



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:07 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 wwPDB EM Validation Summary 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:

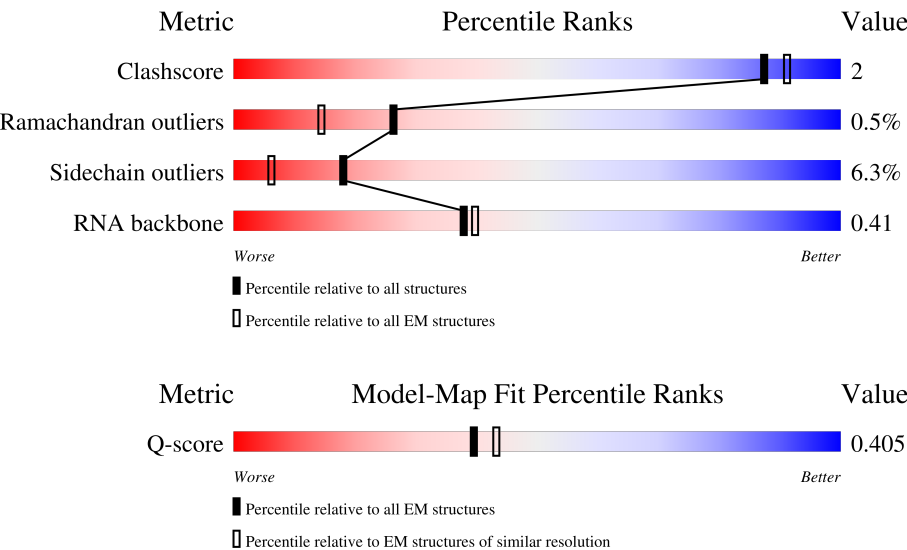
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	89% 89% 8% ..
80	cc	69	83% 77% 12% • 10%
81	dd	56	86% 88% 9% • •
82	ee	133	41% 39% • 59%
83	ff	156	44% 38% 5% • 56%
84	gg	317	98% 92% 6% •
85	hh	8	100% 50% 50%
86	ii	403	92% 84% 8% 8%
87	jj	710	59% 51% 8% • 40%

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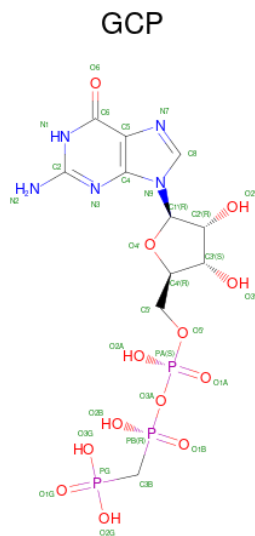
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Mol	Chain	Residues	Atoms		AltConf
88	g	1	Total 1	Mg 1	0
88	j	1	Total 1	Mg 1	0
88	5	176	Total 176	Mg 176	0
88	7	5	Total 5	Mg 5	0
88	8	6	Total 6	Mg 6	0
88	9	66	Total 66	Mg 66	0
88	jj	1	Total 1	Mg 1	0

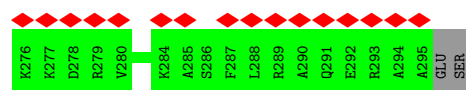
- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

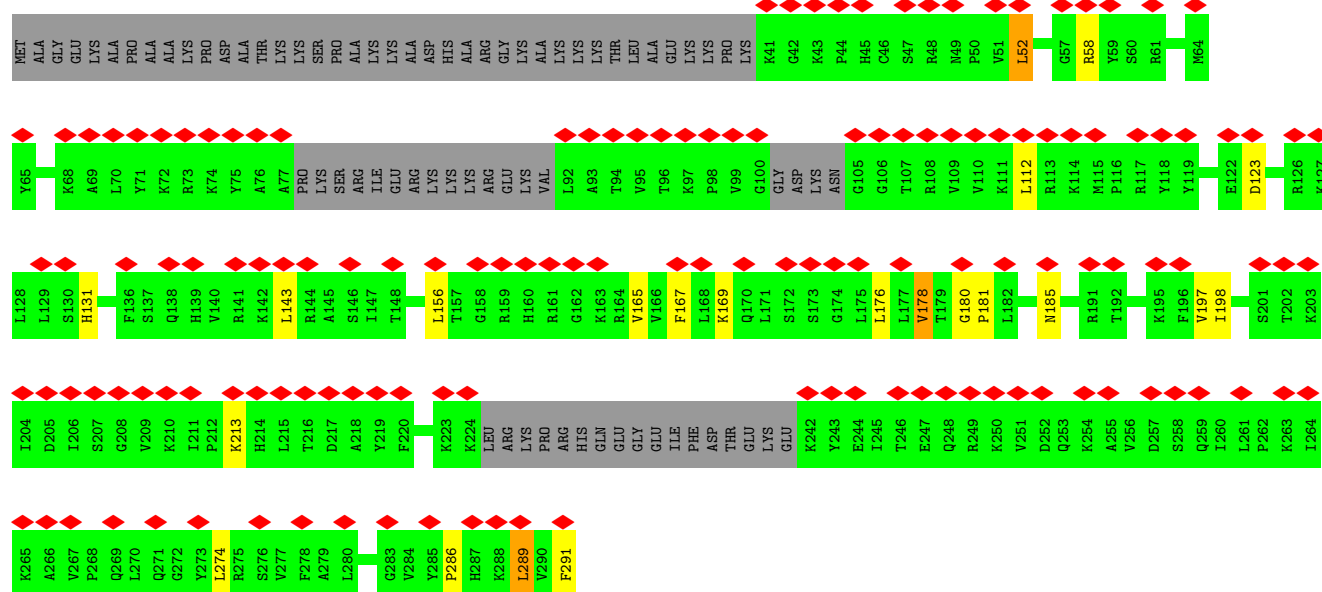
- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



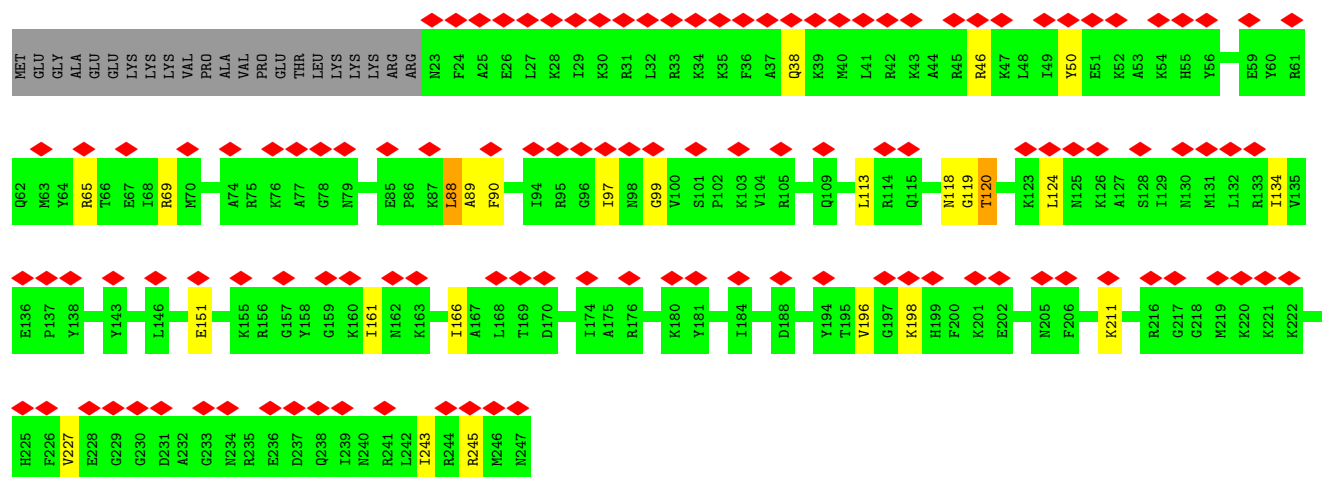
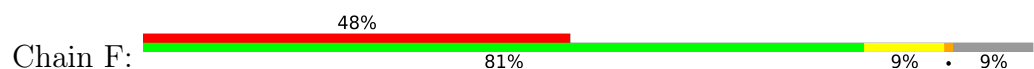
Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	



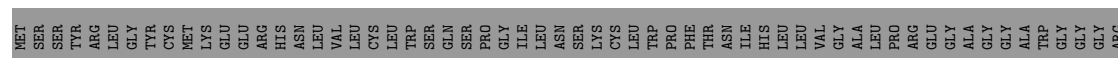
• Molecule 5: 60S ribosomal protein L6

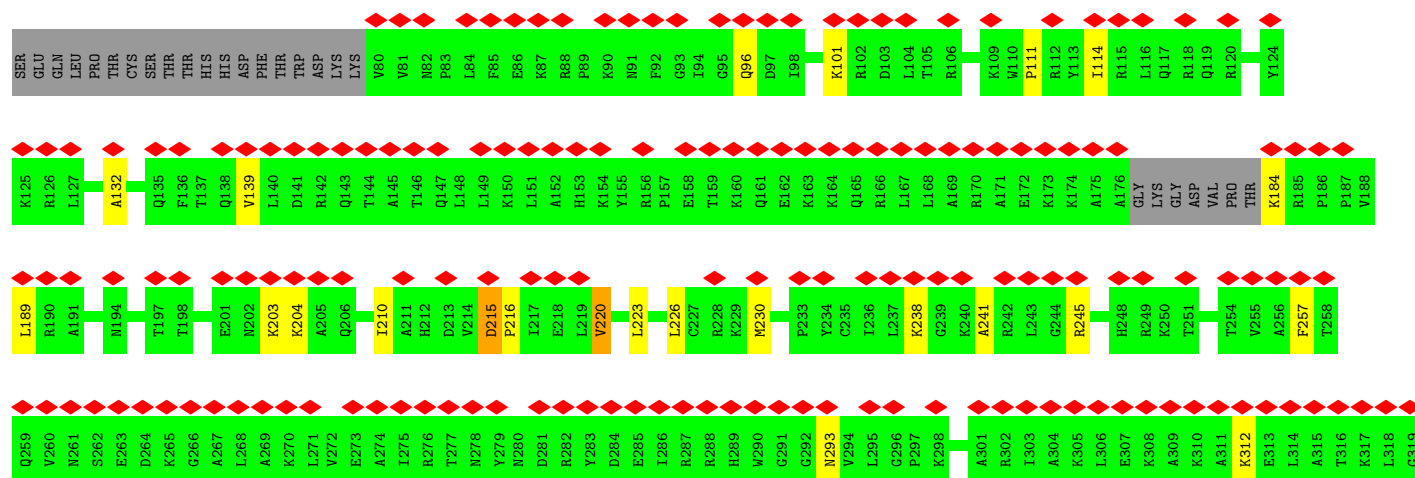


• Molecule 6: uL30

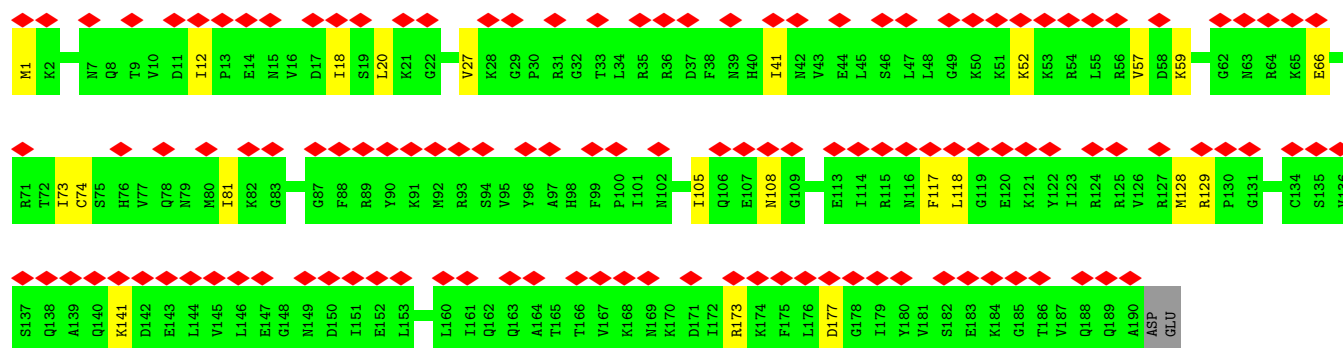
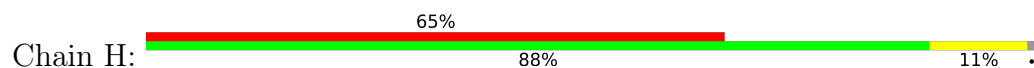


• Molecule 7: eL8

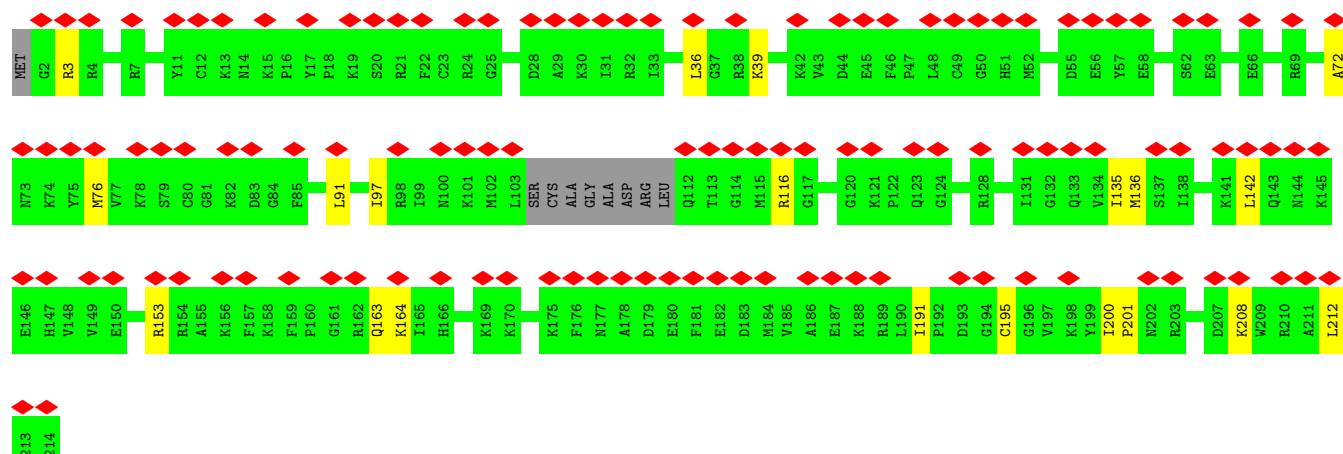
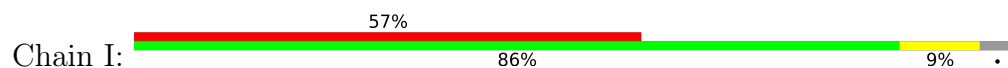




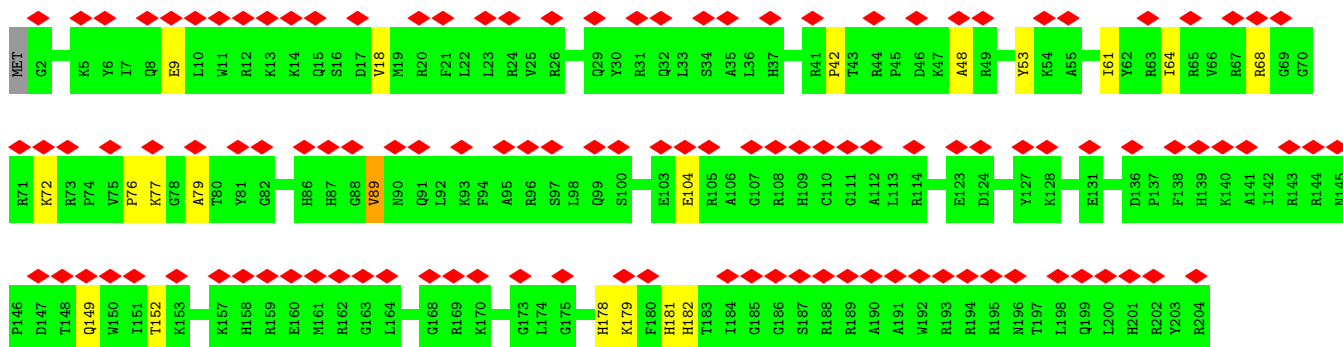
• Molecule 8: uL6



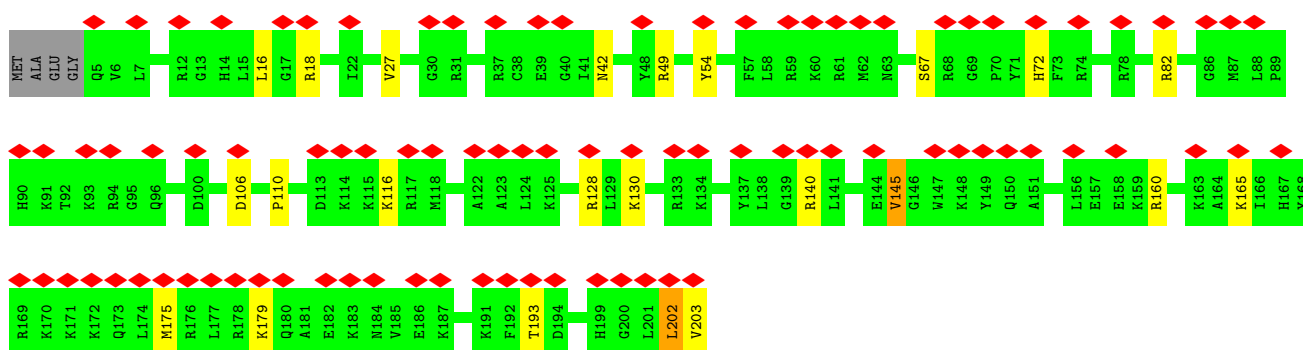
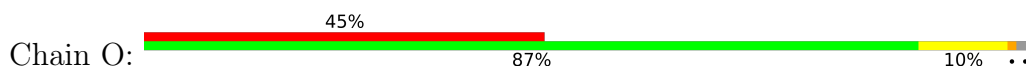
• Molecule 9: Ribosomal protein L10 (Predicted)



