



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:12 AM UTC

PDB ID : 5LZX / pdb_00005lzx
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

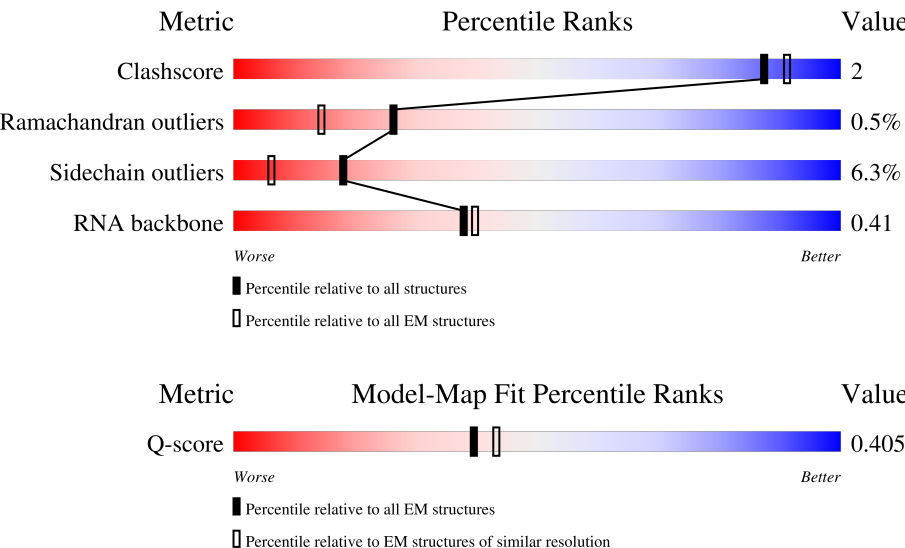
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11424 (3.17 - 4.17)

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

Mol	Chain	Length	Quality of chain
1	A	257	56% 81% 14% • •
2	B	403	53% 87% 11% •
3	C	425	48% 77% 8% • 15%

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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	7	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	8	
86	ii	403	
87	jj	710	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	m	200	-	-	X	-

2 Entry composition

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
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called Ul3.

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

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
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

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

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

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
5	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 6 is a protein called uL30.

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

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
7	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

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
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

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

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

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

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

- Molecule 26 is a protein called uL15.

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

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
27	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

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

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

- Molecule 35 is a protein called Ribosomal protein L37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

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

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

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

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

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

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

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

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

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
72	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

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

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

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

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

- Molecule 86 is a protein called Protein pelota homolog.

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

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
87	jj	425	Total	C	N	O	S	0	0
			3292	2100	565	609	18		

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 (CCD ID: MG) (formula: Mg).

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

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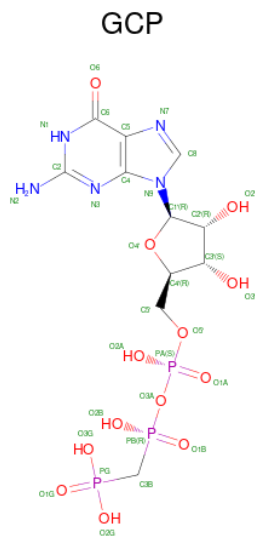
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Mol	Chain	Residues	Atoms		AltConf
88	g	1	Total 1	Mg 1	0
88	j	1	Total 1	Mg 1	0
88	5	176	Total 176	Mg 176	0
88	7	5	Total 5	Mg 5	0
88	8	6	Total 6	Mg 6	0
88	9	66	Total 66	Mg 66	0
88	jj	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

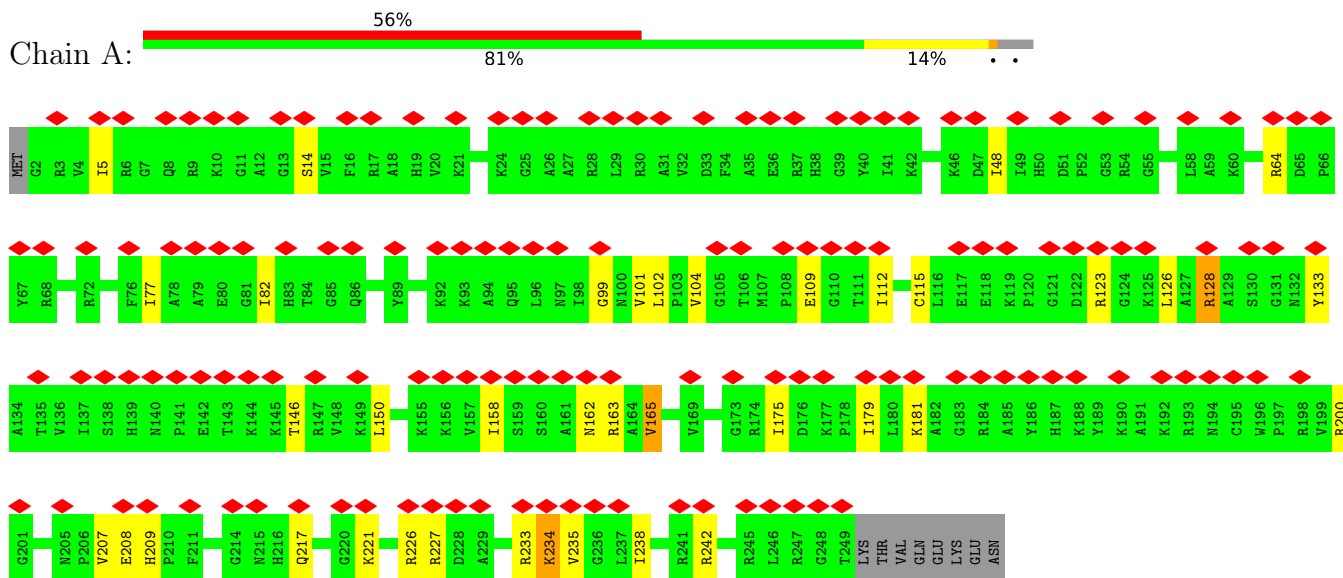


Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

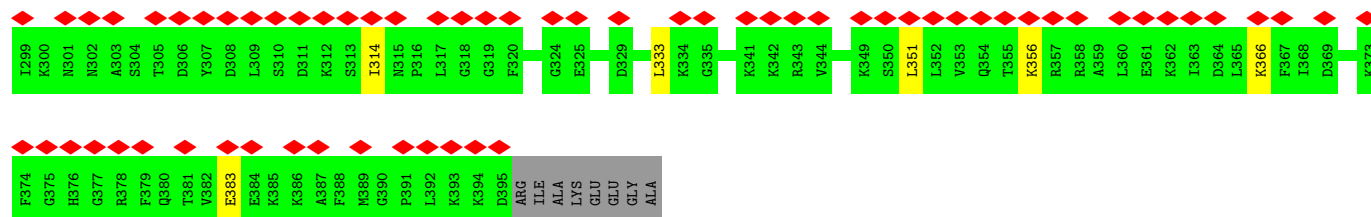
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: uL2

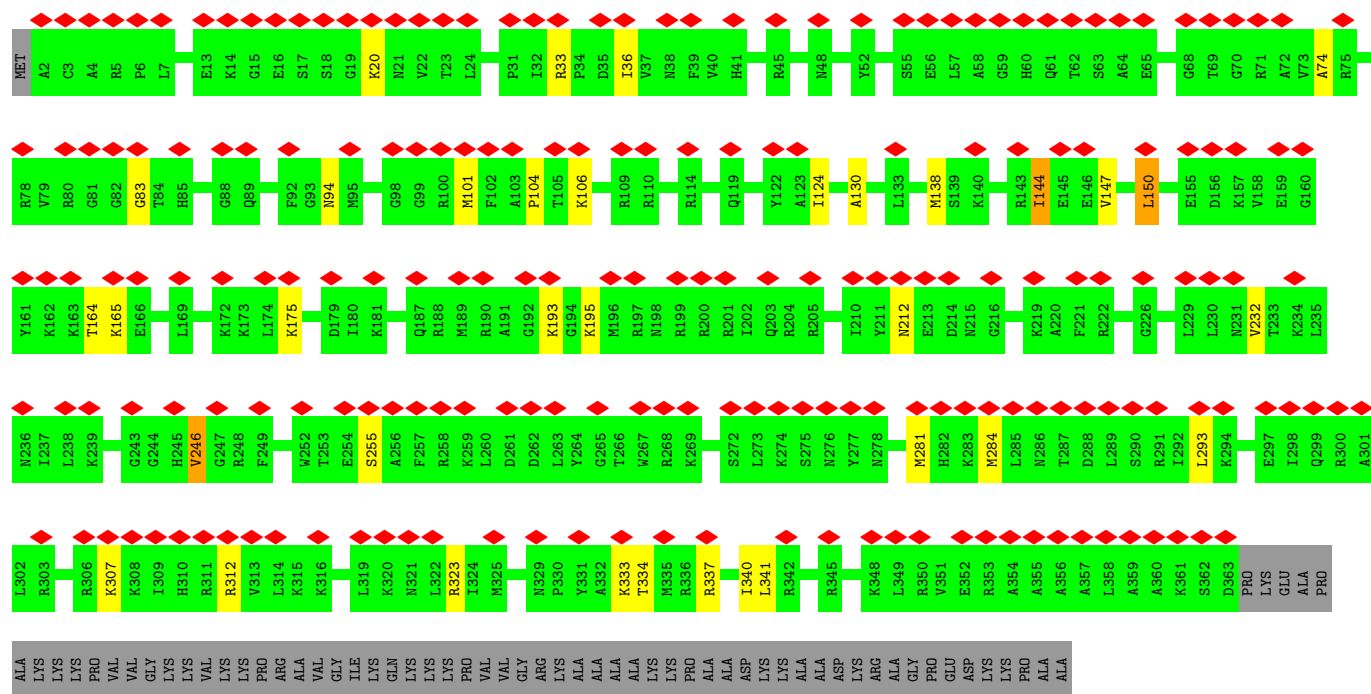
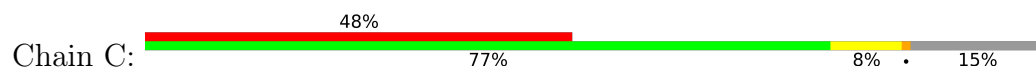


• Molecule 2: U13

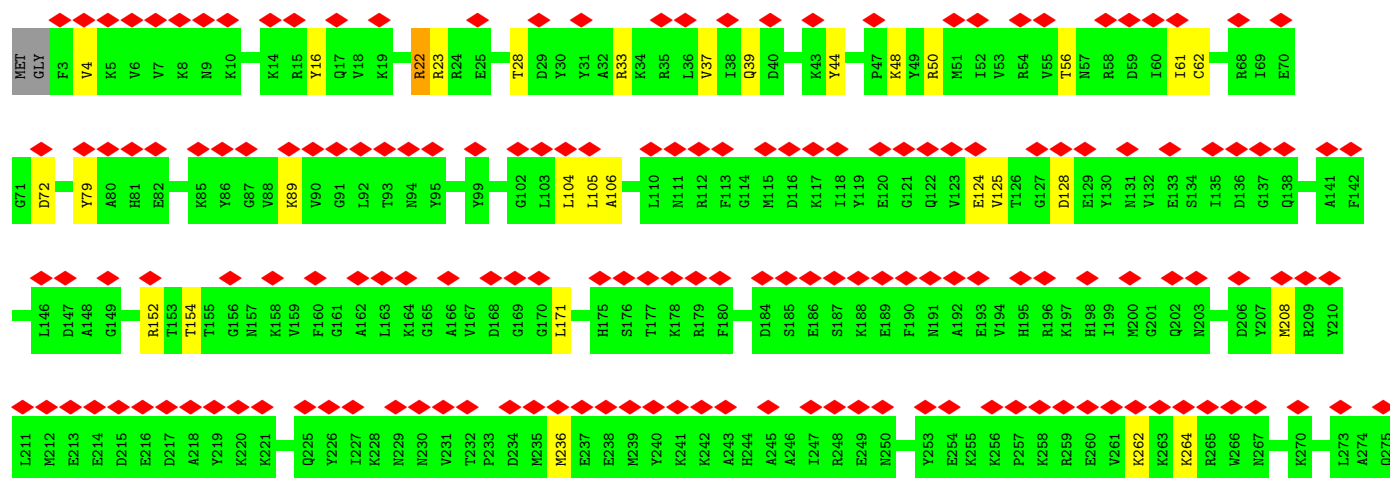
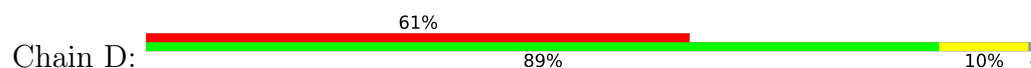


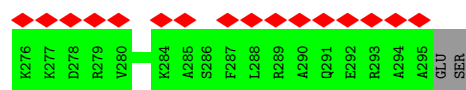


• Molecule 3: uL4

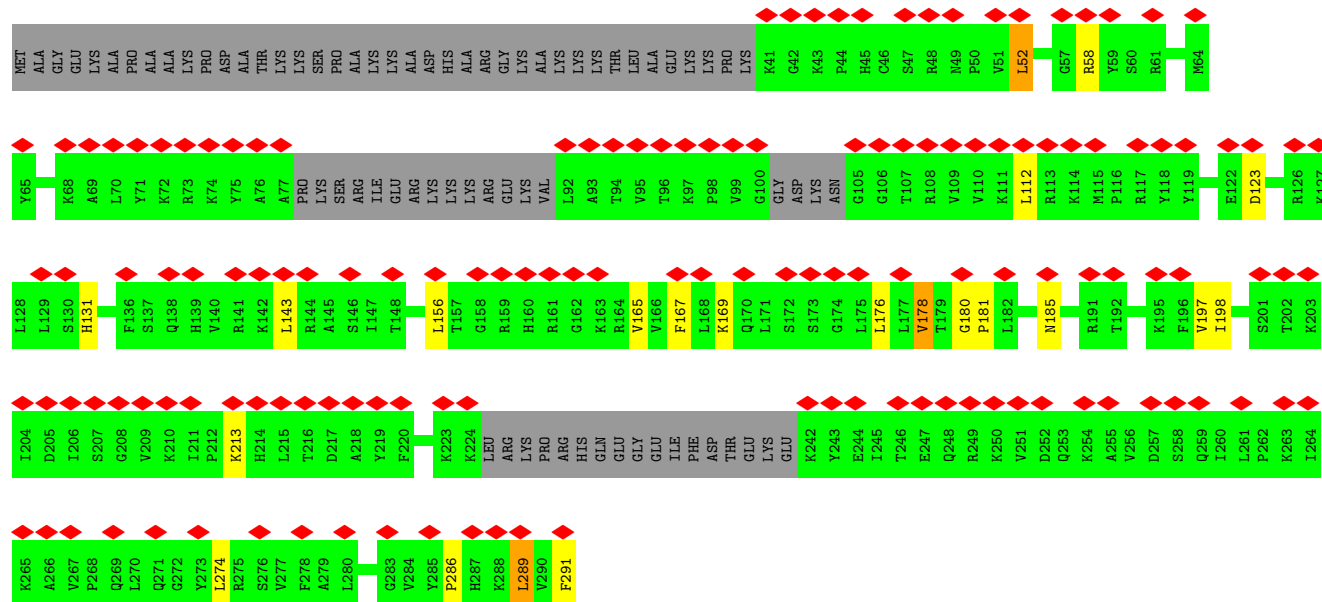


• Molecule 4: 60S ribosomal protein L5

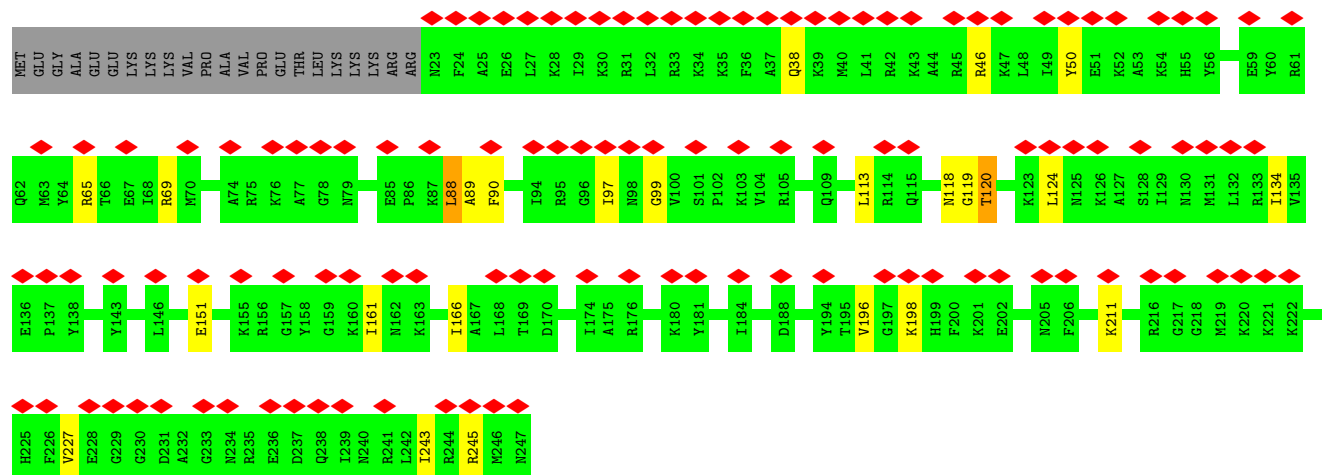
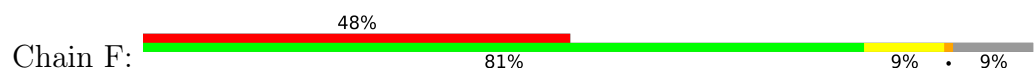




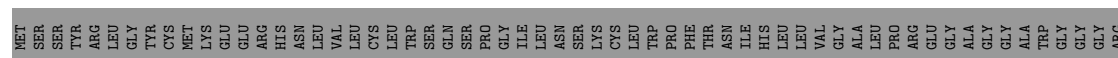
• Molecule 5: 60S ribosomal protein L6

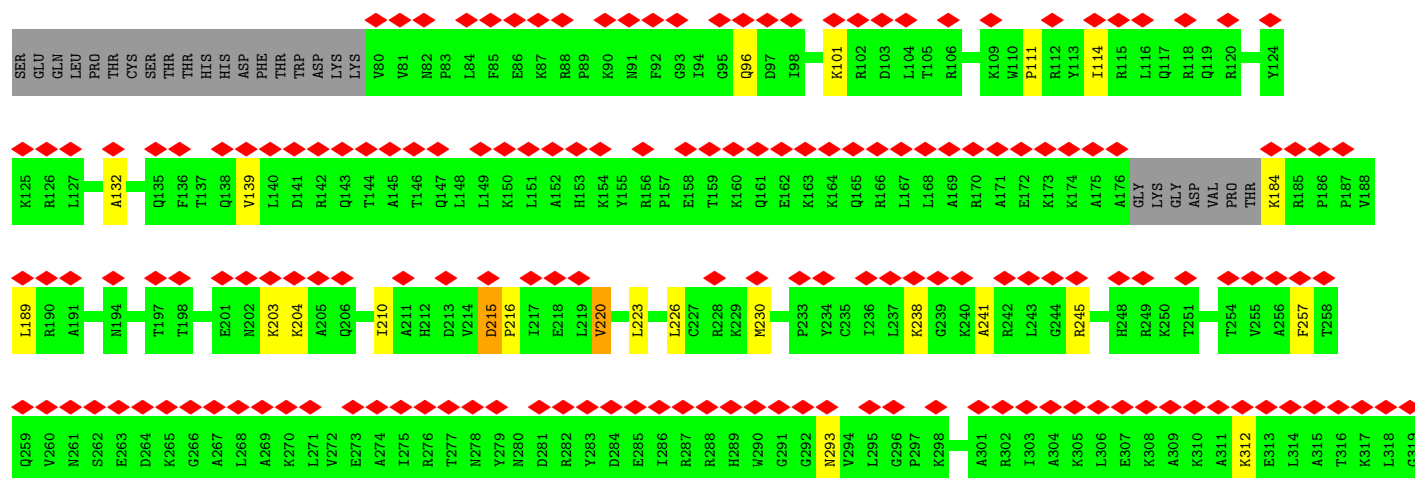


• Molecule 6: uL30

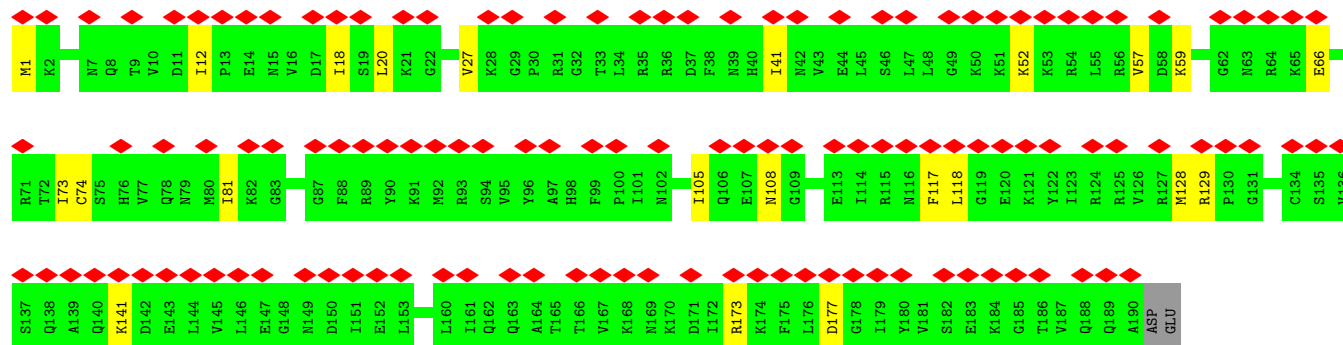
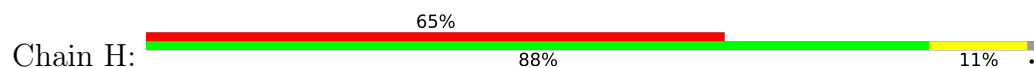


• Molecule 7: eL8

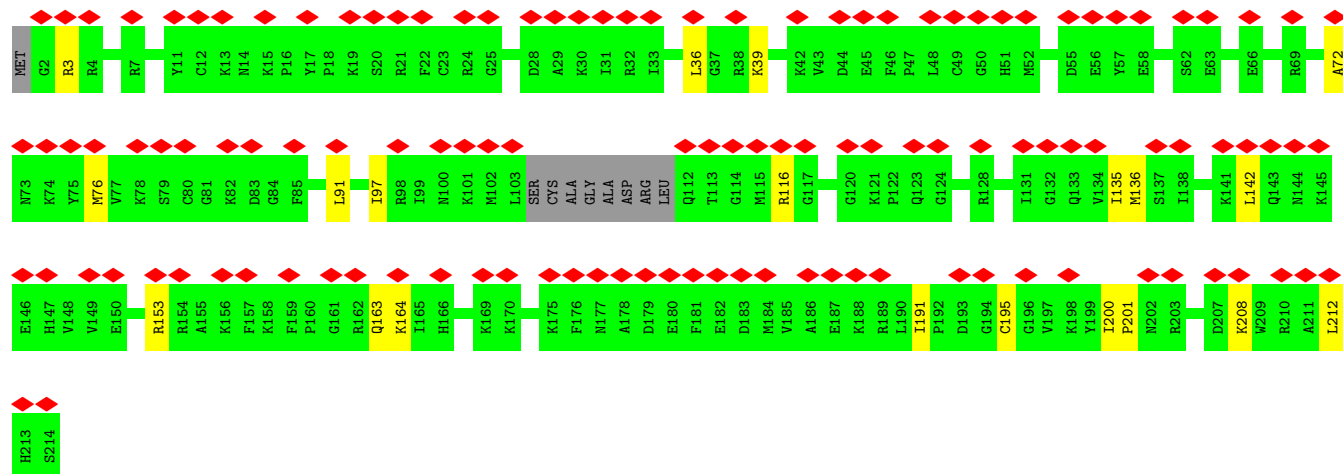
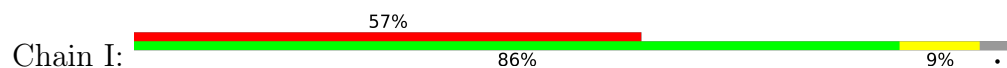




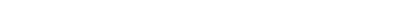
• Molecule 8: uL6

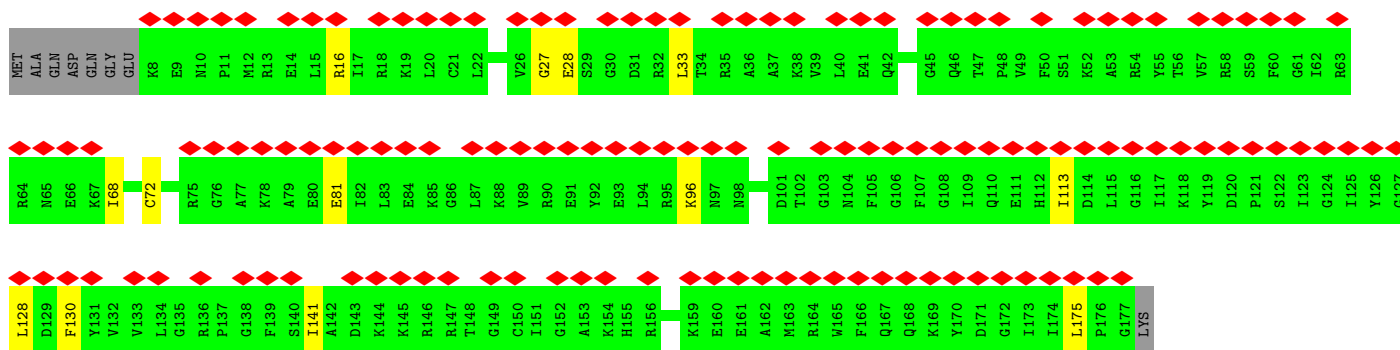


• Molecule 9: Ribosomal protein L10 (Predicted)

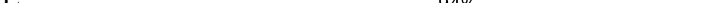


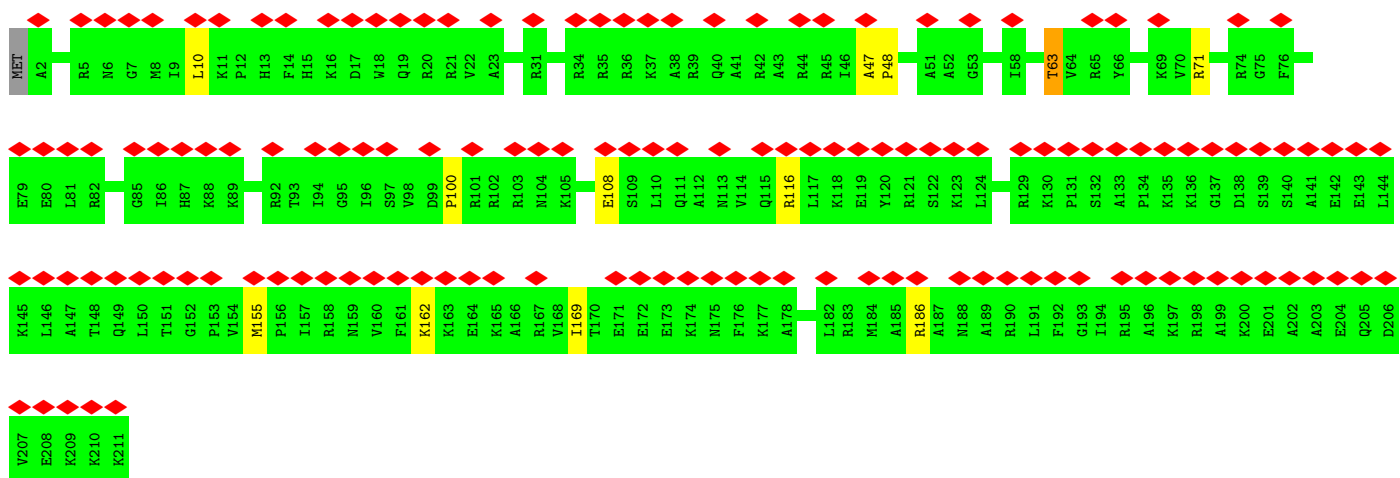
• Molecule 10: uL5

Chain J:  76% 88% 7%

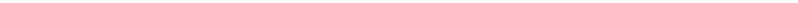


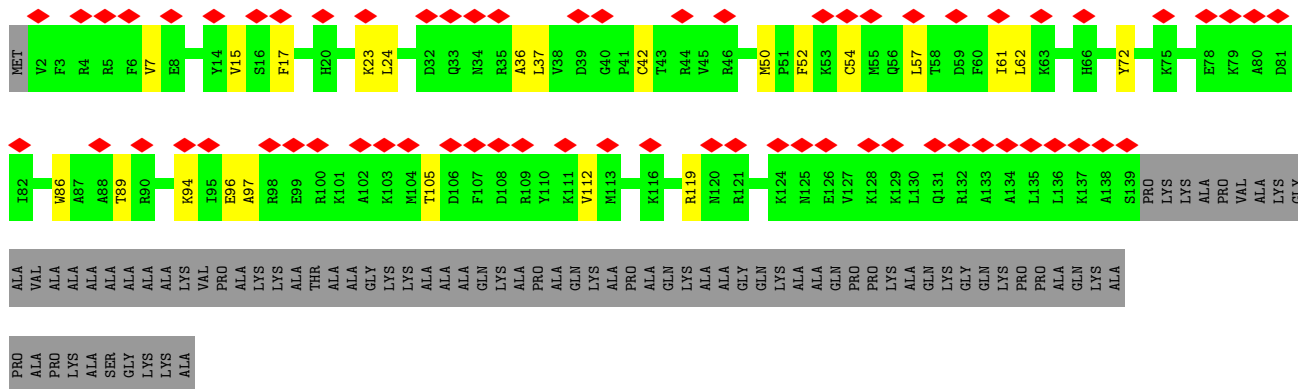
- Molecule 11: eL13

Chain L:  67% 94% 5%

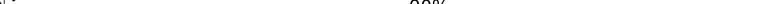


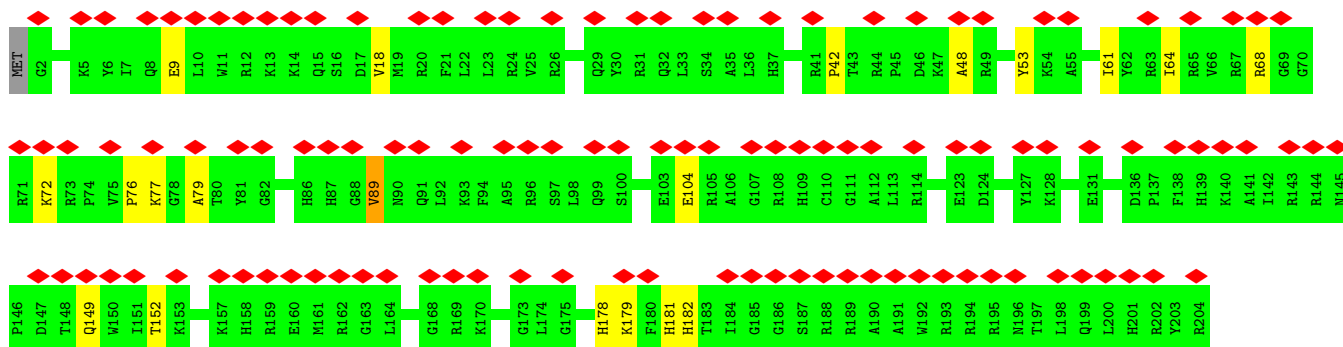
- Molecule 12: eL14

Chain M: 

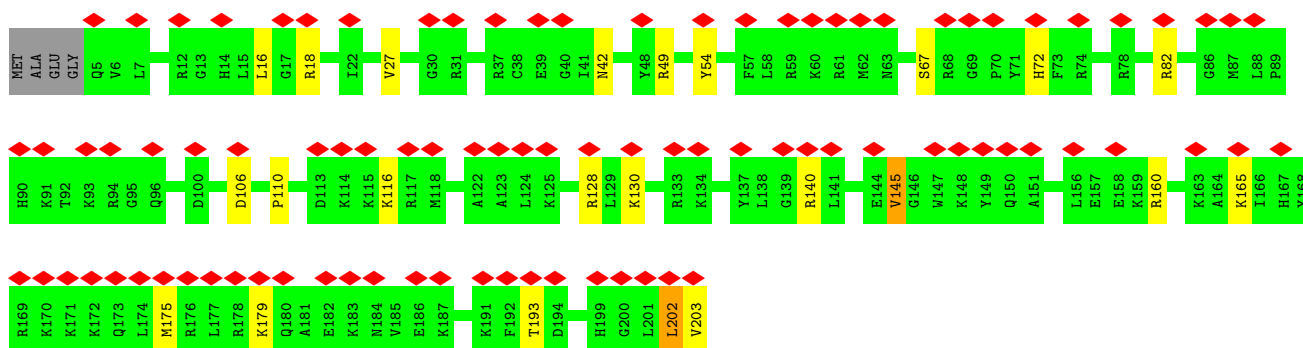
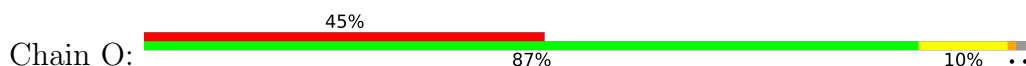


- Molecule 13: Ribosomal protein L15

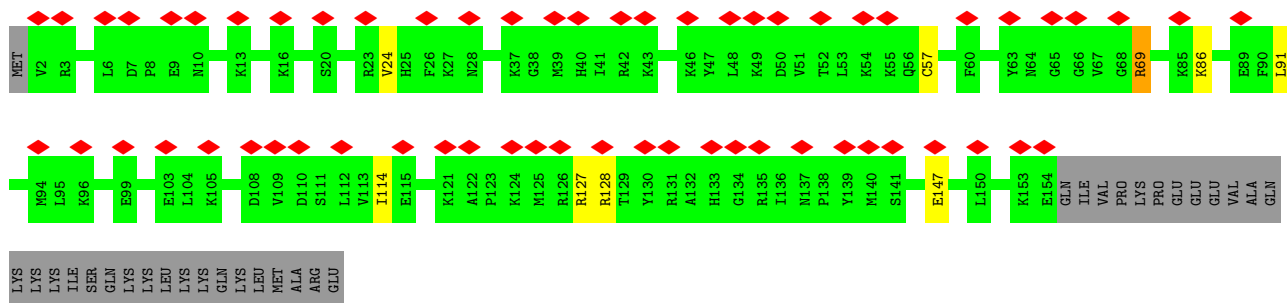
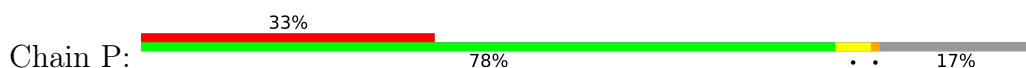
Chain N:  57% 90% 9%



