



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 01:24 pm GMT

PDB ID : 6SGB
EMDB ID : EMD-10180
Title : mt-SSU assemblosome of Trypanosoma brucei
Authors : Saurer, M.; Ramrath, D.J.F.; Niemann, M.; Calderaro, S.; Prange, C.; Mattei, S.; Scaiola, A.; Leitner, A.; Bieri, P.; Horn, E.K.; Leibundgut, M.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2019-08-03
Resolution : 3.30 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:

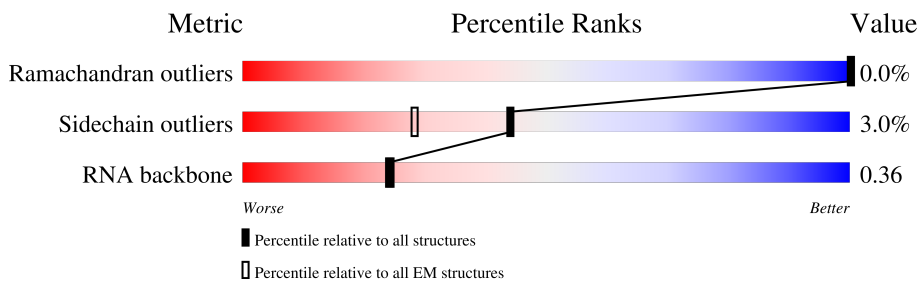
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



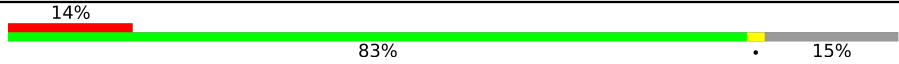

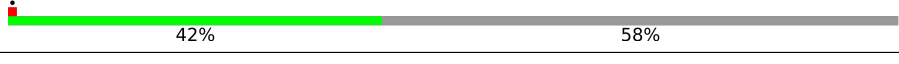

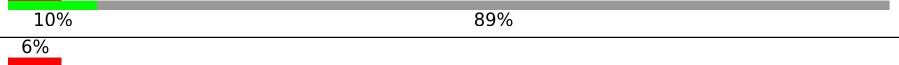
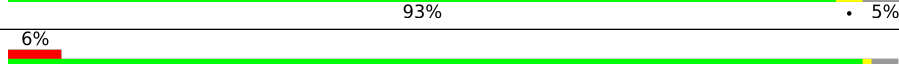
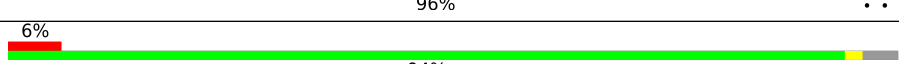
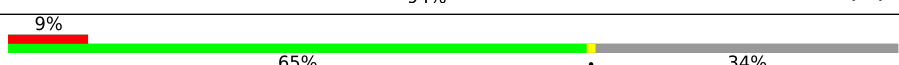
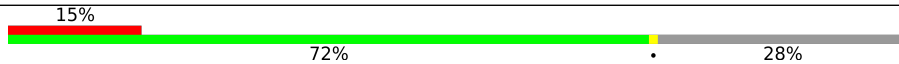

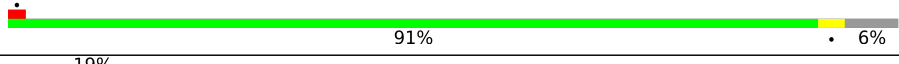
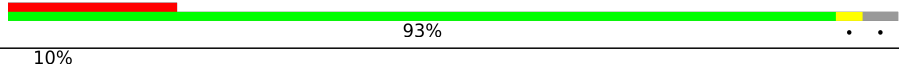


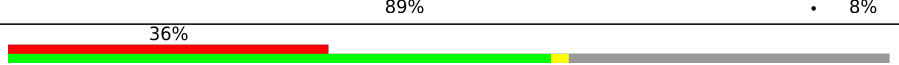

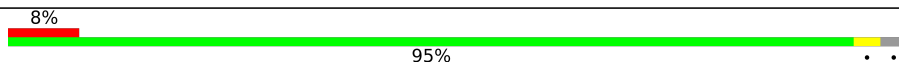








Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	CE	435	
2	CF	160	
3	CH	282	
4	CK	326	
5	CO	429	
6	CP	188	
7	CQ	336	
8	CR	320	

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Mol	Chain	Length	Quality of chain
9	Ca	602	
10	Cb	311	
11	Cd	440	
12	Cj	257	
13	Cn	250	
14	Cp	187	
15	DD	812	
16	DI	407	
17	DL	307	
18	DO	282	
19	DP	274	
20	DR	270	
21	DU	228	
22	DZ	94	
23	F2	1024	
24	F3	966	
25	F5	754	
26	F6	676	
27	F7	679	
28	F8	726	
29	F9	608	
30	FA	642	
31	FB	579	
31	FC	579	
32	FE	553	

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Mol	Chain	Length	Quality of chain
33	FJ	362	22% 95%
34	FM	370	8% 86% 12%
34	FN	370	23% 84% 14%
35	FO	334	5% 95%
36	FP	349	10% 98%
37	FQ	307	16% 82% 16%
37	FR	307	19% 78% 21%
37	FS	307	29% 87% 10%
37	FT	307	18% 73% 24%
37	FU	307	31% 85% 12%
38	FW	263	6% 93% 6%
39	FX	239	92% 8%
40	FY	188	36% 82% 15%
41	FZ	178	72% 73% 25%
42	Fa	171	16% 93% 5%
43	Fb	151	30% 83% 15%
44	Fc	148	15% 53% 43%
45	Fd	143	6% 65% 33%
46	UA	21	67% 100%
47	UB	27	81% 100%
47	Uk	27	44% 100%
48	UC	10	10% 100%
49	UD	9	100%
49	UM	9	22% 100%
49	UQ	9	56% 100%

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Mol	Chain	Length	Quality of chain
49	Uf	9	33% 100%
50	UE	45	62% 100%
50	UP	45	71% 100%
51	UF	11	27% 100%
51	Um	11	45% 100%
52	UG	17	12% 100%
53	UH	5	40% 100%
54	UI	8	25% 100%
54	UN	8	25% 100%
55	UJ	16	56% 100%
56	UK	24	79% 100%
57	UL	22	32% 100%
58	UO	30	37% 100%
59	UY	468	100%
60	CA	620	41% 56% 40% ..
61	CC	74	45% 97% .
62	CI	443	15% 94% . 5%
63	CJ	817	24% 83% . 14%
64	CN	166	70% 86% 7% 8%
65	CS	244	34% 34% . 65%
66	Cg	498	15% 95% ..
67	Ci	181	28% 80% . 19%
68	Ck	874	26% 70% . 27%
69	DB	1181	31% 56% . 43%
70	DC	1165	53% 86% . 12%

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Mol	Chain	Length	Quality of chain
71	DE	747	63% 76% 21%
72	DF	666	24% 72% 26%
73	DG	631	18% 87% 10%
74	DH	581	22% 79% 19%
75	DJ	396	17% 77% 22%
76	DK	324	34% 73% 24%
77	DT	247	16% 87% 11%
78	DV	183	31% 83% 14%
79	DW	179	28% 69% 6% 26%
80	DX	169	58% 68% 32%
81	DY	163	37% 93% 6%
82	F1	1041	21% 82% 15%
83	F4	811	36% 65% 33%
84	FD	579	20% 67% 32%
85	FF	474	18% 84% 14%
86	FG	463	6% 36% 63%
87	FH	457	17% 67% 31%
88	FI	445	21% 76% 22%
89	FK	372	15% 54% 44%
90	FL	353	13% 88% 9%
91	FV	264	11% 76% 20%
92	Fe	123	32% 91% 8%
93	Ua	47	38% 100%
94	Ub	42	64% 100%
95	Uc	12	58% 100%

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Mol	Chain	Length	Quality of chain
96	Ud	59	73% 100%
97	Ue	29	72% 100%
98	Ug	167	57% 100%
99	Uh	255	100% 100%
100	Ui	32	75% 100%
101	Uj	19	63% 100%
102	Ul	14	86% 100%
103	Ux	110	98% 98%

2 Entry composition

There are 110 unique types of molecules in this entry. The entry contains 240624 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 uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CE	392	3147	1992	579	561	15	0	0

- Molecule 2 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CF	159	1317	835	234	242	6	0	0

- Molecule 3 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CH	222	1824	1144	349	321	10	0	0

- Molecule 4 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CK	211	1721	1084	316	311	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7

- Molecule 5 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CO	358	2979	1891	557	514	17	0	0

- Molecule 6 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CP	180	Total	C	N	O	S	0	0
			1489	956	274	250	9		

- Molecule 7 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CQ	219	Total	C	N	O	S	0	0
			1805	1151	340	306	8		

- Molecule 8 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CR	153	Total	C	N	O	S	0	0
			1274	821	233	218	2		

- Molecule 9 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ca	512	Total	C	N	O	S	0	0
			4340	2778	770	771	21		

- Molecule 10 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Cb	153	Total	C	N	O	S	0	0
			1274	819	232	217	6		

- Molecule 11 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Cd	185	Total	C	N	O	S	0	0
			1616	1032	297	279	8		

- Molecule 12 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cj	226	Total	C	N	O	S	0	0
			1792	1138	310	340	4		

- Molecule 13 is a protein called mS38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Cn	27	234	155	44	35	0	0

- Molecule 14 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Cp	178	1506	952	272	277	5	0	0

- Molecule 15 is a protein called mS51 (KRIPP1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	DD	786	6488	4110	1168	1169	41	0	0

- Molecule 16 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	DI	390	3182	2020	554	594	14	0	0

- Molecule 17 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	DL	203	1656	1059	296	291	10	0	0

- Molecule 18 is a protein called mS62 (KRIPP14).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DO	204	1648	1031	300	307	10	0	0

- Molecule 19 is a protein called mS63 (KRIPP16).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	DP	212	1800	1156	321	314	9	0	0

- Molecule 20 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	DR	254	2042	1313	373	346	10	0	0

- Molecule 21 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	DU	219	1738	1095	308	331	4	0	0

- Molecule 22 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	DZ	30	254	167	41	45	1	0	0

- Molecule 23 is a protein called mt-SAF2 (KRIPP2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	F2	915	7274	4570	1281	1384	39	0	0

- Molecule 24 is a protein called mt-SAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	F3	888	6879	4302	1222	1303	52	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	44	THR	ALA	conflict	UNP Q38E61
F3	190	VAL	ILE	conflict	UNP Q38E61
F3	303	ALA	SER	conflict	UNP Q38E61
F3	418	ASP	ASN	conflict	UNP Q38E61

- Molecule 25 is a protein called mt-SAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	F5	480	3474	2167	646	647	14	0	0

- Molecule 26 is a protein called mt-SAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	F6	456	3646	2311	635	686	14	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F6	285	ARG	HIS	conflict	UNP Q38FQ8
F6	291	ILE	THR	conflict	UNP Q38FQ8
F6	602	ALA	VAL	conflict	UNP Q38FQ8
F6	676	CYS	PHE	conflict	UNP Q38FQ8

- Molecule 27 is a protein called mt-SAF7 (KRIPP10).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	F7	662	5225	3322	918	950	35	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F7	36	ILE	THR	conflict	UNP Q57UW6
F7	470	GLU	LYS	conflict	UNP Q57UW6
F7	474	VAL	ALA	conflict	UNP Q57UW6

- Molecule 28 is a protein called mt-SAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	F8	513	3934	2493	721	701	19	0	0

- Molecule 29 is a protein called mt-SAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	F9	216	1755	1088	325	337	5	0	0

- Molecule 30 is a protein called mt-SAF10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	FA	579	4421	2801	785	813	22	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FA	173	ALA	THR	conflict	UNP Q386U1
FA	352	TYR	HIS	conflict	UNP Q386U1

- Molecule 31 is a protein called mt-SAF11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	FB	377	Total	C	N	O	S	0	0
			3055	1928	574	543	10		
31	FC	311	Total	C	N	O	S	0	0
			2572	1629	488	447	8		

- Molecule 32 is a protein called mt-SAF13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FE	434	Total	C	N	O	S	0	0
			3523	2268	611	626	18		

- Molecule 33 is a protein called mt-SAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	FJ	353	Total	C	N	O	S	0	0
			2917	1843	550	516	8		

- Molecule 34 is a protein called mt-SAF21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	FM	326	Total	C	N	O	S	0	0
			2449	1515	449	465	20		
34	FN	319	Total	C	N	O	S	0	0
			2392	1478	436	458	20		

- Molecule 35 is a protein called mt-SAF22 (KRIPP17).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	FO	324	Total	C	N	O	S	0	0
			2671	1674	509	474	14		

- Molecule 36 is a protein called mt-SAF23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	FP	348	2643	1682	464	487	10	0	0

- Molecule 37 is a protein called mt-SAF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	FQ	257	2003	1265	358	373	7	0	0
37	FR	243	1923	1217	344	355	7	0	0
37	FS	277	2198	1389	397	404	8	0	0
37	FT	233	1854	1177	331	339	7	0	0
37	FU	270	2105	1331	380	386	8	0	0

- Molecule 38 is a protein called mt-SAF26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	FW	247	2034	1272	384	371	7	0	0

- Molecule 39 is a protein called mt-SAF27 (KRIPP11).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	FX	220	1741	1093	318	316	14	0	0

- Molecule 40 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	FY	160	1289	819	229	235	6	0	0

- Molecule 41 is a protein called mt-SAF29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	FZ	133	973	605	181	185	2	0	0

- Molecule 42 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Fa	163	1323	860	236	223	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fa	73	ALA	VAL	conflict	UNP Q57VU7

- Molecule 43 is a protein called mt-SAF31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Fb	129	1091	701	198	184	8	0	0

- Molecule 44 is a protein called mt-SAF32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Fc	84	669	427	106	135	1	0	0

- Molecule 45 is a protein called mt-SAF33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Fd	96	758	481	147	122	8	0	0

- Molecule 46 is a protein called UNK-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	UA	21	126	84	21	21	0	0

- Molecule 47 is a protein called UNK-B, UNK-k.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	UB	27	162	108	27	27	0	0
47	Uk	27	162	108	27	27	0	0

- Molecule 48 is a protein called UNK-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	UC	10	Total	C	N	O	0	0
			60	40	10	10		

- Molecule 49 is a protein called UNK-D, UNK-M, UNK-Q, UNK-f.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	UD	9	Total	C	N	O	0	0
			54	36	9	9		
49	UM	9	Total	C	N	O	0	0
			54	36	9	9		
49	UQ	9	Total	C	N	O	0	0
			54	36	9	9		
49	Uf	9	Total	C	N	O	0	0
			54	36	9	9		

- Molecule 50 is a protein called UNK-E, UNK-P.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	UE	45	Total	C	N	O	0	0
			270	180	45	45		
50	UP	45	Total	C	N	O	0	0
			270	180	45	45		

- Molecule 51 is a protein called UNK-F, UNK-m.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	UF	11	Total	C	N	O	0	0
			66	44	11	11		
51	Um	11	Total	C	N	O	0	0
			66	44	11	11		

- Molecule 52 is a protein called UNK-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	UG	17	Total	C	N	O	0	0
			102	68	17	17		

- Molecule 53 is a protein called UNK-H.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	UH	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 54 is a protein called UNK-I, UNK-N.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	UI	8	48	32	8	8	0	0
54	UN	8	48	32	8	8	0	0

- Molecule 55 is a protein called UNK-J.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	UJ	16	96	64	16	16	0	0

- Molecule 56 is a protein called UNK-K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
56	UK	24	144	96	24	24	0	0

- Molecule 57 is a protein called UNK-L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	UL	22	132	88	22	22	0	0

- Molecule 58 is a protein called UNK-O.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	UO	30	180	120	30	30	0	0

- Molecule 59 is a protein called UNK-Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
59	UY	468	2808	1872	468	468	0	0

- Molecule 60 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
60	CA	609	11352	5038	1602	4102	610	0	0

- Molecule 61 is a protein called mS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	CC	74	646	451	96	98	1	0	0

- Molecule 62 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	CI	423	3357	2108	601	631	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 63 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	CJ	701	5709	3605	1017	1064	23	0	0

- Molecule 64 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	CN	153	1285	820	242	216	7	0	0

- Molecule 65 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	CS	85	708	463	121	121	3	0	0

- Molecule 66 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Cg	484	3922	2511	688	703	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	MET	conflict	UNP Q585C2

- Molecule 67 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Ci	147	1222	770	226	218	8	0	0

- Molecule 68 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Ck	638	5123	3220	927	953	23	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 69 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	DB	679	5688	3558	1062	1047	21	0	0

- Molecule 70 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	DC	1028	8223	5194	1453	1546	30	0	0

- Molecule 71 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	DE	590	4639	2957	832	834	16	0	0

- Molecule 72 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	DF	491	3967	2496	745	703	23	0	0

- Molecule 73 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	DG	566	4575	2875	835	834	31	0	0

- Molecule 74 is a protein called mS55 (KRIPP8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	DH	472	3849	2417	720	693	19	0	0

- Molecule 75 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	DJ	308	2521	1612	446	450	13	0	0

- Molecule 76 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	DK	245	1929	1213	349	362	5	0	0

- Molecule 77 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	DT	221	1912	1231	334	337	10	0	0

- Molecule 78 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	DV	157	1323	840	248	231	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 79 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	DW	133	1140	730	216	190	4	0	0

- Molecule 80 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	DX	115	967	612	182	166	7	0	0

- Molecule 81 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	DY	154	1295	829	247	214	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DY	34	HIS	ASP	conflict	UNP Q57YD4

- Molecule 82 is a protein called mt-SAF1 (RSM22).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	F1	889	7194	4493	1372	1289	40	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	707	SER	GLY	conflict	UNP Q385R2
F1	973	THR	MET	conflict	UNP Q385R2

- Molecule 83 is a protein called mt-SAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	F4	541	4382	2783	775	802	22	0	0

- Molecule 84 is a protein called mt-SAF12 (KRIPP18).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	FD	394	3135	2004	546	566	19	0	0

- Molecule 85 is a protein called mt-SAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	FF	408	3265	2052	586	603	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	70	ALA	PRO	conflict	UNP Q57W60
FF	179	PHE	LEU	conflict	UNP Q57W60

- Molecule 86 is a protein called mt-SAF15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	FG	169	1359	852	260	240	7	0	0

- Molecule 87 is a protein called mt-SAF16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	FH	317	2486	1555	440	471	20	0	0

- Molecule 88 is a protein called mt-SAF17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	FI	348	2786	1726	510	537	13	0	0

- Molecule 89 is a protein called mt-SAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
89	FK	208	1699	1084	284	325	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FK	38	HIS	ARG	conflict	UNP Q57XS8

- Molecule 90 is a protein called mt-SAF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
90	FL	320	2555	1609	470	459	17	0	0

- Molecule 91 is a protein called mt-SAF25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
91	FV	210	1636	1039	283	303	11	0	0

- Molecule 92 is a protein called mt-SAF34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
92	Fe	122	1033	642	200	184	7	0	0

- Molecule 93 is a protein called UNK-a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
93	Ua	47	282	188	47	47	0	0

- Molecule 94 is a protein called UNK-b.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
94	Ub	42	252	168	42	42	0	0

- Molecule 95 is a protein called UNK-c.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
95	Uc	12	72	48	12	12	0	0

- Molecule 96 is a protein called UNK-d.

Mol	Chain	Residues	Atoms				AltConf	Trace
96	Ud	59	Total	C	N	O	0	0
			354	236	59	59		

- Molecule 97 is a protein called UNK-e.

Mol	Chain	Residues	Atoms				AltConf	Trace
97	Ue	29	Total	C	N	O	0	0
			174	116	29	29		

- Molecule 98 is a protein called UNK-g.

Mol	Chain	Residues	Atoms				AltConf	Trace
98	Ug	167	Total	C	N	O	0	0
			1002	668	167	167		

- Molecule 99 is a protein called UNK-h.

Mol	Chain	Residues	Atoms				AltConf	Trace
99	Uh	255	Total	C	N	O	0	0
			1530	1020	255	255		

- Molecule 100 is a protein called UNK-i.

Mol	Chain	Residues	Atoms				AltConf	Trace
100	Ui	32	Total	C	N	O	0	0
			192	128	32	32		

- Molecule 101 is a protein called UNK-j.

Mol	Chain	Residues	Atoms				AltConf	Trace
101	Uj	19	Total	C	N	O	0	0
			114	76	19	19		

- Molecule 102 is a protein called UNK-l.

Mol	Chain	Residues	Atoms				AltConf	Trace
102	Ul	14	Total	C	N	O	0	0
			84	56	14	14		

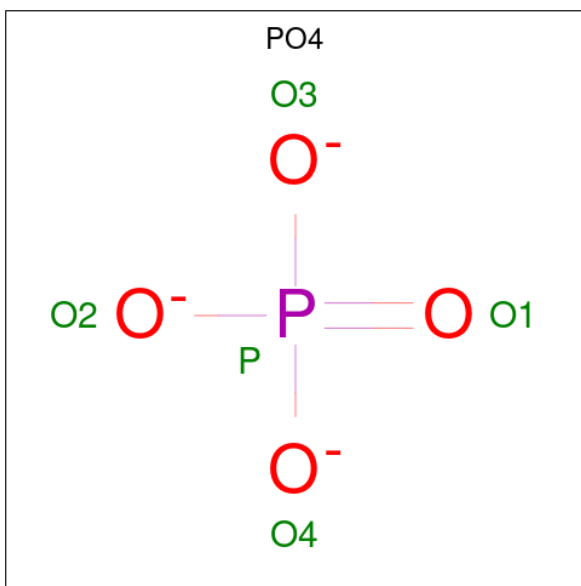
- Molecule 103 is a protein called UNK-x.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
103	Ux	108	648	432	108	108	0	0

- Molecule 104 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

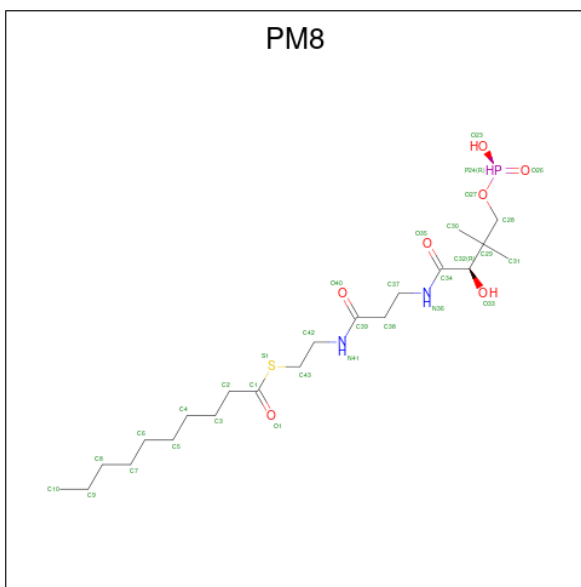
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
104	FP	1	1	1	0
104	FW	1	1	1	0
104	CA	2	2	2	0
104	Cg	1	1	1	0

- Molecule 105 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
105	FW	1	5	4	1	0

- Molecule 106 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: C₂₁H₄₁N₂O₇PS).

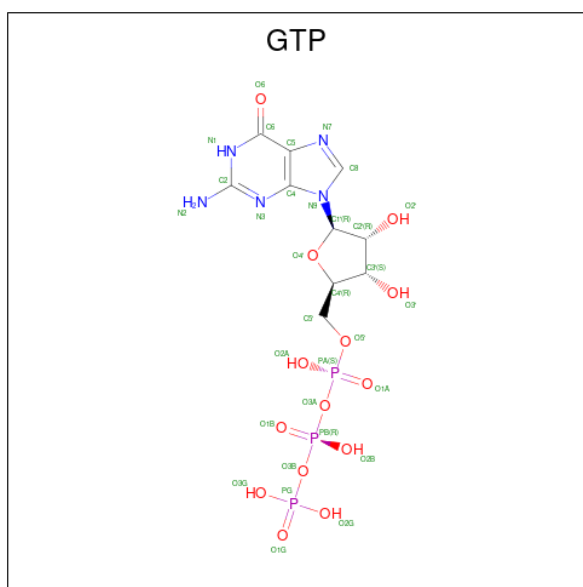


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
106	Fc	1	32	21	2	7	1	1	0

- Molecule 107 is ZINC ION (three-letter code: ZN) (formula: Zn).

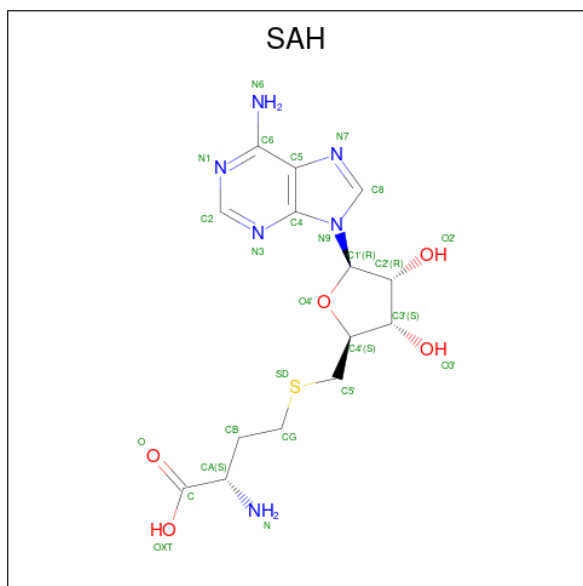
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
107	Fd	1	1	1	0
107	F1	1	1	1	0
107	FG	1	1	1	0
107	FL	2	2	2	0
107	Fe	1	1	1	0

- Molecule 108 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
108	Cg	1	32	10	5	14	3	0

- Molecule 109 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
109	F1	1	26	14	6	5	1	0
109	FF	1	26	14	6	5	1	0

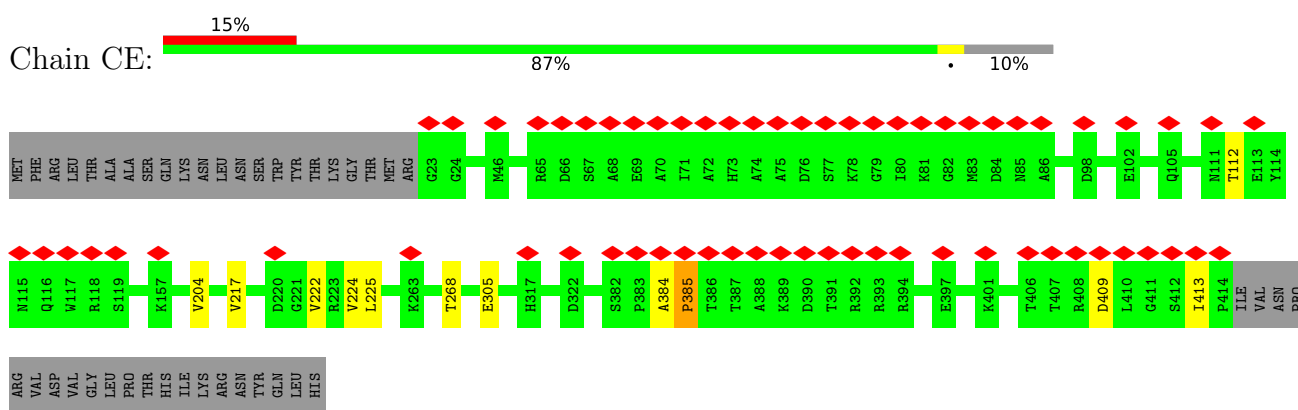
- Molecule 110 is water.