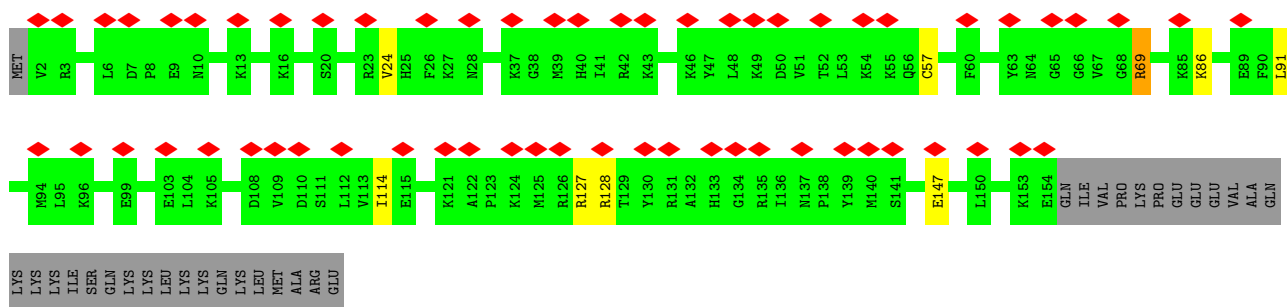
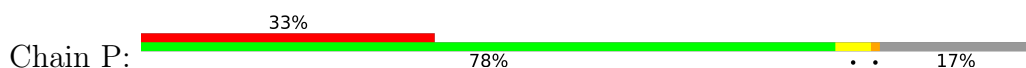
• Molecule 10: uL5



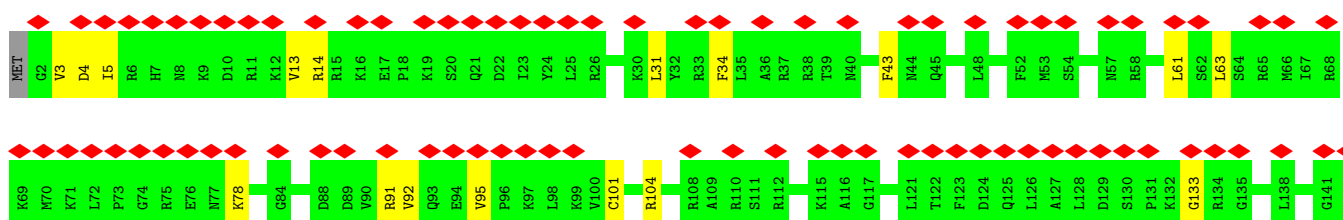
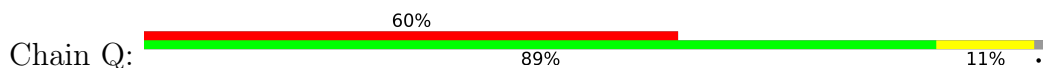
• Molecule 14: uL13

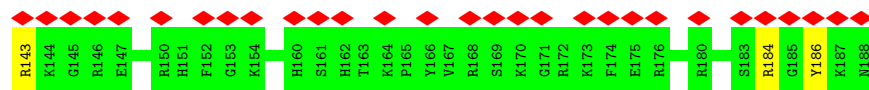


• Molecule 15: uL22

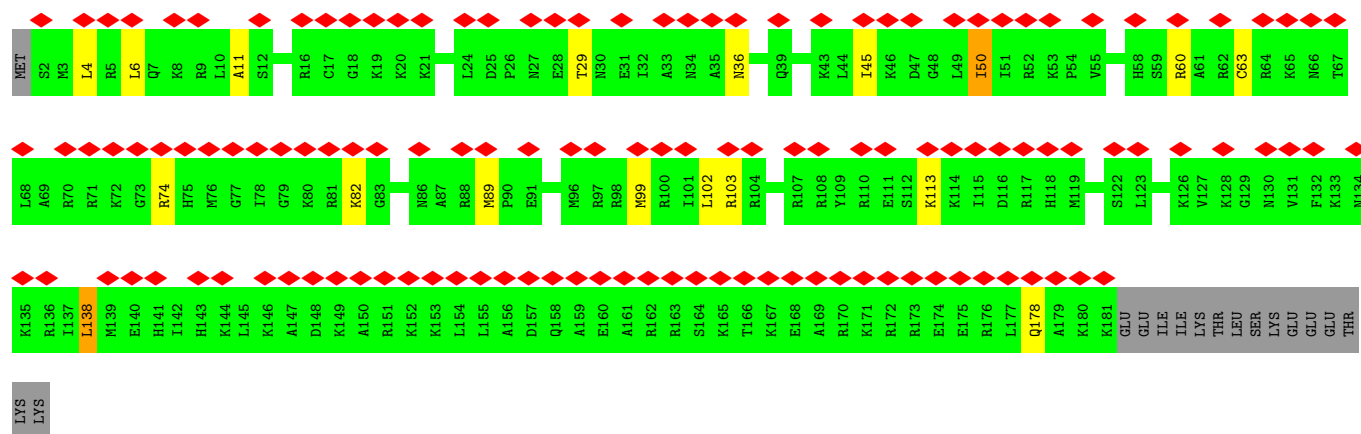
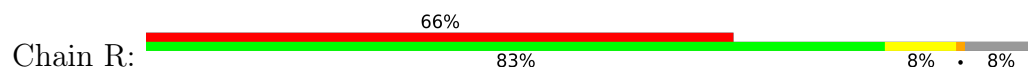


• Molecule 16: eL18

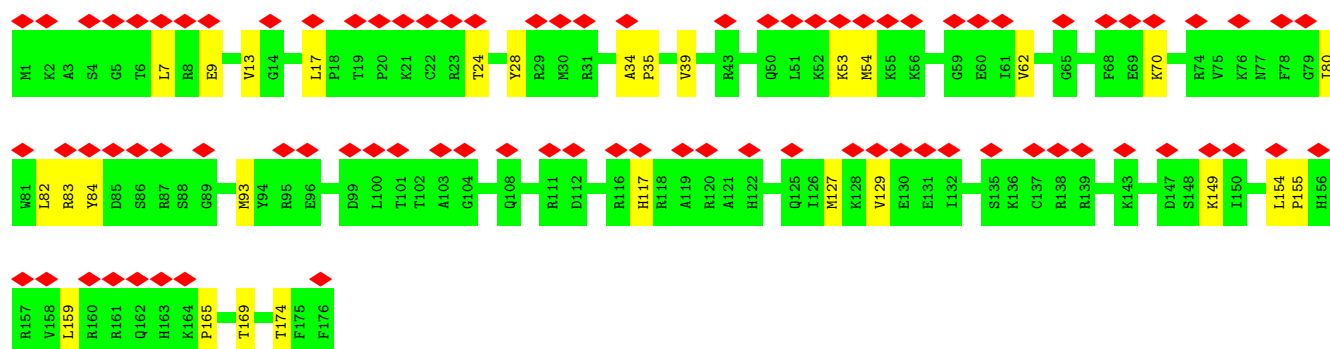
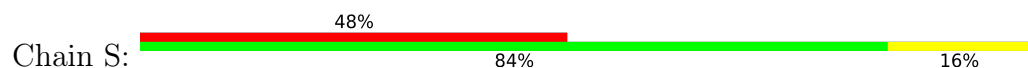




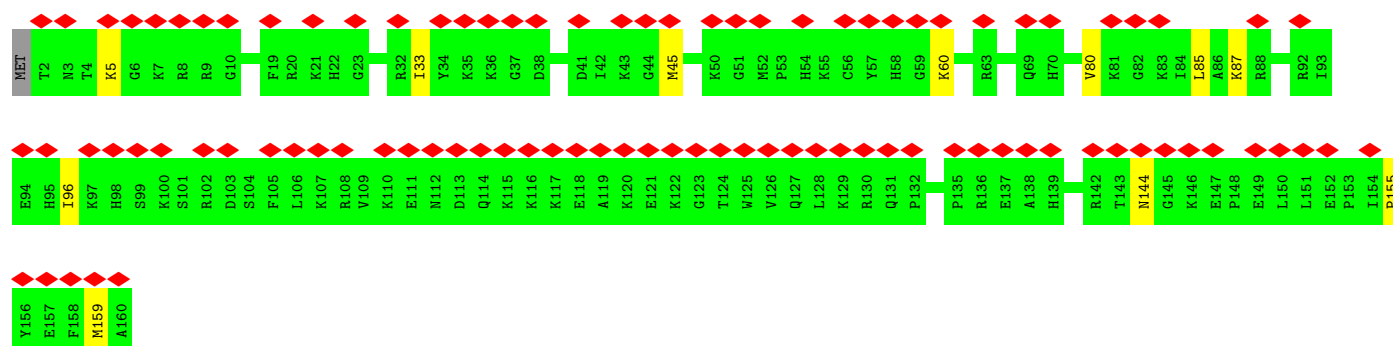
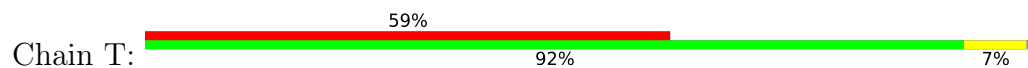
• Molecule 17: eL19



• Molecule 18: eL20

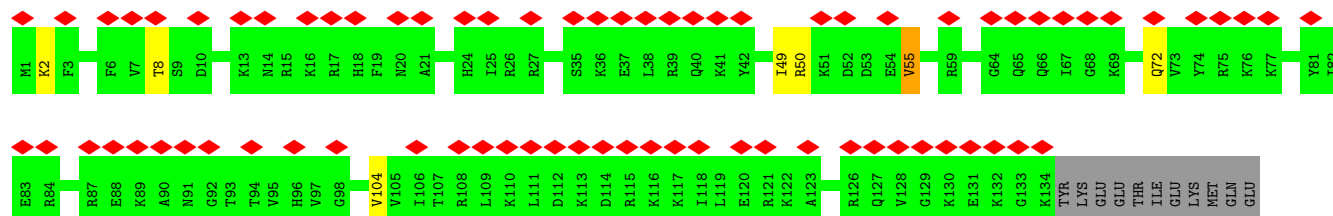
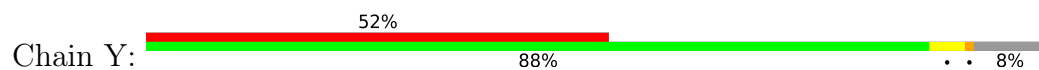


• Molecule 19: eL21

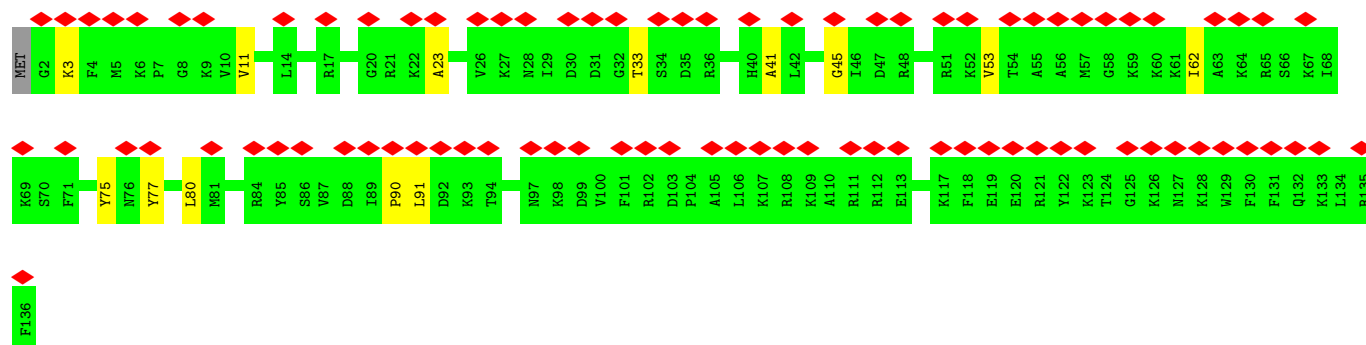
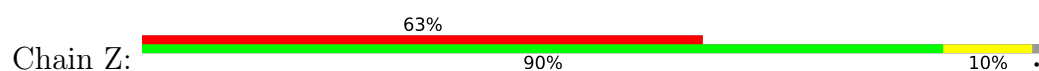




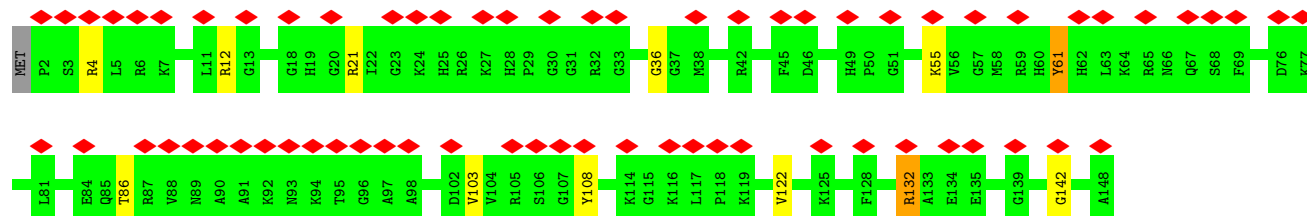
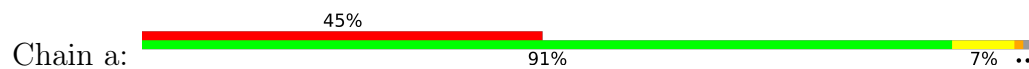
• Molecule 24: uL24



• Molecule 25: 60S ribosomal protein L27



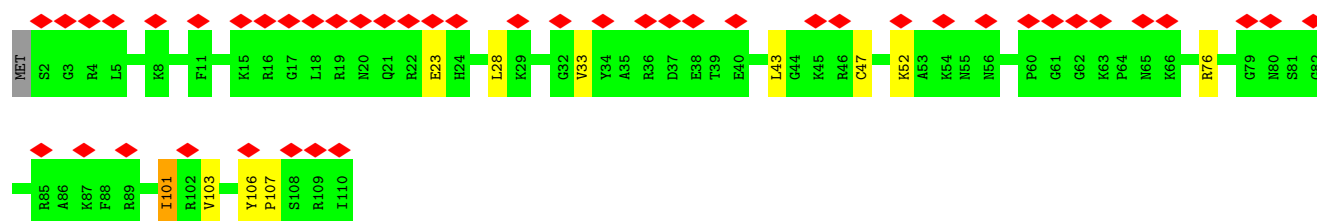
• Molecule 26: uL15



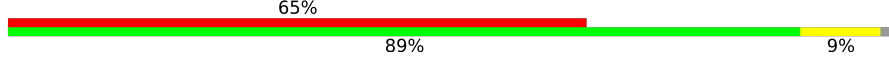
• Molecule 27: eL29

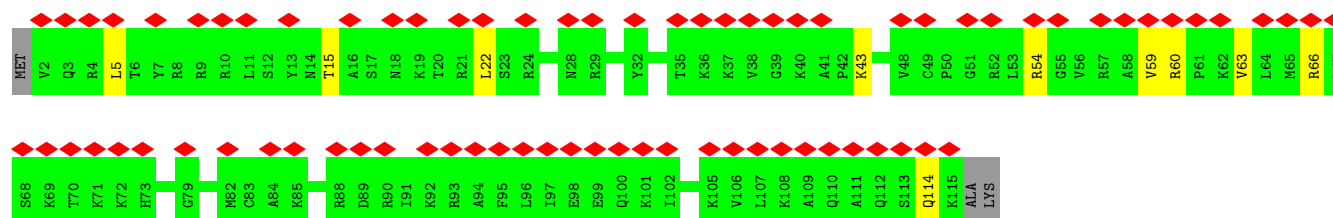


Chain f: 

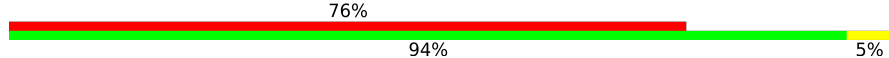


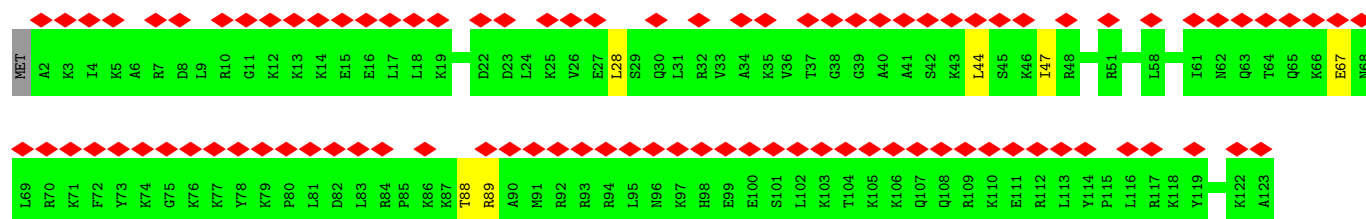
• Molecule 32: eL34

Chain g: 

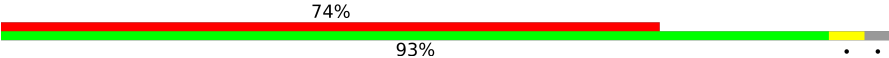


• Molecule 33: uL29

Chain h: 



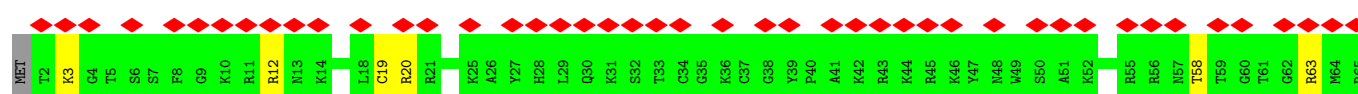
• Molecule 34: 60S ribosomal protein L36

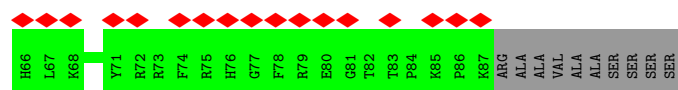
Chain i: 



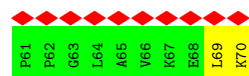
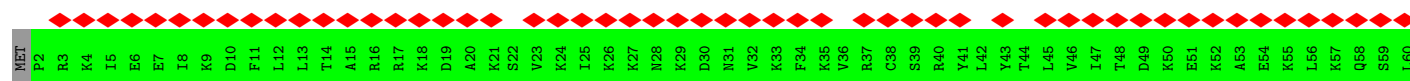
• Molecule 35: Ribosomal protein L37