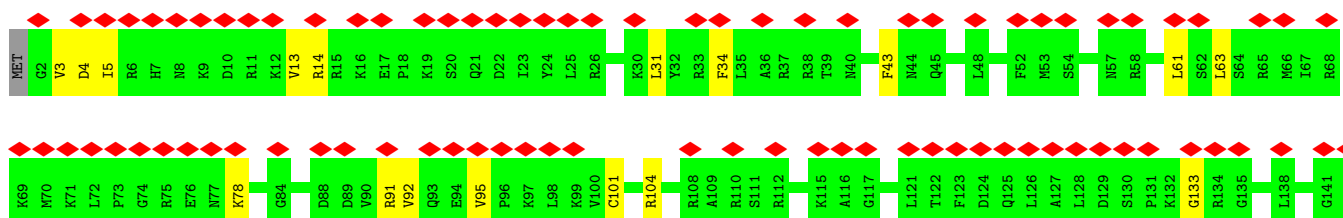
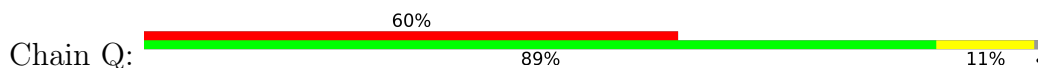
• Molecule 14: uL13

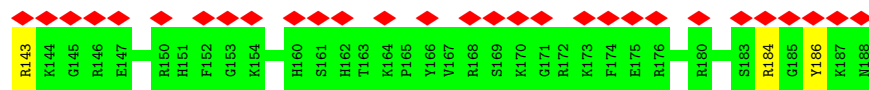


• Molecule 15: uL22

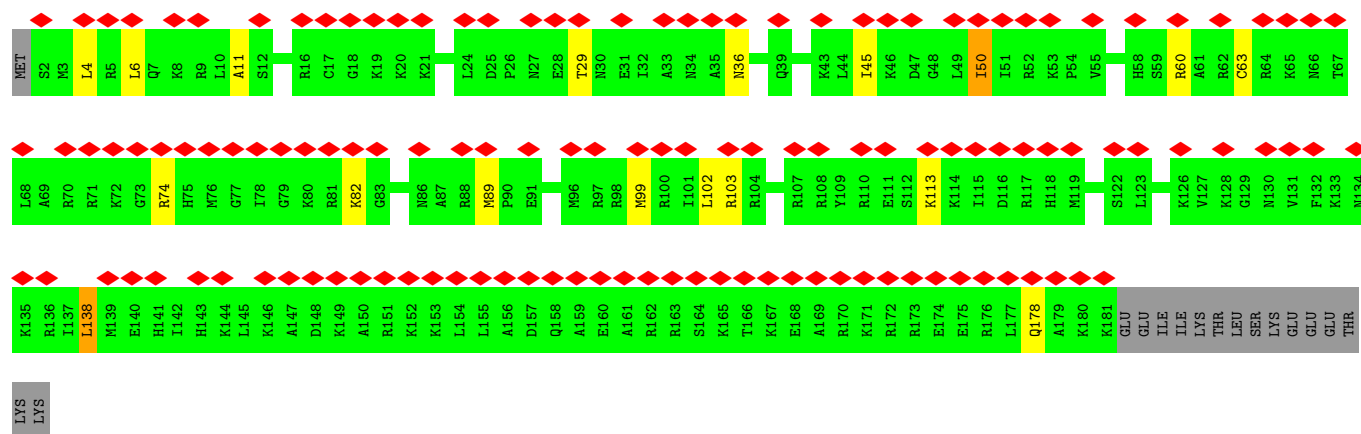
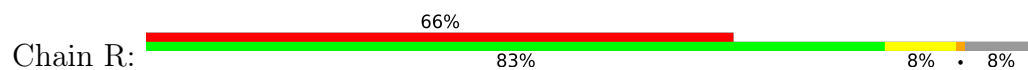


• Molecule 16: eL18

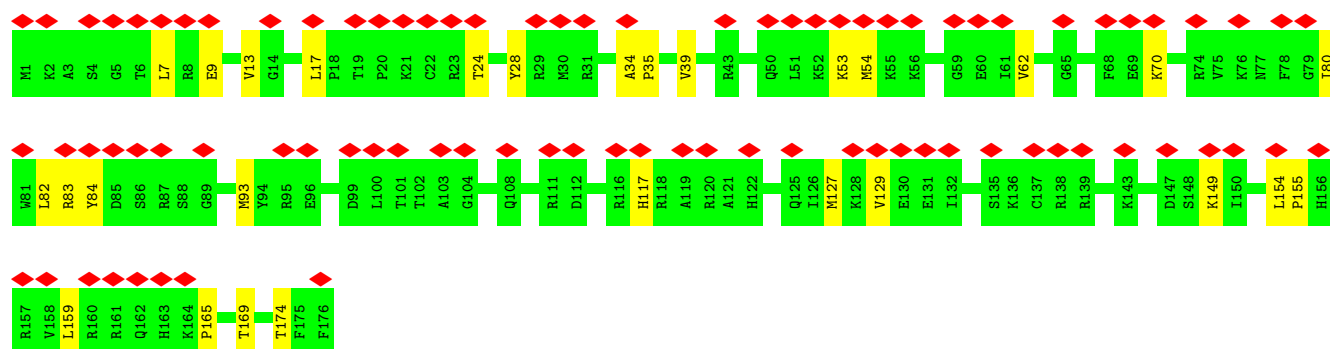
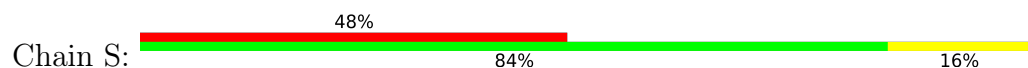




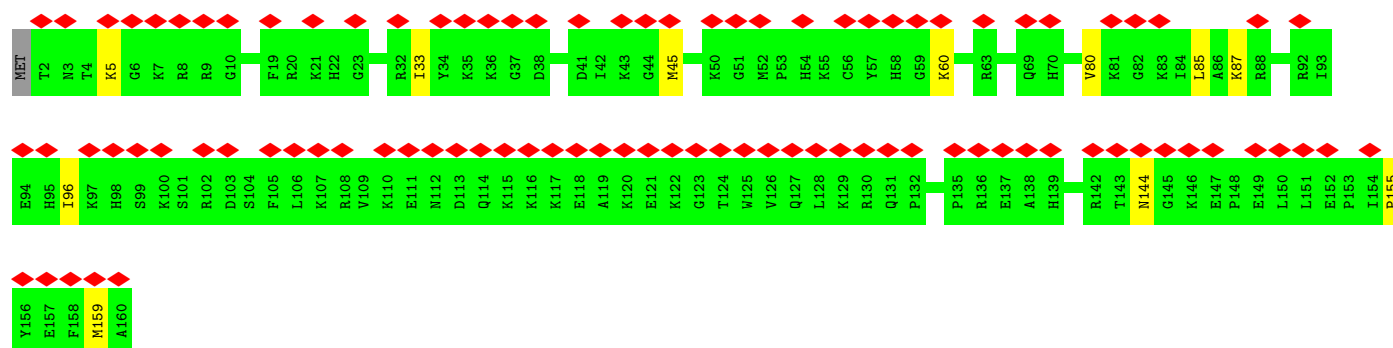
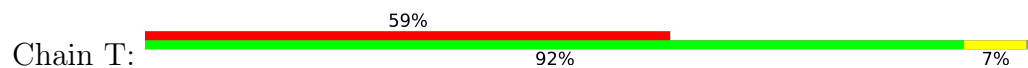
• Molecule 17: eL19



• Molecule 18: eL20

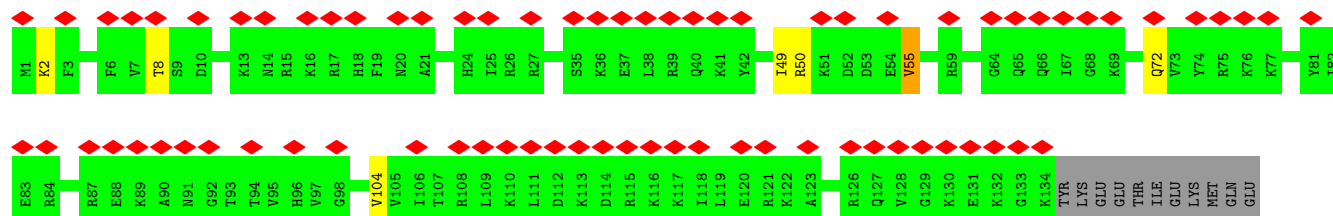
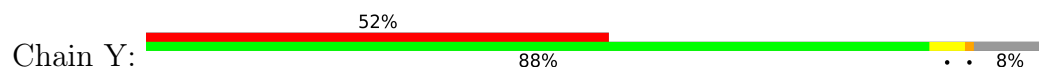


• Molecule 19: eL21

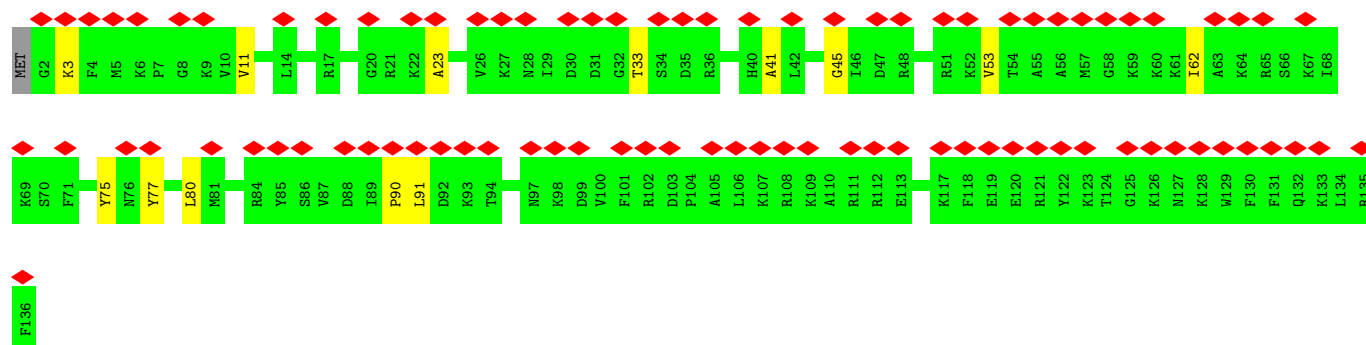
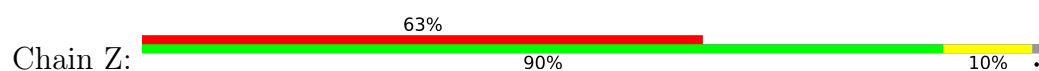




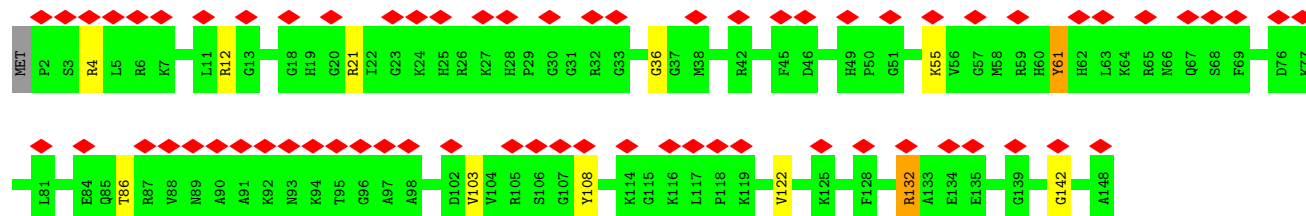
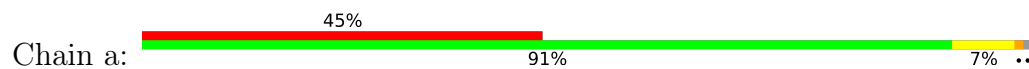
• Molecule 24: uL24



• Molecule 25: 60S ribosomal protein L27



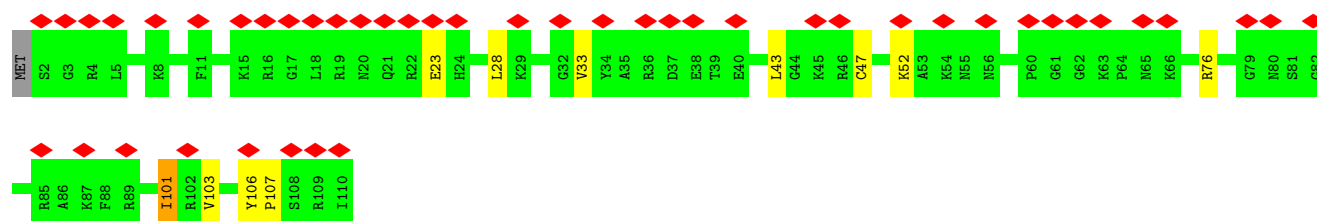
• Molecule 26: uL15



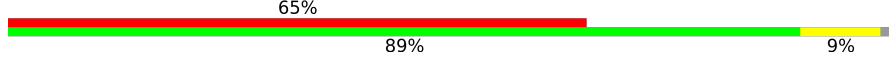
• Molecule 27: eL29

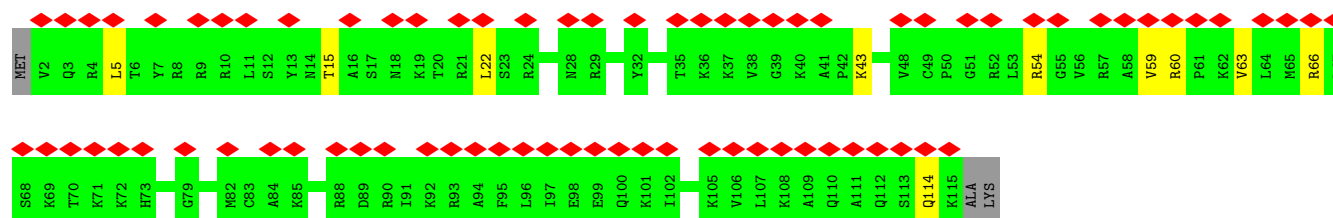


Chain f: 

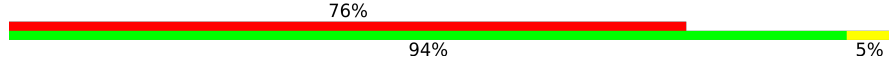


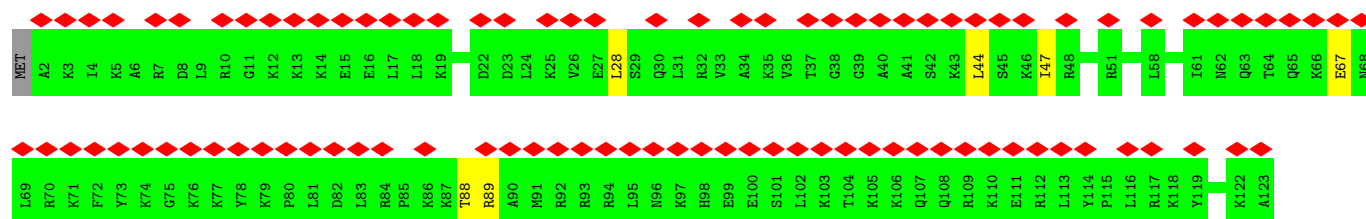
• Molecule 32: eL34

Chain g: 

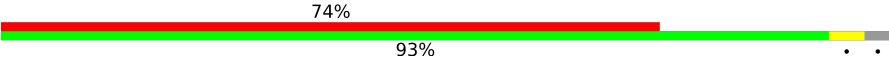


• Molecule 33: uL29

Chain h: 



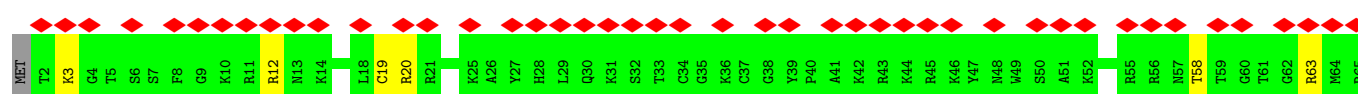
• Molecule 34: 60S ribosomal protein L36

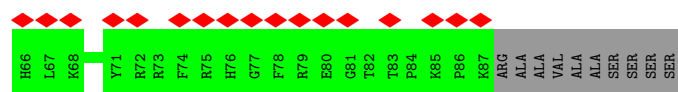
Chain i: 



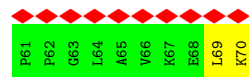
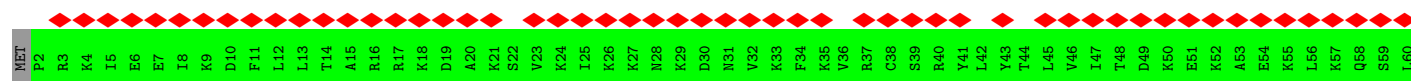
• Molecule 35: Ribosomal protein L37

Chain j: 

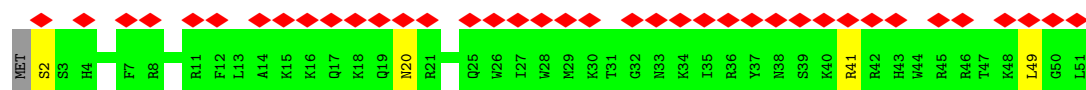
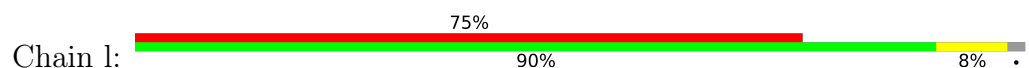




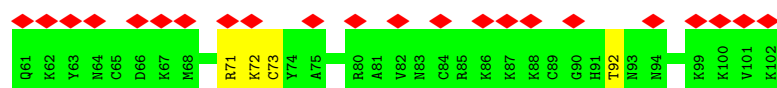
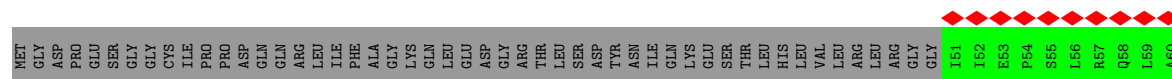
• Molecule 36: eL38



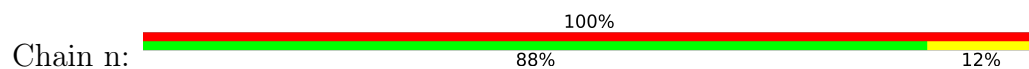
• Molecule 37: eL39



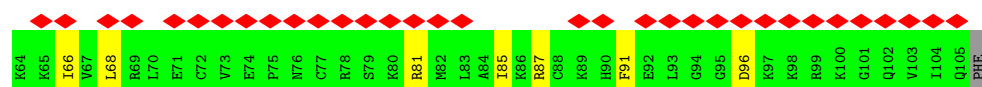
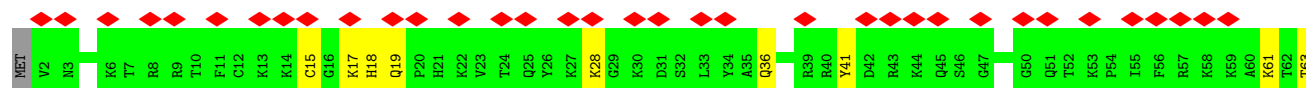
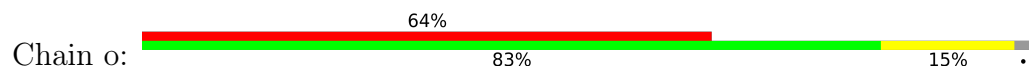
• Molecule 38: eL40



• Molecule 39: eL41



• Molecule 40: eL42

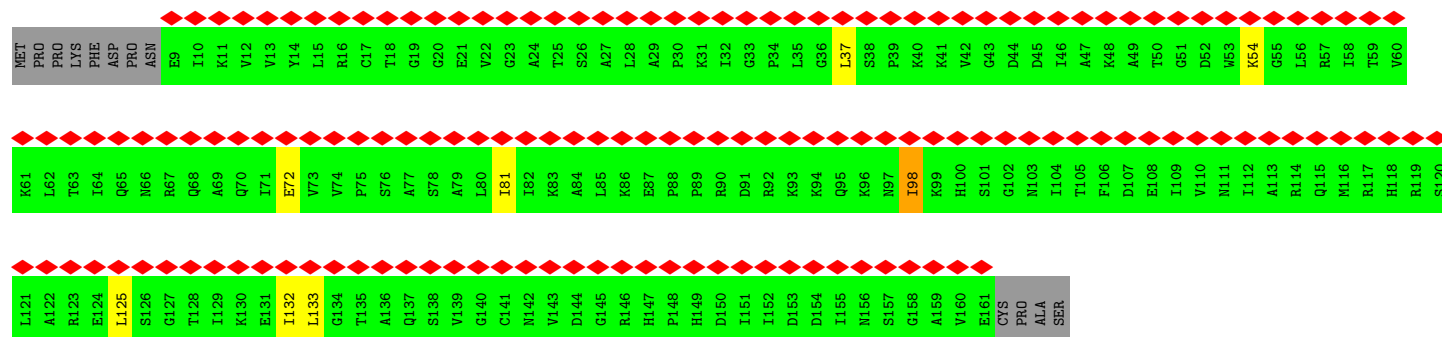


The diagram illustrates the human genome, showing chromosomes 1 through 22, X, and Y. Each chromosome is represented by a colored bar with its name and a list of genes. Red diamond markers indicate specific gene locations. The diagram is organized into two rows: the top row contains chromosomes 1-10, 12-18, 20-22, X, and Y; the bottom row contains chromosomes 11, 19, 21, and 22. The Y chromosome is shown as a small, dark green bar with a few genes.

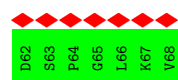
Chromosome	Gene
1	A76, V77, T78, V79, K90, A82, I83, I84, R85, L86, K87, E88, L89, K90, D91, Q92
2	A2, K3, R4, T5, K6, K7, V8, C9, I10, V11, G12
3	R17, Y18, G19
4	L22, R23, K24, M25, V26, K27, K28, I29, E30
5	Q33, H34, A35, K36, Y37, T38
6	F41
7	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
8	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
9	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
10	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
11	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
12	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
13	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
14	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
15	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
16	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
17	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
18	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
19	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
20	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
21	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
22	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
X	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69
Y	T45, K46, M47, K48, R49, R50, A51, V52, G53, I54, V55, H56, C57, G58, S59, C60, M61, V69

ALA	ILE	S181	V121	M61	MET
LYS	ILE	P182	T122	R62	PRO
GLU	ASN	F183	V123	K63	ARG
GLU	GLY	S184	P124	A64	GLU
GLU	TYR	F185	A125	I65	D5
GLU	ARG	G186	Q126	R66	R6
ASP	VAL	L187	N127	G67	A7
LEU	LEU	I188	T128	H68	T8
GLU	ALA	I189	G129	L69	W9
ASP	LEU	Q190	L130	E70	K10
MET	SER	Q191	G131	N71	S11
GLY	VAL	V192	P132	N72	N12
PHE	THR	F193	E133	F73	Y13
LEU	GLU	D194	K134	A74	F14
PHE	THR	N195	T135	L75	L15
PRO	PHE	G196	S136	E76	K16
LEU	PRO	S197	F137	K77	I17
ALA	ALA	I198	F138	L78	I18
GLU	GLY	Q199	G139	L79	Q19
LYS	LYS	N200	A140	P80	L20
VAL	VAL	PRO	L141	H81	L21
LYS	ALA	GLU	G142	I82	D22
ALA	PHE	LEU	I143	R83	D23
LEU	LEU	VAL	T144	G84	Y24
ALA	ALA	ASP	T145	N85	P25
PRO	ASP	ILE	K146	R86	K26
ASP	THR	THR	I147	G87	C27
ALA	ALA	GLU	S148	F88	F28
SER	PHE	ASP	R149	V89	I29
VAL	VAL	LEU	G150	P90	V30
ALA	ALA	HIS	T151	K91	G31
ALA	ALA	SER	I152	K92	A32
PRO	PRO	ARG	E153	E93	D33
GLY	VAL	LEU	I154	D94	N34
ALA	ALA	GLU	L155	L95	V35
ALA	ALA	GLY	S156	T96	G36
SER	SER	VAL	D157	E97	S37
THR	THR	ARG	V158	I98	K38
ALA	ALA	ASN	Q159	R99	Q39
ALA	ALA	ALA	L160	D100	M40
PRO	PRO	SER	I161	M101	Q41
ALA	ALA	VAL	K162	L102	Q42
ALA	ALA	CYS	T163	L103	I43
ALA	ALA	GLN	G164	A104	R44
ALA	ILE	GLY	D165	N105	M45
PRO	PRO	TYR	K166	K106	S46
ALA	LYS	PRO	V167	V107	L47
VAL	VAL	THR	Q168	P108	R48
GLU	ALA	VAL	A169	A109	G49
		SER	S170	A110	K50
		VAL	E171	A111	A51
		PRO	A172	R112	V52
		HIS	T173	A113	V53
		SER	L174	G114	L54
			L175	A115	M55
			N176	I116	G56
			M177	A117	K57
			L178	P118	N58
			N179	C119	T59
			I180	E120	M60

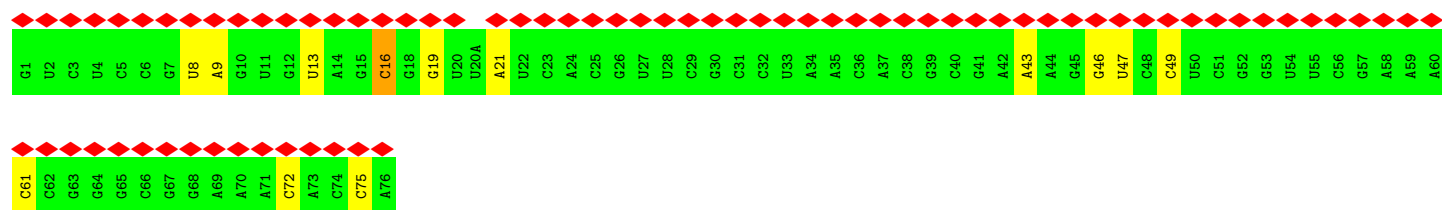
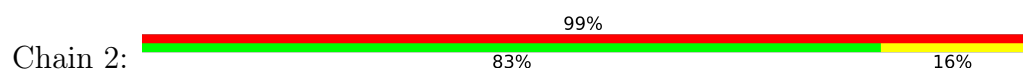
Chain t: 93% 88% 7%



