Full wwPDB EM Validation 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)

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

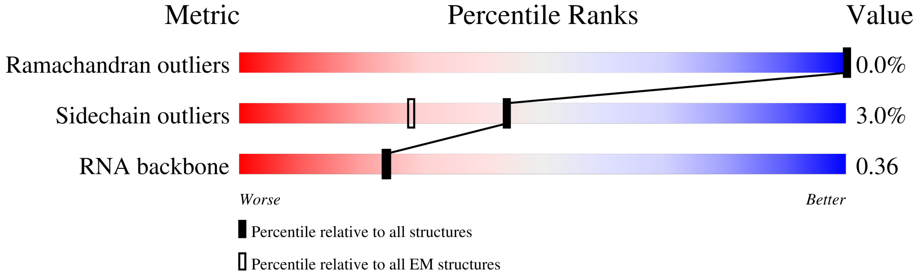
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

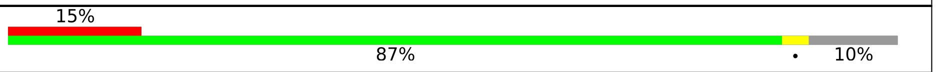
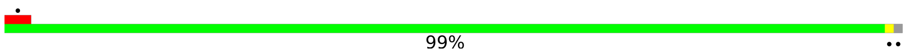
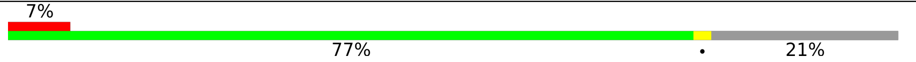
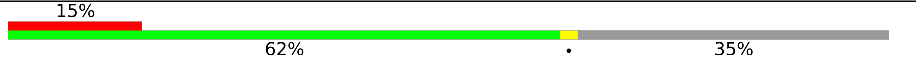
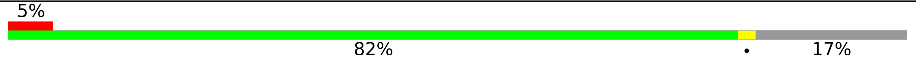
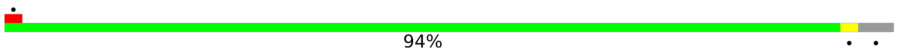
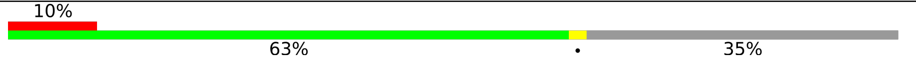
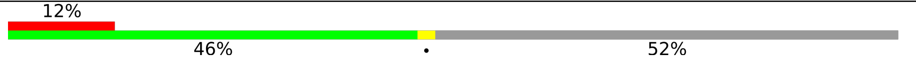
The reported resolution of this entry is 3.30 Å.

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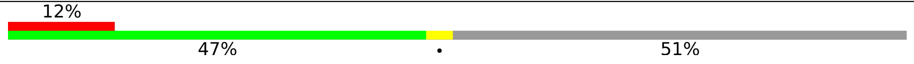
Mol	Chain	Length	Quality of chain
9	Ca	602	
10	Cb	311	
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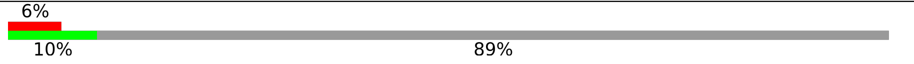
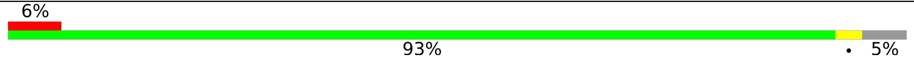
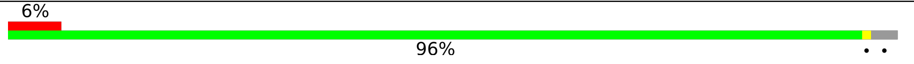
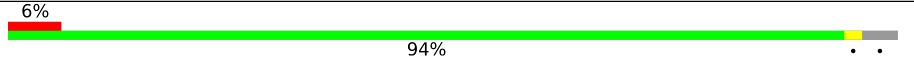
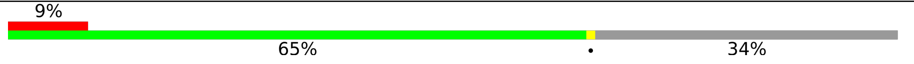
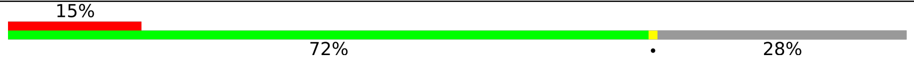
12	Cj	257	
13	Cn	250	
14	Cp	187	
15	DD	812	
16	DI	407	
17	DL	307	
18	DO	282	
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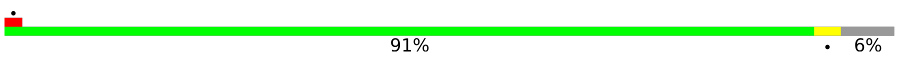
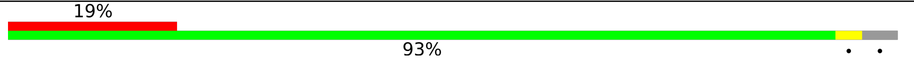
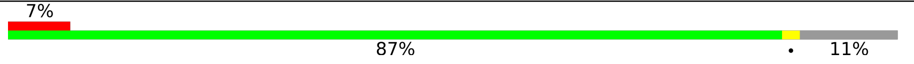
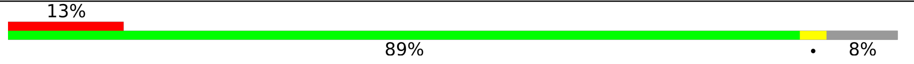
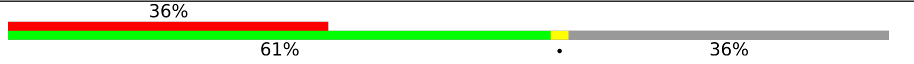
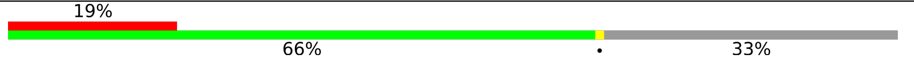
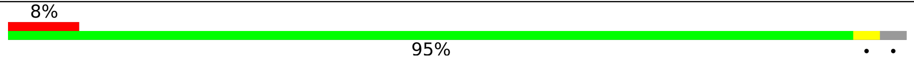
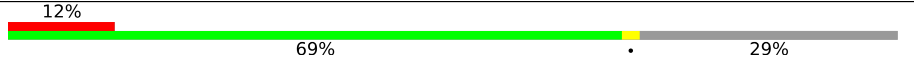
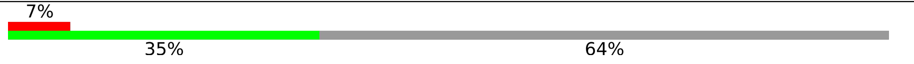
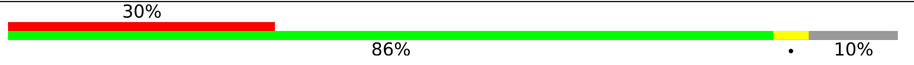
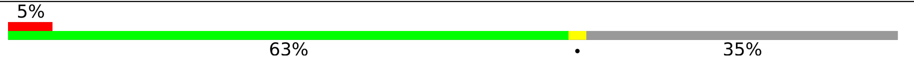
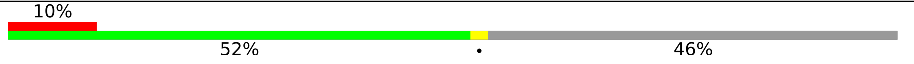
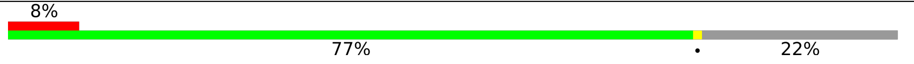
20	DR	270	
21	DU	228	
22	DZ	94	
23	F2	1024	
24	F3	966	
25	F5	754	
26	F6	676	
27	F7	679	
28	F8	726	
29	F9	608	
30	FA	642	
31	FB	579	
31	FC	579	
32	FE	553	

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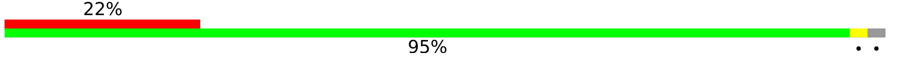
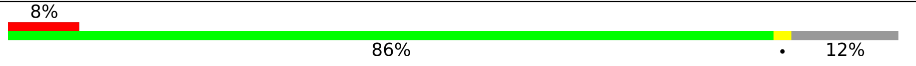
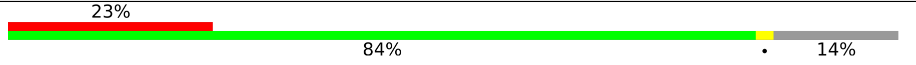
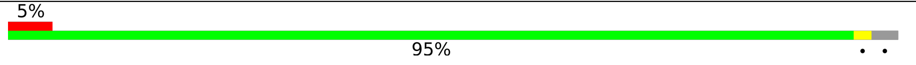
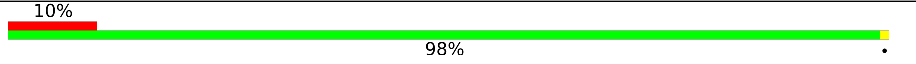
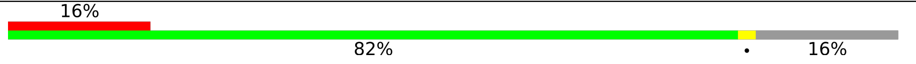
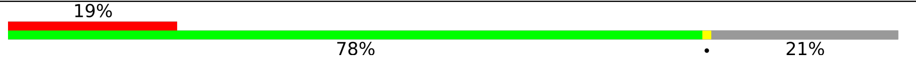
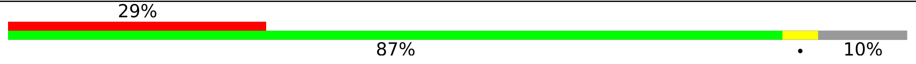
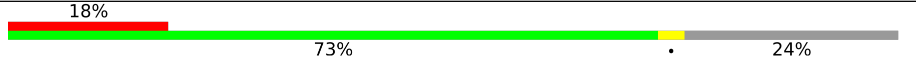
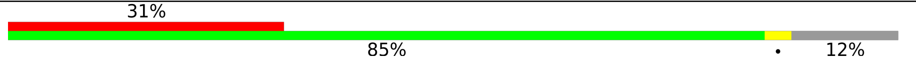
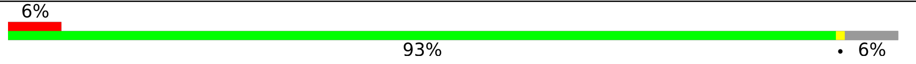
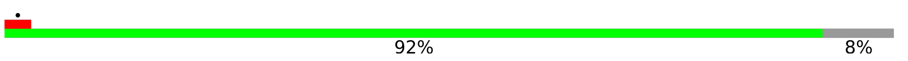
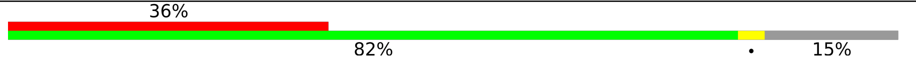
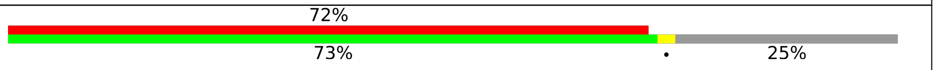
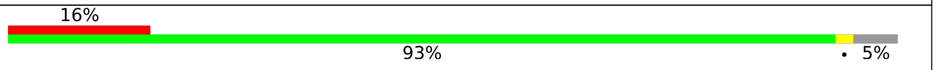
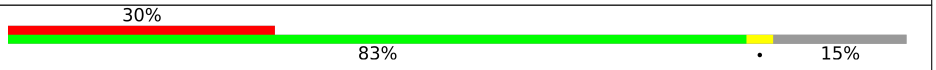
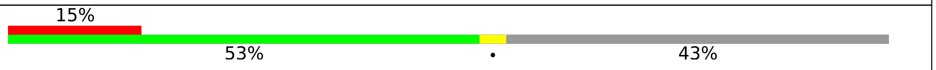
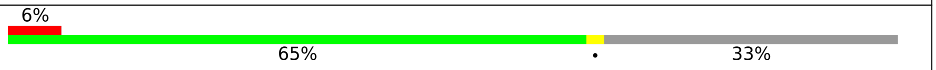
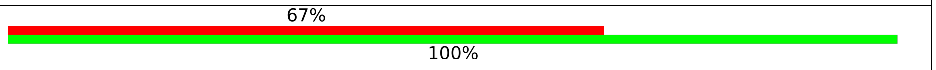
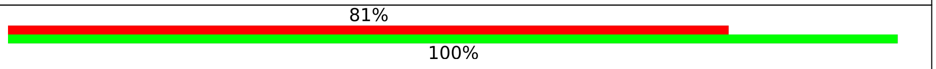
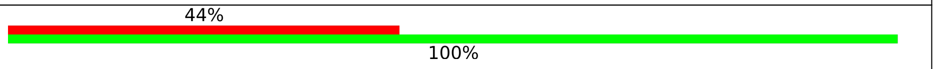
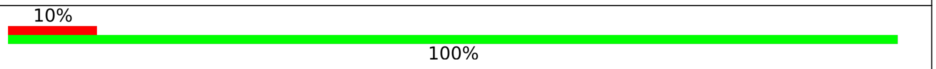
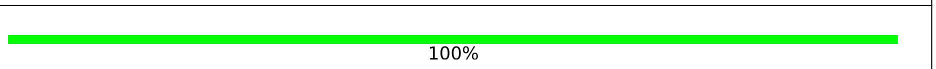
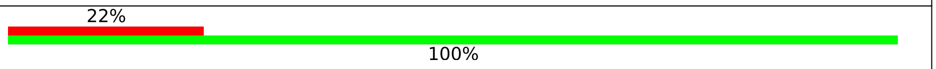
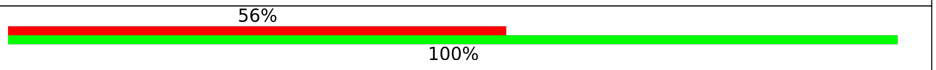
Mol	Chain	Length	Quality of chain
33	FJ	362	
34	FM	370	
34	FN	370	
35	FO	334	
36	FP	349	
37	FQ	307	
37	FR	307	
37	FS	307	
37	FT	307	
37	FU	307	
38	FW	263	
39	FX	239	
40	FY	188	
41	FZ	178	
42	Fa	171	
43	Fb	151	
44	Fc	148	
45	Fd	143	
46	UA	21	
47	UB	27	
47	Uk	27	
48	UC	10	
49	UD	9	
49	UM	9	
49	UQ	9	

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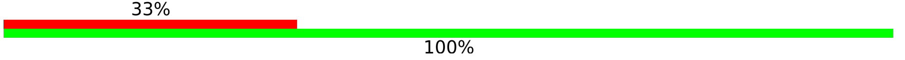
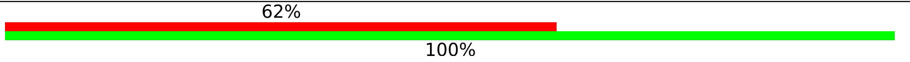
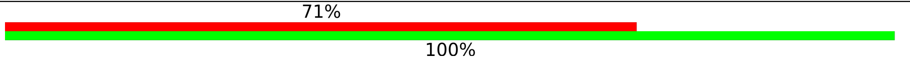
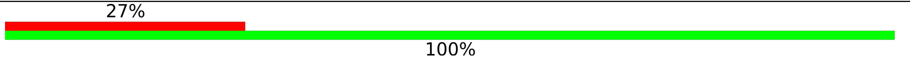
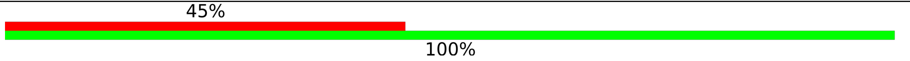
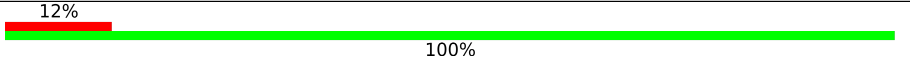
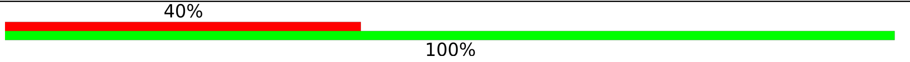
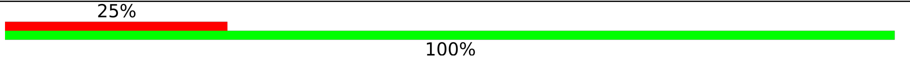
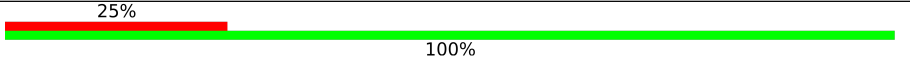
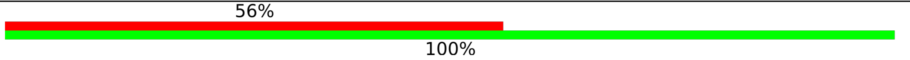
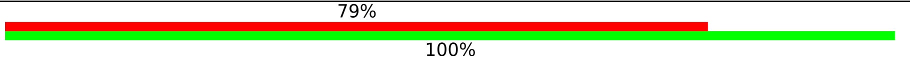
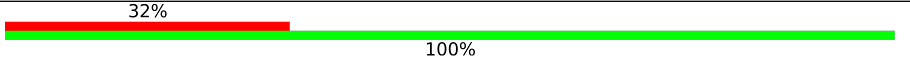
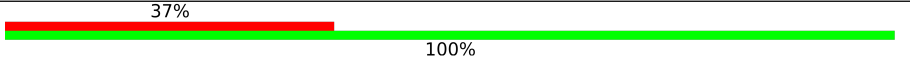
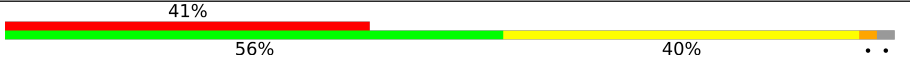
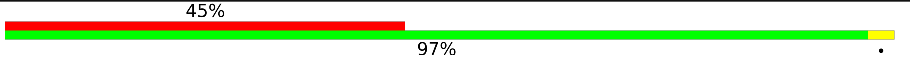
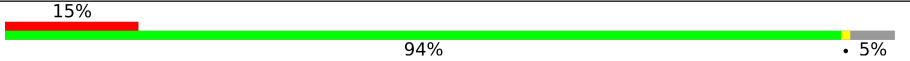
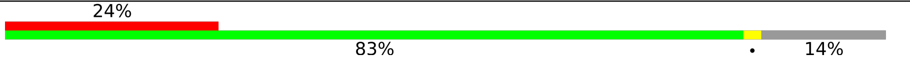
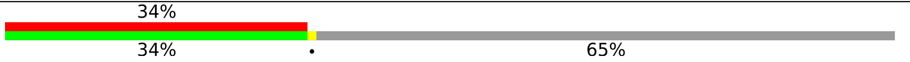
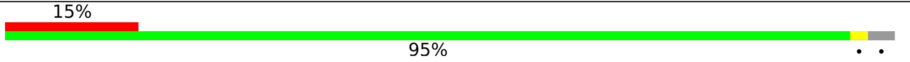
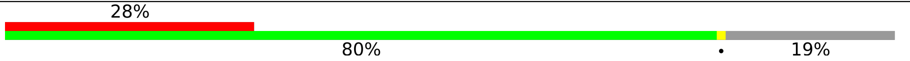
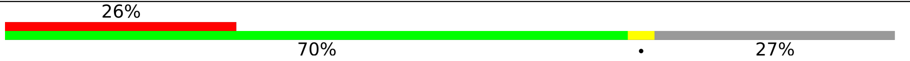
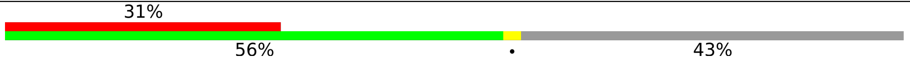
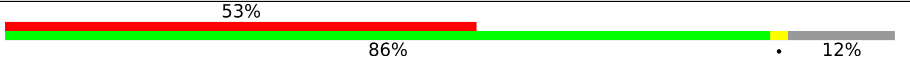
Mol	Chain	Length	Quality of chain
49	Uf	9	
50	UE	45	
50	UP	45	
51	UF	11	
51	Um	11	
52	UG	17	
53	UH	5	
54	UI	8	
54	UN	8	
55	UJ	16	
56	UK	24	
57	UL	22	
58	UO	30	
59	UY	468	
60	CA	620	
61	CC	74	
62	CI	443	
63	CJ	817	
64	CN	166	
65	CS	244	
66	Cg	498	
67	Ci	181	
68	Ck	874	
69	DB	1181	
70	DC	1165	

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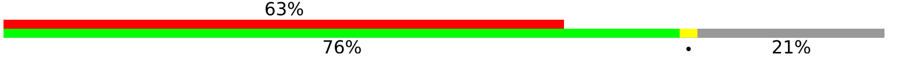
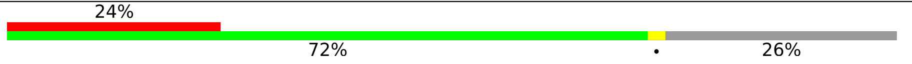
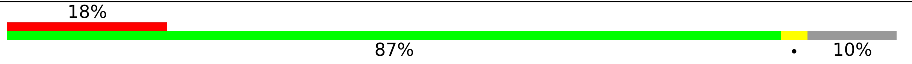
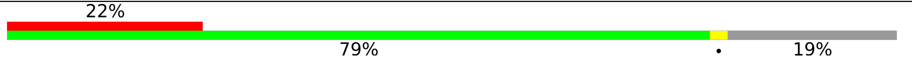
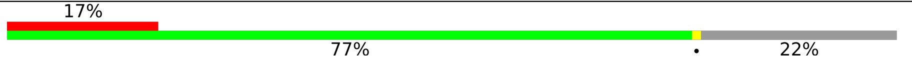
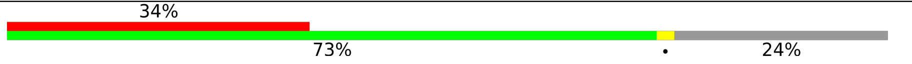
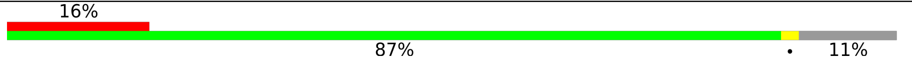
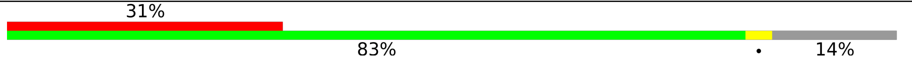
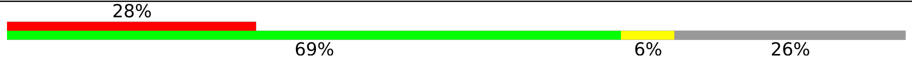
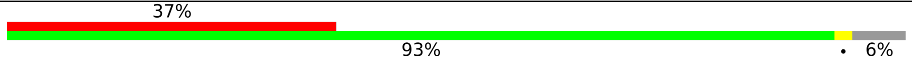
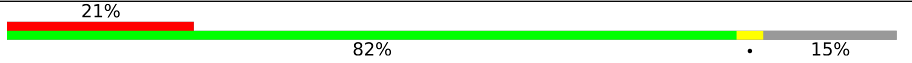
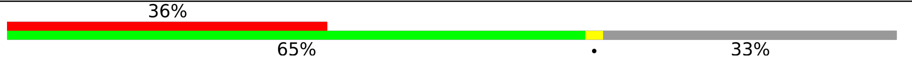
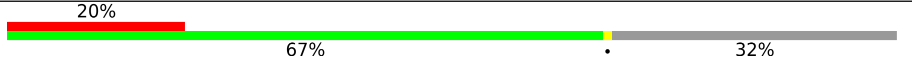
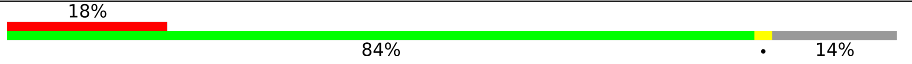
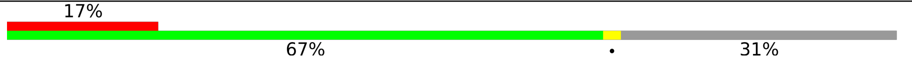
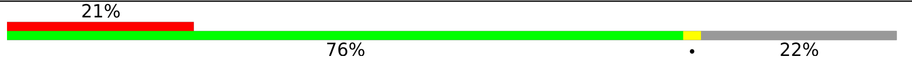
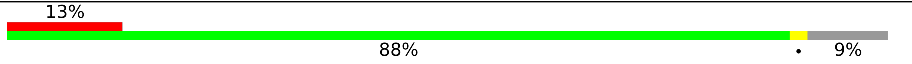
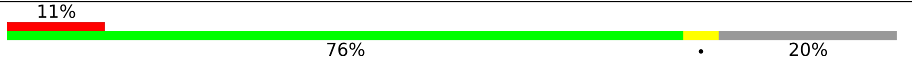
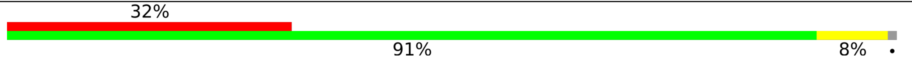
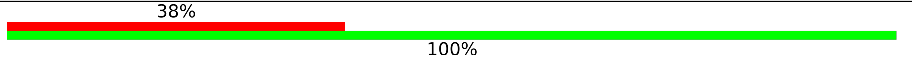
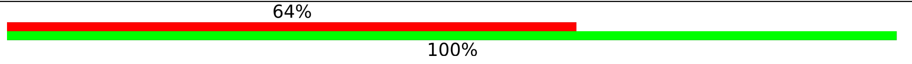
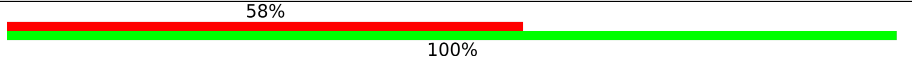
Mol	Chain	Length	Quality of chain
71	DE	747	
72	DF	666	
73	DG	631	
74	DH	581	
75	DJ	396	
76	DK	324	
77	DT	247	
78	DV	183	
79	DW	179	
80	DX	169	
81	DY	163	
82	F1	1041	
83	F4	811	
84	FD	579	
85	FF	474	
86	FG	463	
87	FH	457	
88	FI	445	
89	FK	372	
90	FL	353	
91	FV	264	
92	Fe	123	
93	Ua	47	
94	Ub	42	
95	Uc	12	

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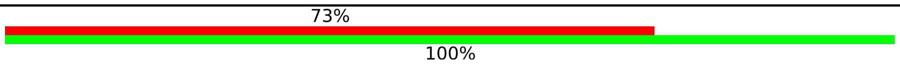
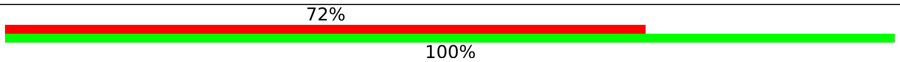
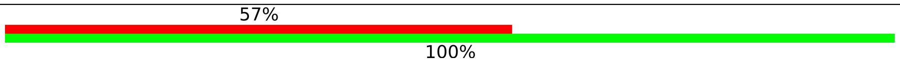
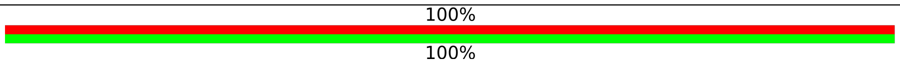
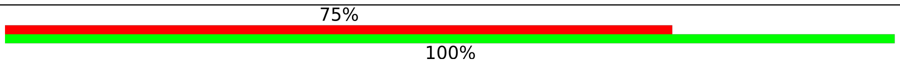
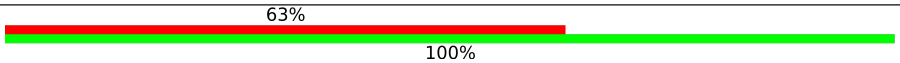
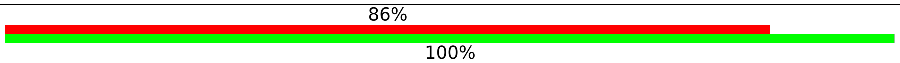
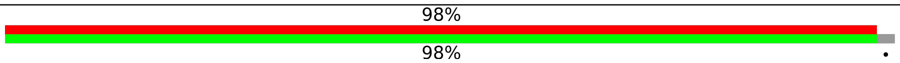
Mol	Chain	Length	Quality of chain
96	Ud	59	
97	Ue	29	
98	Ug	167	
99	Uh	255	
100	Ui	32	
101	Uj	19	
102	Ul	14	
103	Ux	110	

2 Entry composition (i)

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
			Total	C	N	O	S		
6	CP	180	1489	956	274	250	9	0	0

- Molecule 7 is a protein called uS17m.

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

- Molecule 8 is a protein called bS18m.

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

- Molecule 9 is a protein called mS22.

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

- Molecule 10 is a protein called mS23.

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

- Molecule 11 is a protein called mS26.

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

- Molecule 12 is a protein called mS34.

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

- 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
			Total	C	N	O		
47	Uk	27	162	108	27	27	0	0

- Molecule 48 is a protein called UNK-C.

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

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

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

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

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

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

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

- Molecule 52 is a protein called UNK-G.

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

- Molecule 53 is a protein called UNK-H.

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

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

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

- Molecule 55 is a protein called UNK-J.

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

- Molecule 56 is a protein called UNK-K.

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

- Molecule 57 is a protein called UNK-L.

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

- Molecule 58 is a protein called UNK-O.

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

- Molecule 59 is a protein called UNK-Y.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CA	609	Total 11352	C 5038	N 1602	O 4102	P 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
			Total	C	N	O		
96	Ud	59	354	236	59	59	0	0

- Molecule 97 is a protein called UNK-e.

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

- Molecule 98 is a protein called UNK-g.

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

- Molecule 99 is a protein called UNK-h.

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

- Molecule 100 is a protein called UNK-i.

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

- Molecule 101 is a protein called UNK-j.

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

- Molecule 102 is a protein called UNK-l.

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

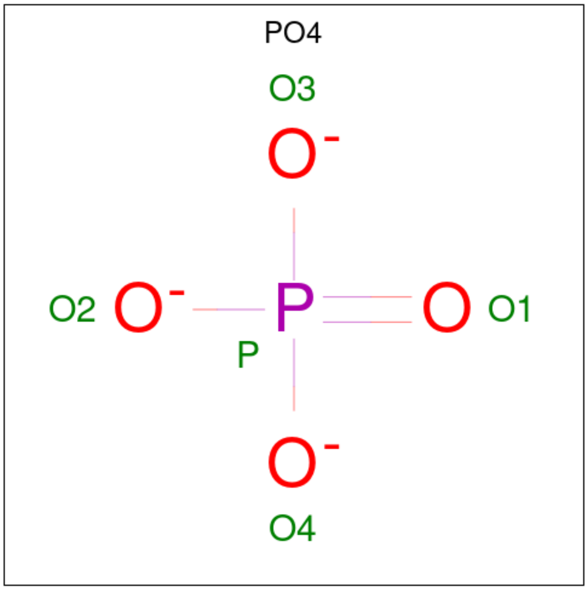
- Molecule 103 is a protein called UNK-x.

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).

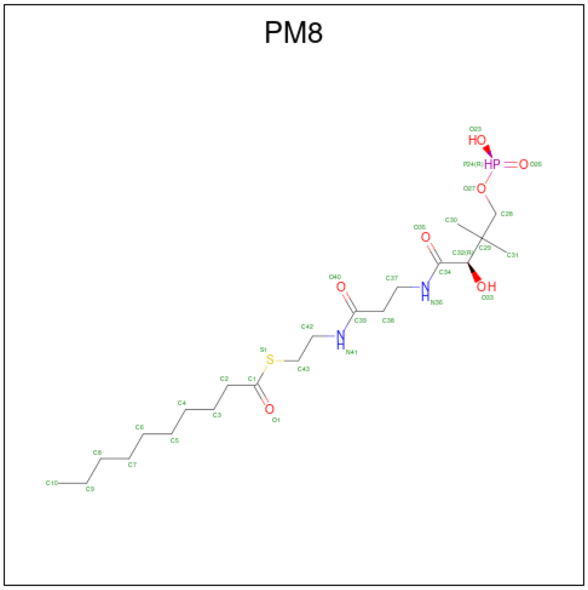
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
104	FP	1	1	1	0
104	FW	1	1	1	0
104	CA	2	2	2	0
104	Cg	1	1	1	0

- Molecule 105 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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: $C_{21}H_{41}N_2O_7PS$).