Chain j: 

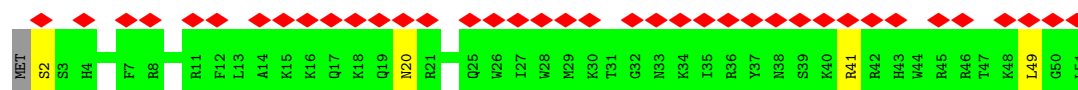
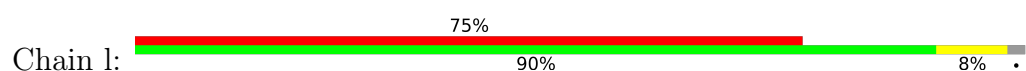




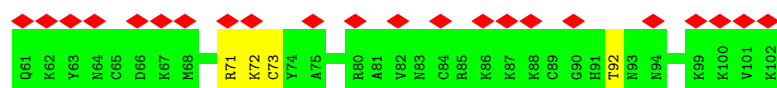
• Molecule 36: eL38



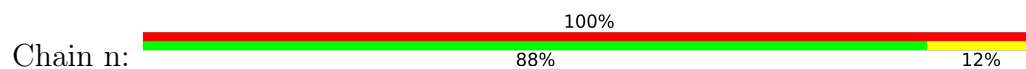
• Molecule 37: eL39



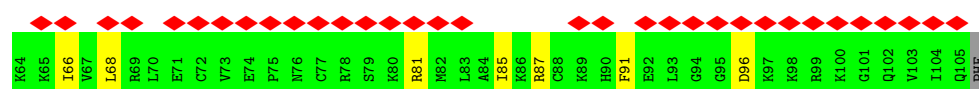
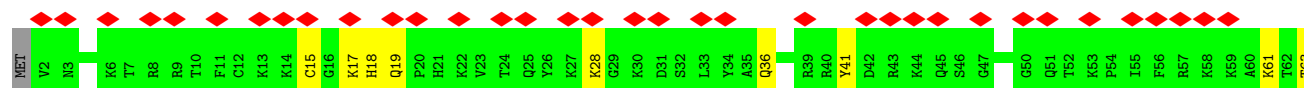
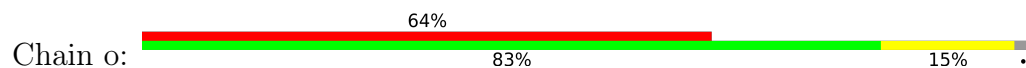
• Molecule 38: eL40

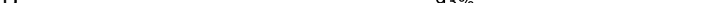


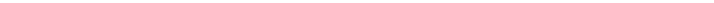
• Molecule 39: eL41

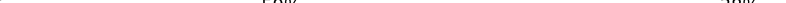


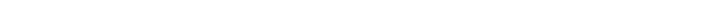
• Molecule 40: eL42

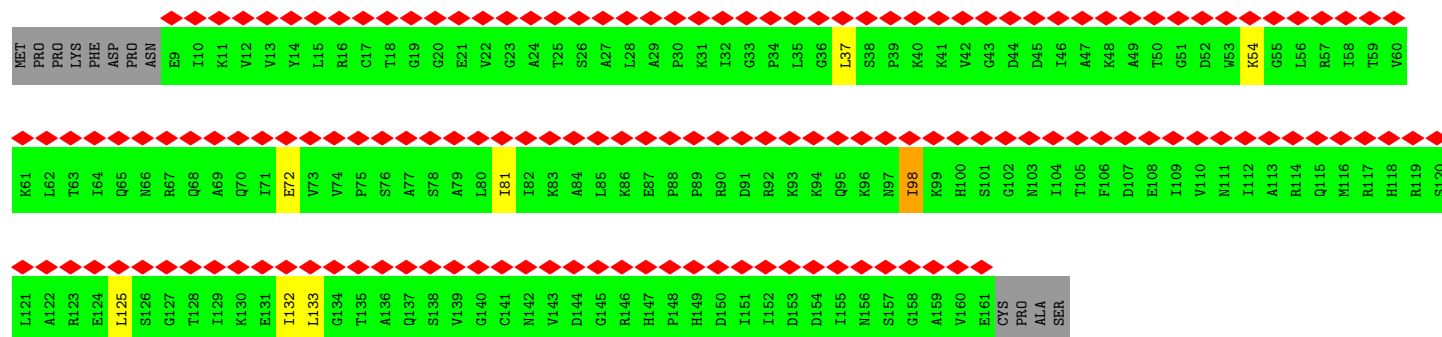


Chain p:  64% 93% 5%

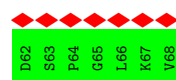
Chain r:  44% 80% 11% 9%

Chain s: 

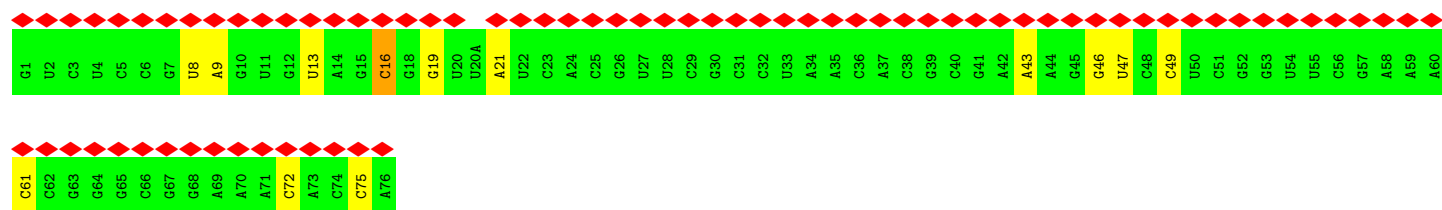
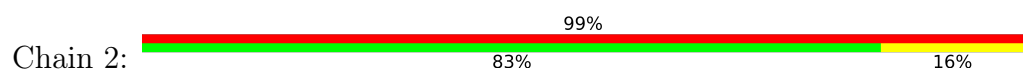
Chain t:  93% 88% 7%



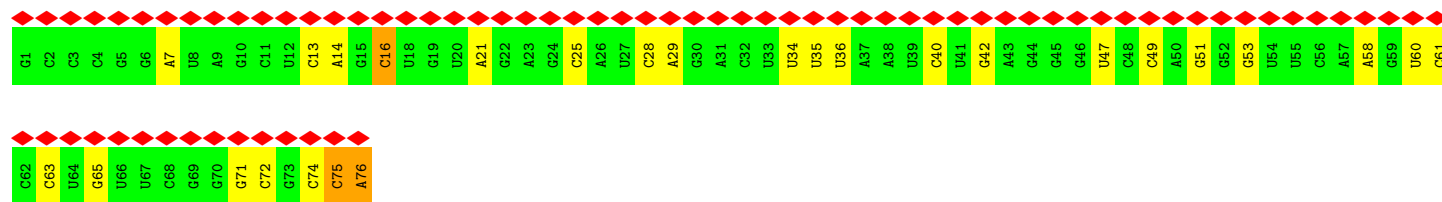
• Molecule 45: Nascent chain



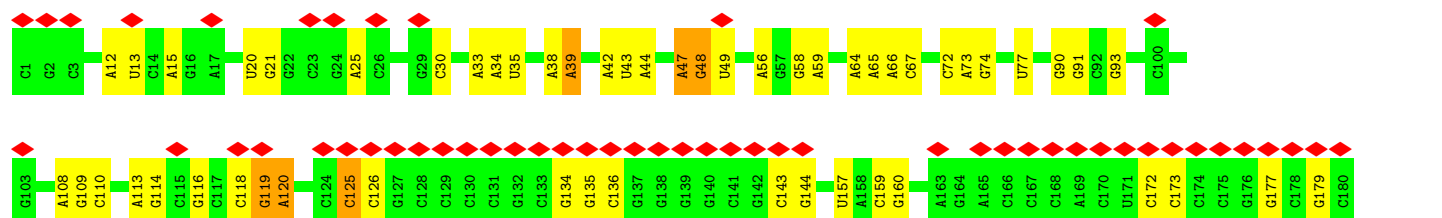
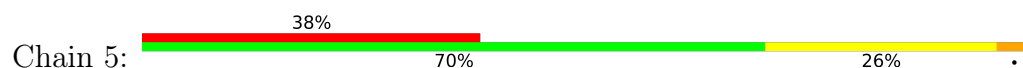
• Molecule 46: P-site tRNA

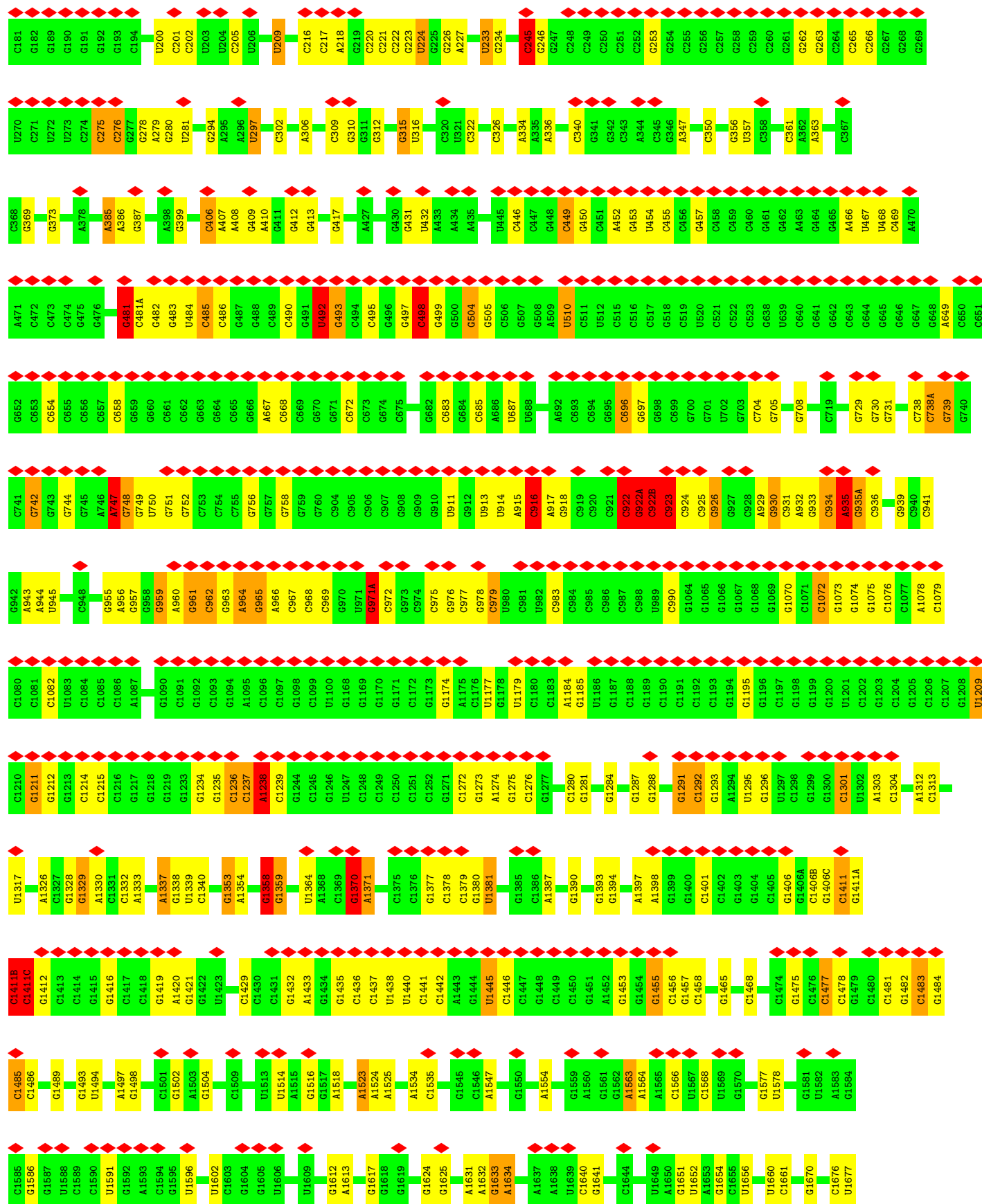


• Molecule 47: E-site tRNA

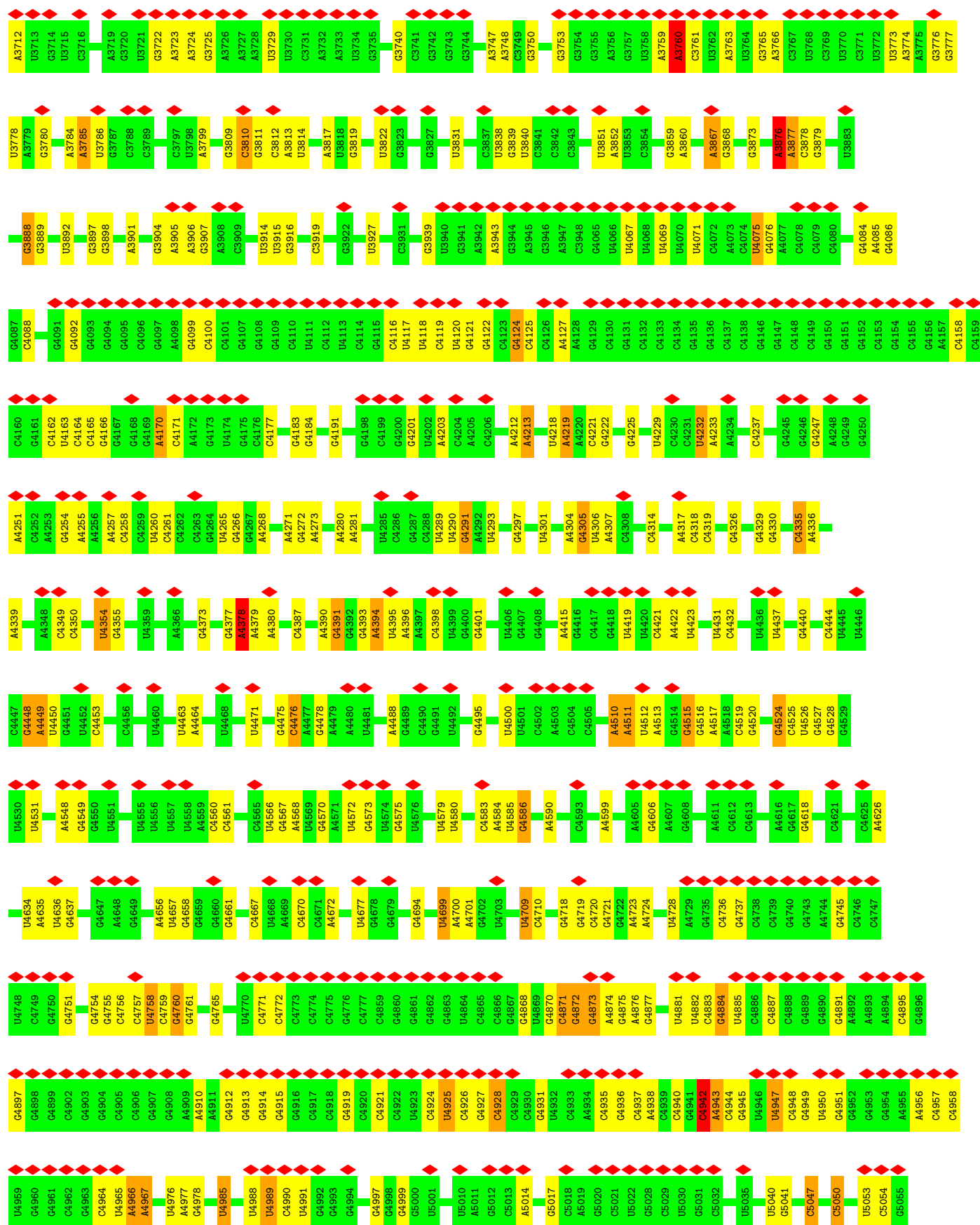


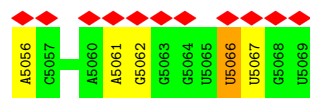
• Molecule 48: 28S ribosomal RNA



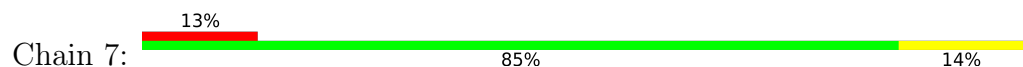




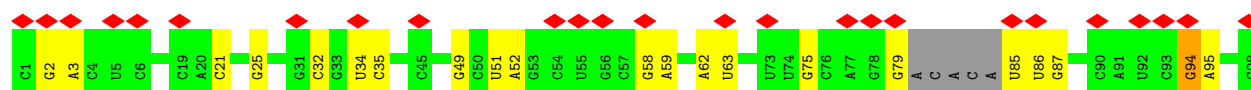




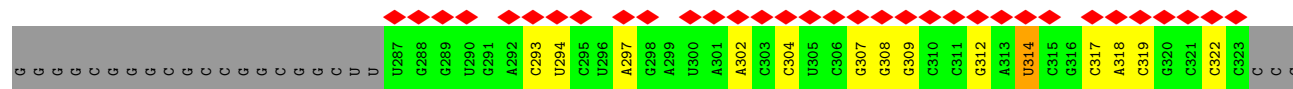
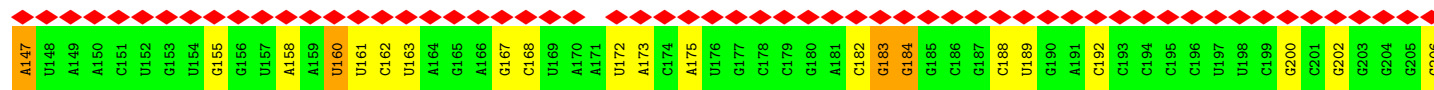
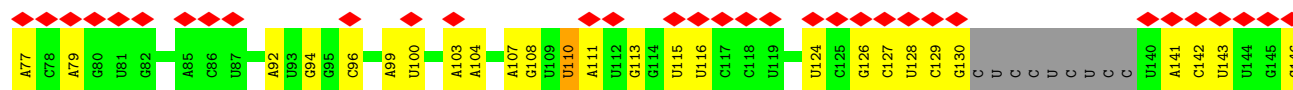
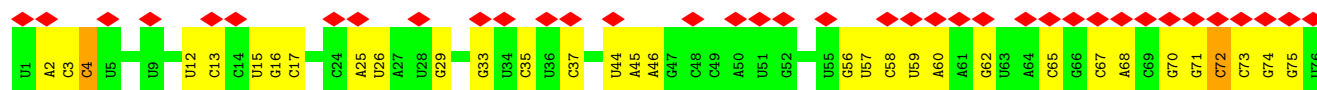
• Molecule 49: 5S ribosomal RNA