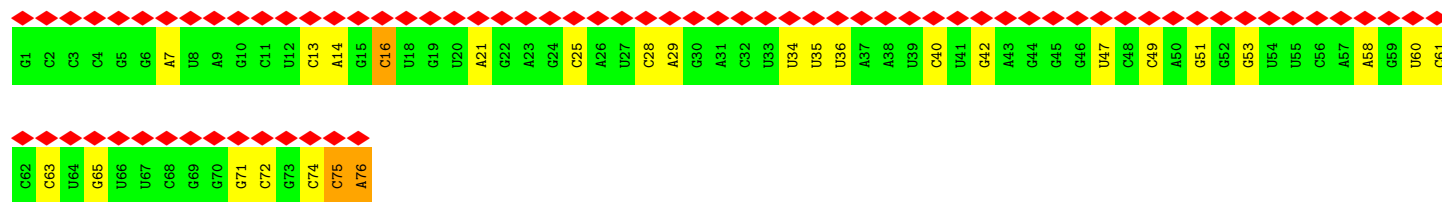
• Molecule 45: Nascent chain



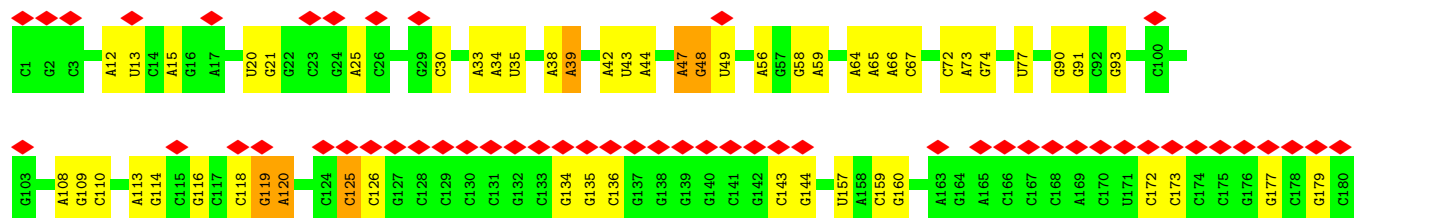
• Molecule 46: P-site tRNA

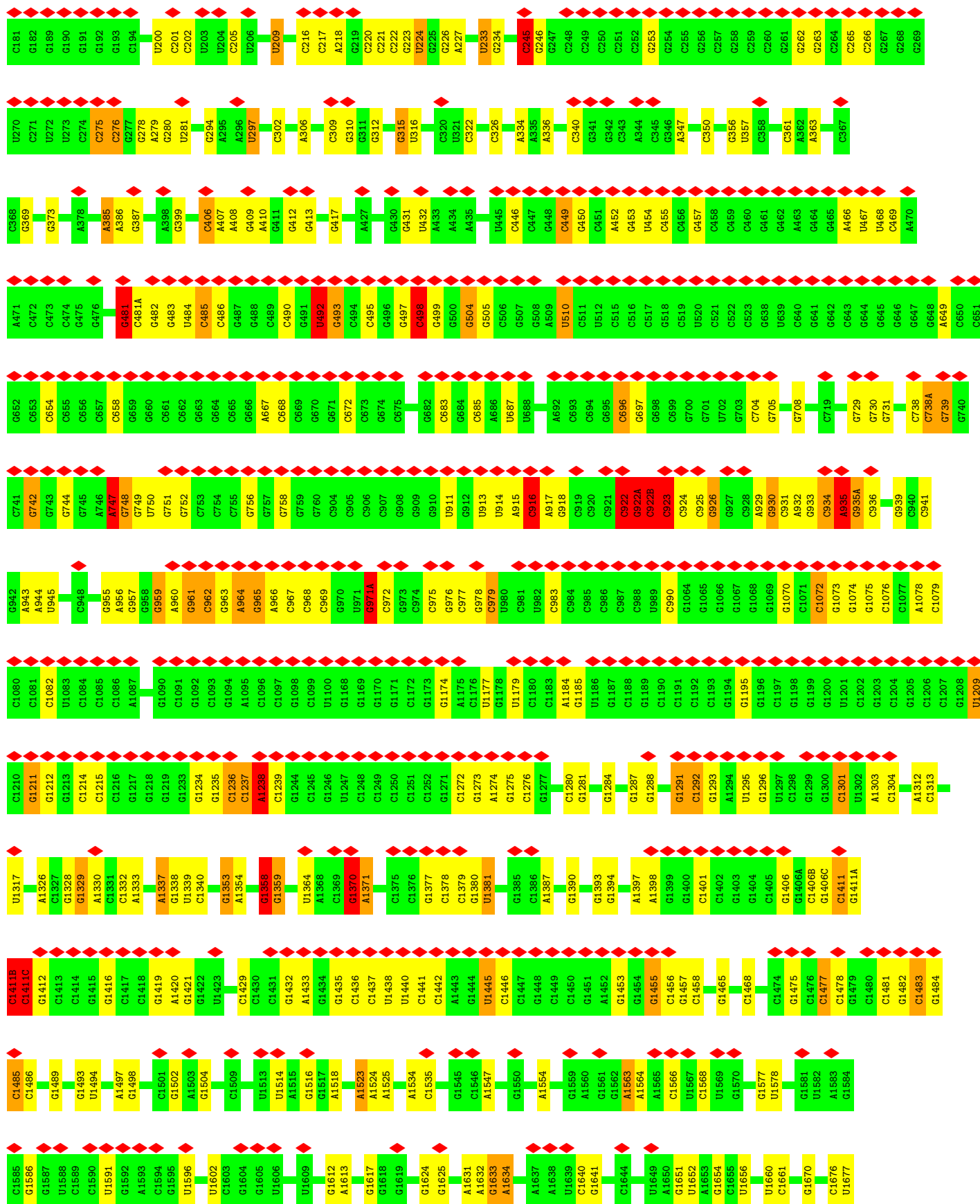


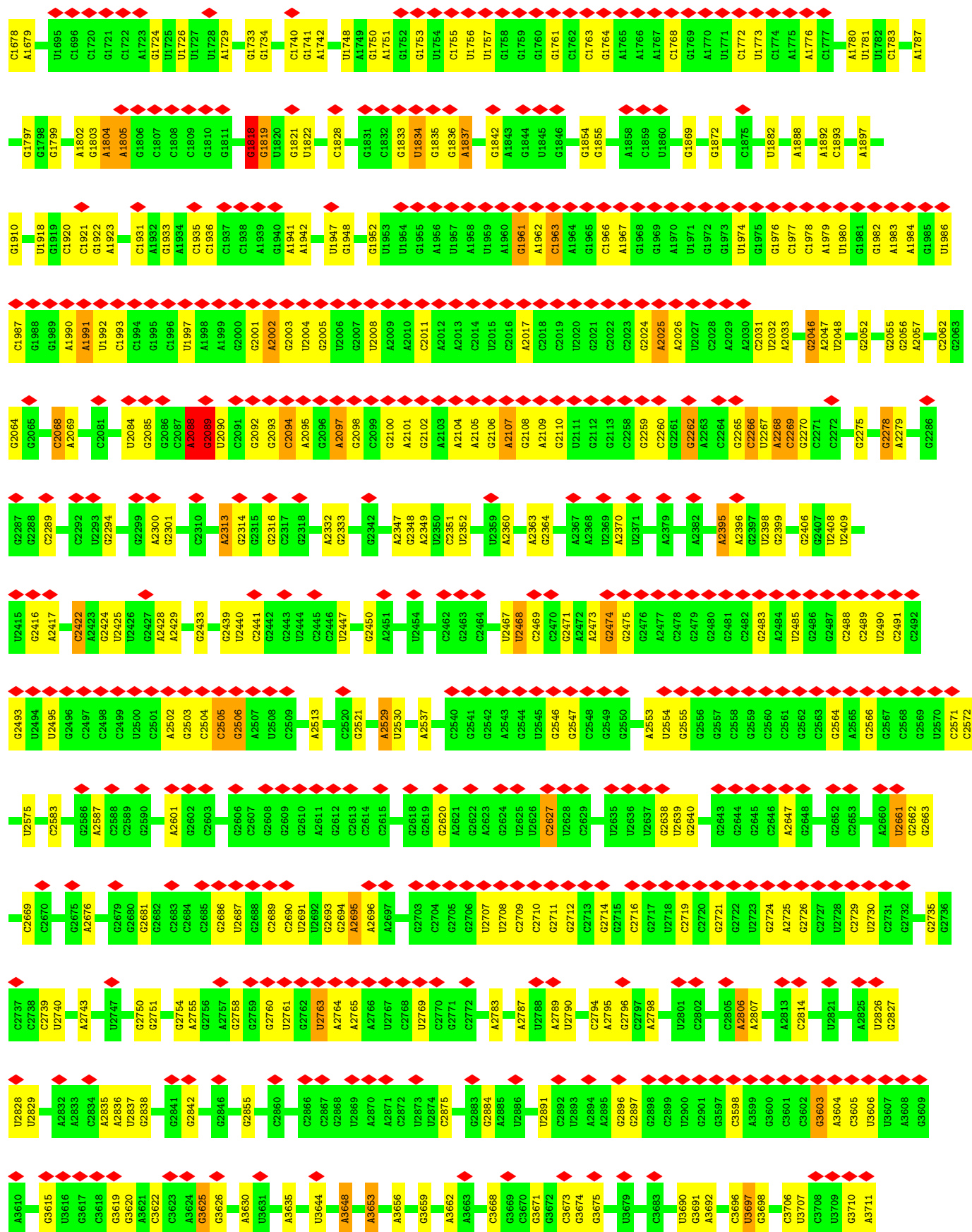
• Molecule 47: E-site tRNA



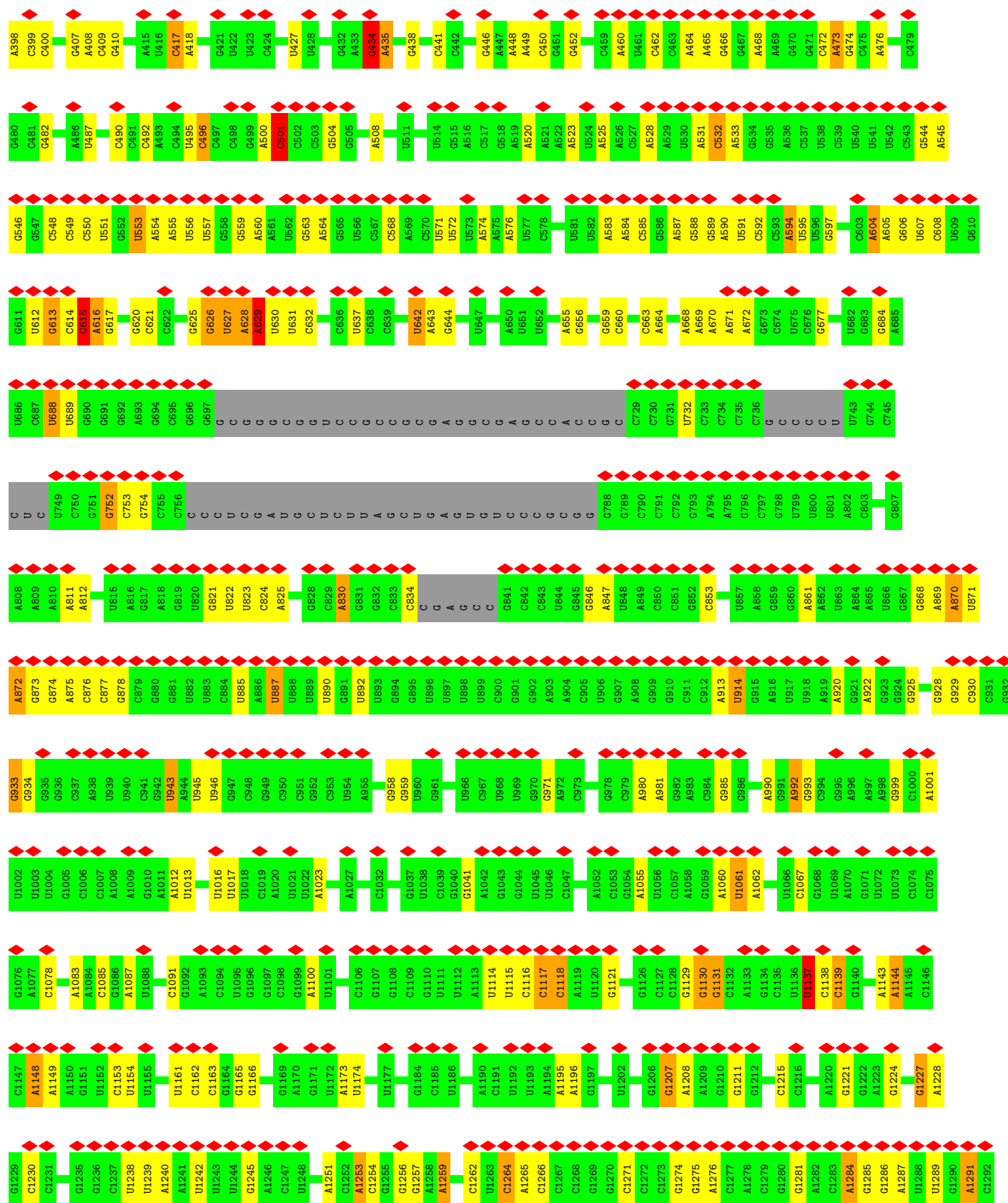
• Molecule 48: 28S ribosomal RNA

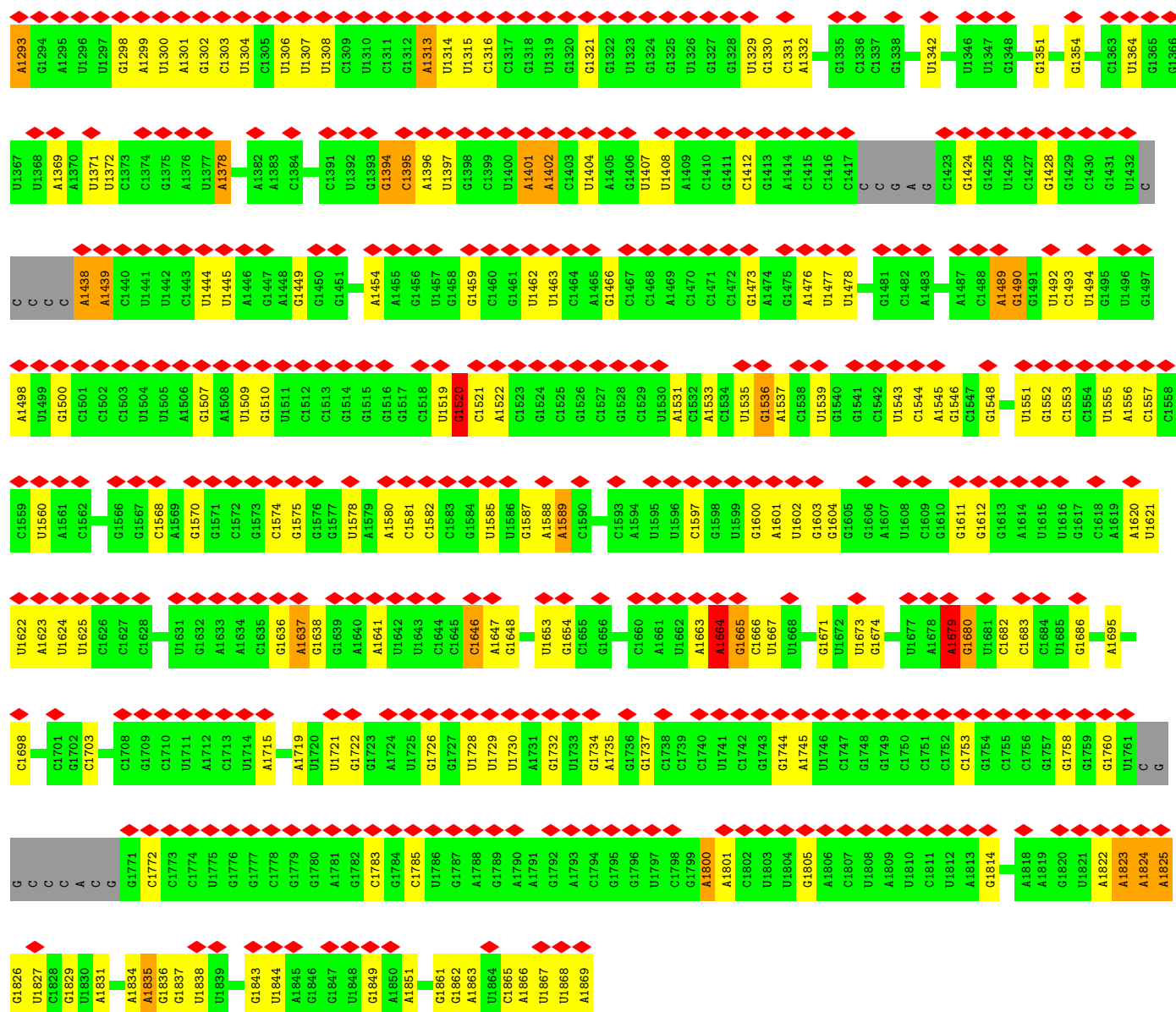




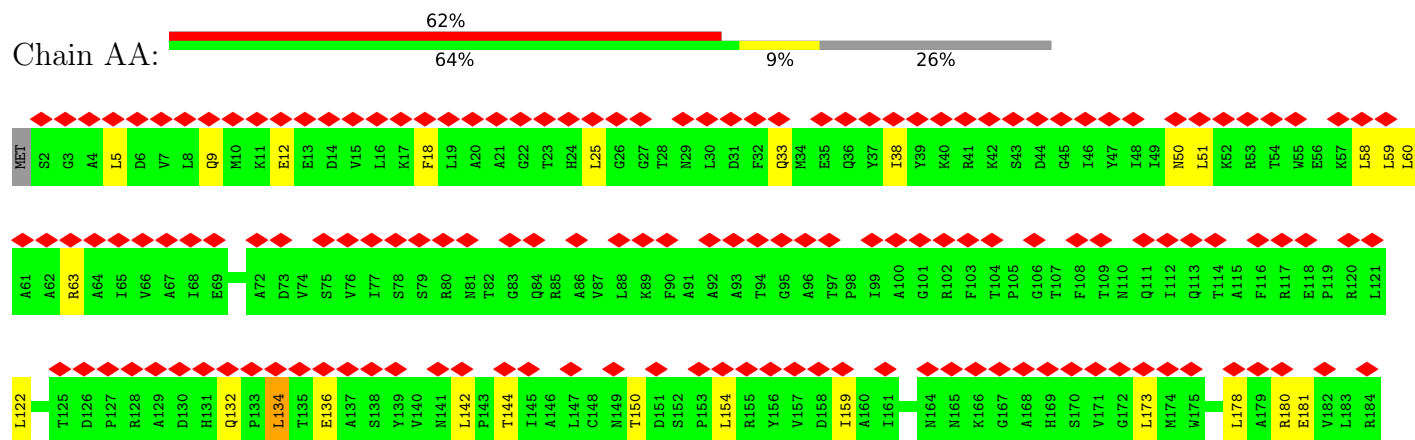




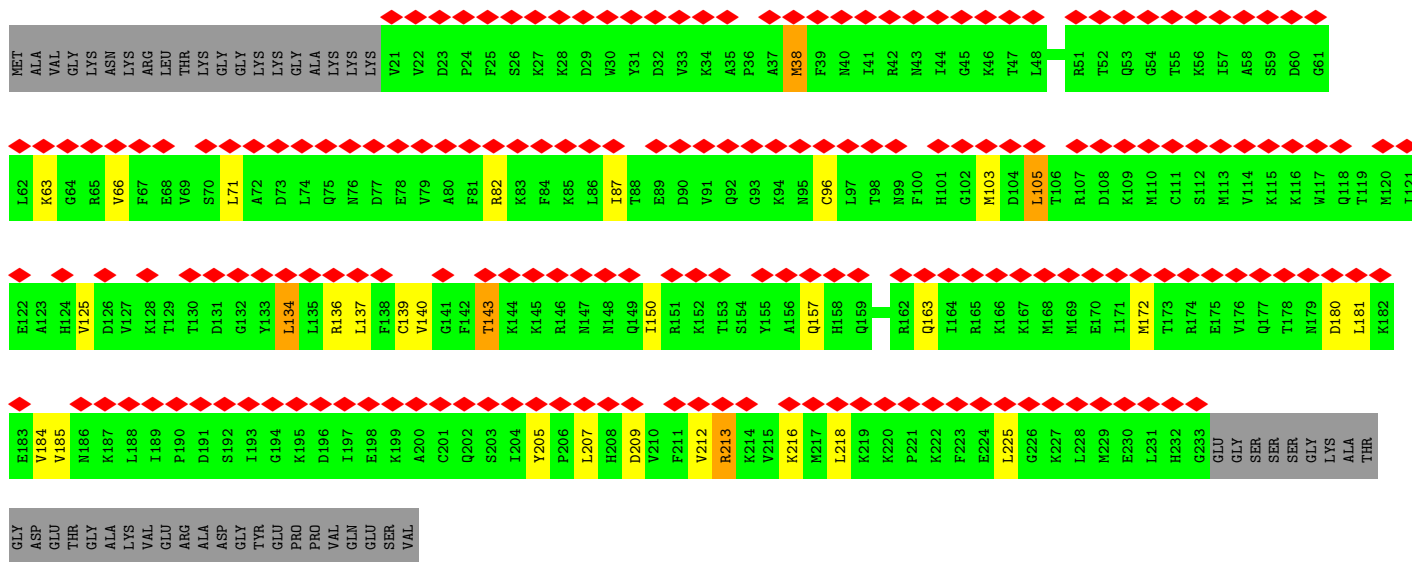
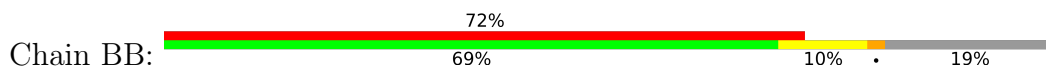




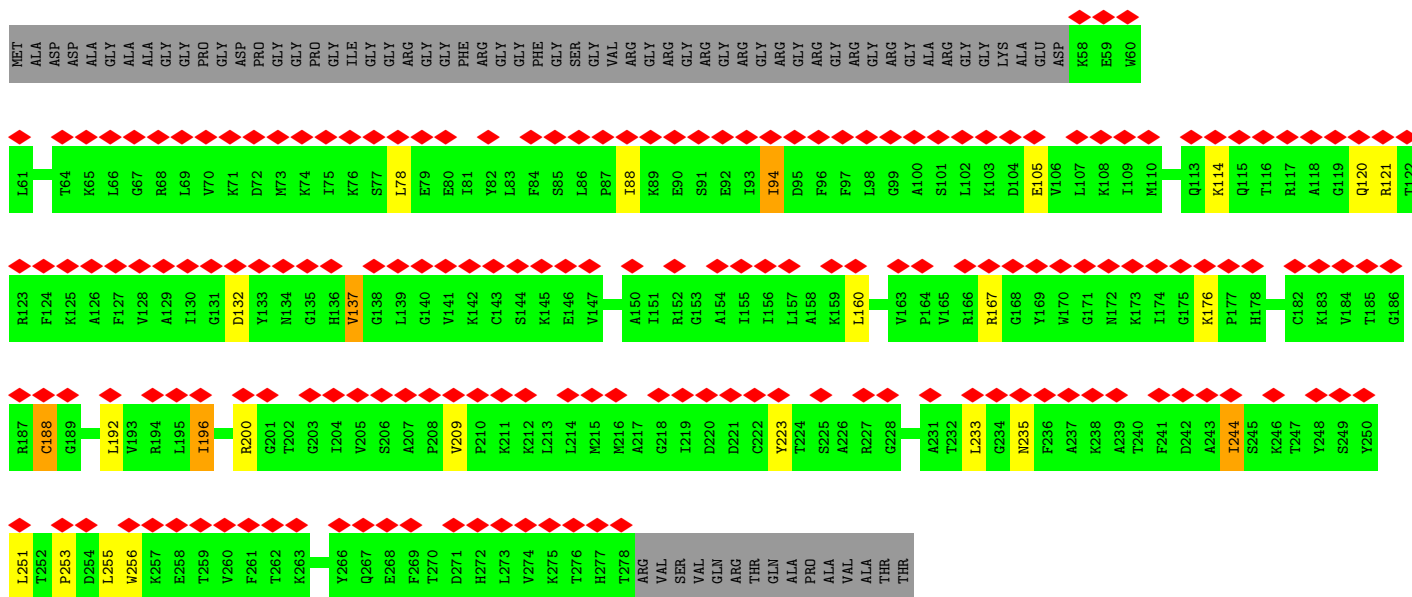
• Molecule 52: uS2



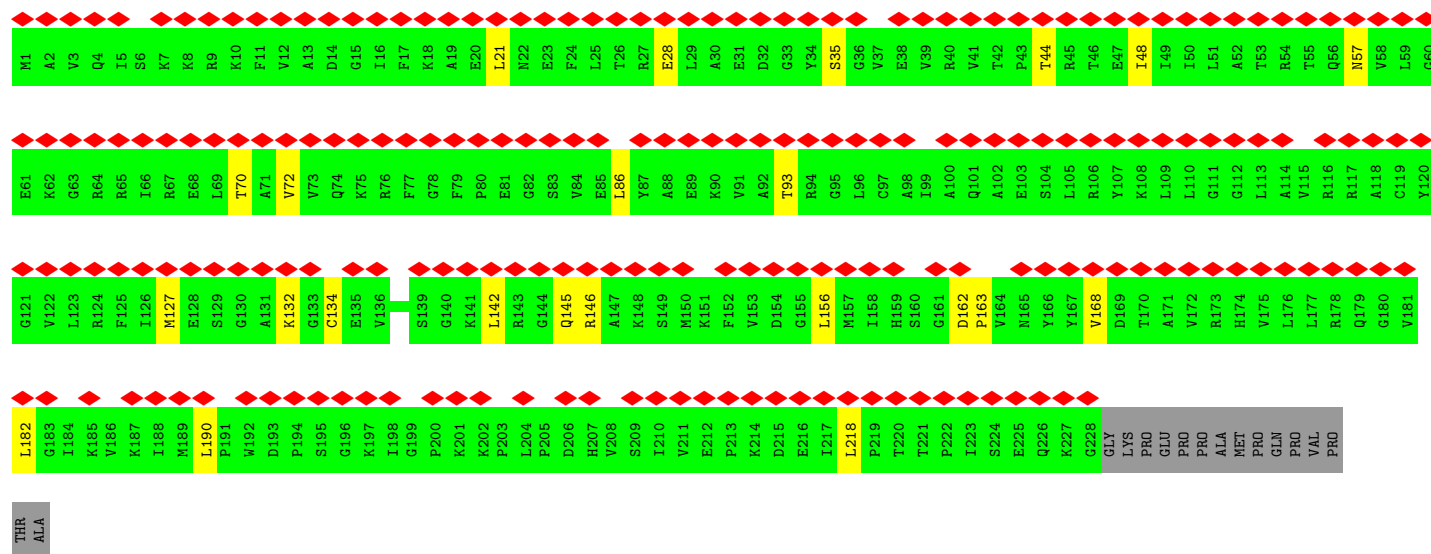
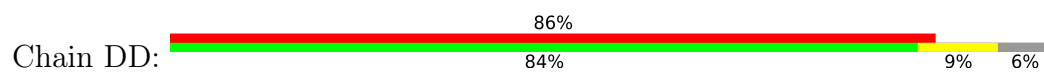
- Molecule 53: 40S ribosomal protein S3a



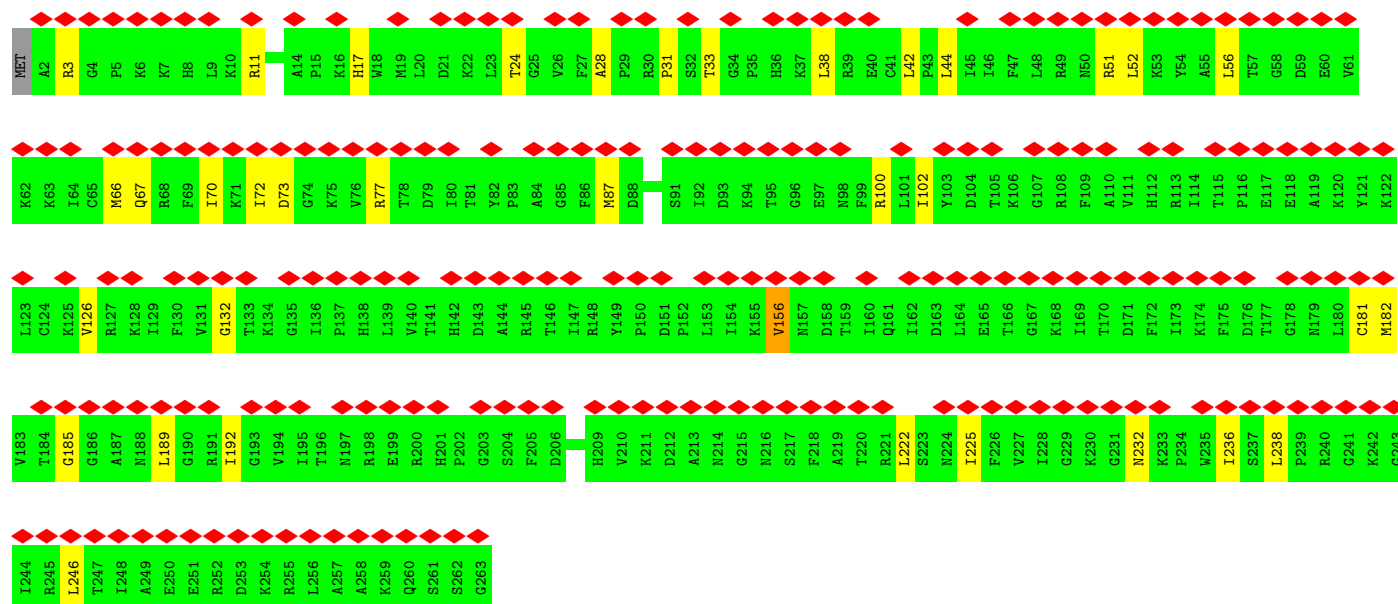
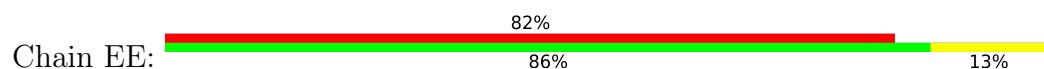
- Molecule 54: uS5



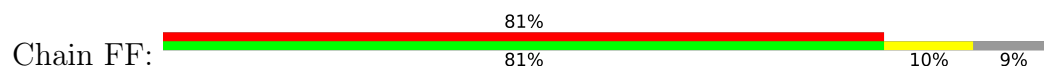
- Molecule 55: uS3

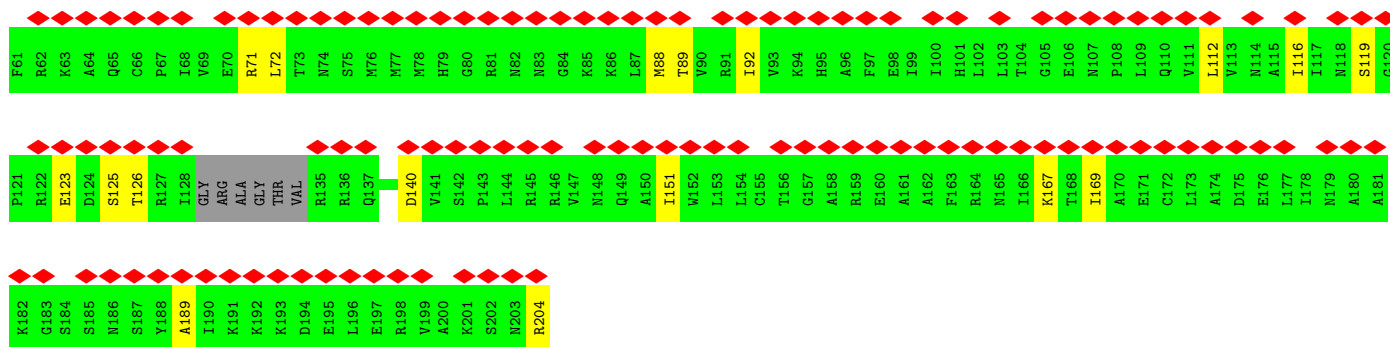


• Molecule 56: eS4

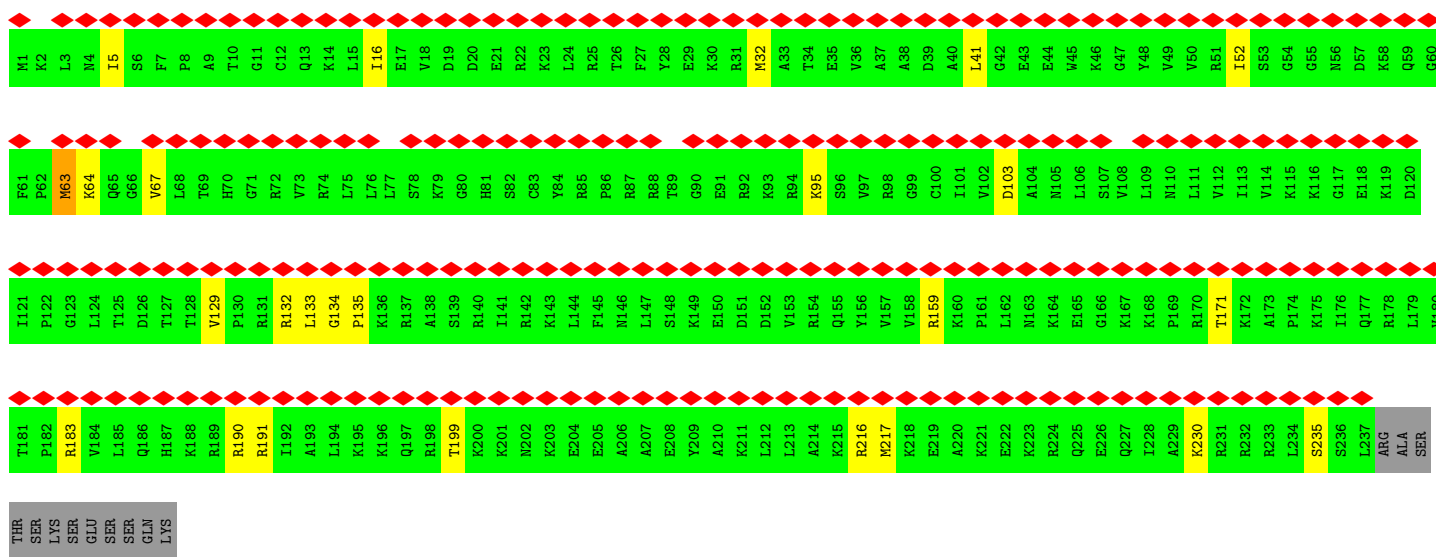
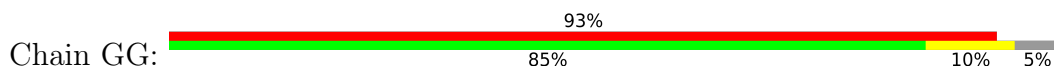


• Molecule 57: uS7

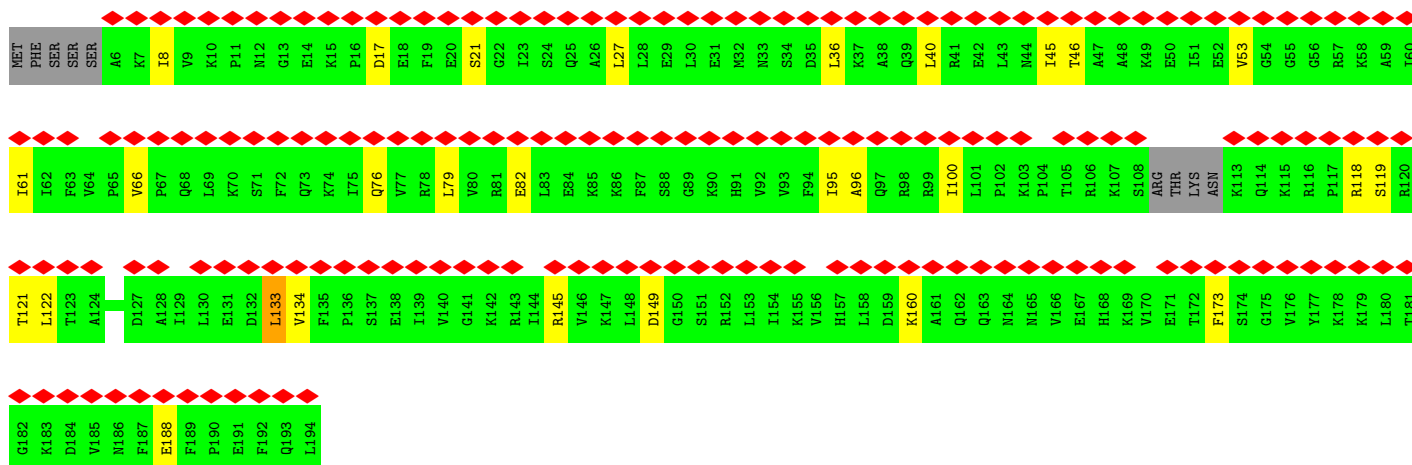
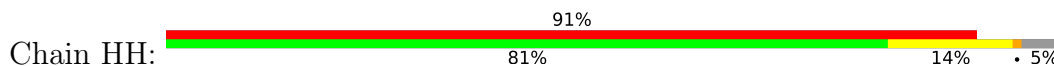




• Molecule 58: 40S ribosomal protein S6



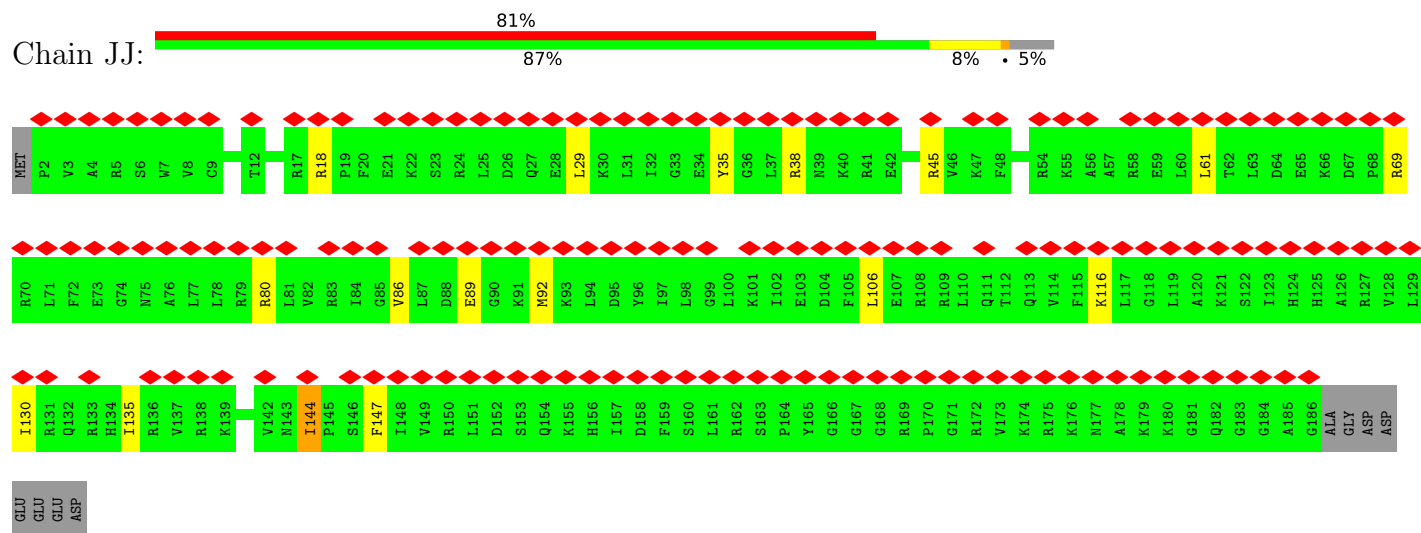
• Molecule 59: eS7



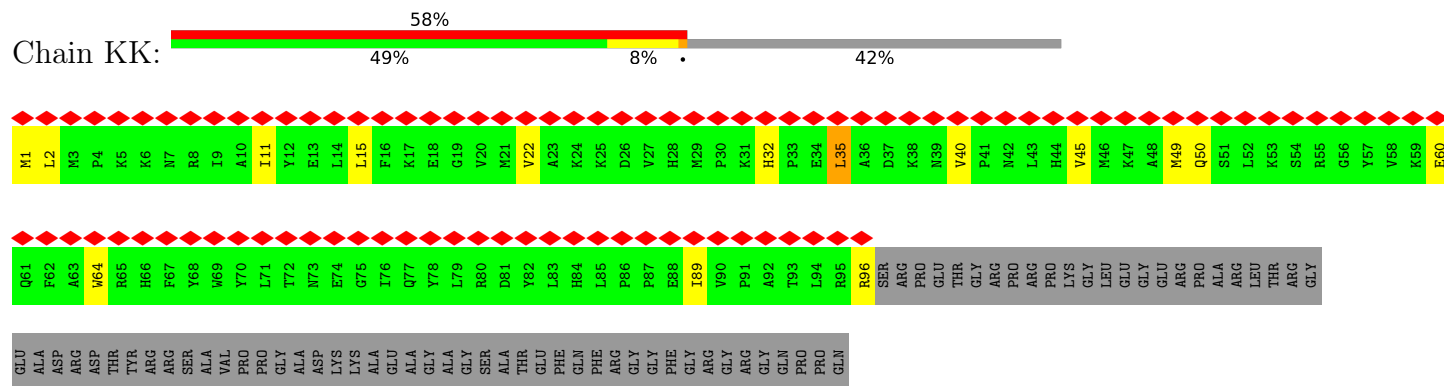
• Molecule 60: eS8



- Molecule 61: Ribosomal protein S9 (Predicted)

