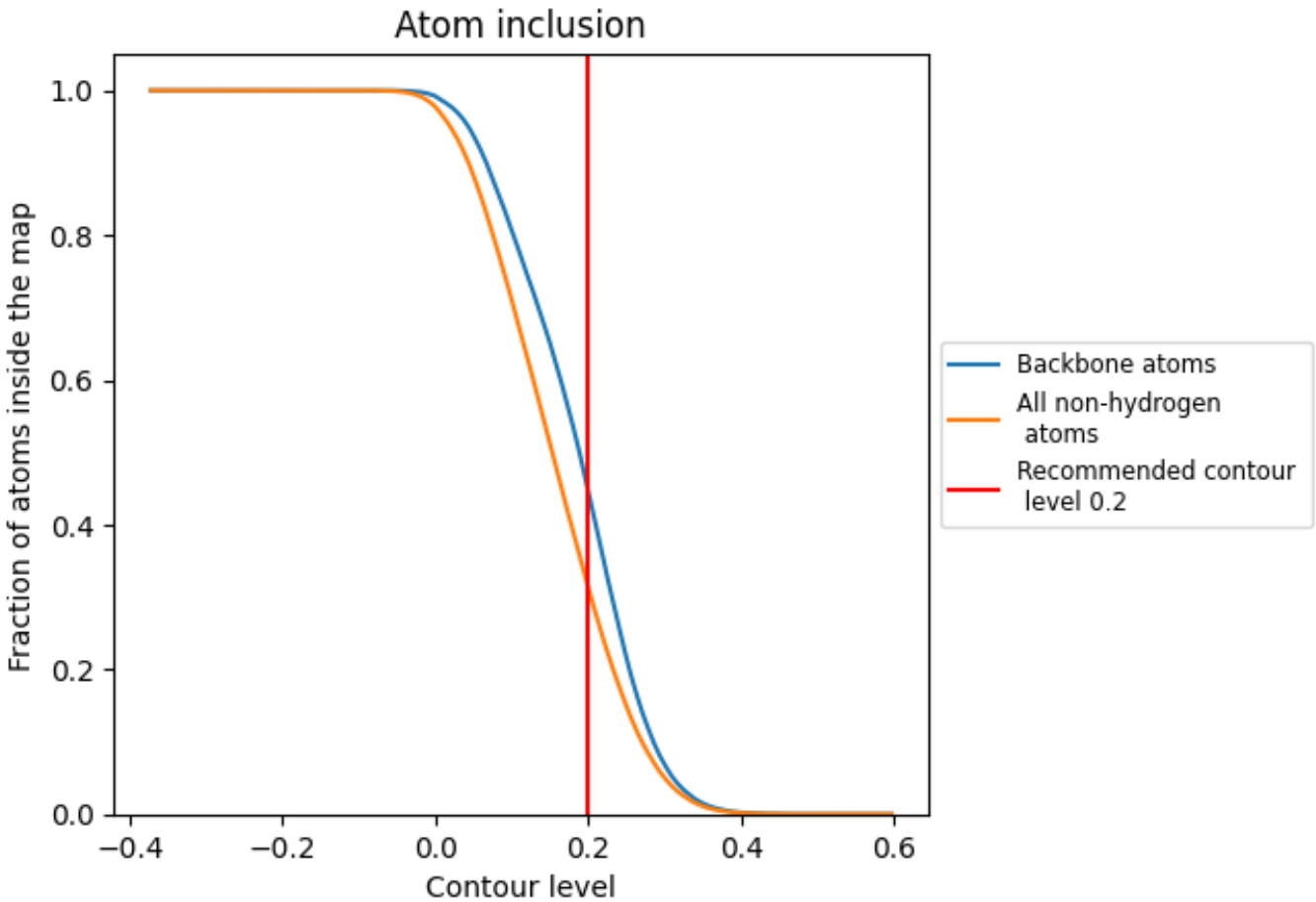
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 31% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3131	0.4050
1	0.0000	0.3250
2	0.0538	0.3660
3	0.0075	0.1760
5	0.3958	0.4120
7	0.5248	0.4510
8	0.4060	0.4200
9	0.3181	0.3880
A	0.3646	0.4720
AA	0.2379	0.4160
B	0.3875	0.4730
BB	0.2019	0.4280
C	0.3811	0.4740
CC	0.2452	0.4380
D	0.3471	0.4350
DD	0.1525	0.3810
E	0.3210	0.4500
EE	0.2519	0.4330
F	0.3980	0.4720
FF	0.2060	0.4190
G	0.2630	0.3960
GG	0.1030	0.3310
H	0.3566	0.4640
HH	0.0869	0.3570
I	0.3585	0.4720
II	0.2090	0.4060
J	0.2559	0.4210
JJ	0.2437	0.4220
KK	0.0595	0.3480
L	0.3303	0.4360
LL	0.2789	0.4420
M	0.4076	0.4580
MM	0.0022	0.1070
N	0.3914	0.4820
NN	0.2333	0.4380

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Chain	Atom inclusion	Q-score
O	0.4274	0.4750
OO	0.2158	0.4430
P	0.4354	0.4800
PP	0.0528	0.3320
Q	0.3497	0.4760
QQ	0.1658	0.4230
R	0.2991	0.4090
RR	0.1667	0.3970
S	0.4070	0.4850
SS	0.0847	0.3710
T	0.3389	0.4660
TT	0.1453	0.3910
U	0.2048	0.4060
UU	0.1344	0.3690
V	0.3100	0.4710
VV	0.2026	0.4320
W	0.1853	0.3140
WW	0.2871	0.4480
X	0.2947	0.4460
XX	0.2530	0.4640
Y	0.3840	0.4490
YY	0.1998	0.4080
Z	0.3141	0.4470
ZZ	0.0995	0.3660
a	0.4119	0.4850
aa	0.2583	0.4360
b	0.1988	0.3940
bb	0.1534	0.3990
c	0.3266	0.4310
cc	0.1638	0.3960
d	0.3734	0.4560
dd	0.1968	0.4330
e	0.3900	0.4840
ee	0.1221	0.3700
f	0.4442	0.4990
ff	0.0000	0.0990
g	0.3065	0.4530
gg	0.0422	0.3420
h	0.2993	0.4290
hh	0.0000	0.2580
i	0.2827	0.4220
ii	0.0249	0.3070

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Chain	Atom inclusion	Q-score
j	0.3205	0.4790
jj	0.0372	0.3130
k	0.1562	0.3940
l	0.3162	0.4710
m	0.3582	0.4670
n	0.0229	0.4110
o	0.3184	0.4640
p	0.3266	0.4500
r	0.4295	0.4860
s	0.0007	0.0370
t	0.0000	0.0010