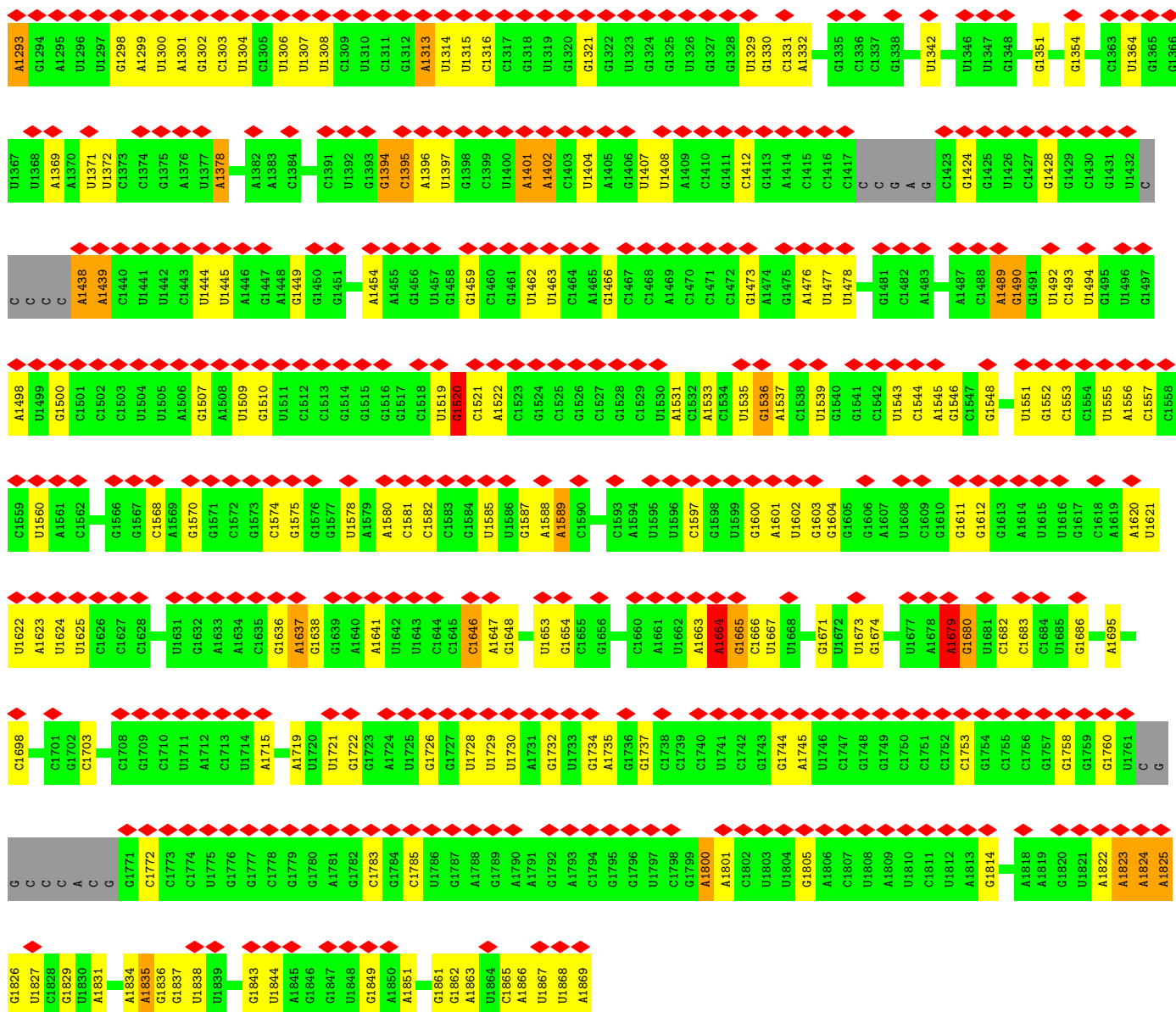
• Molecule 50: 5.8S ribosomal RNA

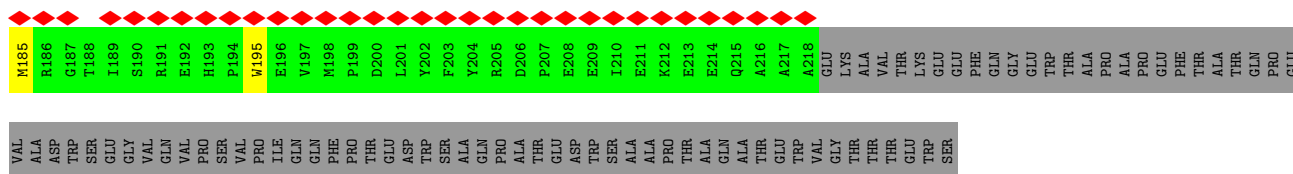


• Molecule 51: 18S ribosomal RNA

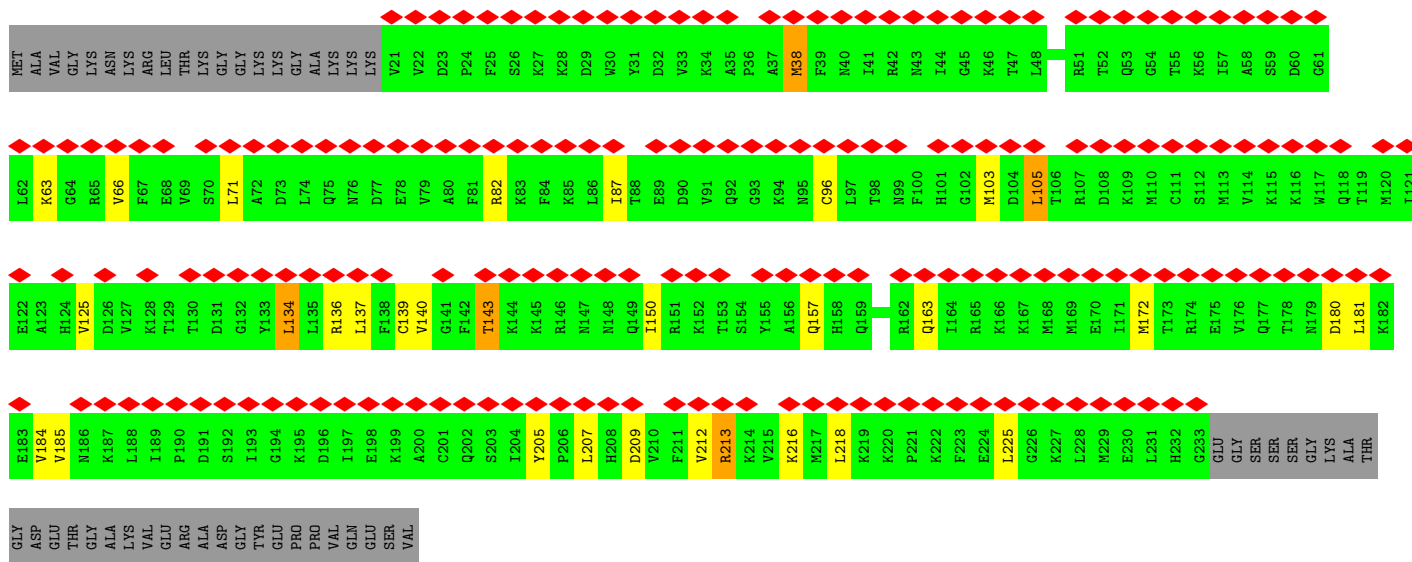
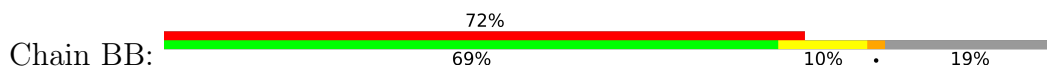




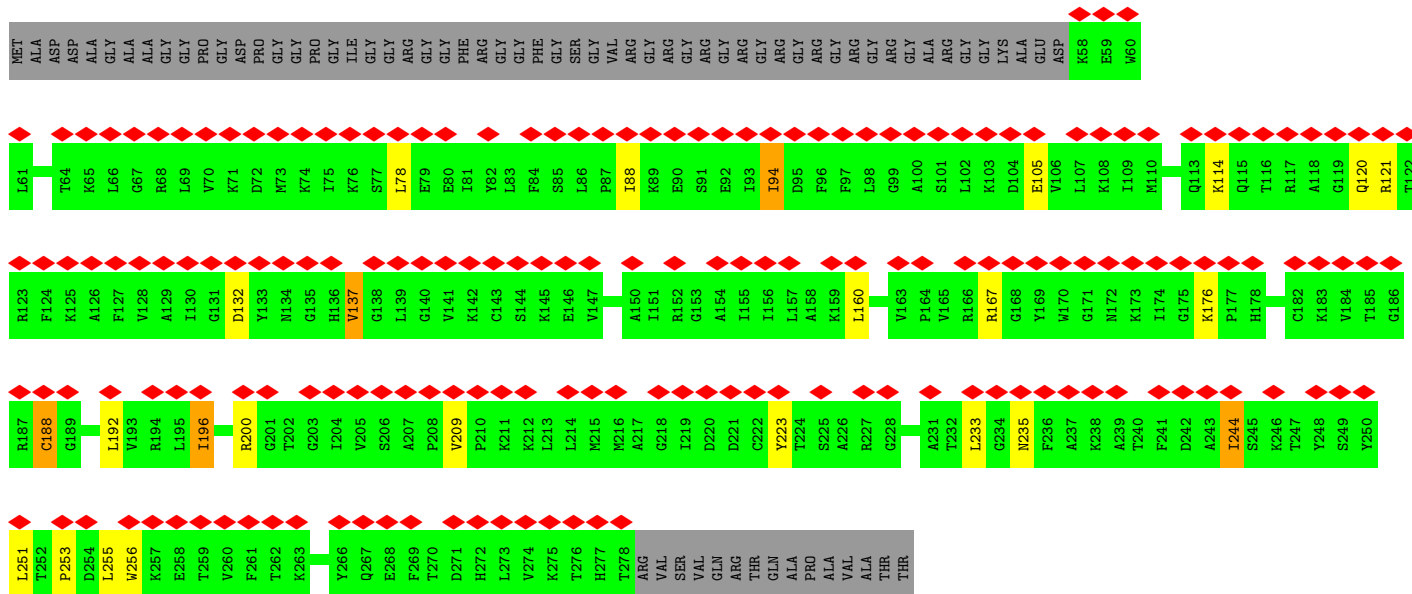




• Molecule 53: 40S ribosomal protein S3a

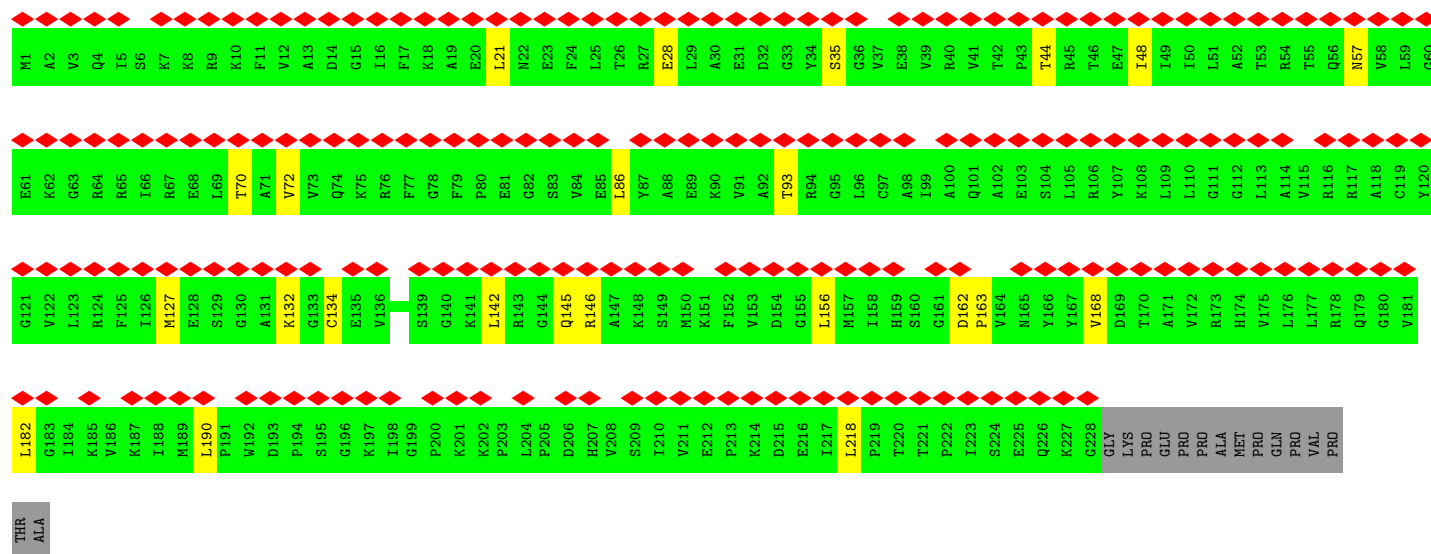


• Molecule 54: uS5



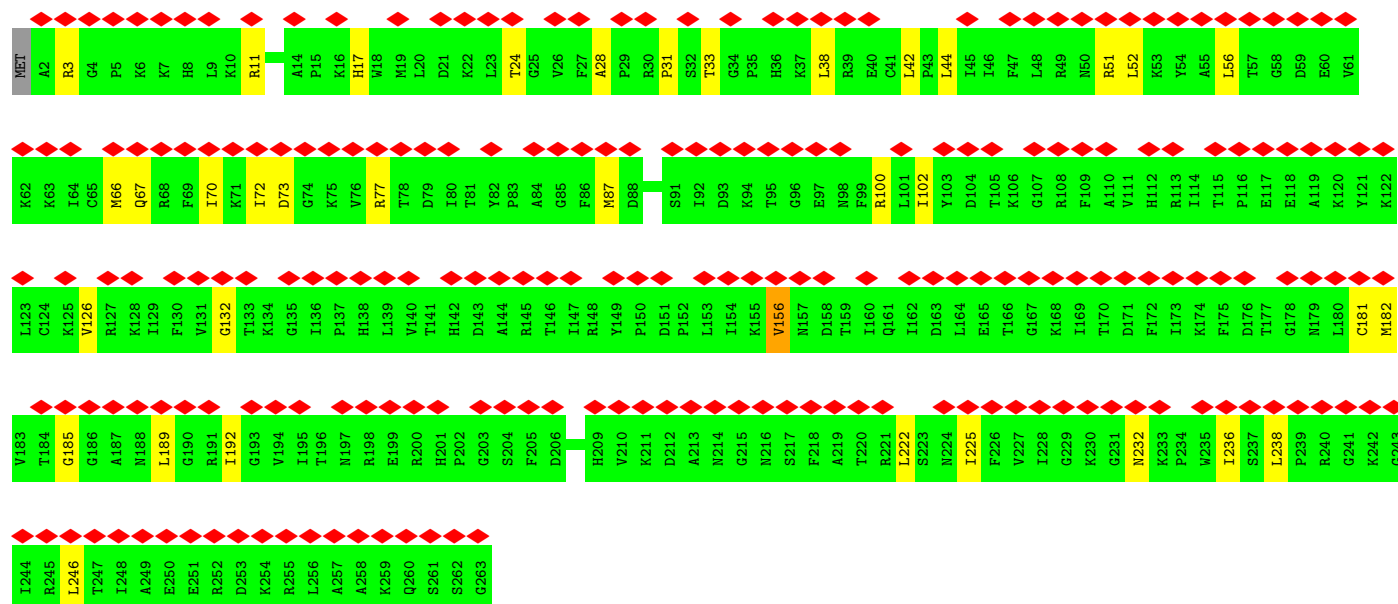
• Molecule 55: uS3

Chain DD: 



• Molecule 56: eS4

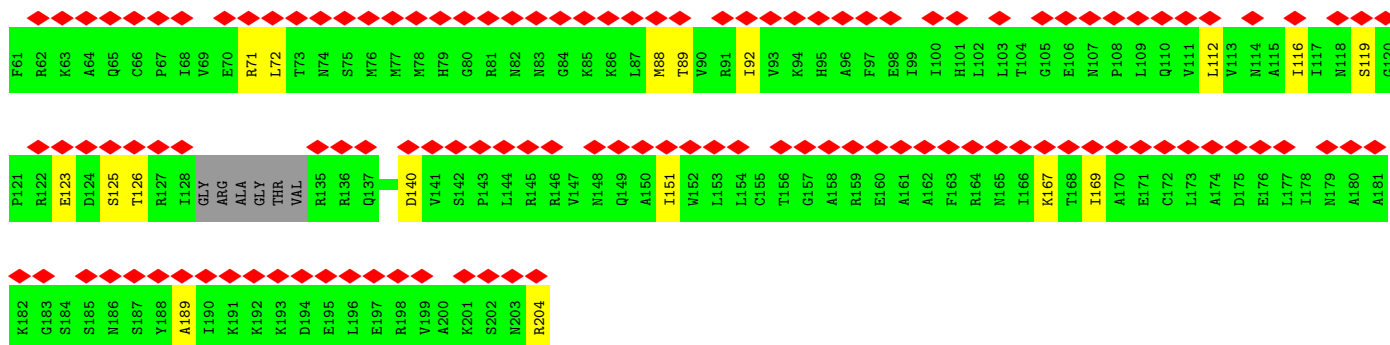
Chain EE: 