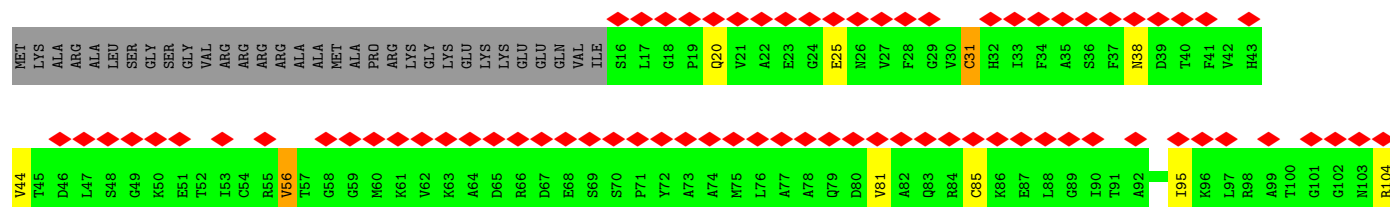


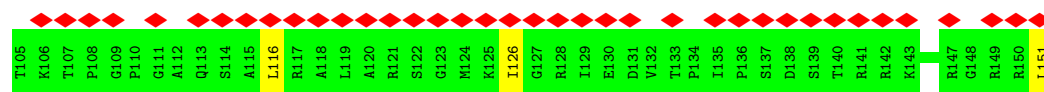
- Molecule 62: eS10



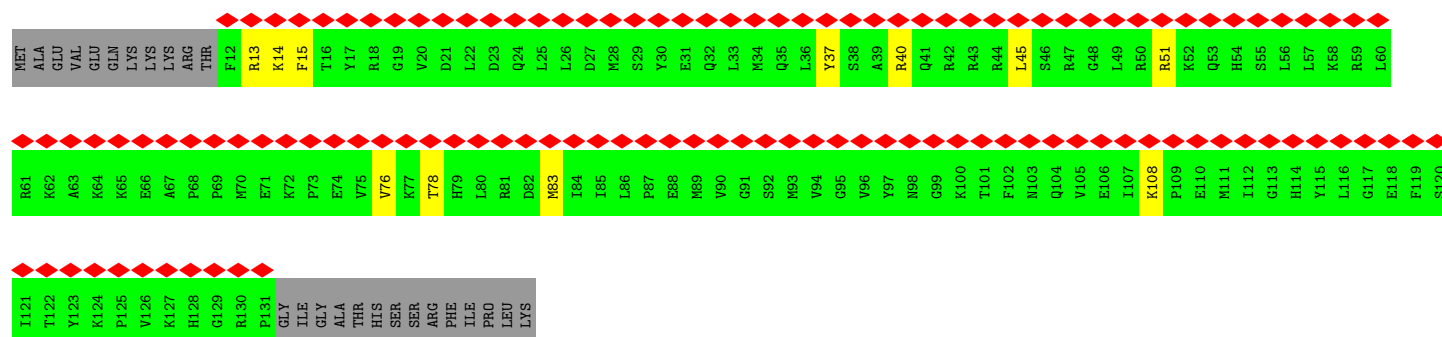
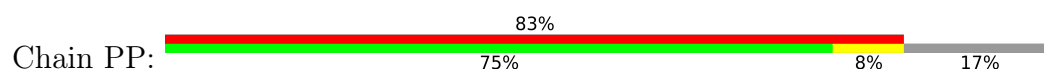
- Molecule 63: uS17



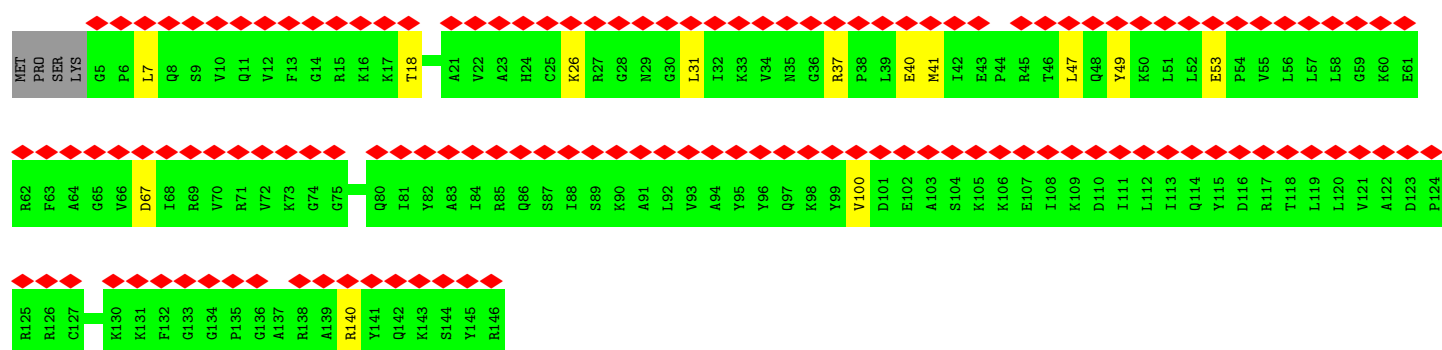
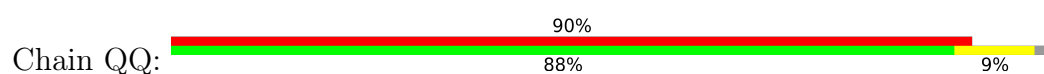




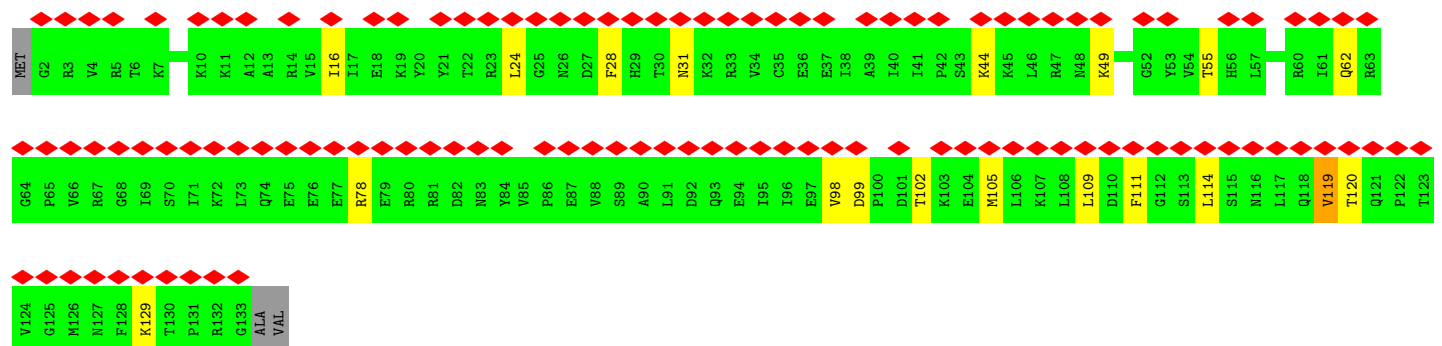
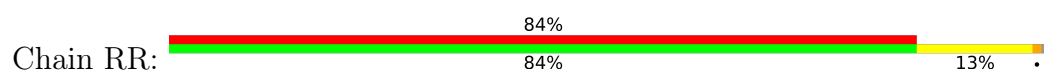
• Molecule 67: uS19



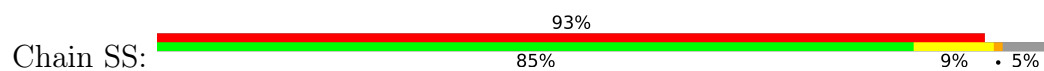
• Molecule 68: uS9

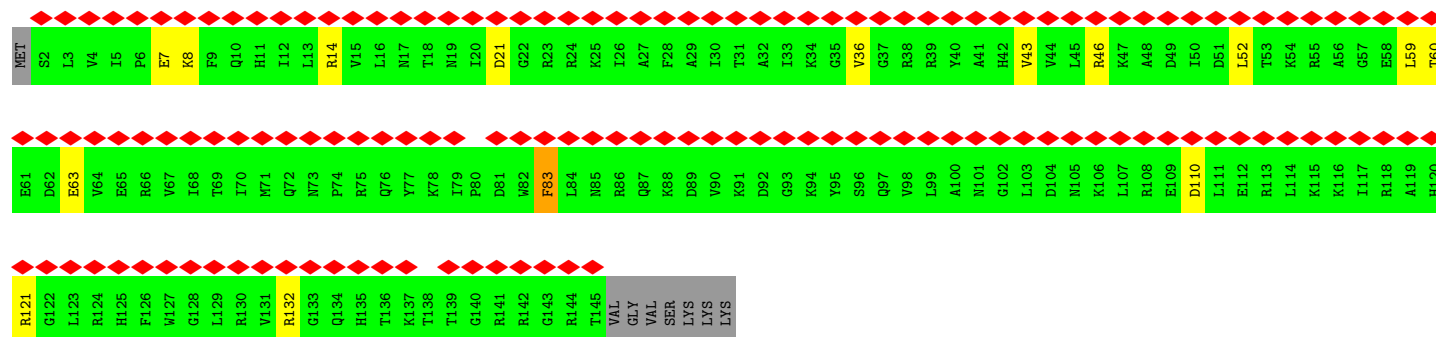


• Molecule 69: eS17

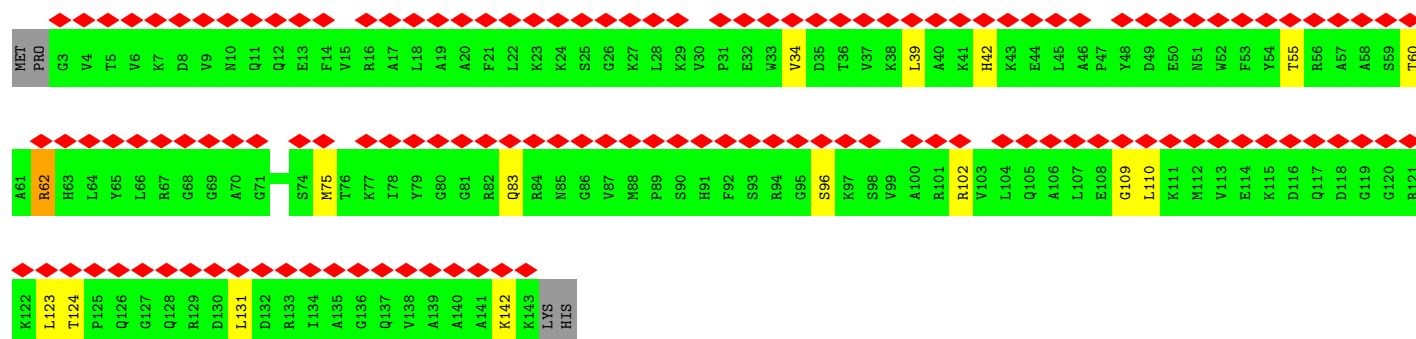


• Molecule 70: uS13

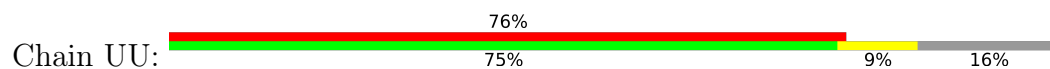




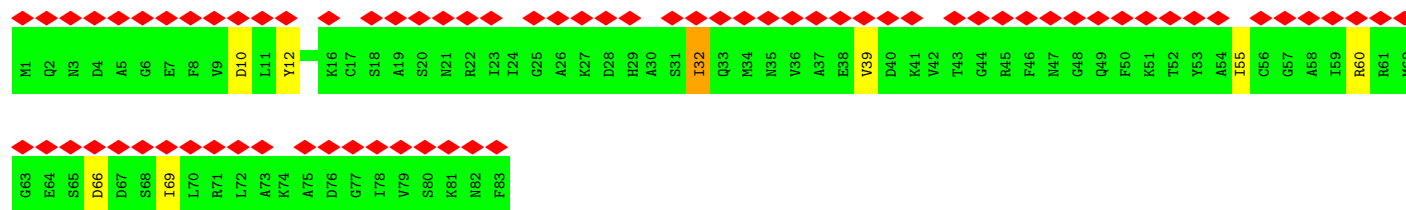
• Molecule 71: eS19



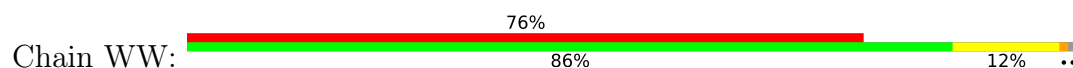
• Molecule 72: uS10

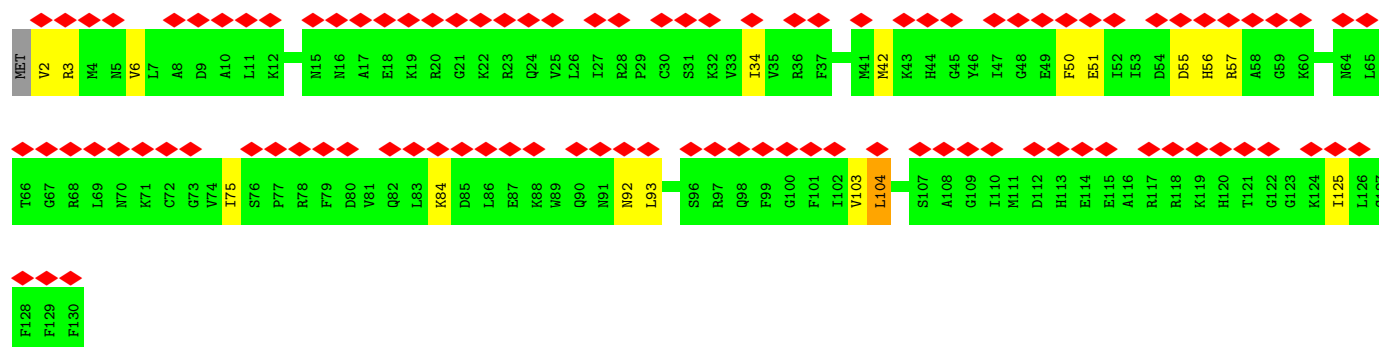


• Molecule 73: eS21

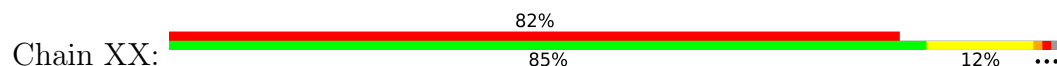


• Molecule 74: uS8

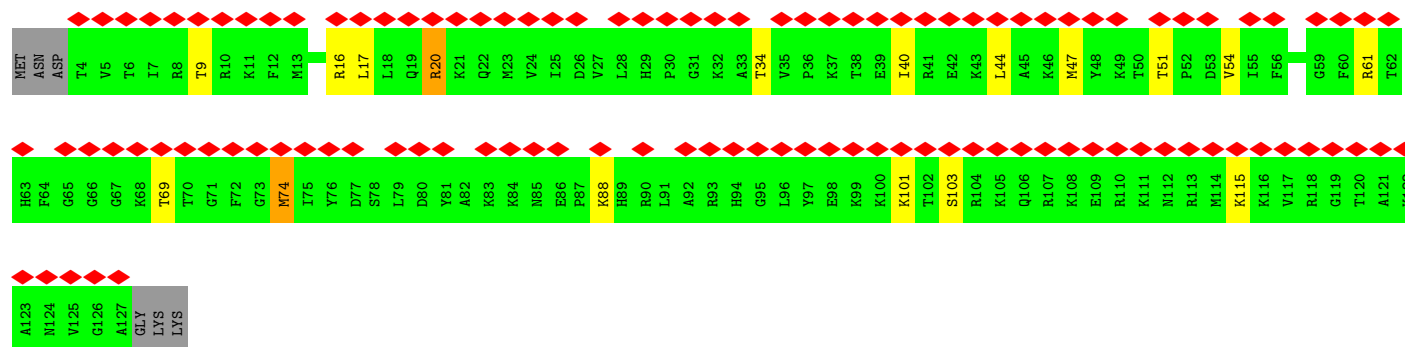
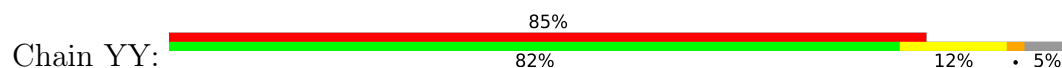




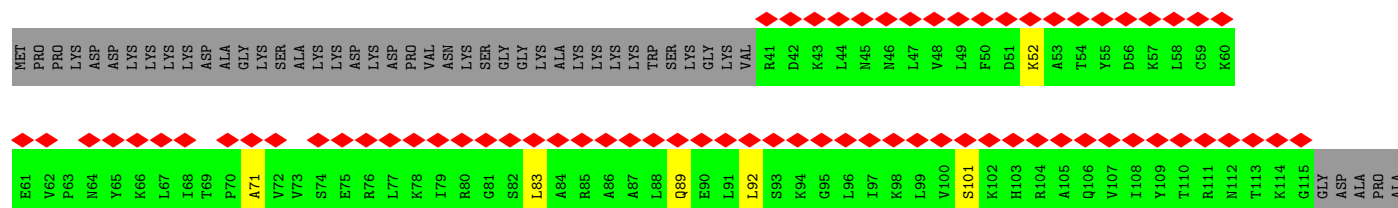
- Molecule 75: uS12



- Molecule 76: eS24



- Molecule 77: eS25



ALA
GLY
GLU
ASP
ALA

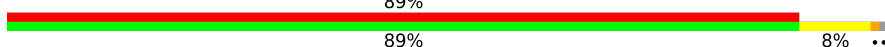
• Molecule 78: eS26

Chain aa: 

MET T2 K3 K4 R5 R6 R7 R8 R9 R10 A11 K12 K13 G16 H17 V18 Q19 P20 I21 R22 N25 C26 A27 R28 C29 V30 P31 K32 D33 K34 A35 I36 K37 K38 F39 V40 I41 I42 R42 N43 I44 V45 E46 A47 A48 A49 V50 R51 D52 I53 S54 E55 A56 S57 V58 F59 D60 A61 Y62

V63 L64 P65 K66 L67 V68 V69 K70 L71 H72 Y73 S76 C77 A78 I79 H80 S81 K82 R85 N86 R87 S88 R89 E90 A91 R92 K93 D94 R95 P98 P99 R100 F101 R102 PRO ALA GLY ALA ALA PRO ARG PRO PRO LYS PRO MET

• Molecule 79: 40S ribosomal protein S27

Chain bb: 

MET P2 L3 A4 K5 D6 L7 L8 H9 P10 S11 P12 E13 E14 E15 K16 K17 K18 H19 K20 K21 K22 R23 L24 V25 Q26 S27 P28 N29 S30 Y31 F32 M33 D34 V35 K36 C37 P38 G39 C40 Y41 K42 I43 T44 T45 V46 F47 S48 H49 A50 Q51 T52 V53 V54 L55 C56 V57 G58 C59 S60

T61 V62 L63 C64 T67 G68 G69 K70 A71 R72 L73 T74 E75 G76 C77 S78 F79 R80 R81 K82 Q83 H84

• Molecule 80: eS28

Chain cc: 

MET ASP THR SER ARG VAL Q7 P8 I9 K10 L11 L12 A12 R13 V14 T15 K16 V17 L18 G19 R20 T21 G22 S23 Q24 Q25 Q26 C27 T28 Q29 V30 R31 V32 E33 F34 M35 D36 D37 T38 S39 R40 S41 I42 I43 R44 M45 V46 K47 G48 P49 V50 R51 E52 G53 D54 V55 L56 T57 L58 L59 E60

S61 E62 R63 E64 A65 R66 R67 L68 ARG

• Molecule 81: uS14

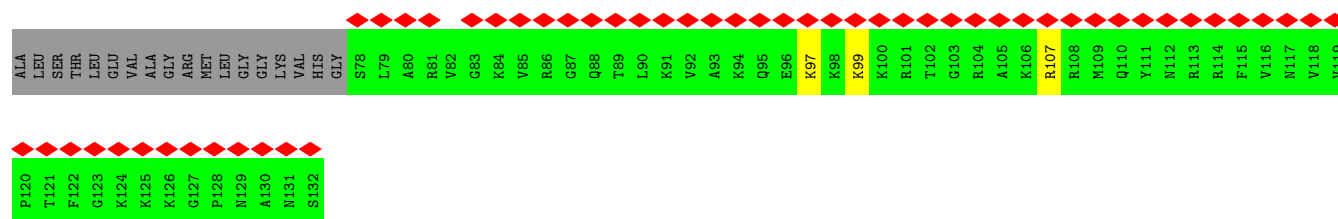
Chain dd: 

MET G2 H3 Q4 Q5 L6 Y7 W8 S9 H10 P11 R12 K13 F14 G15 Q16 G17 S18 R19 S20 C21 R22 V23 C24 S25 N26 R27 H28 G29 L30 I31 R32 K33 M38 C39 R40 Q41 F43 R44 Q45 Y46 A47 K48 D49 I50 G51 F52 I53 K54 L55 D56

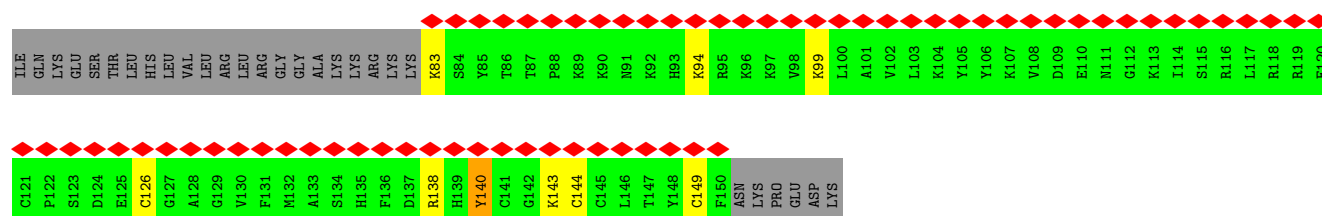
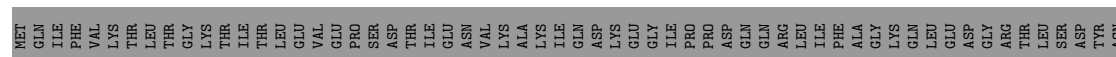
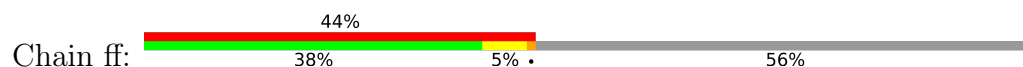
• Molecule 82: eS30

Chain ee: 

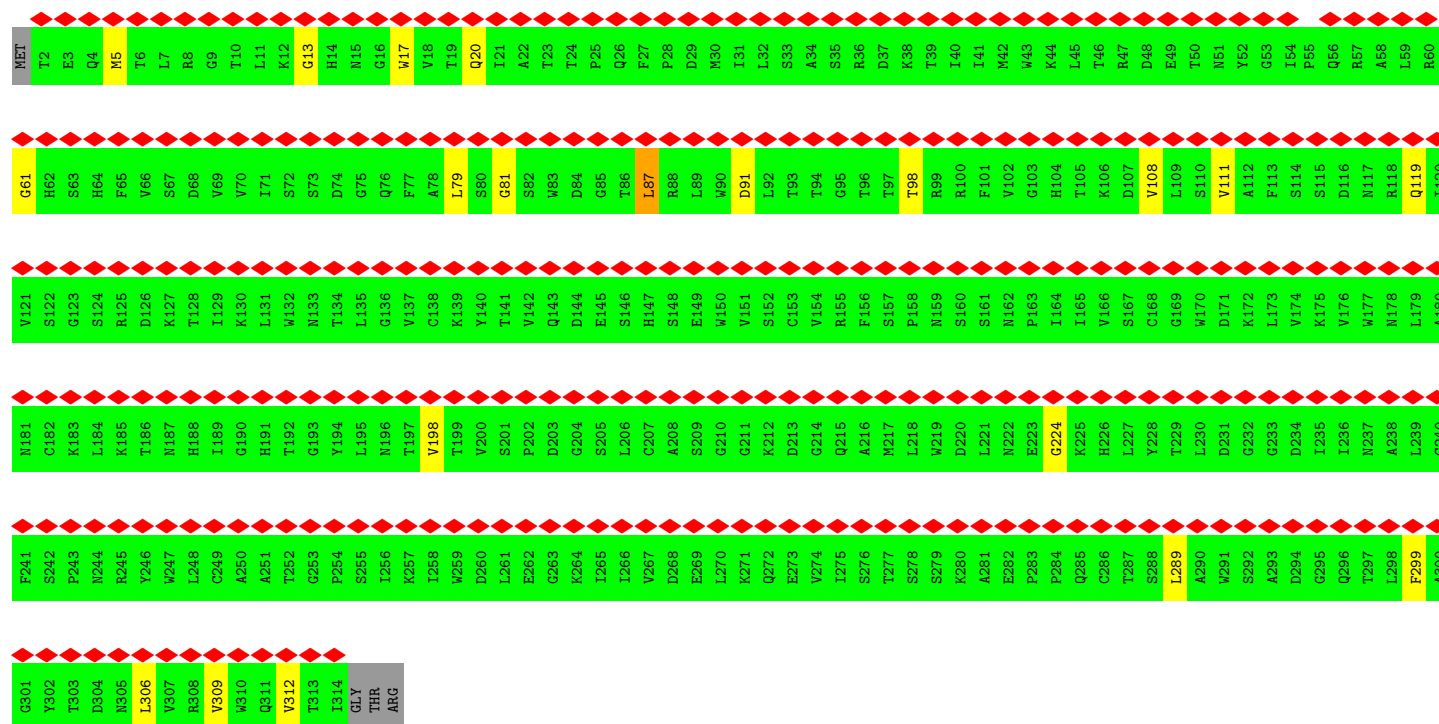
MET GLN LEU PHE VAL ARG ALA GLN LEU LEU HIS THR LEU GLU VAL THR GLY ARG GLU THR VAL ALA GLN ILE LYS ALA HIS VAL R22 ALA SER LEU GLU ILE ALA PRO G29 ASP GLN VAL VAL LEU LEU ALA GLY THR PRO LEU ASP GLU THR LEU GLN CYS GLY VAL GLU



• Molecule 83: eS31



• Molecule 84: RACK1



• Molecule 85: mRNA (UGA stop codon)



L635	L636	K576	Q515	R455	S395	T335	T275
K637	K577	T516	T516	S456	L396	T336	L276
C638	C578	G517	G517	Q457	G397	T337	M277
Q639	T579	D518	D518	S458	V398	K338	G278
M640	R580	R519	R519	S459	T399	V339	H279
F581	A611	L520	L520	E460	Q400	I340	M280
R582	L641	L521	L521	L461	L401	T341	L281
A583	A522	A522	A522	T462	A402	L342	Y282
R584	M523	M523	M523	K463	V403	M343	L283
L585	P524	P524	P524	W464	A404	D344	L284
L586	P525	P525	P525	W465	V405	A345	G285
L587	M526	M526	M526	K466	M406	N286	N286
F588	E527	E527	E527	Q467	K407	G347	I287
N589	T528	T528	T528	L468	M408	H348	N288
I590	C529	C529	C529	Q469	D409	K349	K289
E591	T530	T530	T530	L470	Q410	D350	R290
I592	M531	M531	M531	L471	V411	F351	T291
P593	K532	K532	K532	E472	M412	I352	M292
I594	G533	G533	G533	Q473	W413	P353	H293
T595	I534	I534	I534	L474	Q414	M354	K294
K596	T535	T535	T535	D475	Q415	M355	Y295
G597	L536	L536	L536	S476	E416	I356	E296
F598	H537	H537	H537	F477	R417	T357	Q297
P599	D538	D538	D538	K478	F418	G358	E298
V600	E539	E539	E539	P479	Q419	A359	S299
L601	P540	P540	P540	Q480	E420	A360	K300
L602	V541	V541	V541	Q481	I421	Q361	K301
H603	D542	D542	D542	K482	T422	A362	A302
Y604	K543	K543	K543	S483	G423	D363	G303
Q605	A544	A544	A544	L484	K424	V364	K304
T606	A545	A545	A545	D485	L425	A365	A305
V607	A546	A546	A546	K486	G426	V366	S306
S608	G547	G547	G547	P487	H427	L367	F307
E609	D548	D548	D548	F488	F428	V368	A308
P610	H549	H549	H549	R489	L429	V369	Y309
A611	V550	V550	V550	L490	K430	D370	A310
W612	S551	S551	S551	C491	Q431	A371	W311
I613	L552	L552	L552	W492	A432	S372	V312
K614	T553	T553	T553	S493	G433	R373	L313
R615	L554	L554	L554	D494	F434	G374	D314
L616	V555	V555	V555	W495	K435	E375	E315
I617	G556	G556	G556	F496	E436	F376	T316
S618	M557	M557	M557	K497	D437	E377	G317
V619	D558	D558	D558	P498	D438	A378	E318
L620	I559	I559	I559	Q499	V439	G379	E319
N621	T560	T560	T560	G500	G440	F380	R320
K622	K561	K561	K561	S501	F441	E381	E321
S623	L562	L562	L562	E502	I442	T382	R322
T624	M563	M563	M563	F503	P443	G383	G323
G625	V564	V564	V564	C504	T444	G384	V324
E626	G565	G565	G565	I505	S445	Q385	T325
V627	C566	C566	C566	T506	G446	T386	M326
T628	V627	V627	V627	G507	L447	R387	D327
K629	F628	F628	F628	K508	S448	E388	V328
W630	C569	C569	C569	I509	G449	H389	G329
K631	G570	G570	G570	E510	E450	G390	M330
P632	F571	F571	F571	A511	M451	L391	T331
L633	K572	K572	K572	G512	L452	I392	K332
F634	V573	V573	V573	W513	T453	V393	F333
	P574	P574	P574	L514	T454	R394	F334

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.597	Depositor
Minimum map value	-0.372	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.48	0/1936	0.80	0/2596
2	B	0.47	0/3240	0.79	1/4339 (0.0%)
3	C	0.46	0/2937	0.80	2/3946 (0.1%)
4	D	0.44	0/2437	0.80	0/3264
5	E	0.45	0/1762	0.75	0/2362
6	F	0.46	0/1911	0.81	0/2549
7	G	0.48	0/1910	0.81	0/2569
8	H	0.44	0/1535	0.73	0/2063
9	I	0.45	0/1702	0.78	0/2272
10	J	0.45	0/1385	0.77	0/1852
11	L	0.47	0/1733	0.81	0/2316
12	M	0.47	0/1158	0.86	0/1547
13	N	0.46	0/1746	0.80	0/2338
14	O	0.49	0/1662	0.86	1/2222 (0.0%)
15	P	0.47	0/1268	0.77	0/1700
16	Q	0.47	0/1539	0.80	0/2054
17	R	0.46	0/1524	0.81	0/2013
18	S	0.46	0/1501	0.75	0/2012
19	T	0.46	0/1326	0.74	0/1770
20	U	0.45	0/823	0.73	0/1104
21	V	0.44	0/993	0.76	0/1332
22	W	0.47	0/873	0.80	0/1158
23	X	0.43	0/984	0.79	1/1323 (0.1%)
24	Y	0.40	0/1132	0.76	0/1504
25	Z	0.47	0/1130	0.76	0/1507
26	a	0.45	0/1191	0.80	1/1590 (0.1%)
27	b	0.46	0/861	0.80	0/1138
28	c	0.42	0/771	0.74	0/1034
29	d	0.48	0/903	0.75	0/1216
30	e	0.44	0/1071	0.76	0/1429
31	f	0.51	0/895	0.80	0/1198
32	g	0.45	0/916	0.79	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.42	0/1021	0.81	0/1348
34	i	0.45	0/841	0.77	0/1112
35	j	0.45	0/720	0.80	0/952
36	k	0.42	0/575	0.72	0/761
37	l	0.45	0/459	0.77	0/608
38	m	0.44	0/435	0.78	0/575
39	n	0.44	0/240	0.80	0/305
40	o	0.45	0/864	0.73	0/1140
41	p	0.45	0/718	0.79	0/953
42	r	0.48	0/1010	0.83	0/1354
43	s	0.55	0/1530	0.74	0/2064
44	t	0.59	0/1174	0.82	0/1582
45	1	0.57	0/49	1.05	0/65
46	2	0.36	0/1805	0.67	0/2809
47	3	0.37	0/1777	0.68	0/2763
48	5	0.39	8/84961 (0.0%)	0.76	107/132460 (0.1%)
49	7	0.38	0/2858	0.71	0/4455
50	8	0.37	0/3581	0.70	2/5577 (0.0%)
51	9	0.38	0/40523	0.75	33/63130 (0.1%)
52	AA	0.49	0/1747	0.83	0/2374
53	BB	0.44	0/1756	0.78	0/2350
54	CC	0.47	0/1753	0.83	0/2369
55	DD	0.50	0/1796	0.79	0/2417
56	EE	0.49	0/2118	0.81	1/2849 (0.0%)
57	FF	0.48	0/1492	0.88	0/2005
58	GG	0.51	0/1946	0.81	2/2590 (0.1%)
59	HH	0.51	0/1510	0.79	0/2022
60	II	0.47	0/1715	0.77	0/2287
61	JJ	0.46	0/1550	0.87	1/2069 (0.0%)
62	KK	0.49	0/834	0.81	0/1125
63	LL	0.44	0/1195	0.74	0/1597
64	MM	0.54	0/918	0.84	0/1233
65	NN	0.48	0/1226	0.87	0/1649
66	OO	0.48	0/1029	0.87	0/1380
67	PP	0.54	0/1017	0.83	0/1358
68	QQ	0.48	0/1146	0.79	0/1534
69	RR	0.48	0/1082	0.78	0/1452
70	SS	0.51	0/1208	0.82	0/1618
71	TT	0.51	0/1115	0.85	0/1493
72	UU	0.47	0/805	0.84	2/1081 (0.2%)
73	VV	0.49	0/643	0.84	0/860
74	WW	0.45	0/1051	0.82	0/1406
75	XX	0.47	0/1116	0.82	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.47	0/1028	0.79	0/1366
77	ZZ	0.50	0/604	0.85	0/810
78	aa	0.48	0/828	0.83	0/1109
79	bb	0.49	0/665	0.79	0/891
80	cc	0.45	0/490	0.79	0/656
81	dd	0.48	0/470	0.76	0/623
82	ee	0.47	0/447	0.78	0/587
83	ff	0.52	0/567	0.75	0/753
84	gg	0.47	0/2493	0.68	0/3394
85	hh	0.39	0/188	0.85	0/290
86	ii	0.49	0/2996	0.80	0/4050
87	jj	0.50	0/3352	0.77	1/4523 (0.0%)
All	All	0.43	8/237792 (0.0%)	0.77	155/348210 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	922(A)	G	O3'-P	13.89	1.77	1.61
48	5	1411(B)	C	O3'-P	9.43	1.72	1.61
48	5	1411(C)	C	O5'-C5'	9.29	1.56	1.42
48	5	935	A	C5-C6	-7.99	1.25	1.41
48	5	922	C	O3'-P	6.70	1.69	1.61
48	5	922(B)	C	O5'-C5'	6.22	1.52	1.42
48	5	922(A)	G	C3'-O3'	5.43	1.50	1.42
48	5	922	C	O5'-C5'	5.14	1.50	1.42