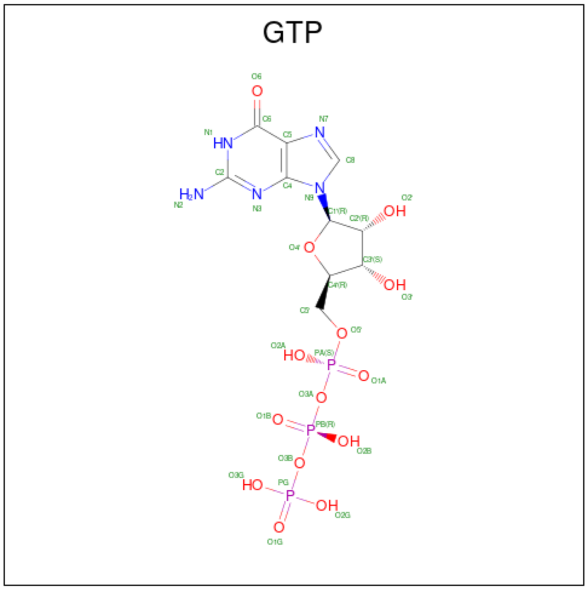


Mol	Chain	Residues	Atoms	AltConf
106	Fc	1	Total C N O P S 32 21 2 7 1 1	0

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

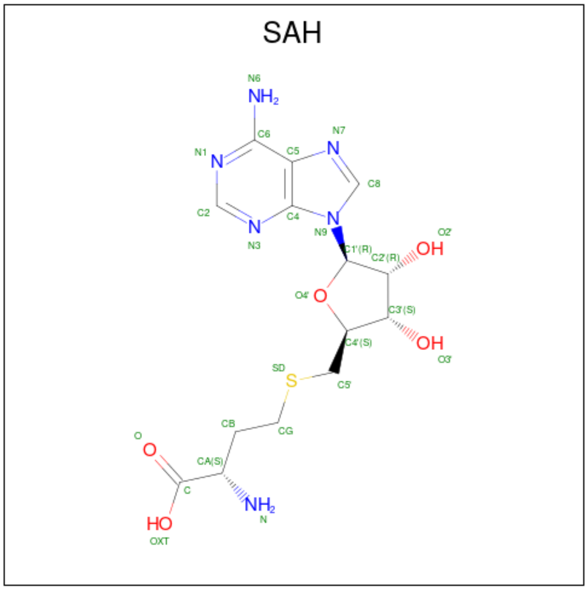
Mol	Chain	Residues	Atoms	AltConf
107	Fd	1	Total Zn 1 1	0
107	F1	1	Total Zn 1 1	0
107	FG	1	Total Zn 1 1	0
107	FL	2	Total Zn 2 2	0
107	Fe	1	Total Zn 1 1	0

- 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
108	Cg	1	Total 32	C 10	N 5	O 14	P 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
109	F1	1	Total 26	C 14	N 6	O 5	S 1	0
109	FF	1	Total 26	C 14	N 6	O 5	S 1	0

- Molecule 110 is water.

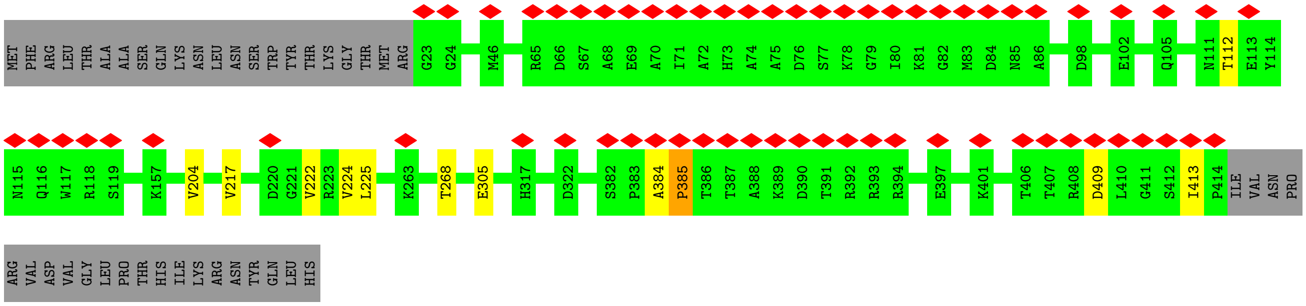
Mol	Chain	Residues	Atoms	AltConf
110	Cg	3	Total O 3 3	0

3 Residue-property plots ⓘ

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

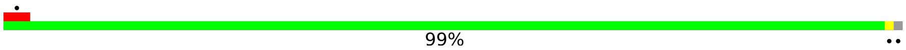
- Molecule 1: uS5m

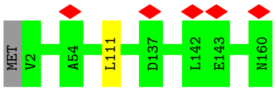
Chain CE:



- Molecule 2: bS6m

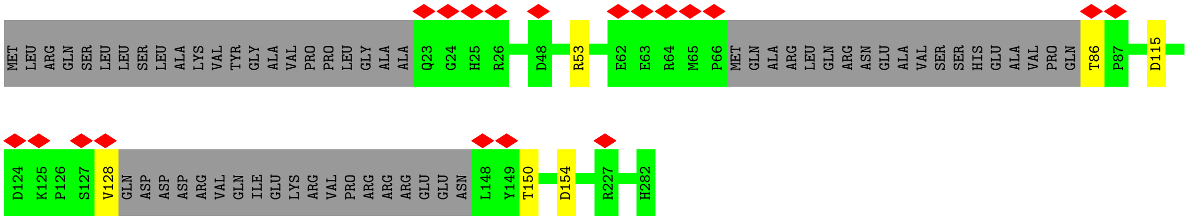
Chain CF:





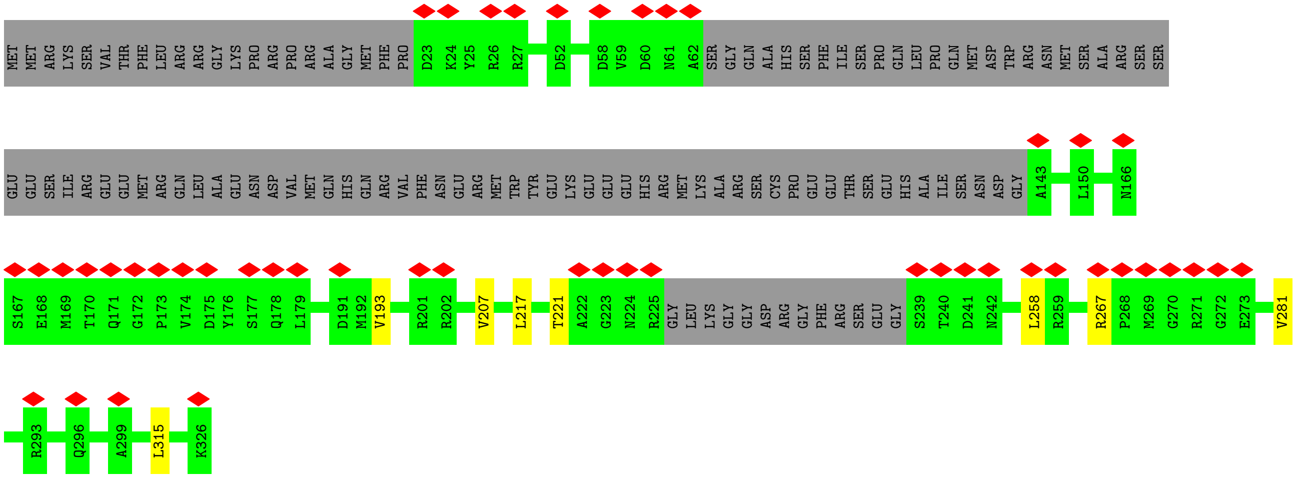
- Molecule 3: uS8m

Chain CH:



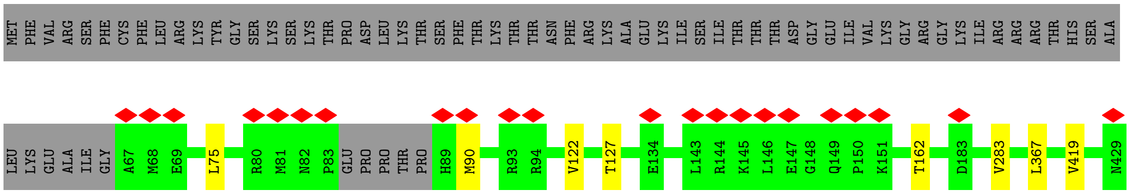
- Molecule 4: uS11m

Chain CK:



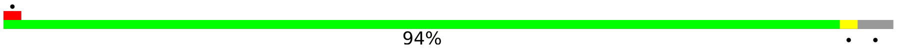
- Molecule 5: uS15m

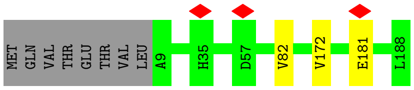
Chain CO:



- Molecule 6: bS16m

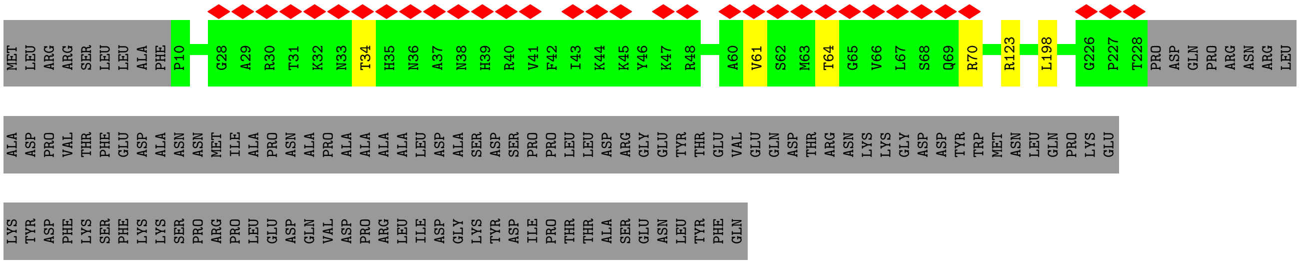
Chain CP:





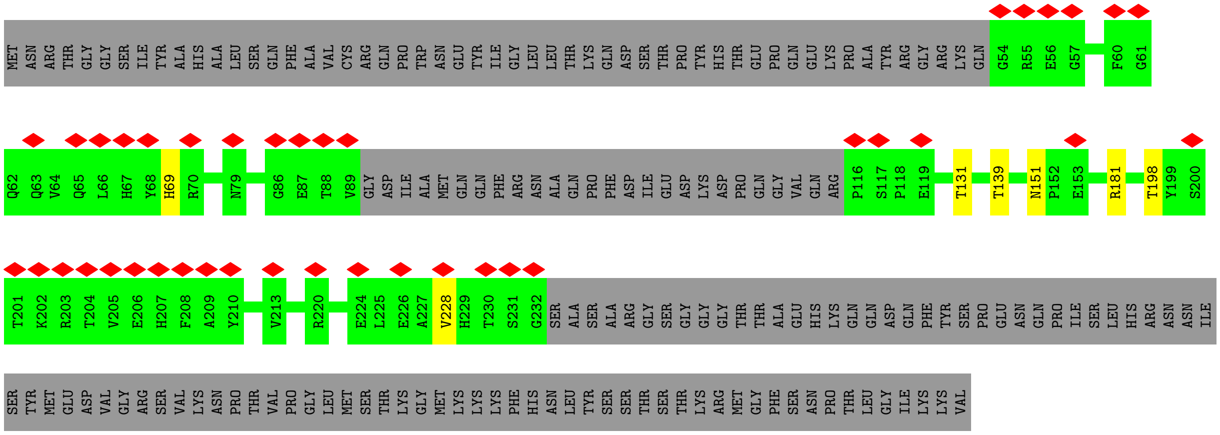
- Molecule 7: uS17m

Chain CQ:



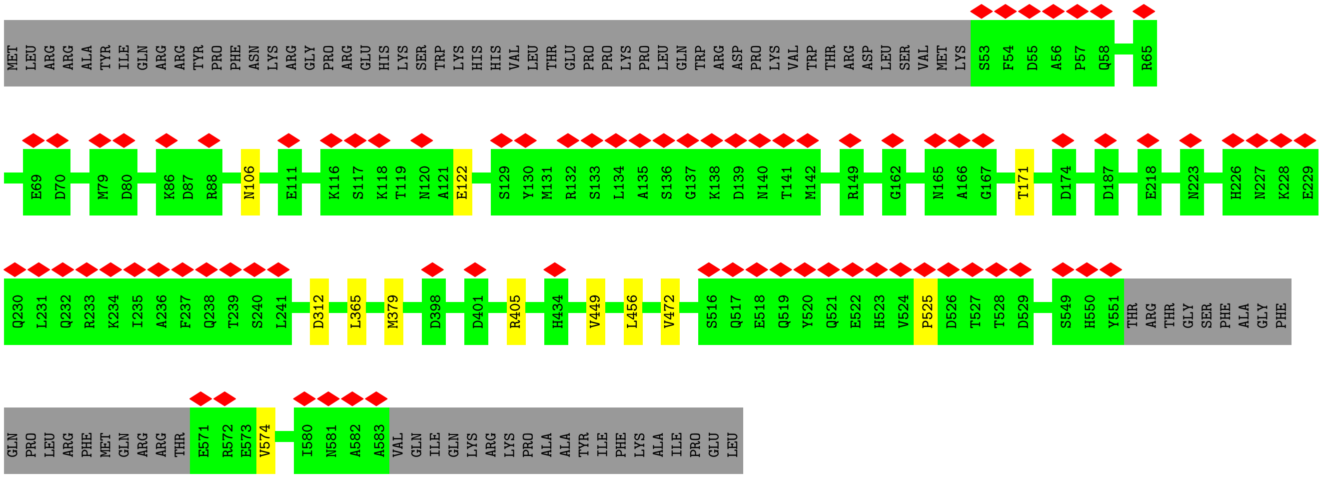
- Molecule 8: bS18m

Chain CR:



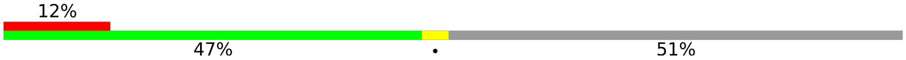
- Molecule 9: mS22

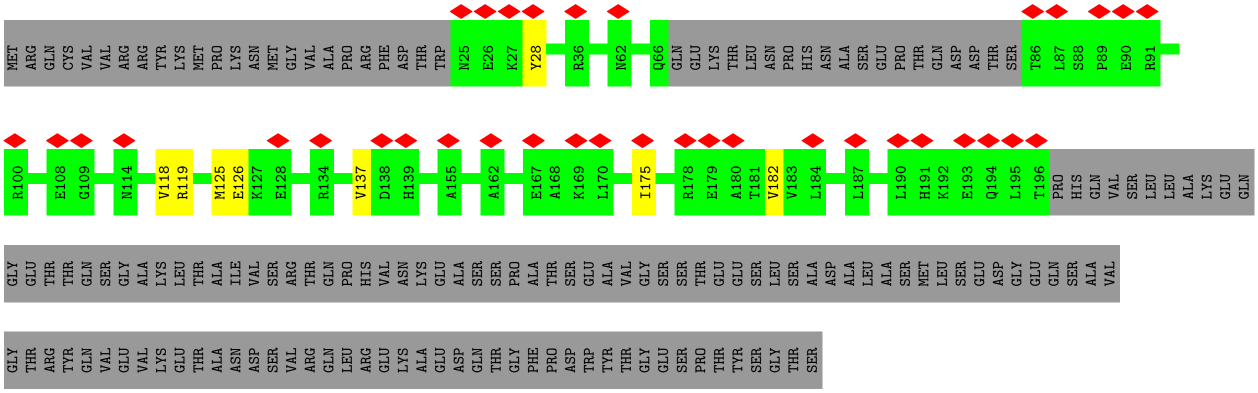
Chain Ca:



- Molecule 10: mS23

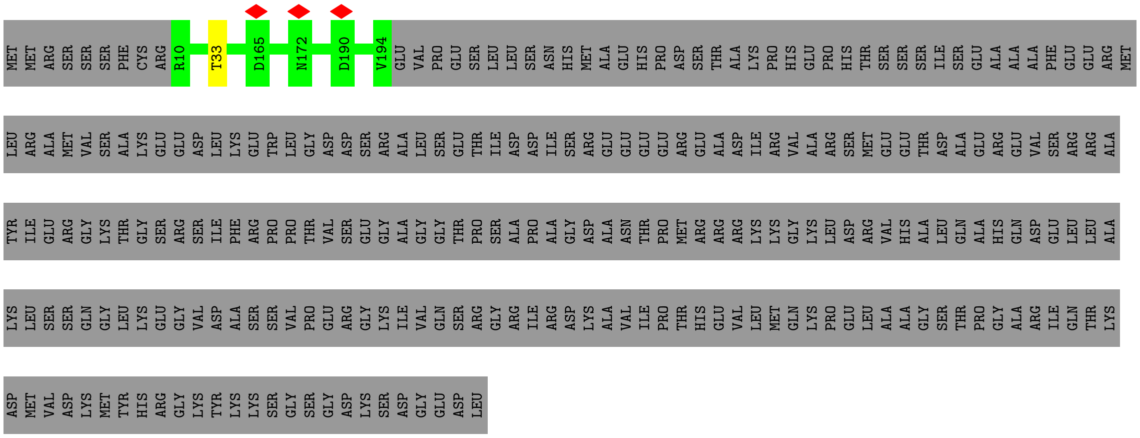
Chain Cb:





- Molecule 11: mS26

Chain Cd:

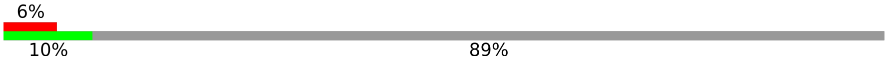


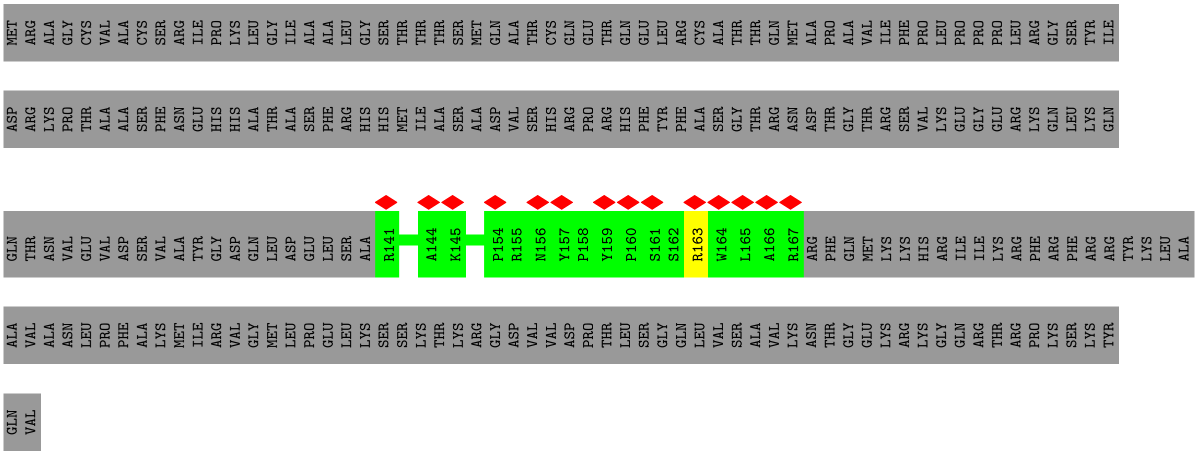
- Molecule 12: mS34

Chain Cj:

- Molecule 13: mS38

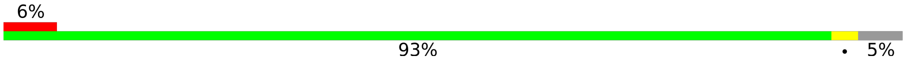
Chain Cn:

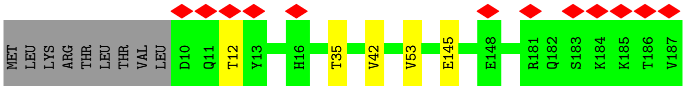




- Molecule 14: mS41

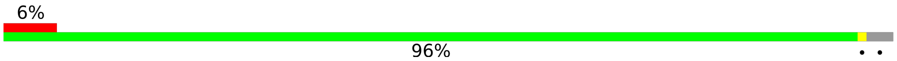
Chain Cp:

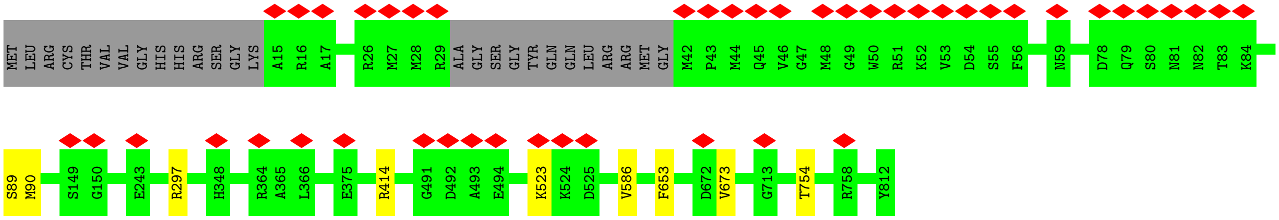




- Molecule 15: mS51 (KRIPP1)

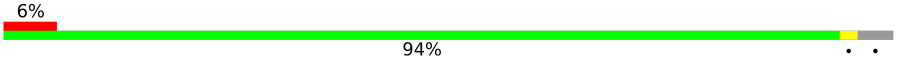
Chain DD:

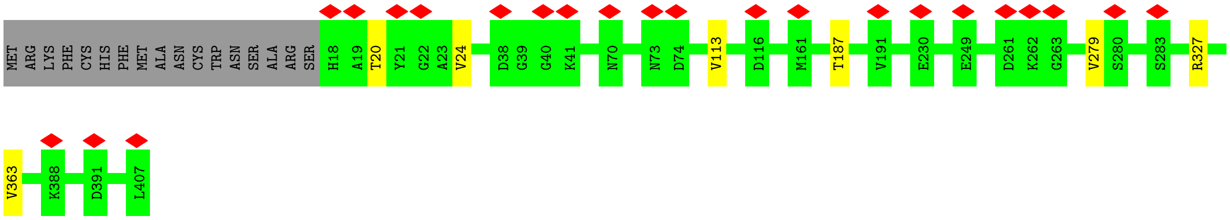




- Molecule 16: mS56

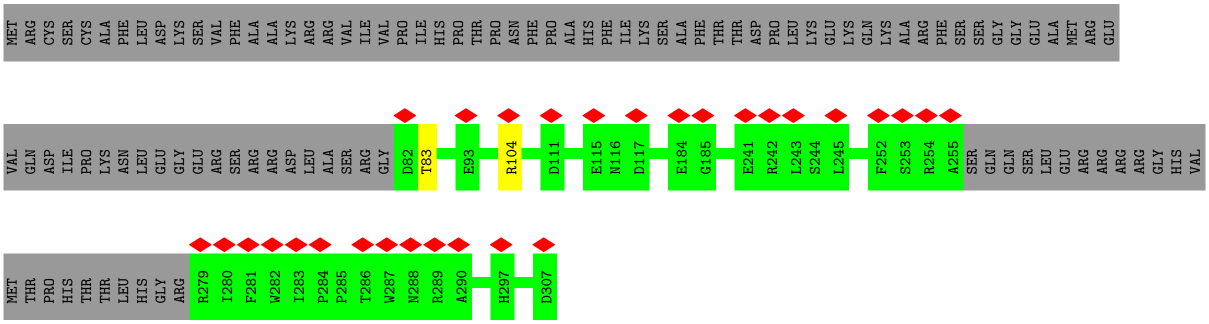
Chain DI:





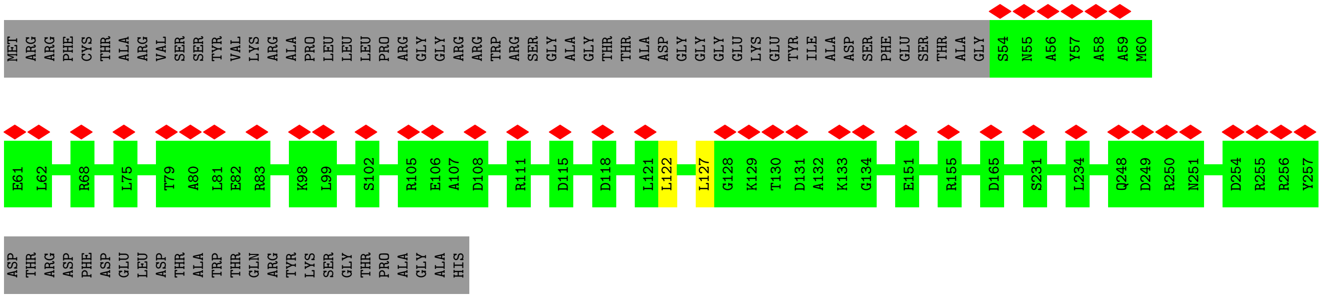
- Molecule 17: mS59

Chain DL:



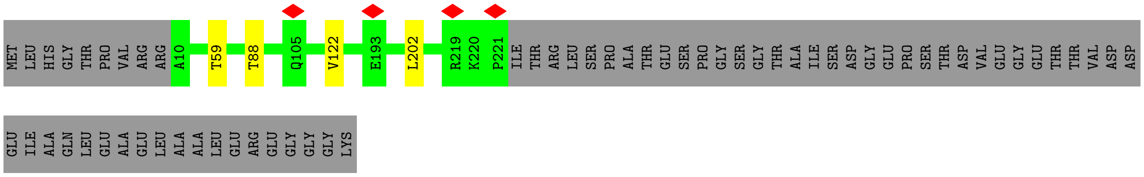
- Molecule 18: mS62 (KRIPP14)

Chain DO:



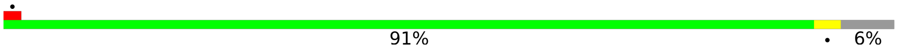
- Molecule 19: mS63 (KRIPP16)

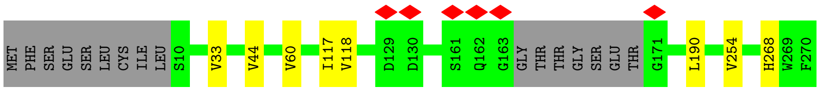
Chain DP:



- Molecule 20: mS65

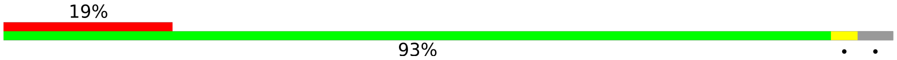
Chain DR:

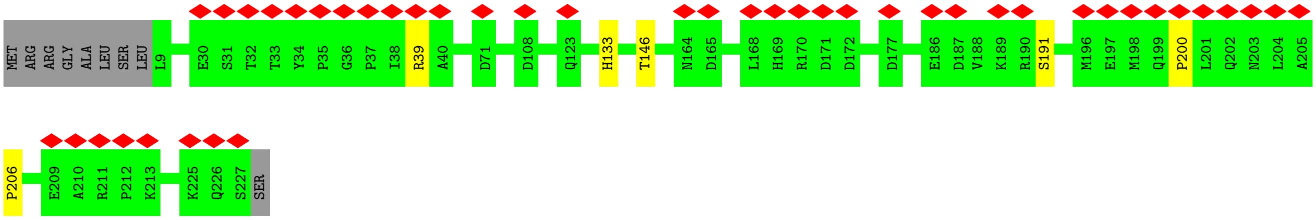




- Molecule 21: mS68

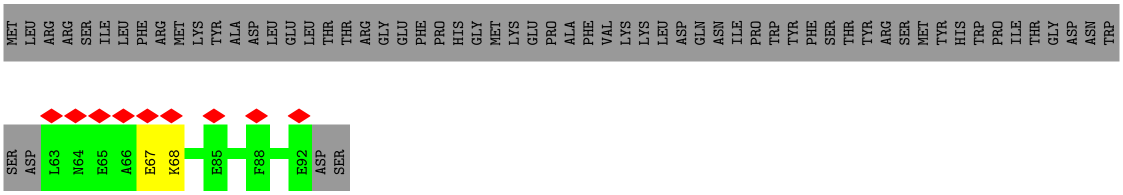
Chain DU:





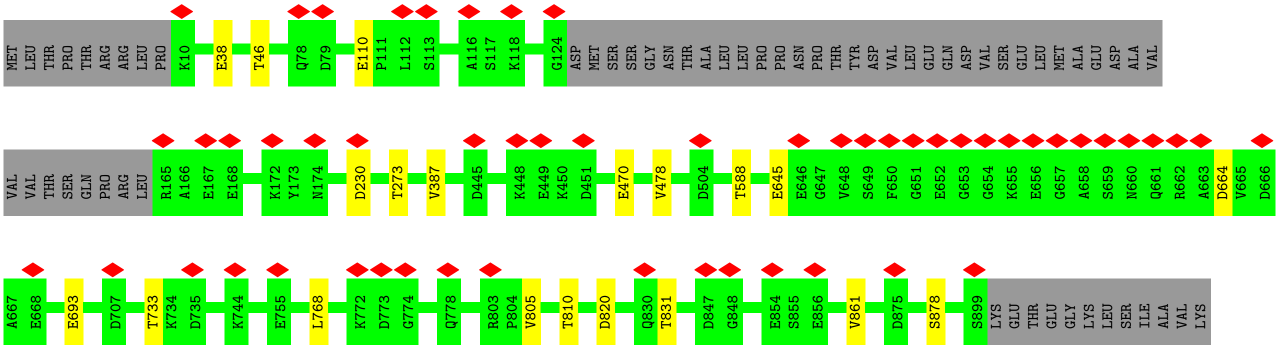
- Molecule 22: mS73

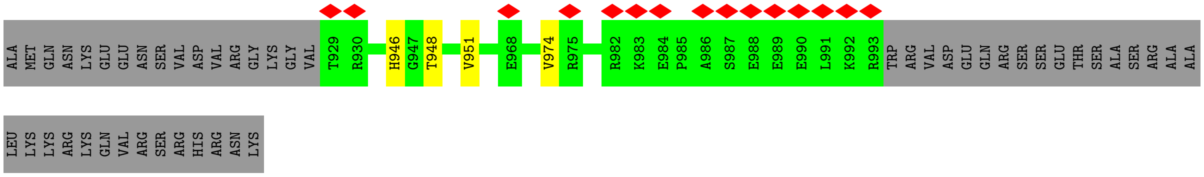
Chain DZ:



- Molecule 23: mt-SAF2 (KRIPP2)

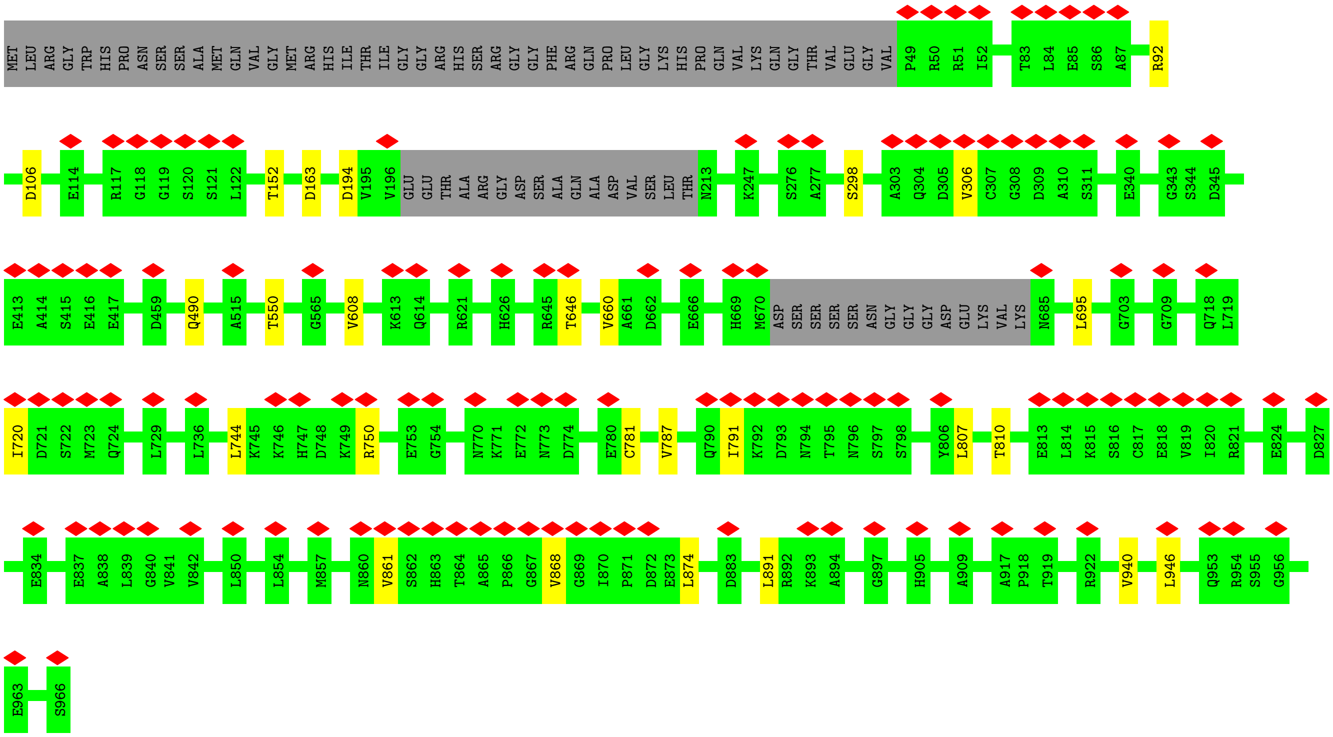
Chain F2:





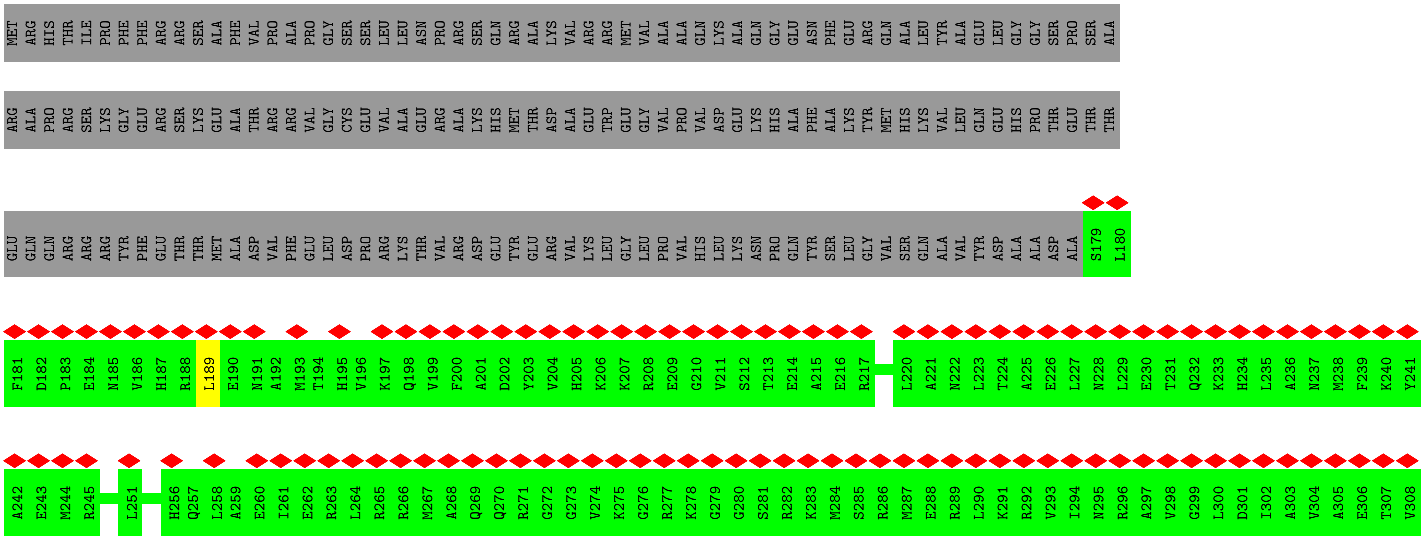
- Molecule 24: mt-SAF3

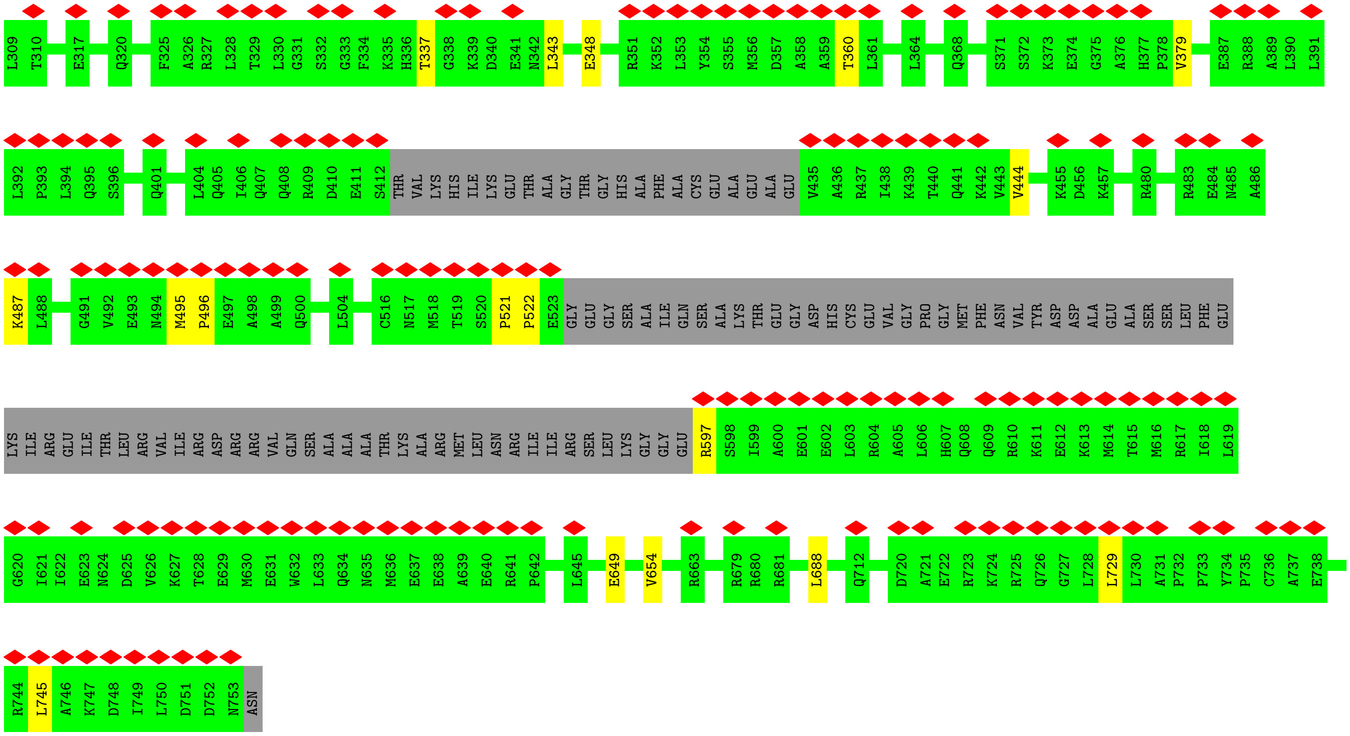
Chain F3:



- Molecule 25: mt-SAF5

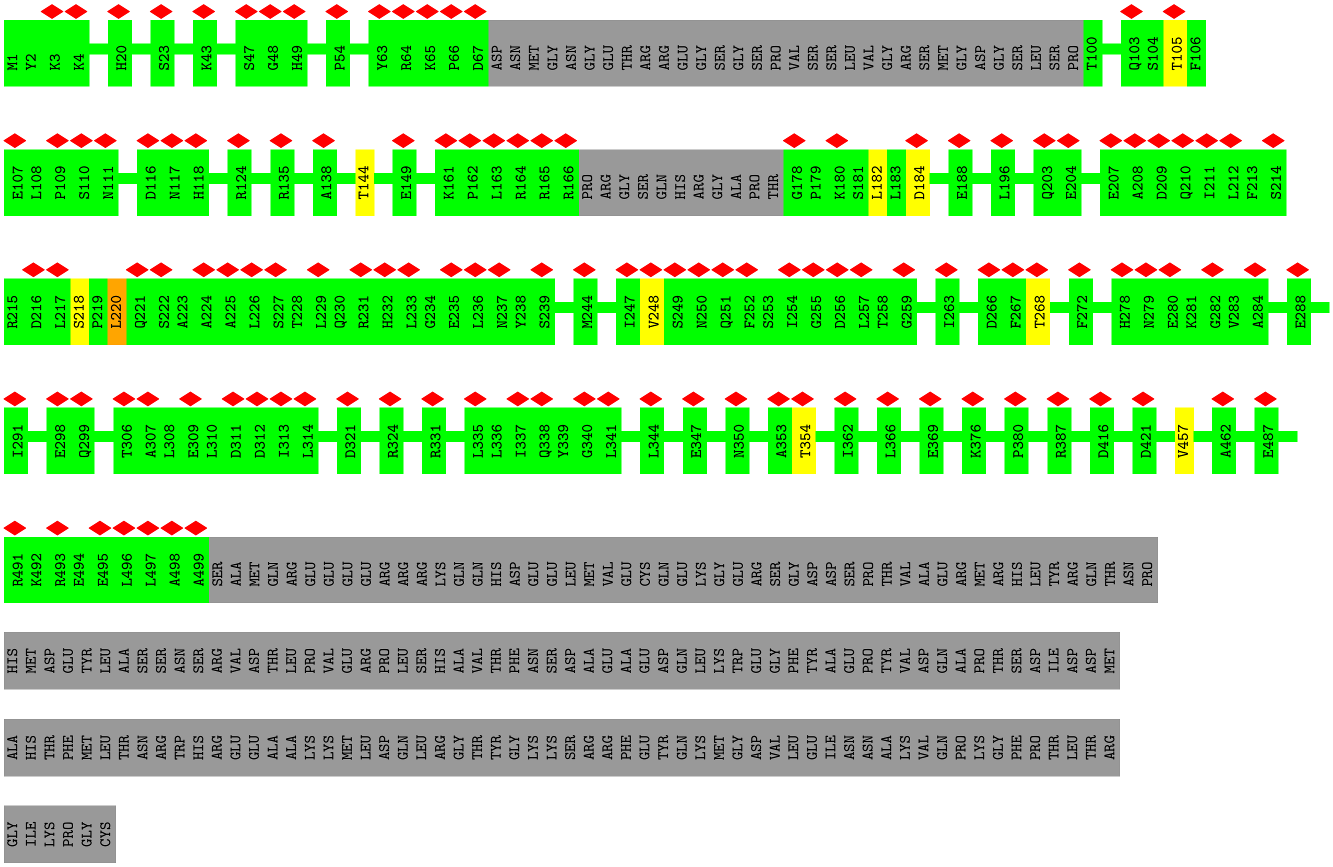
Chain F5:



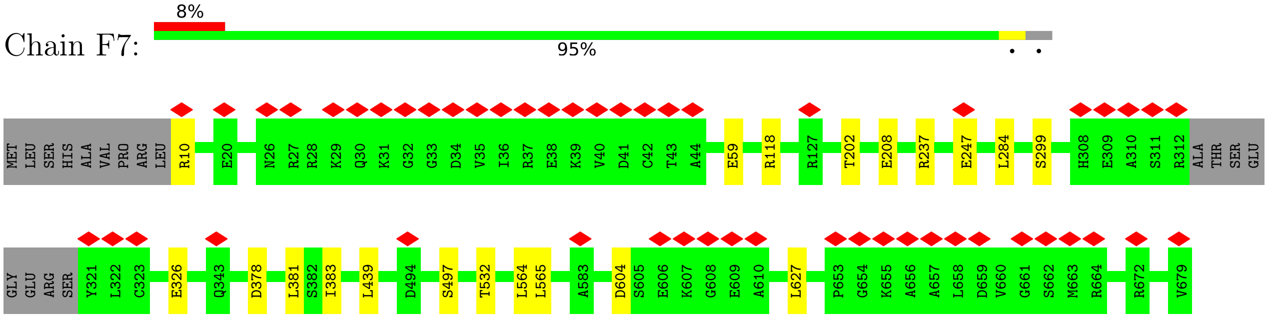


- Molecule 26: mt-SAF6

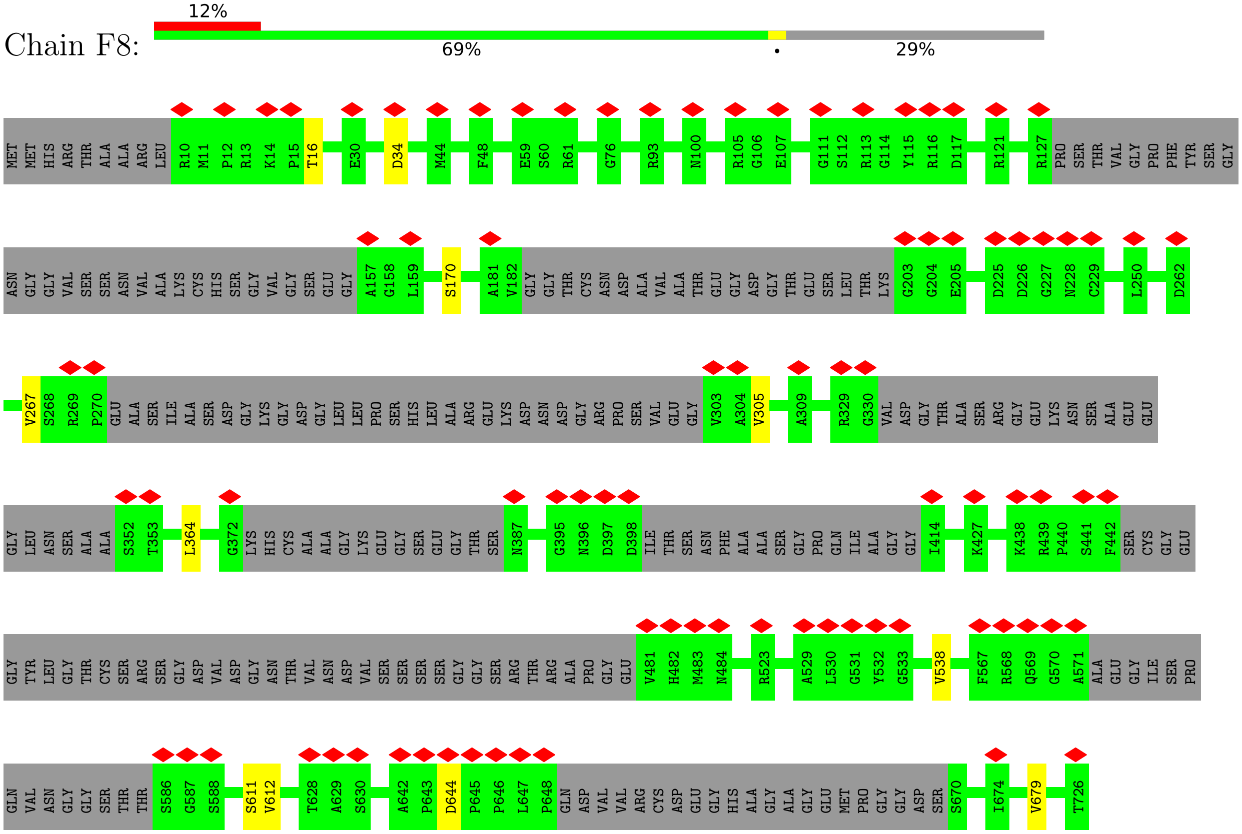
Chain F6:



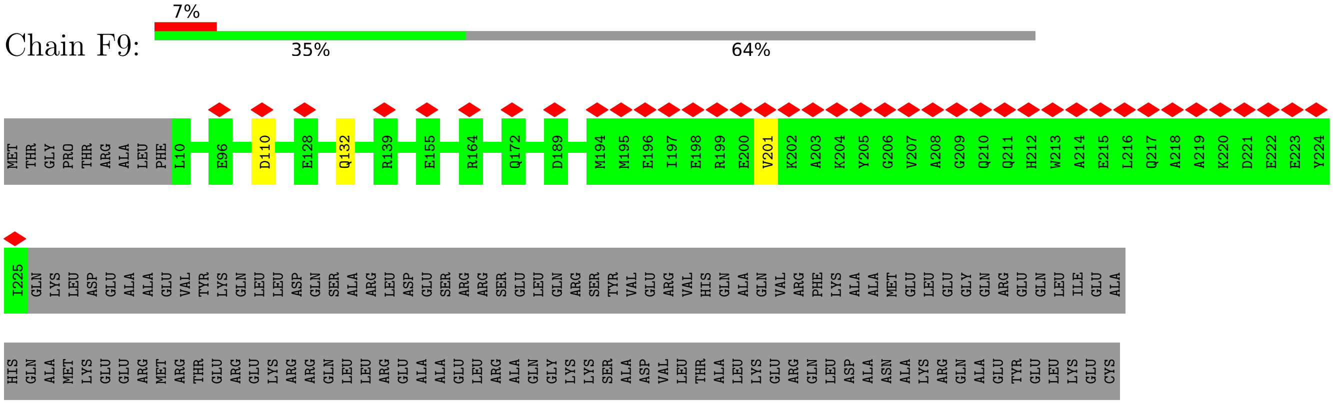
- Molecule 27: mt-SAF7 (KRIPP10)

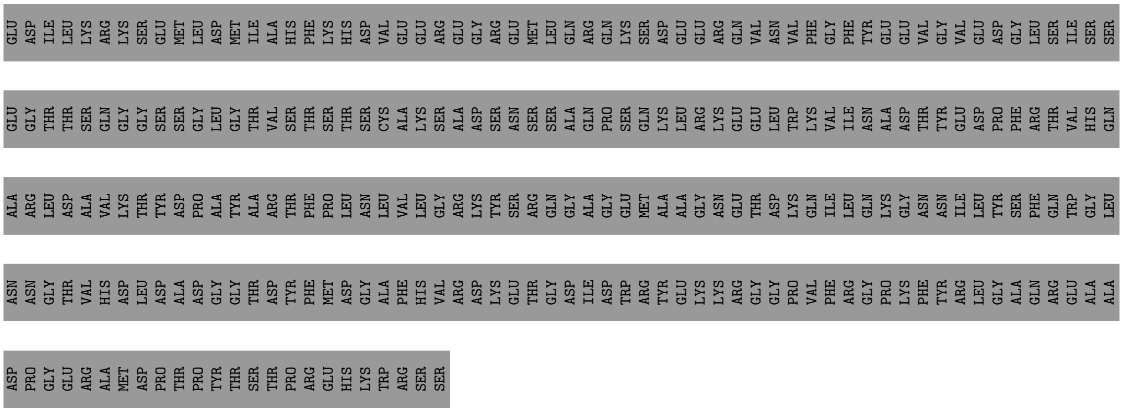


- Molecule 28: mt-SAF8



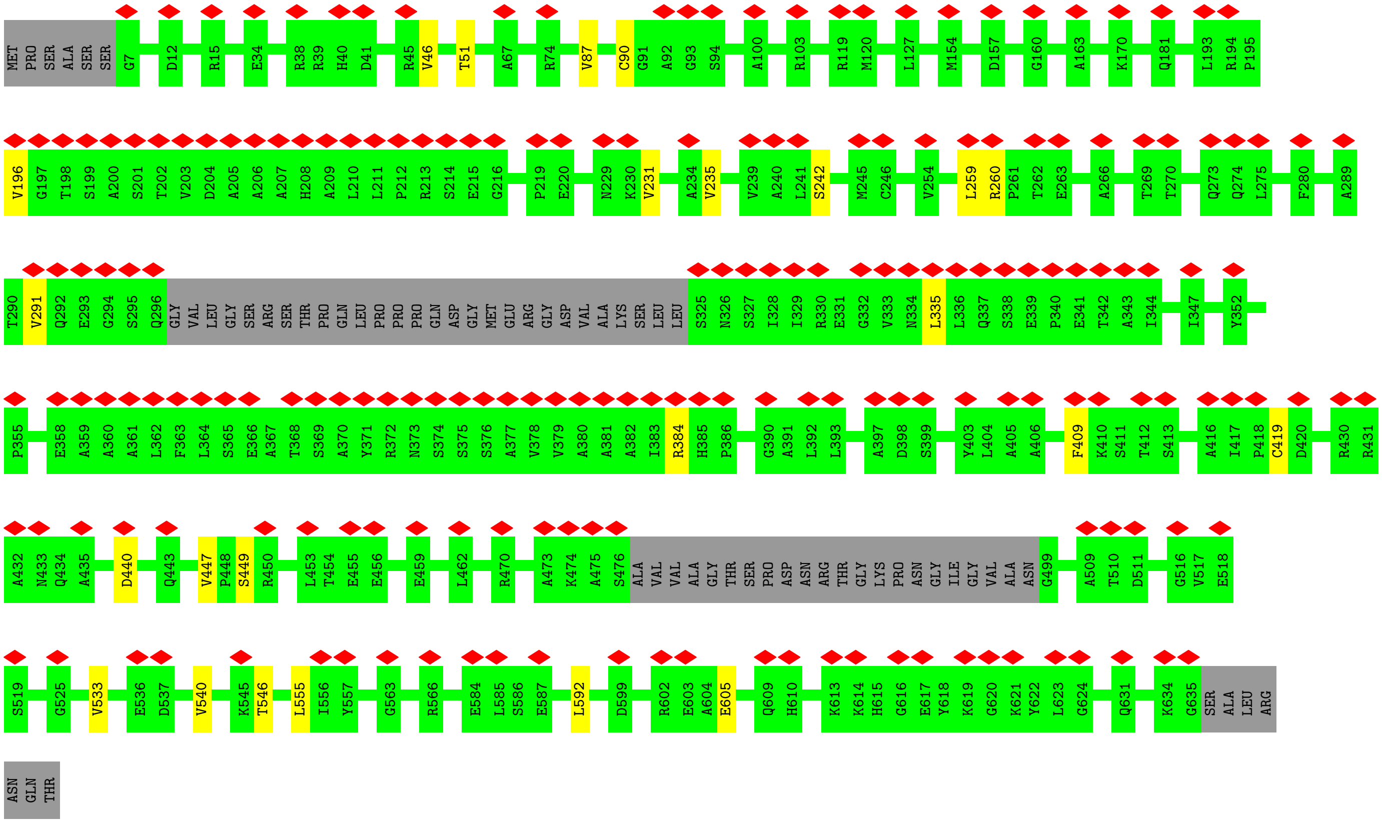
- Molecule 29: mt-SAF9





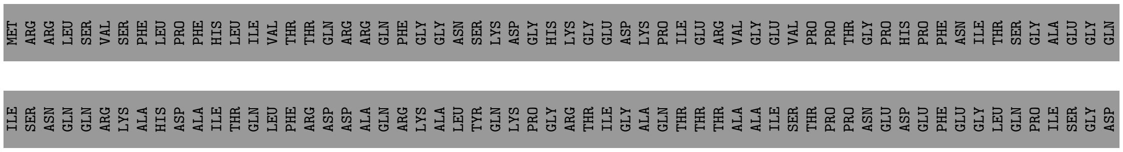
- Molecule 30: mt-SAF10

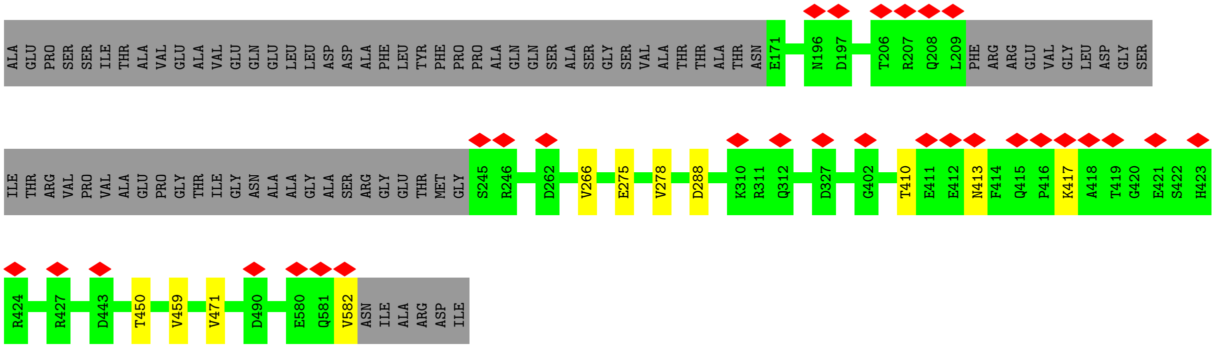
Chain FA:



- Molecule 31: mt-SAF11

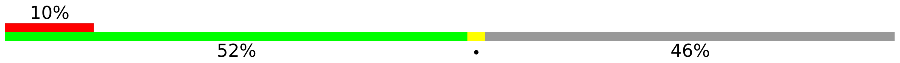
Chain FB:

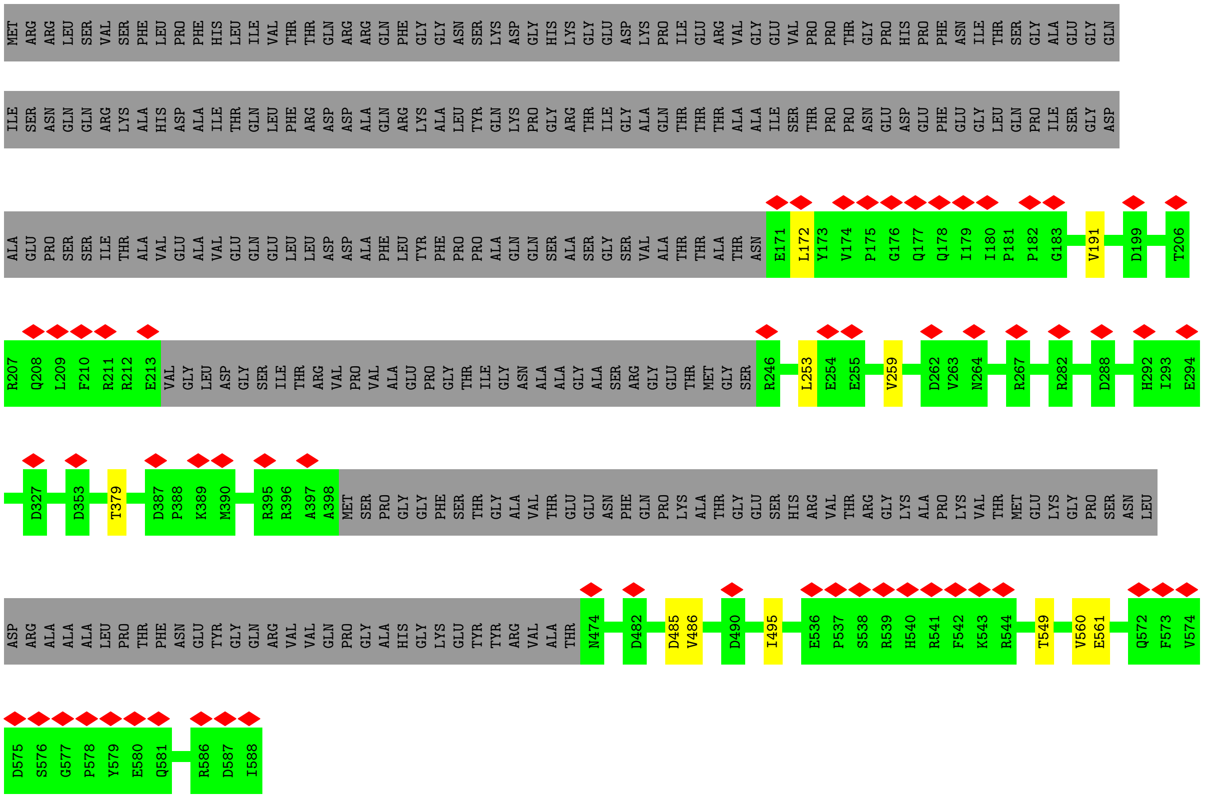




- Molecule 31: mt-SAF11

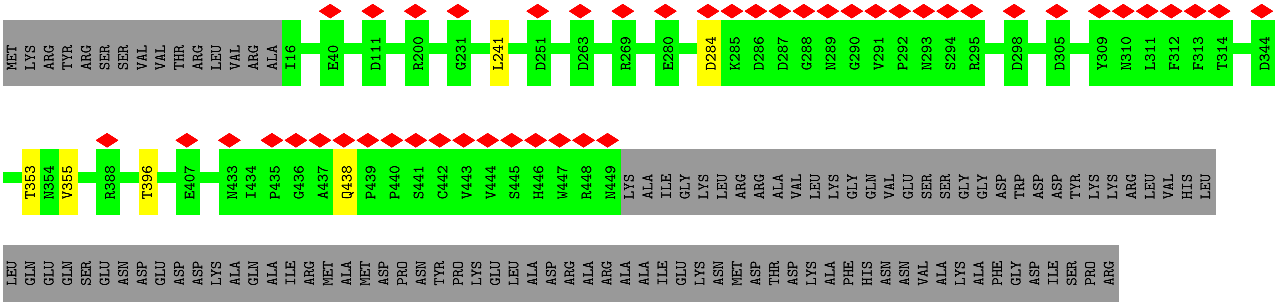
Chain FC:

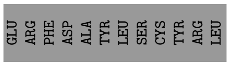




- Molecule 32: mt-SAF13

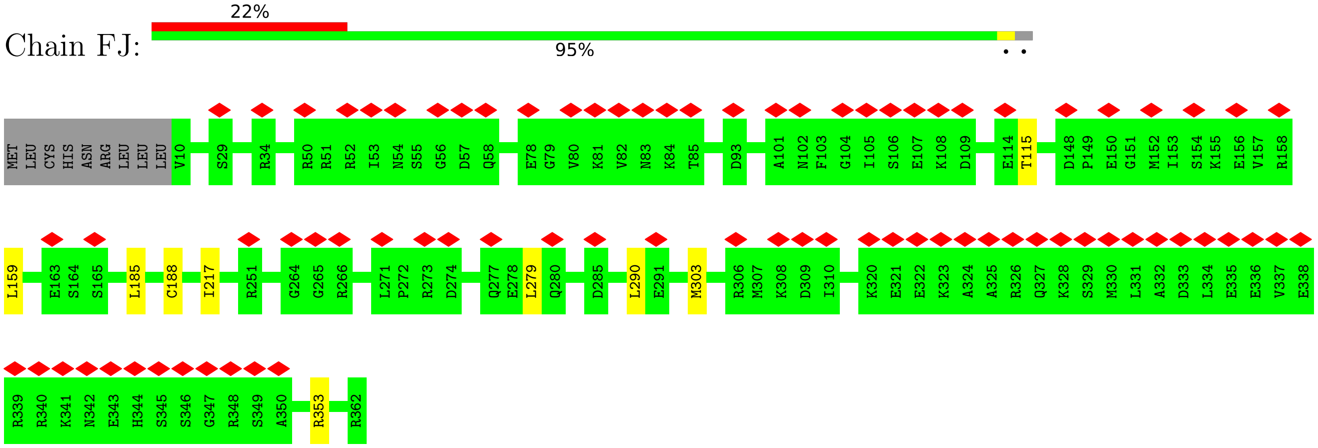
Chain FE:





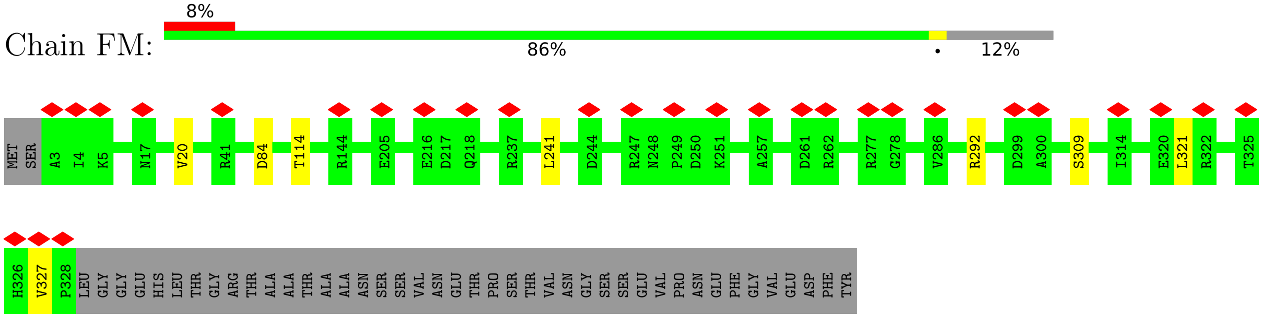
- Molecule 33: mt-SAF18

Chain FJ:



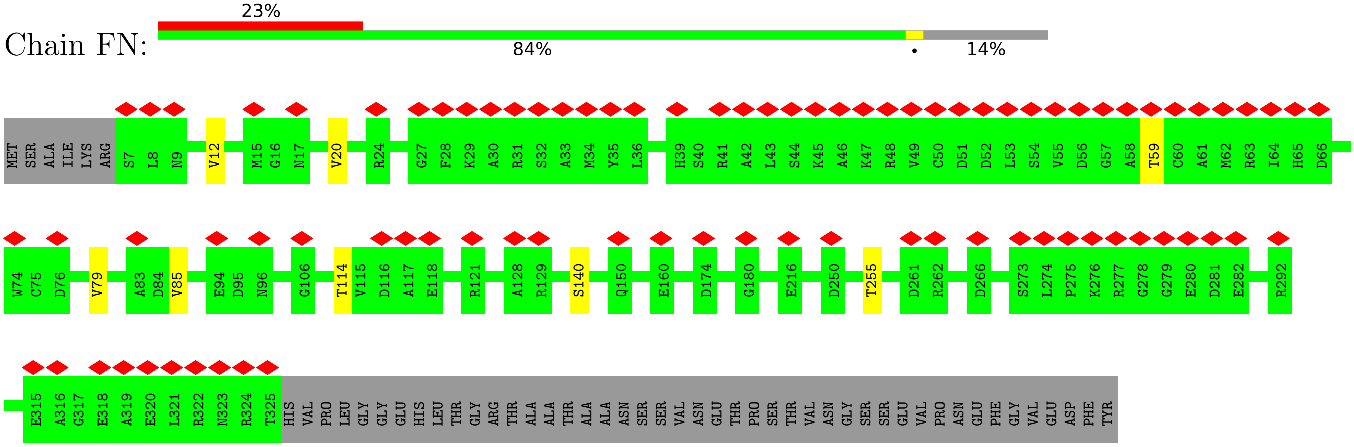
- Molecule 34: mt-SAF21

Chain FM:



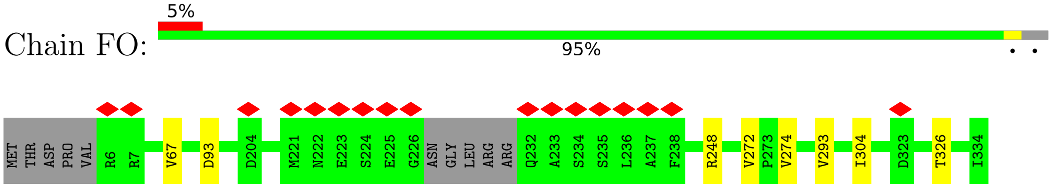
- Molecule 34: mt-SAF21

Chain FN:



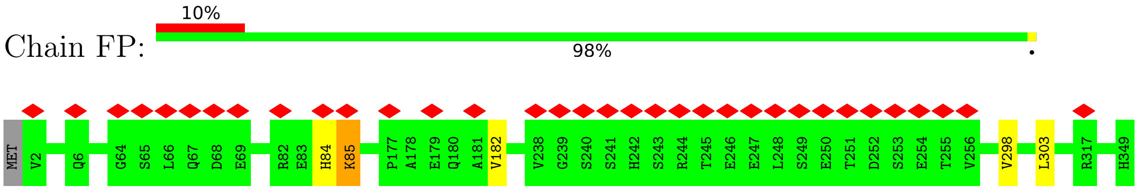
- Molecule 35: mt-SAF22 (KRIPP17)

Chain FO:



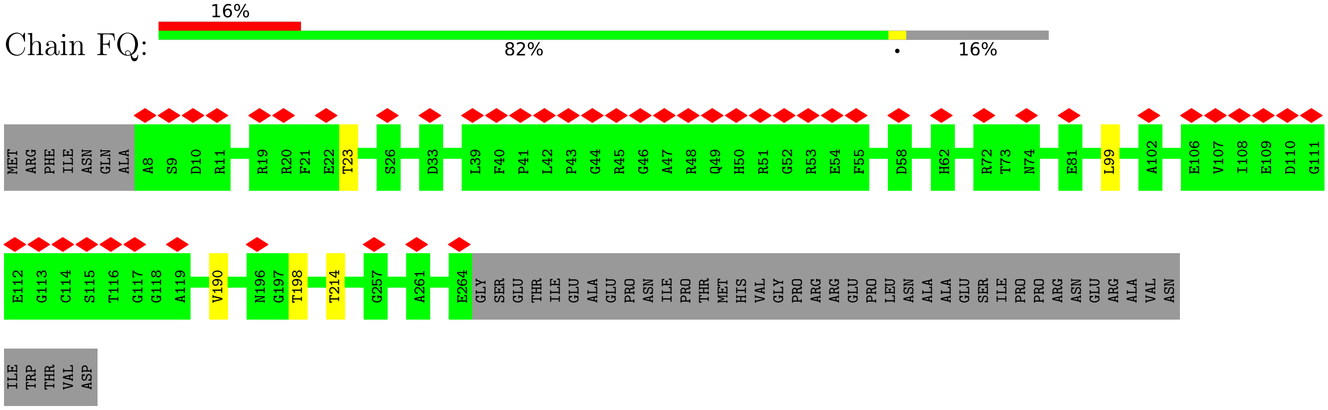
- Molecule 36: mt-SAF23

Chain FP:



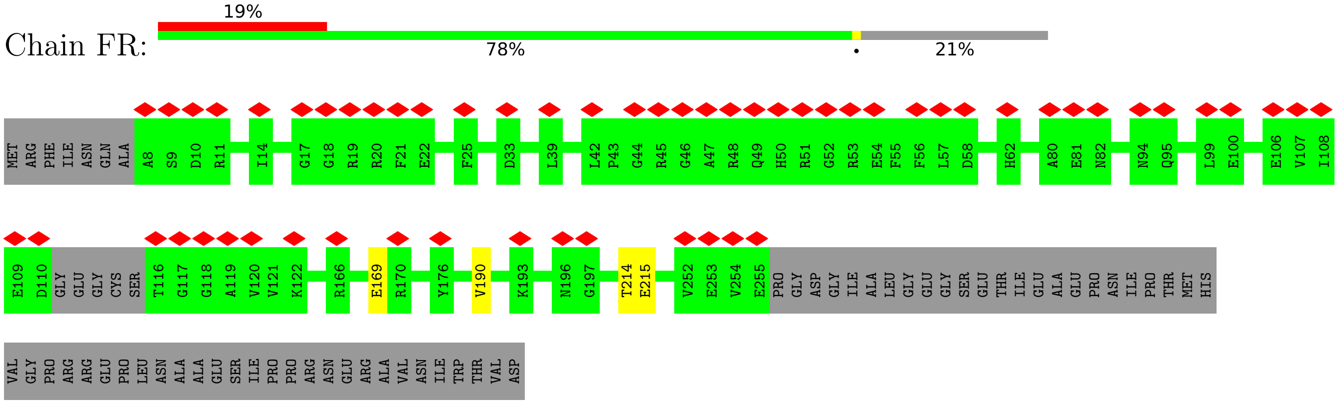
- Molecule 37: mt-SAF24

Chain FQ:



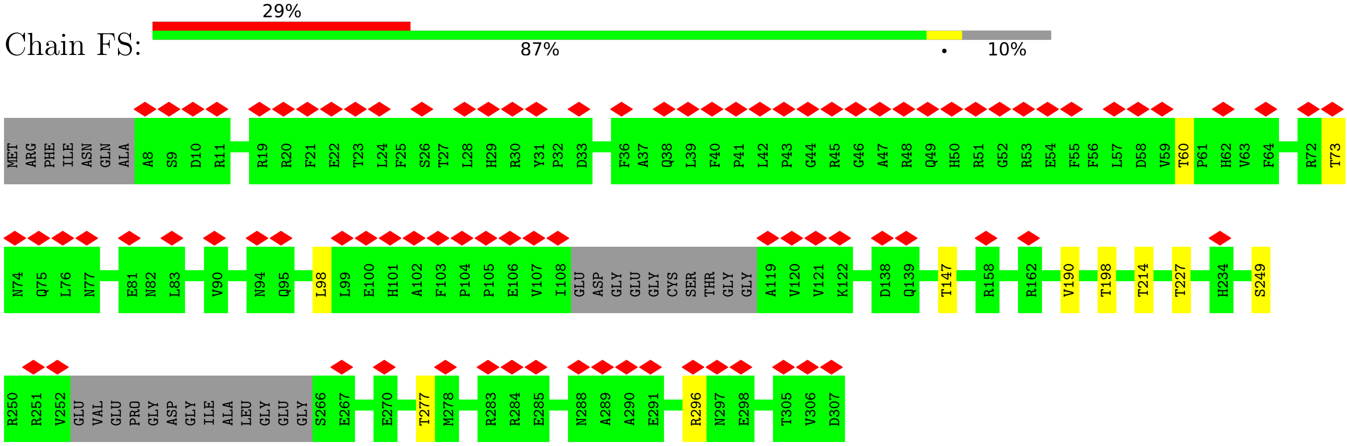
- Molecule 37: mt-SAF24

Chain FR:

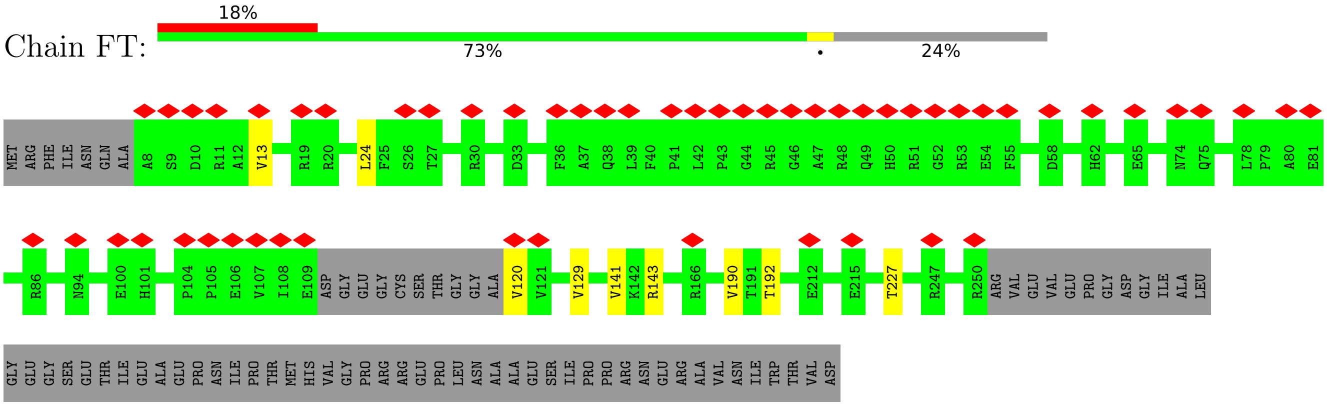


- Molecule 37: mt-SAF24

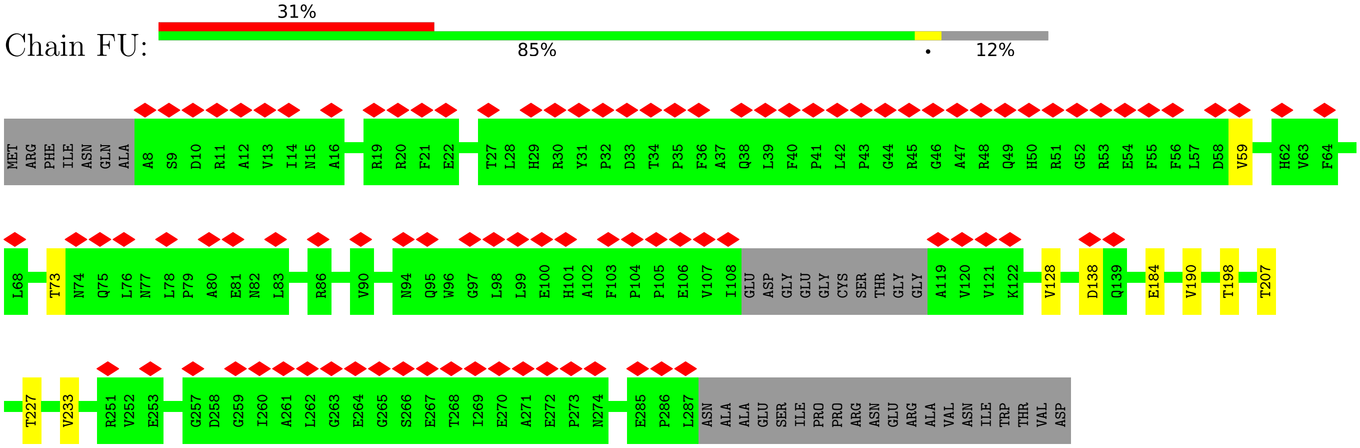
Chain FS:



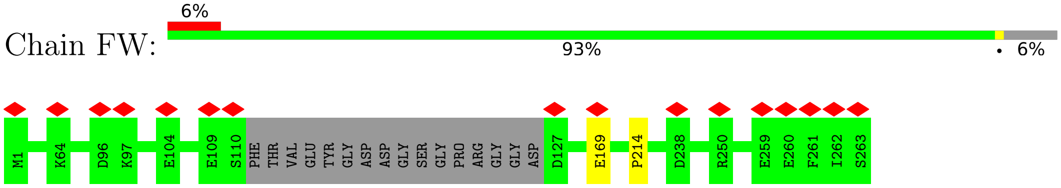
- Molecule 37: mt-SAF24



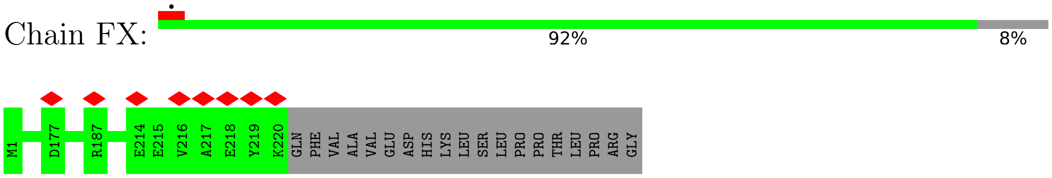
- Molecule 37: mt-SAF24



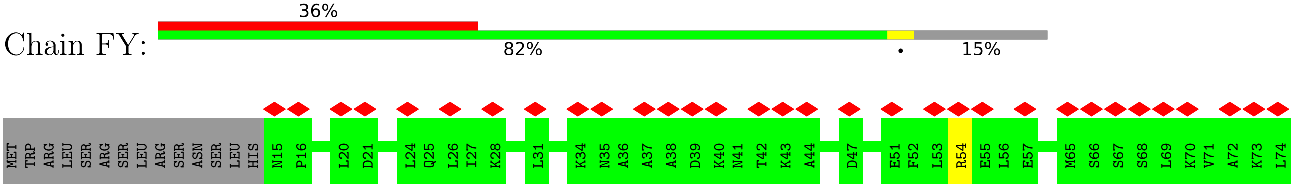
- Molecule 38: mt-SAF26

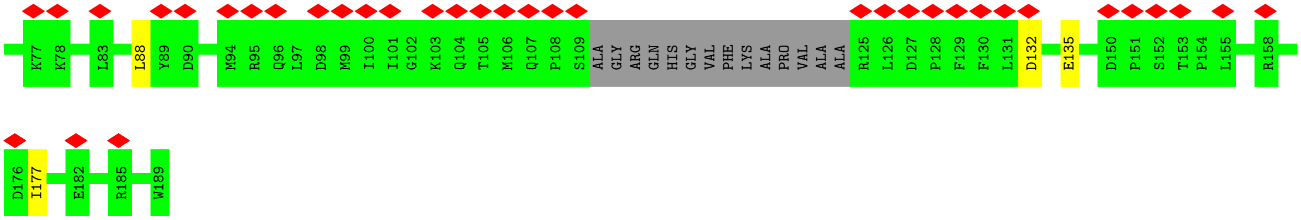


- Molecule 39: mt-SAF27 (KRIPP11)



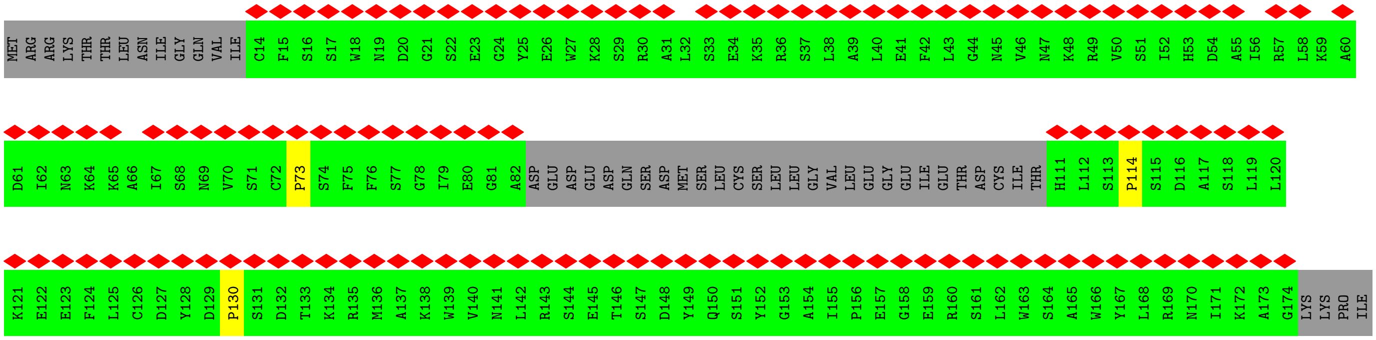
- Molecule 40: mt-SAF28





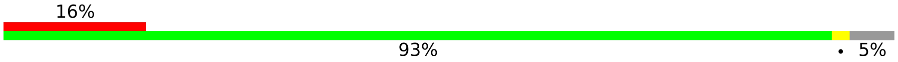
- Molecule 41: mt-SAF29

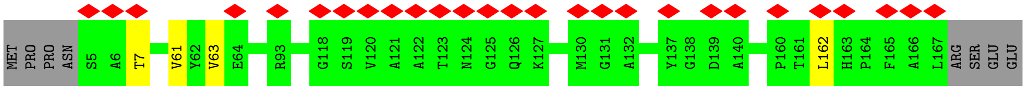
Chain FZ:



- Molecule 42: mt-SAF30

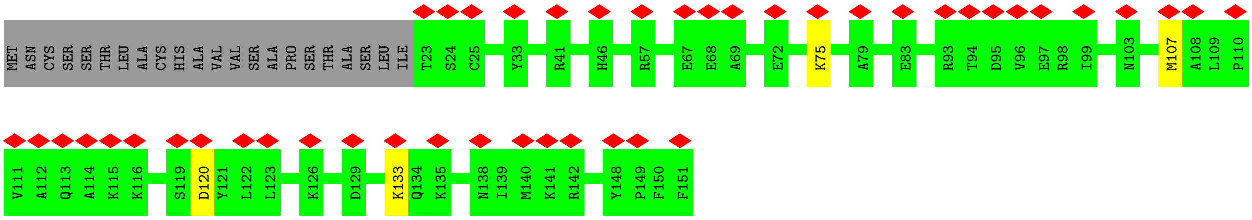
Chain Fa:





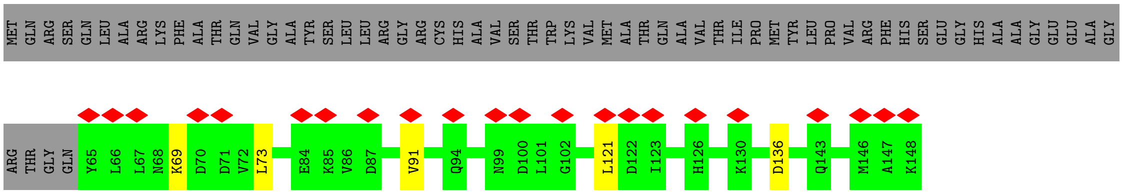
- Molecule 43: mt-SAF31

Chain Fb:



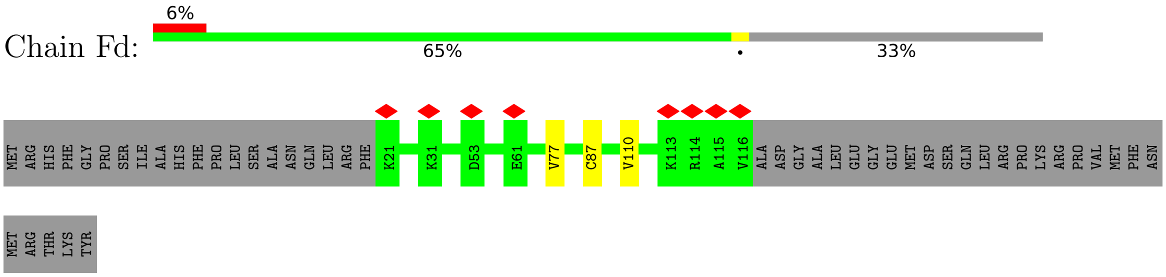
- Molecule 44: mt-SAF32

Chain Fc:



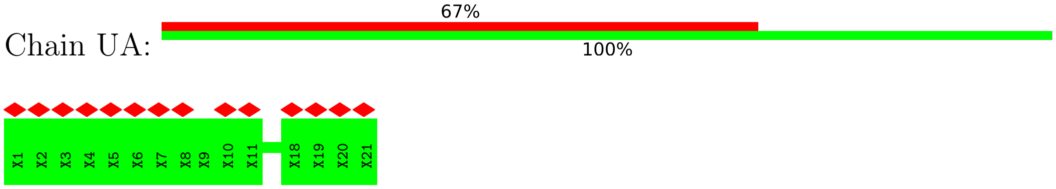
- Molecule 45: mt-SAF33

Chain Fd:



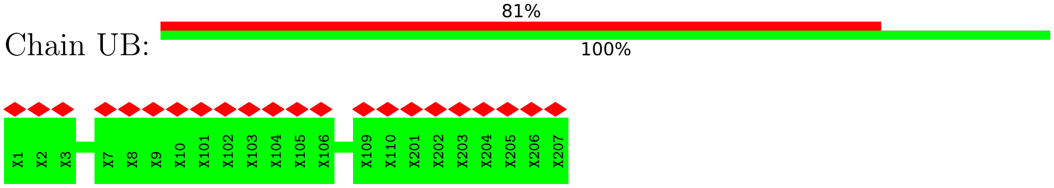
- Molecule 46: UNK-A

Chain UA:



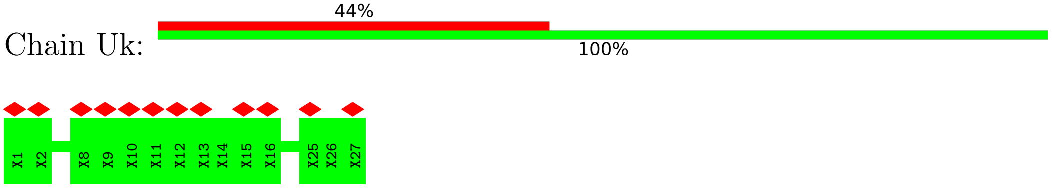
- Molecule 47: UNK-B, UNK-k

Chain UB:



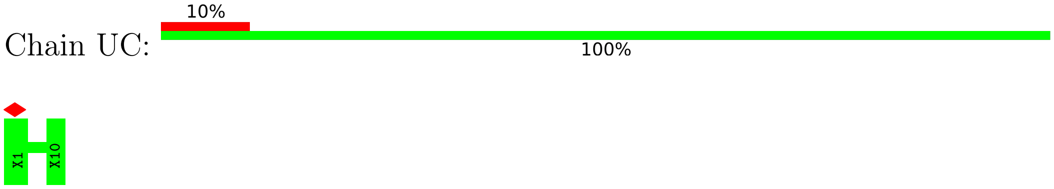
- Molecule 47: UNK-B, UNK-k

Chain Uk:



- Molecule 48: UNK-C

Chain UC:



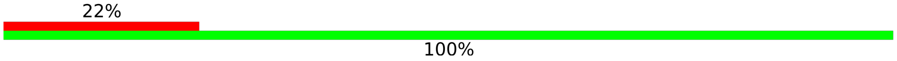
- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f

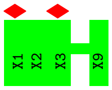
Chain UD:

There are no outlier residues recorded for this chain.

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

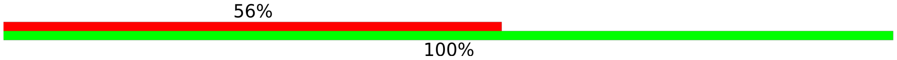
Chain UM:

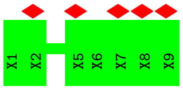




- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f

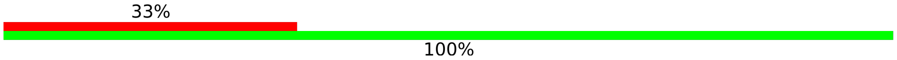
Chain UQ:

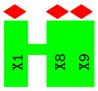




- Molecule 49: UNK-D, UNK-M, UNK-Q, UNK-f

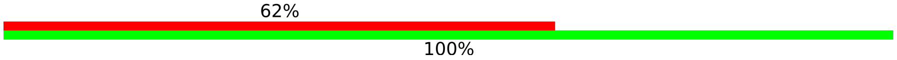
Chain Uf:

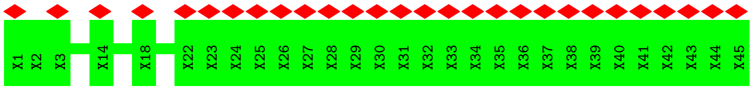




- Molecule 50: UNK-E, UNK-P

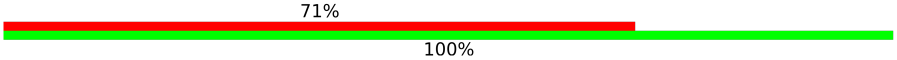
Chain UE:

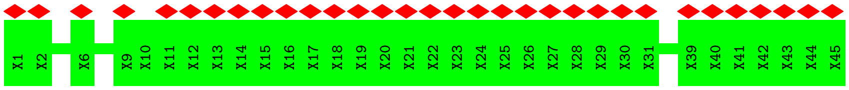




- Molecule 50: UNK-E, UNK-P

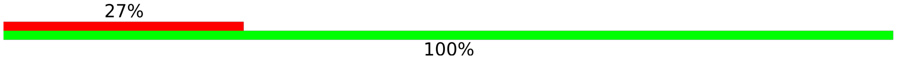
Chain UP:

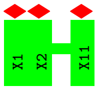




- Molecule 51: UNK-F, UNK-m

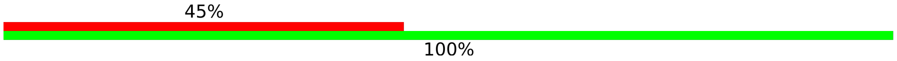
Chain UF:

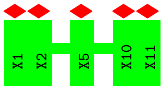




- Molecule 51: UNK-F, UNK-m

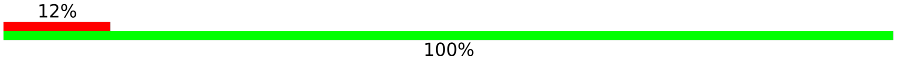
Chain Um:

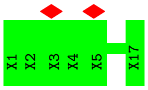




- Molecule 52: UNK-G

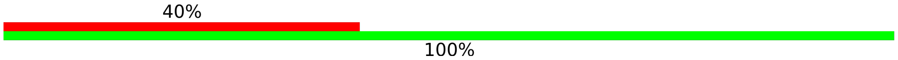
Chain UG:

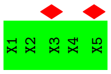




- Molecule 53: UNK-H

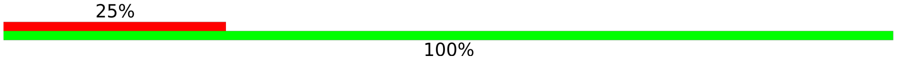
Chain UH:

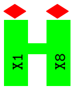




- Molecule 54: UNK-I, UNK-N

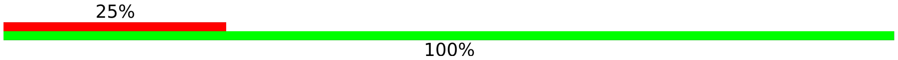
Chain UI:

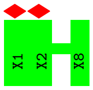




- Molecule 54: UNK-I, UNK-N

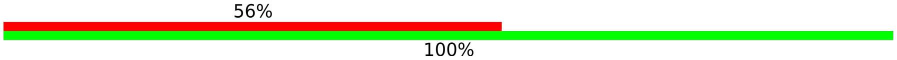
Chain UN:

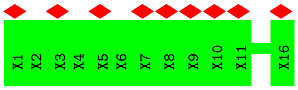




- Molecule 55: UNK-J

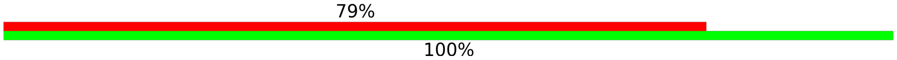
Chain UJ:

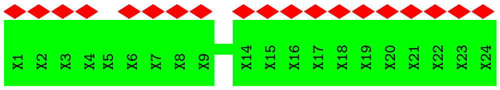




- Molecule 56: UNK-K

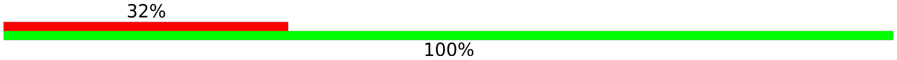
Chain UK:

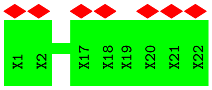




- Molecule 57: UNK-L

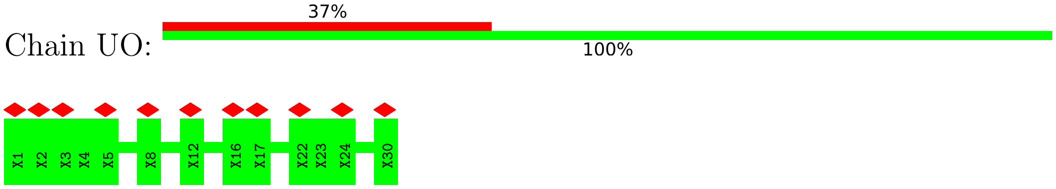
Chain UL:





- Molecule 58: UNK-O

Chain UO:

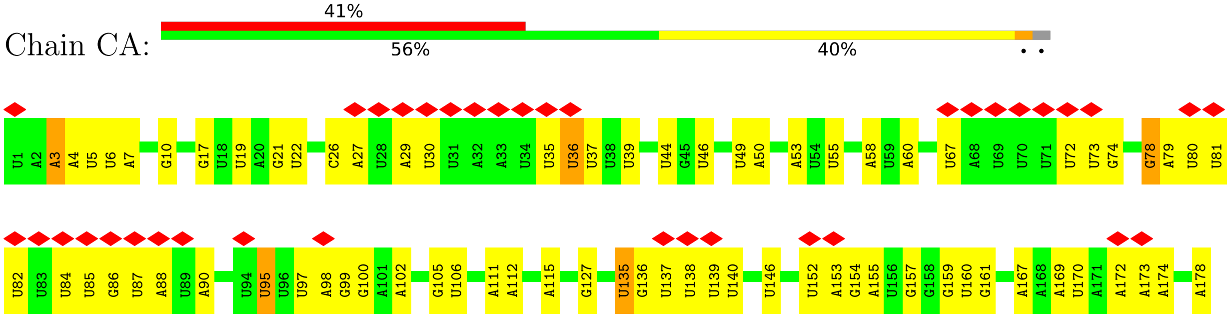


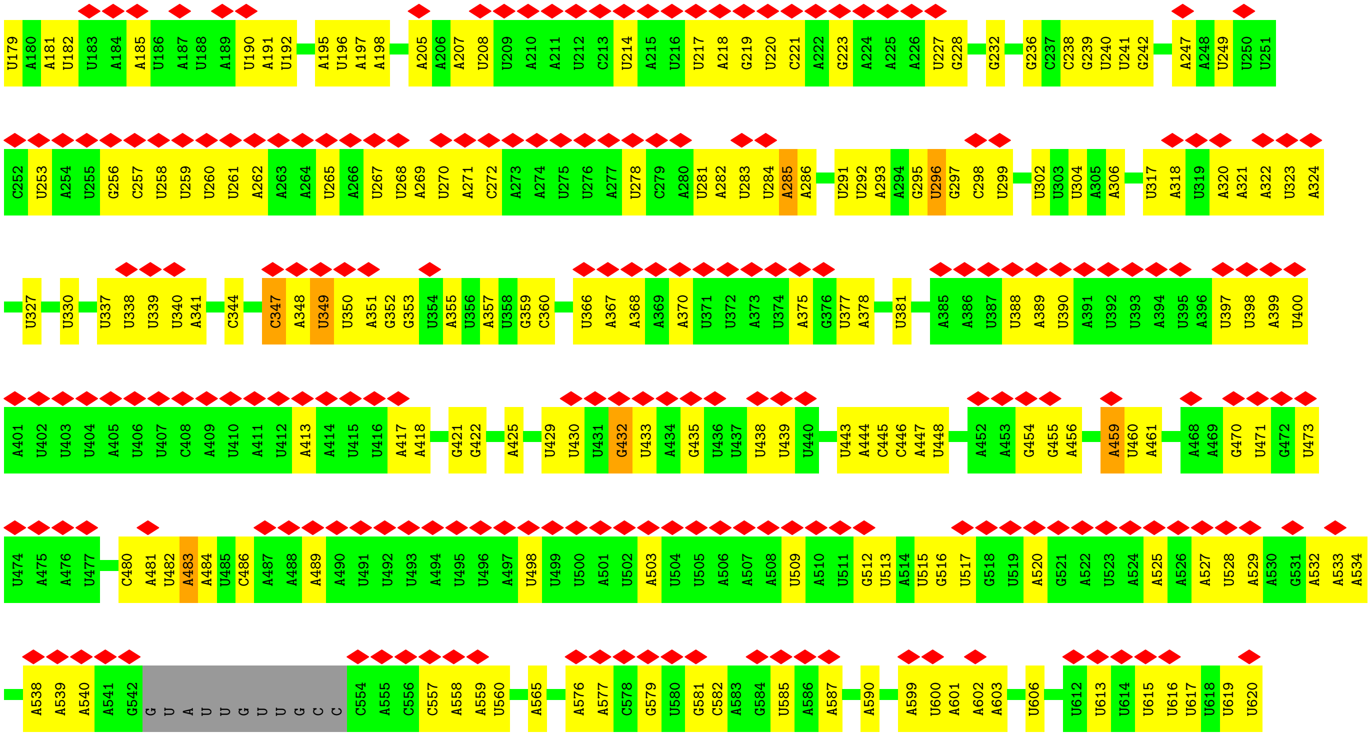
- Molecule 59: UNK-Y

Chain UY:

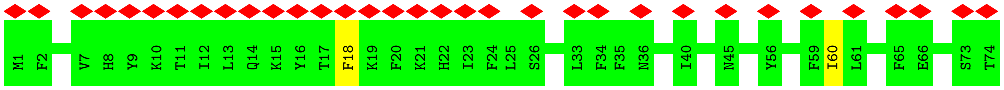
- Molecule 60: 9S rRNA

Chain CA:

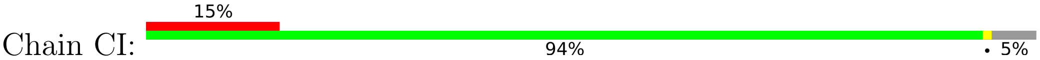


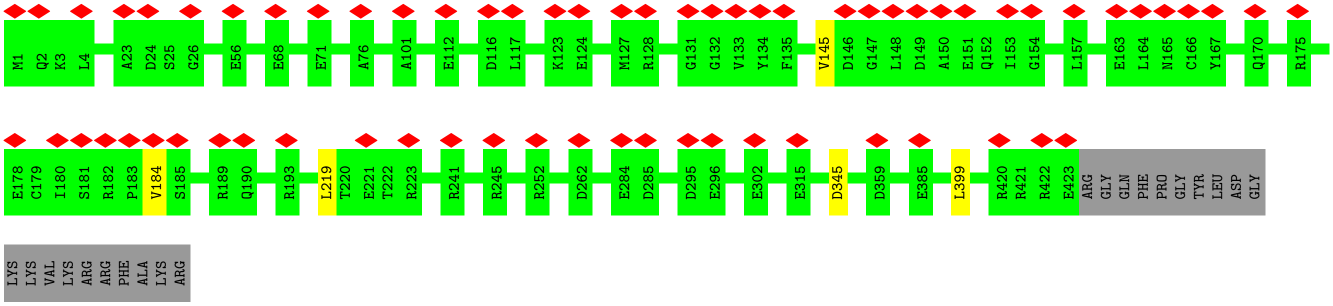


- Molecule 61: mS3m

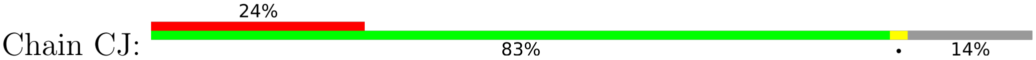


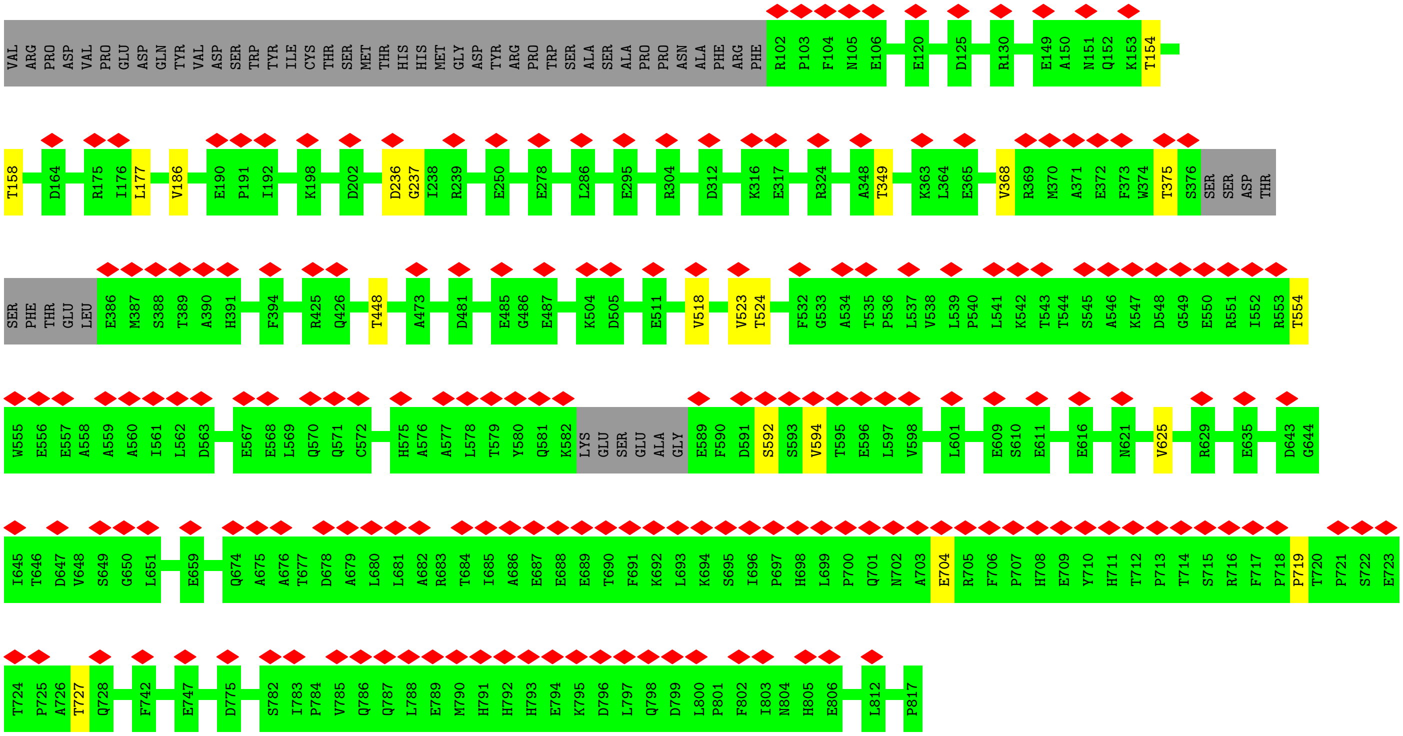
- Molecule 62: uS9m



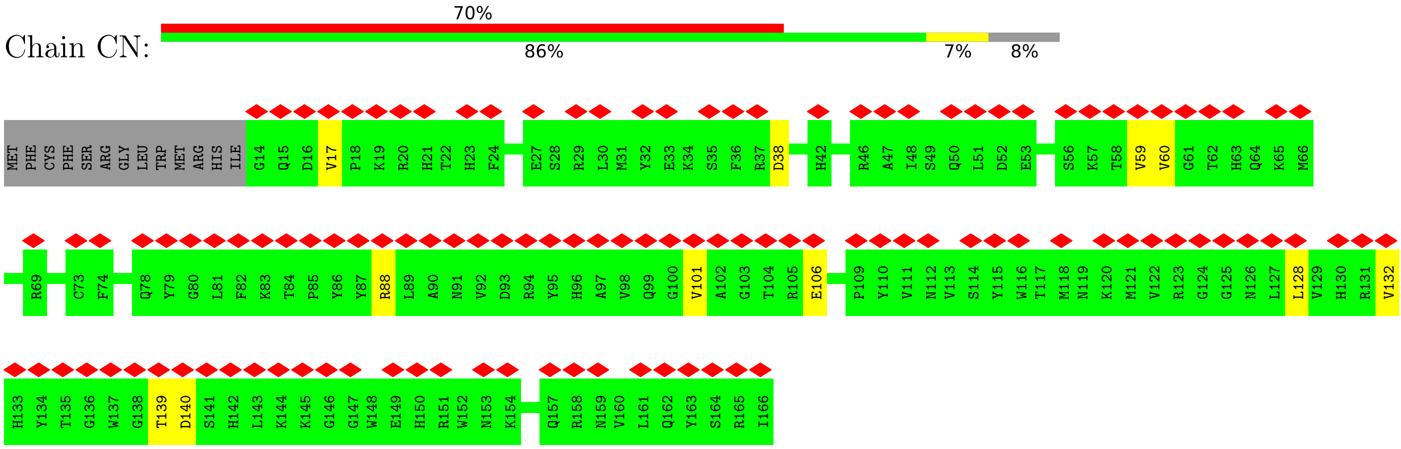


- Molecule 63: uS10m

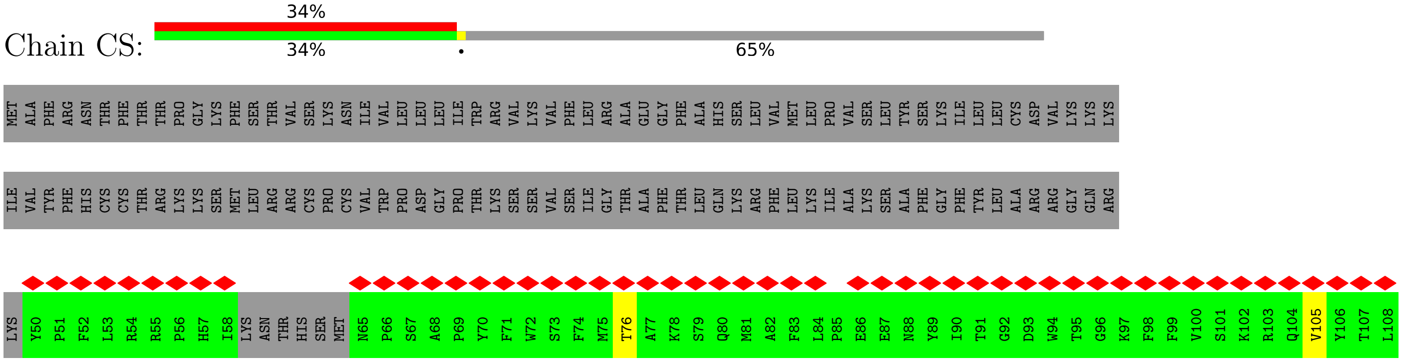


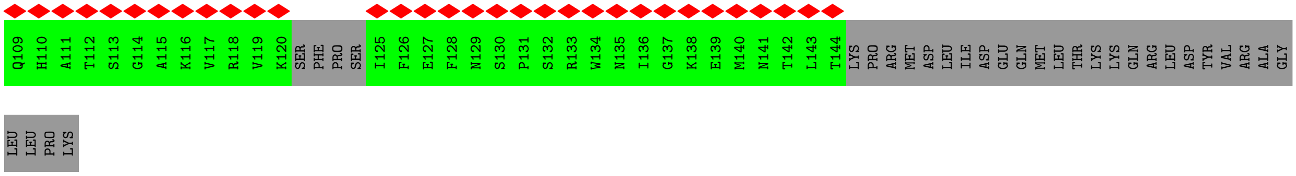


- Molecule 64: uS14m

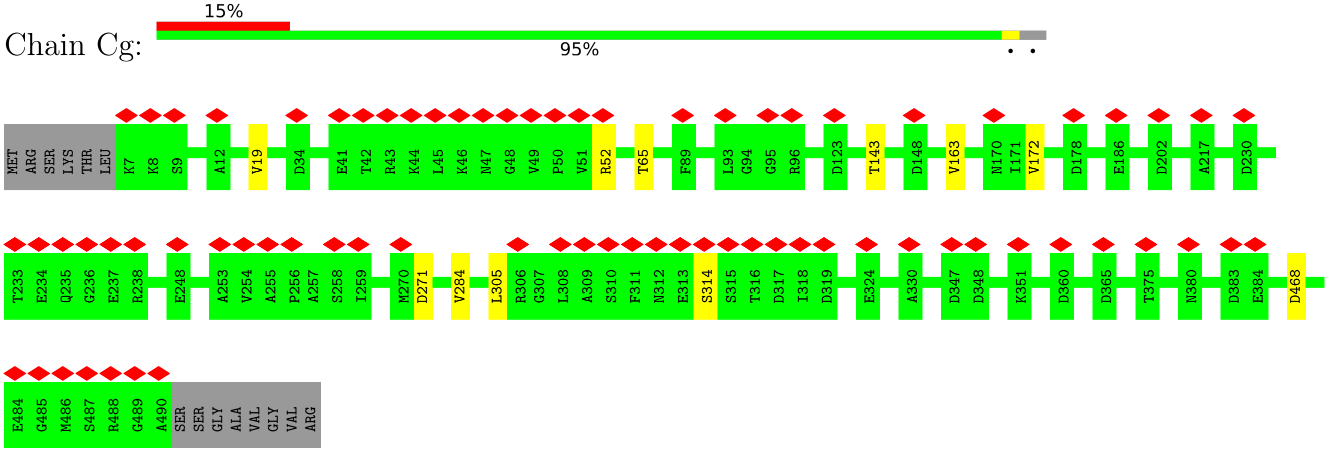


- Molecule 65: uS19m

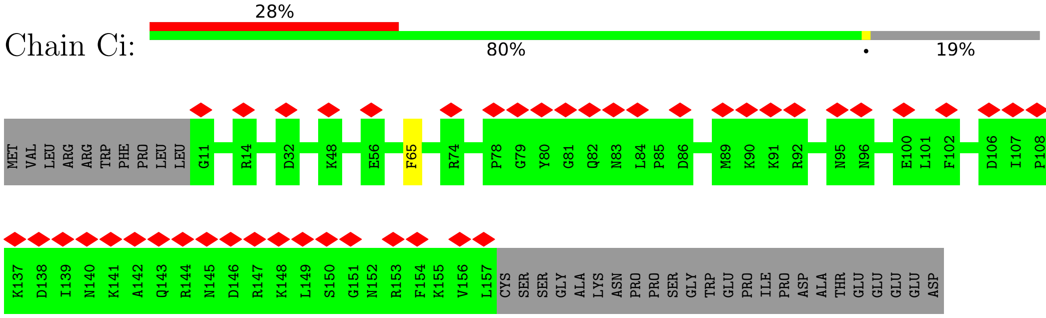




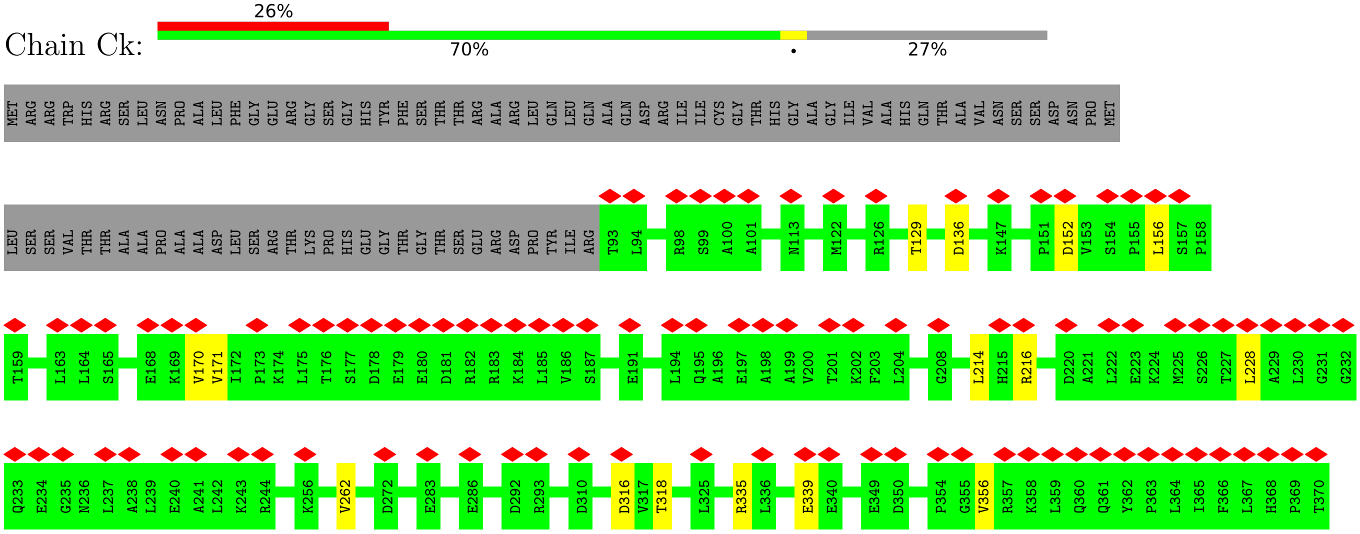
- Molecule 66: mS29

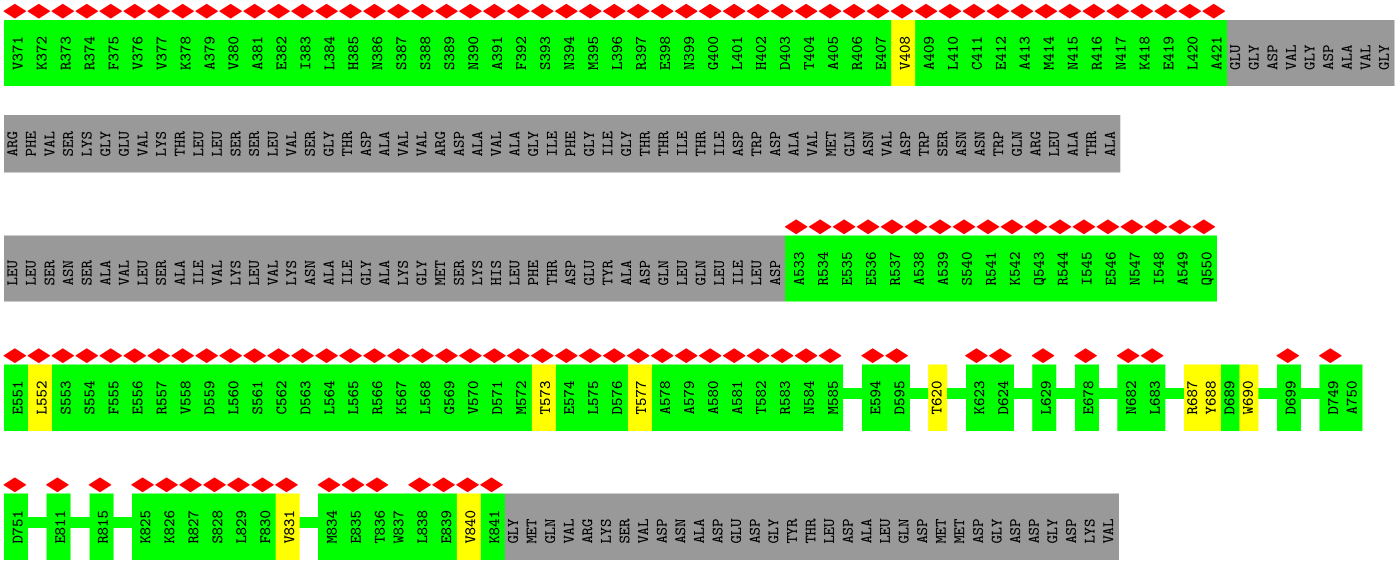


- Molecule 67: mS33



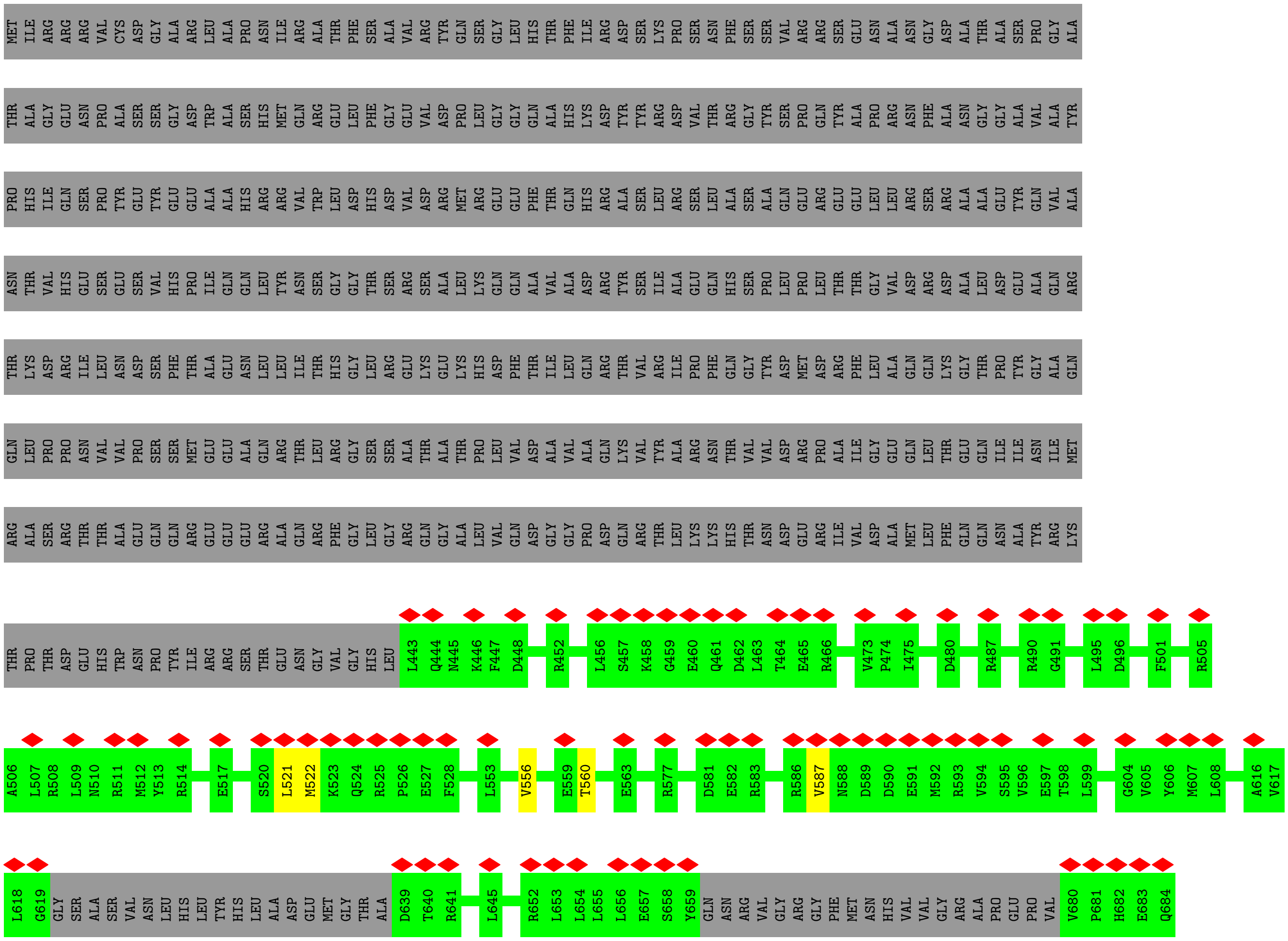
- Molecule 68: mS35

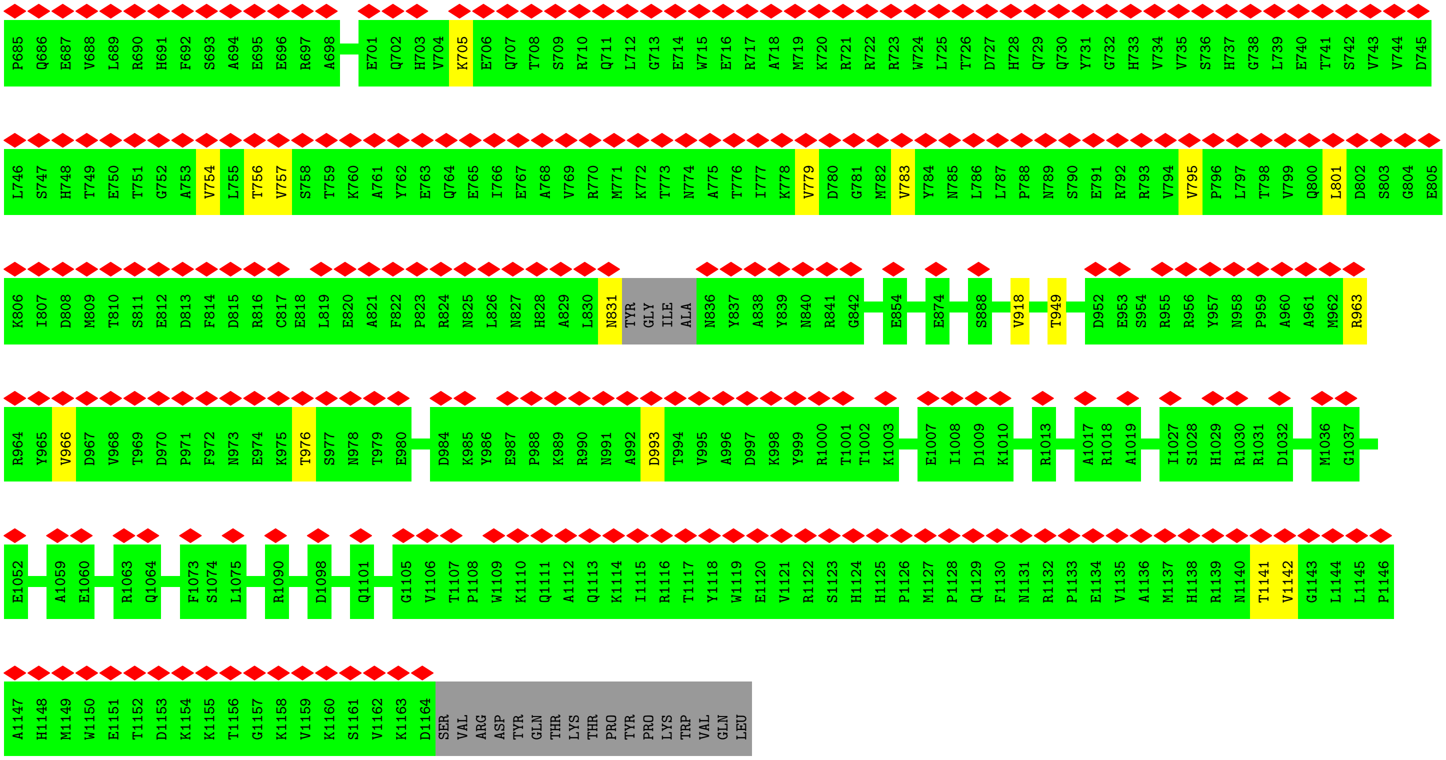




- Molecule 69: mS49

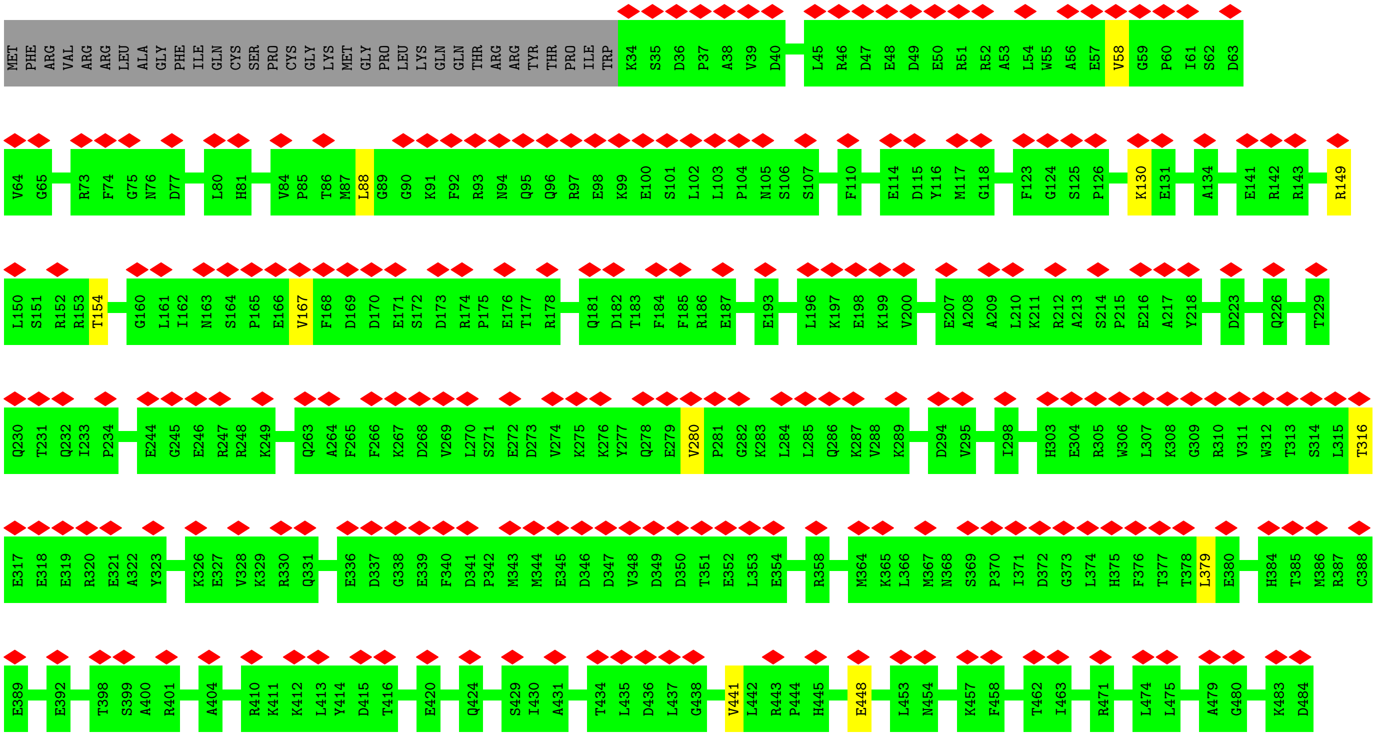
Chain DB:

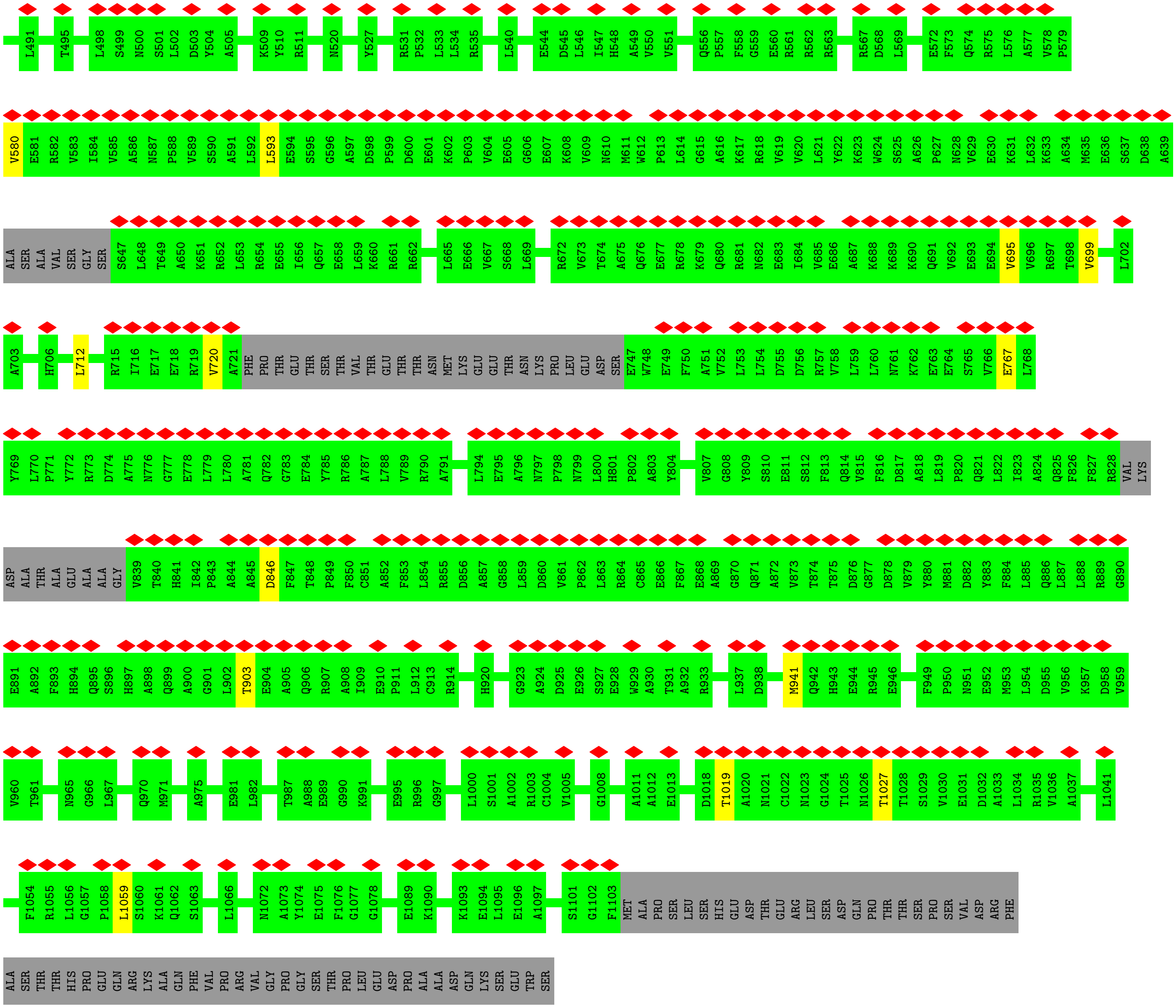




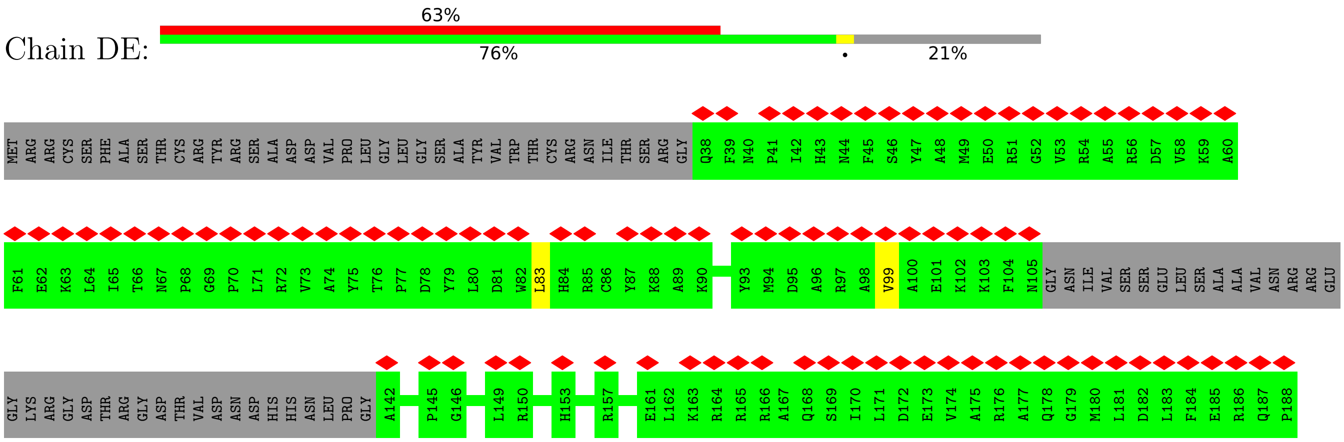
- Molecule 70: mS50

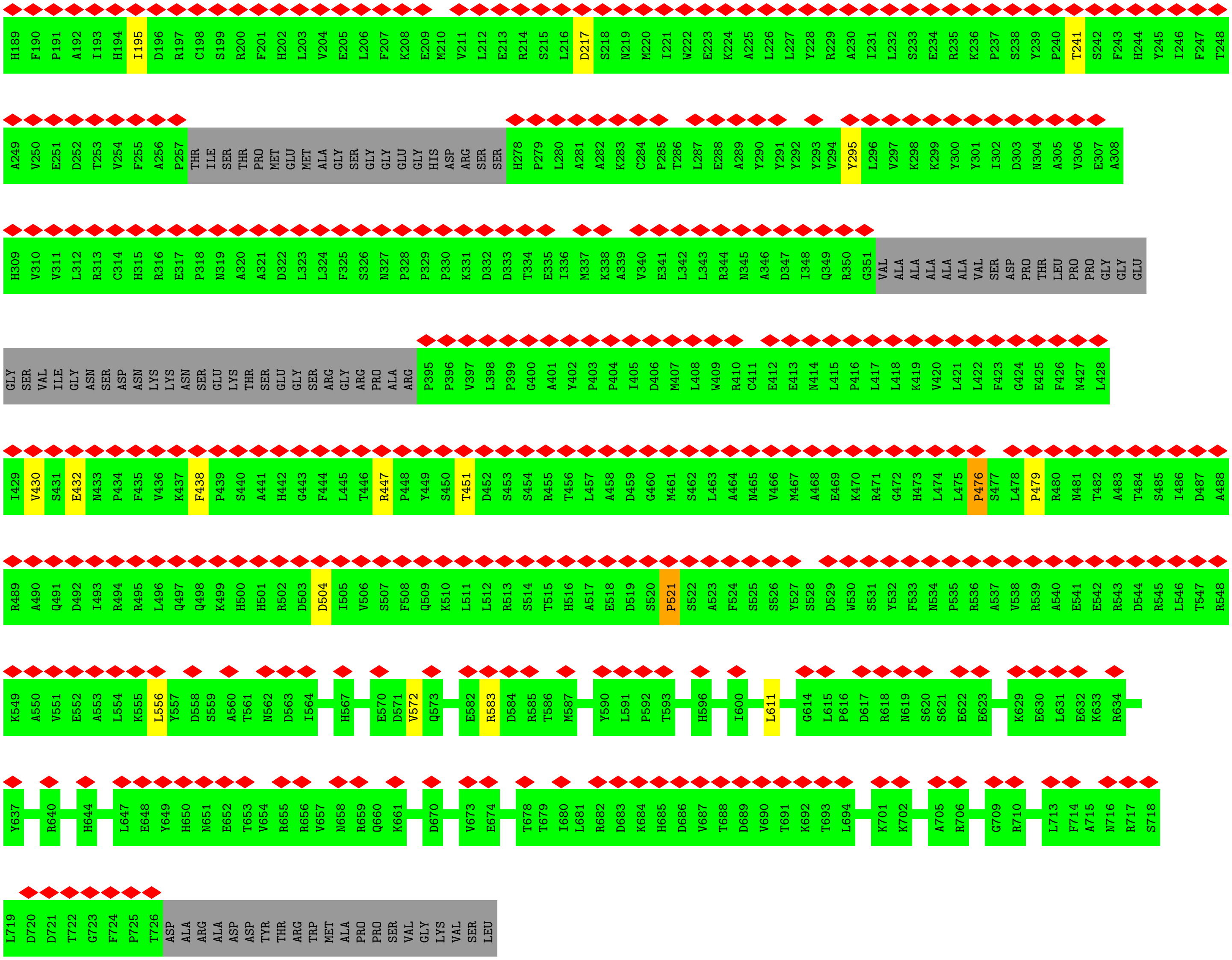
Chain DC:





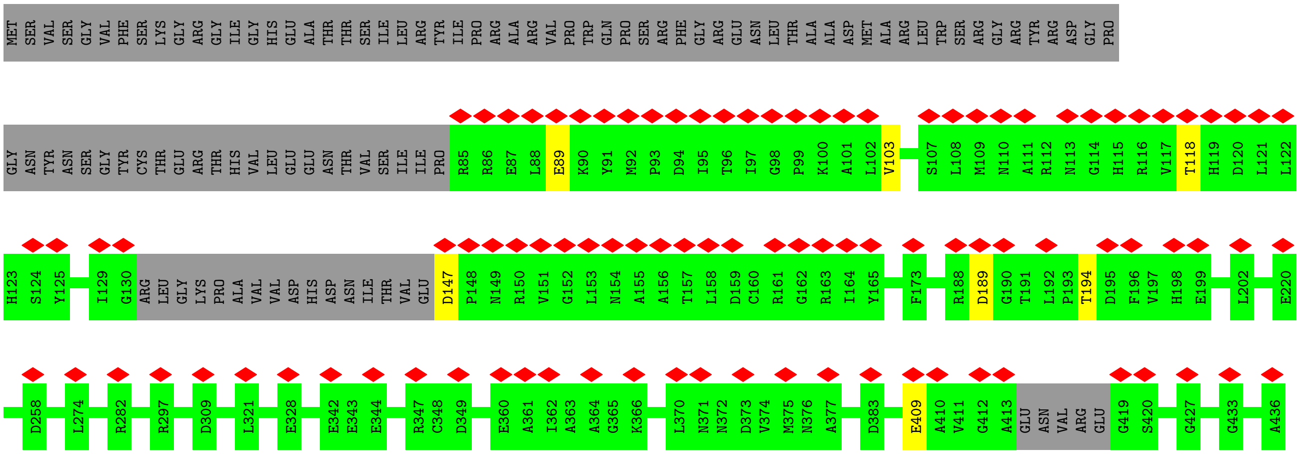
- Molecule 71: mS52

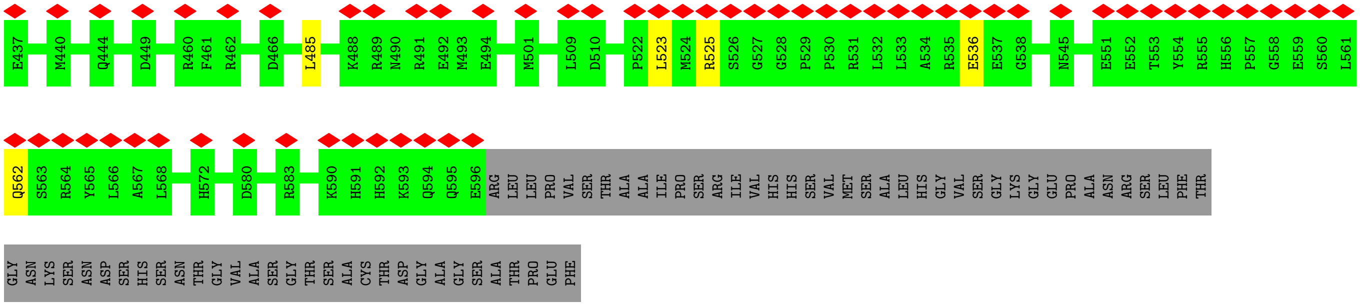




- Molecule 72: mS53

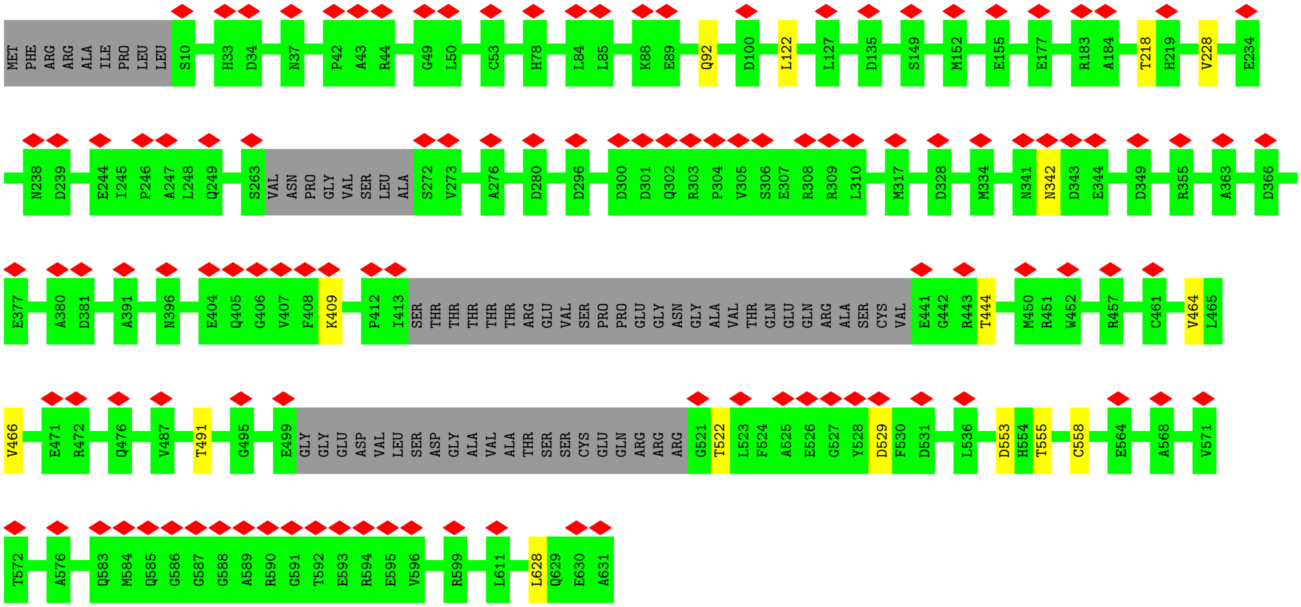
Chain DF:





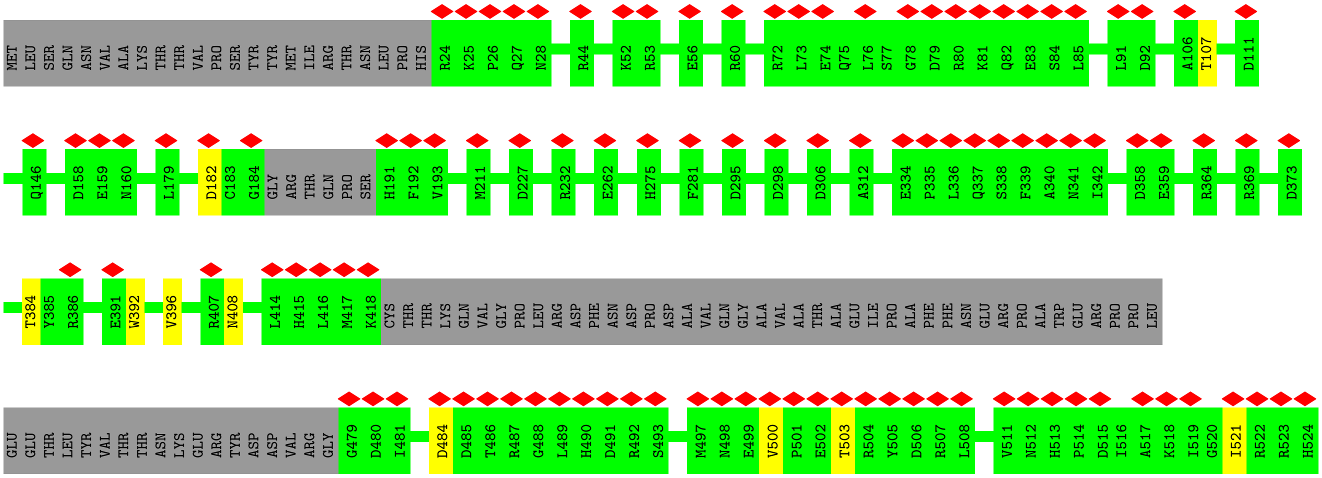
- Molecule 73: mS54

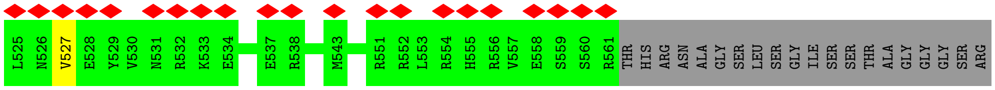
Chain DG:



- Molecule 74: mS55 (KRIPP8)

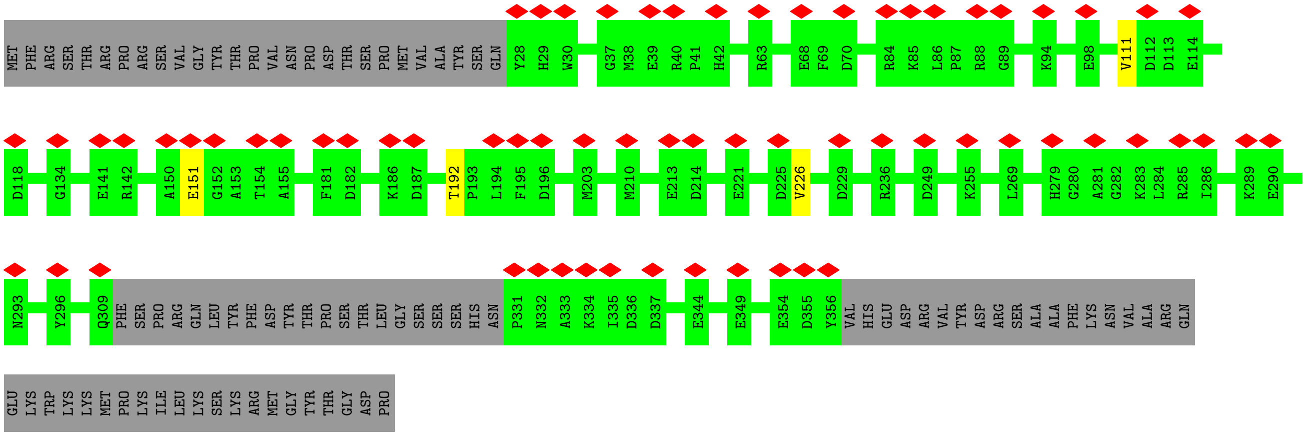
Chain DH:





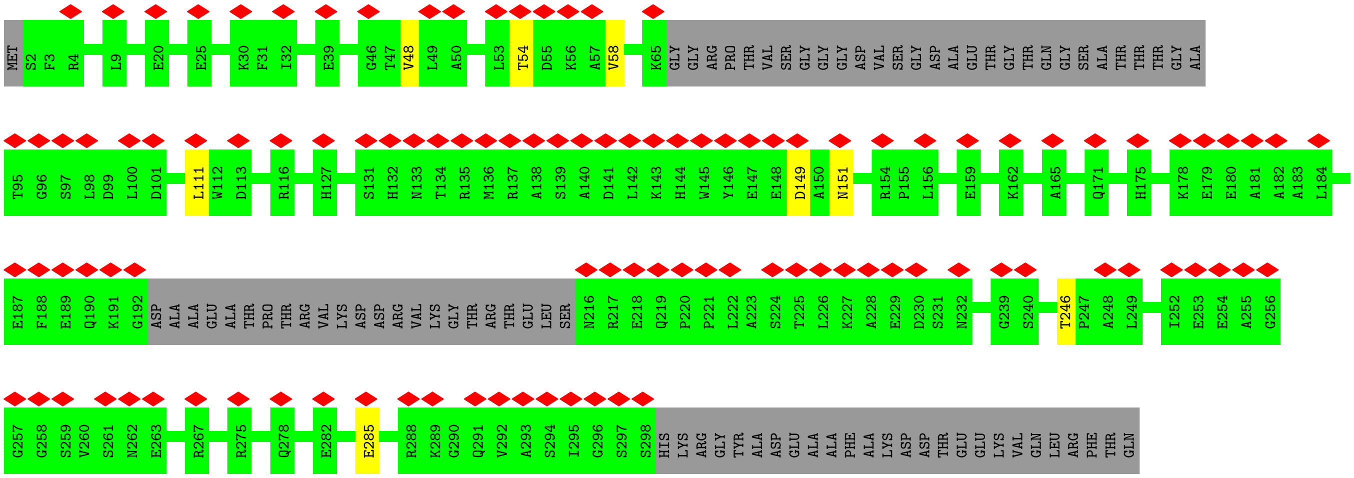
- Molecule 75: mS57

Chain DJ:



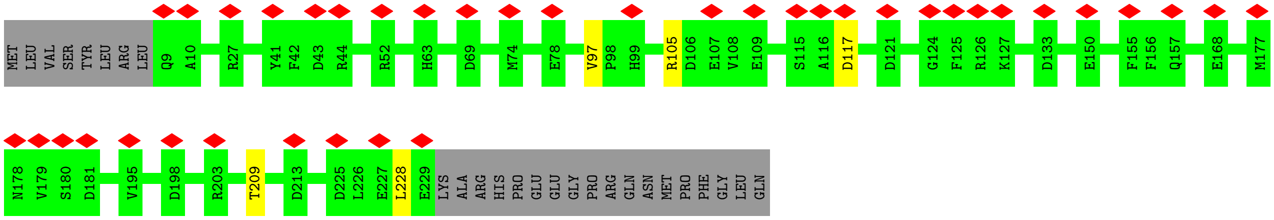
- Molecule 76: mS58

Chain DK:

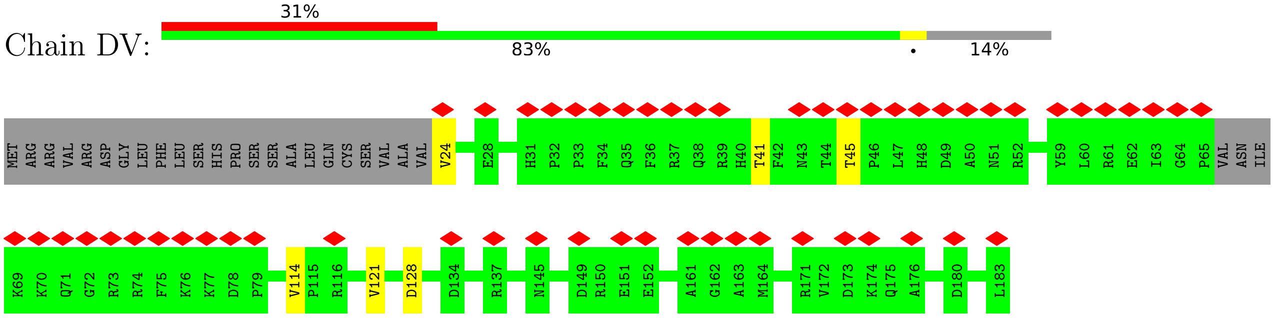


- Molecule 77: mS67

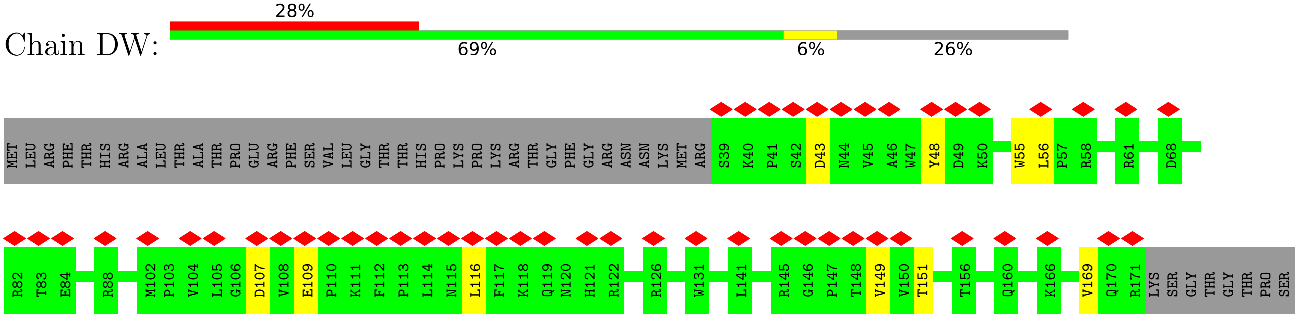
Chain DT:



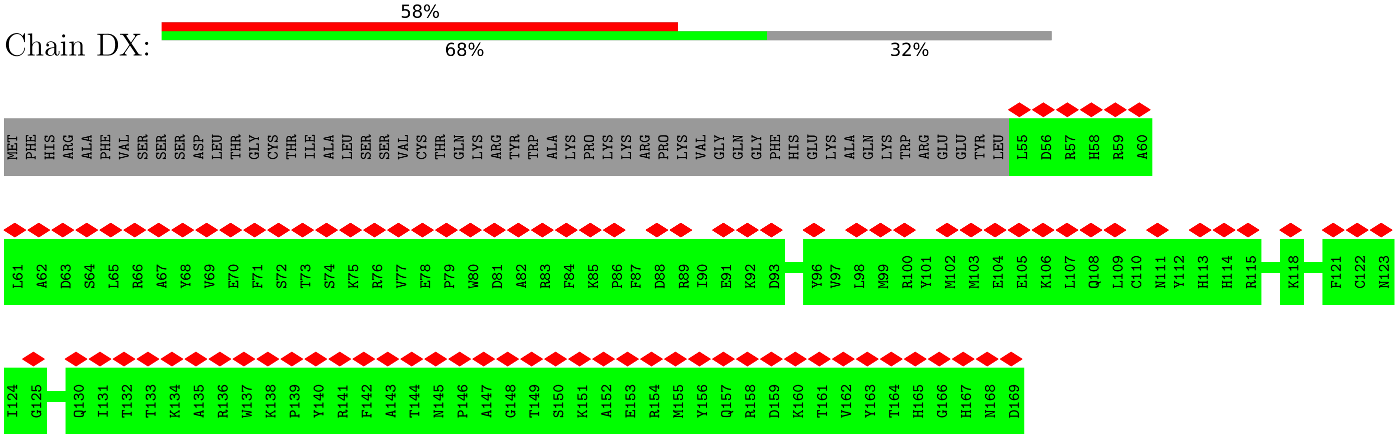
- Molecule 78: mS69



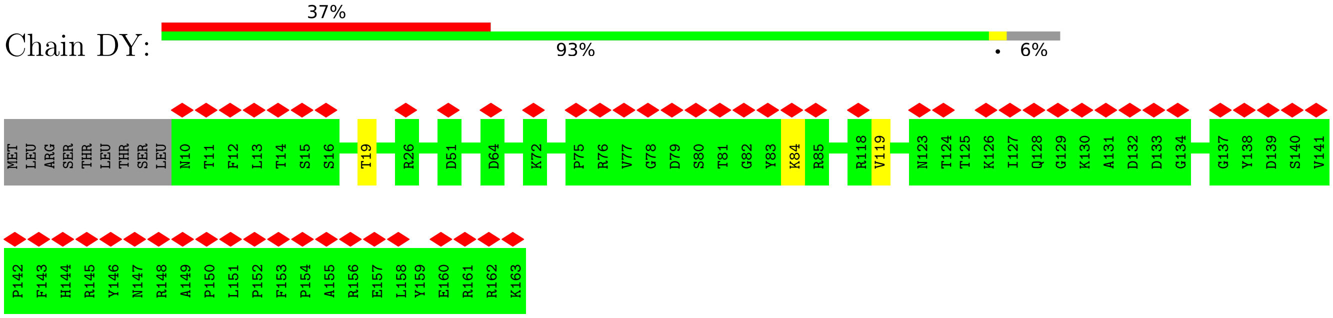
- Molecule 79: mS70



- Molecule 80: mS71

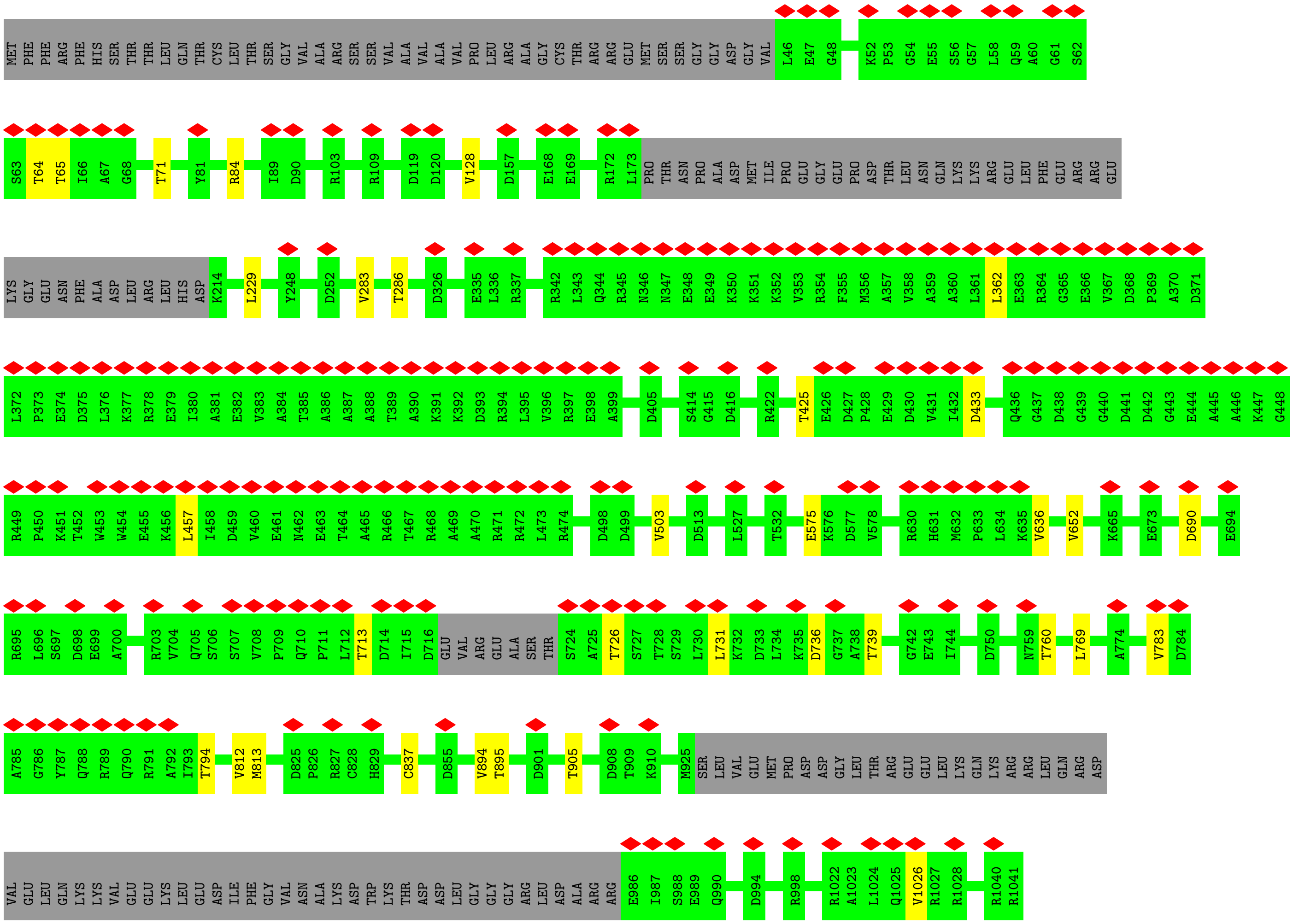


- Molecule 81: mS72



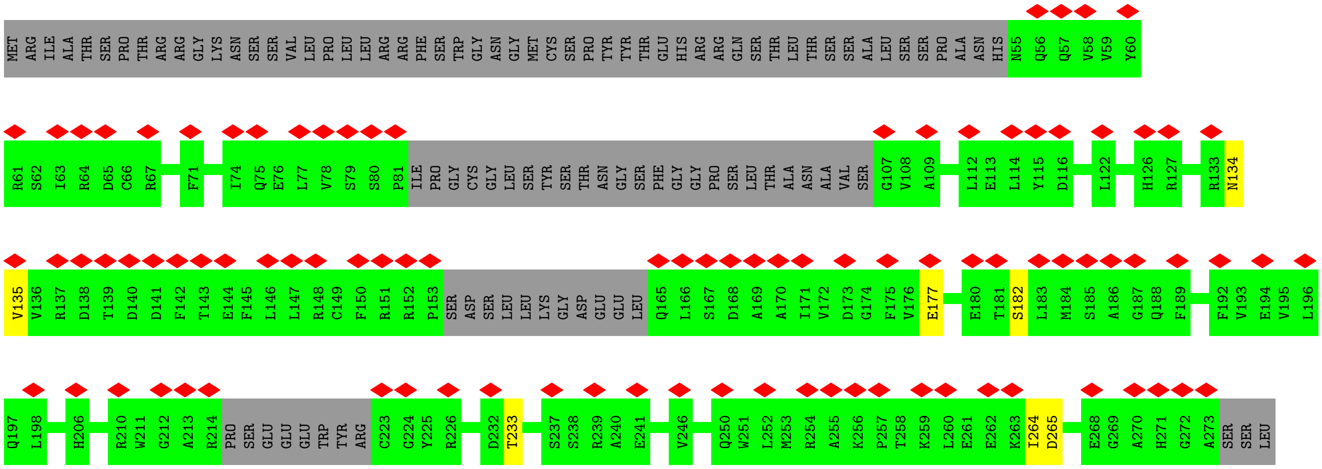
- Molecule 82: mt-SAF1 (RSM22)

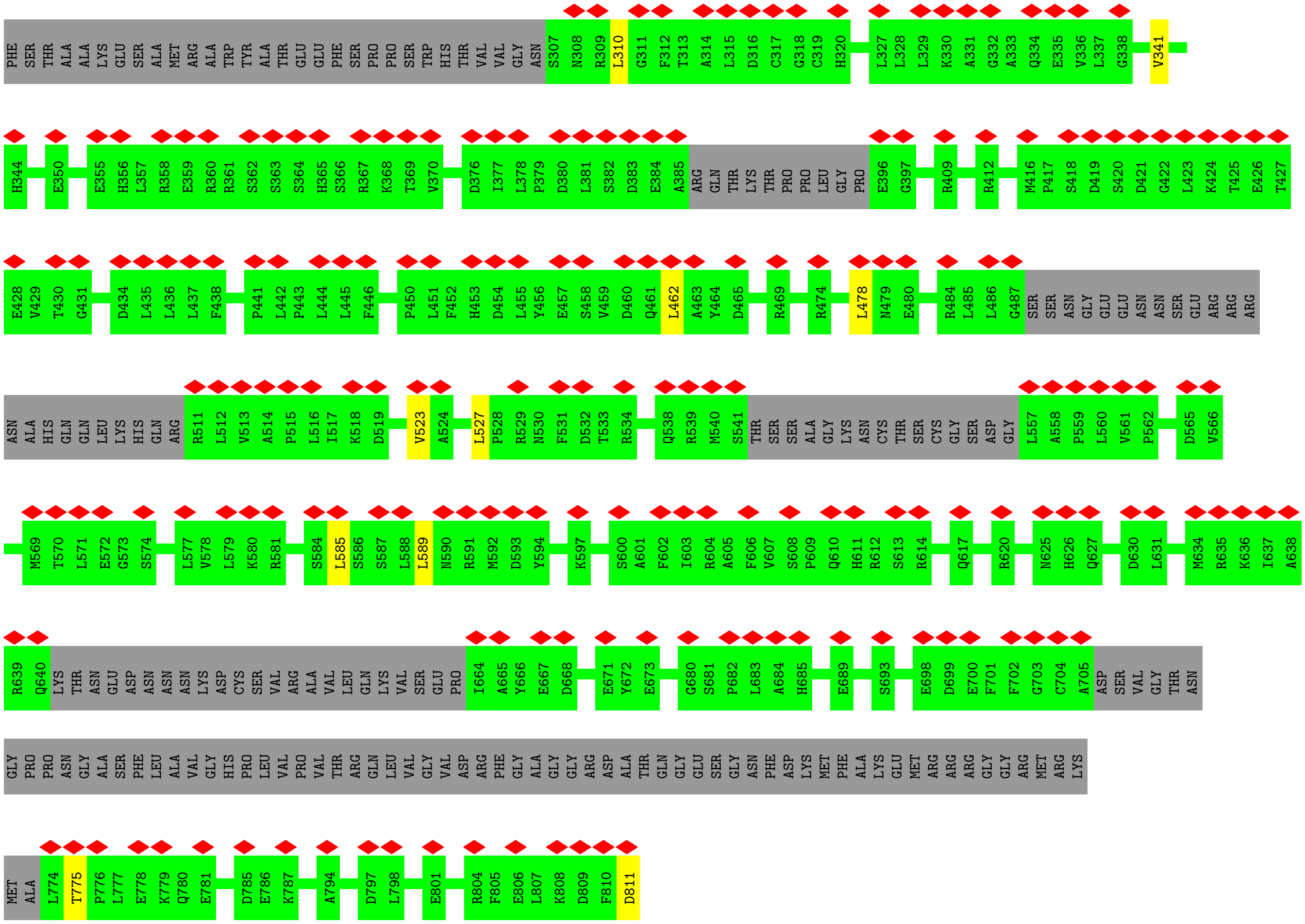
Chain F1:



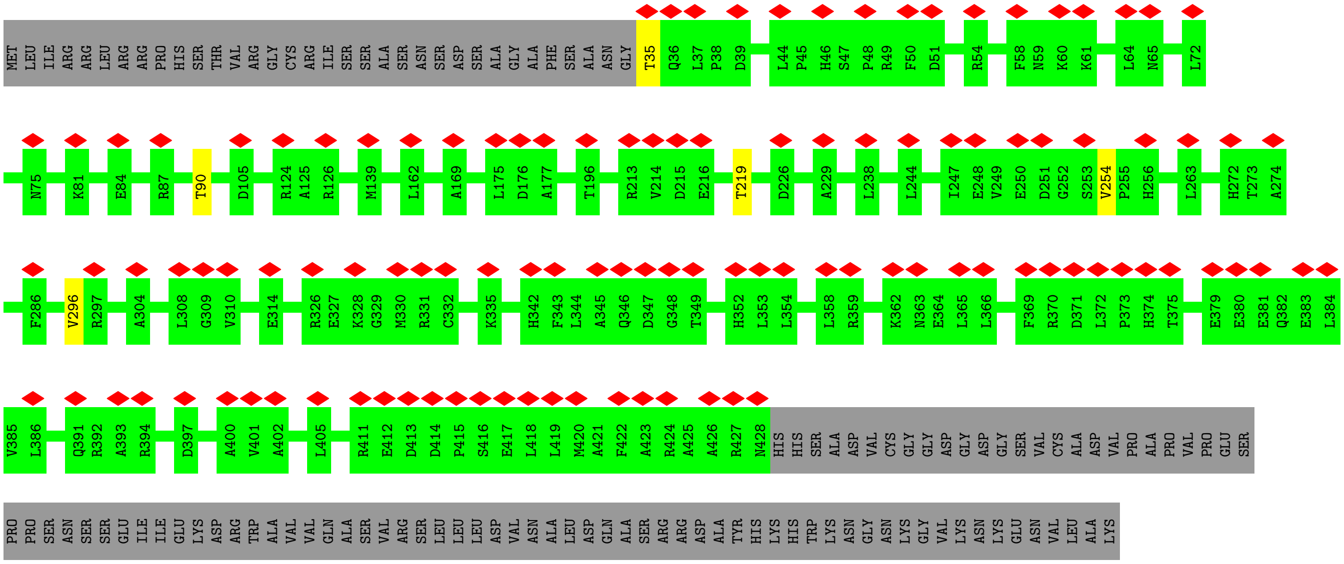
- Molecule 83: mt-SAF4

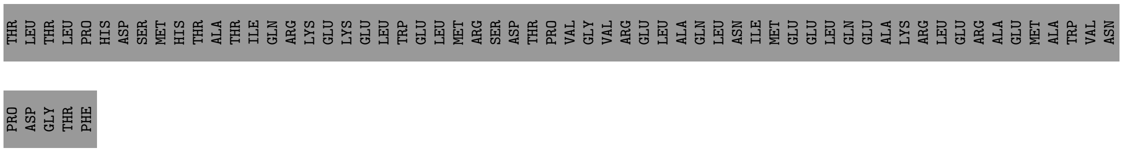
Chain F4:



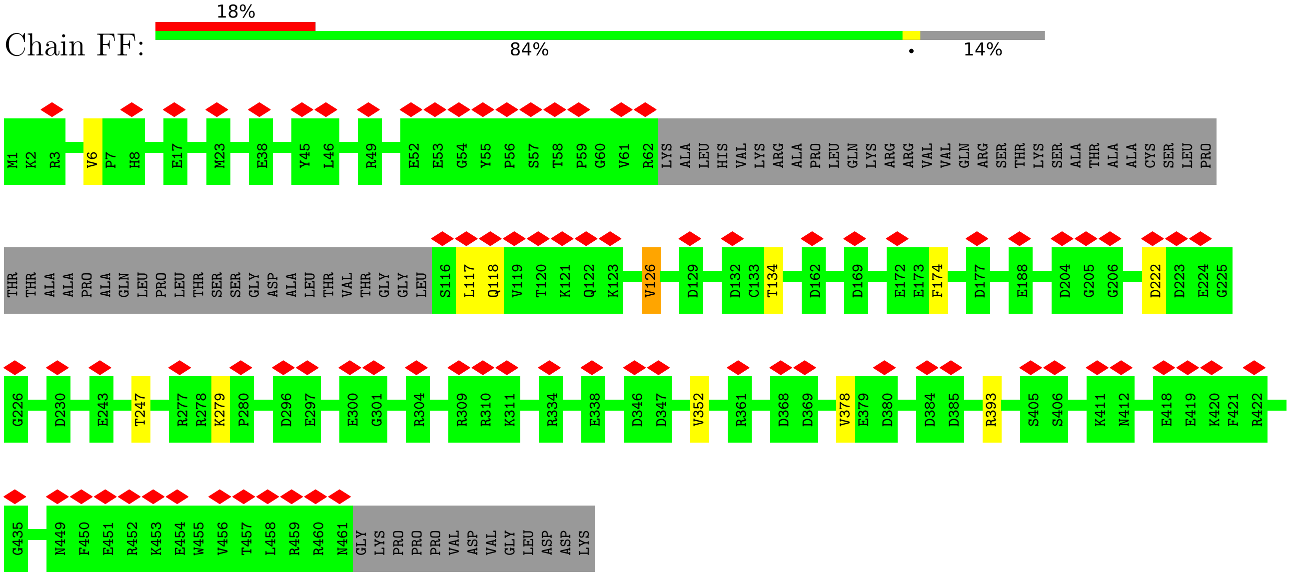


- Molecule 84: mt-SAF12 (KRIPP18)