• Molecule 57: uS7

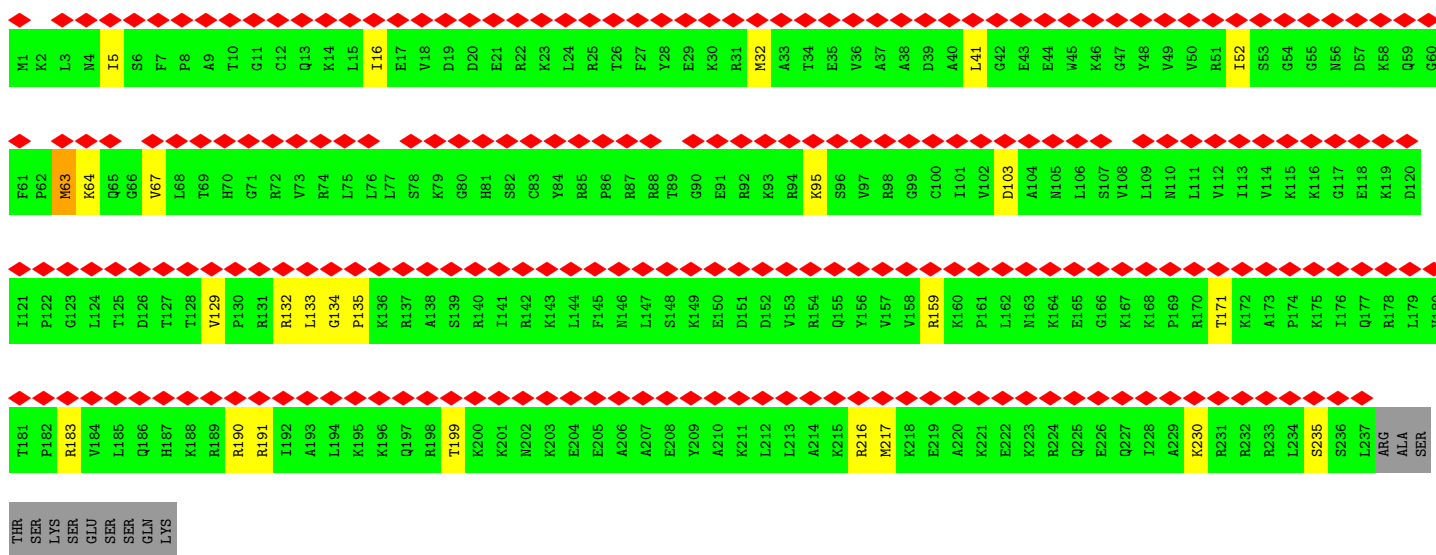
Chain FF: 





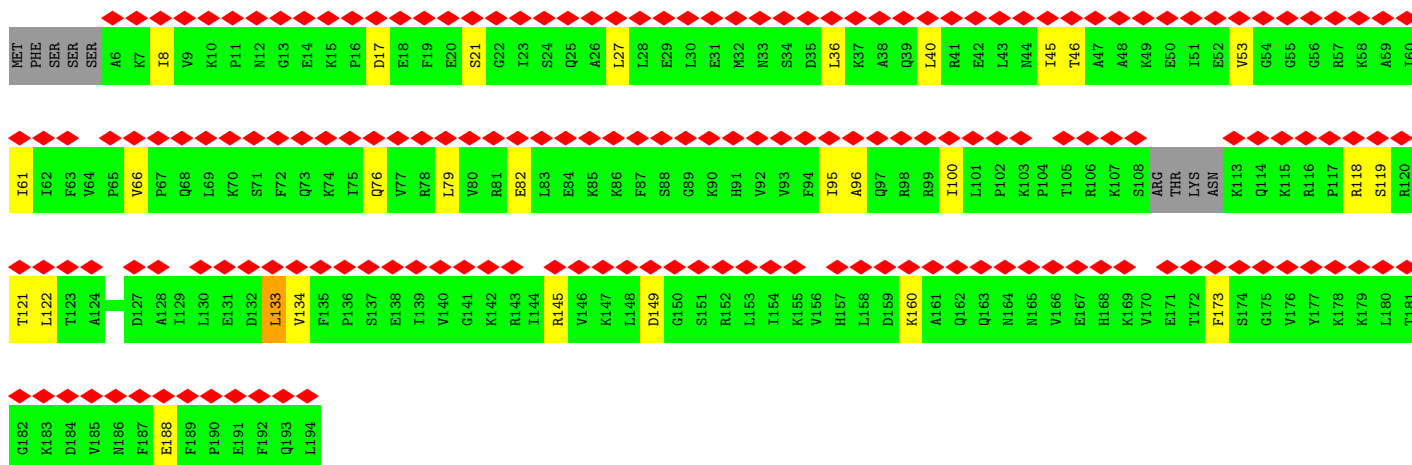
• Molecule 58: 40S ribosomal protein S6

Chain GG: 93%
85% 10% 5%

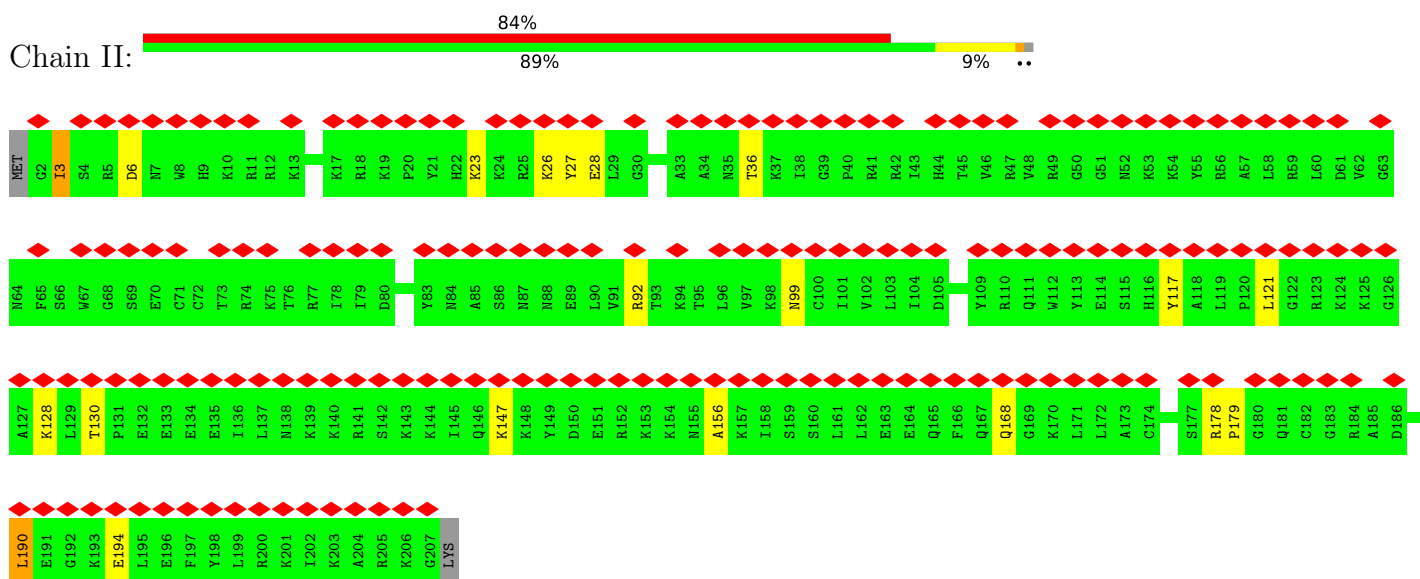


• Molecule 59: eS7

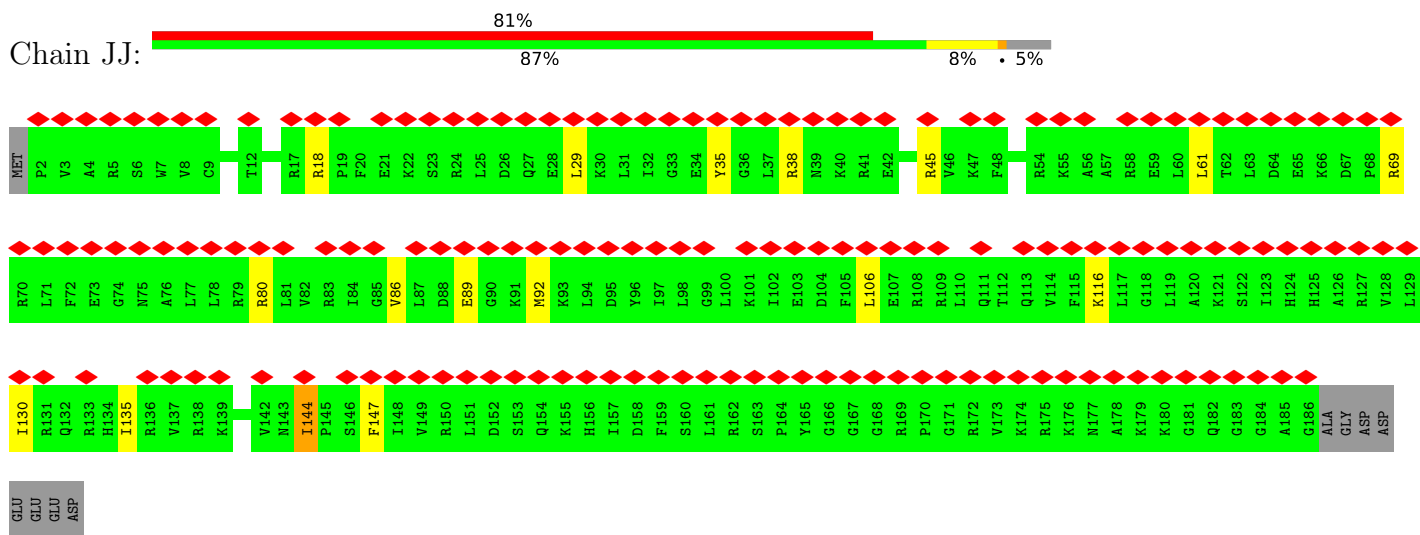
Chain HH: 91%
81% 14% 5%



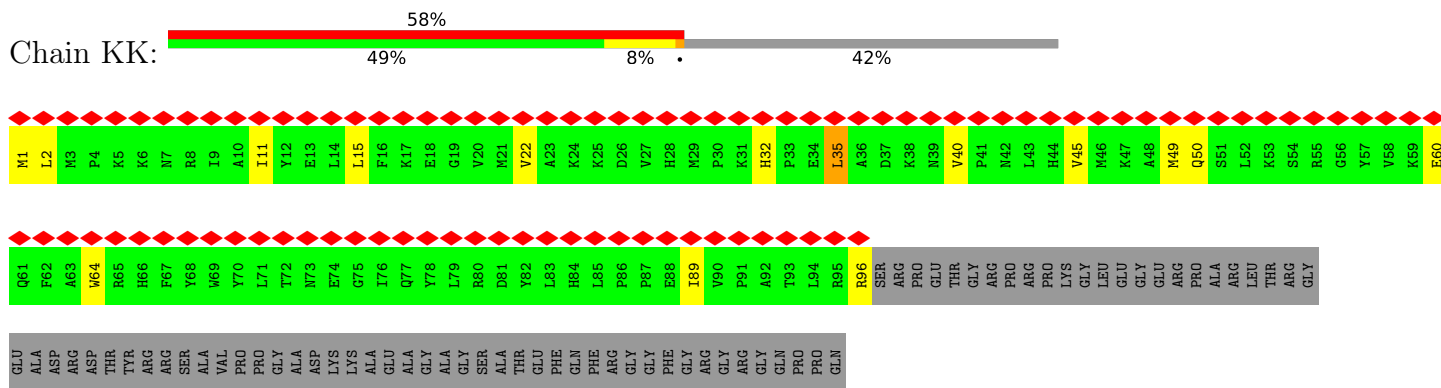
• Molecule 60: eS8



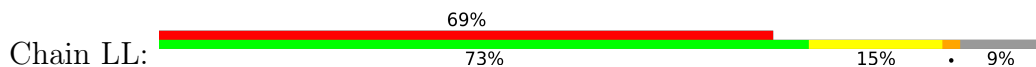
• Molecule 61: Ribosomal protein S9 (Predicted)

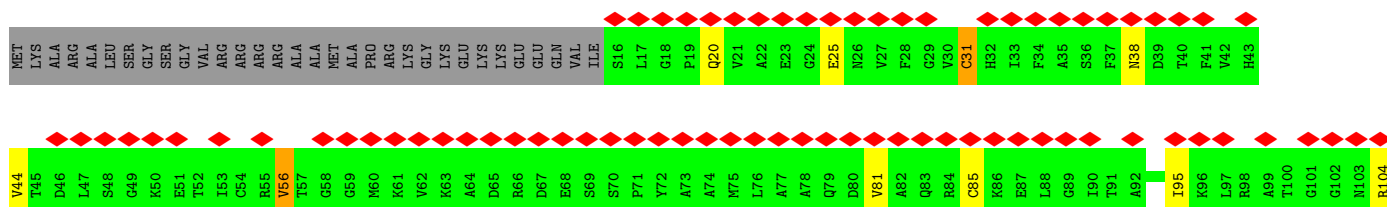


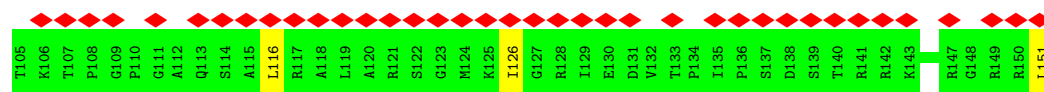
• Molecule 62: eS10



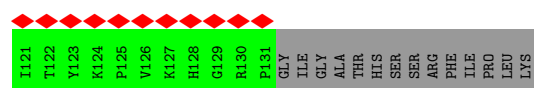
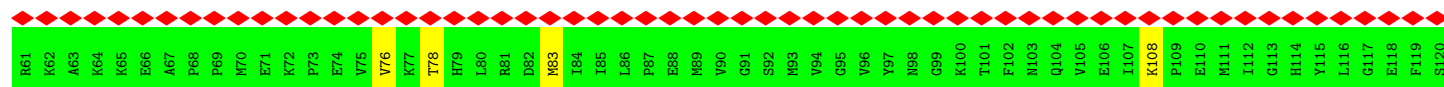
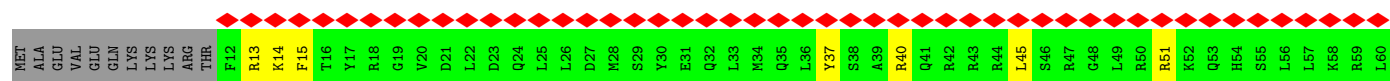
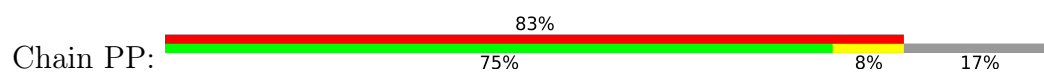
• Molecule 63: uS17



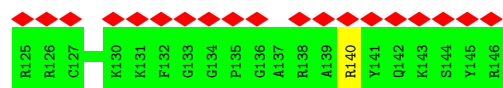
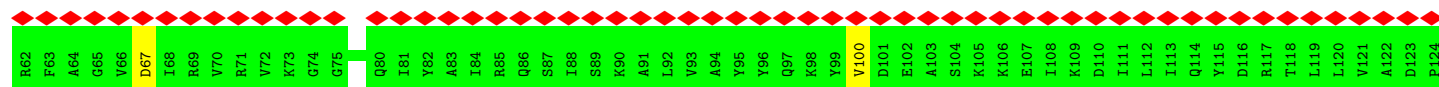
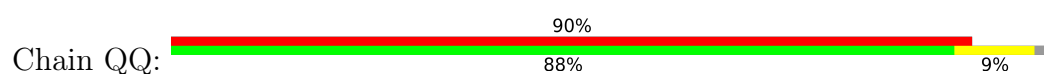




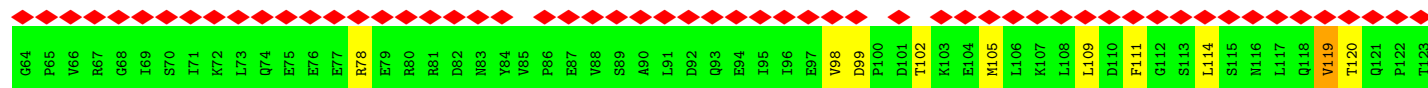
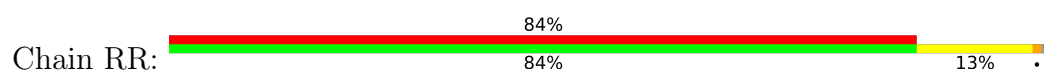
• Molecule 67: uS19