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	C8-N9-C1'	-22.30	60.09	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	922	C	C2'-C3'-O3'	16.55	138.53	113.70
48	5	922(B)	C	C1'-C2'-O2'	-16.18	87.54	111.80
48	5	481	G	N1-C2-N2	-15.53	69.62	116.20
48	5	481	G	N9-C1'-C2'	12.64	132.96	114.00
48	5	935	A	C5-C6-N6	-12.61	85.88	123.70
51	9	1835	A	C2'-C3'-O3'	11.88	127.32	109.50
48	5	1411	C	C4'-C3'-O3'	11.40	130.10	113.00
48	5	1411	C	C2'-C3'-O3'	-10.22	98.37	113.70
48	5	47	A	C4'-C3'-O3'	10.01	124.42	109.40
48	5	385	A	C4'-C3'-O3'	9.82	124.13	109.40
48	5	2046	G	C2'-C3'-O3'	9.37	123.55	109.50
48	5	1411(C)	C	P-O5'-C5'	8.85	134.17	120.90
48	5	922	C	C4'-C3'-C2'	-8.81	93.78	102.60
48	5	2695	A	C2'-C3'-O3'	8.75	122.63	109.50
48	5	3760	A	C2'-C3'-O3'	-8.42	101.07	113.70
48	5	2468	U	C4'-C3'-O3'	8.39	121.99	109.40
51	9	1394	G	C2'-C3'-O3'	8.38	126.26	113.70
48	5	922	C	O4'-C4'-C3'	-8.35	95.65	104.00
48	5	2474	G	C2'-C3'-O3'	8.30	121.96	109.50
14	O	110	PRO	N-CA-C	8.22	120.73	110.70
48	5	1834	U	C2'-C3'-O3'	8.16	121.75	109.50
48	5	48	G	C2'-C3'-O3'	8.12	121.67	109.50
48	5	922	C	C3'-C2'-O2'	7.99	122.69	110.70
48	5	1411	C	C1'-C2'-O2'	7.79	120.09	108.40
51	9	870	A	C4'-C3'-O3'	7.61	120.81	109.40
48	5	2068	C	C4'-C3'-O3'	7.52	120.68	109.40
48	5	3888	G	C2'-C3'-O3'	7.50	124.95	113.70
51	9	1664	A	C4'-C3'-O3'	7.47	120.61	109.40
48	5	4232	U	C4'-C3'-O3'	7.45	120.58	109.40
48	5	922	C	N1-C1'-C2'	-7.38	100.92	112.00
48	5	1411	C	C5'-C4'-C3'	7.38	127.07	116.00
48	5	1485	C	C2'-C3'-O3'	7.37	120.56	109.50
48	5	4942	C	C4'-C3'-O3'	7.37	120.45	109.40
48	5	1477	C	C2'-C3'-O3'	7.34	124.70	113.70
48	5	922(A)	G	N9-C1'-C2'	7.33	123.00	112.00
48	5	481	G	N3-C2-N2	-7.30	98.00	119.90
51	9	1130	G	C4'-C3'-O3'	7.22	120.23	109.40
51	9	434	G	C2'-C3'-O3'	7.18	124.47	113.70
48	5	922(A)	G	P-O3'-C3'	7.17	128.30	119.70
48	5	4170	A	C2'-C3'-O3'	7.14	120.21	109.50
48	5	1370	G	C2'-C3'-O3'	7.08	120.12	109.50
48	5	449	C	C2'-C3'-O3'	7.06	120.08	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2089	G	C2'-C3'-O3'	7.02	120.03	109.50
48	5	747	A	C4'-C3'-O3'	6.92	119.79	109.40
48	5	498	C	C4'-C3'-O3'	6.91	119.76	109.40
51	9	594	A	C4'-C3'-O3'	6.90	119.75	109.40
48	5	935	A	C6-N1-C2	-6.89	97.92	118.60
48	5	935	A	N1-C6-N6	-6.88	97.98	118.60
48	5	4925	U	C2'-C3'-O3'	6.83	119.74	109.50
51	9	72	C	C4'-C3'-O3'	6.79	119.58	109.40
48	5	4448	G	C4'-C3'-O3'	6.78	123.16	113.00
48	5	971(A)	G	C4'-C3'-O3'	6.77	123.15	113.00
51	9	1061	U	C2'-C3'-O3'	-6.76	103.56	113.70
51	9	1646	C	C2'-C3'-O3'	6.70	123.74	113.70
48	5	4947	U	C2'-C3'-O3'	6.66	123.69	113.70
48	5	922	C	C5'-C4'-O4'	6.57	119.66	109.80
48	5	4378	A	C2'-C3'-O3'	6.51	119.27	109.50
51	9	1253	A	C2'-C3'-O3'	6.50	119.24	109.50
48	5	492	U	C2'-C3'-O3'	6.47	119.21	109.50
48	5	2529	A	C2'-C3'-O3'	6.47	119.21	109.50
48	5	2266	C	C2'-C3'-O3'	6.41	119.11	109.50
48	5	3697	U	C2'-C3'-O3'	6.40	123.30	113.70
48	5	406	C	C2'-C3'-O3'	6.39	123.28	113.70
48	5	90	G	C2'-C3'-O3'	6.38	123.28	113.70
58	GG	134	GLY	CA-C-N	6.38	127.82	119.84
58	GG	134	GLY	C-N-CA	6.38	127.82	119.84
51	9	626	G	C4'-C3'-O3'	-6.38	103.44	113.00
48	5	1211	G	C2'-C3'-O3'	6.37	123.25	113.70
48	5	275	C	C2'-C3'-O3'	6.36	123.23	113.70
48	5	2313	A	C2'-C3'-O3'	6.35	119.02	109.50
48	5	125	C	C2'-C3'-O3'	6.32	123.19	113.70
51	9	1520	G	C4'-C3'-O3'	6.27	122.41	113.00
51	9	110	U	C2'-C3'-O3'	6.26	123.10	113.70
51	9	417	C	C4'-C3'-O3'	-6.24	103.64	113.00
48	5	1455	G	C2'-C3'-O3'	6.23	123.04	113.70
48	5	1209	U	C2'-C3'-O3'	-6.22	104.37	113.70
51	9	688	U	C2'-C3'-O3'	6.14	118.72	109.50
48	5	1236	C	C4'-C3'-O3'	6.13	122.19	113.00
48	5	696	C	C2'-C3'-O3'	6.11	118.66	109.50
51	9	752	G	C2'-C3'-O3'	6.06	118.59	109.50
3	C	340	ILE	N-CA-C	-6.00	105.97	111.67
48	5	1818	G	C2'-C3'-O3'	6.00	122.70	113.70
48	5	1411	C	O4'-C4'-C3'	-6.00	98.00	104.00
50	8	124	U	C4'-C3'-O3'	5.93	118.30	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1329	G	C2'-C3'-O3'	5.92	122.58	113.70
51	9	1313	A	C4'-C3'-O3'	5.89	118.24	109.40
48	5	1358	G	C4'-C3'-O3'	5.85	118.17	109.40
51	9	160	U	C4'-C3'-O3'	5.85	118.17	109.40
48	5	3603	G	C4'-C3'-O3'	-5.81	104.28	113.00
48	5	2278	G	C2'-C3'-O3'	5.81	118.21	109.50
48	5	4335	C	C4'-C3'-O3'	-5.79	104.31	113.00
72	UU	72	GLU	N-CA-C	5.78	119.01	107.62
48	5	922(A)	G	C2'-C3'-O3'	5.76	122.33	113.70
48	5	4884	G	C2'-C3'-O3'	5.75	122.33	113.70
48	5	4449	A	C4'-C3'-O3'	5.74	118.01	109.40
48	5	3619	G	C4'-C3'-O3'	-5.71	104.43	113.00
48	5	922(B)	C	C4'-C3'-O3'	5.69	117.93	109.40
48	5	1072	C	C2'-C3'-O3'	5.68	118.03	109.50
51	9	1264	C	C4'-C3'-O3'	5.68	117.92	109.40
51	9	642	U	C4'-C3'-O3'	5.68	121.52	113.00
48	5	245	C	C2'-C3'-O3'	5.68	122.21	113.70
72	UU	93	SER	N-CA-C	5.66	113.11	108.07
48	5	4699	U	C4'-C3'-O3'	5.64	117.86	109.40
48	5	922(B)	C	P-O5'-C5'	5.64	129.36	120.90
48	5	1445	U	C2'-C3'-O3'	5.64	122.16	113.70
48	5	4075	U	C2'-C3'-O3'	5.64	117.96	109.50
50	8	94	G	C2'-C3'-O3'	5.60	117.89	109.50
48	5	959	G	C2'-C3'-O3'	5.59	117.89	109.50
48	5	959	G	C4'-C3'-O3'	5.54	117.70	109.40
48	5	1291	G	C2'-C3'-O3'	5.53	121.99	113.70
48	5	2661	U	C2'-C3'-O3'	5.50	117.75	109.50
51	9	501	C	N1-C1'-C2'	5.47	120.21	112.00
51	9	532	C	C2'-C3'-O3'	5.46	121.89	113.70
3	C	74	ALA	N-CA-C	5.44	119.53	113.01
51	9	1637	A	C2'-C3'-O3'	5.42	117.63	109.50
51	9	629	A	C3'-C2'-O2'	5.42	122.73	114.60
48	5	930	G	C2'-C3'-O3'	5.41	121.81	113.70
48	5	2836	A	C4'-C3'-O3'	-5.41	104.89	113.00
26	a	61	TYR	N-CA-C	5.37	117.00	111.03
2	B	258	HIS	N-CA-C	5.36	121.66	109.81
48	5	916	C	C4'-C3'-O3'	5.34	117.40	109.40
48	5	2088	A	C2'-C3'-O3'	5.32	117.48	109.50
51	9	553	U	C3'-C2'-O2'	5.32	118.68	110.70
48	5	4517	A	C4'-C3'-O3'	-5.26	105.11	113.00
48	5	3603	G	C2'-C3'-O3'	5.26	121.59	113.70
48	5	485	C	C3'-C2'-O2'	5.24	118.56	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	504	G	C2'-C3'-O3'	5.24	121.56	113.70
48	5	38	A	C4'-C3'-O3'	-5.23	105.16	113.00
51	9	1679	A	C2'-C3'-O3'	5.18	117.27	109.50
51	9	1395	C	C4'-C3'-O3'	5.17	120.75	113.00
51	9	677	G	C4'-C3'-O3'	-5.16	105.26	113.00
48	5	90	G	C4'-C3'-O3'	-5.16	105.26	113.00
48	5	922	C	P-O5'-C5'	5.14	128.61	120.90
48	5	1238	A	C2'-C3'-O3'	5.14	121.41	113.70
56	EE	156	VAL	N-CA-C	5.12	115.89	110.72
51	9	1137	U	C2'-C3'-O3'	5.10	121.35	113.70
48	5	3697	U	C3'-C2'-O2'	5.09	118.33	110.70
48	5	3625	G	C2'-C3'-O3'	5.08	121.32	113.70
48	5	923	C	P-O5'-C5'	5.08	128.52	120.90
51	9	553	U	C2'-C3'-O3'	5.08	121.32	113.70
61	JJ	144	ILE	N-CA-C	5.08	113.52	107.73
48	5	1292	C	C2'-C3'-O3'	-5.08	106.08	113.70
48	5	3876	A	C2'-C3'-O3'	5.05	117.07	109.50
48	5	1563	A	C4'-C3'-O3'	5.04	120.56	113.00
51	9	615	C	N1-C1'-C2'	-5.03	104.45	112.00
48	5	922	C	C1'-C2'-O2'	-5.03	100.86	108.40
48	5	1411(C)	C	C5'-C4'-O4'	5.03	117.34	109.80
48	5	4213	A	C4'-C3'-O3'	-5.03	105.46	113.00
48	5	1072	C	C4'-C3'-O3'	5.02	116.94	109.40
87	jj	524	PRO	N-CA-C	5.02	116.83	110.70
48	5	1445	U	C3'-C2'-O2'	5.02	118.23	110.70
23	X	79	PHE	N-CA-C	5.01	112.64	108.13
48	5	1411(B)	C	P-O3'-C3'	5.00	125.70	119.70
51	9	615	C	C3'-C2'-C1'	5.00	106.30	101.30