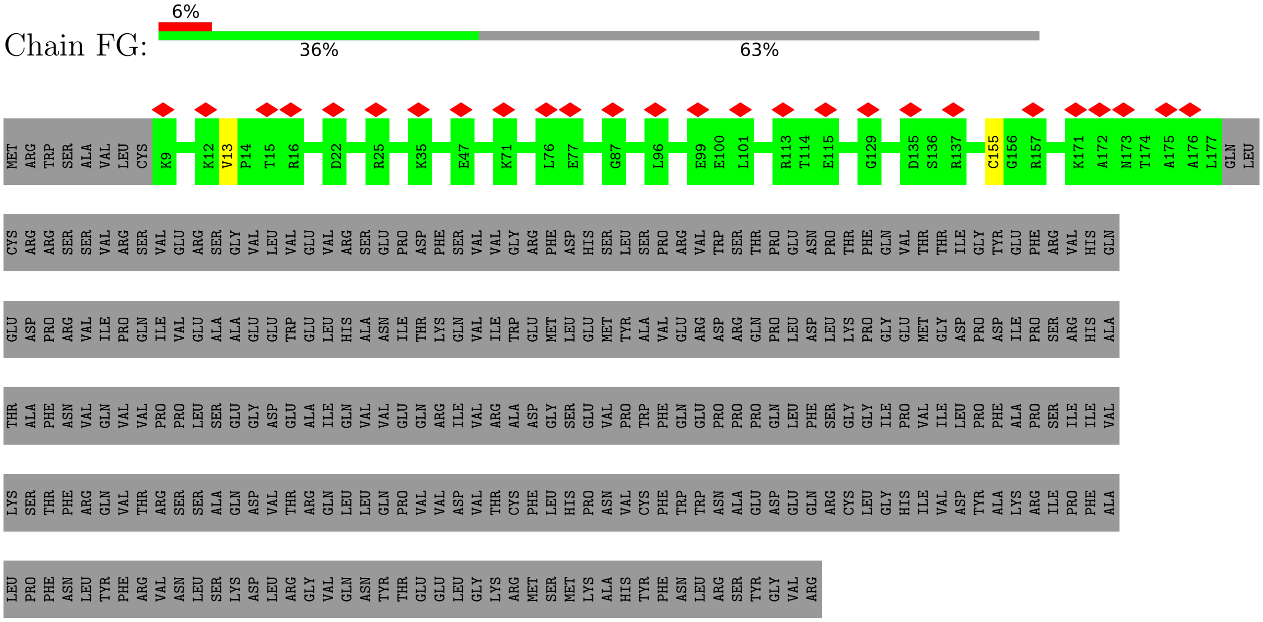




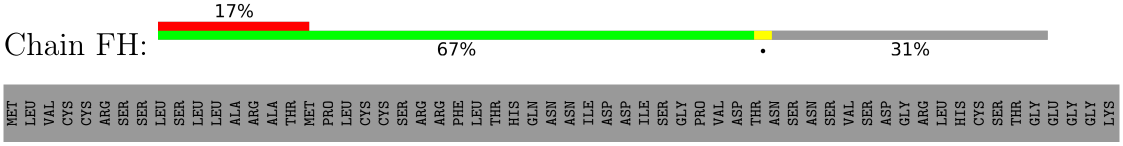
- Molecule 85: mt-SAF14

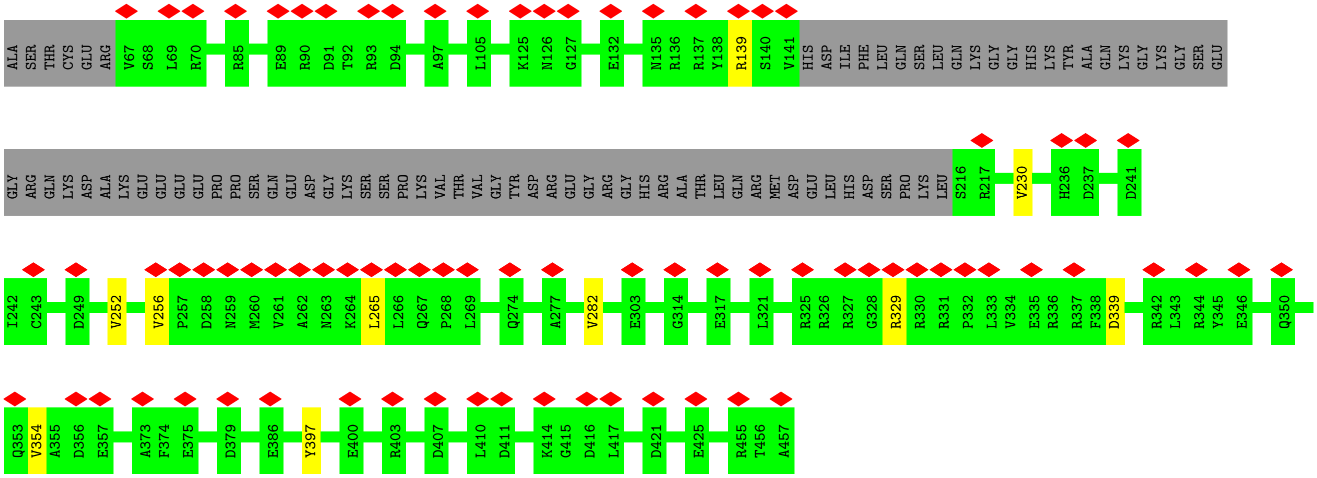


- Molecule 86: mt-SAF15



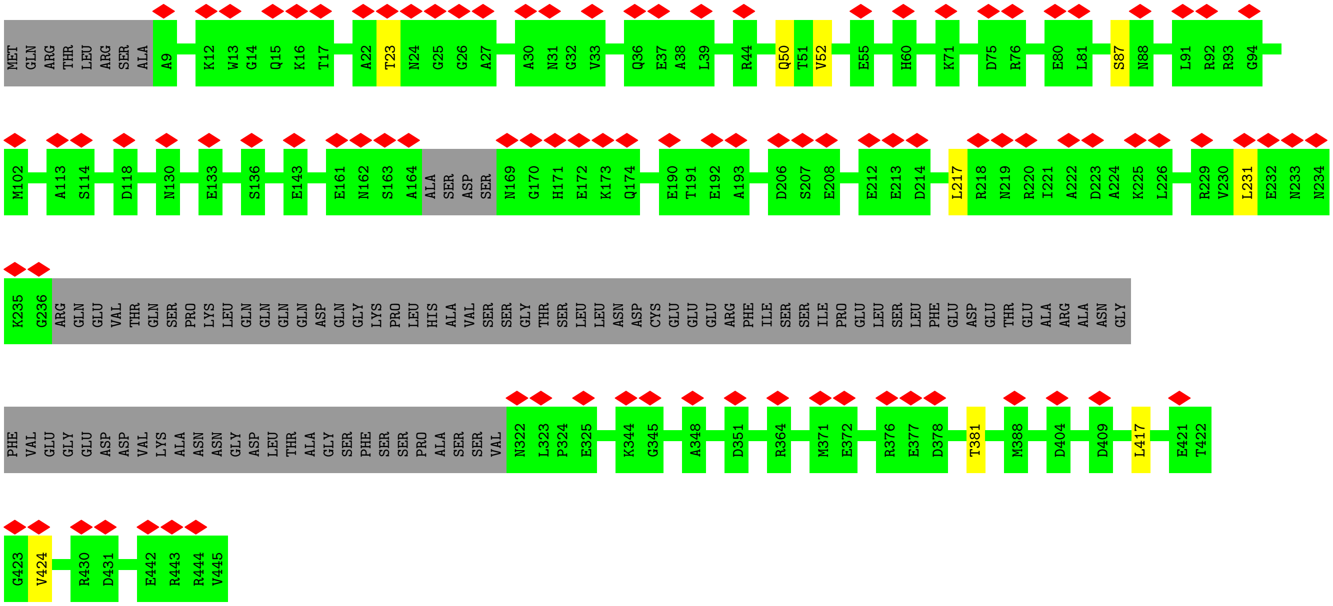
- Molecule 87: mt-SAF16





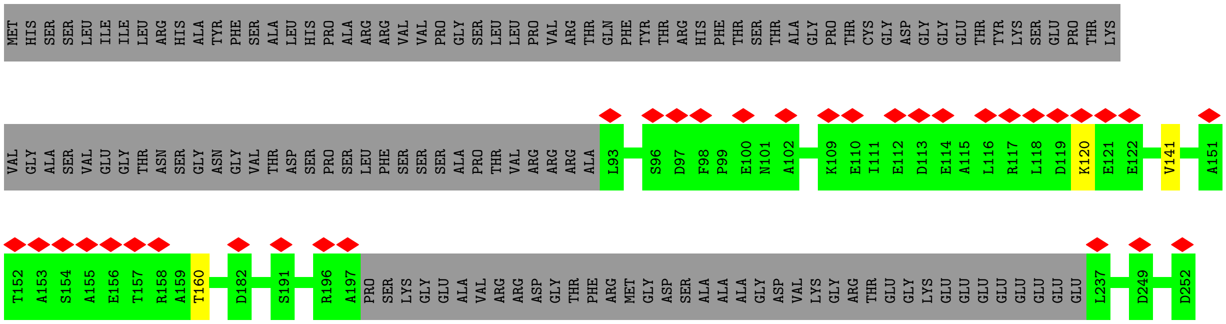
- Molecule 88: mt-SAF17

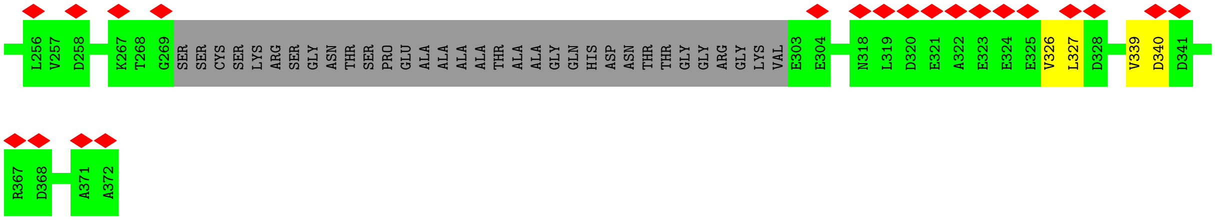
Chain FI:



- Molecule 89: mt-SAF19

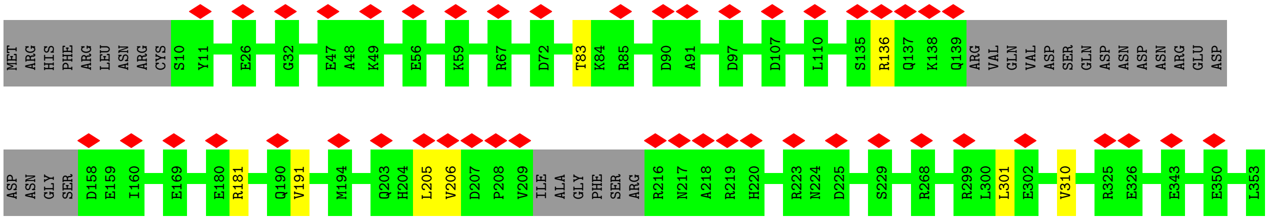
Chain FK:





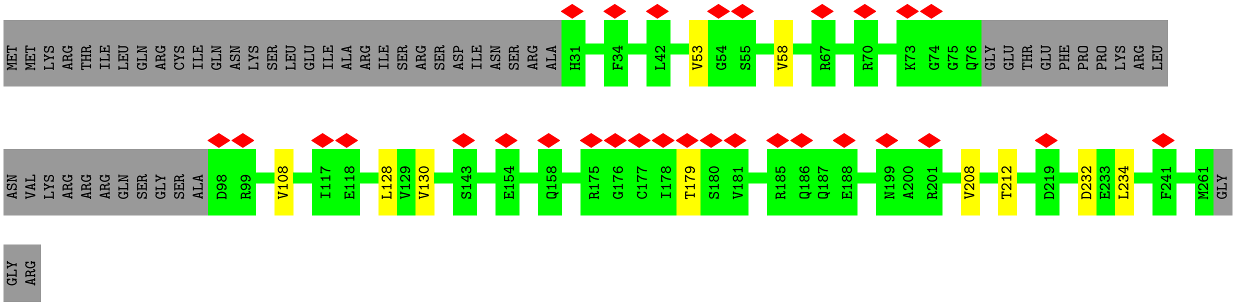
- Molecule 90: mt-SAF20

Chain FL:



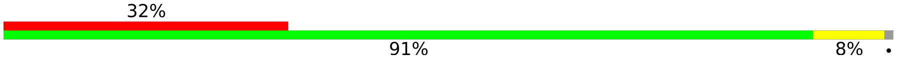
- Molecule 91: mt-SAF25

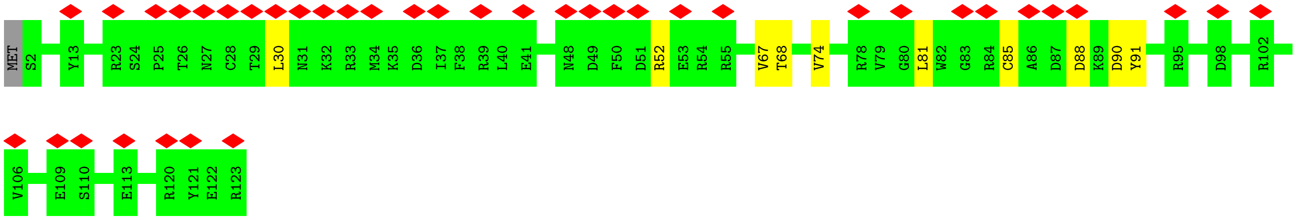
Chain FV:



- Molecule 92: mt-SAF34

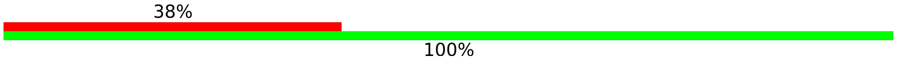
Chain Fe:

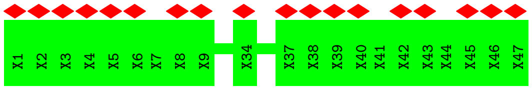




- Molecule 93: UNK-a

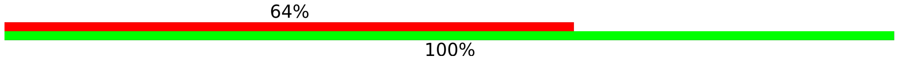
Chain Ua:

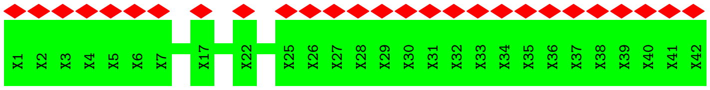




- Molecule 94: UNK-b

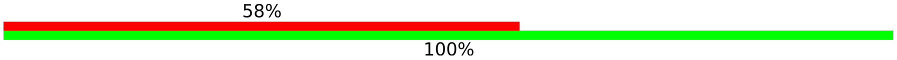
Chain Ub:

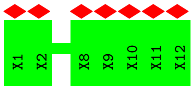




- Molecule 95: UNK-c

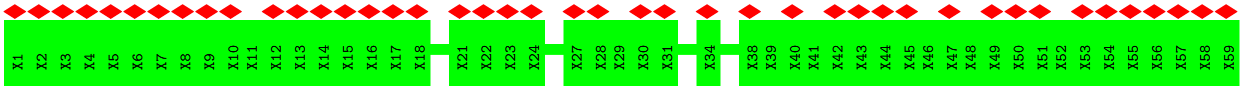
Chain Uc:





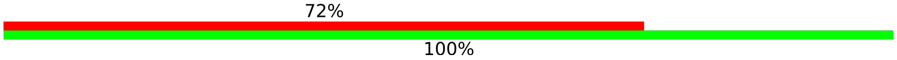
- Molecule 96: UNK-d

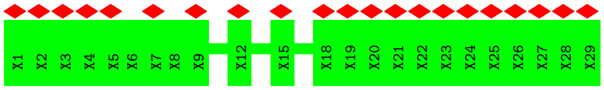
Chain Ud:



- Molecule 97: UNK-e

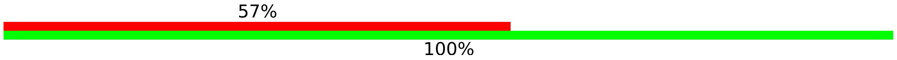
Chain Ue:

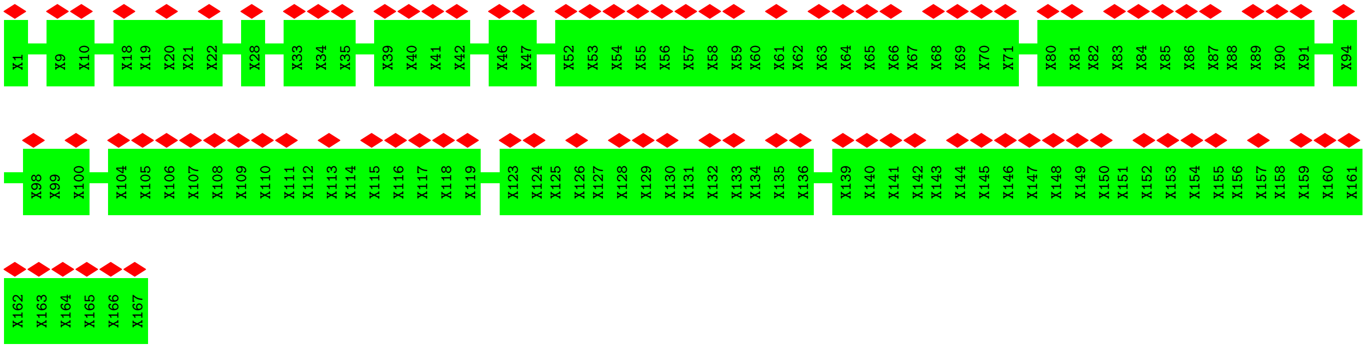




- Molecule 98: UNK-g

Chain Ug:



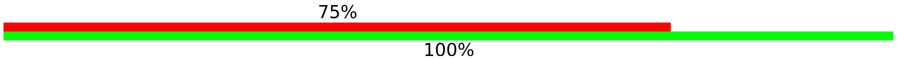


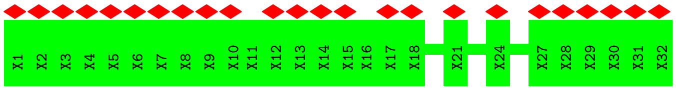
- Molecule 99: UNK-h

Chain Uh:

- Molecule 100: UNK-i

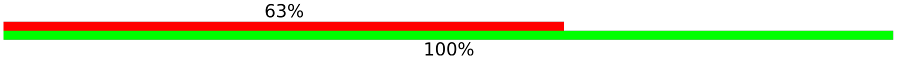
Chain Ui:

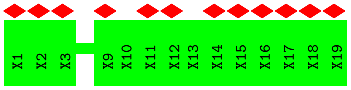




- Molecule 101: UNK-j

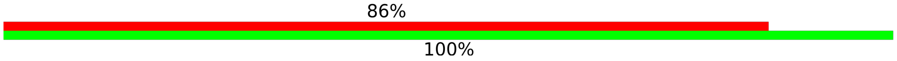
Chain Uj:

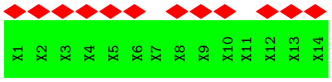




- Molecule 102: UNK-l

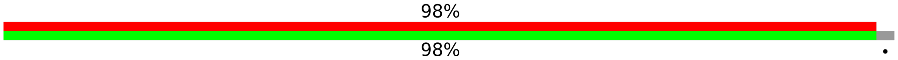
Chain Ul:

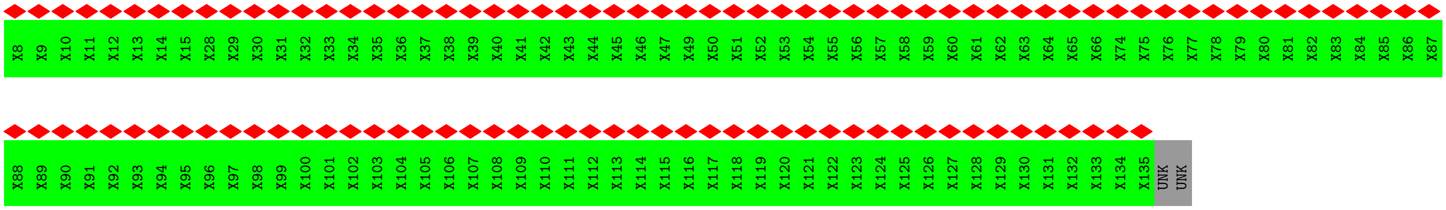




- Molecule 103: UNK-x

Chain Ux:





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 $(e^-/\text{Å}^2)$	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 ⓘ

5.1 Standard geometry ⓘ

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.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
26	F6	220	LEU	CA-CB-CG	7.58	132.73	115.30
60	CA	349	U	OP1-P-O3’	7.28	121.21	105.20
60	CA	99	G	N3-C4-N9	7.25	130.35	126.00
60	CA	99	G	N3-C4-C5	-7.22	124.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	CA	302	U	N1-C2-O2	7.12	127.78	122.80
1	CE	385	PRO	N-CA-CB	7.07	111.78	103.30
60	CA	302	U	N3-C2-O2	-6.94	117.34	122.20
60	CA	349	U	P-O3'-C3'	6.83	127.89	119.70
60	CA	99	G	C8-N9-C1'	-6.73	118.25	127.00
60	CA	344	C	N1-C2-O2	6.61	122.86	118.90
60	CA	512	G	C4-N9-C1'	6.43	134.86	126.50
60	CA	606	U	N3-C2-O2	-6.36	117.75	122.20
60	CA	512	G	N3-C4-C5	-6.20	125.50	128.60
71	DE	479	PRO	N-CA-CB	6.18	110.72	103.30
25	F5	496	PRO	N-CA-CB	6.10	110.62	103.30
9	Ca	525	PRO	N-CA-CB	6.05	110.56	103.30
60	CA	78	G	P-O3'-C3'	6.01	126.91	119.70
21	DU	206	PRO	N-CA-CB	5.91	110.39	103.30
41	FZ	73	PRO	N-CA-CB	5.90	110.38	103.30
60	CA	512	G	N3-C4-N9	5.90	129.54	126.00
21	DU	200	PRO	N-CA-CB	5.88	110.36	103.30
71	DE	476	PRO	N-CA-CB	5.82	110.28	103.30
60	CA	517	U	C2-N1-C1'	5.81	124.67	117.70
5	CO	75	LEU	CA-CB-CG	5.80	128.65	115.30
60	CA	285	A	P-O3'-C3'	5.79	126.65	119.70
60	CA	486	C	C2-N1-C1'	5.76	125.14	118.80
25	F5	521	PRO	N-CA-CB	5.76	110.21	103.30
1	CE	413	ILE	C-N-CD	5.75	140.48	128.40
25	F5	522	PRO	N-CA-CB	5.75	110.19	103.30
41	FZ	114	PRO	N-CA-CB	5.71	110.15	103.30
60	CA	135	U	N1-C2-O2	5.71	126.80	122.80
41	FZ	130	PRO	N-CA-CB	5.71	110.15	103.30
23	F2	946	HIS	C-N-CA	5.66	134.19	122.30
60	CA	135	U	C5-C6-N1	5.65	125.53	122.70
60	CA	459	A	N9-C4-C5	5.61	108.05	105.80
60	CA	19	U	C2-N1-C1'	5.60	124.42	117.70
60	CA	344	C	N3-C2-O2	-5.58	118.00	121.90
71	DE	521	PRO	N-CA-CB	5.55	109.96	103.30
60	CA	19	U	N3-C2-O2	-5.54	118.32	122.20
4	CK	315	LEU	CA-CB-CG	5.54	128.04	115.30
60	CA	456	A	N1-C2-N3	-5.51	126.55	129.30
60	CA	135	U	C2-N1-C1'	5.49	124.28	117.70
60	CA	317	U	C2-N1-C1'	5.47	124.26	117.70
60	CA	95	U	N1-C2-O2	5.45	126.61	122.80
60	CA	348	A	C2-N3-C4	5.43	113.32	110.60
60	CA	615	U	C2-N1-C1'	5.40	124.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	CA	347	C	C5-C6-N1	5.39	123.69	121.00
60	CA	512	G	C8-N9-C1'	-5.38	120.00	127.00
60	CA	3	A	C2-N3-C4	5.38	113.29	110.60
60	CA	36	U	N1-C2-O2	5.33	126.53	122.80
60	CA	296	U	O5'-P-OP2	-5.32	100.91	105.70
60	CA	295	G	OP1-P-O3'	5.27	116.80	105.20
60	CA	360	C	C2-N1-C1'	5.21	124.53	118.80
60	CA	95	U	N3-C2-O2	-5.17	118.58	122.20
60	CA	486	C	N1-C2-O2	5.16	121.99	118.90
60	CA	295	G	P-O3'-C3'	5.15	125.88	119.70
60	CA	347	C	C6-N1-C2	-5.15	118.24	120.30
60	CA	517	U	N1-C2-O2	5.15	126.40	122.80
60	CA	483	A	P-O3'-C3'	5.15	125.88	119.70
60	CA	265	U	N1-C2-O2	5.13	126.39	122.80
60	CA	344	C	C6-N1-C2	-5.12	118.25	120.30
60	CA	347	C	C2-N1-C1'	5.12	124.43	118.80
83	F4	585	LEU	CA-CB-CG	5.11	127.05	115.30
60	CA	55	U	N1-C2-O2	5.11	126.37	122.80
60	CA	317	U	N3-C2-O2	-5.01	118.69	122.20
60	CA	432	G	P-O3'-C3'	5.00	125.71	119.70
60	CA	296	U	O5'-P-OP1	5.00	116.70	110.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	DD	414	ARG	Peptide
74	DH	484	ASP	Peptide
79	DW	55	TRP	Peptide
24	F3	490	GLN	Peptide
27	F7	381	LEU	Peptide
28	F8	644	ASP	Peptide
85	FF	279	LYS	Peptide
36	FP	84	HIS	Peptide
38	FW	214	PRO	Peptide
92	Fe	85	CYS	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CE	385	PRO

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Mol	Chain	Res	Type
36	FP	85	LYS
63	CJ	592	SER
71	DE	521	PRO
1	CE	384	ALA
27	F7	565	LEU
63	CJ	236	ASP
25	F5	495	MET
71	DE	476	PRO
27	F7	383	ILE
63	CJ	237	GLY
85	FF	126	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (696) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CE	112	THR
1	CE	204	VAL
1	CE	217	VAL
1	CE	222	VAL
1	CE	224	VAL
1	CE	225	LEU
1	CE	268	THR
1	CE	305	GLU
1	CE	409	ASP
2	CF	111	LEU
3	CH	53	ARG
3	CH	86	THR
3	CH	115	ASP
3	CH	128	VAL
3	CH	150	THR
3	CH	154	ASP
4	CK	193	VAL
4	CK	207	VAL
4	CK	217	LEU
4	CK	221	THR
4	CK	258	LEU
4	CK	267	ARG
4	CK	281	VAL
5	CO	90	MET
5	CO	122	VAL
5	CO	127	THR
5	CO	162	THR
5	CO	283	VAL
5	CO	367	LEU

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Mol	Chain	Res	Type
5	CO	419	VAL
6	CP	82	VAL
6	CP	172	VAL
6	CP	181	GLU
7	CQ	34	THR
7	CQ	61	VAL
7	CQ	64	THR
7	CQ	70	ARG
7	CQ	123	ARG
7	CQ	198	LEU
8	CR	69	HIS
8	CR	131	THR
8	CR	139	THR
8	CR	151	ASN
8	CR	181	ARG
8	CR	198	THR
8	CR	228	VAL
9	Ca	106	ASN
9	Ca	122	GLU
9	Ca	171	THR
9	Ca	312	ASP
9	Ca	365	LEU
9	Ca	379	MET
9	Ca	405	ARG
9	Ca	449	VAL
9	Ca	456	LEU
9	Ca	472	VAL
9	Ca	574	VAL
10	Cb	28	TYR
10	Cb	118	VAL
10	Cb	119	ARG
10	Cb	125	MET
10	Cb	126	GLU
10	Cb	137	VAL
10	Cb	175	ILE
10	Cb	182	VAL
11	Cd	33	THR
12	Cj	145	THR
12	Cj	161	VAL
12	Cj	167	ASP
12	Cj	234	THR
13	Cn	163	ARG

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Mol	Chain	Res	Type
14	Cp	12	THR
14	Cp	35	THR
14	Cp	42	VAL
14	Cp	53	VAL
14	Cp	145	GLU
15	DD	89	SER
15	DD	90	MET
15	DD	297	ARG
15	DD	523	LYS
15	DD	586	VAL
15	DD	653	PHE
15	DD	673	VAL
15	DD	754	THR
16	DI	20	THR
16	DI	24	VAL
16	DI	113	VAL
16	DI	187	THR
16	DI	279	VAL
16	DI	327	ARG
16	DI	363	VAL
17	DL	83	THR
17	DL	104	ARG
18	DO	122	LEU
18	DO	127	LEU
19	DP	59	THR
19	DP	88	THR
19	DP	122	VAL
19	DP	202	LEU
20	DR	33	VAL
20	DR	44	VAL
20	DR	60	VAL
20	DR	117	ILE
20	DR	118	VAL
20	DR	190	LEU
20	DR	254	VAL
20	DR	268	HIS
21	DU	39	ARG
21	DU	133	HIS
21	DU	146	THR
21	DU	191	SER
22	DZ	67	GLU
22	DZ	68	LYS

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Mol	Chain	Res	Type
23	F2	38	GLU
23	F2	46	THR
23	F2	110	GLU
23	F2	230	ASP
23	F2	273	THR
23	F2	387	VAL
23	F2	470	GLU
23	F2	478	VAL
23	F2	588	THR
23	F2	645	GLU
23	F2	664	ASP
23	F2	693	GLU
23	F2	733	THR
23	F2	768	LEU
23	F2	805	VAL
23	F2	810	THR
23	F2	820	ASP
23	F2	831	THR
23	F2	861	VAL
23	F2	878	SER
23	F2	948	THR
23	F2	951	VAL
23	F2	974	VAL
24	F3	92	ARG
24	F3	106	ASP
24	F3	152	THR
24	F3	163	ASP
24	F3	194	ASP
24	F3	298	SER
24	F3	306	VAL
24	F3	550	THR
24	F3	608	VAL
24	F3	646	THR
24	F3	660	VAL
24	F3	695	LEU
24	F3	720	ILE
24	F3	744	LEU
24	F3	750	ARG
24	F3	781	CYS
24	F3	787	VAL
24	F3	791	ILE
24	F3	807	LEU

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Mol	Chain	Res	Type
24	F3	810	THR
24	F3	861	VAL
24	F3	868	VAL
24	F3	874	LEU
24	F3	891	LEU
24	F3	940	VAL
24	F3	946	LEU
25	F5	189	LEU
25	F5	337	THR
25	F5	343	LEU
25	F5	348	GLU
25	F5	360	THR
25	F5	379	VAL
25	F5	444	VAL
25	F5	487	LYS
25	F5	597	ARG
25	F5	649	GLU
25	F5	654	VAL
25	F5	688	LEU
25	F5	729	LEU
25	F5	745	LEU
26	F6	105	THR
26	F6	144	THR
26	F6	182	LEU
26	F6	184	ASP
26	F6	218	SER
26	F6	220	LEU
26	F6	248	VAL
26	F6	268	THR
26	F6	354	THR
26	F6	457	VAL
27	F7	10	ARG
27	F7	59	GLU
27	F7	118	ARG
27	F7	202	THR
27	F7	208	GLU
27	F7	237	ARG
27	F7	247	GLU
27	F7	284	LEU
27	F7	299	SER
27	F7	326	GLU
27	F7	378	ASP

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Mol	Chain	Res	Type
27	F7	439	LEU
27	F7	497	SER
27	F7	532	THR
27	F7	564	LEU
27	F7	604	ASP
27	F7	627	LEU
28	F8	16	THR
28	F8	34	ASP
28	F8	170	SER
28	F8	267	VAL
28	F8	305	VAL
28	F8	364	LEU
28	F8	538	VAL
28	F8	611	SER
28	F8	612	VAL
28	F8	679	VAL
29	F9	110	ASP
29	F9	132	GLN
29	F9	201	VAL
30	FA	46	VAL
30	FA	51	THR
30	FA	87	VAL
30	FA	90	CYS
30	FA	196	VAL
30	FA	231	VAL
30	FA	235	VAL
30	FA	242	SER
30	FA	259	LEU
30	FA	260	ARG
30	FA	291	VAL
30	FA	335	LEU
30	FA	384	ARG
30	FA	409	PHE
30	FA	419	CYS
30	FA	440	ASP
30	FA	447	VAL
30	FA	449	SER
30	FA	533	VAL
30	FA	540	VAL
30	FA	546	THR
30	FA	555	LEU
30	FA	592	LEU

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Mol	Chain	Res	Type
30	FA	605	GLU
31	FB	266	VAL
31	FB	275	GLU
31	FB	278	VAL
31	FB	288	ASP
31	FB	410	THR
31	FB	413	ASN
31	FB	417	LYS
31	FB	450	THR
31	FB	459	VAL
31	FB	471	VAL
31	FB	582	VAL
31	FC	172	LEU
31	FC	191	VAL
31	FC	253	LEU
31	FC	259	VAL
31	FC	379	THR
31	FC	485	ASP
31	FC	486	VAL
31	FC	495	ILE
31	FC	549	THR
31	FC	560	VAL
31	FC	561	GLU
32	FE	241	LEU
32	FE	284	ASP
32	FE	353	THR
32	FE	355	VAL
32	FE	396	THR
32	FE	438	GLN
33	FJ	115	THR
33	FJ	159	LEU
33	FJ	185	LEU
33	FJ	188	CYS
33	FJ	217	ILE
33	FJ	279	LEU
33	FJ	290	LEU
33	FJ	303	MET
33	FJ	353	ARG
34	FM	20	VAL
34	FM	84	ASP
34	FM	114	THR
34	FM	241	LEU