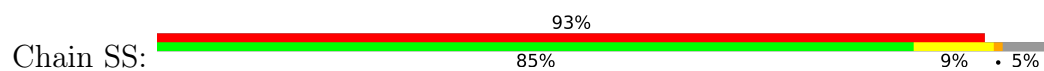
• Molecule 68: uS9

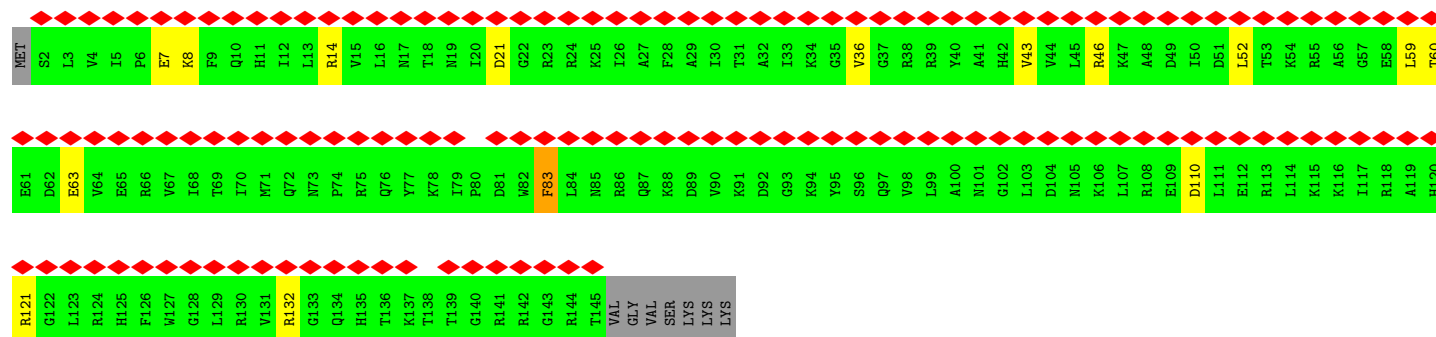


• Molecule 69: eS17

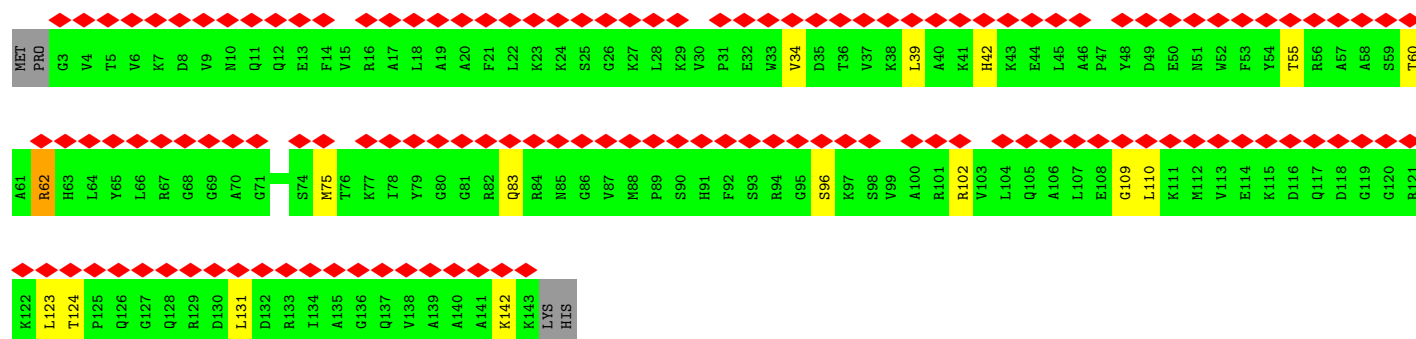


• Molecule 70: uS13

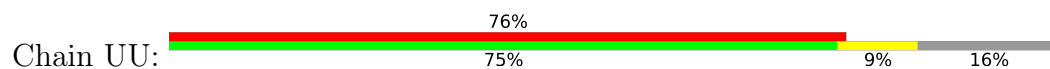




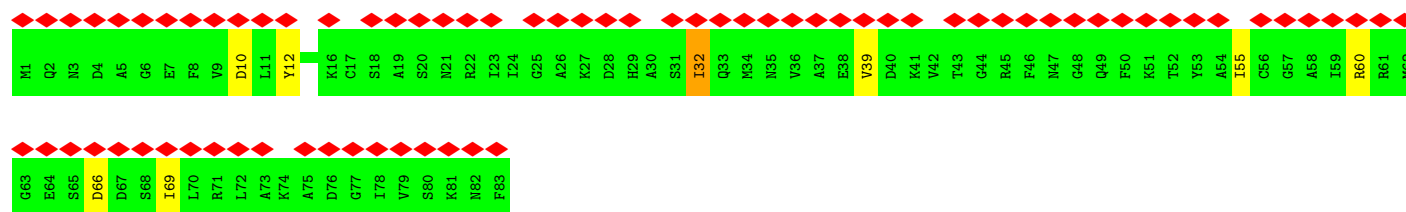
• Molecule 71: eS19



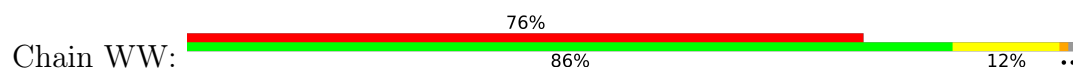
• Molecule 72: uS10



• Molecule 73: eS21



• Molecule 74: uS8



ALA
GLY
GLU
ASP
ALA

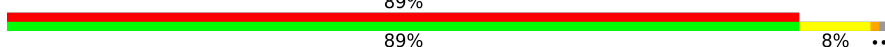
• Molecule 78: eS26

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 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 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 R17 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

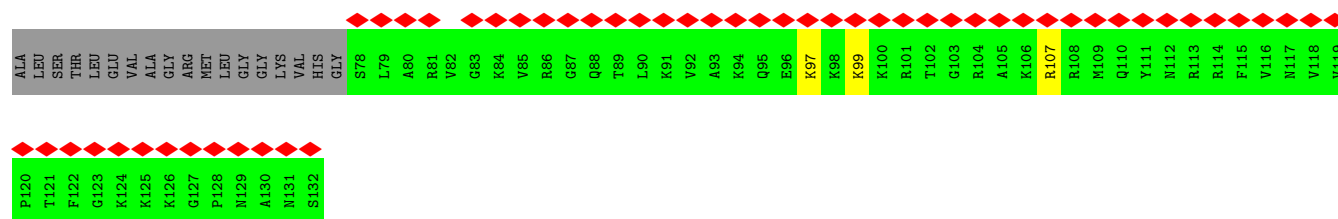
Chain dd: 

MET G2 H3 Q4 Q5 L6 Y7 W8 S9 H10 P11 R12 K13 F14 G15 Q16 G17 S18 R19 S20 C21 R22 V23 S24 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

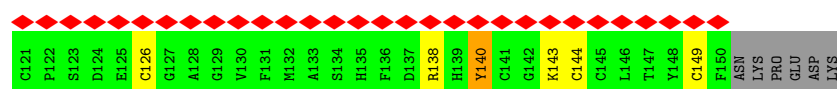
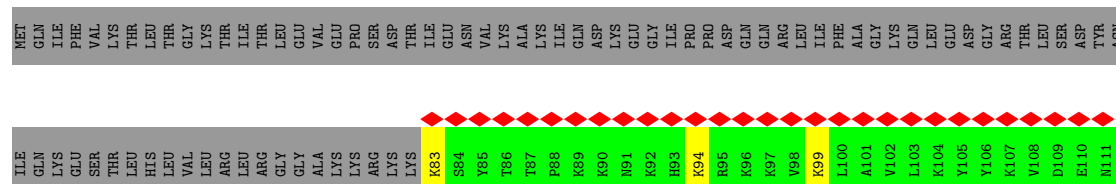
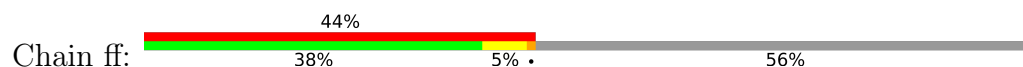
• Molecule 82: eS30

Chain ee: 

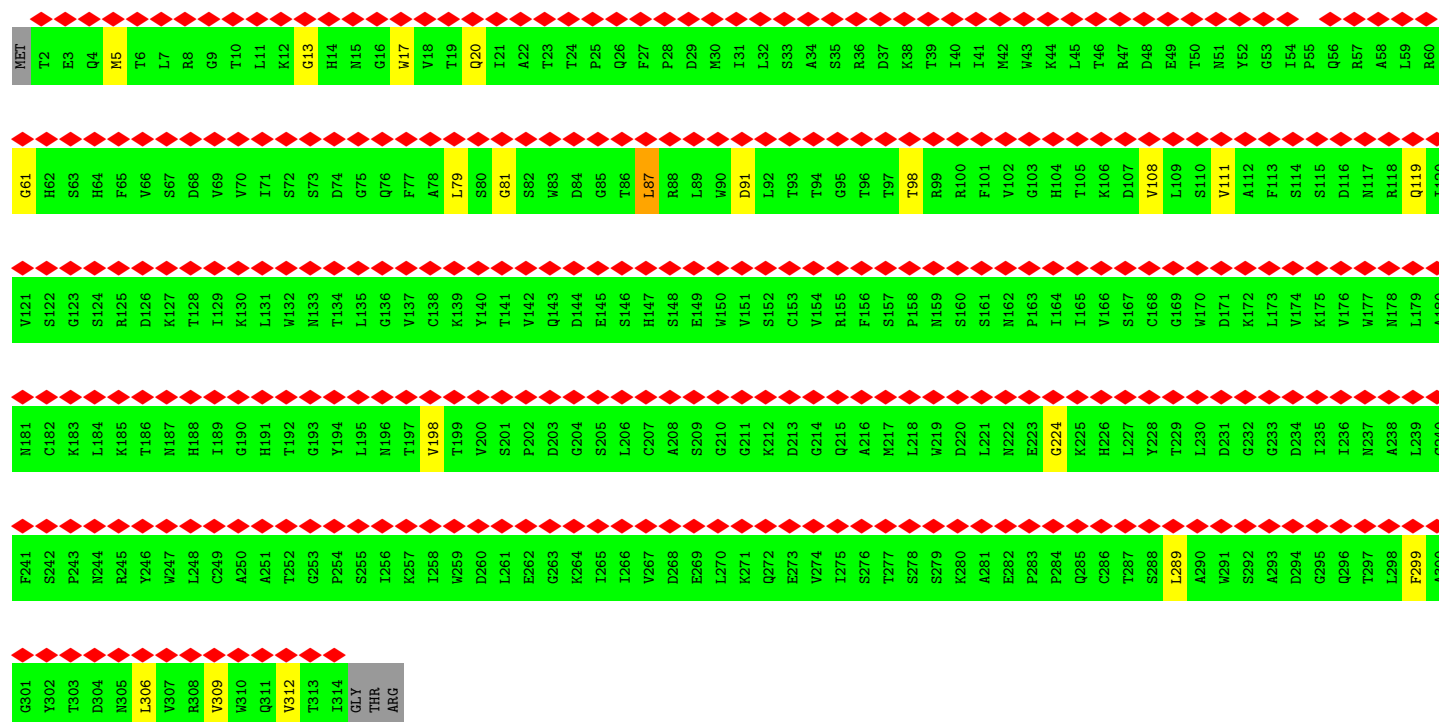
MET GLN LEU PHE VAL ARG ALA GLN LEU LEU HIS THR LEU GLU VAL THR GLY ARG GLU THR VAL ALA GLN ILE LYS ALA HIS VAL R22 ALA SER LEU GLU ILE ALA PRO GLU ASP GLN VAL VAL LEU LEU ALA GLY THR PRO LEU ASP GLU THR LEU GLN CYS GLY VAL GLU



• Molecule 83: eS31



• Molecule 84: RACK1



• Molecule 85: mRNA (UGA stop codon)



L635	L636	K637	G638	Q639	M640	F641	L642	V643	E644	L645	Q646	T647	Q648	R649	P650	I651	A652	L653	E654	L655	V656	K657	D658	F659	K660	E661	L662	G663	R664	F665	N666	L667	R668	Y669	G670	G671	S672	T673	I674	A675	A676	G677	V678	V679	T680	E681	I682	K683	E684												
I576	K576	A577	C578	T579	R580	F581	R582	A583	R584	I585	L586	I587	F588	N589	I590	E591	I592	P593	I594	T595	K596	G597	F598	P599	V600	L601	L602	H603	Y604	Q605	T606	V607	S608	E609	P610	A611	V612	I613	K614	R615	L616	I617	S618	V619	L620	N621	K622	S623	T624	G625	E626	V627	T628	K629	K630	K631	P632	K633	F634		
Q515	T516	G517	D518	R519	L520	L521	A522	M523	P524	P525	N526	E527	T528	C529	T530	V531	K532	G533	I534	T535	L536	H537	D538	E539	P540	V541	D542	H543	A544	A545	A546	G547	D548	H549	V550	S551	L552	T553	L554	V555	G556	M557	D558	I559	I560	K561	I562	N563	V564	G565	C566	I567	F568	C569	G570	P571	K572	V573	P574		
R455	S456	Q457	S458	S459	E460	L461	T462	K463	W464	Y465	K466	G467	L468	C469	L470	L471	E472	Q473	I474	D475	S476	F477	K478	P479	P480	Q481	R482	S483	I484	D485	K486	P487	F488	R489	L490	C491	V492	S493	D494	V495	F496	K497	D498	Q499	G500	S501	G502	F503	C504	I505	T506	G507	K508	I509	E510	A511	G512	Y513	I514		
T335	T336	T337	K338	V339	T399	Q400	L401	A402	V403	A404	V405	N406	K407	M408	D409	Q410	V411	N412	W413	Q414	M354	M355	I356	T357	G358	A359	A360	Q361	A362	D363	V364	A365	V366	L367	V368	V369	D370	A371	A372	A373	G374	E375	F376	E377	A378	G379	F380	E381	T382	G383	G384	Q385	T386	R387	E388	H389	G390	L391	L392	V393	R394
T275	L276	M277	G278	H279	M280	L281	Y282	L283	L284	G285	N286	I287	N288	K289	R290	T291	M292	H293	K294	Y295	E296	Q297	E298	S299	K300	K301	A302	G303	K304	A305	S306	F307	A308	Y309	A310	W311	V312	L313	D314	E315	T316	G317	E318	E319	R320	E321	R322	G323	V324	T325	M326	D327	V328	G329	M330	T331	K332	F333	E334		

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 (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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

The worst 5 of 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

The worst 5 of 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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	N9-C1'-C2'	12.64	132.96	114.00

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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
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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	224 (91%)	19 (8%)	3 (1%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	l	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 678 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	LL	126	VAL
75	XX	115	ILE
64	MM	99	LYS
63	LL	121	GLN
69	RR	62	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
64	MM	19	GLN
81	dd	26	ASN
66	OO	26	ASN
70	SS	10	GLN
86	ii	358	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	27 (37%)	1 (1%)
48	5	3511/3543 (99%)	873 (24%)	165 (4%)
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%)

5 of 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

5 of 259 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	9	1330	G
51	9	1493	C
48	5	2089	G
48	5	2046	G
51	9	1621	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

The worst 5 of 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

The worst 5 of 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

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

Continued on next page...

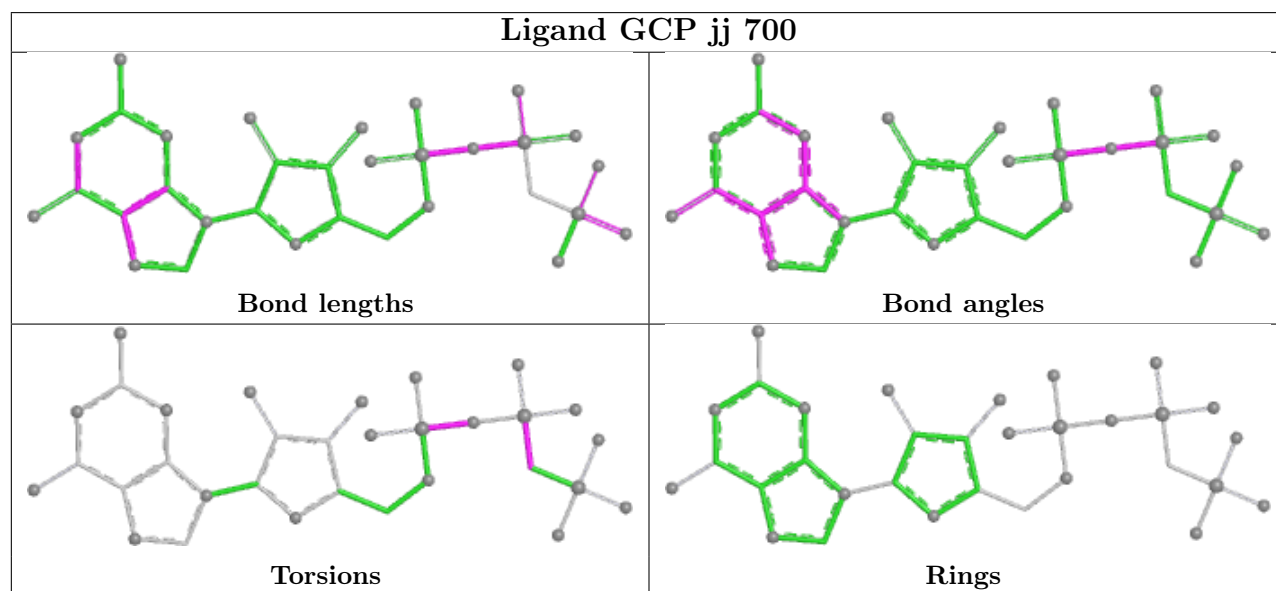
Continued from previous page...

Mol	Chain	Res	Type	Atoms
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 [i](#)

The following chains have linkage breaks:

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

The worst 5 of 54 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

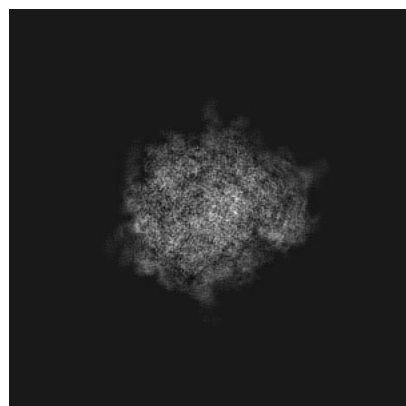
6 Map visualisation [i](#)

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.