Mol	Chain	Residues	Atoms		AltConf
110	Cg	3	Total 3	O 3	0

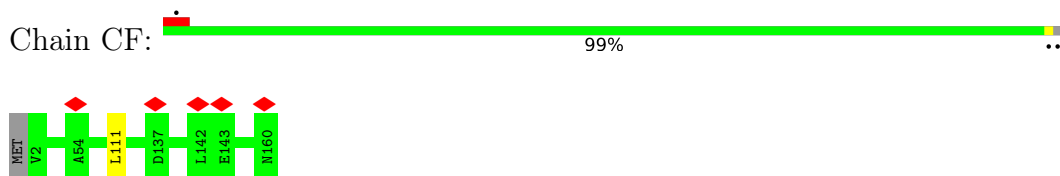
3 Residue-property plots [i](#)

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

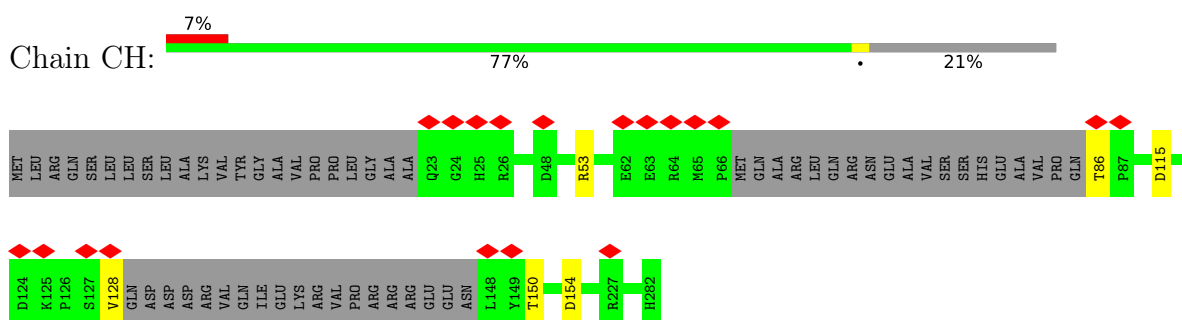
- Molecule 1: uS5m



- Molecule 2: bS6m

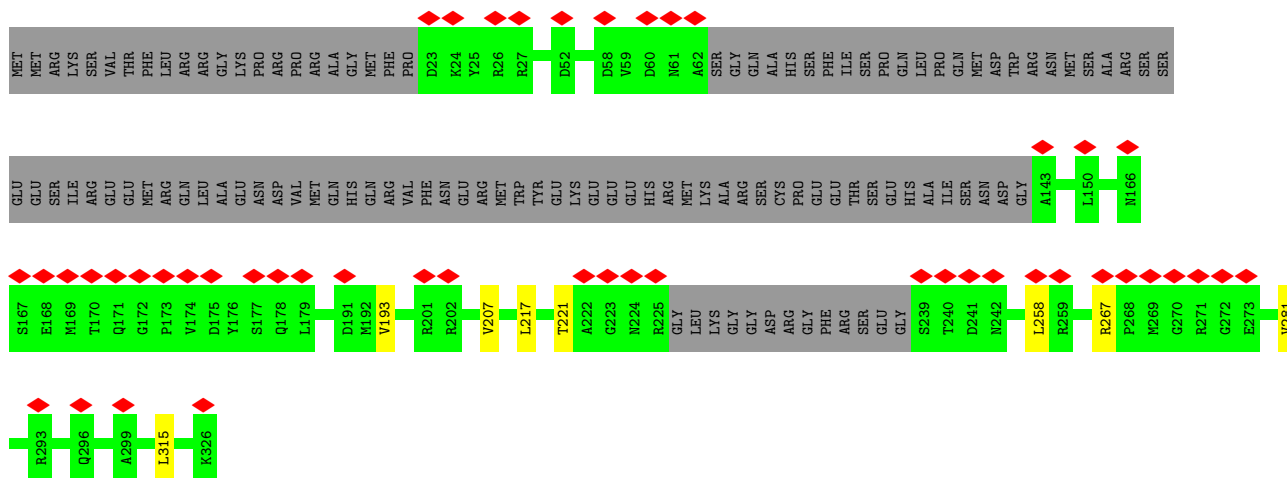


- Molecule 3: uS8m

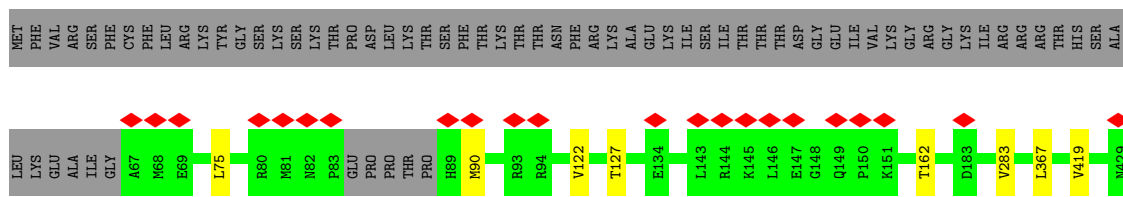
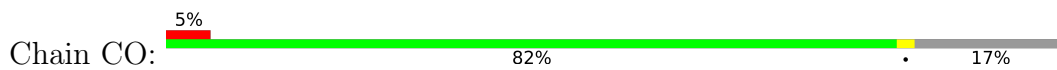


- Molecule 4: uS11m

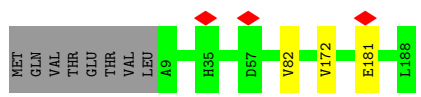




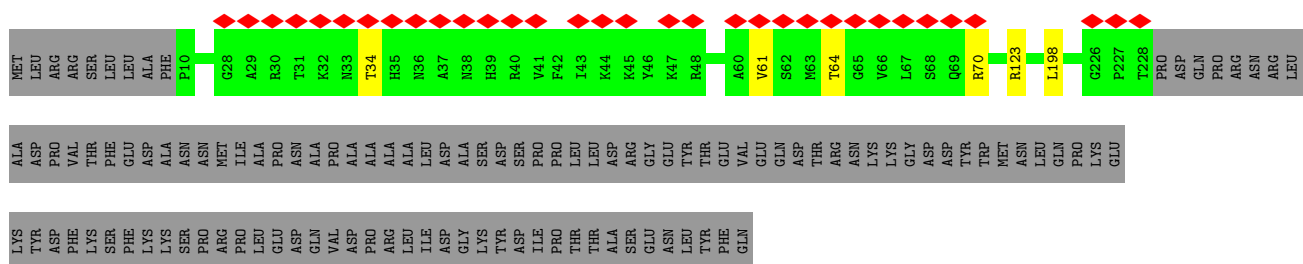
• Molecule 5: uS15m



• Molecule 6: bS16m

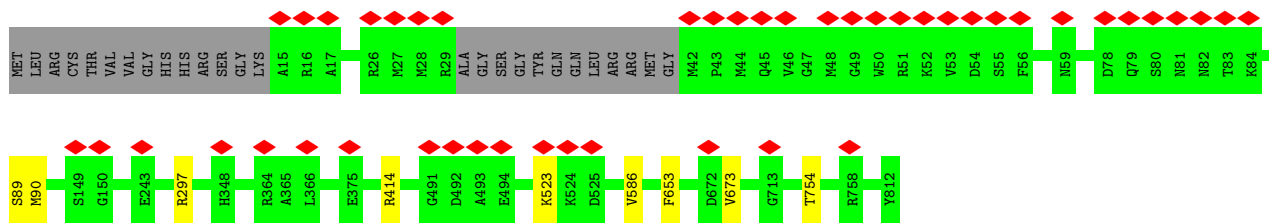


• Molecule 7: uS17m

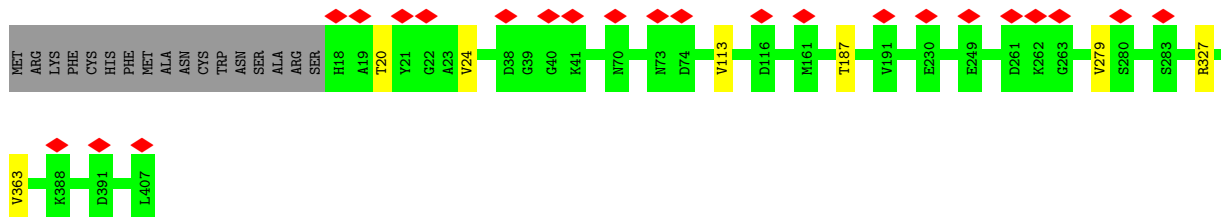


• Molecule 8: bS18m

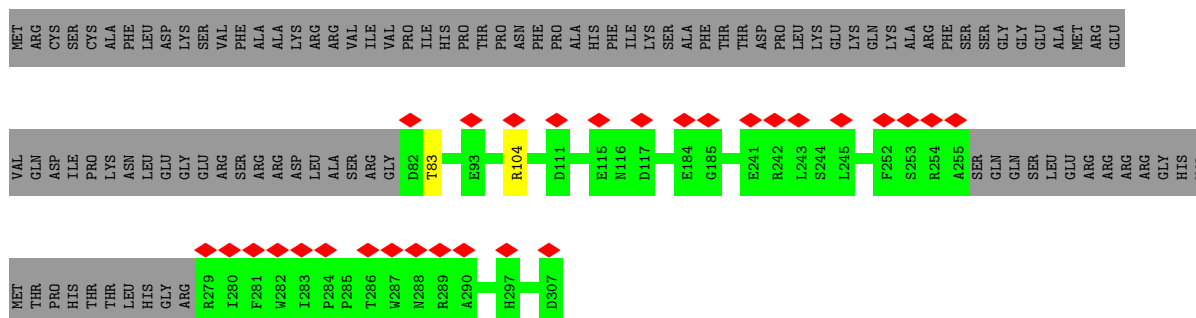




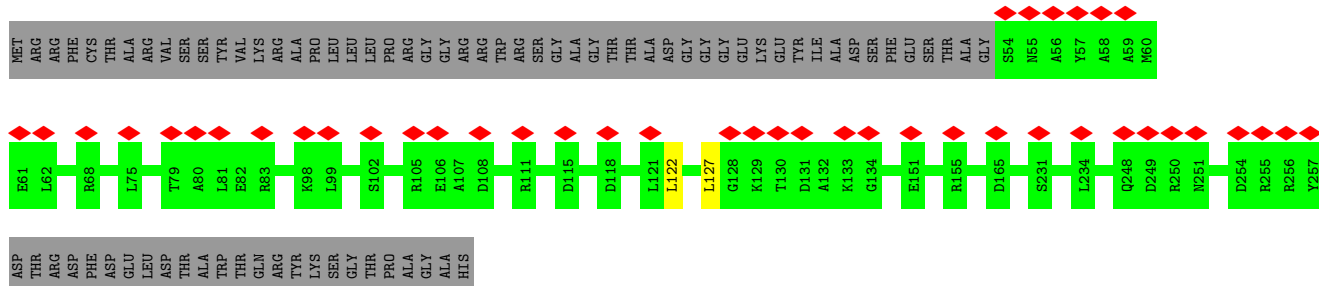
• Molecule 16: mS56



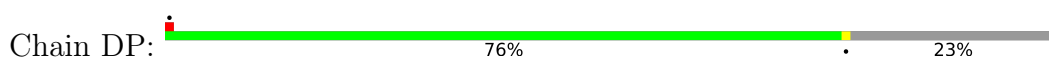
• Molecule 17: mS59

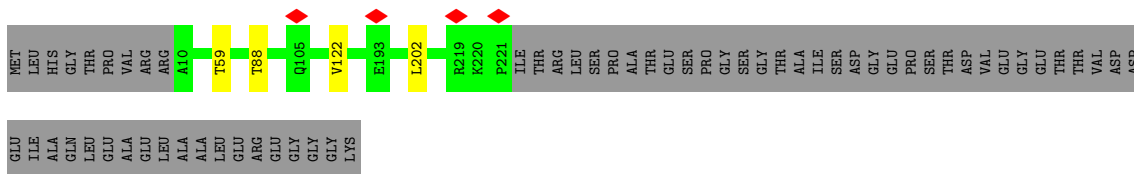


• Molecule 18: mS62 (KRIPP14)

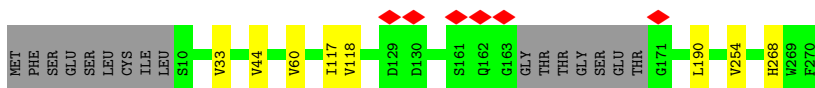


• Molecule 19: mS63 (KRIPP16)

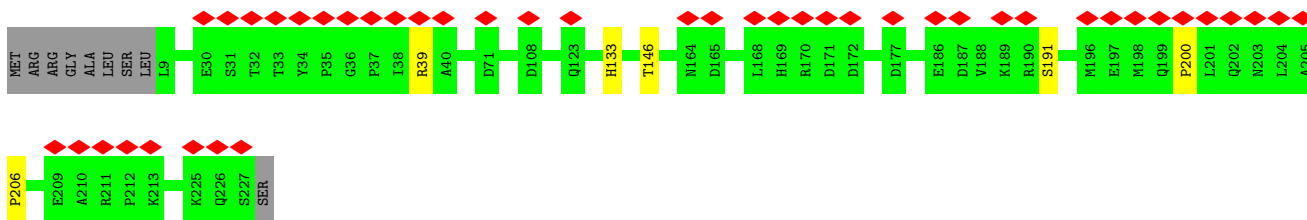




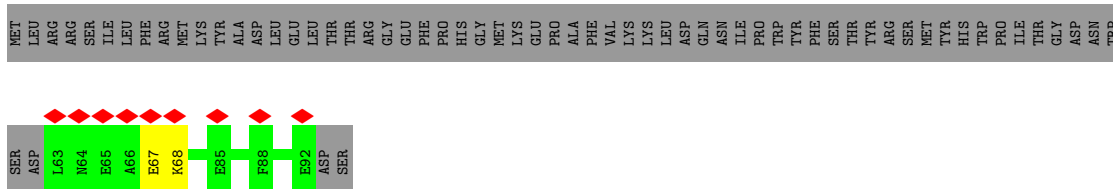
• Molecule 20: mS65



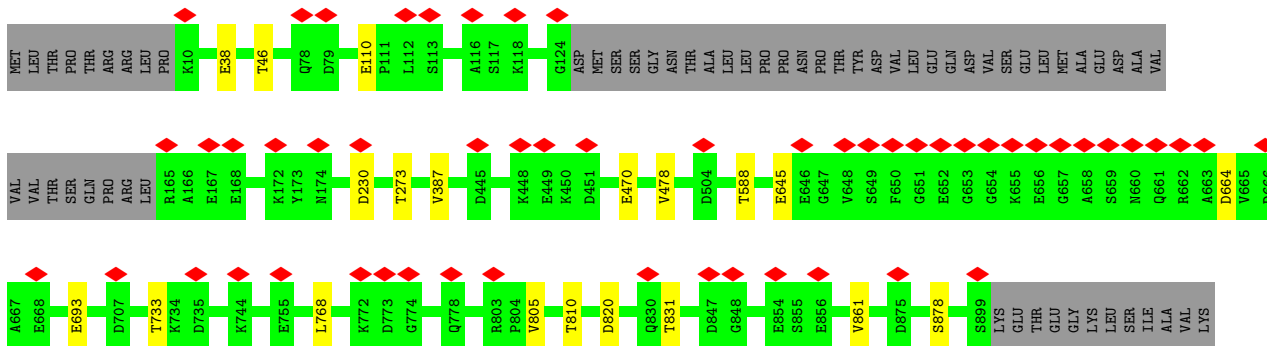
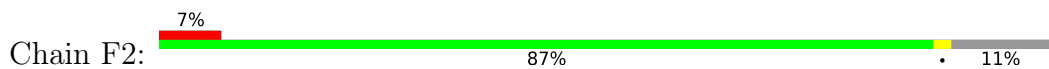
• Molecule 21: mS68

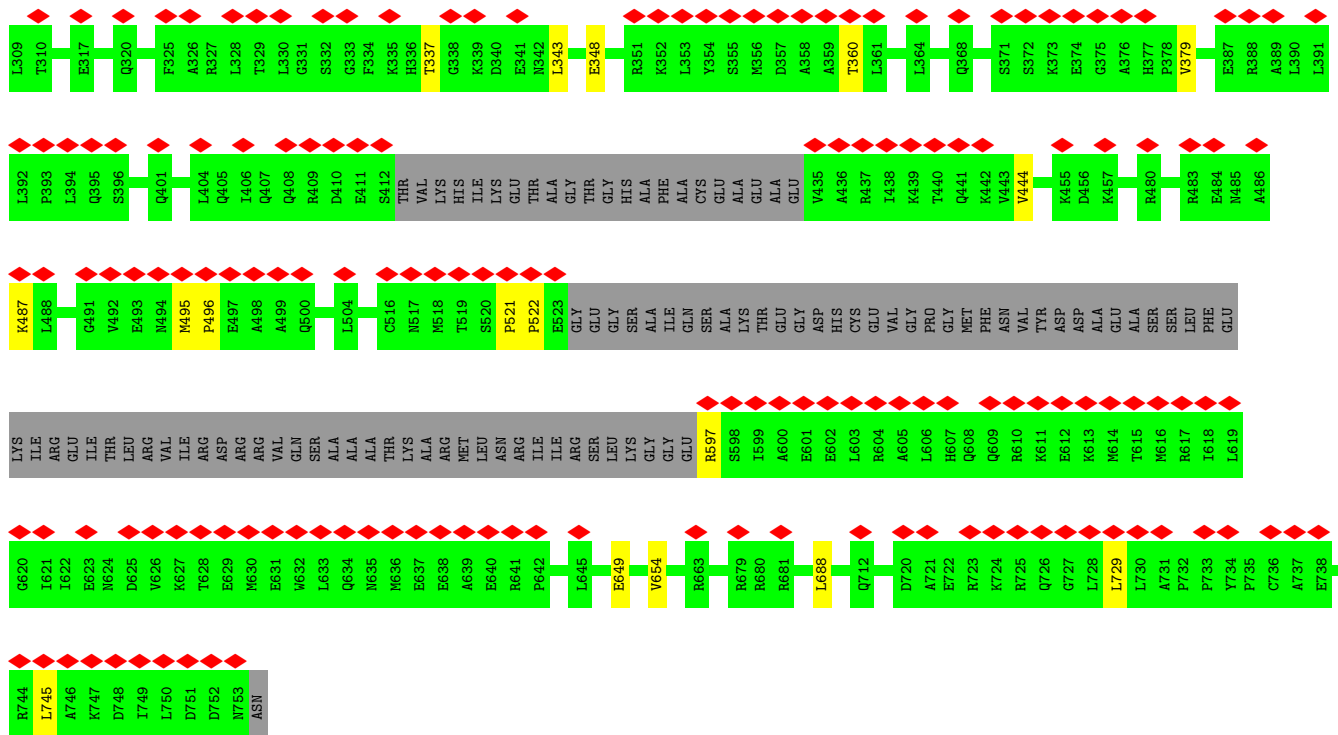


• Molecule 22: mS73

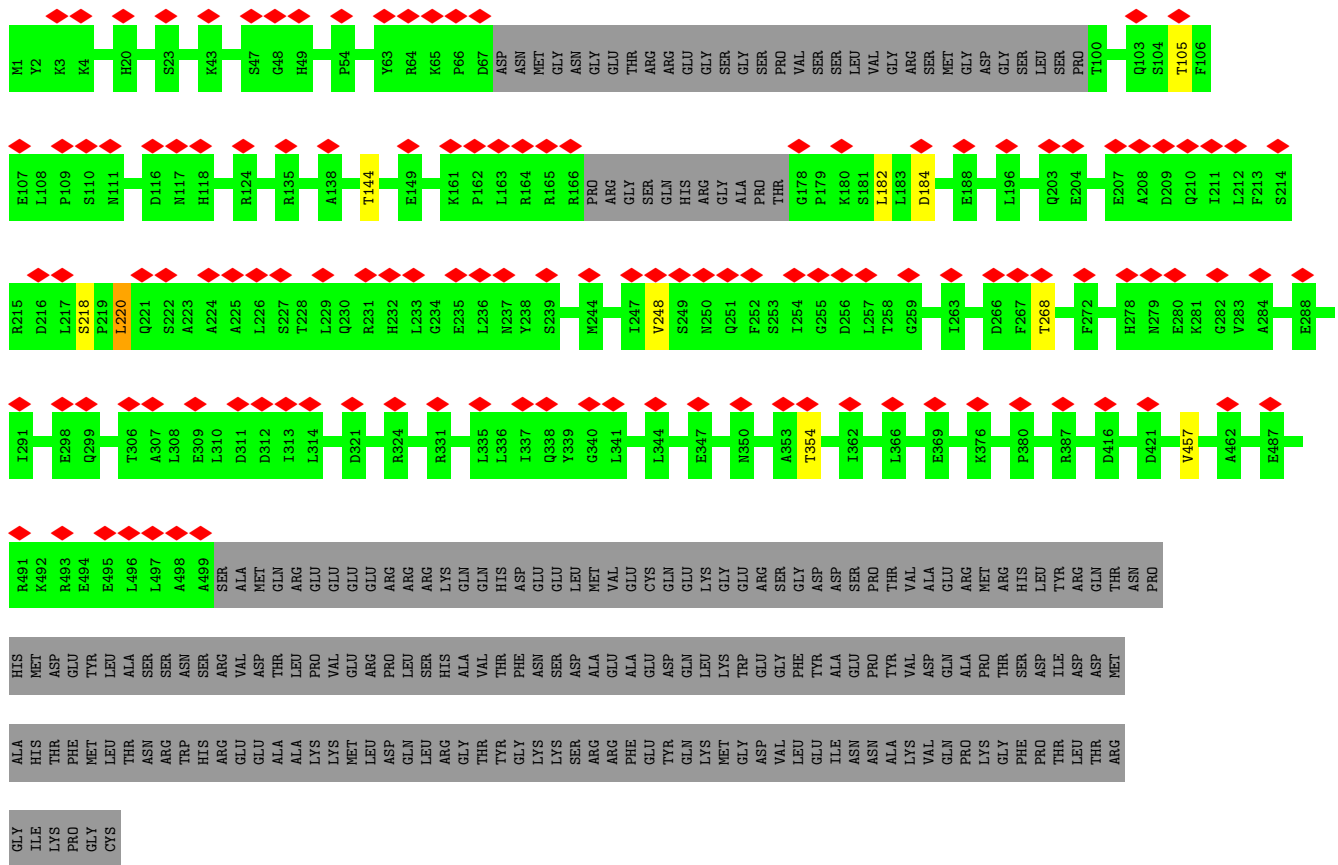


• Molecule 23: mt-SAF2 (KRIPP2)

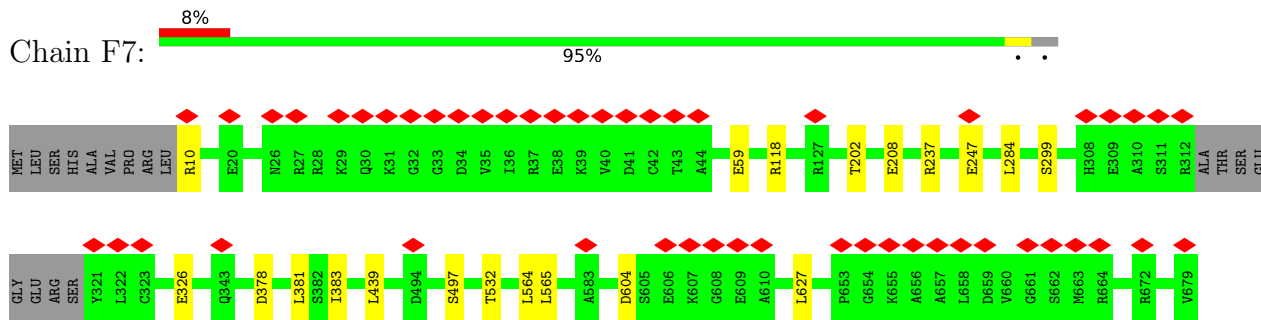




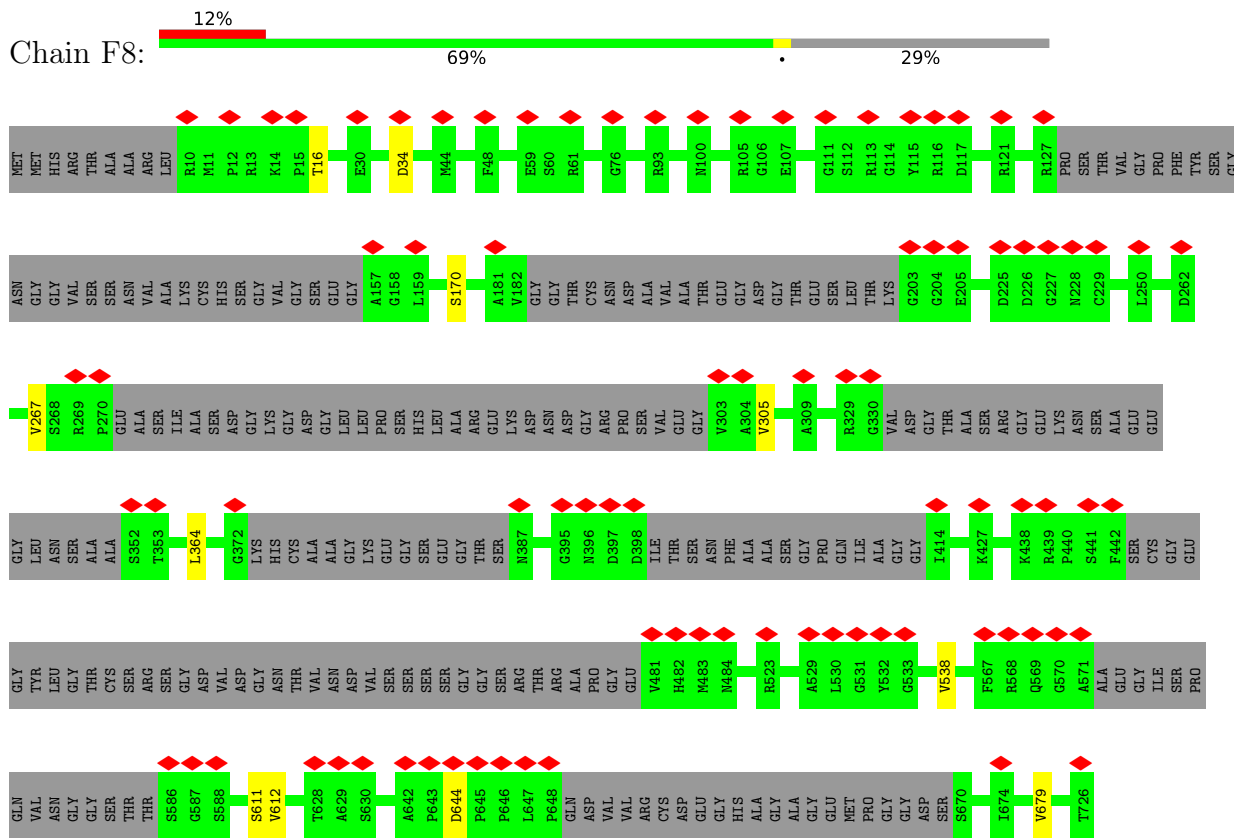
• Molecule 26: mt-SAF6



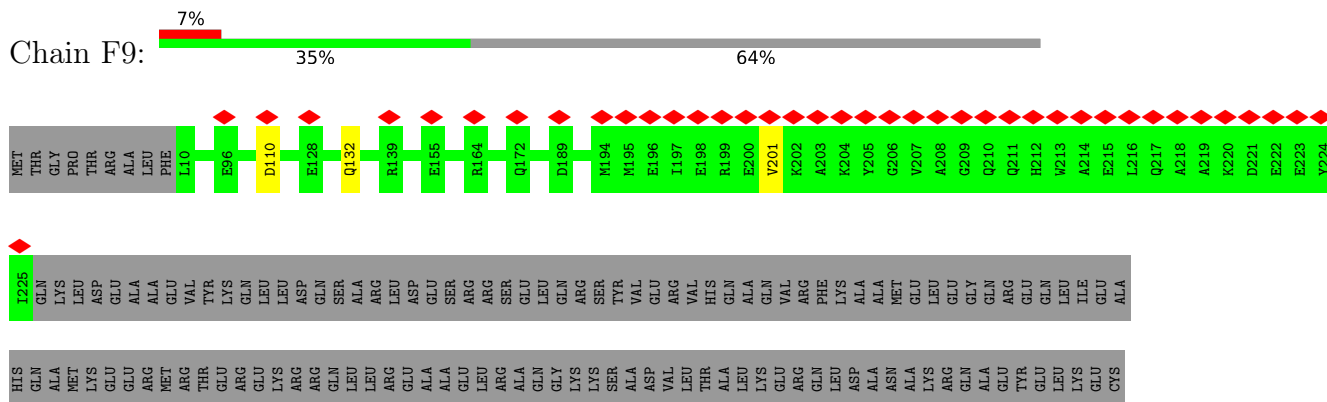
• Molecule 27: mt-SAF7 (KRIPP10)