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	16	0
2	B	3172	0	3310	17	0
3	C	2883	0	3053	14	0
4	D	2391	0	2424	12	0
5	E	1729	0	1887	8	0
6	F	1875	0	1995	11	0
7	G	1879	0	2027	9	0
8	H	1516	0	1597	6	0
9	I	1664	0	1712	4	0
10	J	1362	0	1399	3	0
11	L	1702	0	1820	6	0
12	M	1137	0	1211	10	0
13	N	1701	0	1749	8	0
14	O	1630	0	1778	9	0
15	P	1242	0	1274	2	0
16	Q	1515	0	1634	6	0
17	R	1508	0	1664	6	0
18	S	1462	0	1508	16	0
19	T	1298	0	1366	3	0
20	U	809	0	833	5	0
21	V	979	0	1039	5	0
22	W	860	0	903	3	0
23	X	967	0	1040	1	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	4	0
26	a	1162	0	1209	10	0
27	b	848	0	920	0	0
28	c	761	0	794	4	0
29	d	888	0	930	6	0
30	e	1053	0	1147	4	0
31	f	876	0	912	3	0
32	g	906	0	1000	1	0
33	h	1013	0	1147	1	0
34	i	830	0	916	1	0
35	j	705	0	738	3	0
36	k	569	0	637	0	0
37	l	447	0	480	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	467	2	0
39	n	239	0	289	1	0
40	o	851	0	920	6	0
41	p	708	0	758	3	0
42	r	994	0	1051	2	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	2	0
45	1	49	0	51	0	0
46	2	1616	0	824	1	0
47	3	1593	0	811	3	0
48	5	75972	0	38400	258	0
49	7	2558	0	1296	4	0
50	8	3208	0	1629	4	0
51	9	36249	0	18317	141	0
52	AA	1710	0	1708	9	0
53	BB	1729	0	1803	12	0
54	CC	1716	0	1806	8	0
55	DD	1768	0	1866	6	0
56	EE	2076	0	2177	14	0
57	FF	1471	0	1522	8	0
58	GG	1923	0	2089	5	0
59	HH	1488	0	1582	7	0
60	II	1686	0	1772	5	0
61	JJ	1525	0	1640	5	0
62	KK	810	0	836	6	0
63	LL	1175	0	1249	8	0
64	MM	908	0	939	3	0
65	NN	1202	0	1289	5	0
66	OO	1016	0	1039	7	0
67	PP	997	0	1045	1	0
68	QQ	1128	0	1195	2	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	2	0
71	TT	1097	0	1132	4	0
72	UU	795	0	862	1	0
73	VV	636	0	637	3	0
74	WW	1034	0	1080	7	0
75	XX	1098	0	1167	6	0
76	YY	1011	0	1083	3	0
77	ZZ	598	0	656	1	0
78	aa	814	0	863	4	0
79	bb	651	0	672	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	cc	488	0	514	10	0
81	dd	459	0	448	2	0
82	ee	443	0	492	0	0
83	ff	555	0	567	3	0
84	gg	2436	0	2393	6	0
85	hh	169	0	86	0	0
86	ii	2947	0	2957	18	0
87	jj	3292	0	3371	23	0
88	5	176	0	0	0	0
88	7	5	0	0	0	0
88	8	6	0	0	0	0
88	9	66	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	L	1	0	0	0	0
88	P	2	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	1	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	2	0
89	o	1	0	0	0	0
89	p	1	0	0	1	0
90	jj	32	0	14	0	0
All	All	222005	0	166949	752	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (752) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:C5'	48:5:922(A):G:H3'	1.43	1.44
48:5:3914:U:O4	48:5:4378:A:N1	1.57	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:H5''	48:5:922(B):C:O5'	1.25	1.32
48:5:922:C:H5'	48:5:922(A):G:C3'	1.57	1.31
51:9:1137:U:O4	51:9:1148:A:N1	1.67	1.27
48:5:922:C:H5''	48:5:922(B):C:P	1.74	1.26
48:5:922:C:H2'	48:5:922(B):C:C2	1.67	1.26
83:ff:144:CYS:SG	89:ff:200:ZN:ZN	1.27	1.24
48:5:77:U:O4	48:5:336:A:N1	1.73	1.21
48:5:1524:A:N6	48:5:1652:U:H3	1.36	1.20
48:5:922:C:C5'	48:5:922(B):C:O5'	1.89	1.20
51:9:1137:U:C4	51:9:1148:A:N1	2.10	1.20
48:5:922:C:P	48:5:922(B):C:O5'	2.08	1.12
48:5:922:C:C5'	48:5:922(B):C:P	2.39	1.09
51:9:1293:A:N6	51:9:1306:U:N3	2.03	1.06
48:5:77:U:H3	48:5:336:A:N6	1.54	1.04
48:5:1524:A:N1	48:5:1652:U:O4	1.93	1.01
51:9:613:G:N2	51:9:629:A:OP1	1.92	1.01
51:9:1137:U:O4	51:9:1148:A:C2	2.14	1.00
48:5:1411:C:O4'	48:5:1411(B):C:H2'	1.61	0.99
51:9:628:A:N6	51:9:1500:G:H21	1.61	0.98
48:5:922(B):C:O2'	48:5:923:C:C5'	2.12	0.97
48:5:1411:C:H5'	48:5:1411(B):C:O3'	1.65	0.96
86:ii:45:ARG:NH2	86:ii:94:VAL:HG13	1.81	0.95
38:m:73:CYS:HG	89:m:200:ZN:ZN	0.61	0.94
48:5:2409:U:C4	48:5:2783:A:N1	2.36	0.93
86:ii:44:ILE:HD11	86:ii:62:ARG:NH2	1.81	0.93
48:5:922:C:C2'	48:5:922(B):C:C2	2.52	0.93
48:5:1411:C:H4'	48:5:1411(C):C:O4'	1.68	0.92
41:p:60:CYS:HG	89:p:100:ZN:ZN	0.62	0.89
51:9:872:A:N1	51:9:914:U:O4	2.05	0.89
86:ii:45:ARG:NH1	86:ii:99:TYR:O	2.08	0.86
48:5:922:C:O3'	48:5:922(B):C:C6	2.29	0.86
51:9:1137:U:O4	51:9:1148:A:C6	2.30	0.85
86:ii:45:ARG:HH22	86:ii:94:VAL:HG13	1.40	0.85
48:5:922(B):C:O2'	48:5:923:C:H5''	1.76	0.84
48:5:922:C:H5'	48:5:922(A):G:H3'	0.84	0.83
48:5:922(B):C:O2'	48:5:923:C:O5'	1.97	0.82
48:5:1974:U:N3	48:5:2002:A:C6	2.47	0.82
48:5:922:C:C5'	48:5:922(A):G:C3'	2.31	0.82
48:5:2409:U:O4	48:5:2783:A:N1	2.14	0.81
51:9:1680:G:O2'	80:cc:20:ARG:HD3	1.80	0.81
48:5:922:C:O5'	48:5:922(A):G:H3'	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3914:U:C4	48:5:4378:A:N1	2.50	0.79
48:5:922(B):C:O2'	48:5:923:C:P	2.41	0.77
51:9:612:U:O2	51:9:629:A:N6	2.17	0.76
51:9:872:A:N1	51:9:914:U:C4	2.53	0.76
48:5:922:C:H2'	48:5:922(B):C:N1	2.01	0.75
48:5:922:C:O5'	48:5:922(B):C:O5'	2.05	0.75
51:9:628:A:H62	51:9:1500:G:H21	1.33	0.75
48:5:77:U:C4	48:5:336:A:N1	2.54	0.74
48:5:1411:C:C4'	48:5:1411(C):C:O4'	2.36	0.74
48:5:922:C:P	48:5:922(B):C:P	2.86	0.73
48:5:3914:U:O4	48:5:4378:A:C2	2.41	0.73
48:5:922:C:C6	48:5:922(A):G:C5	2.77	0.73
51:9:1293:A:C6	51:9:1306:U:N3	2.57	0.72
51:9:1137:U:C4	51:9:1148:A:C6	2.78	0.72
38:m:73:CYS:SG	89:m:200:ZN:ZN	1.77	0.71
51:9:1293:A:N6	51:9:1306:U:C2	2.59	0.70
48:5:3914:U:H3	48:5:4378:A:N6	1.88	0.70
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.75	0.69
48:5:3914:U:N3	48:5:4378:A:N6	2.40	0.69
48:5:922:C:H5'	48:5:922(A):G:C2'	2.22	0.68
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.74	0.68
48:5:922:C:C3'	48:5:922(B):C:O4'	2.42	0.68
48:5:738:C:O2'	48:5:738(A):C:O4'	2.05	0.67
48:5:1411:C:HO2'	48:5:1411(C):C:H6	1.41	0.67
48:5:2395:A:O2'	48:5:2806:A:H1'	1.94	0.67
51:9:1679:A:OP1	80:cc:20:ARG:NH1	2.28	0.67
48:5:922:C:C6	48:5:922:C:H3'	2.30	0.66
84:gg:79:LEU:HD22	84:gg:111:VAL:HG21	1.75	0.66
37:l:2:SER:N	48:5:2406:G:N7	2.43	0.66
48:5:922:C:C2'	48:5:922(B):C:N1	2.58	0.66
87:jj:613:ILE:HD12	87:jj:643:VAL:HG21	1.76	0.66
51:9:1293:A:N6	51:9:1306:U:C4	2.56	0.66
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.77	0.66
51:9:613:G:C2	51:9:629:A:OP1	2.48	0.65
80:cc:20:ARG:HH21	80:cc:20:ARG:HG3	1.61	0.65
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.79	0.65
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.70	0.65
48:5:747:A:H4'	48:5:748:G:OP1	1.97	0.65
87:jj:392:LEU:HD23	87:jj:666:MET:HE2	1.78	0.65
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.78	0.65
48:5:922:C:H2'	48:5:922(B):C:N3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:222:C:H2'	48:5:223:G:O4'	1.97	0.64
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.31	0.64
18:S:127:MET:HE1	19:T:155:PRO:HA	1.78	0.63
48:5:1974:U:C4	48:5:2002:A:N6	2.67	0.63
48:5:1411:C:O2'	48:5:1411(C):C:C6	2.51	0.63
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.81	0.63
51:9:613:G:N1	51:9:629:A:OP1	2.30	0.62
48:5:922:C:O5'	48:5:922(A):G:P	2.57	0.62
51:9:1680:G:H4'	80:cc:20:ARG:HD2	1.81	0.62
52:AA:63:ARG:HG3	52:AA:185:MET:HE1	1.81	0.62
86:ii:45:ARG:HH21	86:ii:94:VAL:HG22	1.64	0.62
3:C:341:LEU:HD21	5:E:52:LEU:HD21	1.82	0.62
84:gg:87:LEU:HD21	84:gg:108:VAL:HG11	1.82	0.62
3:C:101:MET:SD	3:C:104:PRO:HA	2.40	0.62
48:5:1411:C:O2'	48:5:1411(C):C:H6	1.83	0.62
51:9:1130:G:H2'	51:9:1130:G:N3	2.14	0.62
51:9:613:G:H22	51:9:629:A:P	2.21	0.61
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.81	0.61
48:5:1370:G:O2'	48:5:1371:A:OP2	2.18	0.61
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.49	0.61
51:9:628:A:N6	51:9:1500:G:N2	2.41	0.61
48:5:922:C:C5'	48:5:922(A):G:O3'	2.49	0.61
51:9:96:C:O2	51:9:473:A:O2'	2.18	0.61
51:9:1680:G:O2'	80:cc:20:ARG:CD	2.49	0.60
51:9:1407:U:H2'	51:9:1408:U:C6	2.35	0.60
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.83	0.60
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.99	0.60
51:9:1293:A:N1	51:9:1306:U:O4	2.33	0.60
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.84	0.60
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.82	0.60
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.82	0.60
86:ii:44:ILE:HD11	86:ii:62:ARG:HH21	1.65	0.60
48:5:922:C:P	48:5:922(B):C:C5'	2.89	0.60
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.34	0.60
48:5:742:G:C2	48:5:922(A):G:C6	2.90	0.60
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	2.01	0.60
48:5:3723:A:H2'	48:5:3724:A:C8	2.37	0.60
48:5:4942:C:H4'	48:5:4943:A:OP1	2.02	0.60
48:5:4510:A:O2'	48:5:4511:A:O4'	2.20	0.60
51:9:183:G:O2'	51:9:184:G:O5'	2.20	0.59
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:872:A:C6	51:9:914:U:O4	2.55	0.59
48:5:922:C:O3'	48:5:922:C:O5'	2.20	0.59
14:O:72:HIS:N	48:5:4586:G:OP1	2.33	0.59
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.85	0.58
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.38	0.58
40:o:68:LEU:HD11	40:o:85:ILE:HD11	1.85	0.58
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.38	0.58
2:B:89:ILE:HD13	2:B:153:MET:HE1	1.86	0.58
87:jj:283:LEU:HB3	87:jj:453:ILE:HD11	1.86	0.58
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.87	0.57
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.69	0.57
18:S:93:MET:HE1	18:S:117:HIS:NE2	2.20	0.57
51:9:29:G:H4'	75:XX:129:SER:HB2	1.86	0.57
51:9:501:C:H2'	51:9:501:C:O2	2.04	0.57
51:9:945:U:H2'	51:9:946:U:C6	2.40	0.57
48:5:961:G:C6	48:5:962:C:C4	2.93	0.57
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.36	0.57
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.86	0.56
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.41	0.56
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.56
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.87	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.23	0.56
48:5:245:C:O4'	48:5:245:C:O2	2.23	0.56
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.39	0.56
48:5:481:G:O6	48:5:481(A):C:H5''	2.05	0.56
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.87	0.56
48:5:1524:A:N6	48:5:1652:U:N3	2.18	0.56
30:e:38:PRO:HD2	30:e:55:MET:HE3	1.88	0.56
48:5:77:U:O4	48:5:336:A:C2	2.57	0.56
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.86	0.56
3:C:334:THR:HG21	6:F:50:TYR:OH	2.06	0.56
11:L:71:ARG:NH2	48:5:74:G:O3'	2.39	0.55
51:9:1401:A:C2	51:9:1402:A:C6	2.94	0.55
48:5:1974:U:N3	48:5:2002:A:N6	2.55	0.55
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.41	0.55
74:WW:3:ARG:HD3	74:WW:6:VAL:HG22	1.88	0.55
18:S:84:TYR:CE1	18:S:93:MET:HE3	2.41	0.55
48:5:738(A):C:H5''	48:5:739:G:H5''	1.89	0.55
48:5:4723:A:H2'	48:5:4724:A:C8	2.42	0.55
51:9:980:A:H2'	51:9:981:A:C8	2.42	0.55
51:9:1824:A:N3	51:9:1824:A:H2'	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2409:U:C4	48:5:2783:A:C2	2.95	0.54
48:5:294:G:O6	48:5:315:G:H1'	2.07	0.54
48:5:922:C:O5'	48:5:922(A):G:C3'	2.49	0.54
48:5:3810:C:O4'	48:5:3810:C:O2	2.25	0.54
51:9:94:G:O2'	51:9:508:A:O2'	2.26	0.54
60:II:27:TYR:CE1	60:II:28:GLU:HG3	2.43	0.54
48:5:922:C:C3'	48:5:922(B):C:C6	2.91	0.54
48:5:922:C:C6	48:5:922:C:C3'	2.91	0.54
48:5:1411:C:HO2'	48:5:1411(C):C:C1'	2.20	0.54
51:9:1589:A:N3	51:9:1653:U:O2'	2.38	0.54
51:9:1438:A:H2'	51:9:1439:A:C8	2.43	0.54
51:9:1012:A:H2'	51:9:1013:U:O4'	2.08	0.54
2:B:14:LEU:HD23	2:B:17:LEU:HD23	1.90	0.54
51:9:872:A:C6	51:9:914:U:C4	2.96	0.54
48:5:2505:C:O2	48:5:2505:C:O4'	2.24	0.54
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.37	0.54
48:5:113:A:H2'	48:5:114:G:O4'	2.08	0.53
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.41	0.53
48:5:1483:C:O2	48:5:1483:C:O4'	2.24	0.53
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.24	0.53
51:9:1535:U:H2'	51:9:1535:U:O2	2.08	0.53
48:5:935:A:N6	48:5:935(A):G:H3'	2.22	0.53
51:9:1117:C:O2'	51:9:1118:C:O4'	2.26	0.53
51:9:1823:A:H3'	51:9:1824:A:H5'	1.90	0.53
48:5:2088:A:O2'	48:5:2089:G:OP2	2.25	0.53
87:jj:534:ILE:HD11	87:jj:544:ALA:HB3	1.91	0.53
6:F:90:PHE:CD2	6:F:243:ILE:HD11	2.44	0.53
48:5:2627:C:O4'	48:5:2627:C:O2	2.27	0.53
51:9:434:G:H2'	51:9:435:A:C8	2.44	0.53
51:9:853:C:O4'	51:9:853:C:O2	2.24	0.53
51:9:1315:U:O2	51:9:1315:U:O4'	2.27	0.53
48:5:1524:A:N1	48:5:1652:U:C4	2.74	0.53
52:AA:38:ILE:HD11	52:AA:150:THR:HG22	1.89	0.53
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.49	0.53
5:E:165:VAL:HG12	5:E:178:VAL:HG22	1.91	0.53
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.39	0.52
7:G:101:LYS:HB3	23:X:42:THR:HG23	1.90	0.52
51:9:1137:U:N3	51:9:1148:A:N6	2.57	0.52
51:9:1139:C:O4'	51:9:1139:C:O2	2.23	0.52
48:5:4989:U:O2	48:5:4989:U:O4'	2.27	0.52
59:HH:27:LEU:HD13	59:HH:45:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:529:CYS:SG	87:jj:556:GLY:N	2.82	0.52
48:5:922:C:H5'	48:5:922(A):G:O3'	2.08	0.52
51:9:501:C:O2	51:9:501:C:C2'	2.58	0.52
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.90	0.52
48:5:1411:C:H1'	48:5:1411(C):C:C6	2.44	0.52
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.92	0.52
48:5:1961:G:O2'	48:5:2025:A:N6	2.43	0.52
2:B:174:ARG:NH1	48:5:4985:U:O2	2.43	0.52
4:D:16:TYR:O	49:7:11:A:N6	2.42	0.52
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.45	0.52
48:5:1411(C):C:H2'	48:5:1412:G:O4'	2.10	0.52
48:5:224:U:O2	48:5:224:U:O4'	2.27	0.52
48:5:738:C:O3'	48:5:738(A):C:H5'	2.10	0.52
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.92	0.52
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.40	0.52
48:5:922:C:H5''	48:5:922(B):C:OP1	2.09	0.52
48:5:1872:G:O2'	48:5:4219:A:N3	2.39	0.52
58:GG:132:ARG:HB3	58:GG:133:LEU:HD12	1.92	0.52
12:M:15:VAL:HG22	12:M:50:MET:HE1	1.92	0.52
40:o:41:TYR:CD1	47:3:75:C:O2	2.63	0.51
48:5:2408:U:O4'	48:5:2409:U:C5	2.63	0.51
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.44	0.51
48:5:934:C:O4'	48:5:935(A):G:O4'	2.28	0.51
51:9:925:G:N2	65:NN:48:SER:OG	2.44	0.51
30:e:31:ILE:HD11	48:5:2347:A:C4	2.45	0.51
51:9:146:G:O2'	51:9:147:A:O5'	2.22	0.51
86:ii:225:ALA:HB2	86:ii:233:LEU:HD23	1.93	0.51
12:M:94:LYS:NZ	48:5:4872:G:OP2	2.43	0.51
48:5:2409:U:O4	48:5:2783:A:C6	2.64	0.51
48:5:4579:U:H2'	48:5:4580:U:C6	2.46	0.51
51:9:1351:G:O2'	51:9:1378:A:N1	2.36	0.51
86:ii:45:ARG:NH2	86:ii:94:VAL:CG1	2.65	0.51
87:jj:619:VAL:HG23	87:jj:632:PRO:HG3	1.93	0.51
51:9:1262:C:O2'	81:dd:12:ARG:NH1	2.40	0.51
48:5:922:C:O5'	48:5:922(A):G:O5'	2.29	0.51
48:5:4305:G:C2'	48:5:4305:G:N3	2.74	0.51
51:9:1364:U:O4'	51:9:1364:U:O2	2.29	0.51
3:C:138:MET:HG2	3:C:144:ILE:HG22	1.93	0.51
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.93	0.51
48:5:922(B):C:C4	48:5:923:C:C5	2.99	0.51
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4871:C:O4'	48:5:4871:C:O2	2.29	0.51
86:ii:150:CYS:SG	86:ii:159:THR:HG22	2.51	0.51
48:5:923:C:C5	48:5:926:G:O4'	2.64	0.51
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.46	0.51
54:CC:253:PRO:HA	54:CC:256:TRP:CD1	2.45	0.51
4:D:208:MET:HE1	4:D:236:MET:HE1	1.93	0.50
48:5:1888:A:N6	48:5:3873:G:O2'	2.44	0.50
48:5:4476:C:O2'	48:5:4478:G:OP2	2.28	0.50
51:9:823:U:O2	51:9:823:U:O4'	2.29	0.50
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.93	0.50
28:c:82:GLY:HA2	28:c:91:VAL:HG12	1.93	0.50
50:8:125:C:O2	50:8:125:C:O4'	2.30	0.50
35:j:19:CYS:SG	35:j:20:ARG:N	2.85	0.50
48:5:1818:G:O2'	48:5:1819:G:OP1	2.21	0.50
48:5:2097:A:OP1	48:5:2107:A:N6	2.45	0.50
51:9:1130:G:O2'	51:9:1131:G:O5'	2.30	0.50
57:FF:126:THR:HG21	80:cc:27:CYS:SG	2.50	0.50
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.93	0.50
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.94	0.50
40:o:81:ARG:NH2	48:5:4293:U:O2'	2.45	0.50
48:5:1381:U:O2	48:5:1381:U:O4'	2.29	0.50
51:9:1444:U:H2'	51:9:1445:U:C6	2.47	0.50
2:B:49:TYR:CE2	2:B:168:MET:HE1	2.46	0.50
53:BB:134:LEU:HD23	53:BB:218:LEU:HD12	1.94	0.50
48:5:3766:A:N1	51:9:1827:U:O2'	2.37	0.50
5:E:185:ASN:ND2	5:E:274:LEU:O	2.45	0.49
31:f:43:LEU:HD22	31:f:76:ARG:HA	1.93	0.49
32:g:59:VAL:HG21	32:g:63:VAL:HG11	1.93	0.49
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.46	0.49
84:gg:81:GLY:HA2	84:gg:87:LEU:HD23	1.95	0.49
87:jj:261:LEU:HD23	87:jj:364:VAL:HG21	1.94	0.49
48:5:2094:C:O2	48:5:2094:C:O4'	2.30	0.49
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.93	0.49
51:9:1129:G:C6	51:9:1130:G:O6	2.65	0.49
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.45	0.49
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.44	0.49
21:V:60:MET:HE1	21:V:78:PRO:HB2	1.95	0.49
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.41	0.49
75:XX:51:VAL:HG22	75:XX:70:VAL:HG11	1.95	0.49
1:A:48:ILE:HG22	41:p:54:ILE:HD12	1.95	0.49
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.94	0.49
51:9:1719:A:N6	51:9:1814:G:O2'	2.44	0.49
54:CC:137:VAL:HG21	54:CC:244:ILE:HD12	1.94	0.49
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.93	0.49
9:I:72:ALA:HB3	9:I:136:MET:HE1	1.94	0.49
13:N:68:ARG:HG2	48:5:302:C:OP1	2.12	0.49
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.43	0.49
48:5:964:A:H2'	48:5:965:G:O4'	2.12	0.49
48:5:1237:C:O2	48:5:1237:C:O4'	2.30	0.49
51:9:107:A:C2	51:9:355:G:C2	3.01	0.49
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.94	0.49
48:5:922:C:O3'	48:5:922(B):C:O4'	2.31	0.49
51:9:584:A:C6	51:9:585:C:C4	3.01	0.49
17:R:102:LEU:HD22	17:R:138:LEU:HD12	1.95	0.49
35:j:63:ARG:NH2	50:8:58:G:N7	2.61	0.49
51:9:604:A:C6	51:9:605:A:N1	2.81	0.49
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.94	0.49
2:B:41:VAL:HA	2:B:187:GLY:HA3	1.95	0.48
2:B:47:LEU:HD23	2:B:166:THR:HG23	1.94	0.48
6:F:161:ILE:HD12	6:F:166:ILE:HB	1.94	0.48
51:9:1520:G:H2'	51:9:1520:G:N3	2.28	0.48
66:OO:116:LEU:HD22	78:aa:53:ILE:HD11	1.94	0.48
2:B:234:ARG:NH2	48:5:4566:U:O2'	2.46	0.48
3:C:130:ALA:HB3	3:C:246:VAL:HG12	1.95	0.48
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.96	0.48
48:5:356:G:O2'	50:8:25:G:N3	2.46	0.48
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.53	0.48
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.95	0.48
48:5:1074:G:C2	48:5:1238:A:C2	3.00	0.48
13:N:179:LYS:O	48:5:297:U:O2'	2.30	0.48
16:Q:184:ARG:NE	26:a:55:LYS:O	2.46	0.48
48:5:2763:U:O2	48:5:2763:U:O4'	2.31	0.48
51:9:612:U:H3	51:9:629:A:H62	1.62	0.48
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.95	0.48
17:R:45:ILE:HG12	17:R:50:ILE:HD11	1.95	0.48
53:BB:105:LEU:HD23	53:BB:213:ARG:HA	1.95	0.48
60:II:190:LEU:HD12	60:II:194:GLU:HB3	1.96	0.48
73:VV:55:ILE:HD11	73:VV:69:ILE:HG12	1.94	0.48
28:c:29:LEU:HD22	28:c:91:VAL:HG21	1.96	0.48
51:9:490:C:O2'	51:9:574:A:N1	2.45	0.48
86:ii:40:ARG:HB3	86:ii:66:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:193:THR:HG23	14:O:202:LEU:HD23	1.96	0.48
48:5:4709:U:C4	48:5:4710:C:C4	3.01	0.48
75:XX:41:PHE:CE1	75:XX:47:ALA:HB3	2.48	0.48
7:G:210:ILE:HG23	7:G:220:VAL:HG11	1.96	0.48
42:r:98:ARG:NH2	48:5:2262:G:OP2	2.46	0.48
51:9:887:U:O2	51:9:887:U:O4'	2.31	0.48
7:G:189:LEU:HD21	7:G:257:PHE:CE1	2.49	0.48
26:a:61:TYR:N	48:5:4354:U:O4	2.46	0.48
63:LL:4:ILE:HD12	63:LL:56:ILE:HD11	1.95	0.48
87:jj:594:ILE:HD11	87:jj:674:ILE:CG2	2.44	0.48
1:A:207:VAL:HG23	1:A:208:GLU:HG3	1.96	0.47
3:C:334:THR:HG22	3:C:337:ARG:HH22	1.79	0.47
26:a:12:ARG:HD3	48:5:1660:U:H2'	1.96	0.47
44:t:98:ILE:HG23	44:t:98:ILE:O	2.14	0.47
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.43	0.47
74:WW:55:ASP:O	74:WW:57:ARG:N	2.47	0.47
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.49	0.47
18:S:80:ILE:HG23	18:S:129:VAL:HG22	1.95	0.47
48:5:1411:C:O5'	48:5:1411(C):C:C5'	2.62	0.47
29:d:36:VAL:HG23	29:d:41:ARG:HG3	1.96	0.47
51:9:1568:C:OP1	71:TT:96:SER:OG	2.29	0.47
48:5:1406:G:C8	48:5:1406(C):G:H2'	2.49	0.47
51:9:1551:U:O2	51:9:1551:U:O4'	2.32	0.47
48:5:922:C:C5	48:5:922(A):G:C5	3.02	0.47
52:AA:18:PHE:HD2	52:AA:51:LEU:HD22	1.79	0.47
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.45	0.47
80:cc:20:ARG:HG3	80:cc:20:ARG:NH2	2.28	0.47
6:F:88:LEU:HD22	6:F:89:ALA:N	2.29	0.47
48:5:2473:A:C2	48:5:2506:G:C2	3.02	0.47
11:L:108:GLU:N	11:L:108:GLU:OE1	2.47	0.47
18:S:13:VAL:HG23	18:S:62:VAL:HB	1.96	0.47
48:5:1411:C:O4'	48:5:1411(B):C:C2'	2.49	0.47
48:5:4524:G:H4'	48:5:4524:G:OP2	2.13	0.47
48:5:4977:A:H2'	48:5:4978:G:O4'	2.14	0.47
51:9:943:U:OP2	53:BB:216:LYS:NZ	2.43	0.47
51:9:1130:G:O2'	51:9:1131:G:P	2.72	0.47
51:9:1624:U:O2	51:9:1624:U:O4'	2.32	0.47
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.96	0.47
48:5:481(A):C:O2	48:5:481(A):C:O4'	2.30	0.47
48:5:1337:A:C2	48:5:2349:A:C2	3.03	0.47
48:5:2268:A:H4'	48:5:2269:C:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1597:C:H4'	51:9:1603:G:O6	2.15	0.47
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.48	0.47
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.96	0.47
51:9:495:U:H2'	51:9:496:C:O4'	2.15	0.47
52:AA:18:PHE:CD1	52:AA:173:LEU:HD11	2.49	0.47
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.49	0.47
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.50	0.47
78:aa:45:VAL:HG11	78:aa:53:ILE:CD1	2.45	0.47
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.44	0.46
40:o:15:CYS:SG	40:o:19:GLN:NE2	2.88	0.46
48:5:1332:C:H2'	48:5:1333:A:C8	2.50	0.46
48:5:1990:A:H3'	48:5:1991:A:H5''	1.97	0.46
63:LL:113:LEU:HD23	63:LL:142:VAL:HG21	1.97	0.46
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.96	0.46
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	1.97	0.46
48:5:4260:U:H2'	48:5:4261:C:C6	2.50	0.46
66:OO:31:CYS:HB2	66:OO:44:VAL:HG22	1.98	0.46
68:QQ:49:TYR:O	68:QQ:53:GLU:N	2.48	0.46
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.97	0.46
48:5:922:C:C6	48:5:922(A):G:C6	3.03	0.46
48:5:1974:U:C4	48:5:2002:A:C6	3.04	0.46
51:9:928:G:H2'	51:9:929:G:C8	2.51	0.46
56:EE:56:LEU:HD11	76:YY:74:MET:HE1	1.98	0.46
66:OO:44:VAL:HG23	66:OO:81:VAL:HG11	1.98	0.46
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.51	0.46
6:F:119:GLY:O	6:F:120:THR:HG23	2.16	0.46
15:P:69:ARG:NH2	48:5:4568:A:N3	2.64	0.46
44:t:81:ILE:HD11	44:t:132:ILE:HG23	1.96	0.46
1:A:179:ILE:O	48:5:3653:A:H4'	2.15	0.46
48:5:3723:A:C2	48:5:3724:A:C6	3.03	0.46
51:9:297:A:H4'	56:EE:132:GLY:O	2.16	0.46
63:LL:37:TYR:CE2	63:LL:51:ILE:HG23	2.51	0.46
83:ff:126:CYS:SG	83:ff:143:LYS:NZ	2.85	0.46
3:C:323:ARG:NH1	48:5:1281:G:C8	2.84	0.46
11:L:100:PRO:O	34:i:25:ARG:NH2	2.46	0.46
12:M:72:TYR:CE1	48:5:738:C:H4'	2.51	0.46
48:5:498:C:O2	48:5:498:C:O4'	2.29	0.46
48:5:1411:C:H1'	48:5:1411(C):C:N1	2.30	0.46
48:5:4390:A:H2'	48:5:4391:G:O4'	2.15	0.46
51:9:627:U:C5	86:ii:99:TYR:HB2	2.51	0.46
51:9:1143:A:C2	51:9:1144:A:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.97	0.46
3:C:195:LYS:NZ	50:8:21:C:OP1	2.46	0.46
8:H:118:LEU:HD21	8:H:177:ASP:HB2	1.98	0.46
29:d:22:THR:HG22	29:d:89:SER:CB	2.46	0.46
48:5:5066:U:H2'	48:5:5067:U:C6	2.50	0.46
51:9:183:G:N3	51:9:183:G:C2'	2.78	0.46
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.98	0.46
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.98	0.46
87:jj:503:PHE:HE1	87:jj:505:ILE:HD12	1.81	0.46
6:F:69:ARG:NH1	48:5:1209:U:O2'	2.49	0.46
48:5:2408:U:C1'	48:5:2409:U:C5	2.99	0.46
86:ii:33:VAL:HG22	86:ii:112:LEU:HD21	1.97	0.46
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.45	0.45
1:A:227:ARG:NH2	48:5:3659:G:O2'	2.49	0.45
13:N:178:HIS:HA	13:N:181:HIS:NE2	2.31	0.45
48:5:922:C:C3'	48:5:922(B):C:N1	2.79	0.45
52:AA:185:MET:HE3	73:VV:39:VAL:HG21	1.98	0.45
2:B:89:ILE:CD1	2:B:153:MET:HE1	2.45	0.45
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.97	0.45
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.49	0.45
51:9:872:A:N6	51:9:914:U:C4	2.85	0.45
51:9:1238:U:H2'	51:9:1239:U:O4'	2.17	0.45
51:9:1834:A:C2'	51:9:1834:A:N3	2.80	0.45
58:GG:52:ILE:HG23	58:GG:52:ILE:O	2.17	0.45
10:J:141:ILE:HD11	49:7:55:A:N3	2.31	0.45
20:U:33:ILE:HD12	20:U:96:LEU:HD22	1.98	0.45
48:5:3867:A:C6	48:5:3868:G:C6	3.04	0.45
51:9:1823:A:C3'	51:9:1824:A:H5'	2.46	0.45
3:C:33:ARG:HD2	3:C:36:ILE:HD12	1.98	0.45
4:D:22:ARG:HG3	4:D:22:ARG:HH11	1.81	0.45
48:5:2439:G:C6	48:5:2440:U:C4	3.04	0.45
80:cc:14:VAL:HG13	80:cc:30:VAL:HG13	1.98	0.45
86:ii:40:ARG:CB	86:ii:66:THR:HG22	2.46	0.45
2:B:14:LEU:HD23	2:B:17:LEU:CD2	2.46	0.45
3:C:144:ILE:HD11	3:C:150:LEU:HD23	1.99	0.45
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.52	0.45
48:5:114:G:N2	48:5:276:C:O2'	2.50	0.45
51:9:1673:U:H2'	51:9:1674:G:O4'	2.17	0.45
58:GG:32:MET:HE2	58:GG:63:MET:HG2	1.99	0.45
26:a:103:VAL:HG12	26:a:108:TYR:HB2	1.97	0.45
28:c:29:LEU:HD23	28:c:94:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.50	0.45
51:9:1303:C:O2	51:9:1303:C:O4'	2.33	0.45
51:9:1329:U:O2'	51:9:1332:A:OP2	2.27	0.45
53:BB:150:ILE:HD13	69:RR:129:LYS:HB2	1.98	0.45
76:YY:20:ARG:CZ	76:YY:74:MET:HE2	2.46	0.45
87:jj:263:LEU:HD23	87:jj:264:VAL:N	2.32	0.45
3:C:212:ASN:HD22	3:C:255:SER:HB2	1.82	0.45
4:D:39:GLN:HG2	4:D:48:LYS:HB2	1.99	0.45
13:N:48:ALA:HB1	13:N:53:TYR:CB	2.46	0.45
13:N:76:PRO:O	13:N:79:ALA:HB3	2.16	0.45
48:5:66:A:O2'	48:5:326:C:O2	2.35	0.45
59:HH:122:LEU:C	59:HH:122:LEU:HD13	2.41	0.45
65:NN:91:LEU:CD1	65:NN:125:LEU:HD12	2.47	0.45
84:gg:91:ASP:HB2	84:gg:98:THR:HG23	1.99	0.45
87:jj:514:ILE:HD12	87:jj:534:ILE:HD12	1.99	0.45
2:B:84:MET:HE1	2:B:183:ILE:HD11	1.98	0.45
11:L:116:ARG:NH1	11:L:155:MET:O	2.50	0.45
48:5:2363:A:C2	48:5:3860:A:C4	3.05	0.45
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.80	0.45
48:5:1751:A:C2	48:5:1780:A:C2	3.05	0.45
48:5:1411:C:C2'	48:5:1411(C):C:O4'	2.65	0.44
57:FF:123:GLU:OE1	57:FF:204:ARG:NH1	2.50	0.44
48:5:1942:A:N3	48:5:4432:C:O2'	2.46	0.44
48:5:4872:G:H4'	48:5:4873:G:H5''	2.00	0.44
51:9:183:G:O2'	51:9:183:G:N3	2.50	0.44
63:LL:82:MET:HB3	63:LL:85:THR:HG23	2.00	0.44
7:G:132:ALA:HB3	13:N:18:VAL:HG22	1.99	0.44
18:S:53:LYS:NZ	49:7:74:A:O2'	2.51	0.44
48:5:4583:C:O2'	48:5:4718:G:N2	2.50	0.44
51:9:399:C:O2	63:LL:106:HIS:ND1	2.51	0.44
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.99	0.44
87:jj:492:VAL:HG23	87:jj:505:ILE:HG23	2.00	0.44
87:jj:587:ILE:HD11	87:jj:635:LEU:HD13	2.00	0.44
48:5:3620:G:OP1	48:5:3622:C:N4	2.50	0.44
62:KK:11:ILE:CD1	62:KK:45:VAL:HG22	2.47	0.44
56:EE:192:ILE:HD13	56:EE:238:LEU:HD23	2.00	0.44
12:M:7:VAL:HG21	18:S:154:LEU:HD21	1.99	0.44
48:5:1411(A):G:C6	48:5:1411(B):C:C4	3.05	0.44
48:5:1854:G:N2	48:5:4394:A:O4'	2.51	0.44
48:5:4928:C:O4'	48:5:4928:C:O2	2.35	0.44
8:H:12:ILE:HG22	8:H:81:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:119:SER:OG	57:FF:189:ALA:HB1	2.17	0.44
5:E:131:HIS:CD2	48:5:1281:G:C5	3.05	0.44
12:M:97:ALA:HB2	14:O:203:VAL:HB	2.00	0.44
74:WW:42:MET:HE3	74:WW:50:PHE:CD2	2.53	0.44
87:jj:266:ILE:CD1	87:jj:393:VAL:HG21	2.48	0.44
7:G:96:GLN:O	48:5:4124:G:N2	2.50	0.44
40:o:63:THR:O	40:o:87:ARG:NH1	2.50	0.44
48:5:1339:U:H2'	48:5:1340:C:C6	2.53	0.44
48:5:2693:G:C6	48:5:2694:G:N1	2.86	0.44
48:5:3760:A:H2	51:9:1825:A:N3	2.16	0.44
51:9:1489:A:H4'	51:9:1490:G:OP2	2.17	0.44
63:LL:99:TYR:O	63:LL:101:ARG:N	2.50	0.44
86:ii:253:LEU:HD22	86:ii:351:VAL:HG21	1.99	0.44
31:f:47:CYS:HB3	31:f:103:VAL:HG12	1.99	0.43
42:r:16:PHE:CE2	42:r:43:LEU:HD11	2.53	0.43
48:5:1358:G:H4'	48:5:1359:G:OP1	2.19	0.43
48:5:2758:G:O2'	48:5:2765:A:N3	2.44	0.43
48:5:3648:A:C4	48:5:3785:A:C6	3.06	0.43
69:RR:28:PHE:HA	69:RR:55:THR:HG21	1.99	0.43
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.99	0.43
48:5:1633:G:H5'	48:5:1634:A:OP1	2.19	0.43
48:5:4423:U:O2	48:5:4423:U:O4'	2.36	0.43
51:9:314:U:O2	51:9:314:U:H2'	2.18	0.43
51:9:958:G:C6	51:9:959:G:C6	3.06	0.43
51:9:992:A:C2	51:9:993:G:C8	3.06	0.43
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.51	0.43
48:5:2729:C:H2'	48:5:2730:U:O4'	2.18	0.43
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	2.01	0.43
69:RR:119:VAL:HG13	69:RR:119:VAL:O	2.18	0.43
6:F:161:ILE:HB	6:F:166:ILE:HD12	1.99	0.43
48:5:978:G:O2'	48:5:979:C:OP2	2.29	0.43
48:5:1411:C:C4	48:5:1411(B):C:C4	3.07	0.43
51:9:628:A:H61	51:9:1500:G:H21	1.55	0.43
53:BB:38:MET:HE3	53:BB:185:VAL:HG11	2.00	0.43
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.99	0.43
1:A:77:ILE:HD13	1:A:128:ARG:HB2	2.00	0.43
3:C:164:THR:HG21	48:5:223:G:H2'	2.00	0.43
22:W:3:VAL:HG21	22:W:12:LYS:CE	2.48	0.43
26:a:12:ARG:NH2	48:5:1338:G:OP2	2.51	0.43
48:5:4758:U:O2	48:5:4758:U:O4'	2.35	0.43
51:9:520:A:O2'	51:9:825:A:N3	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1825:A:N3	86:ii:62:ARG:CD	2.82	0.43
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	2.00	0.43
1:A:181:LYS:HB2	48:5:1577:G:C5	2.54	0.43
22:W:80:ARG:NH2	58:GG:129:VAL:O	2.52	0.43
26:a:86:THR:HG22	48:5:510:U:H5''	2.00	0.43
51:9:92:A:C6	51:9:446:G:C6	3.06	0.43
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.53	0.43
18:S:80:ILE:HG22	18:S:82:LEU:CD2	2.49	0.43
47:3:75:C:H2'	47:3:76:A:H4'	1.99	0.43
48:5:33:A:C6	48:5:34:A:C6	3.06	0.43
48:5:975:C:C5	48:5:976:G:N7	2.87	0.43
48:5:1632:A:H2'	48:5:1632:A:N3	2.33	0.43
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.49	0.43
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.43
66:OO:95:ILE:HD11	66:OO:126:ILE:HD12	2.00	0.43
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.49	0.43
48:5:369:G:N1	48:5:373:G:C6	2.87	0.43
51:9:1291:A:N3	83:ff:140:TYR:OH	2.52	0.43
53:BB:136:ARG:HB2	53:BB:218:LEU:HD11	2.00	0.43
60:II:3:ILE:HG23	60:II:3:ILE:O	2.18	0.43
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	2.01	0.43
79:bb:53:VAL:HG23	79:bb:53:VAL:O	2.19	0.43
87:jj:263:LEU:HD21	87:jj:366:VAL:CG2	2.48	0.43
87:jj:503:PHE:CE1	87:jj:505:ILE:HD12	2.53	0.43
14:O:116:LYS:HD3	18:S:169:THR:HG21	2.01	0.43
17:R:60:ARG:NH1	17:R:63:CYS:SG	2.91	0.43
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	2.01	0.43
48:5:77:U:H3	48:5:336:A:H61	0.71	0.43
48:5:922:C:H5'	48:5:922(B):C:P	2.47	0.43
48:5:922(B):C:N3	48:5:923:C:C5	2.87	0.43
48:5:3690:U:H2'	48:5:3691:G:O4'	2.19	0.43
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.54	0.43
81:dd:18:SER:OG	81:dd:19:ARG:N	2.52	0.43
87:jj:489:ARG:NH2	87:jj:573:VAL:O	2.51	0.43
12:M:17:PHE:CE1	12:M:54:CYS:HA	2.54	0.43
25:Z:23:ALA:HA	25:Z:45:GLY:HA2	2.01	0.43
48:5:1390:G:N2	48:5:1393:G:OP2	2.49	0.43
51:9:1666:C:H2'	51:9:1667:U:O4'	2.19	0.43
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.54	0.43
40:o:66:ILE:HD13	40:o:91:PHE:CZ	2.54	0.42
51:9:1664:A:H4'	51:9:1665:G:OP1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:87:MET:HE1	56:EE:236:ILE:HD13	2.00	0.42
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.19	0.42
59:HH:133:LEU:HD22	59:HH:173:PHE:CD1	2.54	0.42
84:gg:299:PHE:CD2	84:gg:309:VAL:HG12	2.54	0.42
4:D:33:ARG:NH1	4:D:72:ASP:OD2	2.52	0.42
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.01	0.42
48:5:750:U:H2'	48:5:751:G:O4'	2.18	0.42
51:9:107:A:C6	51:9:108:G:C6	3.07	0.42
55:DD:48:ILE:HG23	55:DD:86:LEU:HD12	2.01	0.42
71:TT:42:HIS:HB2	71:TT:83:GLN:HA	2.01	0.42
5:E:167:PHE:CE1	5:E:176:LEU:HD22	2.54	0.42
9:I:191:ILE:HD11	9:I:212:LEU:HD11	2.00	0.42
14:O:42:ASN:OD1	14:O:42:ASN:N	2.52	0.42
26:a:36:GLY:N	48:5:39:A:OP2	2.52	0.42
48:5:209:U:C4	48:5:233:U:C4	3.08	0.42
48:5:2750:G:H2'	48:5:2751:G:O4'	2.19	0.42
49:7:14:C:C4	49:7:66:G:N2	2.87	0.42
51:9:830:A:OP2	51:9:846:G:N2	2.52	0.42
51:9:933:G:H1'	51:9:1001:A:O4'	2.19	0.42
57:FF:34:SER:HA	80:cc:55:VAL:HB	2.01	0.42
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.54	0.42
20:U:84:LYS:HA	20:U:87:THR:HG22	2.02	0.42
48:5:1493:G:C6	48:5:1494:U:C2	3.07	0.42
48:5:3656:A:O4'	48:5:3747:A:C2	2.72	0.42
48:5:4305:G:N3	48:5:4305:G:H2'	2.33	0.42
80:cc:30:VAL:HG12	80:cc:32:VAL:HG13	2.01	0.42
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.51	0.42
30:e:44:ARG:NH2	48:5:1312:A:O2'	2.52	0.42
48:5:67:C:OP2	48:5:312:G:N2	2.52	0.42
48:5:916:C:O2	48:5:916:C:O4'	2.37	0.42
51:9:615:C:H2'	51:9:616:A:C8	2.54	0.42
5:E:180:GLY:O	5:E:181:PRO:C	2.62	0.42
30:e:126:ASN:OD1	30:e:126:ASN:N	2.53	0.42
51:9:62:G:H4'	51:9:172:U:C5	2.55	0.42
51:9:625:G:H4'	51:9:629:A:C4	2.55	0.42
53:BB:137:LEU:HB3	53:BB:172:MET:HE3	2.01	0.42
64:MM:49:LEU:C	64:MM:49:LEU:HD13	2.44	0.42
78:aa:11:ALA:HB3	78:aa:33:ASP:HB2	2.02	0.42
1:A:207:VAL:HG11	48:5:1633:G:C6	2.54	0.42
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.54	0.42
48:5:3724:A:N6	48:5:3725:G:C6	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4291:G:H5''	48:5:4291:G:N3	2.35	0.42
48:5:4966:A:C2	48:5:4967:A:C2	3.08	0.42
51:9:1245:G:O2'	51:9:1492:U:OP1	2.28	0.42
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.49	0.42
56:EE:185:GLY:N	56:EE:189:LEU:HD13	2.35	0.42
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.19	0.42
87:jj:263:LEU:HD21	87:jj:366:VAL:HG23	2.02	0.42
1:A:101:VAL:HB	1:A:165:VAL:HG12	2.02	0.42
21:V:64:THR:HG21	48:5:3799:A:OP1	2.19	0.42
48:5:4525:C:H2'	48:5:4526:U:O4'	2.20	0.42
87:jj:352:ILE:N	87:jj:353:PRO:CD	2.82	0.42
18:S:28:TYR:CD2	18:S:54:MET:HE1	2.55	0.42
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.49	0.42
51:9:183:G:O2'	51:9:184:G:O4'	2.36	0.42
60:II:36:THR:HG21	60:II:179:PRO:HB2	2.01	0.42
62:KK:35:LEU:CD1	62:KK:40:VAL:HG21	2.49	0.42
87:jj:266:ILE:HG23	87:jj:389:HIS:HB3	2.01	0.42
87:jj:396:LEU:C	87:jj:396:LEU:HD23	2.45	0.42
29:d:33:ILE:O	29:d:36:VAL:HG22	2.20	0.41
35:j:12:ARG:NH2	48:5:1617:G:O3'	2.53	0.41
51:9:57:U:OP1	51:9:504:G:O2'	2.32	0.41
51:9:1825:A:N1	86:ii:108:ARG:HG2	2.35	0.41
53:BB:103:MET:HE1	53:BB:212:VAL:HG23	2.01	0.41
53:BB:212:VAL:HG23	53:BB:212:VAL:O	2.20	0.41
13:N:42:PRO:HD3	13:N:61:ILE:HD12	2.01	0.41
48:5:2031:C:O3'	48:5:2032:U:P	2.78	0.41
48:5:4515:G:C2	48:5:4516:G:C8	3.09	0.41
51:9:35:C:O2	51:9:520:A:N1	2.53	0.41
51:9:1843:G:H2'	51:9:1844:U:O4'	2.20	0.41
56:EE:181:CYS:SG	56:EE:225:ILE:HG23	2.60	0.41
75:XX:105:PHE:CG	75:XX:112:VAL:HG21	2.55	0.41
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.56	0.41
4:D:61:ILE:HG23	4:D:79:TYR:CE2	2.55	0.41
18:S:83:ARG:HB2	18:S:127:MET:HE3	2.02	0.41
48:5:976:G:N2	48:5:977:C:C2	2.88	0.41
48:5:1301:C:O2	48:5:1301:C:O4'	2.34	0.41
51:9:1162:C:H2'	51:9:1163:C:O4'	2.20	0.41
84:gg:5:MET:HE1	84:gg:312:VAL:HG22	2.02	0.41
2:B:36:ASP:OD1	2:B:36:ASP:N	2.53	0.41
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.51	0.41
12:M:23:LYS:HE3	48:5:935:A:H3'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922(A):G:OP1	48:5:922(B):C:C5	2.74	0.41
48:5:961:G:C6	48:5:971(A):G:C4	3.09	0.41
48:5:5047:C:O2'	48:5:5050:C:OP2	2.36	0.41
51:9:1137:U:H3	51:9:1148:A:N6	2.18	0.41
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.02	0.41
2:B:91:GLY:CA	2:B:153:MET:HE3	2.50	0.41
2:B:92:TYR:HB3	2:B:99:LEU:HD21	2.02	0.41
7:G:241:ALA:O	7:G:245:ARG:N	2.54	0.41
17:R:11:ALA:HB1	17:R:50:ILE:HD13	2.03	0.41
25:Z:41:ALA:HB2	25:Z:77:TYR:HE1	1.85	0.41
26:a:132:ARG:NH1	48:5:1468:C:OP1	2.48	0.41
29:d:36:VAL:HG23	29:d:41:ARG:CG	2.49	0.41
48:5:492:U:O2'	48:5:493:G:P	2.78	0.41
48:5:1411:C:O2'	48:5:1411(C):C:H3'	2.21	0.41
48:5:3876:A:O2'	48:5:3877:A:P	2.79	0.41
51:9:1734:G:O2'	51:9:1800:A:N6	2.52	0.41
56:EE:31:PRO:HD2	56:EE:38:LEU:CD1	2.50	0.41
63:LL:96:ILE:N	63:LL:96:ILE:HD12	2.35	0.41
74:WW:104:LEU:HB3	74:WW:125:ILE:HA	2.01	0.41
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.60	0.41
6:F:113:LEU:HD22	6:F:118:ASN:O	2.20	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.01	0.41
26:a:21:ARG:NH1	48:5:1317:U:OP1	2.53	0.41
48:5:922:C:C2'	48:5:922(B):C:C1'	2.98	0.41
48:5:1411:C:C1'	48:5:1411(C):C:O4'	2.69	0.41
56:EE:182:MET:CE	56:EE:192:ILE:HD11	2.50	0.41
69:RR:111:PHE:HB3	69:RR:114:LEU:HD21	2.03	0.41
16:Q:43:PHE:CD2	16:Q:133:GLY:HA3	2.56	0.41
33:h:44:LEU:O	33:h:47:ILE:HG22	2.20	0.41
48:5:1651:G:N1	48:5:1652:U:C4	2.89	0.41
51:9:1520:G:N3	51:9:1520:G:C2'	2.83	0.41
57:FF:116:ILE:HD12	57:FF:151:ILE:HG13	2.01	0.41
87:jj:539:GLU:N	87:jj:540:PRO:CD	2.84	0.41
20:U:23:LEU:HD11	20:U:83:LEU:HD23	2.03	0.41
51:9:15:U:H2'	51:9:16:G:O4'	2.21	0.41
51:9:1276:A:N6	51:9:1321:G:O2'	2.54	0.41
55:DD:132:LYS:HE3	55:DD:156:LEU:HD23	2.01	0.41
87:jj:604:TYR:O	87:jj:605:GLN:C	2.64	0.41
48:5:119:G:H3'	48:5:120:A:C5'	2.50	0.41
48:5:1523:A:N7	48:5:1652:U:C4	2.89	0.41
48:5:1804:A:O2'	48:5:1805:A:OP2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:427:U:O2	51:9:427:U:O4'	2.38	0.41
51:9:1735:A:C4	51:9:1800:A:C2	3.08	0.41
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	2.02	0.41
54:CC:188:CYS:SG	54:CC:235:ASN:HA	2.61	0.41
86:ii:65:LEU:HD21	86:ii:94:VAL:HG21	2.02	0.41
86:ii:313:ILE:N	86:ii:313:ILE:HD13	2.36	0.41
3:C:144:ILE:HG12	3:C:147:VAL:HG21	2.02	0.41
6:F:97:ILE:HD11	16:Q:4:ASP:CG	2.46	0.41
28:c:52:CYS:HB2	28:c:92:CYS:SG	2.60	0.41
48:5:922:C:O2'	48:5:922(B):C:C2	2.74	0.41
48:5:1411:C:C4	48:5:1411(B):C:C5	3.09	0.41
48:5:2690:C:H2'	48:5:2691:U:O4'	2.21	0.41
48:5:3668:C:C2	48:5:3675:G:C2	3.09	0.41
51:9:1259:A:H3'	51:9:1259:A:N3	2.35	0.41
57:FF:167:LYS:HA	77:ZZ:71:ALA:HB1	2.02	0.41
48:5:1963:C:N4	48:5:4694:G:O6	2.54	0.40
48:5:3706:C:H2'	48:5:3707:U:O4'	2.21	0.40
48:5:4289:U:H2'	48:5:4290:U:C6	2.56	0.40
51:9:398:A:H5'	51:9:398:A:C8	2.56	0.40
51:9:1207:G:C6	51:9:1837:G:C6	3.09	0.40
51:9:1834:A:N3	51:9:1834:A:H2'	2.36	0.40
37:l:20:ASN:O	37:l:41:ARG:NE	2.54	0.40
41:p:52:VAL:HG21	48:5:2739:C:H4'	2.03	0.40
48:5:1802:A:O2'	48:5:1837:A:OP1	2.39	0.40
48:5:3765:G:O2'	48:5:3766:A:N7	2.54	0.40
51:9:12:U:H2'	51:9:13:C:C6	2.57	0.40
51:9:571:U:C5	51:9:572:U:C5	3.09	0.40
51:9:1130:G:N3	51:9:1130:G:C2'	2.82	0.40
51:9:1620:A:O2'	67:PP:40:ARG:NH2	2.54	0.40
53:BB:143:THR:HG22	53:BB:205:TYR:CD1	2.56	0.40
56:EE:100:ARG:HD2	56:EE:102:ILE:HD11	2.02	0.40
18:S:35:PRO:HD2	18:S:39:VAL:HG21	2.02	0.40
29:d:33:ILE:HD11	29:d:41:ARG:CB	2.52	0.40
51:9:1536:G:H2'	51:9:1537:A:C8	2.56	0.40
56:EE:44:LEU:HD21	56:EE:70:ILE:HG21	2.03	0.40
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	2.03	0.40
66:OO:116:LEU:HD22	78:aa:53:ILE:CD1	2.51	0.40
2:B:86:VAL:HG13	2:B:162:VAL:HG22	2.04	0.40
4:D:4:VAL:HG11	48:5:4247:G:C5'	2.51	0.40
13:N:149:GLN:O	13:N:152:THR:OG1	2.35	0.40
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922(B):C:C2	48:5:923:C:C6	3.10	0.40
48:5:3851:U:H2'	48:5:3852:A:O4'	2.21	0.40
1:A:82:ILE:HD11	1:A:99:GLY:HA3	2.04	0.40
5:E:156:LEU:HD11	5:E:198:ILE:HG13	2.02	0.40
7:G:139:VAL:HG11	7:G:238:LYS:HG3	2.04	0.40
18:S:80:ILE:HG22	18:S:82:LEU:HD22	2.02	0.40
39:n:11:ARG:NH2	51:9:1844:U:OP1	2.52	0.40
48:5:1748:U:C2	48:5:1783:C:C2	3.09	0.40
51:9:584:A:N6	51:9:585:C:N4	2.69	0.40
51:9:1173:A:H2'	51:9:1174:U:O4'	2.21	0.40
51:9:1227:G:C2	51:9:1228:A:C8	3.10	0.40
62:KK:32:HIS:CD2	62:KK:45:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	10	39
2	B	392/403 (97%)	367 (94%)	24 (6%)	1 (0%)	36	65
3	C	360/425 (85%)	338 (94%)	20 (6%)	2 (1%)	21	52
4	D	291/297 (98%)	279 (96%)	10 (3%)	2 (1%)	18	50
5	E	208/291 (72%)	190 (91%)	18 (9%)	0	100	100
6	F	223/247 (90%)	210 (94%)	11 (5%)	2 (1%)	14	45
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%)	24	56
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	24	56
12	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
13	N	201/204 (98%)	186 (92%)	14 (7%)	1 (0%)	24	56
14	O	197/203 (97%)	183 (93%)	14 (7%)	0	100	100
15	P	151/184 (82%)	142 (94%)	8 (5%)	1 (1%)	18	50
16	Q	185/188 (98%)	168 (91%)	15 (8%)	2 (1%)	11	41
17	R	178/196 (91%)	170 (96%)	8 (4%)	0	100	100
18	S	174/176 (99%)	163 (94%)	9 (5%)	2 (1%)	11	41
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	10 (10%)	1 (1%)	12	43
21	V	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	12	43
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%)	8	35
26	a	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
27	b	100/245 (41%)	92 (92%)	7 (7%)	1 (1%)	12	43
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	90 (86%)	14 (13%)	1 (1%)	12	43
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	6	32
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%)	12	43
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	11	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	r	122/137 (89%)	109 (89%)	11 (9%)	2 (2%)	7	34
43	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	12	43
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	9	38
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	198 (92%)	16 (7%)	1 (0%)	24	56
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%)	14	45
56	EE	260/263 (99%)	248 (95%)	11 (4%)	1 (0%)	30	60
57	FF	181/204 (89%)	169 (93%)	10 (6%)	2 (1%)	11	41
58	GG	235/249 (94%)	226 (96%)	8 (3%)	1 (0%)	30	60
59	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
60	II	204/208 (98%)	190 (93%)	13 (6%)	1 (0%)	24	56
61	JJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	24	56
62	KK	94/165 (57%)	87 (93%)	6 (6%)	1 (1%)	11	41
63	LL	139/158 (88%)	127 (91%)	11 (8%)	1 (1%)	18	50
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%)	18	50
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%)	16	47
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	18	50
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%)	16	47
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	5	29
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%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	bb	81/84 (96%)	70 (86%)	10 (12%)	1 (1%)	10	39
80	cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	4 (8%)	1 (2%)	6	32
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	282 (91%)	26 (8%)	3 (1%)	12	43
86	ii	370/403 (92%)	342 (92%)	27 (7%)	1 (0%)	36	65
87	jj	423/710 (60%)	388 (92%)	31 (7%)	4 (1%)	14	45
All	All	12317/14495 (85%)	11449 (93%)	804 (6%)	64 (0%)	26	56