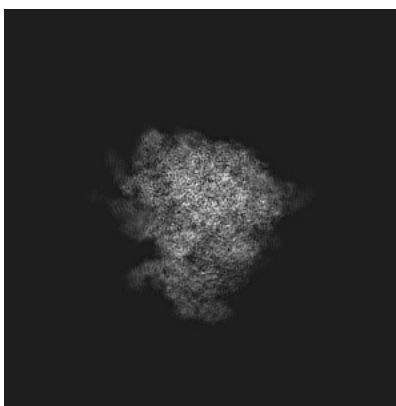
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

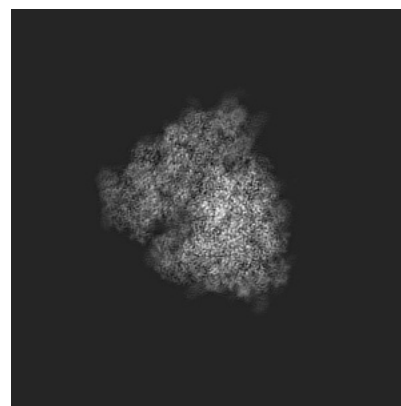
6.1.1 Primary map



X

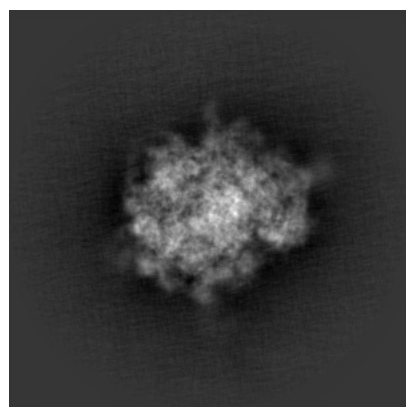


Y

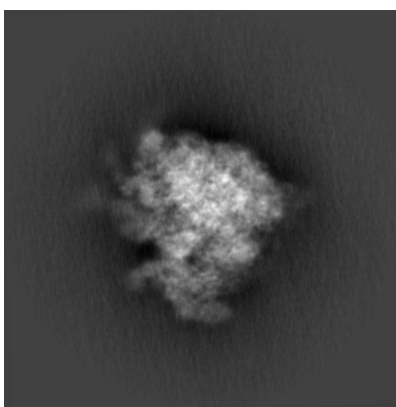


Z

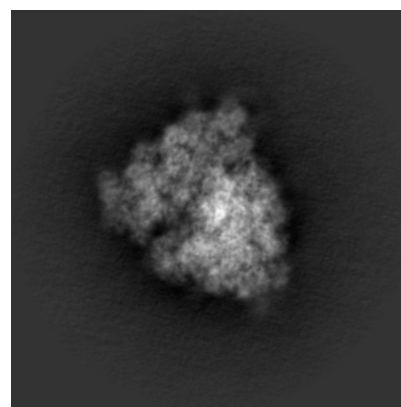
6.1.2 Raw map



X



Y

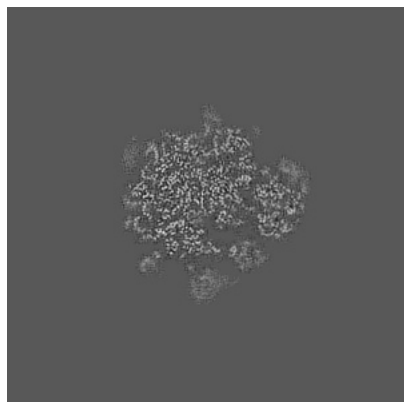


Z

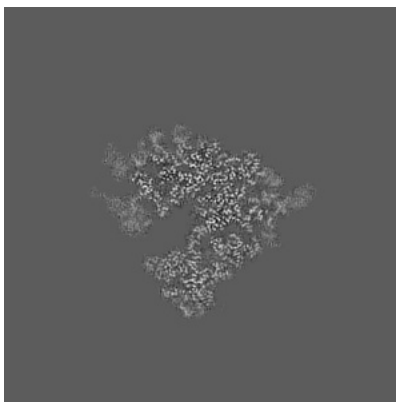
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

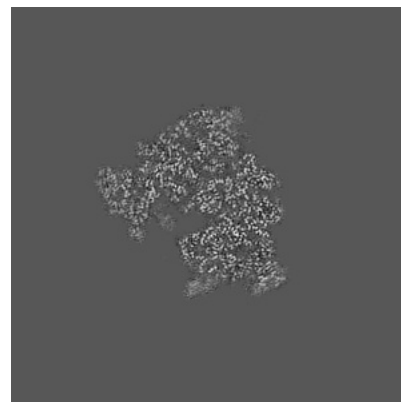
6.2.1 Primary map



X Index: 210

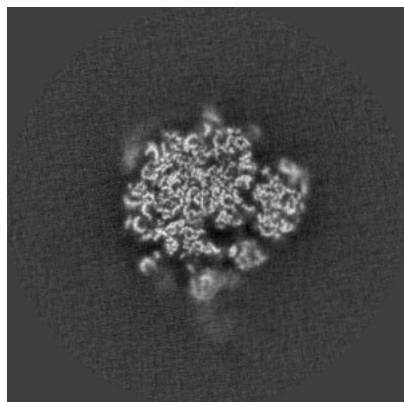


Y Index: 210

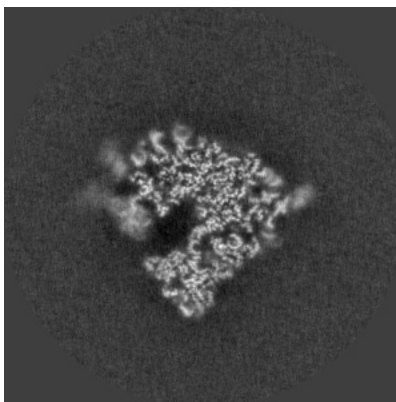


Z Index: 210

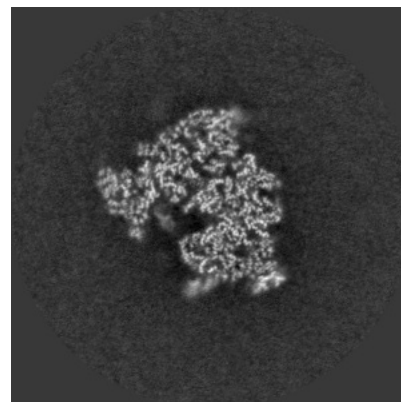
6.2.2 Raw map



X Index: 210



Y Index: 210

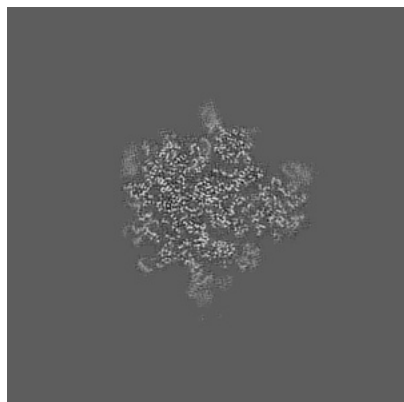


Z Index: 210

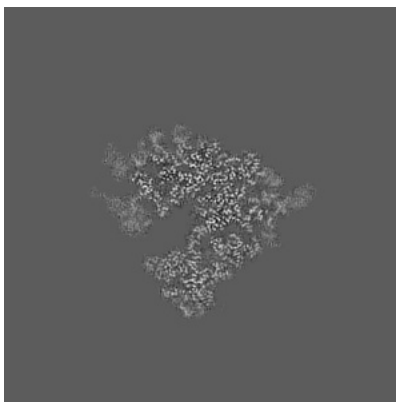
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

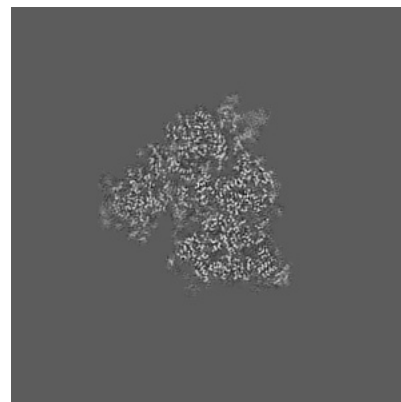
6.3.1 Primary map



X Index: 216

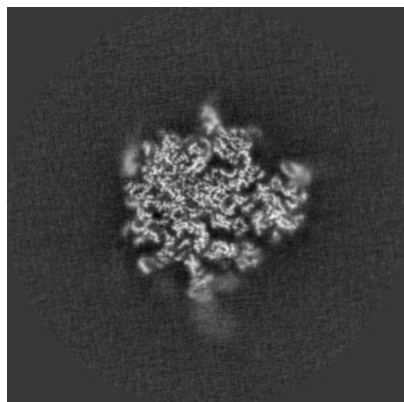


Y Index: 210

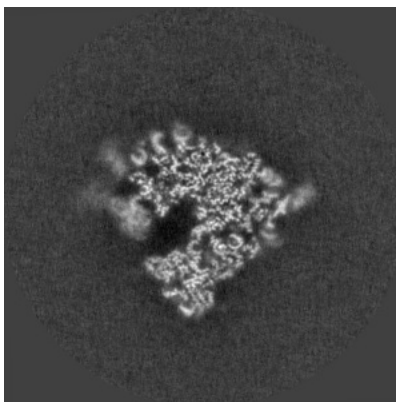


Z Index: 202

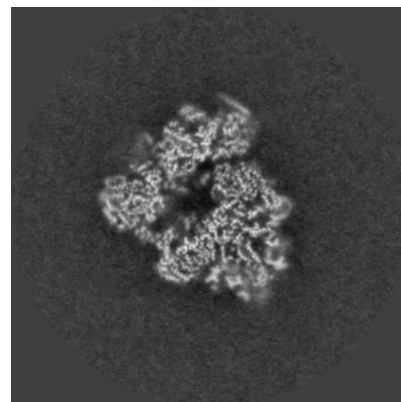
6.3.2 Raw map



X Index: 215



Y Index: 211

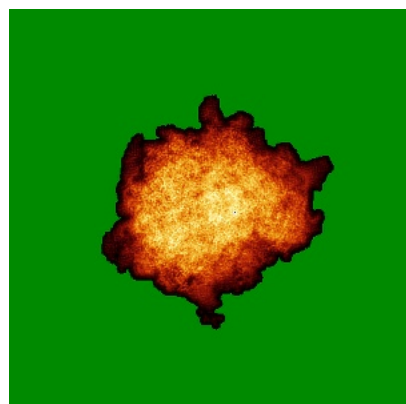


Z Index: 187

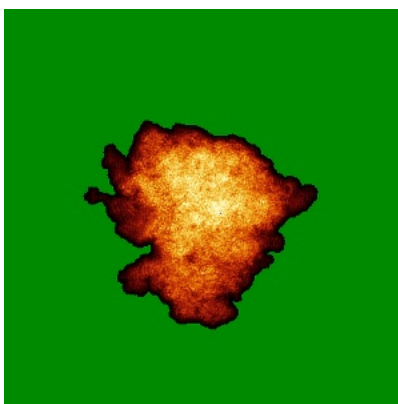
The images above show the largest variance slices of the map in three orthogonal directions.

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

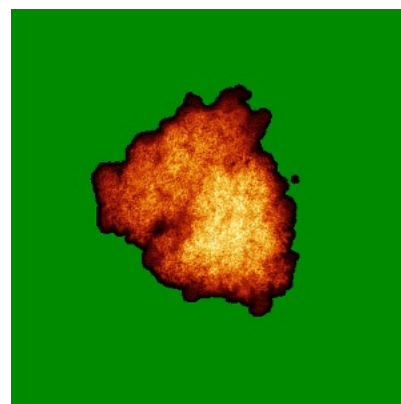
6.4.1 Primary map



X

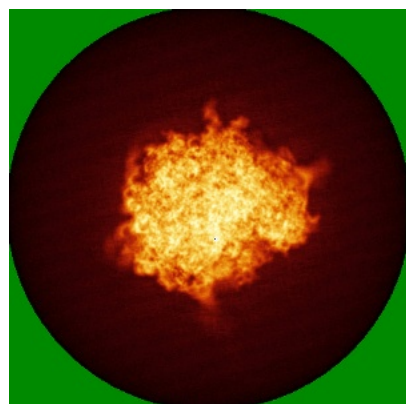


Y

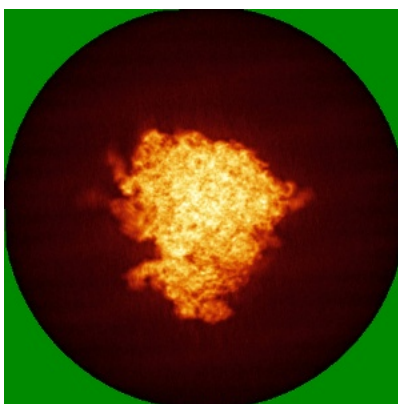


Z

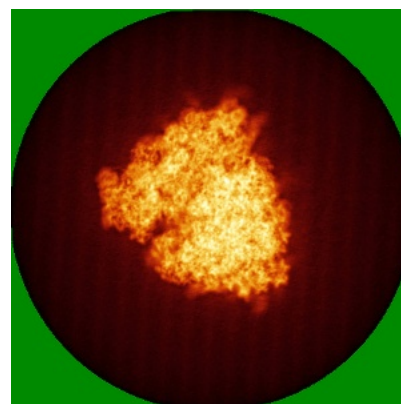
6.4.2 Raw map



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.

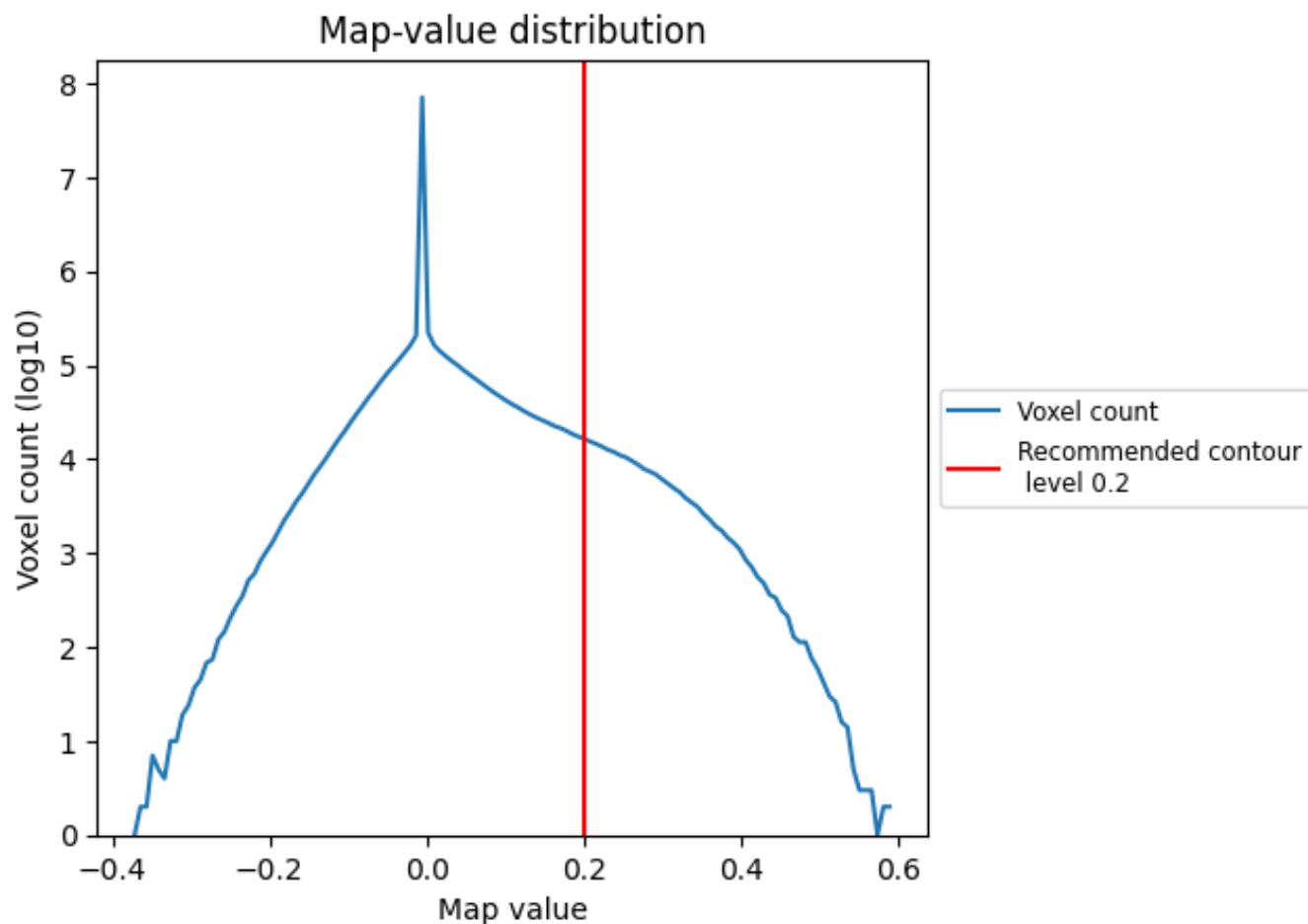
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

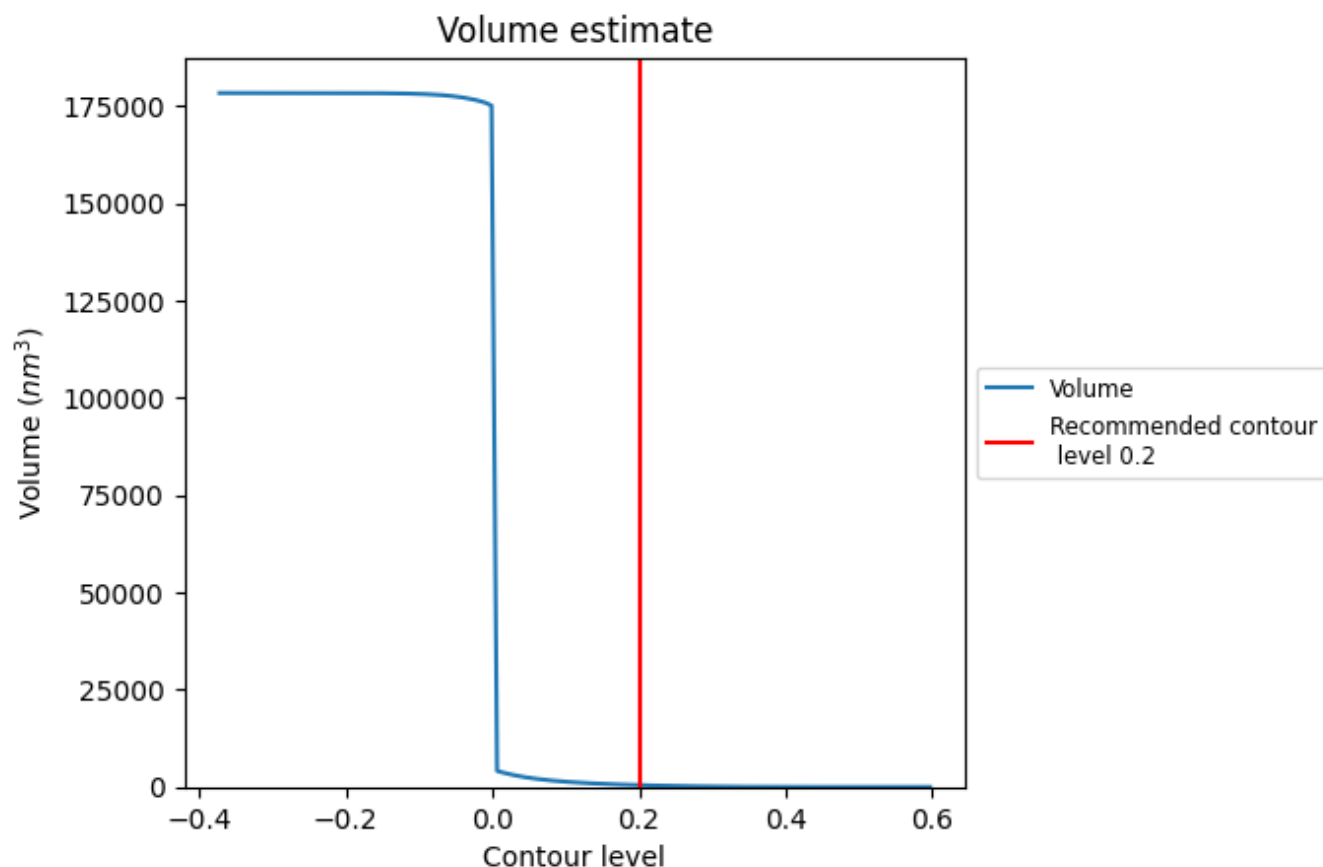
This section contains the results of statistical analysis of the map.