• Molecule 28: mt-SAF8

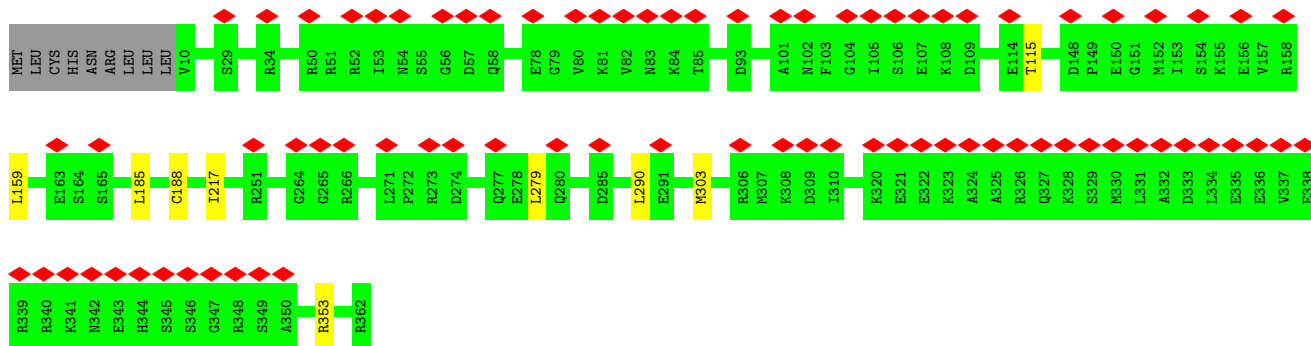


• Molecule 29: mt-SAF9

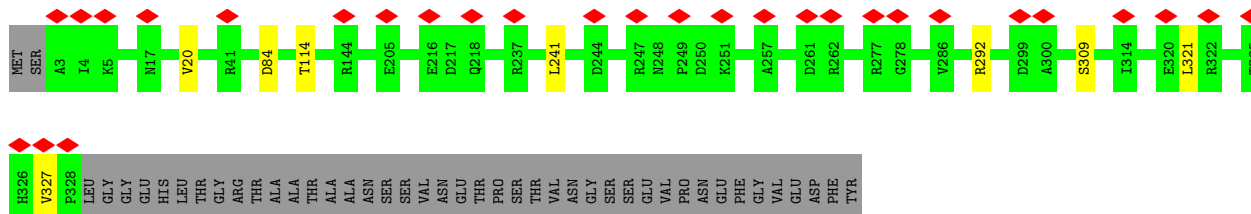
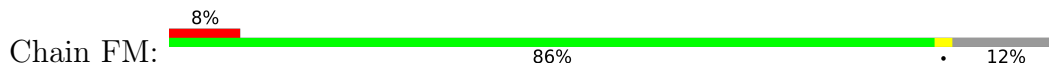


GLU
ARG
LEU
PHE
ASP
ALA
TVR
LEU
SER
CYS
TVR
ARG
LEU

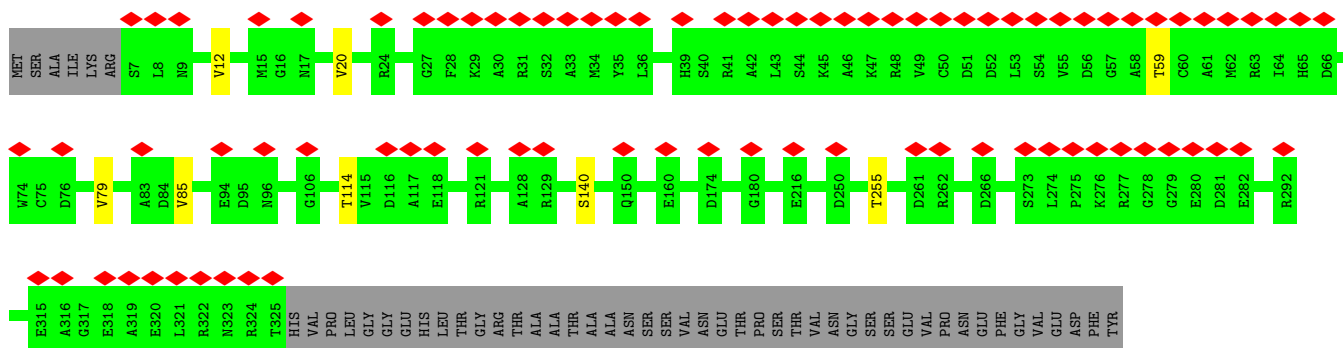
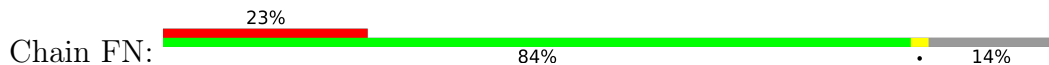
• Molecule 33: mt-SAF18



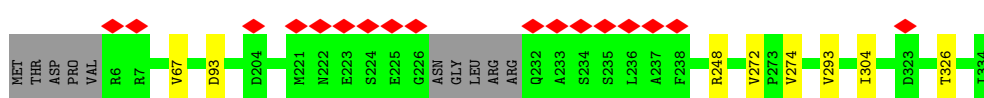
• Molecule 34: mt-SAF21



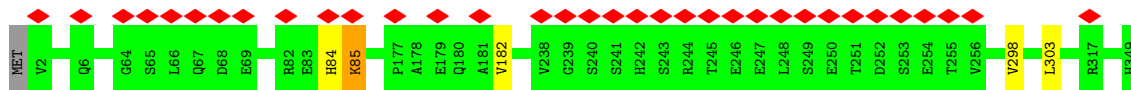
• Molecule 34: mt-SAF21



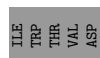
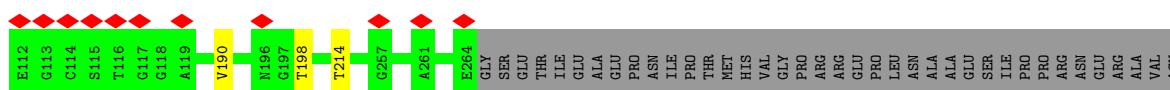
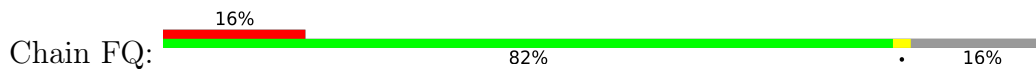
• Molecule 35: mt-SAF22 (KRIPP17)



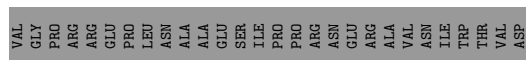
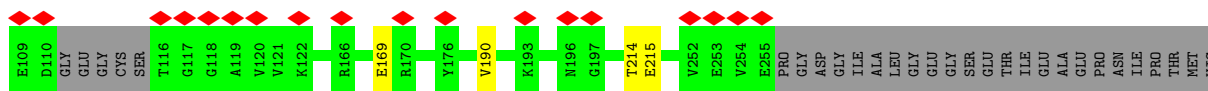
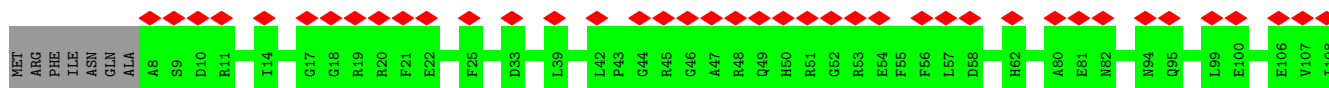
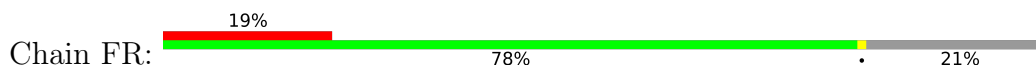
- Molecule 36: mt-SAF23



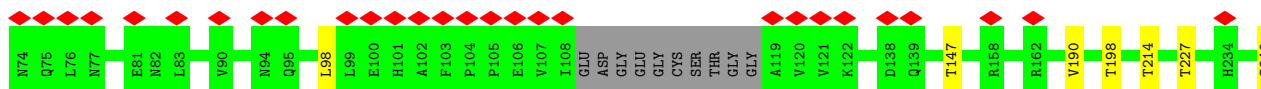
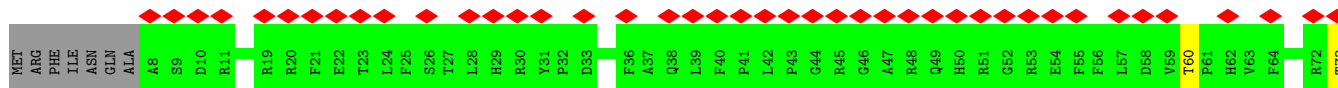
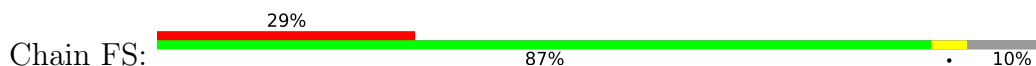
- Molecule 37: mt-SAF24



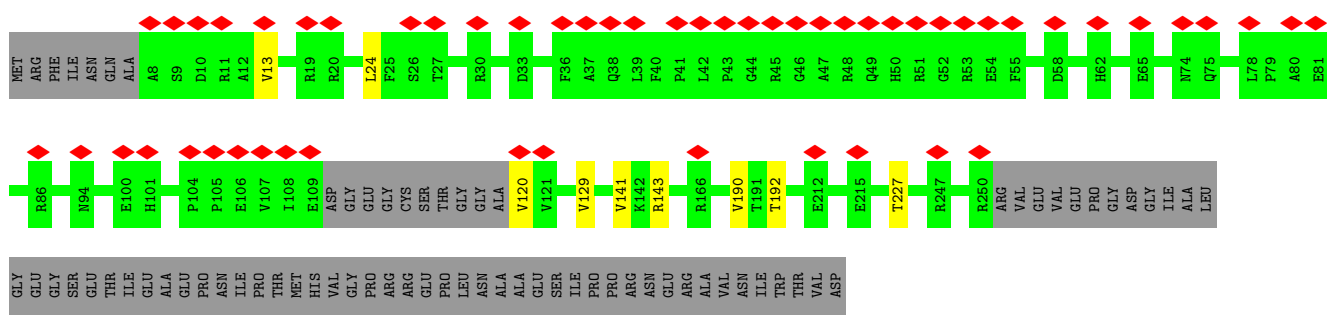
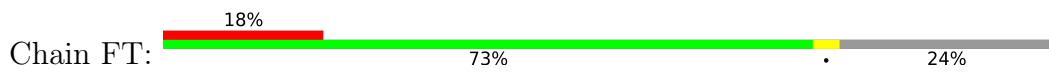
- Molecule 37: mt-SAF24



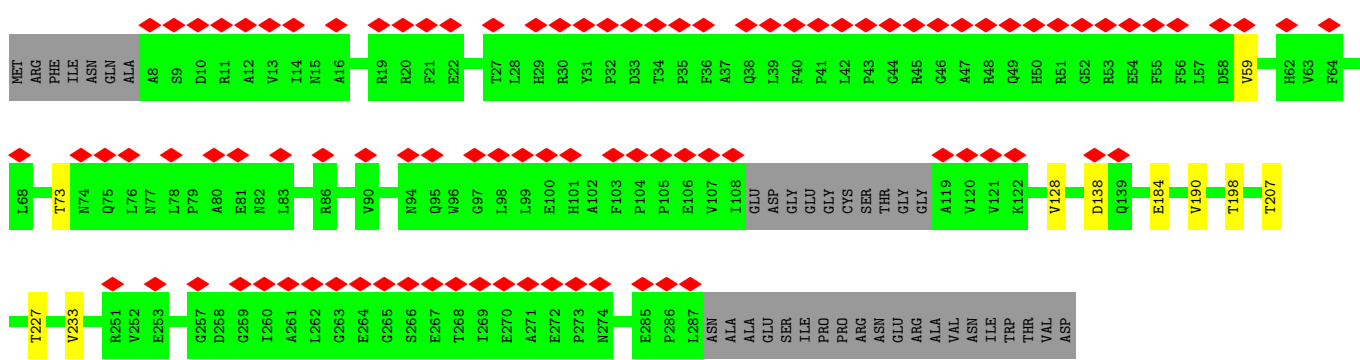
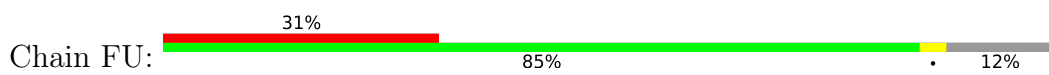
- Molecule 37: mt-SAF24



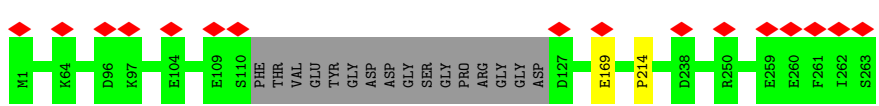
- Molecule 37: mt-SAF24



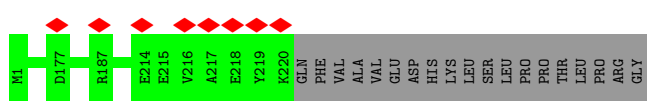
• Molecule 37: mt-SAF24



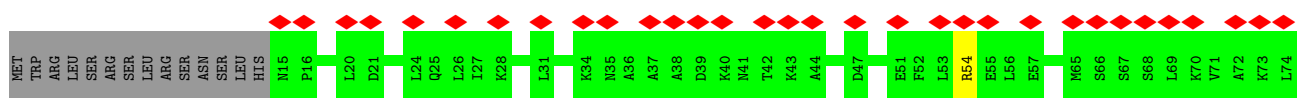
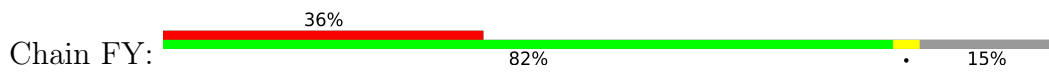
• Molecule 38: mt-SAF26

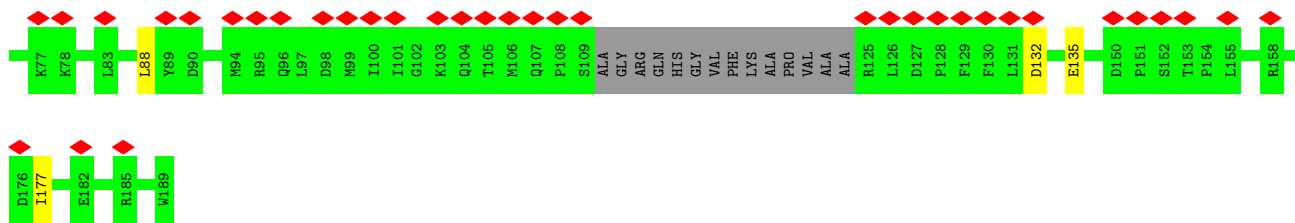


• Molecule 39: mt-SAF27 (KRIPP11)

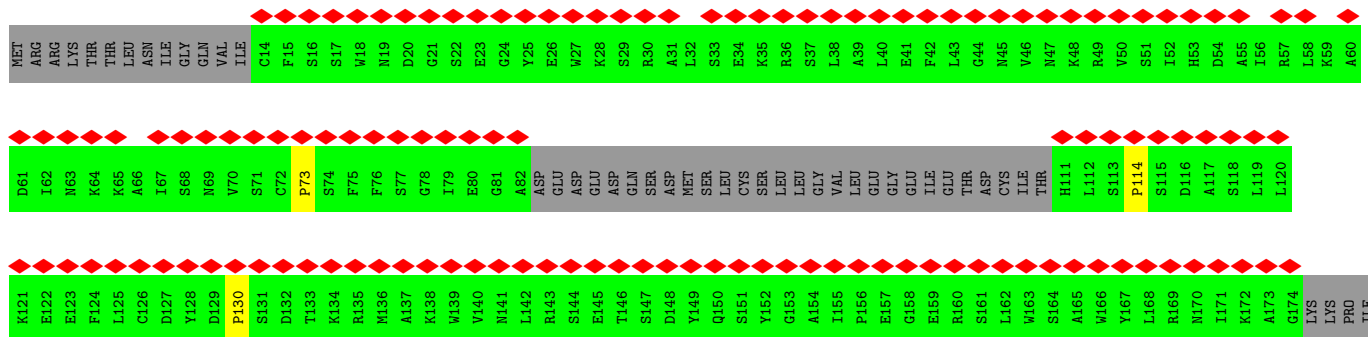
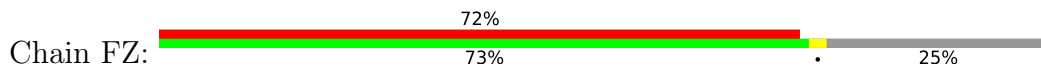


• Molecule 40: mt-SAF28

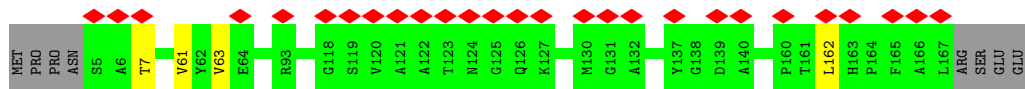




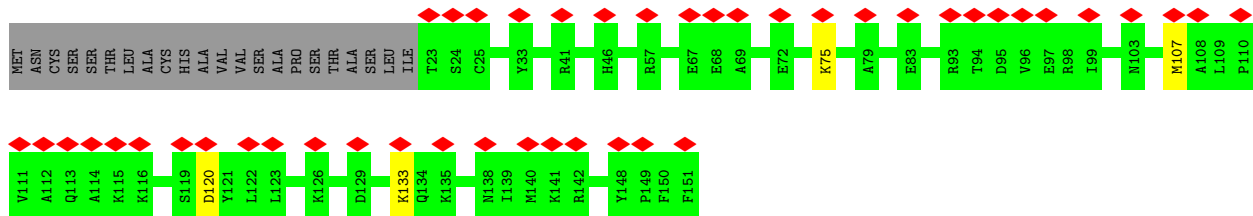
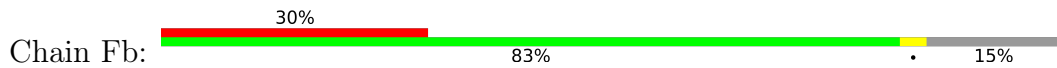
• Molecule 41: mt-SAF29



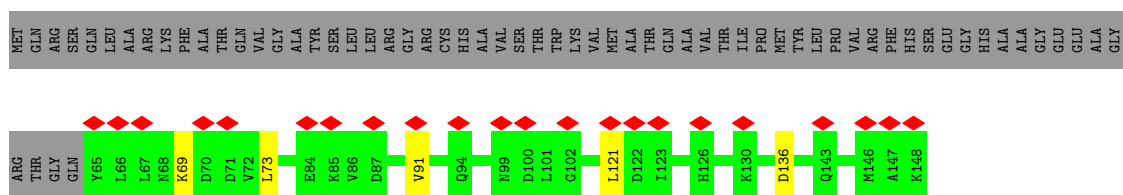
• Molecule 42: mt-SAF30



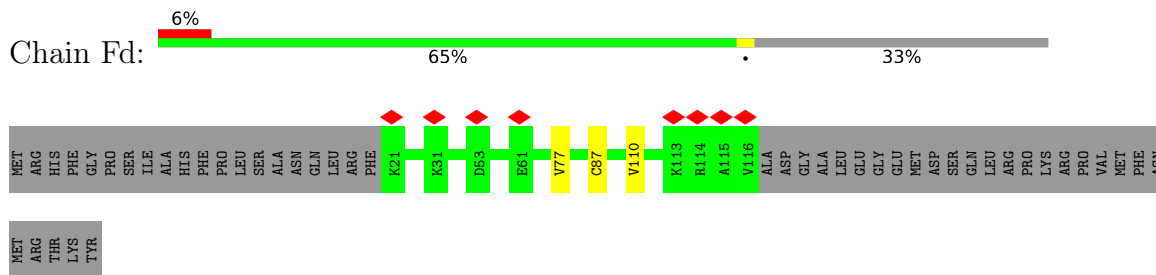
• Molecule 43: mt-SAF31



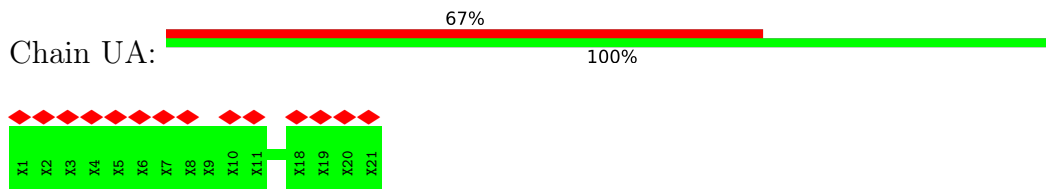
• Molecule 44: mt-SAF32



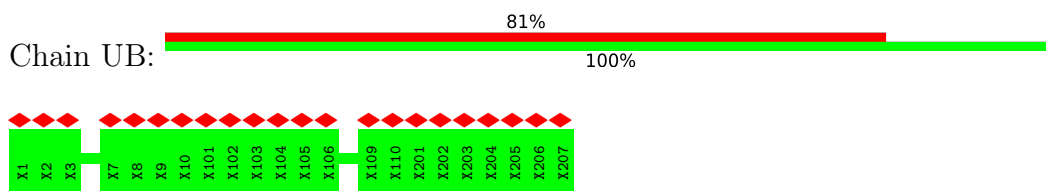
- Molecule 45: mt-SAF33



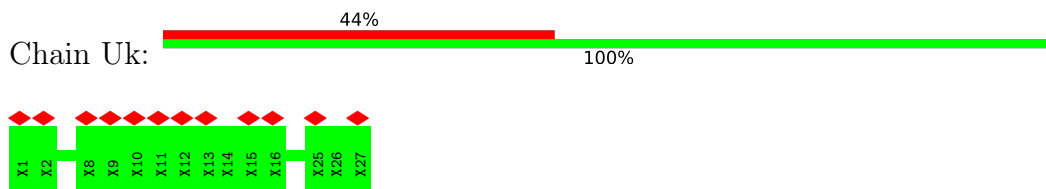
- Molecule 46: UNK-A



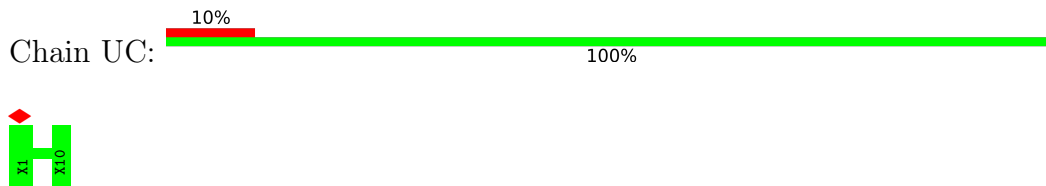
- Molecule 47: UNK-B, UNK-k



- Molecule 47: UNK-B, UNK-k



- Molecule 48: UNK-C



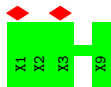
- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f



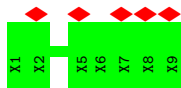
There are no outlier residues recorded for this chain.

- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f





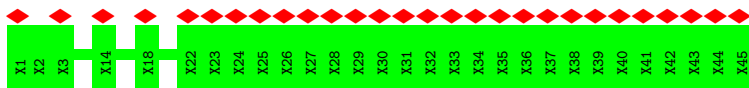
- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f



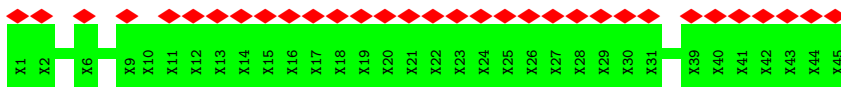
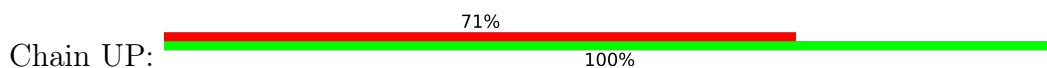
- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f



- Molecule 50: UNK-E, UNK-P



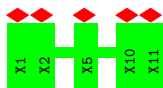
- Molecule 50: UNK-E, UNK-P



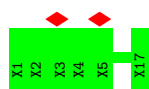
- Molecule 51: UNK-F, UNK-m



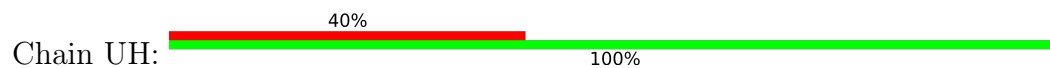
- Molecule 51: UNK-F, UNK-m



- Molecule 52: UNK-G



- Molecule 53: UNK-H



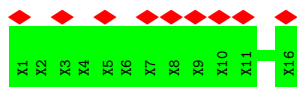
- Molecule 54: UNK-I, UNK-N



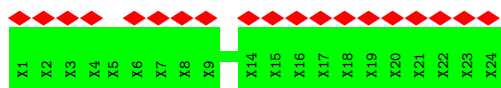
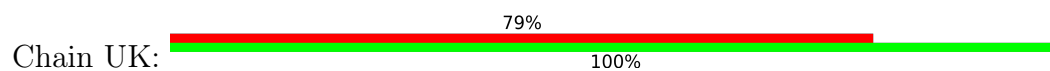
- Molecule 54: UNK-I, UNK-N



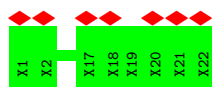
- Molecule 55: UNK-J



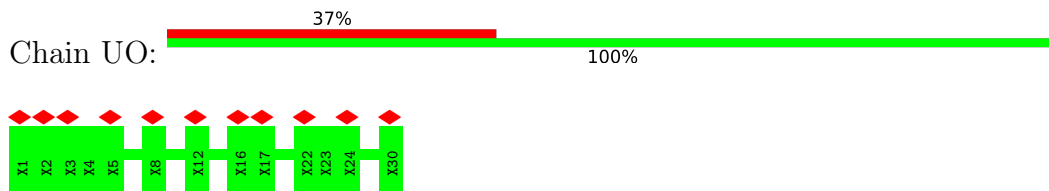
- Molecule 56: UNK-K



- Molecule 57: UNK-L



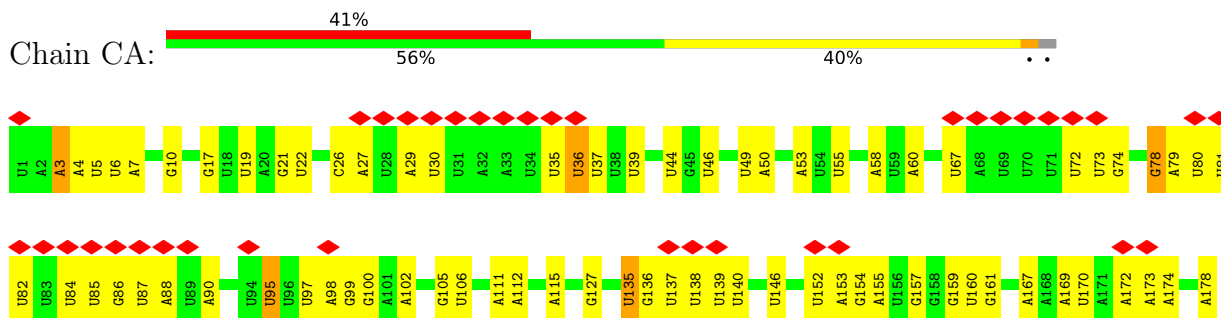
• Molecule 58: UNK-O

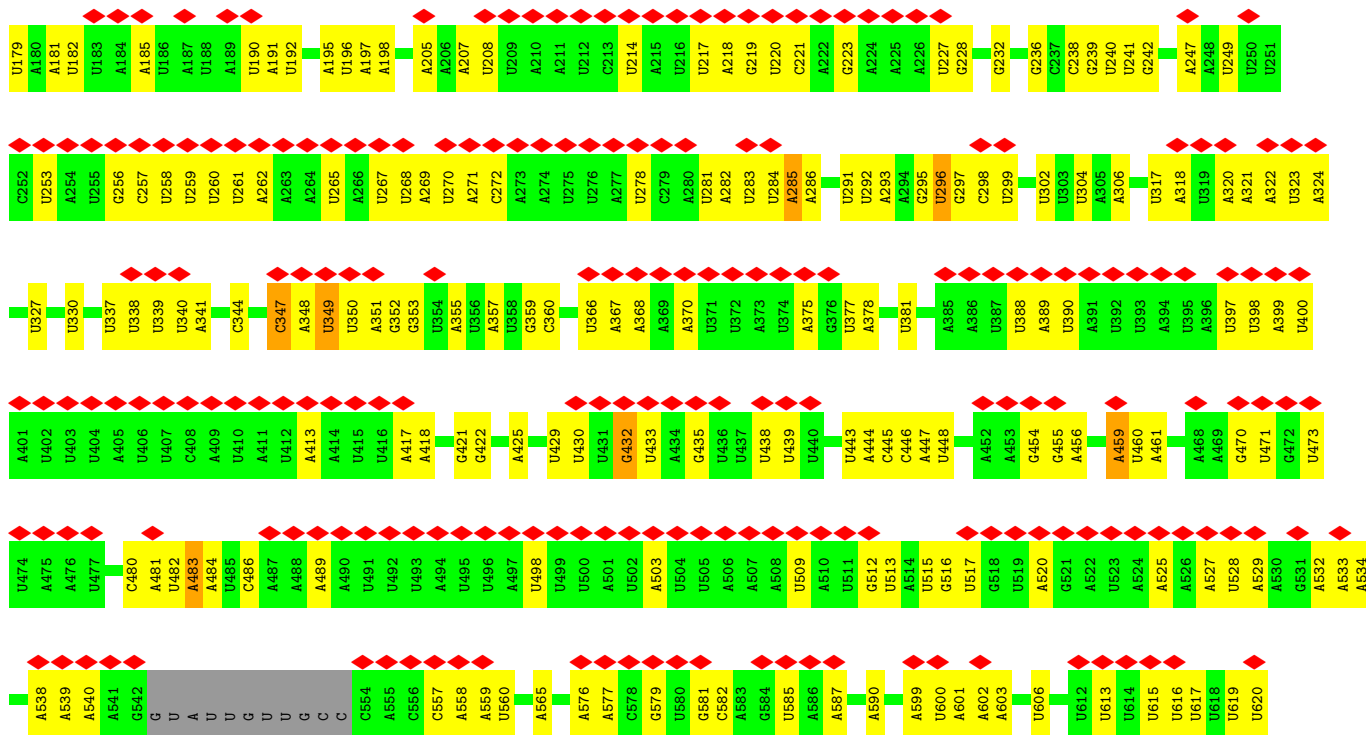


• Molecule 59: UNK-Y

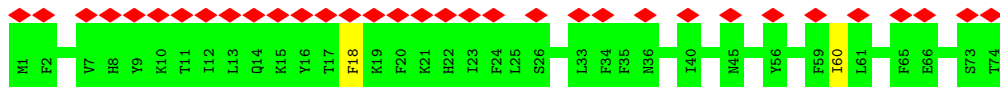


• Molecule 60: 9S rRNA

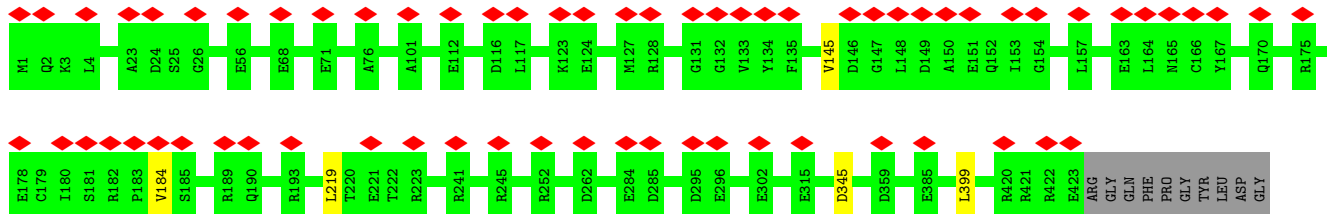




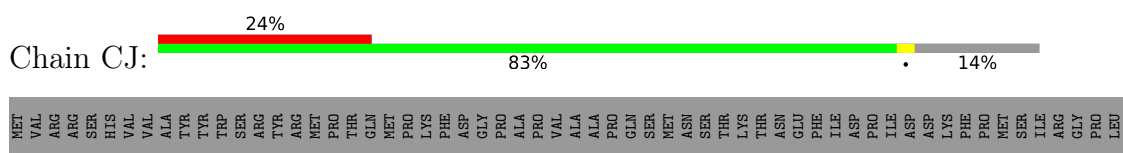
• Molecule 61: mS3m

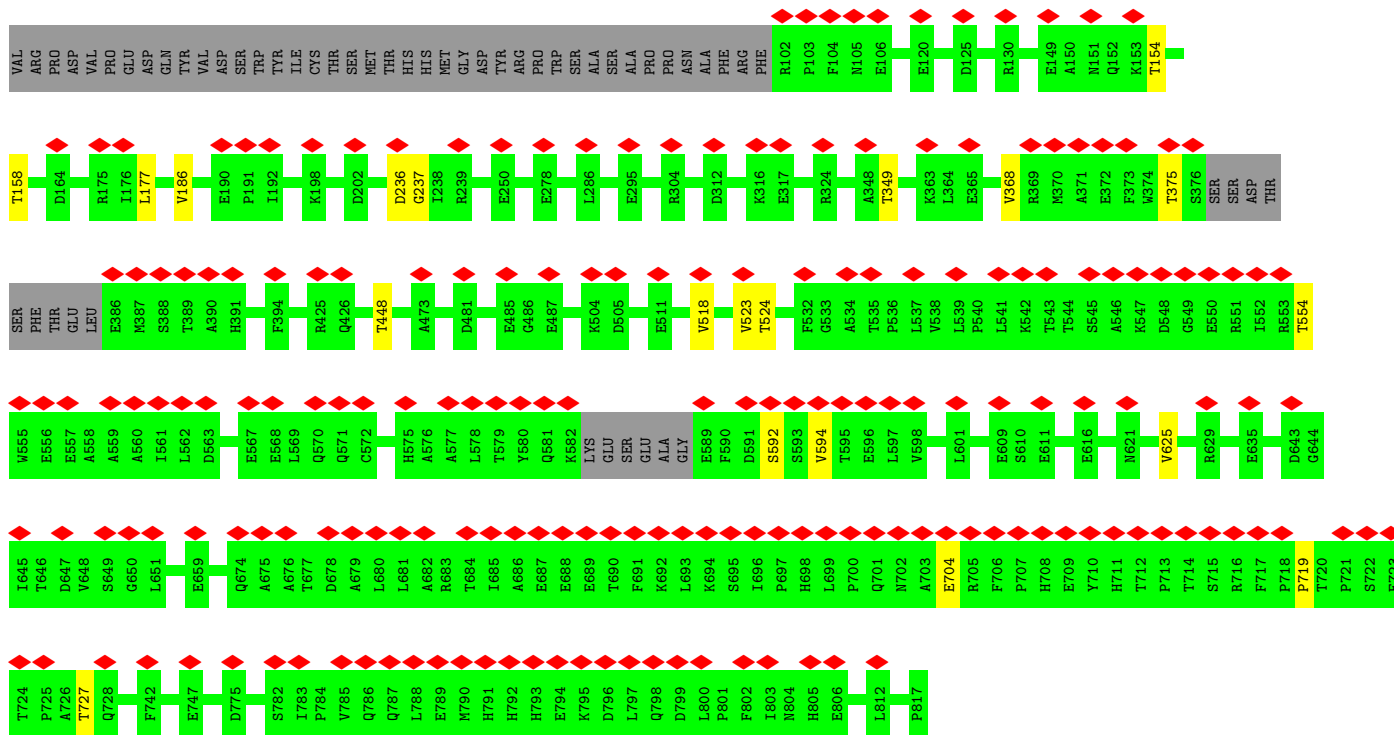


• Molecule 62: uS9m

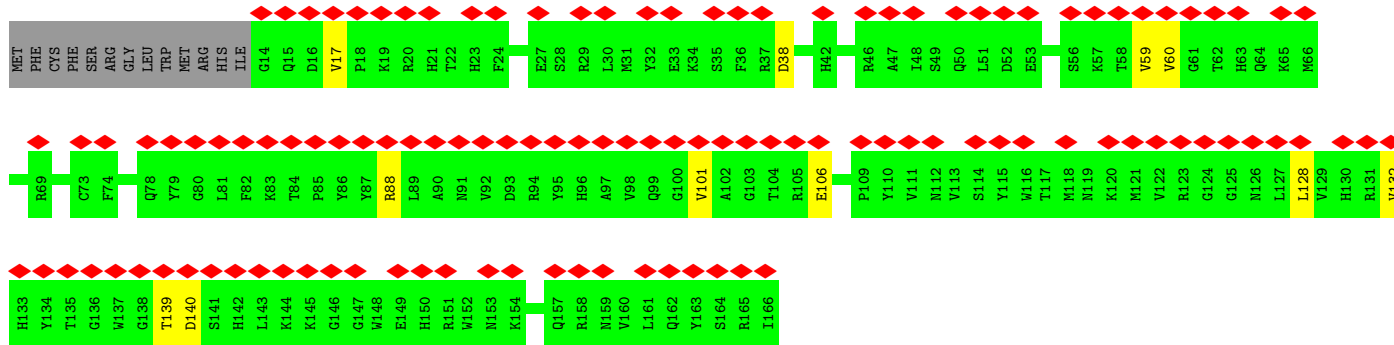
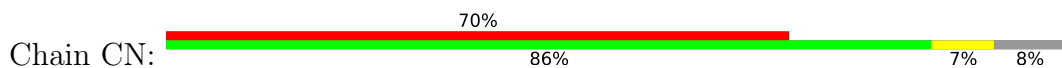


• Molecule 63: uS10m

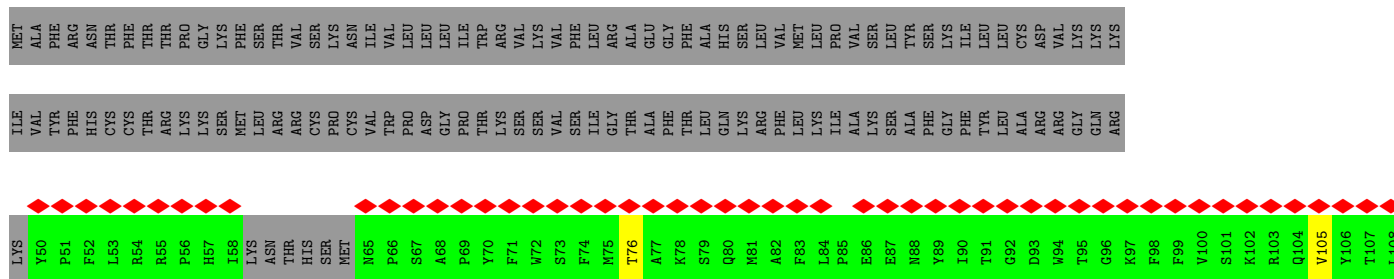


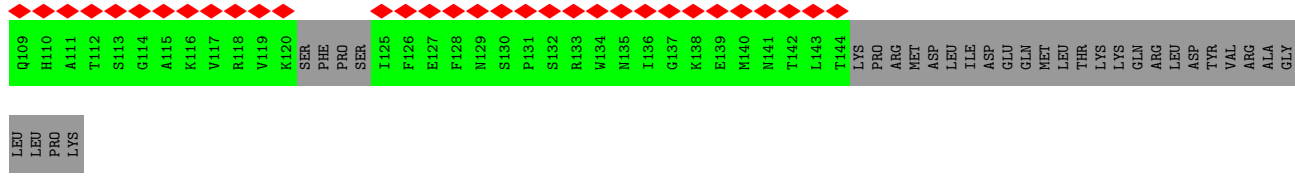


• Molecule 64: uS14m

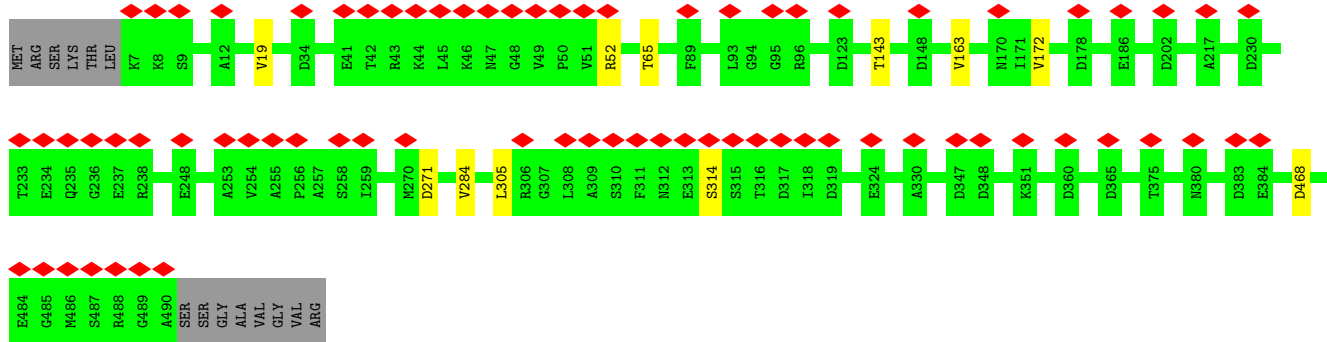


• Molecule 65: uS19m

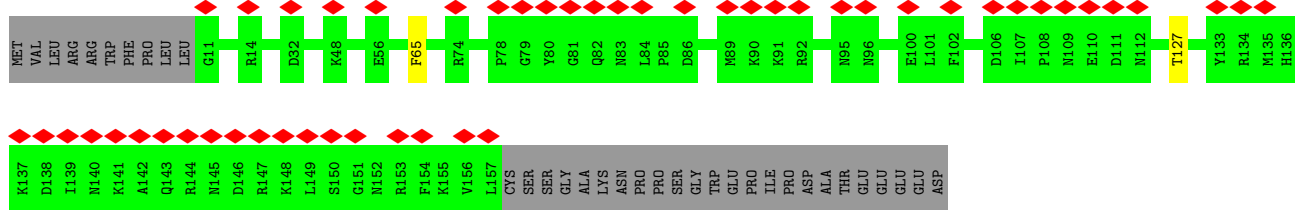
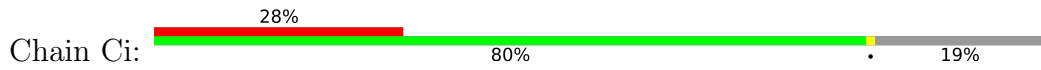




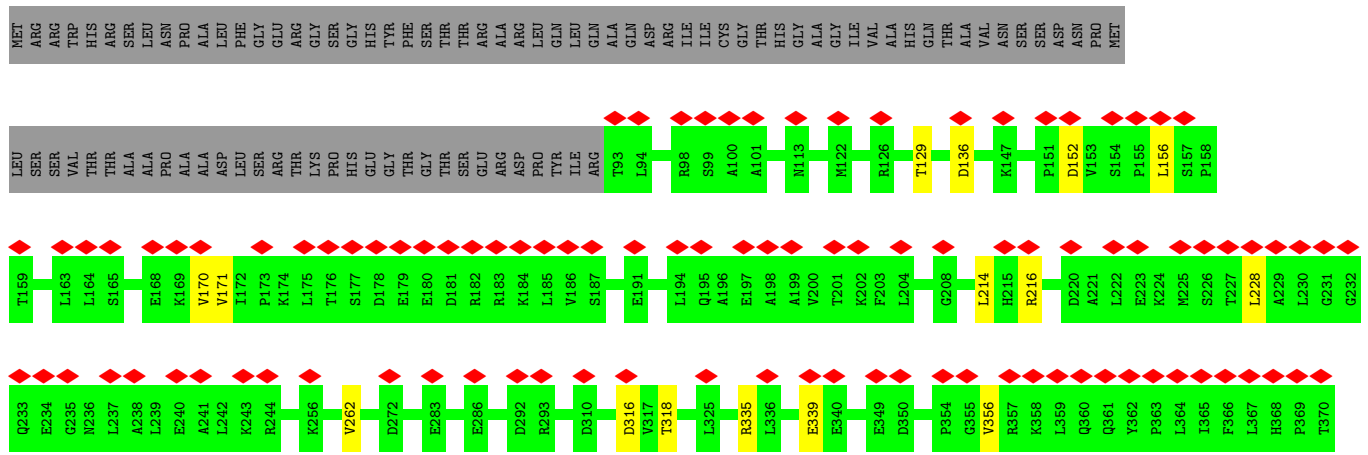
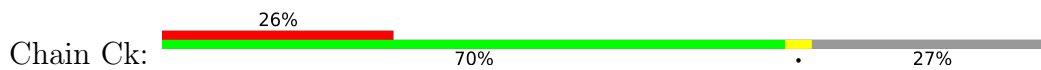
• Molecule 66: mS29

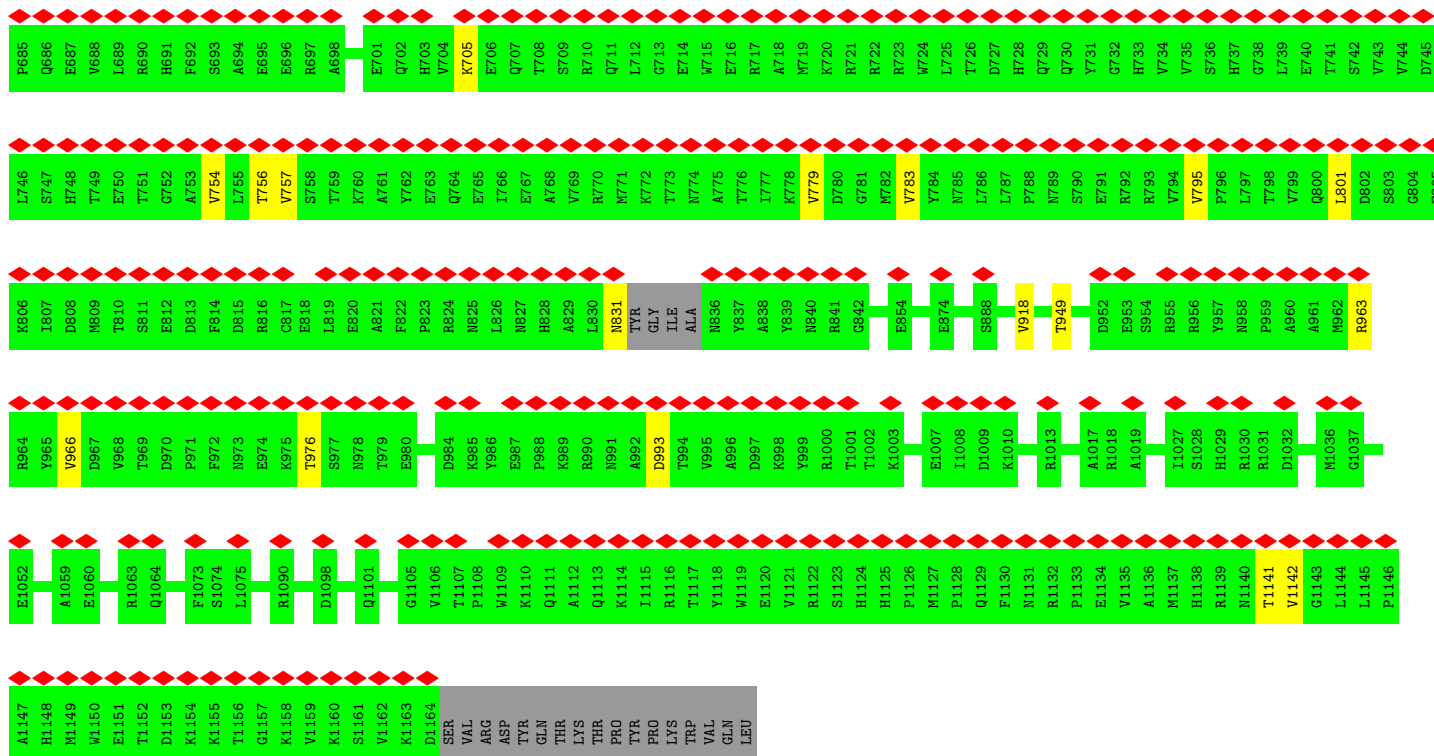


• Molecule 67: mS33

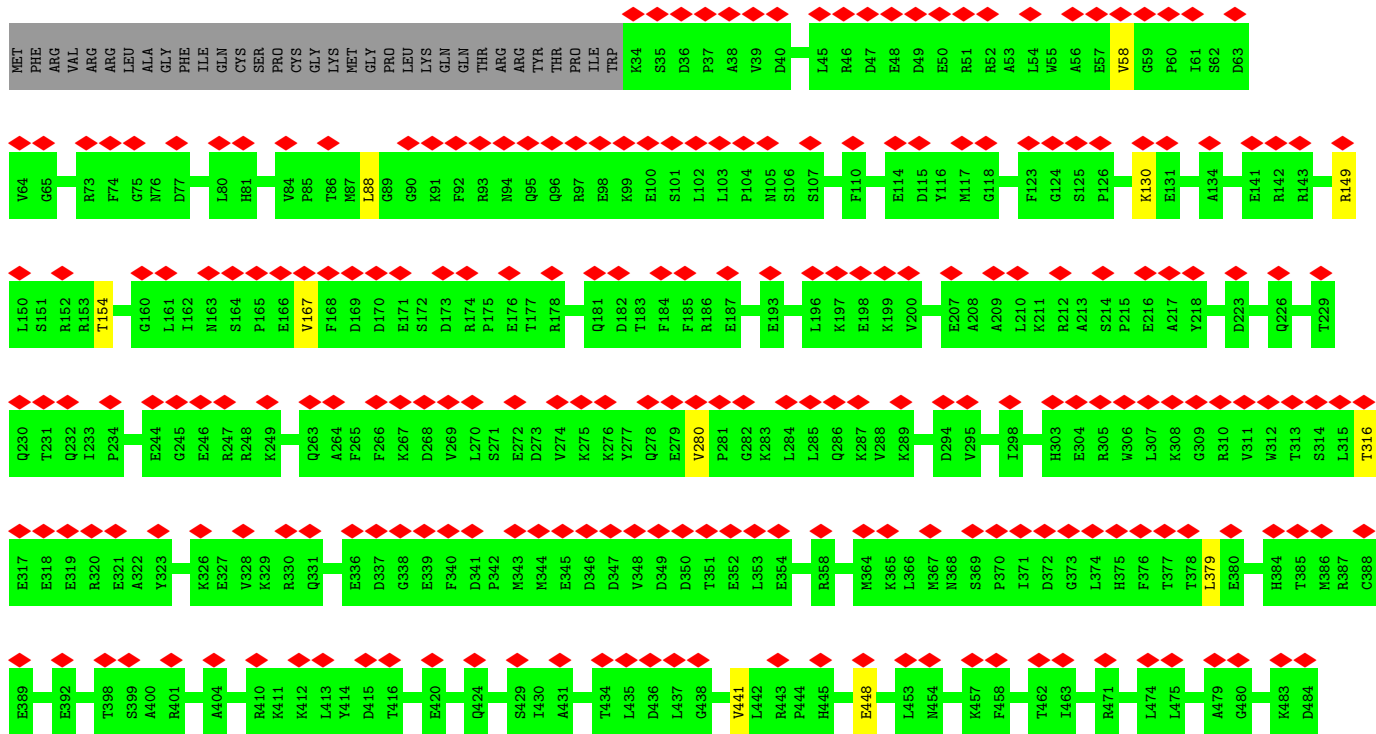
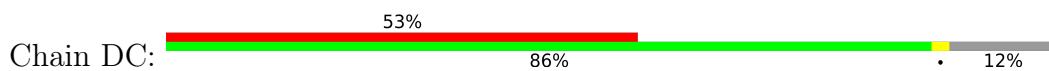