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

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Mol	Chain	Res	Type
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
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 ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	174 (92%)	16 (8%)	10	34
2	B	342/348 (98%)	323 (94%)	19 (6%)	19	45
3	C	302/347 (87%)	287 (95%)	15 (5%)	22	47
4	D	247/250 (99%)	237 (96%)	10 (4%)	28	52
5	E	190/251 (76%)	179 (94%)	11 (6%)	18	44
6	F	196/215 (91%)	186 (95%)	10 (5%)	21	47
7	G	200/272 (74%)	190 (95%)	10 (5%)	22	47
8	H	169/171 (99%)	156 (92%)	13 (8%)	12	37
9	I	175/181 (97%)	163 (93%)	12 (7%)	14	41
10	J	143/149 (96%)	135 (94%)	8 (6%)	19	45
11	L	175/176 (99%)	171 (98%)	4 (2%)	44	62
12	M	117/161 (73%)	108 (92%)	9 (8%)	12	37
13	N	171/172 (99%)	164 (96%)	7 (4%)	27	51
14	O	171/173 (99%)	157 (92%)	14 (8%)	10	35
15	P	134/163 (82%)	127 (95%)	7 (5%)	21	46
16	Q	164/165 (99%)	153 (93%)	11 (7%)	15	42
17	R	159/175 (91%)	149 (94%)	10 (6%)	16	43
18	S	157/157 (100%)	149 (95%)	8 (5%)	21	47
19	T	139/140 (99%)	132 (95%)	7 (5%)	22	47
20	U	89/114 (78%)	87 (98%)	2 (2%)	45	62
21	V	101/107 (94%)	88 (87%)	13 (13%)	4	20
22	W	86/126 (68%)	86 (100%)	0	100	100
23	X	106/134 (79%)	101 (95%)	5 (5%)	23	48
24	Y	124/135 (92%)	118 (95%)	6 (5%)	23	48
25	Z	117/118 (99%)	114 (97%)	3 (3%)	40	59
26	a	119/120 (99%)	116 (98%)	3 (2%)	42	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	84/184 (46%)	81 (96%)	3 (4%)	31	54
28	c	84/98 (86%)	82 (98%)	2 (2%)	43	61
29	d	98/110 (89%)	91 (93%)	7 (7%)	13	40
30	e	114/121 (94%)	103 (90%)	11 (10%)	8	30
31	f	88/89 (99%)	84 (96%)	4 (4%)	24	49
32	g	98/100 (98%)	90 (92%)	8 (8%)	10	35
33	h	109/110 (99%)	105 (96%)	4 (4%)	30	53
34	i	86/89 (97%)	83 (96%)	3 (4%)	32	54
35	j	73/80 (91%)	71 (97%)	2 (3%)	39	58
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	56
37	l	47/48 (98%)	46 (98%)	1 (2%)	47	63
38	m	48/90 (53%)	45 (94%)	3 (6%)	16	43
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	35
40	o	92/94 (98%)	87 (95%)	5 (5%)	20	46
41	p	74/75 (99%)	73 (99%)	1 (1%)	59	70
42	r	108/121 (89%)	98 (91%)	10 (9%)	8	31
43	s	164/258 (64%)	158 (96%)	6 (4%)	30	53
44	t	126/137 (92%)	122 (97%)	4 (3%)	34	55
45	1	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	165 (92%)	15 (8%)	10	35
53	BB	194/231 (84%)	176 (91%)	18 (9%)	8	31
54	CC	187/225 (83%)	171 (91%)	16 (9%)	10	34
55	DD	190/202 (94%)	177 (93%)	13 (7%)	14	41
56	EE	224/225 (100%)	212 (95%)	12 (5%)	20	46
57	FF	158/170 (93%)	153 (97%)	5 (3%)	34	55
58	GG	207/218 (95%)	191 (92%)	16 (8%)	12	37
59	HH	165/174 (95%)	148 (90%)	17 (10%)	7	29
60	II	178/180 (99%)	166 (93%)	12 (7%)	15	42
61	JJ	161/168 (96%)	151 (94%)	10 (6%)	16	43
62	KK	87/136 (64%)	79 (91%)	8 (9%)	8	32
63	LL	130/142 (92%)	115 (88%)	15 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	MM	99/108 (92%)	87 (88%)	12 (12%)	5	22
65	NN	130/131 (99%)	119 (92%)	11 (8%)	10	34
66	OO	106/130 (82%)	100 (94%)	6 (6%)	18	45
67	PP	109/130 (84%)	99 (91%)	10 (9%)	8	32
68	QQ	117/121 (97%)	107 (92%)	10 (8%)	10	34
69	RR	119/121 (98%)	108 (91%)	11 (9%)	8	32
70	SS	125/132 (95%)	112 (90%)	13 (10%)	7	28
71	TT	111/115 (96%)	101 (91%)	10 (9%)	9	32
72	UU	92/107 (86%)	85 (92%)	7 (8%)	12	38
73	VV	67/67 (100%)	63 (94%)	4 (6%)	17	44
74	WW	112/113 (99%)	107 (96%)	5 (4%)	24	49
75	XX	113/115 (98%)	104 (92%)	9 (8%)	11	36
76	YY	107/112 (96%)	92 (86%)	15 (14%)	3	18
77	ZZ	66/103 (64%)	61 (92%)	5 (8%)	12	38
78	aa	88/98 (90%)	80 (91%)	8 (9%)	9	32
79	bb	75/76 (99%)	68 (91%)	7 (9%)	8	31
80	cc	55/62 (89%)	51 (93%)	4 (7%)	13	39
81	dd	48/49 (98%)	45 (94%)	3 (6%)	16	43
82	ee	46/106 (43%)	43 (94%)	3 (6%)	15	42
83	ff	61/140 (44%)	55 (90%)	6 (10%)	7	30
84	gg	272/275 (99%)	265 (97%)	7 (3%)	40	59
86	ii	326/353 (92%)	308 (94%)	18 (6%)	19	45
87	jj	358/608 (59%)	332 (93%)	26 (7%)	13	39
All	All	10733/12306 (87%)	10055 (94%)	678 (6%)	18	43

All (678) 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	123	ARG
1	A	128	ARG

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Mol	Chain	Res	Type
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	66	LYS
2	B	74	GLU
2	B	95	THR
2	B	135	LYS
2	B	248	LEU
2	B	262	VAL
2	B	279	GLU
2	B	294	LYS
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	366	LYS
2	B	383	GLU
3	C	20	LYS
3	C	106	LYS
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS

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Mol	Chain	Res	Type
3	C	312	ARG
3	C	333	LYS
4	D	22	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	262	LYS
4	D	264	LYS
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	123	ASP
5	E	143	LEU
5	E	169	LYS
5	E	178	VAL
5	E	197	VAL
5	E	213	LYS
5	E	289	LEU
5	E	291	PHE
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	88	LEU
6	F	120	THR
6	F	134	ILE
6	F	151	GLU
6	F	198	LYS
6	F	211	LYS
6	F	245	ARG
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	215	ASP
7	G	220	VAL
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	293	ASN

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Mol	Chain	Res	Type
7	G	312	LYS
8	H	1	MET
8	H	20	LEU
8	H	52	LYS
8	H	57	VAL
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	129	ARG
8	H	141	LYS
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	76	MET
9	I	97	ILE
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	200	ILE
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	96	LYS
10	J	113	ILE
10	J	175	LEU
11	L	10	LEU
11	L	63	THR
11	L	162	LYS
11	L	186	ARG
12	M	37	LEU
12	M	42	CYS
12	M	57	LEU
12	M	61	ILE

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Mol	Chain	Res	Type
12	M	62	LEU
12	M	89	THR
12	M	96	GLU
12	M	105	THR
12	M	112	VAL
13	N	9	GLU
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	89	VAL
13	N	104	GLU
13	N	182	HIS
14	O	16	LEU
14	O	27	VAL
14	O	49	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	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	24	VAL
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	31	LEU
16	Q	61	LEU
16	Q	63	LEU
16	Q	78	LYS
16	Q	91	ARG
16	Q	95	VAL

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Mol	Chain	Res	Type
16	Q	101	CYS
16	Q	143	ARG
17	R	6	LEU
17	R	36	ASN
17	R	50	ILE
17	R	82	LYS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	138	LEU
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	70	LYS
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	45	MET
19	T	60	LYS
19	T	96	ILE
19	T	144	ASN
19	T	159	MET
20	U	33	ILE
20	U	83	LEU
21	V	15	ARG
21	V	16	ILE
21	V	18	LEU
21	V	35	LYS
21	V	41	SER
21	V	45	ILE
21	V	60	MET
21	V	69	LYS
21	V	71	GLU
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS

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Mol	Chain	Res	Type
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	55	VAL
24	Y	72	GLN
24	Y	104	VAL
25	Z	3	LYS
25	Z	11	VAL
25	Z	33	THR
26	a	4	ARG
26	a	122	VAL
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	48	GLU
29	d	78	ARG
29	d	90	ARG
29	d	98	SER
29	d	102	LEU
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	113	GLU
30	e	126	ASN
30	e	128	ARG
31	f	23	GLU
31	f	33	VAL

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Mol	Chain	Res	Type
31	f	52	LYS
31	f	101	ILE
32	g	5	LEU
32	g	15	THR
32	g	22	LEU
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	28	LEU
33	h	67	GLU
33	h	88	THR
33	h	89	ARG
34	i	33	LEU
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	18	HIS
40	o	28	LYS
40	o	36	GLN
40	o	61	LYS
41	p	8	VAL
42	r	8	MET
42	r	18	ILE
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

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Mol	Chain	Res	Type
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	72	GLU
44	t	98	ILE
44	t	133	LEU
52	AA	5	LEU
52	AA	9	GLN
52	AA	12	GLU
52	AA	25	LEU
52	AA	50	ASN
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	122	LEU
52	AA	132	GLN
52	AA	134	LEU
52	AA	136	GLU
52	AA	142	LEU
52	AA	178	LEU
52	AA	181	GLU
53	BB	38	MET
53	BB	63	LYS
53	BB	71	LEU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	125	VAL
53	BB	134	LEU
53	BB	143	THR
53	BB	157	GLN
53	BB	163	GLN
53	BB	180	ASP
53	BB	181	LEU
53	BB	184	VAL
53	BB	207	LEU
53	BB	209	ASP

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Mol	Chain	Res	Type
53	BB	213	ARG
53	BB	225	LEU
54	CC	78	LEU
54	CC	94	ILE
54	CC	105	GLU
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	132	ASP
54	CC	137	VAL
54	CC	160	LEU
54	CC	167	ARG
54	CC	188	CYS
54	CC	192	LEU
54	CC	196	ILE
54	CC	244	ILE
54	CC	251	LEU
54	CC	255	LEU
55	DD	28	GLU
55	DD	35	SER
55	DD	57	ASN
55	DD	72	VAL
55	DD	127	MET
55	DD	134	CYS
55	DD	142	LEU
55	DD	145	GLN
55	DD	146	ARG
55	DD	168	VAL
55	DD	182	LEU
55	DD	190	LEU
55	DD	218	LEU
56	EE	17	HIS
56	EE	24	THR
56	EE	33	THR
56	EE	42	LEU
56	EE	51	ARG
56	EE	52	LEU
56	EE	66	MET
56	EE	67	GLN
56	EE	77	ARG
56	EE	222	LEU
56	EE	232	ASN

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Mol	Chain	Res	Type
56	EE	246	LEU
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	125	SER
57	FF	140	ASP
58	GG	41	LEU
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	95	LYS
58	GG	103	ASP
58	GG	159	ARG
58	GG	171	THR
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	199	THR
58	GG	216	ARG
58	GG	217	MET
58	GG	230	LYS
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	133	LEU
59	HH	145	ARG
59	HH	149	ASP
59	HH	160	LYS
59	HH	188	GLU
60	II	6	ASP
60	II	23	LYS
60	II	26	LYS

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Mol	Chain	Res	Type
60	II	92	ARG
60	II	99	ASN
60	II	121	LEU
60	II	128	LYS
60	II	130	THR
60	II	147	LYS
60	II	168	GLN
60	II	178	ARG
60	II	190	LEU
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	80	ARG
61	JJ	86	VAL
61	JJ	89	GLU
61	JJ	92	MET
61	JJ	116	LYS
62	KK	1	MET
62	KK	2	LEU
62	KK	22	VAL
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
63	LL	153	LYS

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Mol	Chain	Res	Type
64	MM	22	LEU
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	85	LEU
64	MM	99	LYS
64	MM	101	ARG
64	MM	112	LYS
64	MM	129	LYS
65	NN	27	LYS
65	NN	29	THR
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	86	GLU
65	NN	107	LYS
65	NN	110	ASP
65	NN	125	LEU
65	NN	132	LYS
66	OO	25	GLU
66	OO	31	CYS
66	OO	38	ASN
66	OO	56	VAL
66	OO	104	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	45	LEU
67	PP	51	ARG
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	108	LYS
68	QQ	7	LEU
68	QQ	26	LYS
68	QQ	31	LEU

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Mol	Chain	Res	Type
68	QQ	37	ARG
68	QQ	40	GLU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	67	ASP
68	QQ	100	VAL
68	QQ	140	ARG
69	RR	31	ASN
69	RR	44	LYS
69	RR	49	LYS
69	RR	62	GLN
69	RR	78	ARG
69	RR	98	VAL
69	RR	99	ASP
69	RR	102	THR
69	RR	105	MET
69	RR	109	LEU
69	RR	120	THR
70	SS	7	GLU
70	SS	8	LYS
70	SS	14	ARG
70	SS	21	ASP
70	SS	36	VAL
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	63	GLU
70	SS	83	PHE
70	SS	110	ASP
70	SS	132	ARG
71	TT	34	VAL
71	TT	39	LEU
71	TT	55	THR
71	TT	62	ARG
71	TT	102	ARG
71	TT	110	LEU
71	TT	123	LEU
71	TT	124	THR
71	TT	131	LEU
71	TT	142	LYS
72	UU	18	HIS

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Mol	Chain	Res	Type
72	UU	25	THR
72	UU	56	MET
72	UU	60	THR
72	UU	76	THR
72	UU	88	LEU
72	UU	106	ILE
73	VV	10	ASP
73	VV	12	TYR
73	VV	32	ILE
73	VV	66	ASP
74	WW	51	GLU
74	WW	84	LYS
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
75	XX	7	LEU
75	XX	8	ARG
75	XX	15	SER
75	XX	29	LYS
75	XX	45	SER
75	XX	67	ARG
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	44	LEU
76	YY	47	MET
76	YY	51	THR
76	YY	54	VAL
76	YY	61	ARG
76	YY	74	MET
76	YY	88	LYS
76	YY	101	LYS
76	YY	103	SER
76	YY	115	LYS
77	ZZ	52	LYS
77	ZZ	83	LEU
77	ZZ	89	GLN

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Mol	Chain	Res	Type
77	ZZ	92	LEU
77	ZZ	101	SER
78	aa	12	LYS
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	41	ILE
78	aa	42	ARG
78	aa	55	GLU
78	aa	87	ARG
79	bb	17	ARG
79	bb	37	CYS
79	bb	42	LYS
79	bb	64	CYS
79	bb	78	SER
79	bb	80	ARG
79	bb	81	ARG
80	cc	30	VAL
80	cc	40	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	18	SER
81	dd	48	LYS
81	dd	49	ASP
82	ee	97	LYS
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	87	LEU
84	gg	119	GLN
84	gg	198	VAL
84	gg	289	LEU
84	gg	306	LEU
86	ii	8	ILE
86	ii	40	ARG

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Mol	Chain	Res	Type
86	ii	68	CYS
86	ii	81	LEU
86	ii	107	ASN
86	ii	148	HIS
86	ii	149	ILE
86	ii	170	LYS
86	ii	172	LYS
86	ii	183	GLU
86	ii	198	HIS
86	ii	205	ILE
86	ii	243	VAL
86	ii	258	CYS
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	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	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	534	ILE
87	jj	557	MET
87	jj	590	ILE
87	jj	600	VAL
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 (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	97	ASN
1	A	100	ASN
1	A	140	ASN
1	A	162	ASN
1	A	194	ASN
1	A	205	ASN
1	A	215	ASN
2	B	109	HIS
2	B	158	GLN
2	B	167	GLN
2	B	204	GLN
2	B	271	GLN
3	C	38	ASN
3	C	212	ASN
4	D	9	ASN
4	D	57	ASN
4	D	291	GLN
5	E	131	HIS
5	E	253	GLN
5	E	269	GLN
6	F	79	ASN
7	G	135	GLN
7	G	143	GLN
7	G	147	GLN
7	G	206	GLN
7	G	248	HIS
7	G	261	ASN
8	H	8	GLN
8	H	98	HIS
8	H	108	ASN
9	I	95	HIS
9	I	123	GLN
9	I	144	ASN
10	J	112	HIS
11	L	19	GLN
11	L	28	GLN
11	L	87	HIS
11	L	113	ASN
11	L	115	GLN
12	M	48	GLN

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Mol	Chain	Res	Type
12	M	70	GLN
13	N	15	GLN
13	N	139	HIS
13	N	149	GLN
13	N	182	HIS
14	O	65	ASN
14	O	150	GLN
15	P	75	GLN
17	R	34	ASN
17	R	40	GLN
17	R	130	ASN
17	R	141	HIS
18	S	50	GLN
18	S	125	GLN
19	T	58	HIS
19	T	70	HIS
19	T	90	ASN
22	W	30	GLN
22	W	48	GLN
23	X	57	GLN
23	X	73	HIS
23	X	93	ASN
23	X	105	ASN
23	X	108	GLN
24	Y	18	HIS
24	Y	56	GLN
24	Y	72	GLN
26	a	60	HIS
26	a	62	HIS
27	b	60	ASN
28	c	73	HIS
28	c	78	ASN
29	d	34	HIS
29	d	100	ASN
30	e	68	HIS
33	h	65	GLN
33	h	108	GLN
37	l	38	ASN
38	m	91	HIS
40	o	19	GLN
40	o	36	GLN
42	r	70	GLN

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Mol	Chain	Res	Type
42	r	85	ASN
42	r	103	HIS
42	r	121	GLN
43	s	34	ASN
43	s	126	GLN
43	s	179	ASN
43	s	200	ASN
44	t	65	GLN
44	t	95	GLN
52	AA	111	GLN
52	AA	113	GLN
53	BB	163	GLN
54	CC	235	ASN
55	DD	101	GLN
56	EE	157	ASN
56	EE	161	GLN
56	EE	188	ASN
56	EE	260	GLN
57	FF	79	HIS
57	FF	83	ASN
58	GG	13	GLN
58	GG	105	ASN
58	GG	177	GLN
58	GG	186	GLN
58	GG	197	GLN
60	II	138	ASN
61	JJ	111	GLN
61	JJ	113	GLN
61	JJ	156	HIS
62	KK	42	ASN
62	KK	84	HIS
63	LL	100	ASN
64	MM	19	GLN
64	MM	55	ASN
65	NN	90	HIS
66	OO	20	GLN
66	OO	26	ASN
66	OO	38	ASN
66	OO	79	GLN
67	PP	79	HIS
67	PP	114	HIS
68	QQ	35	ASN

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Mol	Chain	Res	Type
68	QQ	48	GLN
68	QQ	142	GLN
69	RR	26	ASN
69	RR	62	GLN
69	RR	127	ASN
70	SS	10	GLN
70	SS	19	ASN
70	SS	97	GLN
73	VV	49	GLN
74	WW	92	ASN
75	XX	16	HIS
75	XX	77	ASN
76	YY	85	ASN
78	aa	19	GLN
78	aa	86	ASN
79	bb	26	GLN
79	bb	49	HIS
81	dd	4	GLN
81	dd	26	ASN
84	gg	64	HIS
84	gg	196	ASN
84	gg	222	ASN
86	ii	87	ASN
86	ii	109	GLN
86	ii	355	GLN
86	ii	358	GLN
87	jj	268	HIS
87	jj	361	GLN
87	jj	499	GLN
87	jj	526	ASN
87	jj	537	HIS
87	jj	549	HIS
87	jj	605	GLN
87	jj	639	GLN

5.3.3 RNA ⓘ

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	3511/3543 (99%)	873 (24%)	165 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	7	119/120 (99%)	13 (10%)	2 (1%)
50	8	150/156 (96%)	35 (23%)	7 (4%)
51	9	1683/1869 (90%)	428 (25%)	84 (4%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5616/5847 (96%)	1393 (24%)	259 (4%)

All (1393) 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

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Mol	Chain	Res	Type
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
48	5	20	U
48	5	21	G
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	125	C
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C

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Mol	Chain	Res	Type
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
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	275	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	752	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

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Mol	Chain	Res	Type
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
48	5	963	G
48	5	964	A
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

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Mol	Chain	Res	Type
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
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	1329	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

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Mol	Chain	Res	Type
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	1440	U
48	5	1441	C
48	5	1442	C
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

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Mol	Chain	Res	Type
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
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	1678	C
48	5	1679	A
48	5	1724	G
48	5	1726	U
48	5	1729	A
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G

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Mol	Chain	Res	Type
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
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	1935	C

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Mol	Chain	Res	Type
48	5	1936	C
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	1979	A
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2429	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2467	U
48	5	2468	U
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	3809	G
48	5	3810	C
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	4221	C
48	5	4222	G
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
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

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Mol	Chain	Res	Type
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	4463	U
48	5	4464	A
48	5	4471	U
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

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Mol	Chain	Res	Type
48	5	4520	G
48	5	4524	G
48	5	4527	G
48	5	4528	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	4572	U
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	109	U
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
51	9	873	G
51	9	874	G
51	9	875	A
51	9	876	C
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	1016	U
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
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G

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Mol	Chain	Res	Type
51	9	1131	G
51	9	1137	U
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
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1291	A

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Mol	Chain	Res	Type
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
51	9	1477	U
51	9	1478	U
51	9	1489	A
51	9	1490	G

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Mol	Chain	Res	Type
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
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G

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Mol	Chain	Res	Type
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
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A

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Mol	Chain	Res	Type
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
48	5	315	G
48	5	385	A
48	5	406	C
48	5	408	A

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Mol	Chain	Res	Type
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
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G

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Mol	Chain	Res	Type
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
48	5	2313	A
48	5	2396	A
48	5	2398	U
48	5	2428	A

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Mol	Chain	Res	Type
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
48	5	4272	G
48	5	4291	G
48	5	4378	A
48	5	4395	U

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Mol	Chain	Res	Type
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
51	9	369	C
51	9	434	G
51	9	465	A
51	9	500	A

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Mol	Chain	Res	Type
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
51	9	1285	G
51	9	1286	G
51	9	1313	A
51	9	1330	G

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Mol	Chain	Res	Type
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 oligosaccharides 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	32,34,34	1.49	8 (25%)	49,54,54	1.76	7 (14%)

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	-	4/19/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C5-C4	3.29	1.47	1.38
90	jj	700	GCP	PG-O3G	2.90	1.61	1.55
90	jj	700	GCP	PG-O2G	2.90	1.61	1.55
90	jj	700	GCP	PB-O3A	2.77	1.61	1.58
90	jj	700	GCP	C5-N7	-2.14	1.34	1.39
90	jj	700	GCP	PB-O2B	2.10	1.61	1.56
90	jj	700	GCP	C6-N1	-2.08	1.35	1.38
90	jj	700	GCP	PA-O3A	2.07	1.61	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C5-C4-N3	-6.07	118.72	128.39
90	jj	700	GCP	C2-N3-C4	5.13	121.13	112.30
90	jj	700	GCP	N9-C4-N3	4.55	135.05	125.95
90	jj	700	GCP	C6-C5-N7	3.31	136.31	130.29
90	jj	700	GCP	C4-C5-N7	-2.60	106.55	110.67
90	jj	700	GCP	PB-O3A-PA	-2.25	125.02	132.37
90	jj	700	GCP	O6-C6-C5	-2.13	120.92	126.53

There are no chirality outliers.

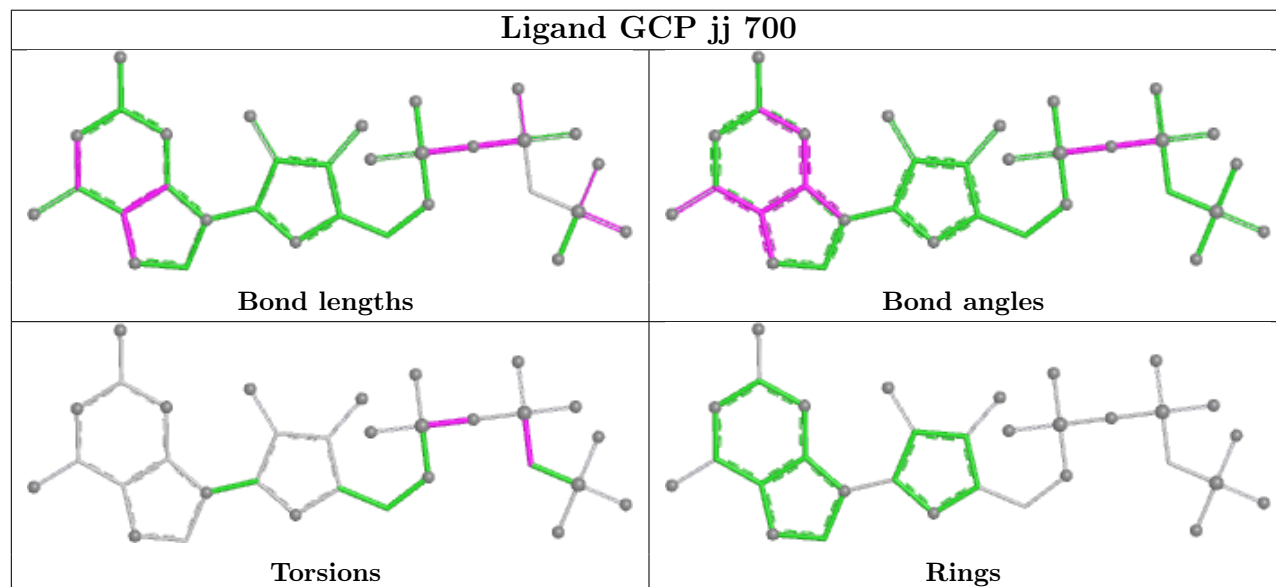
All (4) torsion outliers are listed below:

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

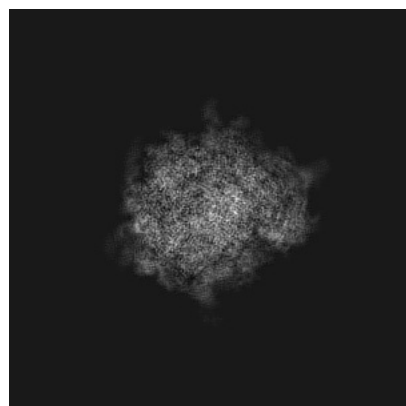
6 Map visualisation [i](#)

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.

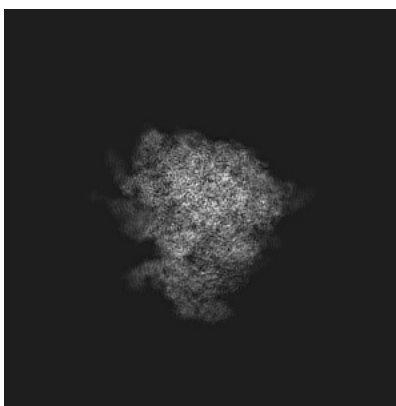
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

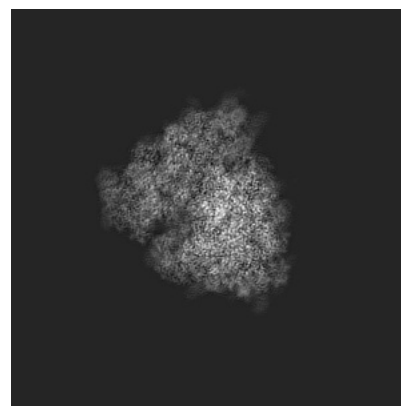
6.1.1 Primary map



X

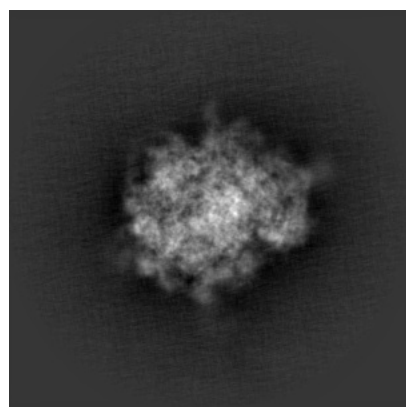


Y

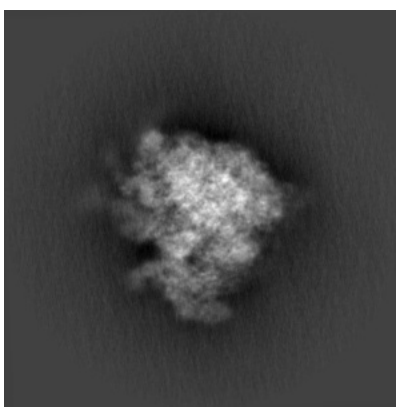


Z

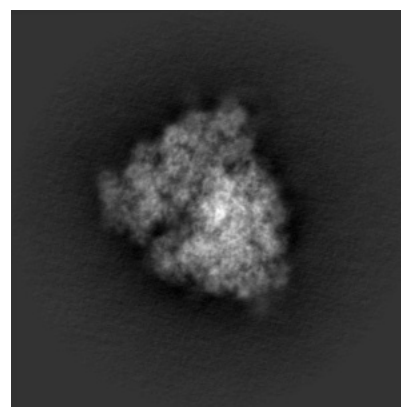
6.1.2 Raw map



X



Y

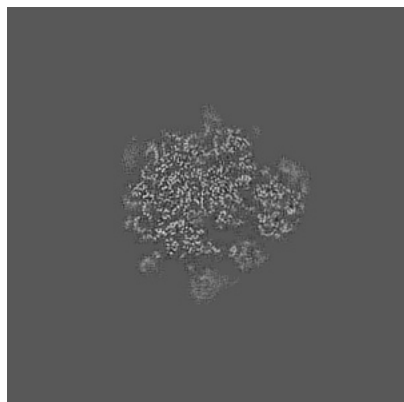


Z

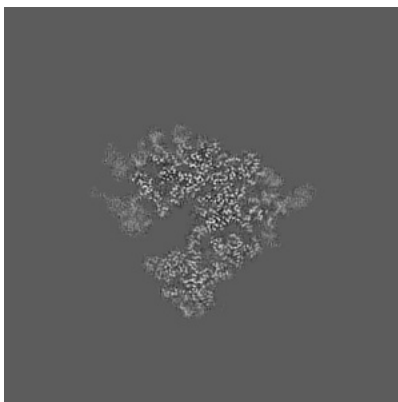
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

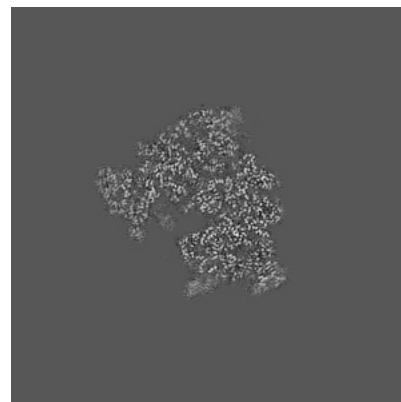
6.2.1 Primary map



X Index: 210

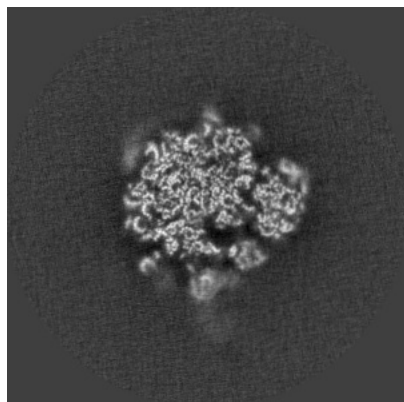


Y Index: 210

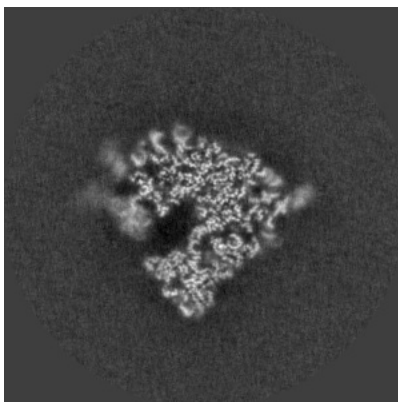


Z Index: 210

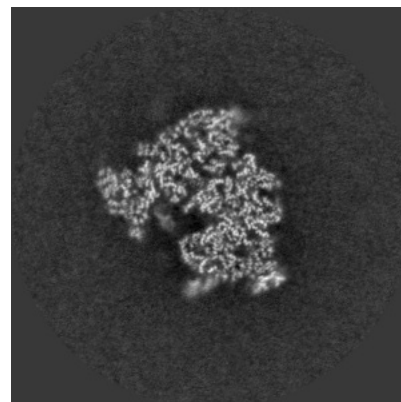
6.2.2 Raw map



X Index: 210



Y Index: 210

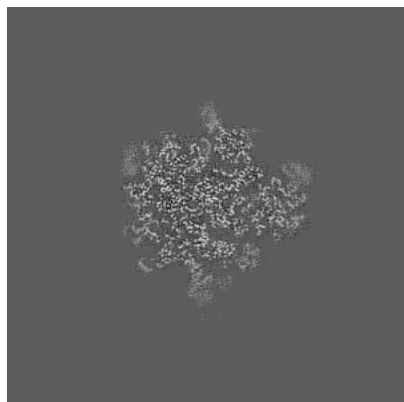


Z Index: 210

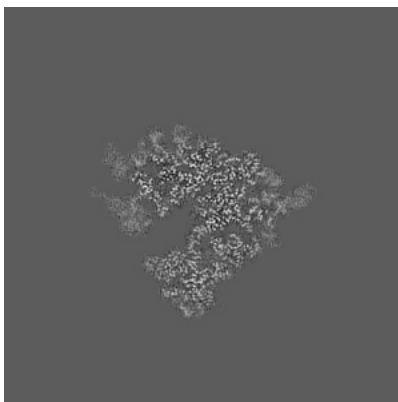
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