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.

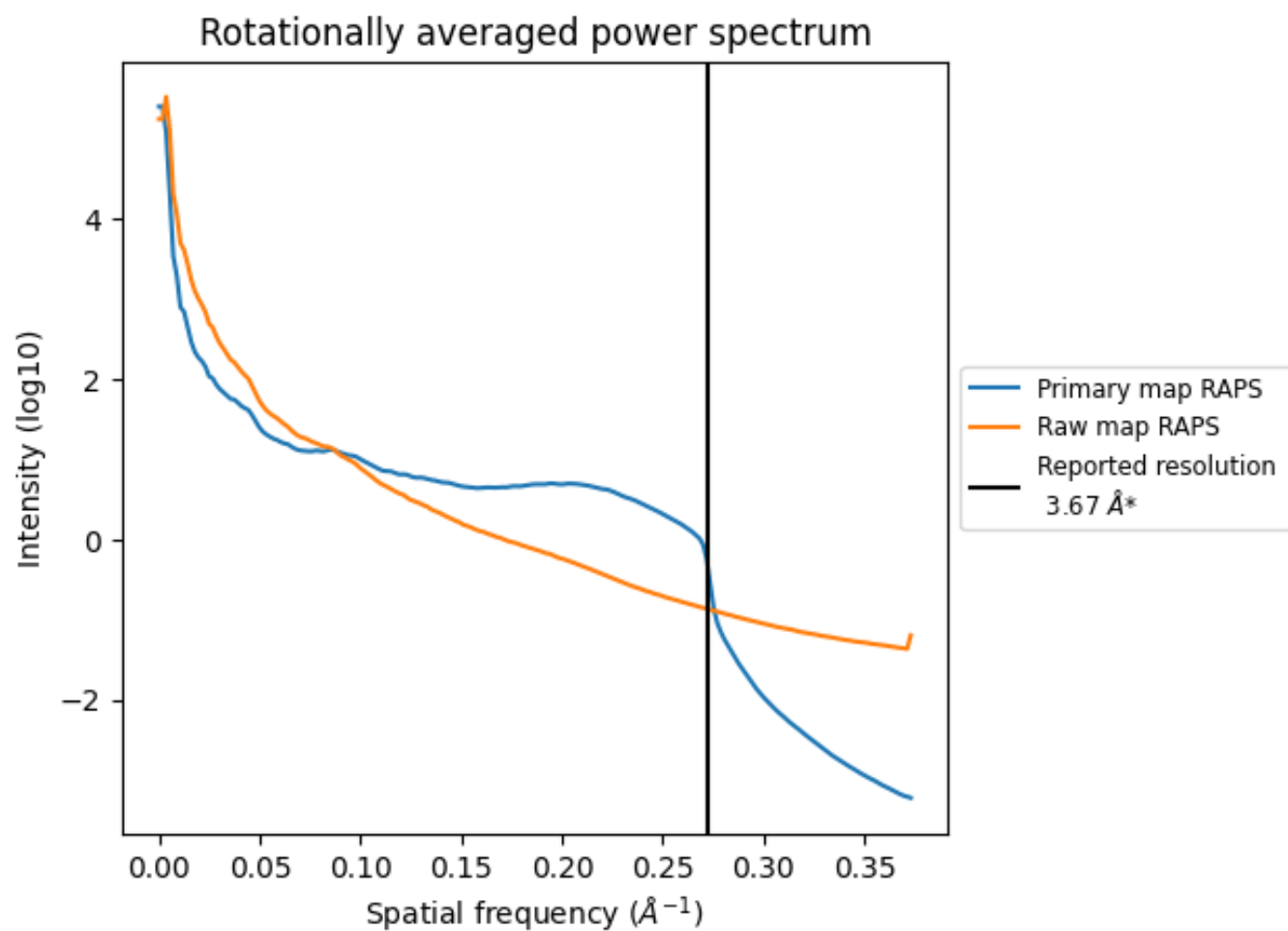
7.2 Volume estimate [i](#)



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 ⓘ

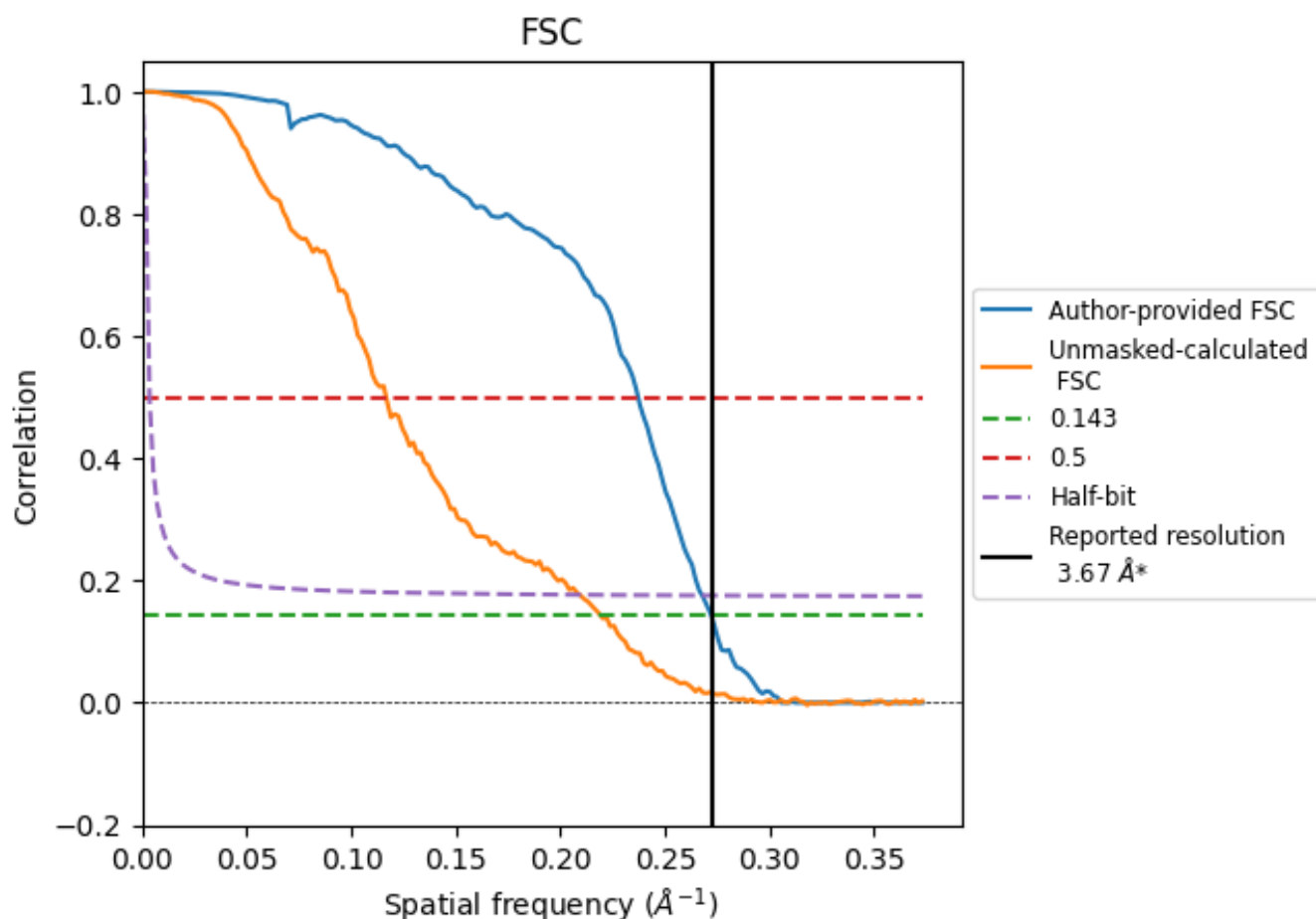


*Reported resolution corresponds to spatial frequency of $0.272 \text{ \AA}^{-1}$

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

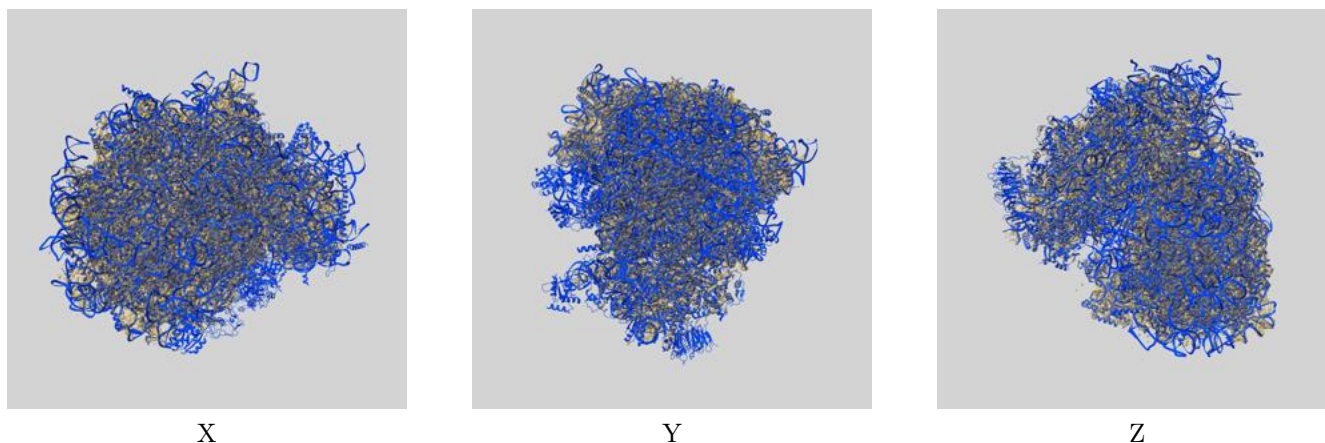
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.68	4.22	3.73
Unmasked-calculated*	4.56	8.57	4.78

*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](#)

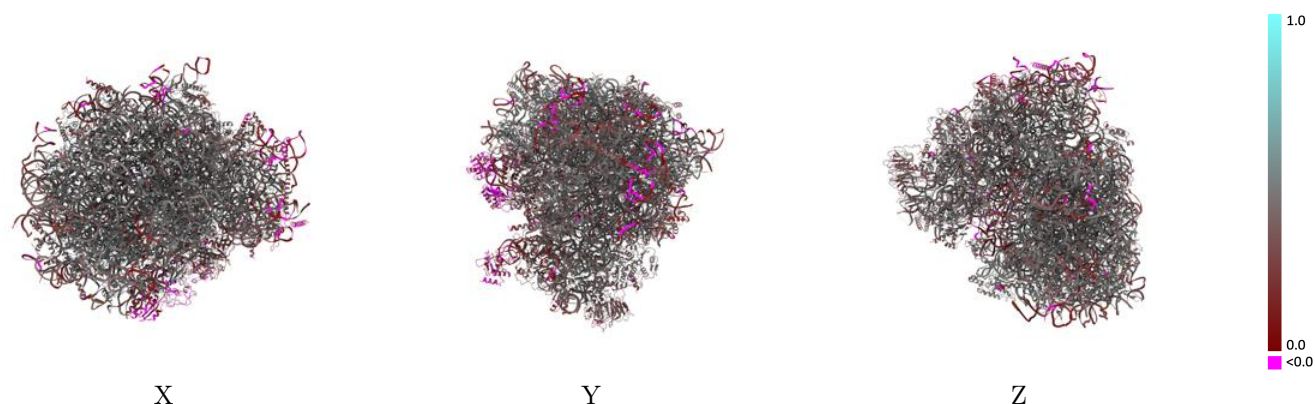
This section contains information regarding the fit between EMDB map EMD-4135 and PDB model 5LZX. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



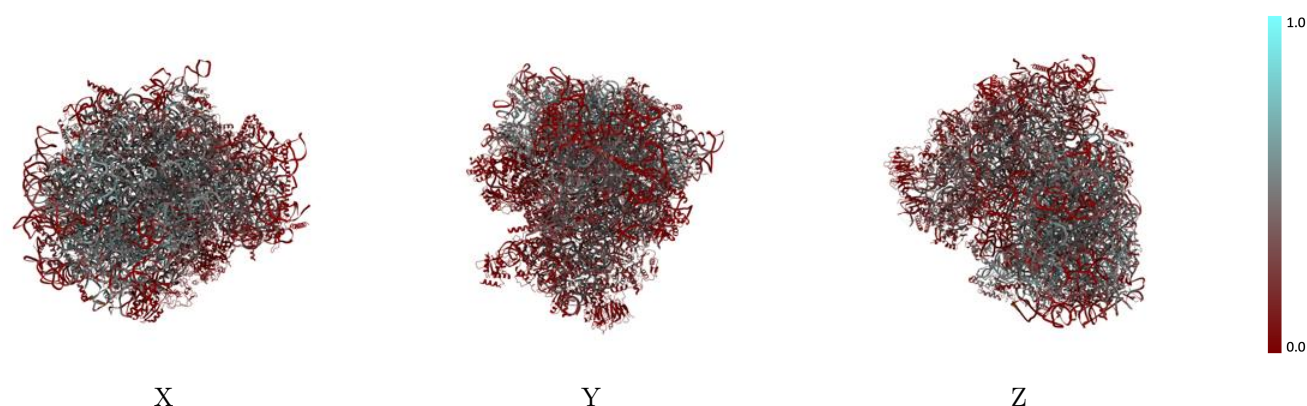
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



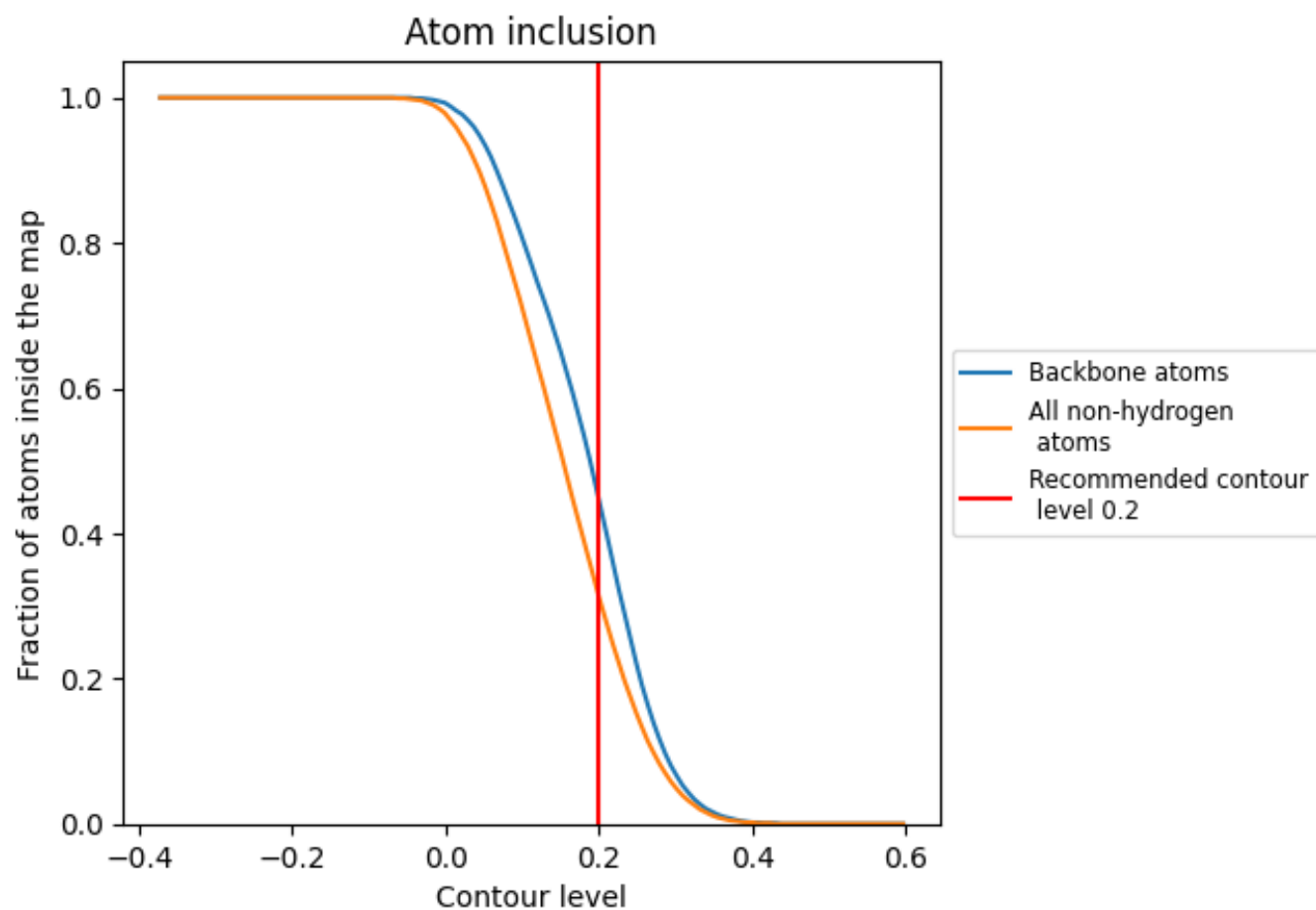
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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