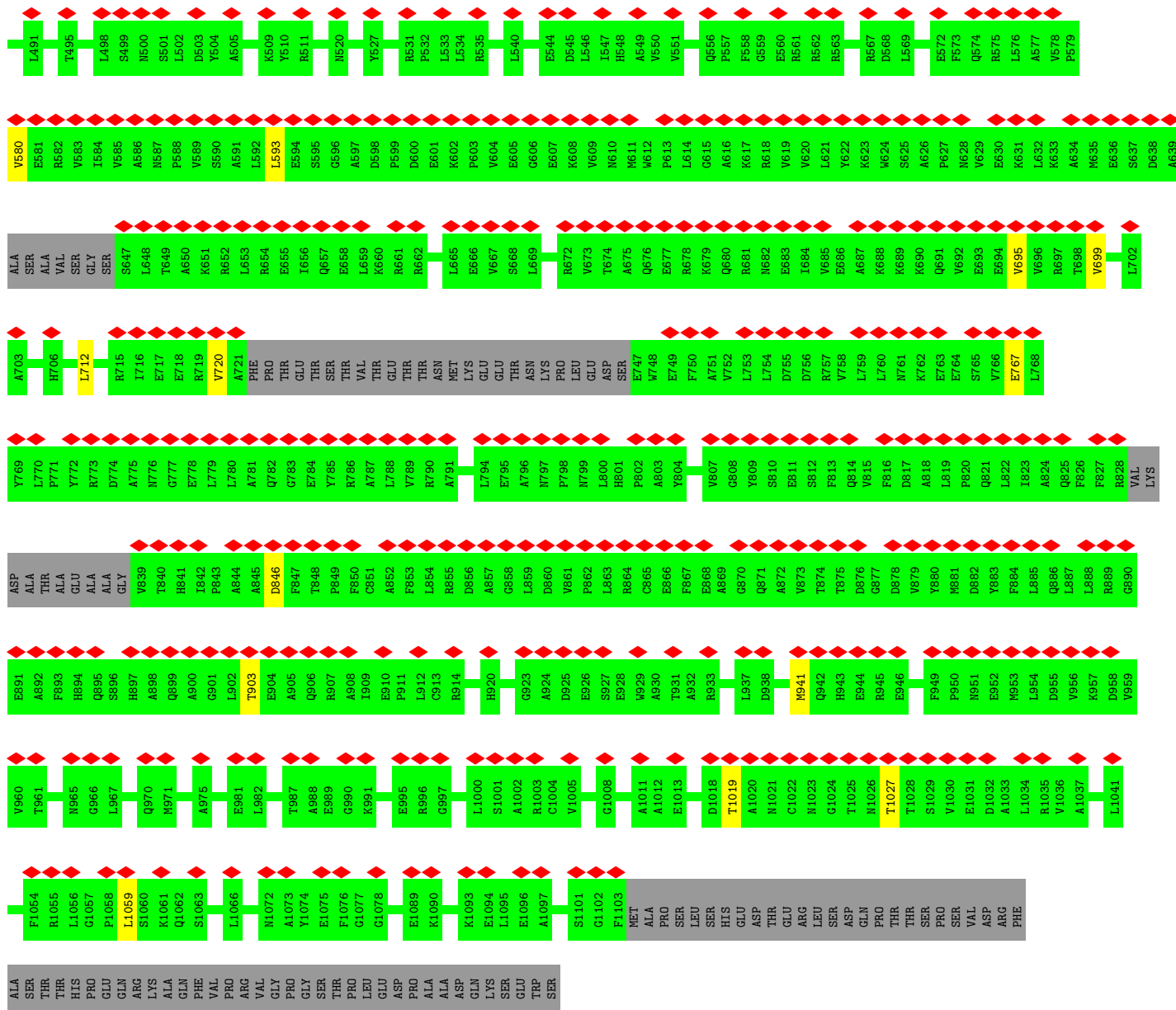
• Molecule 68: mS35



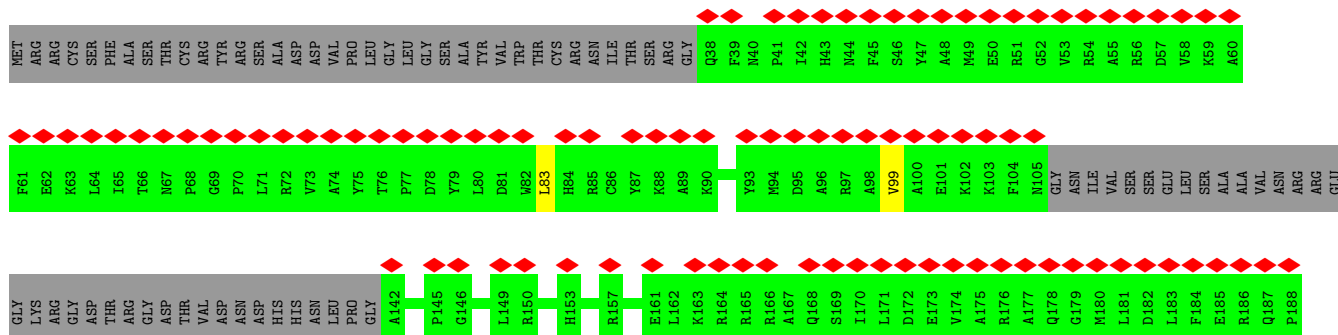
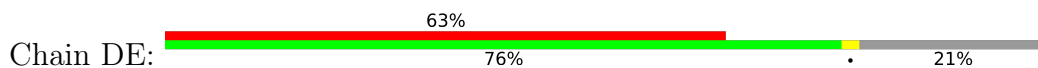


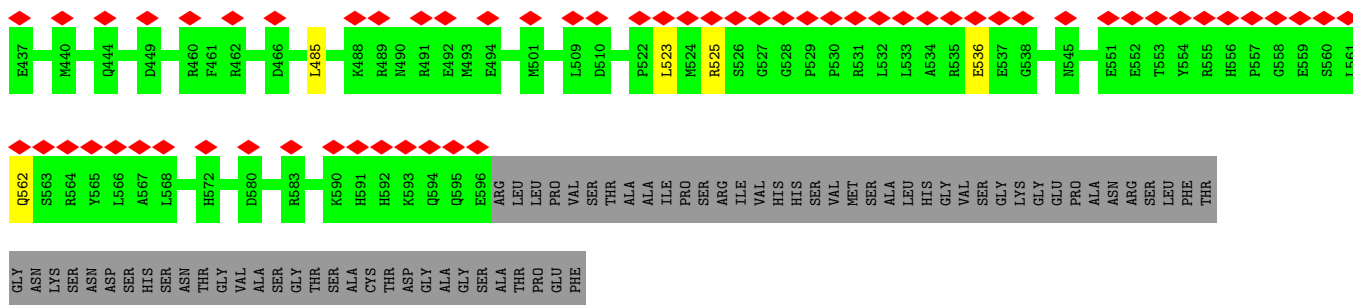
• Molecule 70: mS50



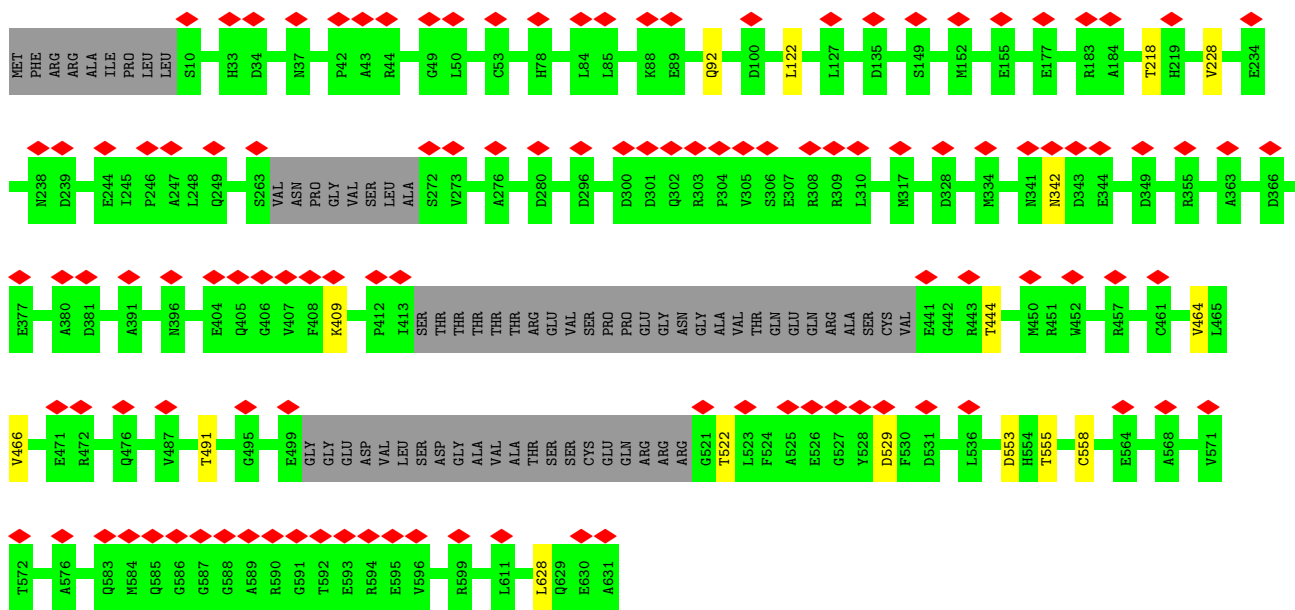
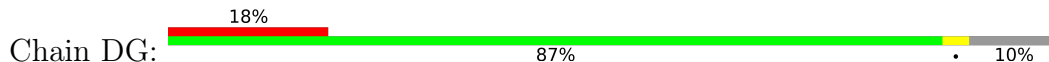


- Molecule 71: mS52

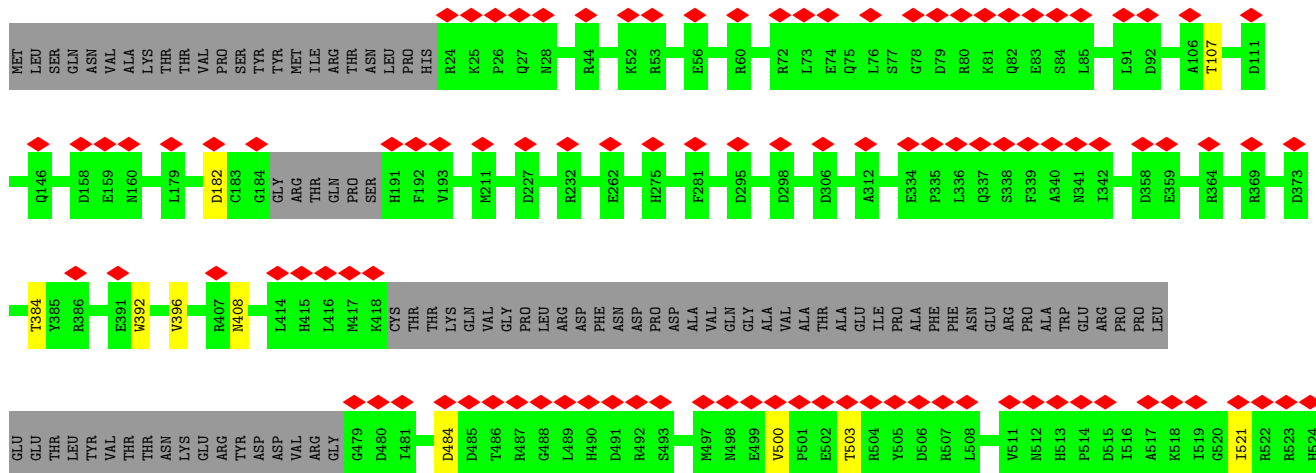
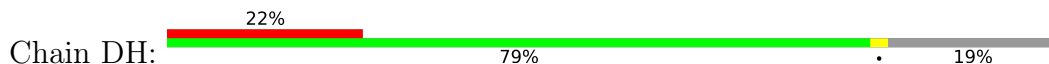


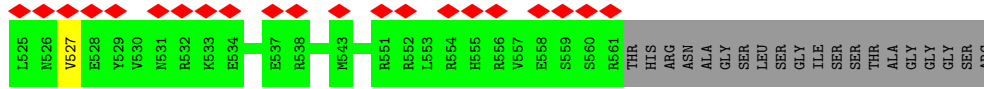


• Molecule 73: mS54

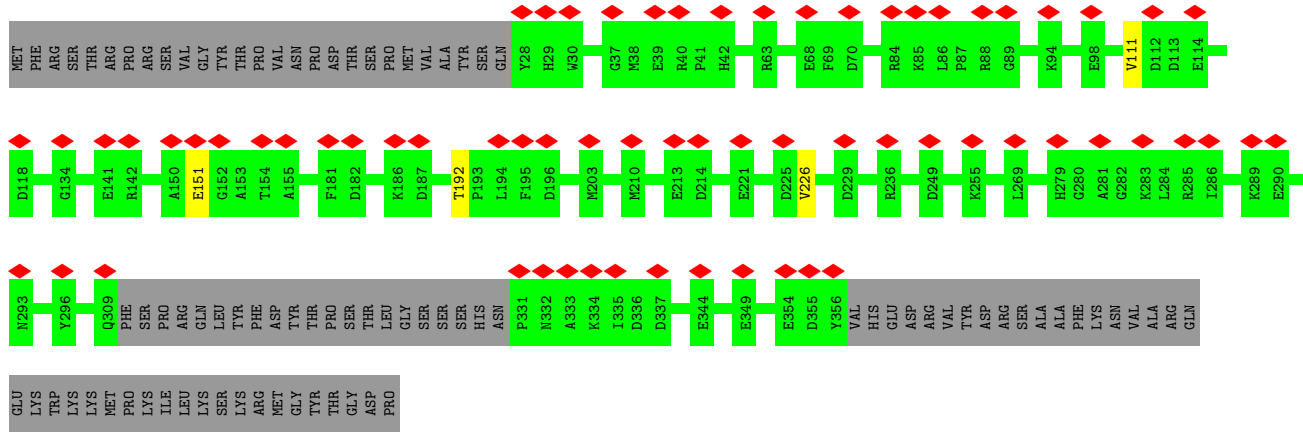
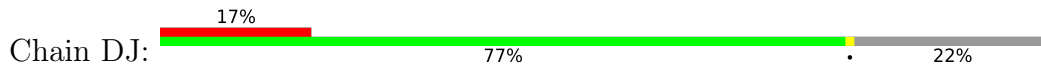


• Molecule 74: mS55 (KRIPP8)

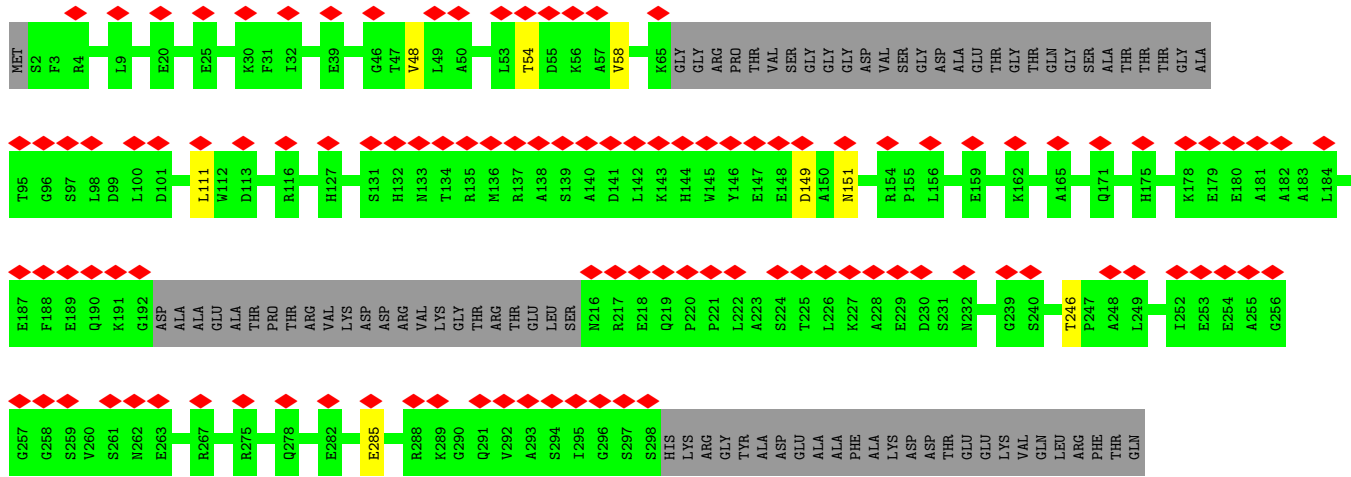
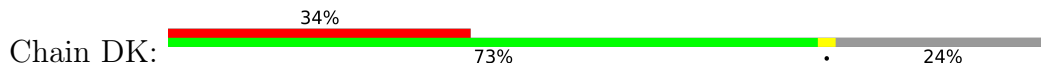




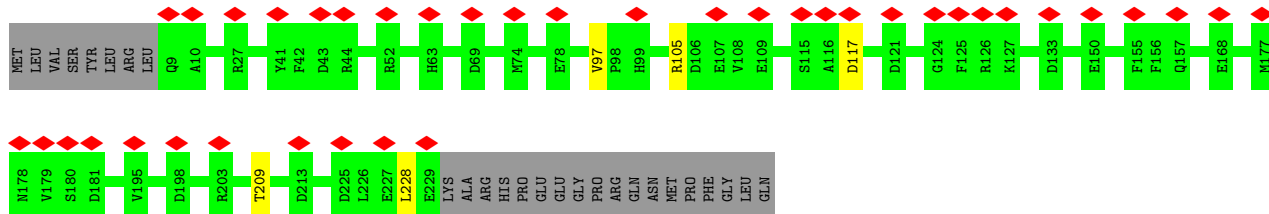
• Molecule 75: mS57



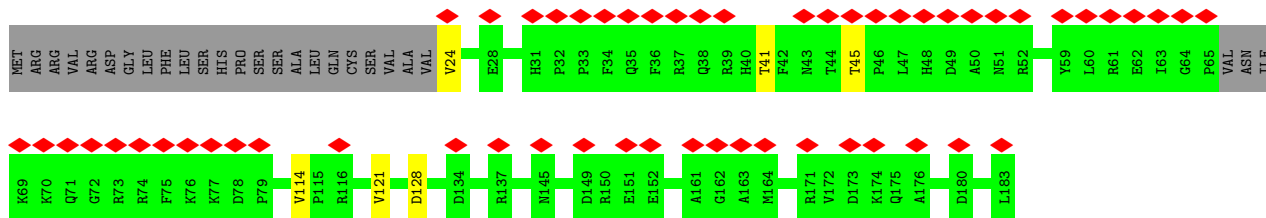
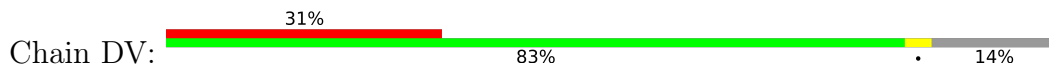
• Molecule 76: mS58



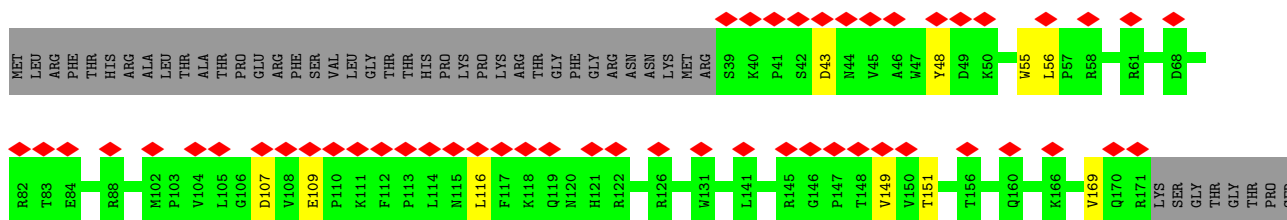
• Molecule 77: mS67



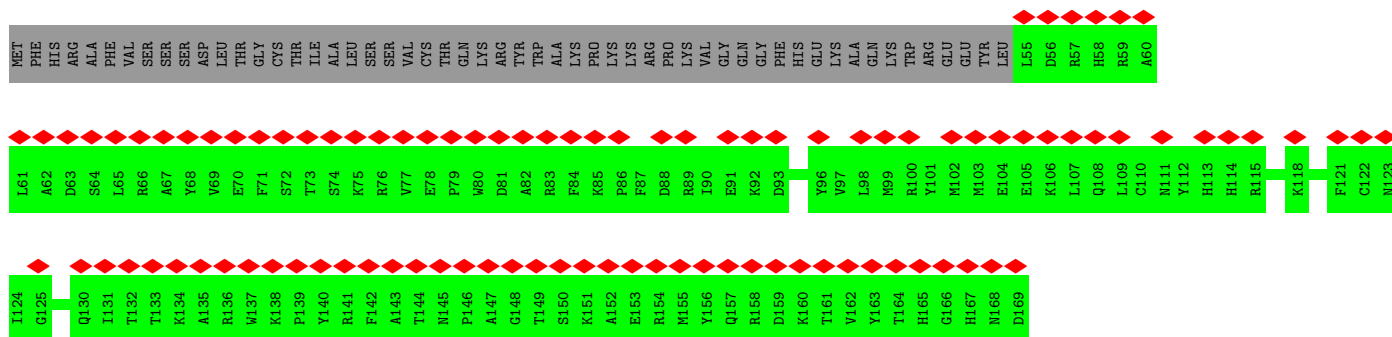
• Molecule 78: mS69



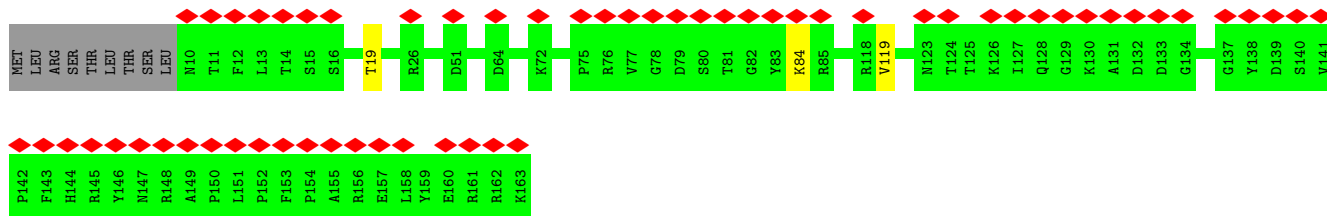
• Molecule 79: mS70



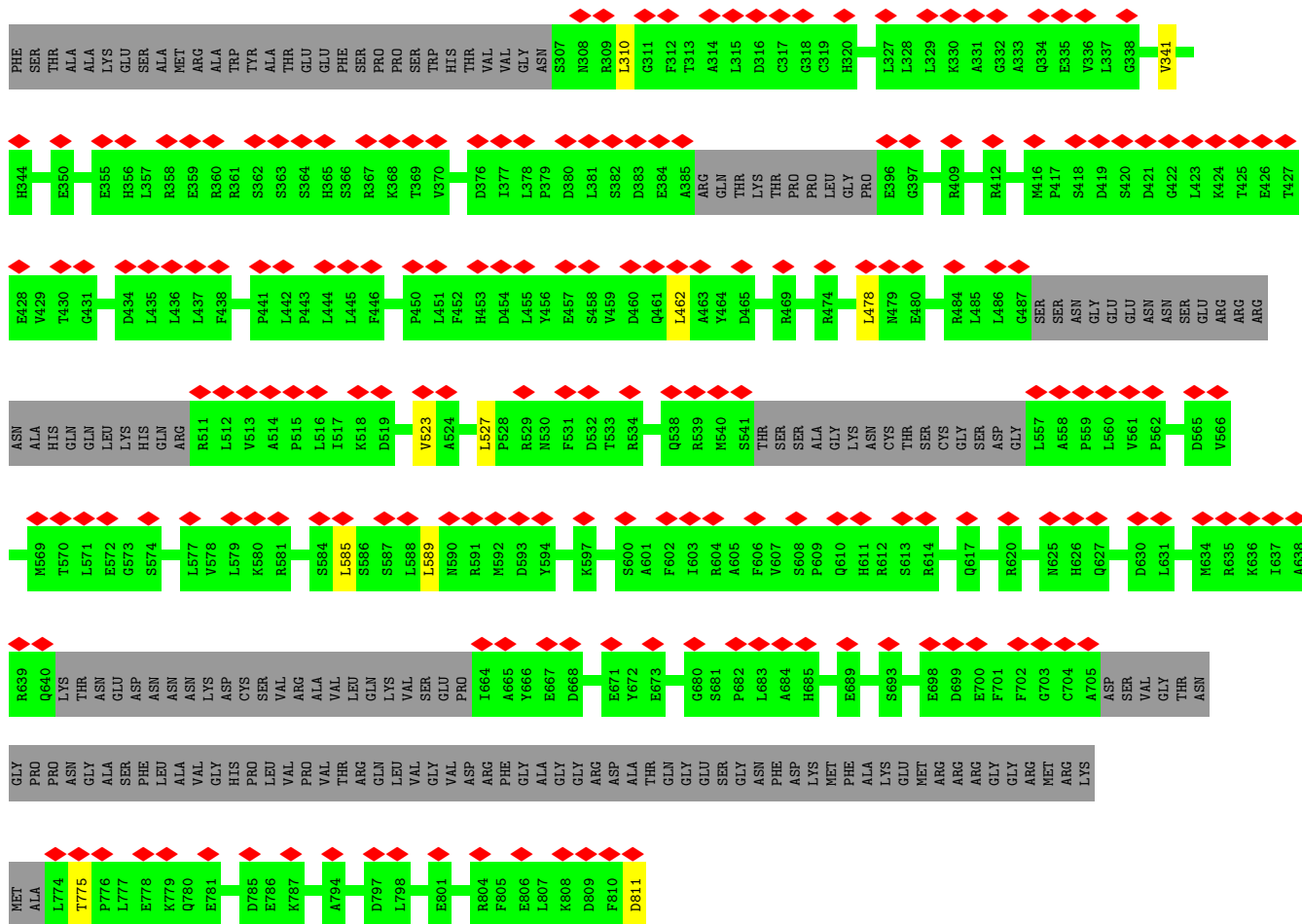
• Molecule 80: mS71



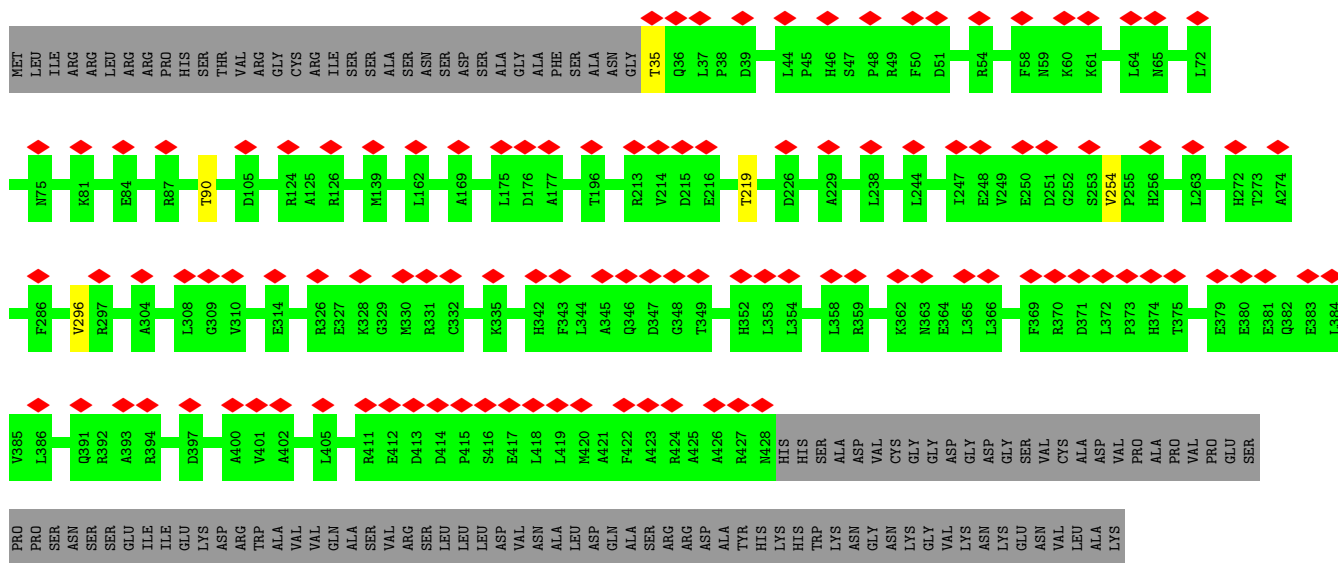
• Molecule 81: mS72

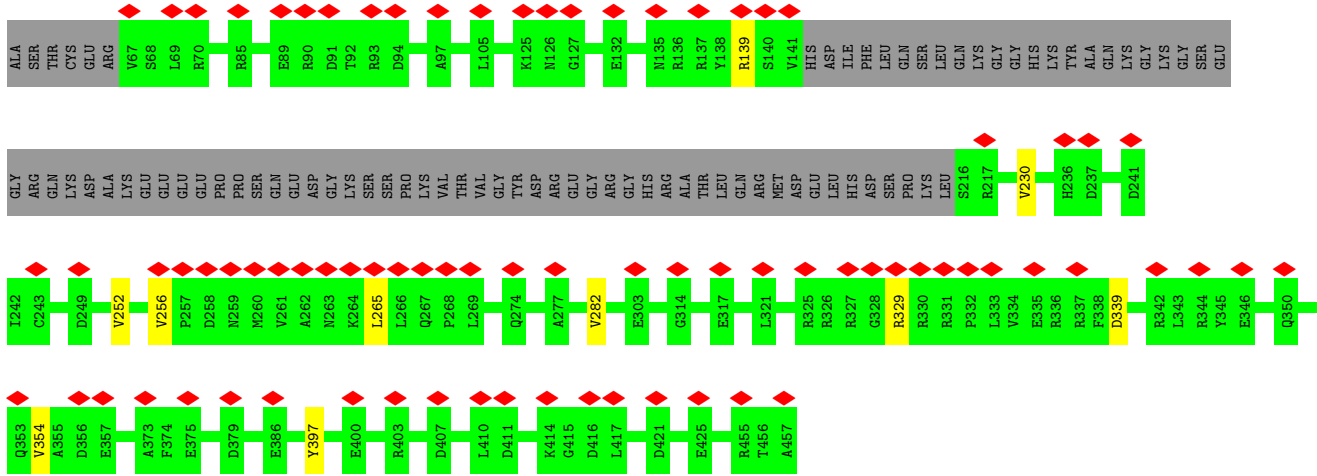


• Molecule 82: mt-SAF1 (RSM22)