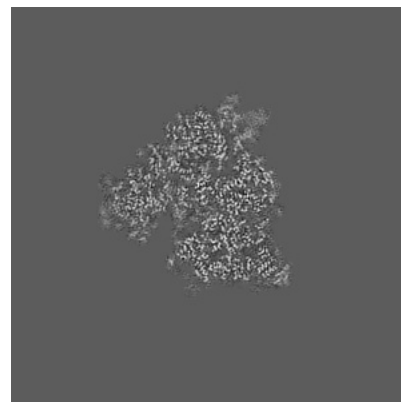
6.3.1 Primary map



X Index: 216

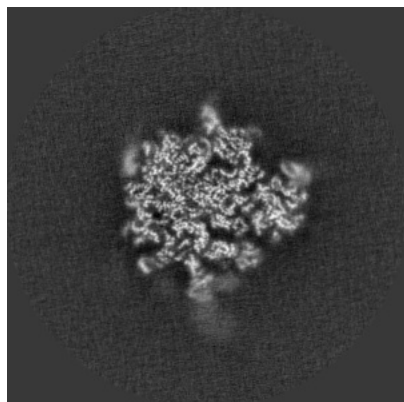


Y Index: 210

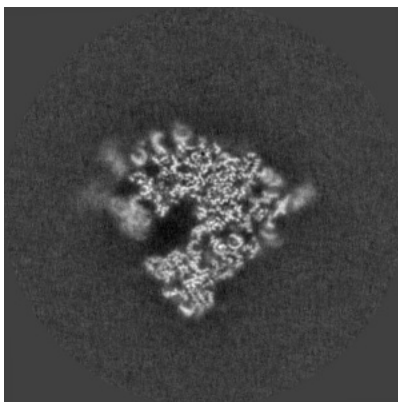


Z Index: 202

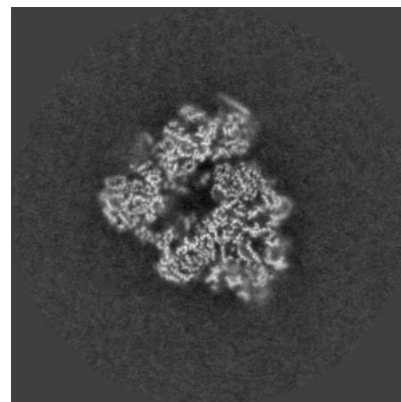
6.3.2 Raw map



X Index: 215



Y Index: 211

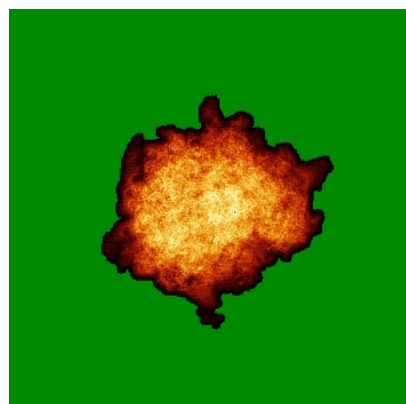


Z Index: 187

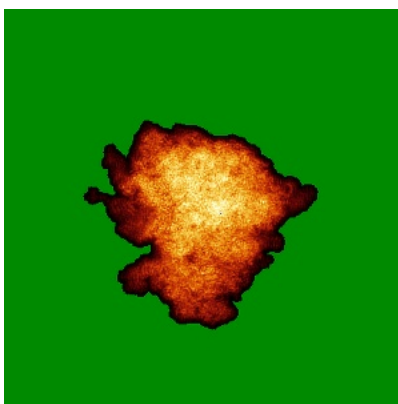
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

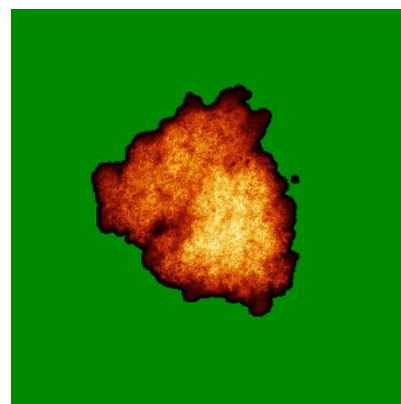
6.4.1 Primary map



X

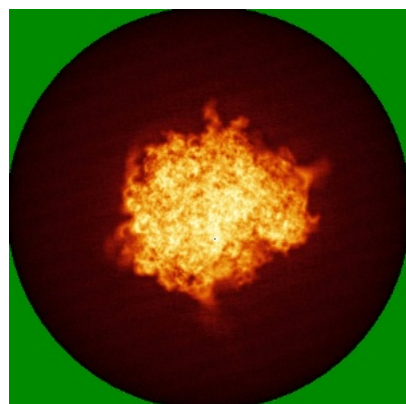


Y

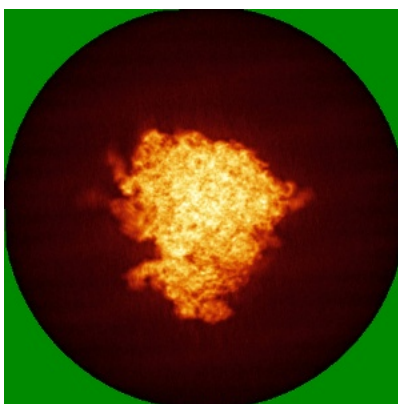


Z

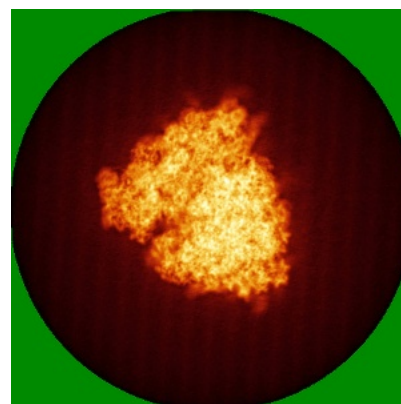
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

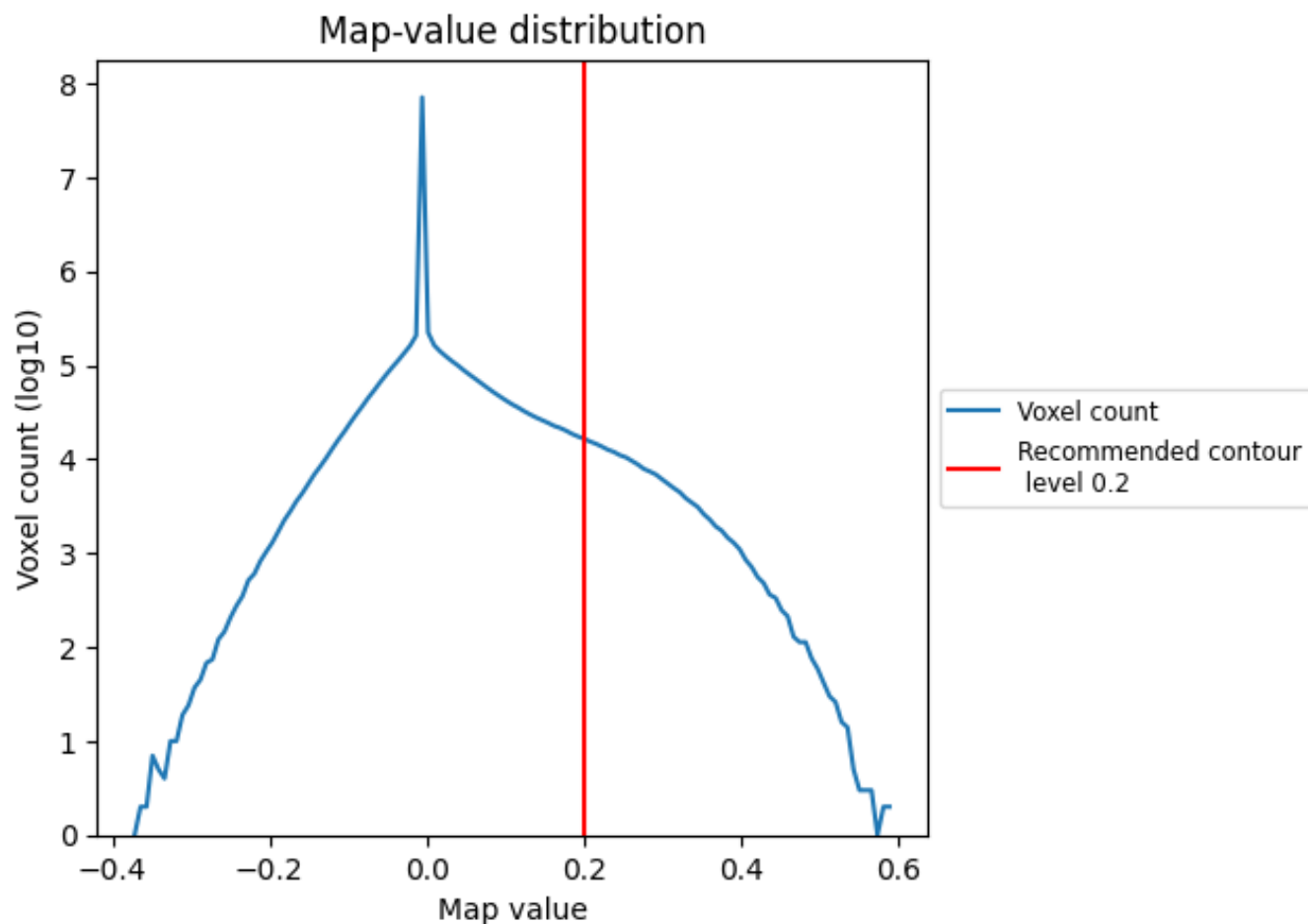
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

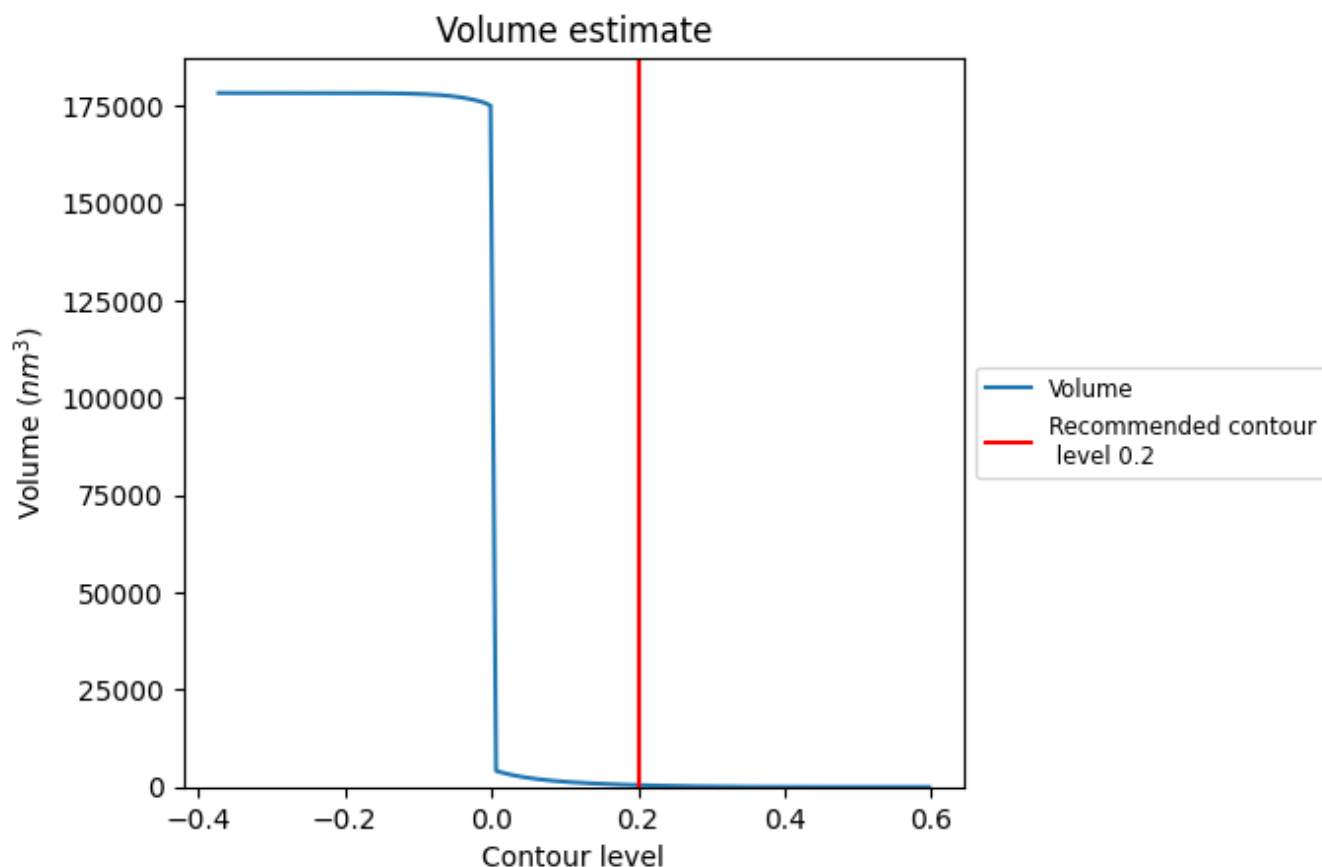
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

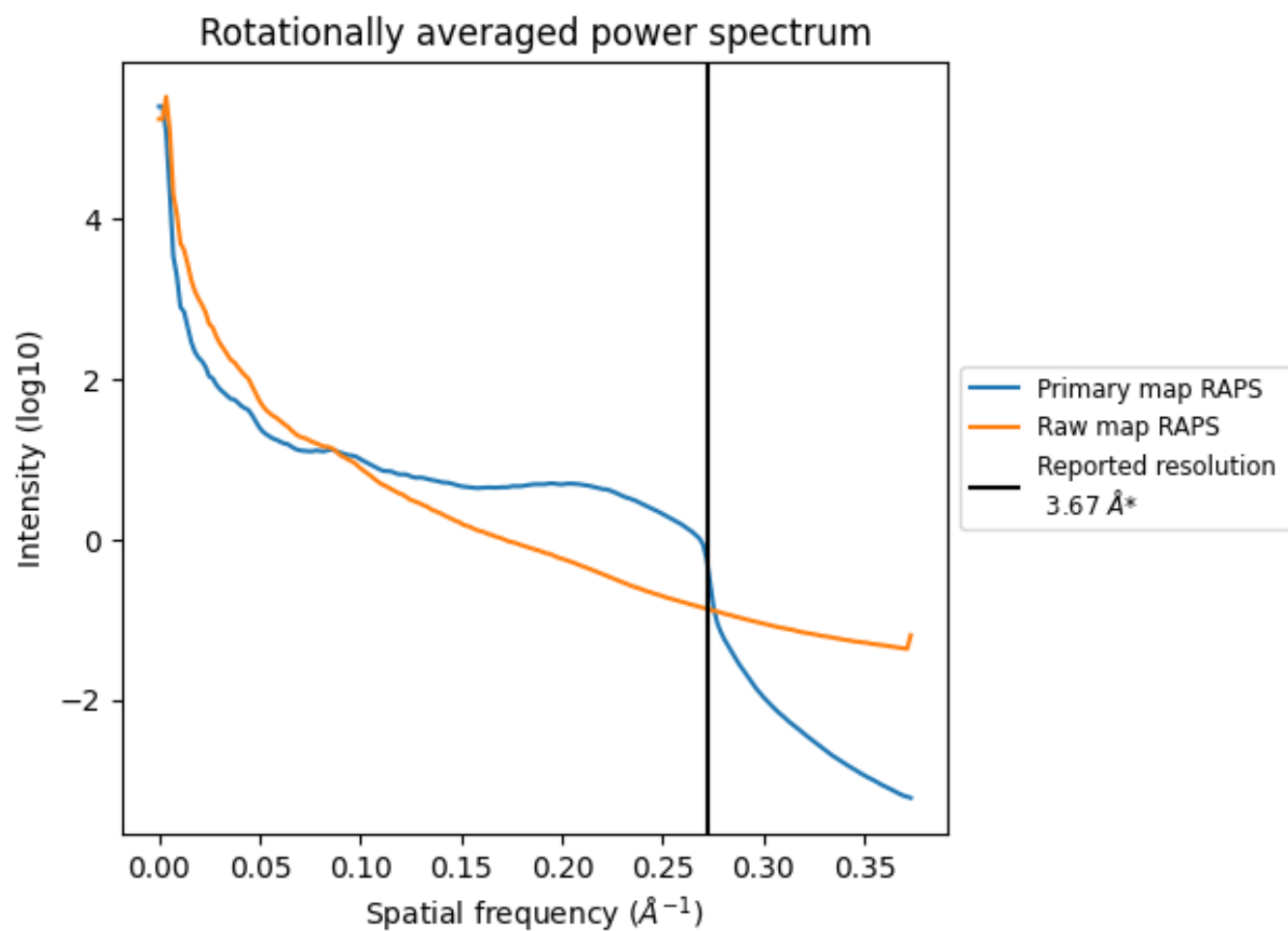
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 470 nm³; 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 ⓘ

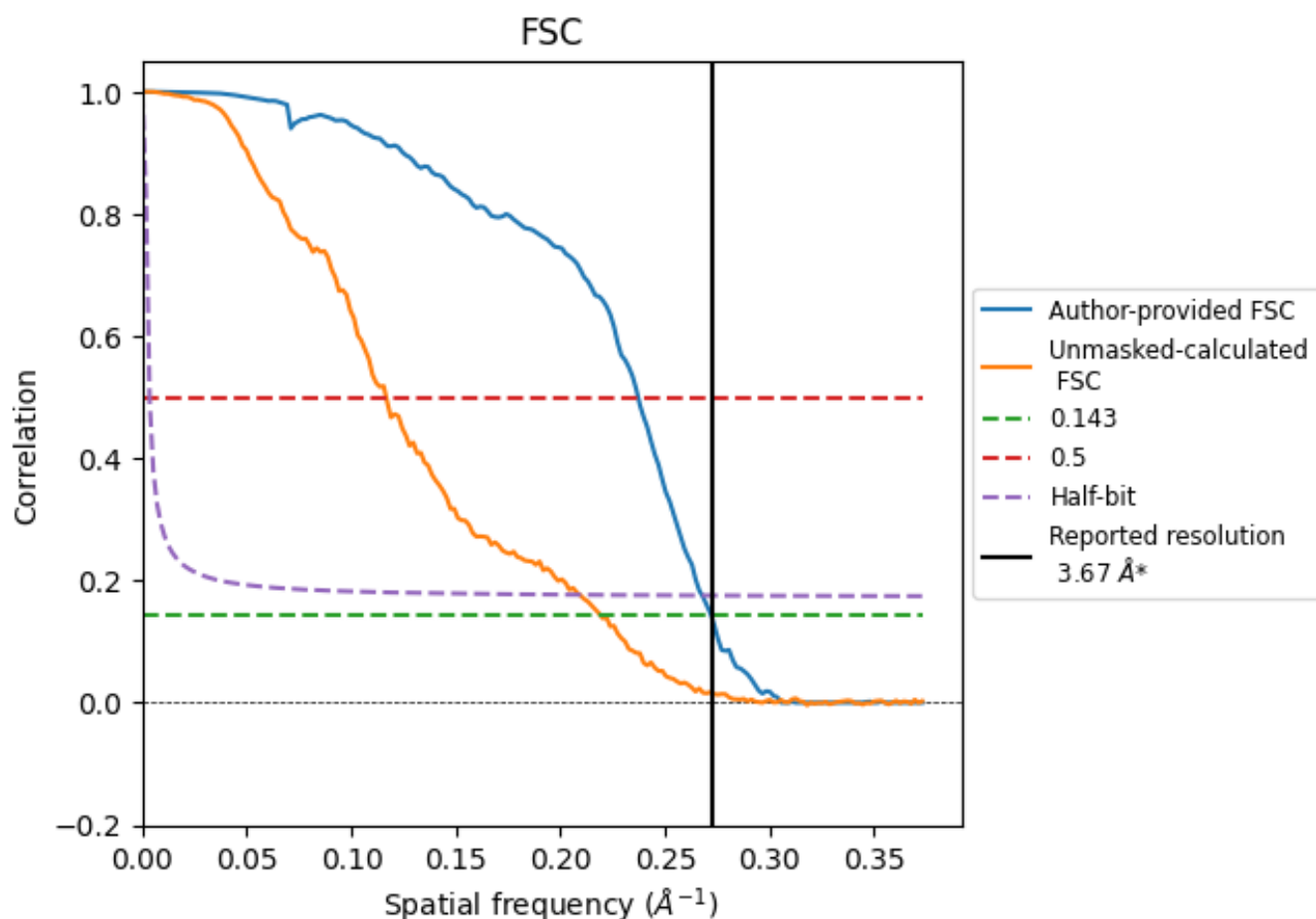


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates

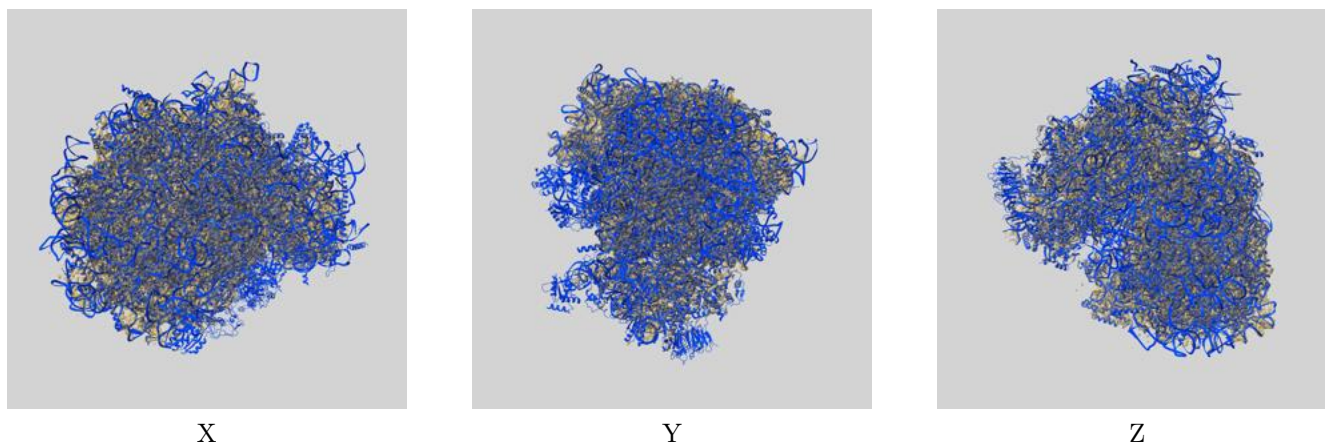
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.68	4.22	3.73
Unmasked-calculated*	4.56	8.57	4.78

*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](#)

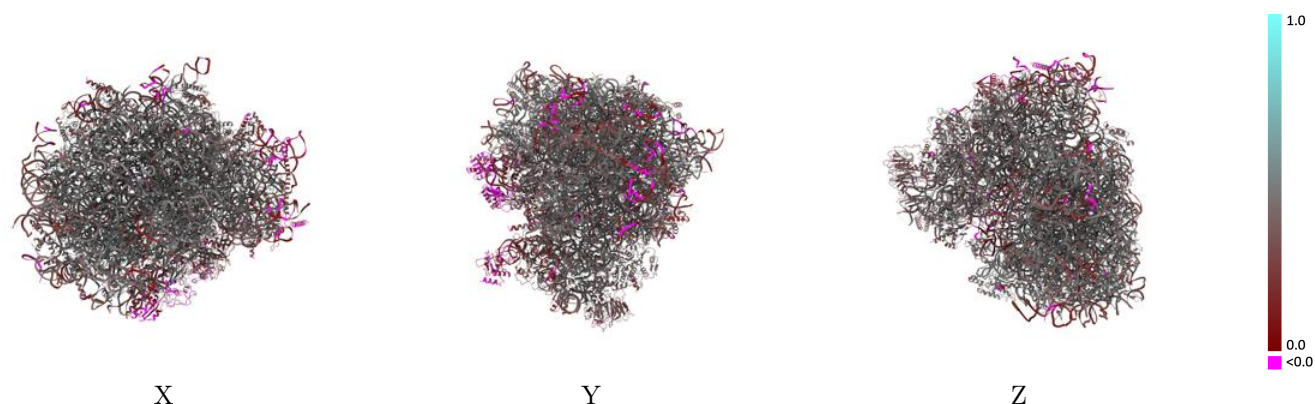
This section contains information regarding the fit between EMDB map EMD-4135 and PDB model 5LZX. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



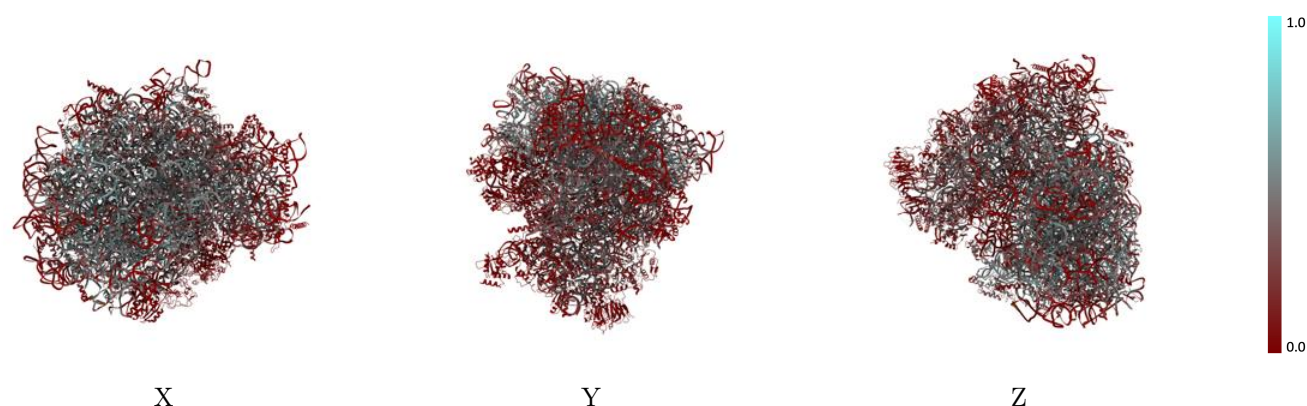
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



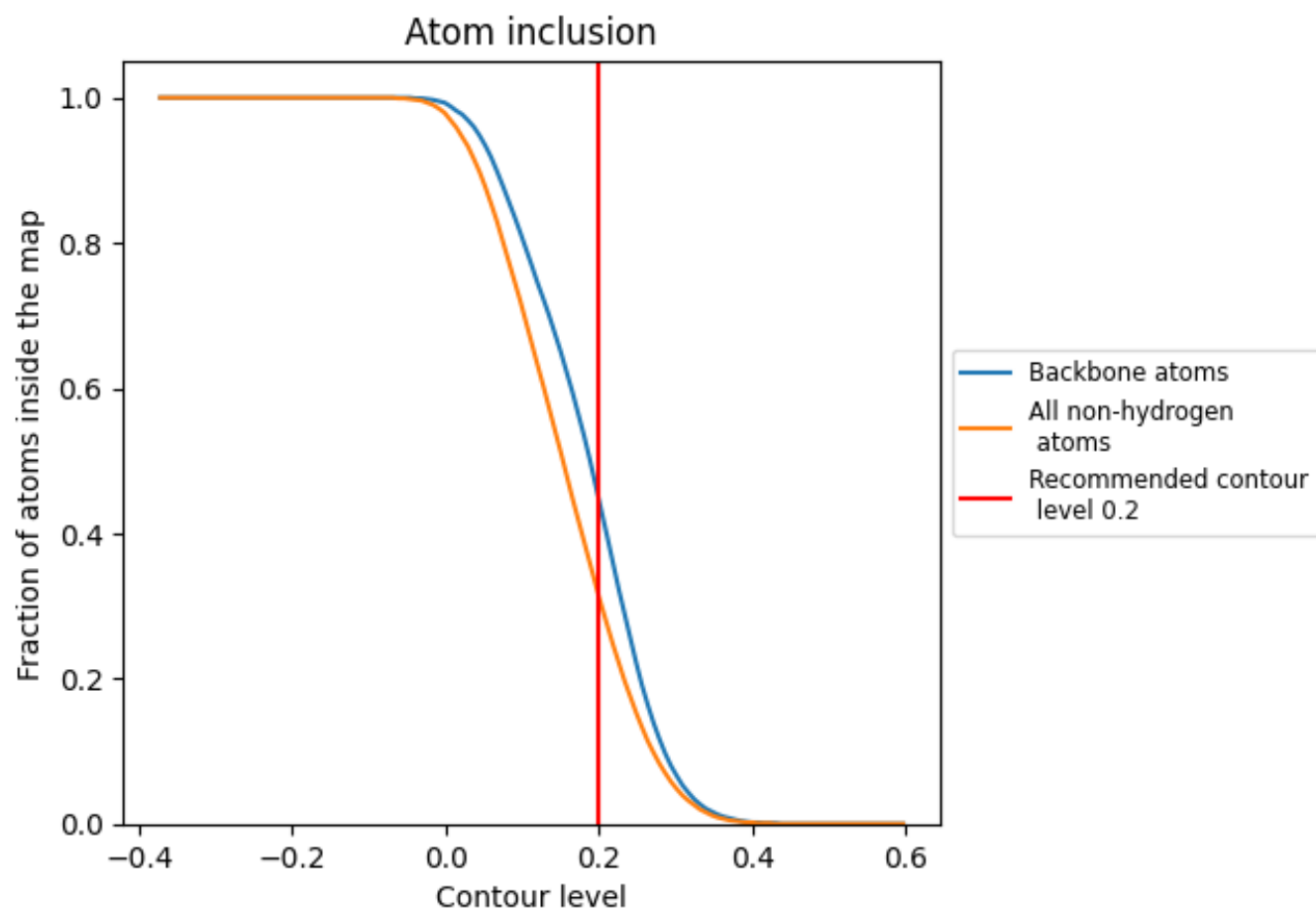
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

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 ⓘ

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	 0.3130	 0.4050
1	 0.0000	 0.3250
2	 0.0540	 0.3660
3	 0.0070	 0.1760
5	 0.3960	 0.4120
7	 0.5250	 0.4510
8	 0.4060	 0.4200
9	 0.3180	 0.3880
A	 0.3650	 0.4720
AA	 0.2380	 0.4160
B	 0.3880	 0.4730
BB	 0.2020	 0.4280
C	 0.3810	 0.4740
CC	 0.2450	 0.4380
D	 0.3470	 0.4350
DD	 0.1520	 0.3810
E	 0.3210	 0.4500
EE	 0.2520	 0.4330
F	 0.3980	 0.4720
FF	 0.2060	 0.4190
G	 0.2630	 0.3960
GG	 0.1030	 0.3310
H	 0.3570	 0.4640
HH	 0.0870	 0.3570
I	 0.3580	 0.4720
II	 0.2090	 0.4060
J	 0.2560	 0.4210
JJ	 0.2440	 0.4220
KK	 0.0590	 0.3480
L	 0.3300	 0.4360
LL	 0.2790	 0.4420
M	 0.4080	 0.4580
MM	 0.0020	 0.1070
N	 0.3910	 0.4820
NN	 0.2330	 0.4380



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Chain	Atom inclusion	Q-score
O	 0.4270	 0.4750
OO	 0.2160	 0.4430
P	 0.4350	 0.4800
PP	 0.0530	 0.3320
Q	 0.3500	 0.4760
QQ	 0.1660	 0.4230
R	 0.2990	 0.4090
RR	 0.1670	 0.3970
S	 0.4070	 0.4850
SS	 0.0850	 0.3710
T	 0.3390	 0.4660
TT	 0.1450	 0.3910
U	 0.2050	 0.4060
UU	 0.1340	 0.3690
V	 0.3100	 0.4710
VV	 0.2030	 0.4320
W	 0.1850	 0.3140
WW	 0.2870	 0.4480
X	 0.2950	 0.4460
XX	 0.2530	 0.4640
Y	 0.3840	 0.4490
YY	 0.2000	 0.4080
Z	 0.3140	 0.4470
ZZ	 0.1000	 0.3660
a	 0.4120	 0.4850
aa	 0.2580	 0.4360
b	 0.1990	 0.3940
bb	 0.1530	 0.3990
c	 0.3270	 0.4310
cc	 0.1640	 0.3960
d	 0.3730	 0.4560
dd	 0.1970	 0.4330
e	 0.3900	 0.4840
ee	 0.1220	 0.3700
f	 0.4440	 0.4990
ff	 0.0000	 0.0990
g	 0.3060	 0.4530
gg	 0.0420	 0.3420
h	 0.2990	 0.4290
hh	 0.0000	 0.2580
i	 0.2830	 0.4220
ii	 0.0250	 0.3070

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Chain	Atom inclusion	Q-score
j	 0.3210	 0.4790
jj	 0.0370	 0.3130
k	 0.1560	 0.3940
l	 0.3160	 0.4710
m	 0.3580	 0.4670
n	 0.0230	 0.4110
o	 0.3180	 0.4640
p	 0.3270	 0.4500
r	 0.4290	 0.4860
s	 0.0010	 0.0370
t	 0.0000	 0.0010