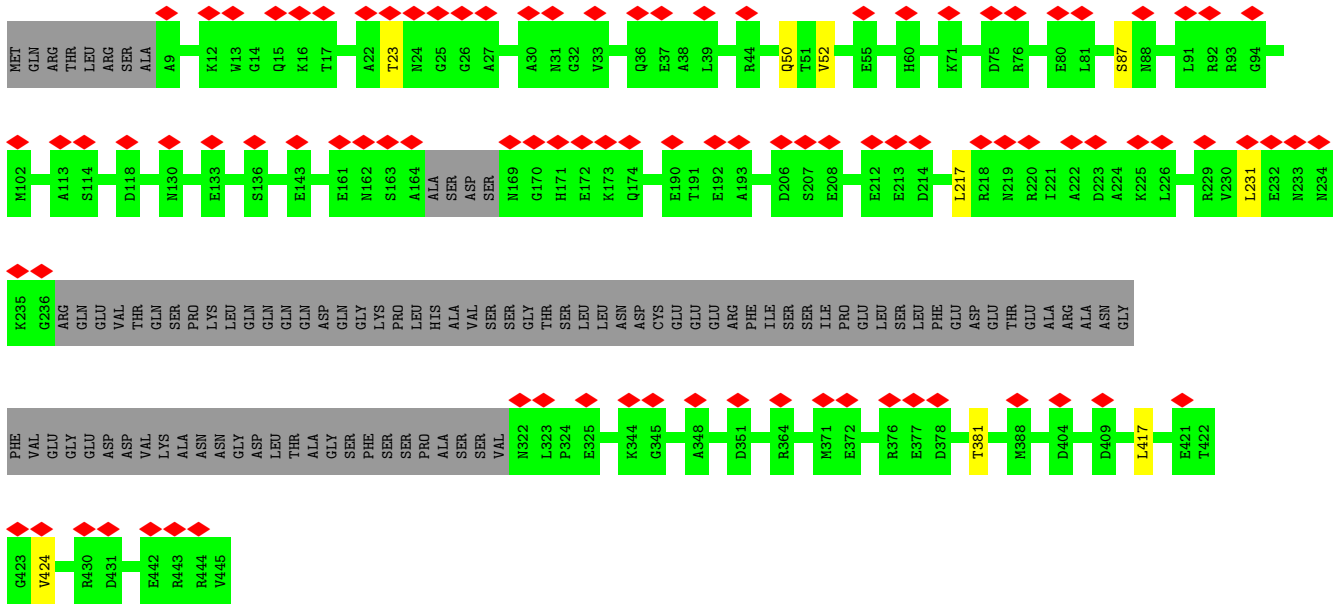
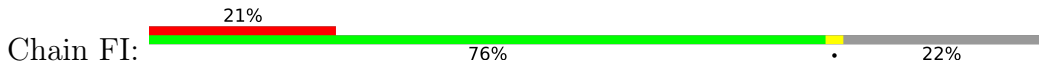


● Molecule 84: mt-SAF12 (KRIPP18)

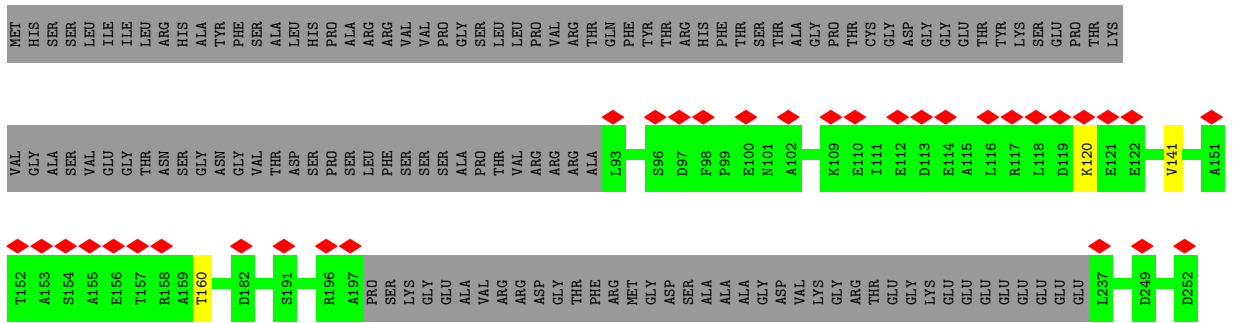


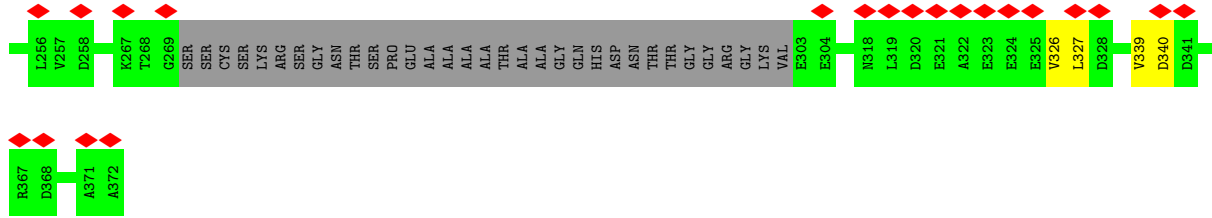


• Molecule 88: mt-SAF17

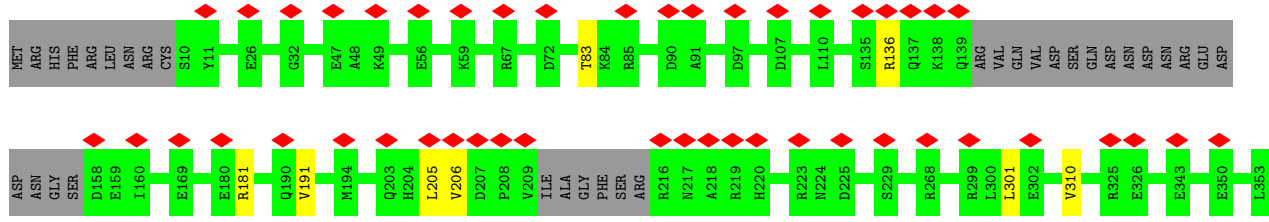
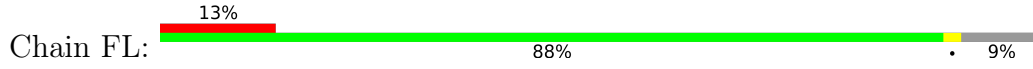


• Molecule 89: mt-SAF19

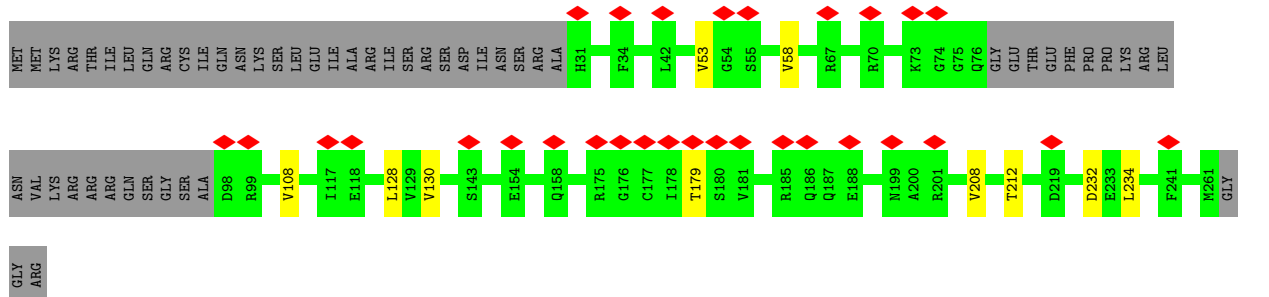
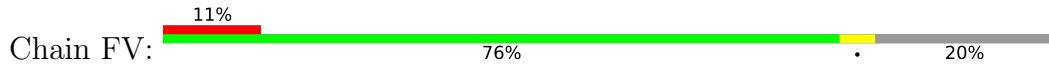




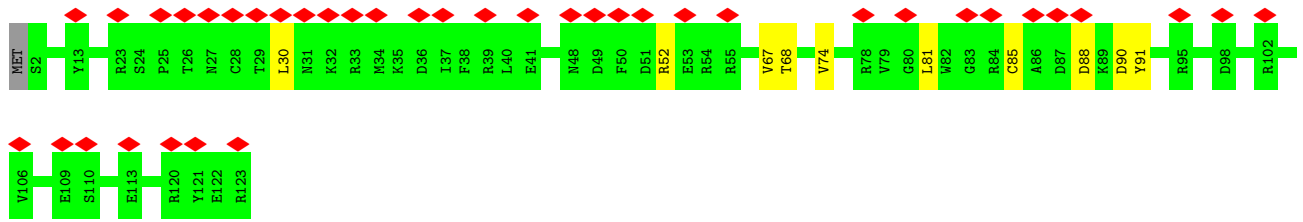
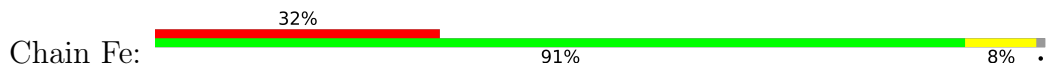
• Molecule 90: mt-SAF20



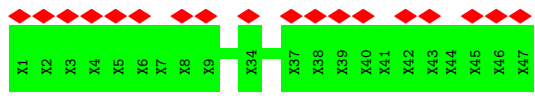
• Molecule 91: mt-SAF25



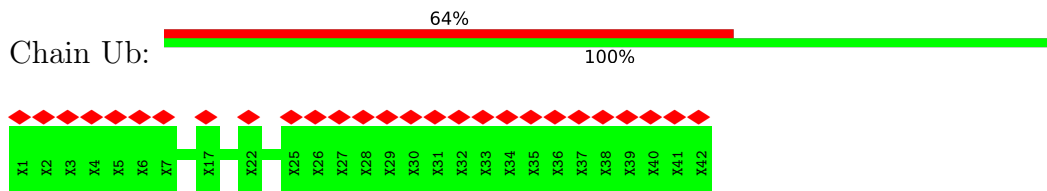
• Molecule 92: mt-SAF34



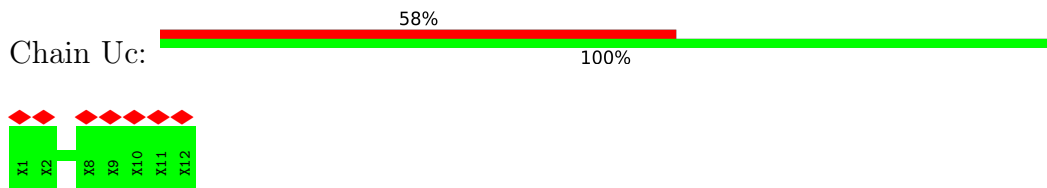
• Molecule 93: UNK-a



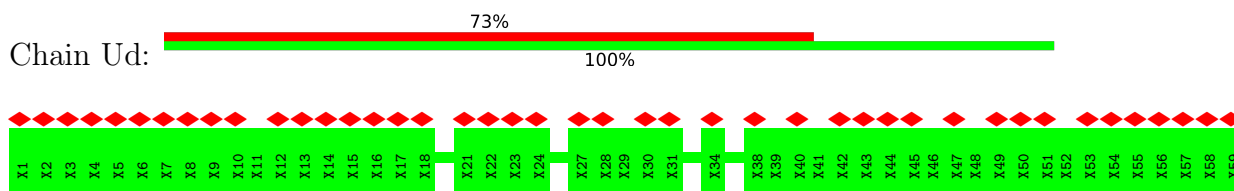
• Molecule 94: UNK-b



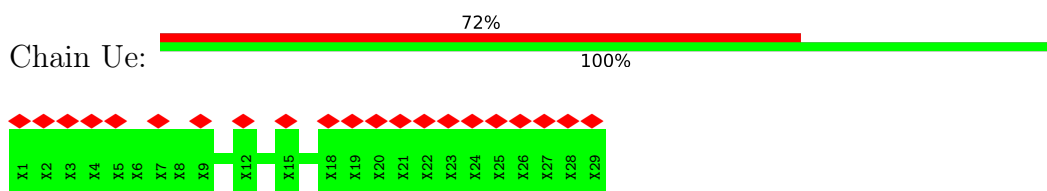
• Molecule 95: UNK-c



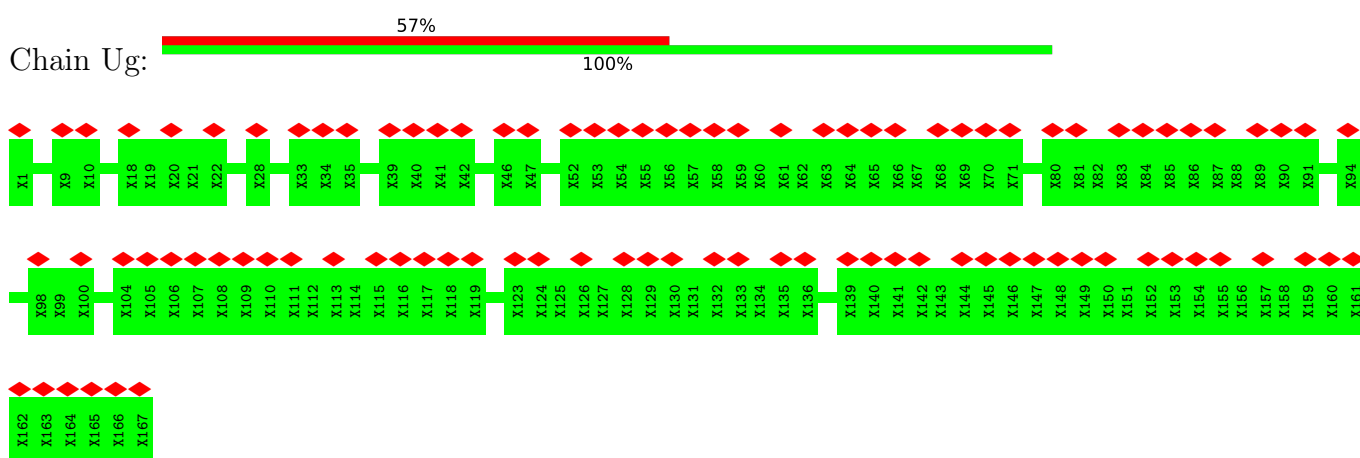
• Molecule 96: UNK-d



• Molecule 97: UNK-e

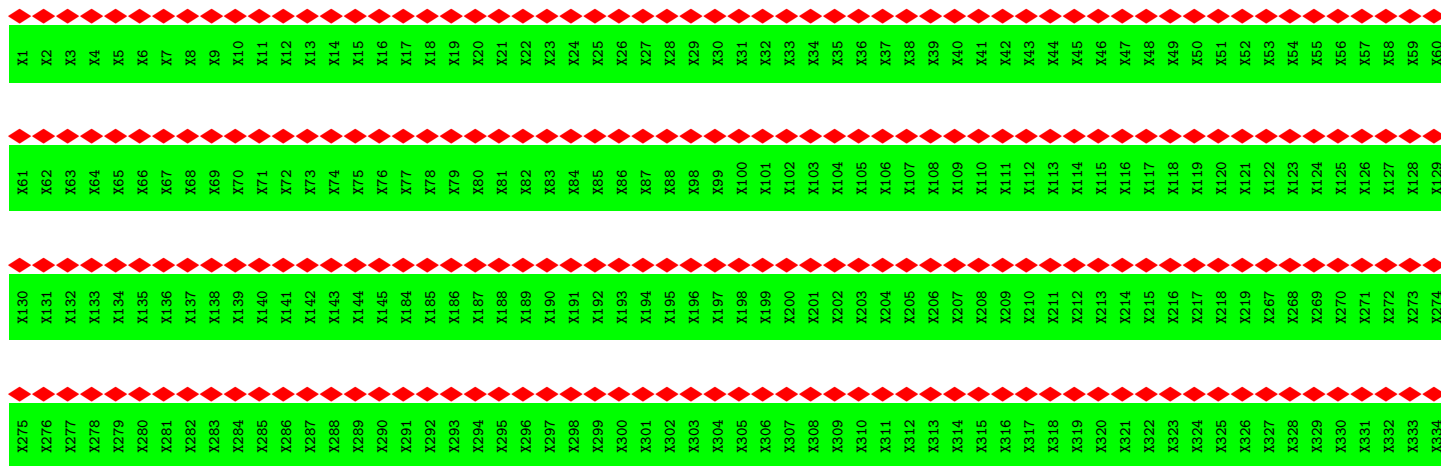


• Molecule 98: UNK-g

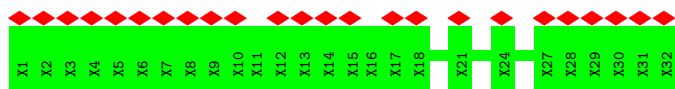
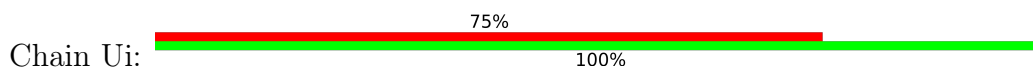


• Molecule 99: UNK-h

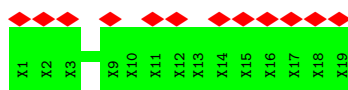




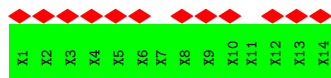
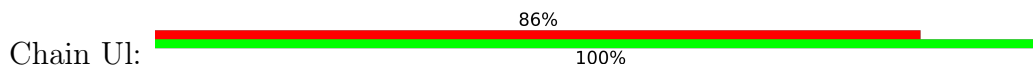
• Molecule 100: UNK-i



• Molecule 101: UNK-j



• Molecule 102: UNK-l



• Molecule 103: UNK-x



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; On the fly in RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.613	Depositor
Minimum map value	-0.285	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, UBD, SAH, GTP, ZN, MG, PM8

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	CE	0.26	0/3226	0.47	2/4364 (0.0%)
2	CF	0.25	0/1344	0.44	0/1813
3	CH	0.25	0/1864	0.44	0/2511
4	CK	0.27	0/1760	0.48	1/2372 (0.0%)
5	CO	0.25	0/3057	0.44	1/4121 (0.0%)
6	CP	0.26	0/1533	0.48	0/2074
7	CQ	0.27	0/1856	0.45	0/2509
8	CR	0.26	0/1315	0.46	0/1785
9	Ca	0.26	0/4474	0.44	1/6052 (0.0%)
10	Cb	0.26	0/1304	0.45	0/1751
11	Cd	0.30	0/1662	0.40	0/2234
12	Cj	0.26	0/1842	0.45	0/2511
13	Cn	0.28	0/245	0.49	0/333
14	Cp	0.25	0/1551	0.42	0/2103
15	DD	0.26	0/6678	0.43	0/9051
16	DI	0.25	0/3248	0.42	0/4401
17	DL	0.26	0/1699	0.43	0/2293
18	DO	0.23	0/1680	0.39	0/2265
19	DP	0.24	0/1854	0.43	0/2511
20	DR	0.26	0/2107	0.47	0/2871
21	DU	0.26	0/1780	0.51	2/2416 (0.1%)
22	DZ	0.25	0/263	0.45	0/355
23	F2	0.25	0/7432	0.44	1/10042 (0.0%)
24	F3	0.25	0/6999	0.44	0/9472
25	F5	0.26	0/3533	0.43	3/4798 (0.1%)
26	F6	0.26	0/3728	0.47	1/5060 (0.0%)
27	F7	0.26	0/5342	0.45	0/7236
28	F8	0.26	0/4025	0.44	0/5450
29	F9	0.24	0/1785	0.39	0/2399
30	FA	0.26	0/4507	0.47	0/6139
31	FB	0.26	0/3132	0.45	0/4248
31	FC	0.25	0/2635	0.45	0/3572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	FE	0.26	0/3629	0.44	0/4935
33	FJ	0.29	0/2986	0.49	0/4030
34	FM	0.26	0/2489	0.46	0/3365
34	FN	0.24	0/2430	0.43	0/3285
35	FO	0.26	0/2733	0.44	0/3692
36	FP	0.26	0/2710	0.45	0/3709
37	FQ	0.26	0/2048	0.45	0/2786
37	FR	0.25	0/1966	0.45	0/2673
37	FS	0.25	0/2249	0.46	0/3063
37	FT	0.25	0/1897	0.45	0/2580
37	FU	0.25	0/2154	0.45	0/2933
38	FW	0.24	0/2077	0.43	0/2805
39	FX	0.25	0/1783	0.41	0/2410
40	FY	0.27	0/1321	0.45	0/1788
41	FZ	0.23	0/989	0.49	3/1336 (0.2%)
42	Fa	0.26	0/1363	0.43	0/1853
43	Fb	0.24	0/1123	0.40	0/1513
44	Fc	0.24	0/679	0.41	0/923
45	Fd	0.25	0/779	0.43	0/1054
60	CA	0.30	0/12605	1.00	53/19567 (0.3%)
61	CC	0.28	0/666	0.47	0/900
62	CI	0.24	0/3424	0.42	0/4626
63	CJ	0.25	0/5865	0.44	0/7974
64	CN	0.23	0/1323	0.41	0/1790
65	CS	0.26	0/731	0.43	0/987
66	Cg	0.26	0/4043	0.42	0/5489
67	Ci	0.24	0/1256	0.43	0/1695
68	Ck	0.24	0/5215	0.44	0/7050
69	DB	0.24	0/5830	0.44	0/7889
70	DC	0.25	0/8409	0.42	0/11399
71	DE	0.24	0/4756	0.44	3/6462 (0.0%)
72	DF	0.24	0/4056	0.44	0/5493
73	DG	0.24	0/4674	0.41	0/6333
74	DH	0.23	0/3935	0.42	0/5321
75	DJ	0.24	0/2591	0.42	0/3508
76	DK	0.24	0/1965	0.42	0/2652
77	DT	0.25	0/1982	0.43	0/2686
78	DV	0.26	0/1358	0.43	0/1836
79	DW	0.28	0/1182	0.49	0/1613
80	DX	0.24	0/993	0.43	0/1336
81	DY	0.25	0/1337	0.41	0/1814
82	F1	0.25	0/7334	0.45	0/9883
83	F4	0.24	0/4483	0.45	1/6061 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
84	FD	0.24	0/3216	0.42	0/4380
85	FF	0.25	0/3335	0.45	0/4498
86	FG	0.24	0/1386	0.45	0/1869
87	FH	0.25	0/2537	0.42	0/3442
88	FI	0.25	0/2834	0.43	0/3821
89	FK	0.25	0/1748	0.43	0/2378
90	FL	0.25	0/2613	0.45	0/3538
91	FV	0.26	0/1680	0.43	0/2281
92	Fe	0.25	0/1057	0.46	0/1421
All	All	0.26	0/237284	0.49	72/323837 (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
15	DD	0	1
24	F3	0	1
27	F7	0	1
28	F8	0	1
36	FP	0	1
38	FW	0	1
74	DH	0	1
79	DW	0	1
85	FF	0	1
92	Fe	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CA	146	U	N3-C2-O2	-9.25	115.72	122.20
60	CA	146	U	N1-C2-O2	9.16	129.21	122.80
60	CA	99	G	C4-N9-C1'	8.02	136.93	126.50
60	CA	146	U	C2-N1-C1'	7.67	126.91	117.70
60	CA	302	U	C2-N1-C1'	7.62	126.84	117.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	DD	414	ARG	Peptide
24	F3	490	GLN	Peptide
27	F7	381	LEU	Peptide
28	F8	644	ASP	Peptide
36	FP	84	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	390/435 (90%)	375 (96%)	13 (3%)	2 (0%)	29	61
2	CF	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	CH	216/282 (77%)	211 (98%)	5 (2%)	0	100	100
4	CK	205/326 (63%)	190 (93%)	15 (7%)	0	100	100
5	CO	354/429 (82%)	345 (98%)	9 (2%)	0	100	100
6	CP	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
7	CQ	217/336 (65%)	209 (96%)	8 (4%)	0	100	100
8	CR	149/320 (47%)	141 (95%)	8 (5%)	0	100	100
9	Ca	508/602 (84%)	490 (96%)	18 (4%)	0	100	100
10	Cb	149/311 (48%)	145 (97%)	4 (3%)	0	100	100
11	Cd	183/440 (42%)	182 (100%)	1 (0%)	0	100	100
12	Cj	224/257 (87%)	219 (98%)	5 (2%)	0	100	100
13	Cn	25/250 (10%)	23 (92%)	2 (8%)	0	100	100
14	Cp	176/187 (94%)	171 (97%)	5 (3%)	0	100	100
15	DD	782/812 (96%)	756 (97%)	26 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	DI	388/407 (95%)	378 (97%)	10 (3%)	0	100	100
17	DL	199/307 (65%)	192 (96%)	7 (4%)	0	100	100
18	DO	202/282 (72%)	200 (99%)	2 (1%)	0	100	100
19	DP	210/274 (77%)	206 (98%)	4 (2%)	0	100	100
20	DR	250/270 (93%)	241 (96%)	9 (4%)	0	100	100
21	DU	217/228 (95%)	203 (94%)	14 (6%)	0	100	100
22	DZ	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
23	F2	909/1024 (89%)	886 (98%)	23 (2%)	0	100	100
24	F3	882/966 (91%)	857 (97%)	25 (3%)	0	100	100
25	F5	474/754 (63%)	461 (97%)	12 (2%)	1 (0%)	47	77
26	F6	450/676 (67%)	436 (97%)	14 (3%)	0	100	100
27	F7	658/679 (97%)	615 (94%)	41 (6%)	2 (0%)	41	71
28	F8	493/726 (68%)	475 (96%)	18 (4%)	0	100	100
29	F9	214/608 (35%)	213 (100%)	1 (0%)	0	100	100
30	FA	573/642 (89%)	553 (96%)	20 (4%)	0	100	100
31	FB	373/579 (64%)	363 (97%)	10 (3%)	0	100	100
31	FC	305/579 (53%)	294 (96%)	11 (4%)	0	100	100
32	FE	432/553 (78%)	416 (96%)	16 (4%)	0	100	100
33	FJ	351/362 (97%)	333 (95%)	18 (5%)	0	100	100
34	FM	324/370 (88%)	320 (99%)	4 (1%)	0	100	100
34	FN	317/370 (86%)	311 (98%)	6 (2%)	0	100	100
35	FO	320/334 (96%)	306 (96%)	14 (4%)	0	100	100
36	FP	346/349 (99%)	332 (96%)	13 (4%)	1 (0%)	41	71
37	FQ	255/307 (83%)	250 (98%)	5 (2%)	0	100	100
37	FR	239/307 (78%)	234 (98%)	5 (2%)	0	100	100
37	FS	271/307 (88%)	261 (96%)	10 (4%)	0	100	100
37	FT	229/307 (75%)	224 (98%)	5 (2%)	0	100	100
37	FU	266/307 (87%)	258 (97%)	8 (3%)	0	100	100
38	FW	243/263 (92%)	237 (98%)	6 (2%)	0	100	100
39	FX	218/239 (91%)	211 (97%)	7 (3%)	0	100	100
40	FY	156/188 (83%)	145 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	FZ	129/178 (72%)	125 (97%)	4 (3%)	0	100	100
42	Fa	161/171 (94%)	158 (98%)	3 (2%)	0	100	100
43	Fb	127/151 (84%)	124 (98%)	3 (2%)	0	100	100
44	Fc	82/148 (55%)	82 (100%)	0	0	100	100
45	Fd	94/143 (66%)	93 (99%)	1 (1%)	0	100	100
61	CC	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
62	CI	421/443 (95%)	409 (97%)	12 (3%)	0	100	100
63	CJ	695/817 (85%)	659 (95%)	33 (5%)	3 (0%)	34	66
64	CN	151/166 (91%)	149 (99%)	2 (1%)	0	100	100
65	CS	79/244 (32%)	77 (98%)	2 (2%)	0	100	100
66	Cg	482/498 (97%)	461 (96%)	21 (4%)	0	100	100
67	Ci	145/181 (80%)	143 (99%)	2 (1%)	0	100	100
68	Ck	634/874 (72%)	606 (96%)	28 (4%)	0	100	100
69	DB	671/1181 (57%)	651 (97%)	20 (3%)	0	100	100
70	DC	1020/1165 (88%)	997 (98%)	23 (2%)	0	100	100
71	DE	582/747 (78%)	566 (97%)	14 (2%)	2 (0%)	41	71
72	DF	485/666 (73%)	466 (96%)	19 (4%)	0	100	100
73	DG	558/631 (88%)	546 (98%)	12 (2%)	0	100	100
74	DH	466/581 (80%)	447 (96%)	19 (4%)	0	100	100
75	DJ	304/396 (77%)	298 (98%)	6 (2%)	0	100	100
76	DK	239/324 (74%)	229 (96%)	10 (4%)	0	100	100
77	DT	219/247 (89%)	211 (96%)	8 (4%)	0	100	100
78	DV	153/183 (84%)	147 (96%)	6 (4%)	0	100	100
79	DW	131/179 (73%)	120 (92%)	11 (8%)	0	100	100
80	DX	113/169 (67%)	106 (94%)	7 (6%)	0	100	100
81	DY	152/163 (93%)	149 (98%)	3 (2%)	0	100	100
82	F1	881/1041 (85%)	849 (96%)	32 (4%)	0	100	100
83	F4	521/811 (64%)	497 (95%)	24 (5%)	0	100	100
84	FD	392/579 (68%)	384 (98%)	8 (2%)	0	100	100
85	FF	404/474 (85%)	388 (96%)	15 (4%)	1 (0%)	47	77
86	FG	167/463 (36%)	162 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	FH	313/457 (68%)	303 (97%)	10 (3%)	0	100	100
88	FI	342/445 (77%)	333 (97%)	9 (3%)	0	100	100
89	FK	202/372 (54%)	202 (100%)	0	0	100	100
90	FL	314/353 (89%)	299 (95%)	15 (5%)	0	100	100
91	FV	206/264 (78%)	198 (96%)	8 (4%)	0	100	100
92	Fe	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
All	All	26932/35095 (77%)	26033 (97%)	887 (3%)	12 (0%)	100	100

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CE	385	PRO
36	FP	85	LYS
63	CJ	592	SER
71	DE	521	PRO
1	CE	384	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CE	325/372 (87%)	316 (97%)	9 (3%)	43	70
2	CF	143/144 (99%)	142 (99%)	1 (1%)	84	90
3	CH	195/246 (79%)	189 (97%)	6 (3%)	40	67
4	CK	184/284 (65%)	177 (96%)	7 (4%)	33	62
5	CO	314/377 (83%)	307 (98%)	7 (2%)	52	74
6	CP	160/168 (95%)	157 (98%)	3 (2%)	57	77
7	CQ	194/297 (65%)	188 (97%)	6 (3%)	40	67
8	CR	130/279 (47%)	123 (95%)	7 (5%)	22	53
9	Ca	449/543 (83%)	438 (98%)	11 (2%)	49	73
10	Cb	132/267 (49%)	124 (94%)	8 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Cd	168/381 (44%)	167 (99%)	1 (1%)	86	91
12	Cj	193/219 (88%)	189 (98%)	4 (2%)	53	75
13	Cn	22/210 (10%)	21 (96%)	1 (4%)	27	58
14	Cp	166/175 (95%)	161 (97%)	5 (3%)	41	68
15	DD	691/711 (97%)	683 (99%)	8 (1%)	71	83
16	DI	350/365 (96%)	343 (98%)	7 (2%)	55	76
17	DL	173/263 (66%)	171 (99%)	2 (1%)	71	83
18	DO	170/229 (74%)	168 (99%)	2 (1%)	71	83
19	DP	191/239 (80%)	187 (98%)	4 (2%)	53	75
20	DR	221/235 (94%)	213 (96%)	8 (4%)	35	63
21	DU	179/201 (89%)	175 (98%)	4 (2%)	52	74
22	DZ	25/84 (30%)	23 (92%)	2 (8%)	12	37
23	F2	763/867 (88%)	740 (97%)	23 (3%)	41	68
24	F3	748/809 (92%)	722 (96%)	26 (4%)	36	64
25	F5	293/642 (46%)	279 (95%)	14 (5%)	25	56
26	F6	401/590 (68%)	391 (98%)	10 (2%)	47	72
27	F7	554/577 (96%)	537 (97%)	17 (3%)	40	67
28	F8	410/561 (73%)	400 (98%)	10 (2%)	49	73
29	F9	175/504 (35%)	172 (98%)	3 (2%)	60	78
30	FA	477/526 (91%)	453 (95%)	24 (5%)	24	55
31	FB	322/483 (67%)	311 (97%)	11 (3%)	37	65
31	FC	272/483 (56%)	261 (96%)	11 (4%)	31	61
32	FE	386/486 (79%)	380 (98%)	6 (2%)	62	79
33	FJ	314/323 (97%)	305 (97%)	9 (3%)	42	69
34	FM	257/292 (88%)	249 (97%)	8 (3%)	40	67
34	FN	251/292 (86%)	243 (97%)	8 (3%)	39	67
35	FO	281/290 (97%)	273 (97%)	8 (3%)	43	70
36	FP	270/286 (94%)	266 (98%)	4 (2%)	65	81
37	FQ	211/264 (80%)	206 (98%)	5 (2%)	49	73
37	FR	206/264 (78%)	202 (98%)	4 (2%)	57	77
37	FS	238/264 (90%)	227 (95%)	11 (5%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	FT	200/264 (76%)	191 (96%)	9 (4%)	27	58
37	FU	222/264 (84%)	212 (96%)	10 (4%)	27	58
38	FW	223/234 (95%)	222 (100%)	1 (0%)	91	95
39	FX	178/195 (91%)	178 (100%)	0	100	100
40	FY	141/163 (86%)	136 (96%)	5 (4%)	36	64
41	FZ	86/156 (55%)	86 (100%)	0	100	100
42	Fa	141/149 (95%)	137 (97%)	4 (3%)	43	70
43	Fb	117/135 (87%)	113 (97%)	4 (3%)	37	65
44	Fc	78/127 (61%)	73 (94%)	5 (6%)	17	46
45	Fd	79/119 (66%)	76 (96%)	3 (4%)	33	62
61	CC	73/73 (100%)	71 (97%)	2 (3%)	44	71
62	CI	355/371 (96%)	350 (99%)	5 (1%)	67	82
63	CJ	619/723 (86%)	602 (97%)	17 (3%)	44	71
64	CN	138/150 (92%)	127 (92%)	11 (8%)	12	37
65	CS	76/220 (34%)	74 (97%)	2 (3%)	46	71
66	Cg	426/437 (98%)	415 (97%)	11 (3%)	46	71
67	Ci	130/160 (81%)	128 (98%)	2 (2%)	65	81
68	Ck	557/747 (75%)	532 (96%)	25 (4%)	27	58
69	DB	613/1030 (60%)	591 (96%)	22 (4%)	35	63
70	DC	867/985 (88%)	843 (97%)	24 (3%)	43	70
71	DE	464/644 (72%)	448 (97%)	16 (3%)	37	65
72	DF	417/560 (74%)	405 (97%)	12 (3%)	42	69
73	DG	490/543 (90%)	474 (97%)	16 (3%)	38	66
74	DH	413/504 (82%)	403 (98%)	10 (2%)	49	73
75	DJ	267/347 (77%)	263 (98%)	4 (2%)	65	81
76	DK	203/261 (78%)	195 (96%)	8 (4%)	32	62
77	DT	205/228 (90%)	200 (98%)	5 (2%)	49	73
78	DV	142/165 (86%)	136 (96%)	6 (4%)	30	60
79	DW	124/163 (76%)	115 (93%)	9 (7%)	14	41
80	DX	102/149 (68%)	102 (100%)	0	100	100
81	DY	137/146 (94%)	134 (98%)	3 (2%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	F1	764/895 (85%)	731 (96%)	33 (4%)	29	59
83	F4	479/703 (68%)	463 (97%)	16 (3%)	38	66
84	FD	338/494 (68%)	333 (98%)	5 (2%)	65	81
85	FF	348/400 (87%)	337 (97%)	11 (3%)	39	67
86	FG	147/414 (36%)	145 (99%)	2 (1%)	67	82
87	FH	270/390 (69%)	260 (96%)	10 (4%)	34	63
88	FI	297/380 (78%)	288 (97%)	9 (3%)	41	68
89	FK	181/308 (59%)	174 (96%)	7 (4%)	32	62
90	FL	279/309 (90%)	271 (97%)	8 (3%)	42	69
91	FV	184/231 (80%)	174 (95%)	10 (5%)	22	53
92	Fe	114/115 (99%)	105 (92%)	9 (8%)	12	37
All	All	23288/30143 (77%)	22592 (97%)	696 (3%)	44	68

5 of 696 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	DC	58	VAL
81	DY	19	THR
70	DC	695	VAL
69	DB	1142	VAL
73	DG	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

Mol	Chain	Res	Type
77	DT	219	GLN
91	FV	147	GLN
80	DX	58	HIS
84	FD	374	HIS
31	FB	329	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
60	CA	605/620 (97%)	240 (39%)	7 (1%)

5 of 240 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
60	CA	3	A
60	CA	4	A
60	CA	5	U
60	CA	6	U
60	CA	7	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
60	CA	285	A
60	CA	296	U
60	CA	483	A
60	CA	349	U
60	CA	173	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
60	UBD	CA	620	-	23,25,26	0.63	0	31,37,40	0.62	1 (3%)

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
60	UBD	CA	620	-	-	2/12/30/31	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CA	620	UBD	O4P-P2-O5P	2.35	119.86	110.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	CA	620	UBD	O4'-C4'-C5'-O5'
60	CA	620	UBD	C3'-O3'-P2-O4P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 11 are monoatomic - leaving 5 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
106	PM8	Fc	201	44	25,31,31	0.76	1 (4%)	30,38,38	0.91	1 (3%)
109	SAH	FF	501	-	24,28,28	1.20	3 (12%)	25,40,40	1.78	5 (20%)
108	GTP	Cg	501	104	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
105	PO4	FW	301	-	4,4,4	0.99	0	6,6,6	0.45	0
109	SAH	F1	1102	-	24,28,28	1.21	3 (12%)	25,40,40	1.73	5 (20%)

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
109	SAH	F1	1102	-	-	3/11/31/31	0/3/3/3
106	PM8	Fc	201	44	-	2/36/38/38	-
109	SAH	FF	501	-	-	1/11/31/31	0/3/3/3
108	GTP	Cg	501	104	-	5/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
108	Cg	501	GTP	C5-C6	-4.12	1.39	1.47
109	F1	1102	SAH	C2-N3	3.91	1.38	1.32
109	FF	501	SAH	C2-N3	3.91	1.38	1.32
106	Fc	201	PM8	C2-C1	2.58	1.53	1.50
109	F1	1102	SAH	C2-N1	2.43	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
109	F1	1102	SAH	N3-C2-N1	-5.48	120.11	128.68
109	FF	501	SAH	N3-C2-N1	-5.47	120.13	128.68
109	FF	501	SAH	C5'-SD-CG	-4.45	88.92	102.27
109	F1	1102	SAH	C5'-SD-CG	-3.99	90.28	102.27
108	Cg	501	GTP	PA-O3A-PB	-3.95	119.28	132.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

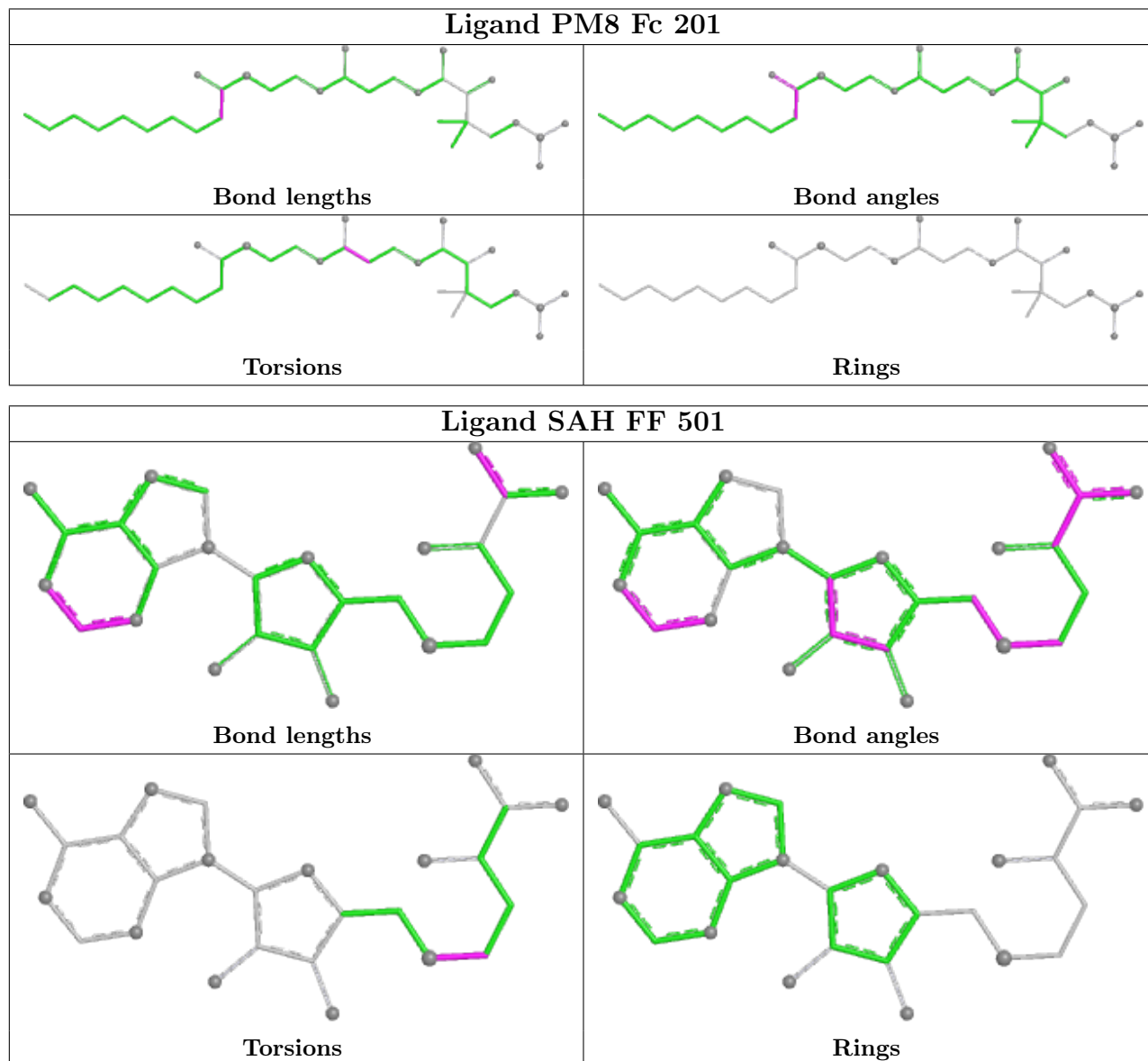
Mol	Chain	Res	Type	Atoms
108	Cg	501	GTP	C5'-O5'-PA-O3A
108	Cg	501	GTP	C5'-O5'-PA-O1A
108	Cg	501	GTP	C5'-O5'-PA-O2A
108	Cg	501	GTP	C3'-C4'-C5'-O5'
106	Fc	201	PM8	C37-C38-C39-O40

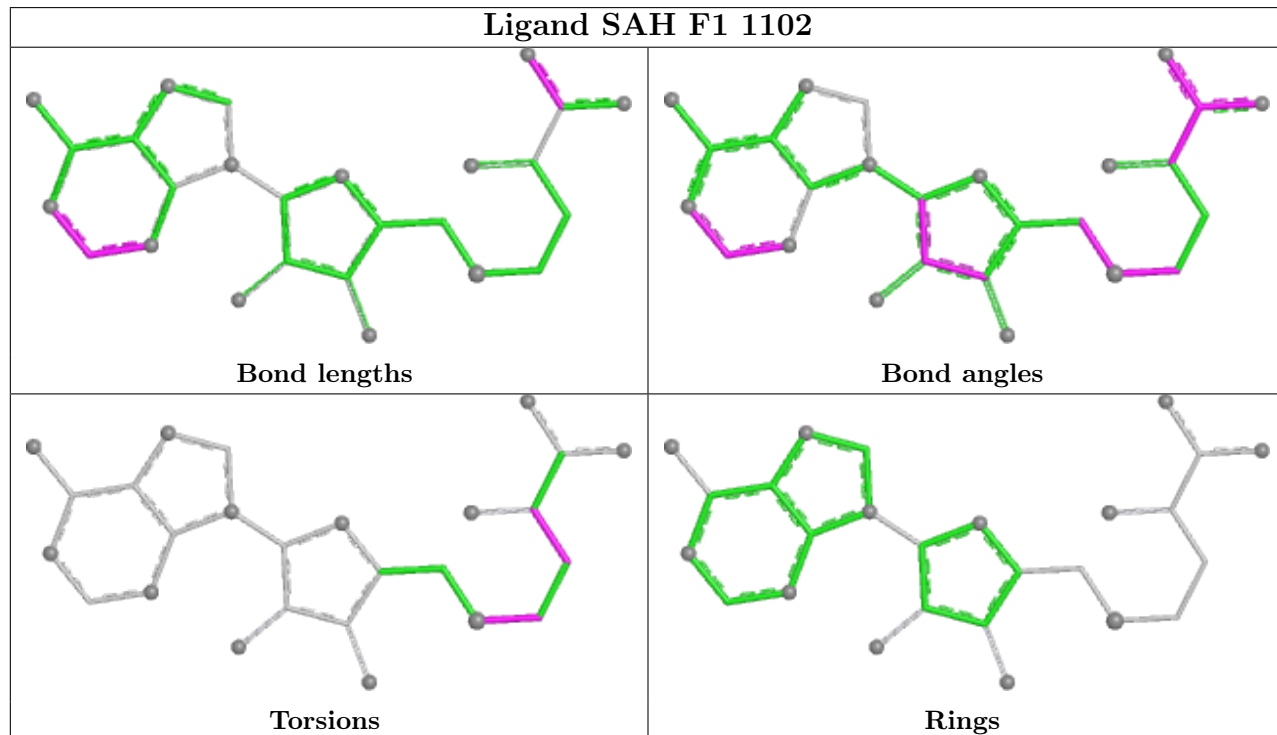
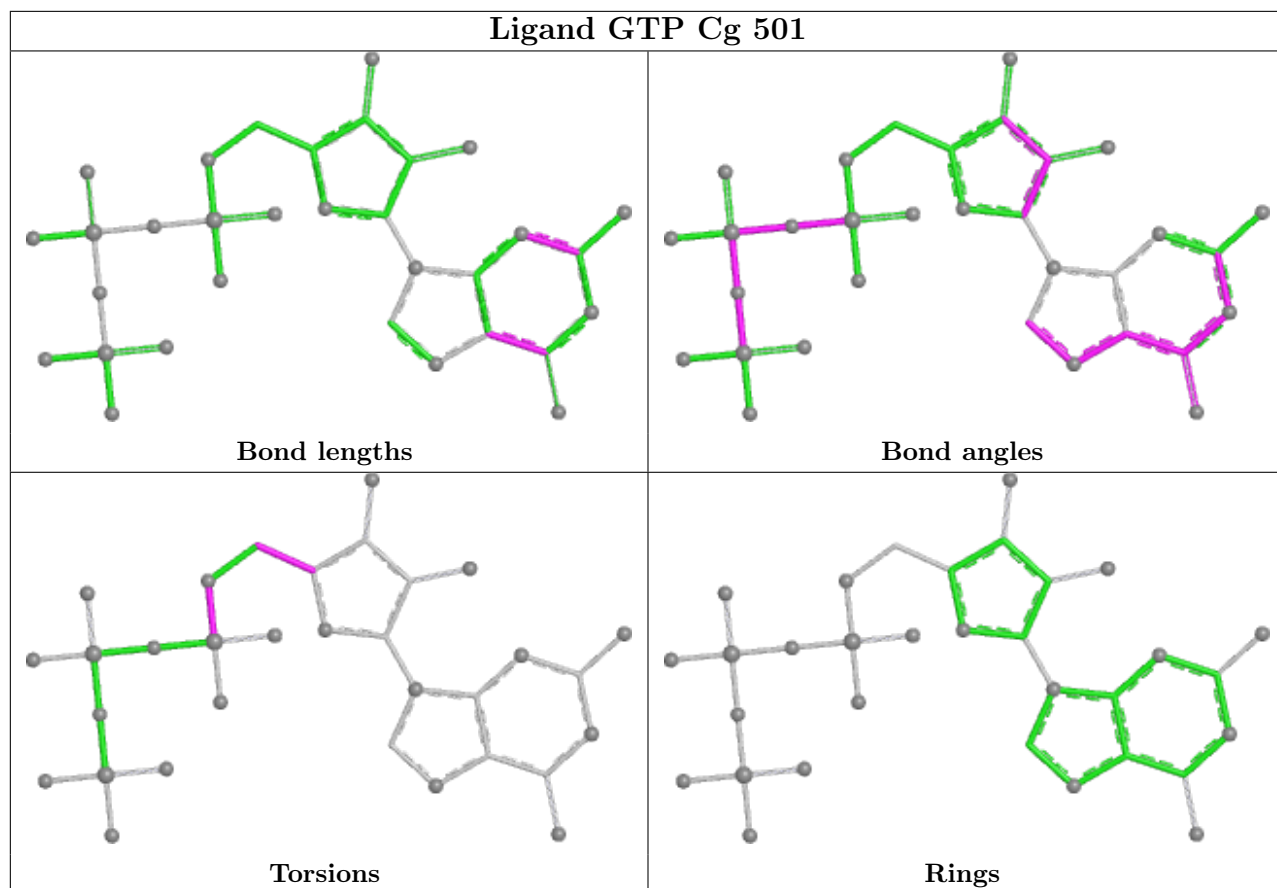
There are no ring outliers.

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
59	UY	13
99	Uh	11
98	Ug	10
103	Ux	3
47	UB	2
60	CA	1

The worst 5 of 40 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UY	347:UNK	C	348:UNK	N	76.88
1	UY	439:UNK	C	440:UNK	N	65.92
1	Uh	219:UNK	C	267:UNK	N	52.49
1	Uh	13:UNK	C	14:UNK	N	49.20
1	UB	10:UNK	C	101:UNK	N	45.40

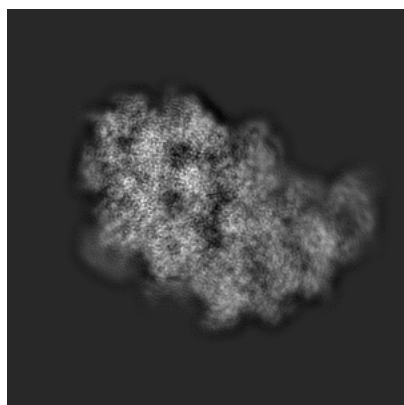
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10180. These allow visual inspection of the internal detail of the map and identification of artifacts.

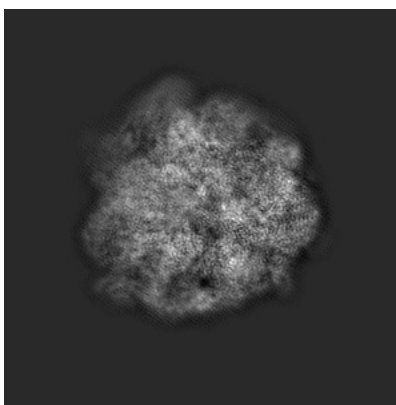
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

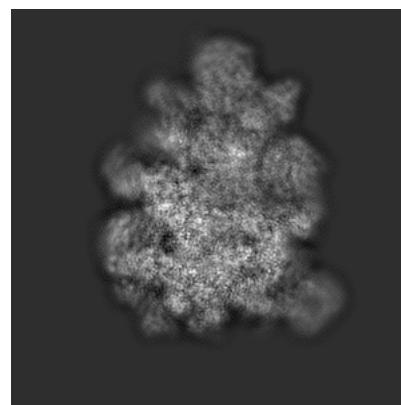
6.1.1 Primary map



X



Y

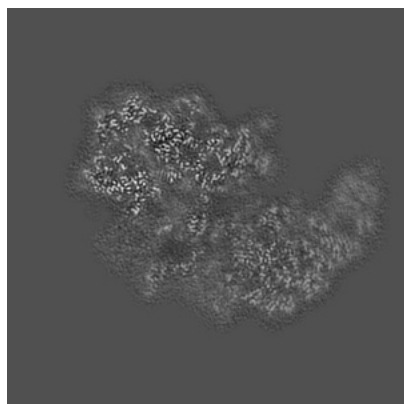


Z

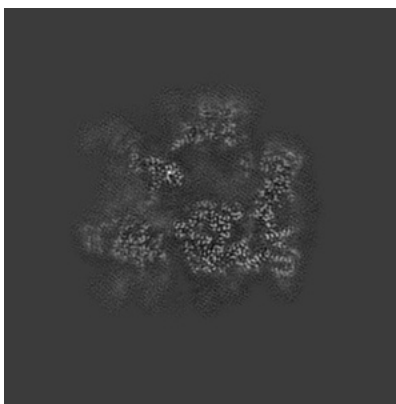
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

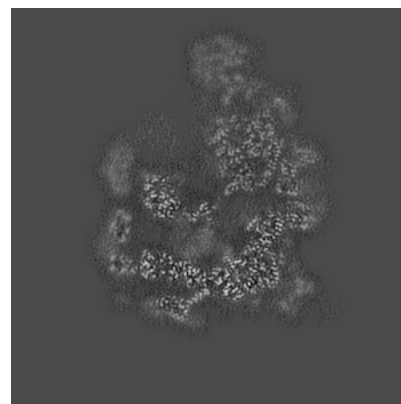
6.2.1 Primary map



X Index: 160



Y Index: 160

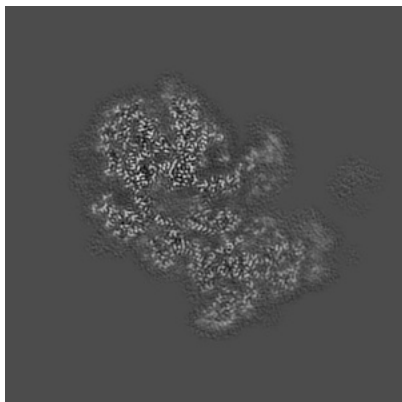


Z Index: 160

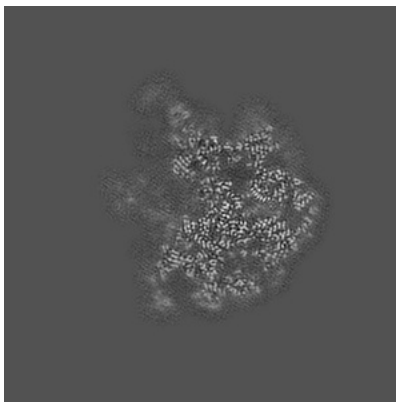
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

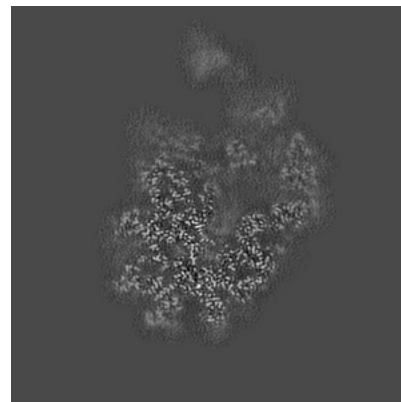
6.3.1 Primary map



X Index: 137



Y Index: 109

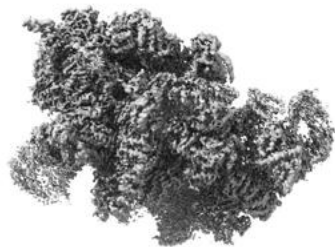


Z Index: 181

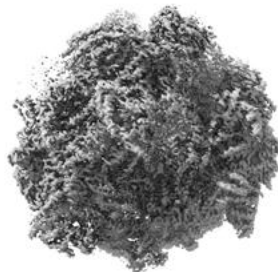
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

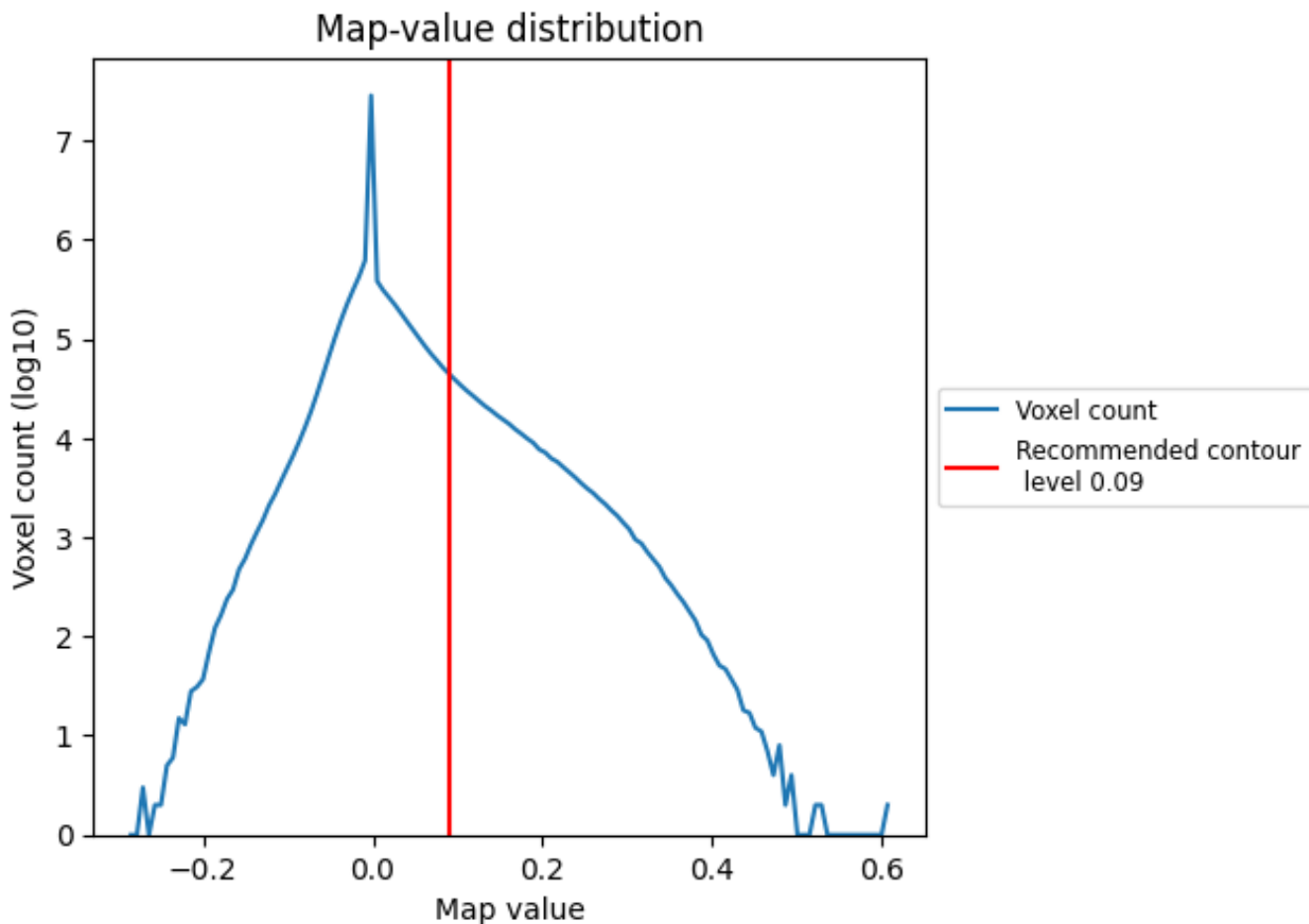
6.5 Mask visualisation

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

7 Map analysis [i](#)

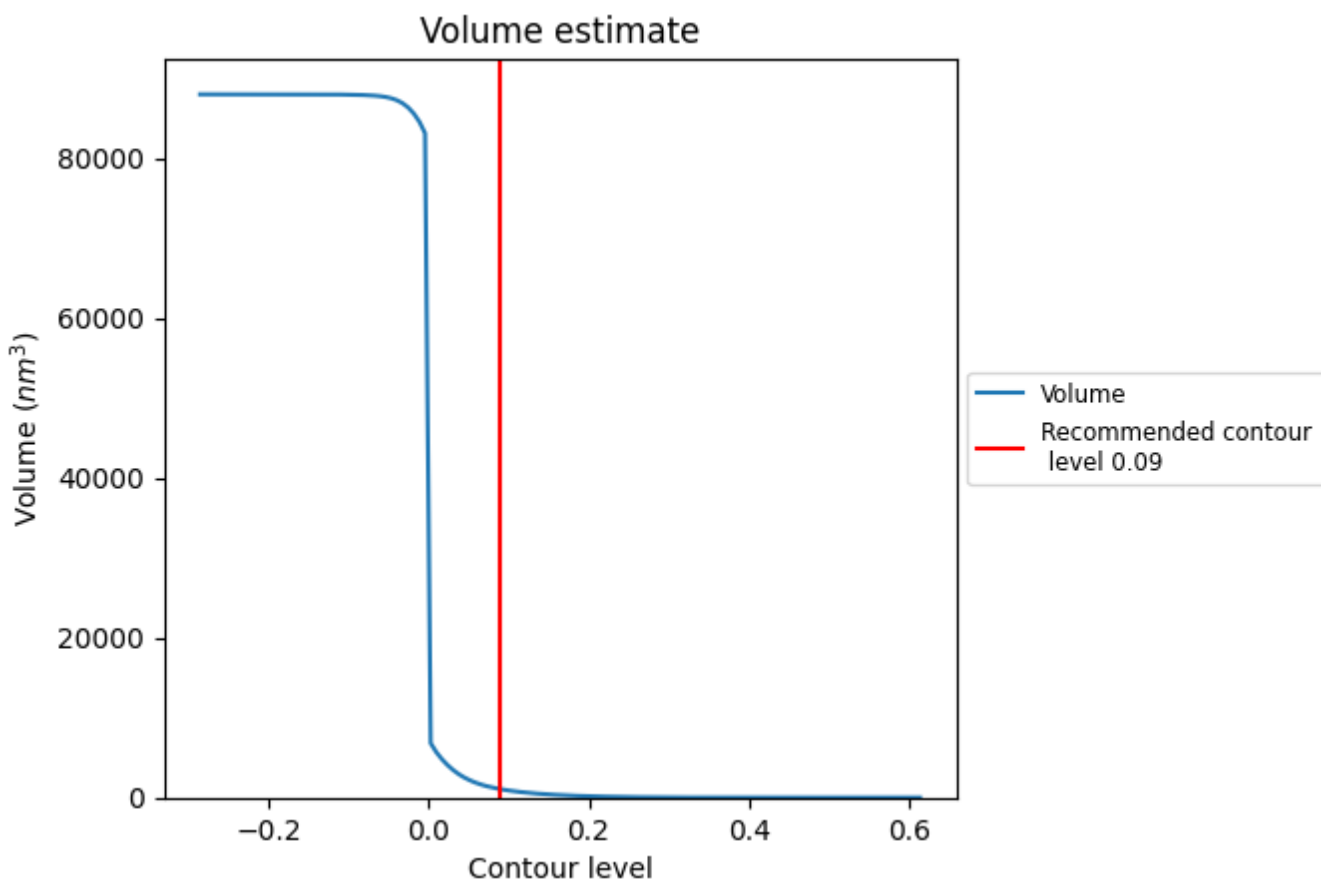
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

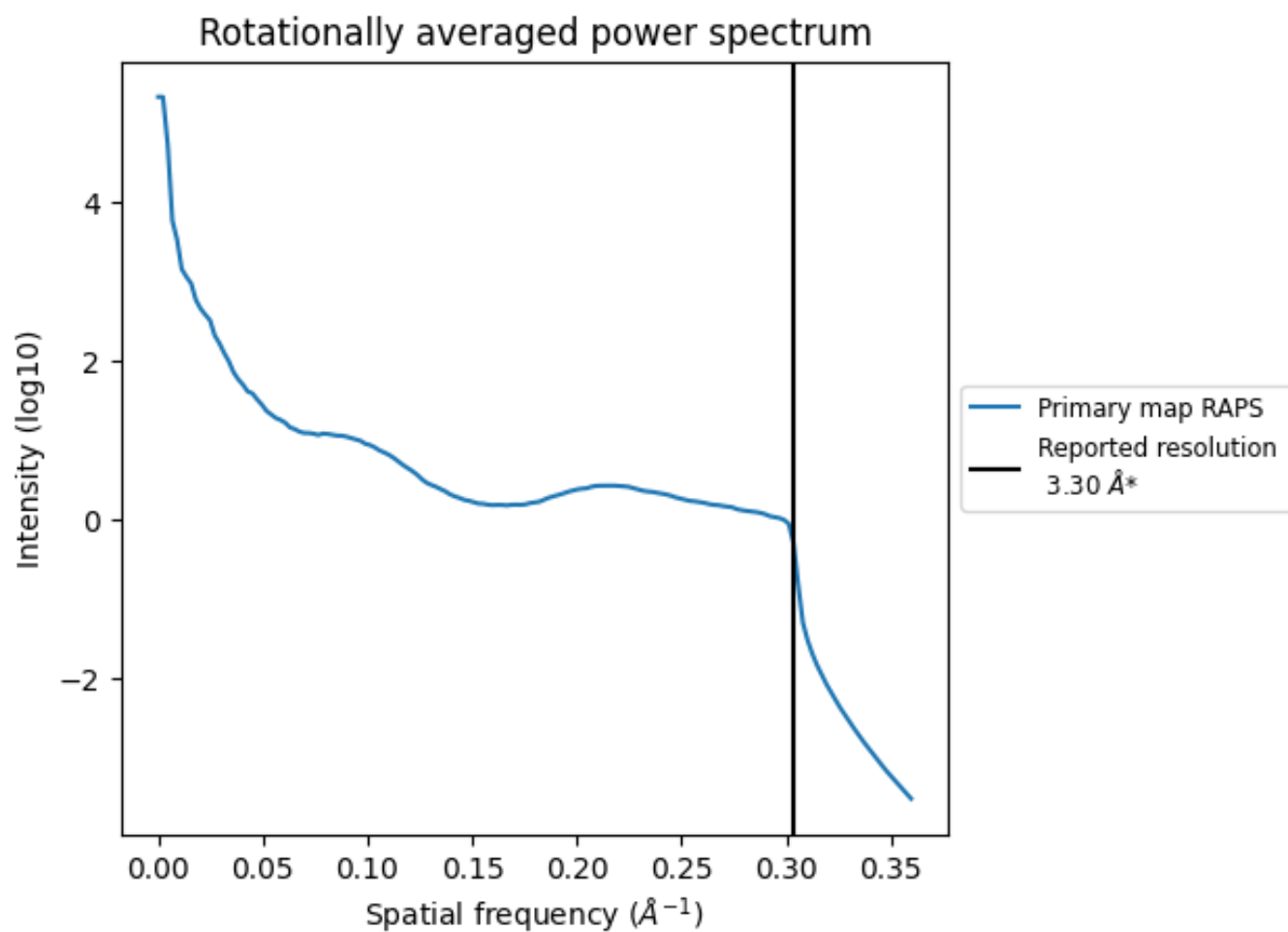
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 10511 nm^3 ; this corresponds to an approximate mass of 949 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

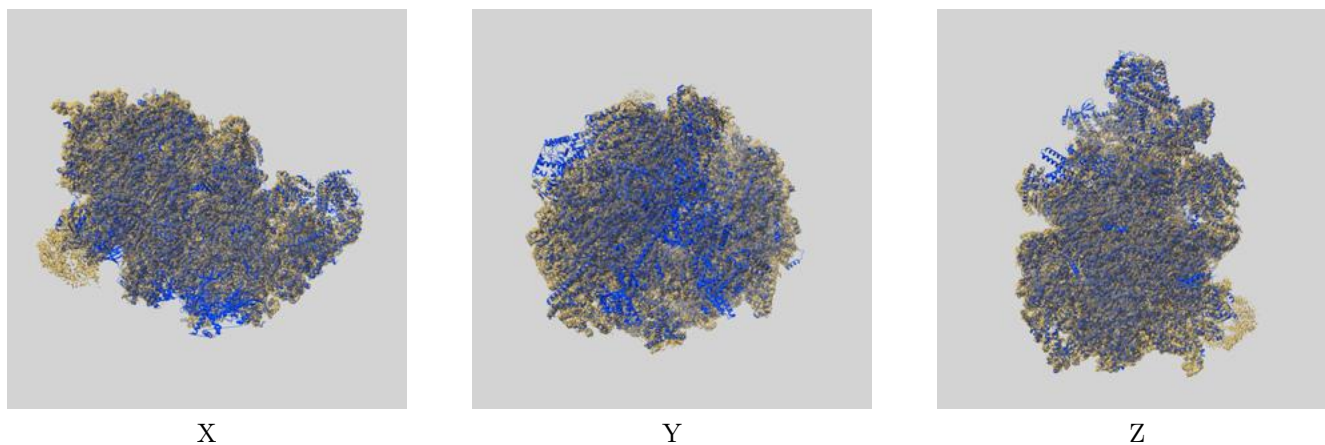
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

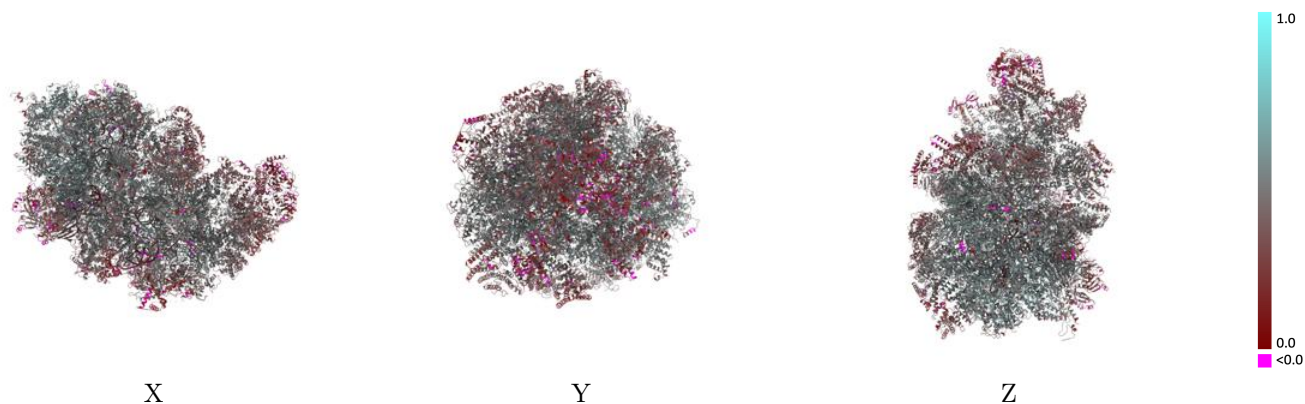
This section contains information regarding the fit between EMDB map EMD-10180 and PDB model 6SGB. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



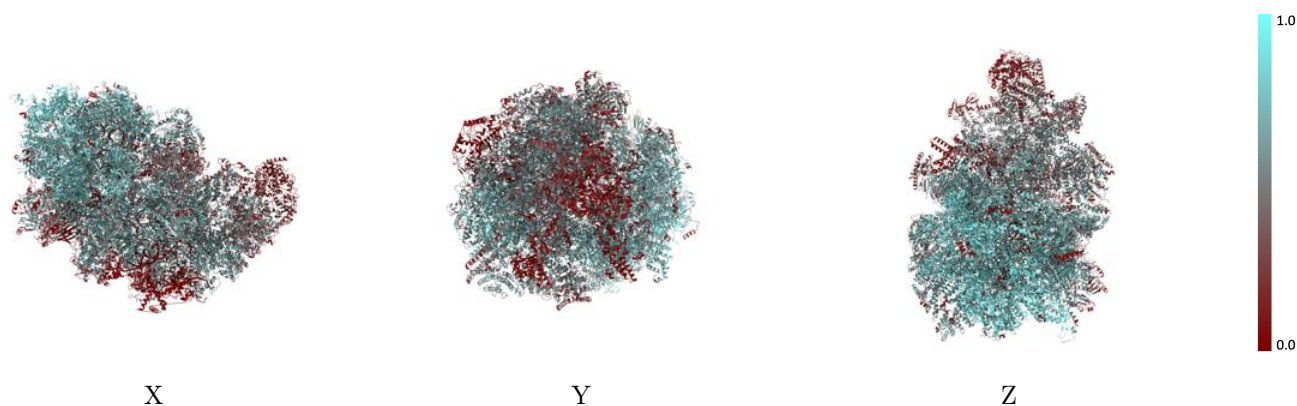
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



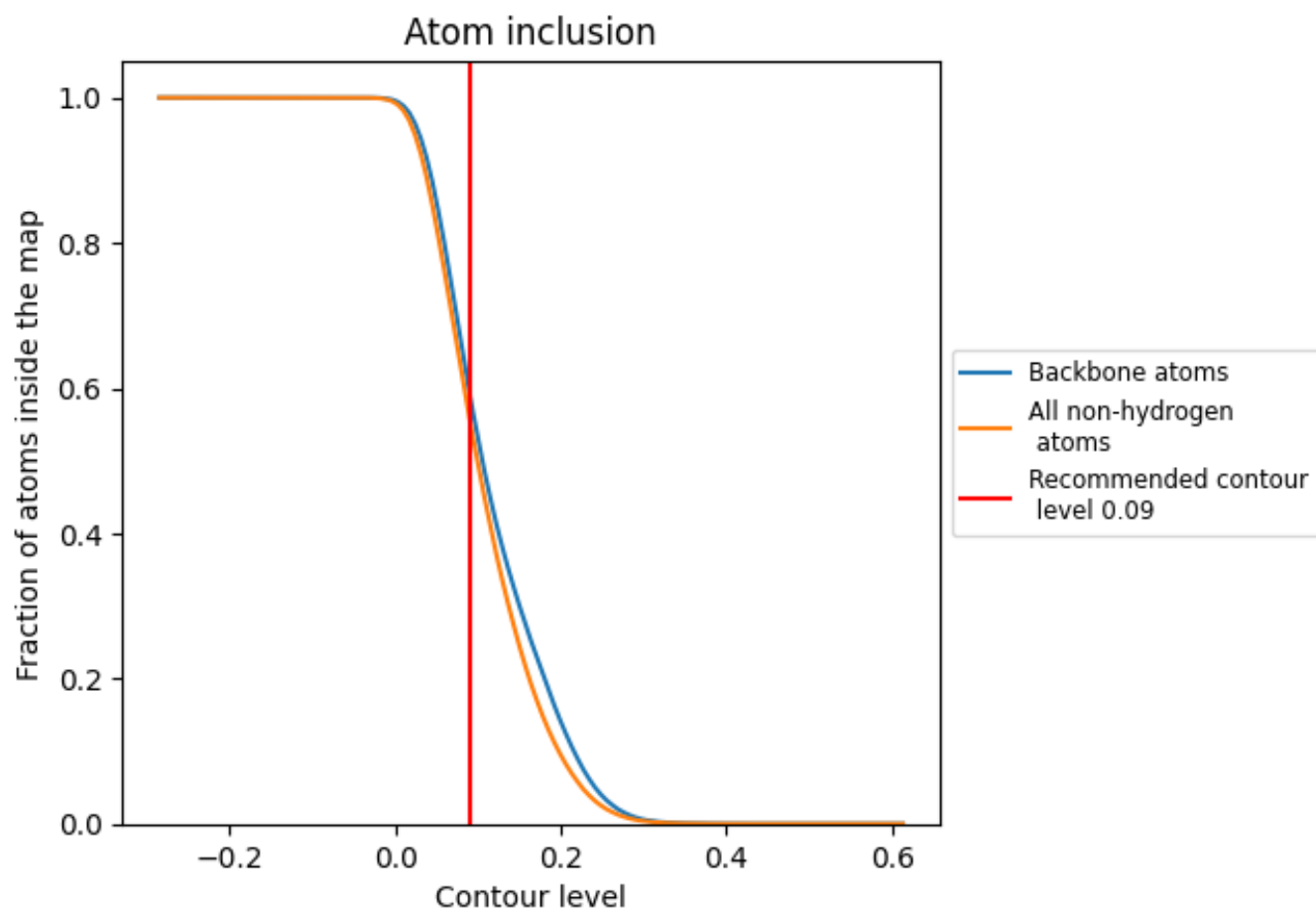
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 56% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5569	 0.4390
CA	 0.5675	 0.3950
CC	 0.4031	 0.4580
CE	 0.6658	 0.5010
CF	 0.7271	 0.5020
CH	 0.7425	 0.5320
CI	 0.6266	 0.4750
CJ	 0.5468	 0.4650
CK	 0.5812	 0.4280
CN	 0.2607	 0.4540
CO	 0.7469	 0.5240
CP	 0.7950	 0.5350
CQ	 0.7051	 0.5330
CR	 0.5780	 0.4330
CS	 0.0087	 0.3310
Ca	 0.6687	 0.4820
Cb	 0.5572	 0.4100
Cd	 0.7917	 0.5140
Cg	 0.6225	 0.4630
Ci	 0.5059	 0.4880
Cj	 0.8284	 0.5330
Ck	 0.4811	 0.3990
Cn	 0.3710	 0.4220
Cp	 0.7321	 0.5110
DB	 0.3632	 0.3750
DC	 0.3517	 0.3270
DD	 0.7861	 0.5270
DE	 0.2112	 0.2450
DF	 0.5016	 0.4460
DG	 0.5738	 0.4040
DH	 0.5161	 0.4690
DI	 0.7383	 0.4930
DJ	 0.5576	 0.4450
DK	 0.4151	 0.4110
DL	 0.6592	 0.5020



















































































Continued on next page...

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Chain	Atom inclusion	Q-score
DO	 0.6011	 0.4040
DP	 0.8118	 0.4880
DR	 0.8116	 0.5200
DT	 0.5783	 0.4970
DU	 0.6665	 0.4940
DV	 0.5121	 0.4570
DW	 0.5023	 0.4300
DX	 0.1749	 0.3900
DY	 0.4940	 0.4530
DZ	 0.5020	 0.4430
F1	 0.5612	 0.4700
F2	 0.7169	 0.4830
F3	 0.6659	 0.4390
F4	 0.4002	 0.3780
F5	 0.3746	 0.3270
F6	 0.5402	 0.3490
F7	 0.7253	 0.4830
F8	 0.6431	 0.4750
F9	 0.6176	 0.4850
FA	 0.4949	 0.4040
FB	 0.7008	 0.5080
FC	 0.6293	 0.4310
FD	 0.5056	 0.4300
FE	 0.6908	 0.5100
FF	 0.5668	 0.4750
FG	 0.6245	 0.4950
FH	 0.5387	 0.4560
FI	 0.5050	 0.4660
FJ	 0.5849	 0.4700
FK	 0.5561	 0.4710
FL	 0.6006	 0.5180
FM	 0.6810	 0.4770
FN	 0.5262	 0.3790
FO	 0.7813	 0.5300
FP	 0.7495	 0.4830
FQ	 0.6332	 0.4440
FR	 0.5861	 0.4360
FS	 0.5325	 0.4180
FT	 0.6007	 0.4180
FU	 0.5178	 0.3810
FV	 0.5876	 0.4660
FW	 0.7342	 0.5020

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Chain	Atom inclusion	Q-score
FX	 0.7801	 0.4820
FY	 0.4667	 0.3860
FZ	 0.1276	 0.3860
Fa	 0.6371	 0.5130
Fb	 0.5358	 0.3440
Fc	 0.5165	 0.3280
Fd	 0.7304	 0.4900
Fe	 0.4808	 0.4460
UA	 0.3175	 0.2380
UB	 0.2037	 0.3200
UC	 0.7333	 0.4270
UD	 0.8519	 0.5070
UE	 0.2926	 0.2610
UF	 0.5606	 0.4540
UG	 0.7255	 0.4700
UH	 0.4000	 0.4990
UI	 0.6250	 0.4210
UJ	 0.3542	 0.3170
UK	 0.2431	 0.3550
UL	 0.5227	 0.3640
UM	 0.5741	 0.4650
UN	 0.5208	 0.3820
UO	 0.4444	 0.2880
UP	 0.2889	 0.2850
UQ	 0.4444	 0.3130
UY	 0.0025	 0.2760
Ua	 0.4433	 0.4270
Ub	 0.2540	 0.4040
Uc	 0.2778	 0.4630
Ud	 0.2825	 0.3520
Ue	 0.2759	 0.3380
Uf	 0.4815	 0.5010
Ug	 0.3723	 0.2800
Uh	 0.0196	 0.2690
Ui	 0.2292	 0.2920
Uj	 0.2982	 0.3120
Uk	 0.4012	 0.4580
Ul	 0.1786	 0.2220
Um	 0.3939	 0.4370
Ux	 0.0108	 0.2830