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Mol	Chain	Res	Type
34	FM	292	ARG
34	FM	309	SER
34	FM	321	LEU
34	FM	327	VAL
34	FN	12	VAL
34	FN	20	VAL
34	FN	59	THR
34	FN	79	VAL
34	FN	85	VAL
34	FN	114	THR
34	FN	140	SER
34	FN	255	THR
35	FO	67	VAL
35	FO	93	ASP
35	FO	248	ARG
35	FO	272	VAL
35	FO	274	VAL
35	FO	293	VAL
35	FO	304	ILE
35	FO	326	THR
36	FP	85	LYS
36	FP	182	VAL
36	FP	298	VAL
36	FP	303	LEU
37	FQ	23	THR
37	FQ	99	LEU
37	FQ	190	VAL
37	FQ	198	THR
37	FQ	214	THR
37	FR	169	GLU
37	FR	190	VAL
37	FR	214	THR
37	FR	215	GLU
37	FS	60	THR
37	FS	73	THR
37	FS	98	LEU
37	FS	147	THR
37	FS	190	VAL
37	FS	198	THR
37	FS	214	THR
37	FS	227	THR
37	FS	249	SER

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Mol	Chain	Res	Type
37	FS	277	THR
37	FS	296	ARG
37	FT	13	VAL
37	FT	24	LEU
37	FT	120	VAL
37	FT	129	VAL
37	FT	141	VAL
37	FT	143	ARG
37	FT	190	VAL
37	FT	192	THR
37	FT	227	THR
37	FU	59	VAL
37	FU	73	THR
37	FU	128	VAL
37	FU	138	ASP
37	FU	184	GLU
37	FU	190	VAL
37	FU	198	THR
37	FU	207	THR
37	FU	227	THR
37	FU	233	VAL
38	FW	169	GLU
40	FY	54	ARG
40	FY	88	LEU
40	FY	132	ASP
40	FY	135	GLU
40	FY	177	ILE
42	Fa	7	THR
42	Fa	61	VAL
42	Fa	63	VAL
42	Fa	162	LEU
43	Fb	75	LYS
43	Fb	107	MET
43	Fb	120	ASP
43	Fb	133	LYS
44	Fc	69	LYS
44	Fc	73	LEU
44	Fc	91	VAL
44	Fc	121	LEU
44	Fc	136	ASP
45	Fd	77	VAL
45	Fd	87	CYS

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Mol	Chain	Res	Type
45	Fd	110	VAL
61	CC	18	PHE
61	CC	60	ILE
62	CI	145	VAL
62	CI	184	VAL
62	CI	219	LEU
62	CI	345	ASP
62	CI	399	LEU
63	CJ	154	THR
63	CJ	158	THR
63	CJ	177	LEU
63	CJ	186	VAL
63	CJ	349	THR
63	CJ	368	VAL
63	CJ	375	THR
63	CJ	448	THR
63	CJ	518	VAL
63	CJ	523	VAL
63	CJ	524	THR
63	CJ	554	THR
63	CJ	594	VAL
63	CJ	625	VAL
63	CJ	704	GLU
63	CJ	719	PRO
63	CJ	727	THR
64	CN	17	VAL
64	CN	38	ASP
64	CN	59	VAL
64	CN	60	VAL
64	CN	88	ARG
64	CN	101	VAL
64	CN	106	GLU
64	CN	128	LEU
64	CN	132	VAL
64	CN	139	THR
64	CN	140	ASP
65	CS	76	THR
65	CS	105	VAL
66	Cg	19	VAL
66	Cg	52	ARG
66	Cg	65	THR
66	Cg	143	THR

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Mol	Chain	Res	Type
66	Cg	163	VAL
66	Cg	172	VAL
66	Cg	271	ASP
66	Cg	284	VAL
66	Cg	305	LEU
66	Cg	314	SER
66	Cg	468	ASP
67	Ci	65	PHE
67	Ci	127	THR
68	Ck	129	THR
68	Ck	136	ASP
68	Ck	152	ASP
68	Ck	156	LEU
68	Ck	170	VAL
68	Ck	171	VAL
68	Ck	214	LEU
68	Ck	216	ARG
68	Ck	228	LEU
68	Ck	262	VAL
68	Ck	316	ASP
68	Ck	318	THR
68	Ck	335	ARG
68	Ck	339	GLU
68	Ck	356	VAL
68	Ck	408	VAL
68	Ck	552	LEU
68	Ck	573	THR
68	Ck	577	THR
68	Ck	620	THR
68	Ck	687	ARG
68	Ck	688	TYR
68	Ck	690	TRP
68	Ck	831	VAL
68	Ck	840	VAL
69	DB	521	LEU
69	DB	522	MET
69	DB	556	VAL
69	DB	560	THR
69	DB	587	VAL
69	DB	705	LYS
69	DB	754	VAL
69	DB	756	THR

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Mol	Chain	Res	Type
69	DB	757	VAL
69	DB	779	VAL
69	DB	783	VAL
69	DB	795	VAL
69	DB	801	LEU
69	DB	831	ASN
69	DB	918	VAL
69	DB	949	THR
69	DB	963	ARG
69	DB	966	VAL
69	DB	976	THR
69	DB	993	ASP
69	DB	1141	THR
69	DB	1142	VAL
70	DC	58	VAL
70	DC	88	LEU
70	DC	130	LYS
70	DC	149	ARG
70	DC	154	THR
70	DC	167	VAL
70	DC	280	VAL
70	DC	316	THR
70	DC	379	LEU
70	DC	441	VAL
70	DC	448	GLU
70	DC	580	VAL
70	DC	593	LEU
70	DC	695	VAL
70	DC	699	VAL
70	DC	712	LEU
70	DC	720	VAL
70	DC	767	GLU
70	DC	846	ASP
70	DC	903	THR
70	DC	941	MET
70	DC	1019	THR
70	DC	1027	THR
70	DC	1059	LEU
71	DE	83	LEU
71	DE	99	VAL
71	DE	195	ILE
71	DE	217	ASP

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Mol	Chain	Res	Type
71	DE	241	THR
71	DE	295	TYR
71	DE	430	VAL
71	DE	432	GLU
71	DE	438	PHE
71	DE	447	ARG
71	DE	451	THR
71	DE	504	ASP
71	DE	556	LEU
71	DE	572	VAL
71	DE	583	ARG
71	DE	611	LEU
72	DF	89	GLU
72	DF	103	VAL
72	DF	118	THR
72	DF	147	ASP
72	DF	189	ASP
72	DF	194	THR
72	DF	409	GLU
72	DF	485	LEU
72	DF	523	LEU
72	DF	525	ARG
72	DF	536	GLU
72	DF	562	GLN
73	DG	92	GLN
73	DG	122	LEU
73	DG	218	THR
73	DG	228	VAL
73	DG	342	ASN
73	DG	409	LYS
73	DG	444	THR
73	DG	464	VAL
73	DG	466	VAL
73	DG	491	THR
73	DG	522	THR
73	DG	529	ASP
73	DG	553	ASP
73	DG	555	THR
73	DG	558	CYS
73	DG	628	LEU
74	DH	107	THR
74	DH	182	ASP

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Mol	Chain	Res	Type
74	DH	384	THR
74	DH	392	TRP
74	DH	396	VAL
74	DH	408	ASN
74	DH	500	VAL
74	DH	503	THR
74	DH	521	ILE
74	DH	527	VAL
75	DJ	111	VAL
75	DJ	151	GLU
75	DJ	192	THR
75	DJ	226	VAL
76	DK	48	VAL
76	DK	54	THR
76	DK	58	VAL
76	DK	111	LEU
76	DK	149	ASP
76	DK	151	ASN
76	DK	246	THR
76	DK	285	GLU
77	DT	97	VAL
77	DT	105	ARG
77	DT	117	ASP
77	DT	209	THR
77	DT	228	LEU
78	DV	24	VAL
78	DV	41	THR
78	DV	45	THR
78	DV	114	VAL
78	DV	121	VAL
78	DV	128	ASP
79	DW	43	ASP
79	DW	48	TYR
79	DW	56	LEU
79	DW	107	ASP
79	DW	109	GLU
79	DW	116	LEU
79	DW	149	VAL
79	DW	151	THR
79	DW	169	VAL
81	DY	19	THR
81	DY	84	LYS

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Mol	Chain	Res	Type
81	DY	119	VAL
82	F1	64	THR
82	F1	65	THR
82	F1	71	THR
82	F1	84	ARG
82	F1	128	VAL
82	F1	229	LEU
82	F1	283	VAL
82	F1	286	THR
82	F1	362	LEU
82	F1	425	THR
82	F1	433	ASP
82	F1	457	LEU
82	F1	503	VAL
82	F1	575	GLU
82	F1	636	VAL
82	F1	652	VAL
82	F1	690	ASP
82	F1	713	THR
82	F1	726	THR
82	F1	731	LEU
82	F1	736	ASP
82	F1	739	THR
82	F1	760	THR
82	F1	769	LEU
82	F1	783	VAL
82	F1	794	THR
82	F1	812	VAL
82	F1	813	MET
82	F1	837	CYS
82	F1	894	VAL
82	F1	895	THR
82	F1	905	THR
82	F1	1026	VAL
83	F4	134	ASN
83	F4	135	VAL
83	F4	177	GLU
83	F4	182	SER
83	F4	233	THR
83	F4	264	ILE
83	F4	265	ASP
83	F4	310	LEU

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Mol	Chain	Res	Type
83	F4	341	VAL
83	F4	462	LEU
83	F4	478	LEU
83	F4	523	VAL
83	F4	527	LEU
83	F4	589	LEU
83	F4	775	THR
83	F4	811	ASP
84	FD	35	THR
84	FD	90	THR
84	FD	219	THR
84	FD	254	VAL
84	FD	296	VAL
85	FF	6	VAL
85	FF	117	LEU
85	FF	118	GLN
85	FF	126	VAL
85	FF	134	THR
85	FF	174	PHE
85	FF	222	ASP
85	FF	247	THR
85	FF	352	VAL
85	FF	378	VAL
85	FF	393	ARG
86	FG	13	VAL
86	FG	155	CYS
87	FH	139	ARG
87	FH	230	VAL
87	FH	252	VAL
87	FH	256	VAL
87	FH	265	LEU
87	FH	282	VAL
87	FH	329	ARG
87	FH	339	ASP
87	FH	354	VAL
87	FH	397	TYR
88	FI	23	THR
88	FI	50	GLN
88	FI	52	VAL
88	FI	87	SER
88	FI	217	LEU
88	FI	231	LEU

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Mol	Chain	Res	Type
88	FI	381	THR
88	FI	417	LEU
88	FI	424	VAL
89	FK	120	LYS
89	FK	141	VAL
89	FK	160	THR
89	FK	326	VAL
89	FK	327	LEU
89	FK	339	VAL
89	FK	340	ASP
90	FL	83	THR
90	FL	136	ARG
90	FL	181	ARG
90	FL	191	VAL
90	FL	205	LEU
90	FL	206	VAL
90	FL	301	LEU
90	FL	310	VAL
91	FV	53	VAL
91	FV	58	VAL
91	FV	108	VAL
91	FV	128	LEU
91	FV	130	VAL
91	FV	179	THR
91	FV	208	VAL
91	FV	212	THR
91	FV	232	ASP
91	FV	234	LEU
92	Fe	30	LEU
92	Fe	52	ARG
92	Fe	67	VAL
92	Fe	68	THR
92	Fe	74	VAL
92	Fe	81	LEU
92	Fe	88	ASP
92	Fe	90	ASP
92	Fe	91	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (291) such sidechains are listed below:

Mol	Chain	Res	Type
1	CE	132	HIS

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Mol	Chain	Res	Type
1	CE	159	HIS
1	CE	333	ASN
2	CF	86	HIS
3	CH	29	HIS
3	CH	54	GLN
3	CH	55	GLN
3	CH	111	GLN
3	CH	247	HIS
4	CK	252	ASN
5	CO	135	GLN
5	CO	281	HIS
6	CP	19	GLN
6	CP	87	HIS
7	CQ	20	GLN
7	CQ	90	GLN
7	CQ	146	HIS
8	CR	69	HIS
8	CR	183	GLN
8	CR	193	ASN
9	Ca	76	GLN
9	Ca	105	GLN
11	Cd	119	HIS
11	Cd	144	ASN
11	Cd	155	GLN
11	Cd	159	HIS
12	Cj	153	HIS
14	Cp	113	GLN
14	Cp	154	GLN
14	Cp	182	GLN
15	DD	76	ASN
15	DD	79	GLN
15	DD	156	GLN
15	DD	176	HIS
15	DD	273	HIS
15	DD	300	GLN
15	DD	353	HIS
15	DD	387	GLN
15	DD	402	GLN
15	DD	507	GLN
16	DI	18	HIS
16	DI	30	GLN
16	DI	175	GLN

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Mol	Chain	Res	Type
16	DI	250	ASN
16	DI	285	GLN
16	DI	320	GLN
16	DI	370	GLN
16	DI	372	ASN
17	DL	99	GLN
18	DO	159	HIS
18	DO	251	ASN
19	DP	116	HIS
19	DP	143	ASN
20	DR	68	HIS
20	DR	145	HIS
20	DR	179	HIS
21	DU	19	GLN
21	DU	63	HIS
21	DU	155	GLN
23	F2	56	GLN
23	F2	307	ASN
23	F2	337	GLN
23	F2	461	HIS
23	F2	698	HIS
24	F3	182	HIS
24	F3	405	ASN
24	F3	468	GLN
24	F3	654	GLN
24	F3	691	GLN
24	F3	747	HIS
24	F3	849	GLN
24	F3	905	HIS
25	F5	401	GLN
25	F5	609	GLN
26	F6	19	HIS
26	F6	203	GLN
26	F6	210	GLN
26	F6	363	ASN
27	F7	61	HIS
27	F7	103	HIS
27	F7	109	ASN
27	F7	214	HIS
27	F7	232	ASN
28	F8	68	HIS
28	F8	219	HIS

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Mol	Chain	Res	Type
28	F8	499	GLN
29	F9	51	ASN
29	F9	210	GLN
30	FA	30	HIS
30	FA	147	ASN
30	FA	181	GLN
30	FA	238	GLN
30	FA	385	HIS
30	FA	609	GLN
31	FB	192	GLN
31	FB	194	GLN
31	FB	248	HIS
31	FB	329	HIS
31	FB	357	GLN
31	FB	441	ASN
31	FB	532	GLN
31	FC	177	GLN
31	FC	326	GLN
31	FC	345	ASN
31	FC	474	ASN
32	FE	119	ASN
32	FE	136	GLN
32	FE	143	GLN
32	FE	215	ASN
32	FE	242	ASN
33	FJ	41	HIS
33	FJ	180	HIS
33	FJ	236	GLN
33	FJ	238	ASN
34	FM	200	ASN
34	FN	312	HIS
35	FO	46	HIS
35	FO	94	HIS
35	FO	135	ASN
35	FO	147	ASN
35	FO	157	GLN
35	FO	181	ASN
35	FO	303	HIS
35	FO	306	ASN
36	FP	15	ASN
36	FP	116	GLN
36	FP	293	HIS

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Mol	Chain	Res	Type
37	FQ	74	ASN
37	FQ	139	GLN
37	FQ	178	GLN
37	FR	213	HIS
37	FS	178	GLN
37	FS	213	HIS
37	FS	288	ASN
37	FT	242	HIS
37	FU	29	HIS
37	FU	213	HIS
38	FW	77	GLN
38	FW	99	GLN
38	FW	178	HIS
38	FW	221	HIS
39	FX	154	GLN
39	FX	164	HIS
40	FY	80	HIS
40	FY	166	HIS
41	FZ	53	HIS
43	Fb	134	GLN
44	Fc	96	HIS
45	Fd	42	HIS
45	Fd	59	HIS
45	Fd	76	HIS
45	Fd	78	GLN
61	CC	31	ASN
62	CI	136	GLN
62	CI	174	GLN
62	CI	229	HIS
63	CJ	441	HIS
63	CJ	450	HIS
63	CJ	460	HIS
63	CJ	476	ASN
63	CJ	571	GLN
63	CJ	619	HIS
63	CJ	761	GLN
63	CJ	791	HIS
63	CJ	792	HIS
63	CJ	793	HIS
63	CJ	804	ASN
64	CN	96	HIS
64	CN	153	ASN

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Mol	Chain	Res	Type
65	CS	65	ASN
65	CS	135	ASN
66	Cg	47	ASN
66	Cg	87	GLN
66	Cg	99	GLN
66	Cg	184	HIS
66	Cg	453	GLN
66	Cg	474	GLN
67	Ci	19	HIS
68	Ck	644	HIS
68	Ck	679	GLN
68	Ck	728	GLN
69	DB	524	GLN
69	DB	562	GLN
69	DB	643	HIS
69	DB	940	GLN
69	DB	1064	GLN
70	DC	81	HIS
70	DC	227	GLN
70	DC	303	HIS
70	DC	539	ASN
70	DC	574	GLN
70	DC	682	ASN
70	DC	691	GLN
70	DC	799	ASN
70	DC	821	GLN
70	DC	871	GLN
70	DC	1026	ASN
70	DC	1062	GLN
71	DE	202	HIS
71	DE	345	ASN
71	DE	703	GLN
72	DF	175	GLN
72	DF	214	HIS
72	DF	572	HIS
72	DF	587	GLN
73	DG	26	ASN
73	DG	71	ASN
73	DG	170	ASN
73	DG	191	GLN
73	DG	200	GLN
73	DG	230	ASN

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Mol	Chain	Res	Type
73	DG	476	GLN
73	DG	477	GLN
73	DG	557	GLN
74	DH	100	HIS
74	DH	123	HIS
74	DH	160	ASN
74	DH	255	GLN
74	DH	356	GLN
75	DJ	29	HIS
75	DJ	42	HIS
75	DJ	82	GLN
75	DJ	174	ASN
75	DJ	301	HIS
76	DK	132	HIS
76	DK	163	HIS
76	DK	171	GLN
77	DT	72	HIS
77	DT	91	GLN
77	DT	99	HIS
77	DT	192	GLN
77	DT	219	GLN
78	DV	40	HIS
78	DV	51	ASN
78	DV	71	GLN
79	DW	71	GLN
79	DW	121	HIS
79	DW	154	HIS
80	DX	58	HIS
81	DY	106	GLN
82	F1	331	HIS
82	F1	332	GLN
82	F1	344	GLN
82	F1	462	ASN
82	F1	517	GLN
82	F1	762	HIS
82	F1	763	ASN
82	F1	776	HIS
82	F1	862	HIS
82	F1	1025	GLN
83	F4	266	ASN
83	F4	320	HIS
83	F4	348	ASN

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Mol	Chain	Res	Type
83	F4	470	HIS
83	F4	472	HIS
83	F4	626	HIS
83	F4	686	HIS
84	FD	65	ASN
84	FD	195	GLN
84	FD	240	GLN
84	FD	374	HIS
85	FF	122	GLN
85	FF	335	GLN
85	FF	370	HIS
86	FG	133	GLN
86	FG	162	ASN
87	FH	111	HIS
87	FH	134	ASN
88	FI	15	GLN
88	FI	36	GLN
88	FI	97	HIS
88	FI	120	GLN
88	FI	153	GLN
88	FI	219	ASN
88	FI	228	GLN
88	FI	340	HIS
89	FK	169	GLN
89	FK	195	GLN
89	FK	312	ASN
90	FL	70	ASN
90	FL	80	ASN
90	FL	137	GLN
90	FL	189	HIS
90	FL	335	GLN
91	FV	63	ASN
91	FV	76	GLN
91	FV	147	GLN
91	FV	194	HIS
91	FV	207	HIS
92	Fe	42	ASN
92	Fe	101	GLN

5.3.3 RNA ⓘ

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

All (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
60	CA	10	G
60	CA	17	G
60	CA	21	G
60	CA	22	U
60	CA	26	C
60	CA	27	A
60	CA	29	A
60	CA	30	U
60	CA	35	U
60	CA	36	U
60	CA	37	U
60	CA	39	U
60	CA	44	U
60	CA	46	U
60	CA	49	U
60	CA	50	A
60	CA	53	A
60	CA	58	A
60	CA	60	A
60	CA	67	U
60	CA	72	U
60	CA	73	U
60	CA	74	G
60	CA	78	G
60	CA	79	A
60	CA	80	U
60	CA	81	U
60	CA	82	U
60	CA	84	U
60	CA	85	U
60	CA	86	G
60	CA	87	U
60	CA	88	A

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Mol	Chain	Res	Type
60	CA	90	A
60	CA	95	U
60	CA	97	U
60	CA	98	A
60	CA	100	G
60	CA	102	A
60	CA	105	G
60	CA	106	U
60	CA	111	A
60	CA	112	A
60	CA	115	A
60	CA	127	G
60	CA	135	U
60	CA	136	G
60	CA	137	U
60	CA	138	U
60	CA	139	U
60	CA	140	U
60	CA	152	U
60	CA	153	A
60	CA	154	G
60	CA	155	A
60	CA	157	G
60	CA	159	G
60	CA	160	U
60	CA	161	G
60	CA	167	A
60	CA	169	A
60	CA	170	U
60	CA	172	A
60	CA	173	A
60	CA	174	A
60	CA	178	A
60	CA	179	U
60	CA	181	A
60	CA	182	U
60	CA	185	A
60	CA	190	U
60	CA	191	A
60	CA	192	U
60	CA	195	A
60	CA	196	U

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Mol	Chain	Res	Type
60	CA	197	A
60	CA	198	A
60	CA	205	A
60	CA	207	A
60	CA	208	U
60	CA	214	U
60	CA	217	U
60	CA	218	A
60	CA	219	G
60	CA	220	U
60	CA	221	C
60	CA	223	G
60	CA	227	U
60	CA	228	G
60	CA	232	G
60	CA	236	G
60	CA	238	C
60	CA	239	G
60	CA	240	U
60	CA	241	U
60	CA	242	G
60	CA	247	A
60	CA	249	U
60	CA	253	U
60	CA	256	G
60	CA	257	C
60	CA	258	U
60	CA	259	U
60	CA	260	U
60	CA	261	U
60	CA	262	A
60	CA	267	U
60	CA	268	U
60	CA	269	A
60	CA	270	U
60	CA	271	A
60	CA	272	C
60	CA	278	U
60	CA	281	U
60	CA	282	A
60	CA	283	U
60	CA	284	U

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Mol	Chain	Res	Type
60	CA	285	A
60	CA	286	A
60	CA	291	U
60	CA	292	U
60	CA	293	A
60	CA	296	U
60	CA	297	G
60	CA	298	C
60	CA	299	U
60	CA	304	U
60	CA	306	A
60	CA	318	A
60	CA	320	A
60	CA	321	A
60	CA	322	A
60	CA	323	U
60	CA	324	A
60	CA	327	U
60	CA	330	U
60	CA	337	U
60	CA	338	U
60	CA	339	U
60	CA	340	U
60	CA	341	A
60	CA	347	C
60	CA	350	U
60	CA	351	A
60	CA	352	G
60	CA	353	G
60	CA	355	A
60	CA	357	A
60	CA	359	G
60	CA	366	U
60	CA	367	A
60	CA	368	A
60	CA	370	A
60	CA	375	A
60	CA	377	U
60	CA	378	A
60	CA	381	U
60	CA	388	U
60	CA	389	A

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Mol	Chain	Res	Type
60	CA	390	U
60	CA	397	U
60	CA	398	U
60	CA	399	A
60	CA	400	U
60	CA	413	A
60	CA	417	A
60	CA	418	A
60	CA	421	G
60	CA	422	G
60	CA	425	A
60	CA	429	U
60	CA	430	U
60	CA	432	G
60	CA	433	U
60	CA	435	G
60	CA	438	U
60	CA	439	U
60	CA	443	U
60	CA	444	A
60	CA	445	C
60	CA	446	C
60	CA	447	A
60	CA	448	U
60	CA	454	G
60	CA	455	G
60	CA	459	A
60	CA	460	U
60	CA	461	A
60	CA	470	G
60	CA	471	U
60	CA	473	U
60	CA	480	C
60	CA	481	A
60	CA	482	U
60	CA	484	A
60	CA	489	A
60	CA	498	U
60	CA	503	A
60	CA	509	U
60	CA	513	U
60	CA	515	U

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Mol	Chain	Res	Type
60	CA	516	G
60	CA	520	A
60	CA	525	A
60	CA	527	A
60	CA	528	U
60	CA	529	A
60	CA	532	A
60	CA	533	A
60	CA	534	A
60	CA	538	A
60	CA	539	A
60	CA	540	A
60	CA	557	C
60	CA	558	A
60	CA	559	A
60	CA	560	U
60	CA	565	A
60	CA	576	A
60	CA	577	A
60	CA	579	G
60	CA	581	G
60	CA	582	C
60	CA	585	U
60	CA	587	A
60	CA	590	A
60	CA	599	A
60	CA	600	U
60	CA	601	A
60	CA	602	A
60	CA	603	A
60	CA	613	U
60	CA	616	U
60	CA	617	U
60	CA	619	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
60	CA	78	G
60	CA	160	U
60	CA	173	A
60	CA	285	A

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

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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(^{o})	Ideal(^{o})
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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
109	FF	501	SAH	C2-N1	2.39	1.38	1.33
109	F1	1102	SAH	OXT-C	-2.21	1.23	1.30
109	FF	501	SAH	OXT-C	-2.12	1.23	1.30
108	Cg	501	GTP	C2-N3	2.02	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
108	Cg	501	GTP	C3'-C2'-C1'	3.47	106.20	100.98
108	Cg	501	GTP	C5-C6-N1	3.18	119.56	113.95
108	Cg	501	GTP	PB-O3B-PG	-3.02	122.45	132.83
108	Cg	501	GTP	C8-N7-C5	2.86	108.44	102.99
108	Cg	501	GTP	C2-N1-C6	-2.79	119.96	125.10
109	F1	1102	SAH	C3'-C2'-C1'	2.69	105.02	100.98
109	FF	501	SAH	OXT-C-O	-2.68	117.99	124.09
109	F1	1102	SAH	OXT-C-O	-2.66	118.06	124.09
109	FF	501	SAH	C3'-C2'-C1'	2.63	104.93	100.98
106	Fc	201	PM8	O1-C1-C2	-2.25	121.33	123.99
109	FF	501	SAH	OXT-C-CA	2.24	121.02	113.38
109	F1	1102	SAH	OXT-C-CA	2.20	120.88	113.38
108	Cg	501	GTP	O6-C6-C5	-2.18	120.12	124.37

There are no chirality outliers.

All (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
108	Cg	501	GTP	O4'-C4'-C5'-O5'
109	F1	1102	SAH	C-CA-CB-CG

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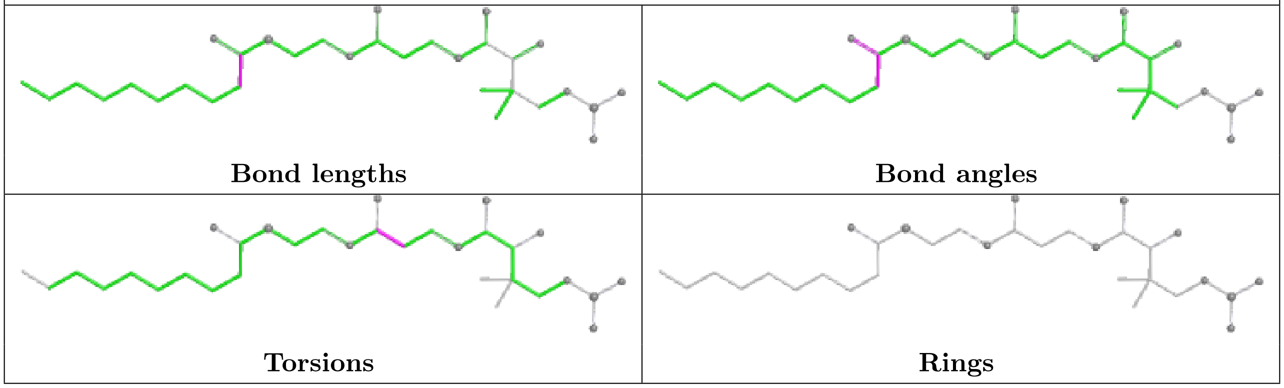
Mol	Chain	Res	Type	Atoms
106	Fc	201	PM8	C37-C38-C39-N41
109	F1	1102	SAH	CB-CG-SD-C5'
109	FF	501	SAH	CB-CG-SD-C5'
109	F1	1102	SAH	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand PM8 Fc 201



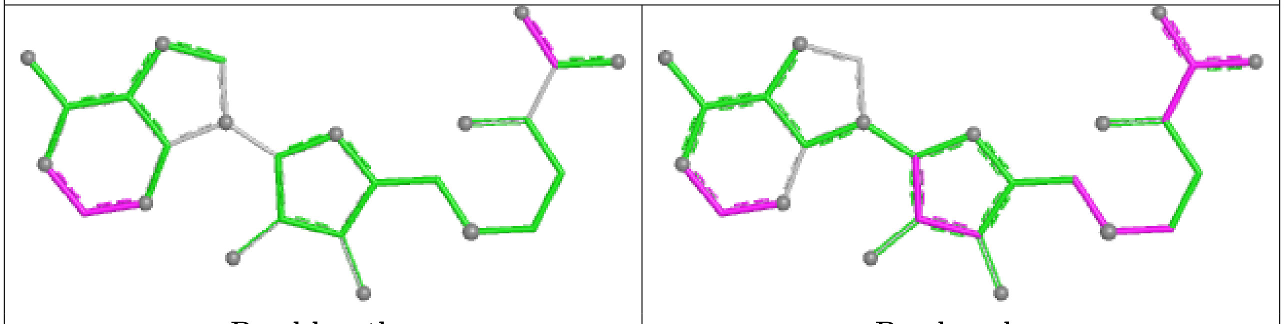
Bond lengths

Bond angles

Torsions

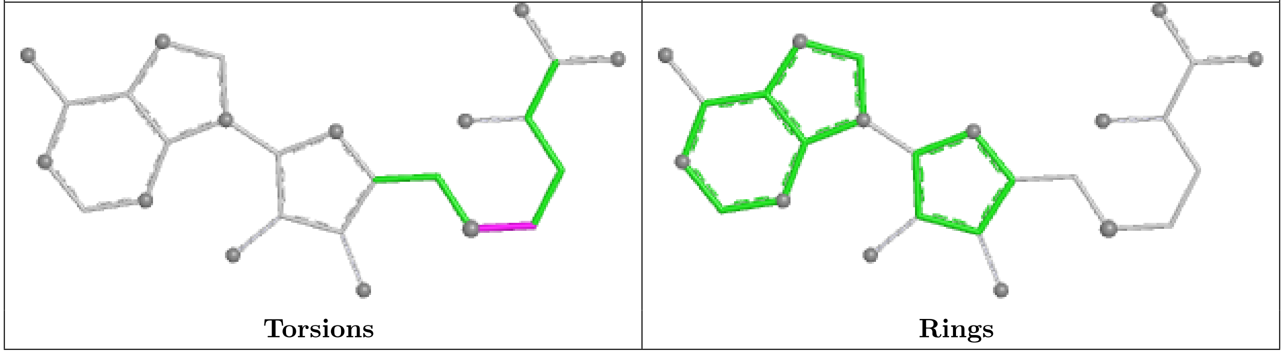
Rings

Ligand SAH FF 501



Bond lengths

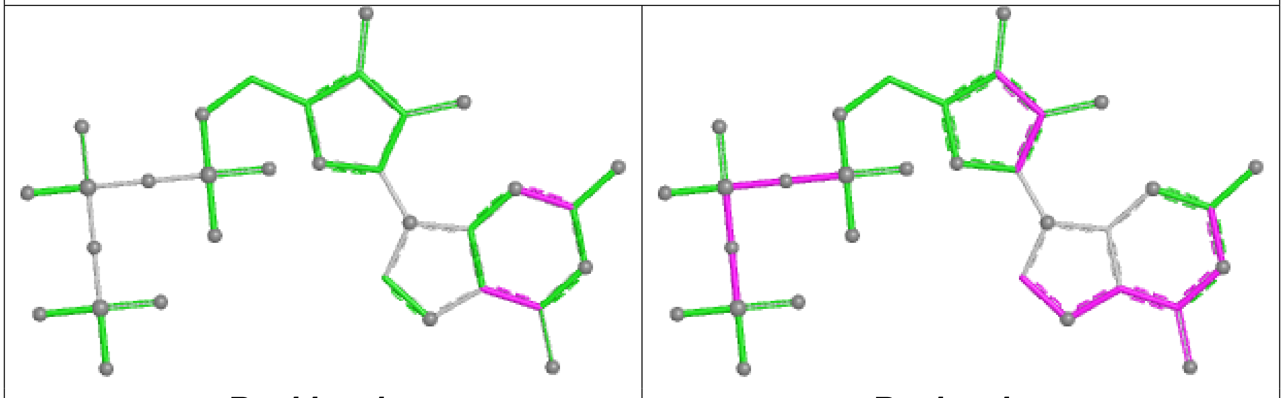
Bond angles



Torsions

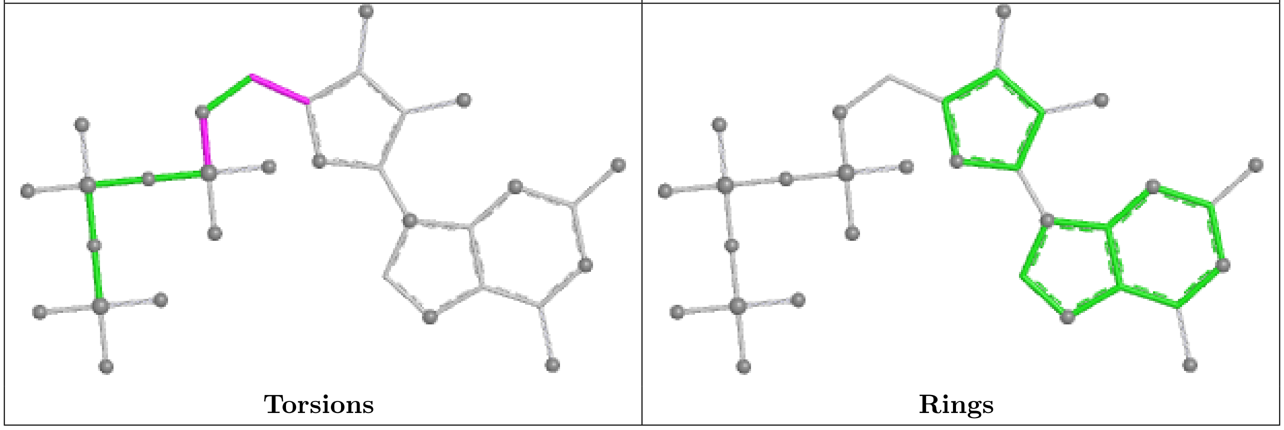
Rings

Ligand GTP Cg 501



Bond lengths

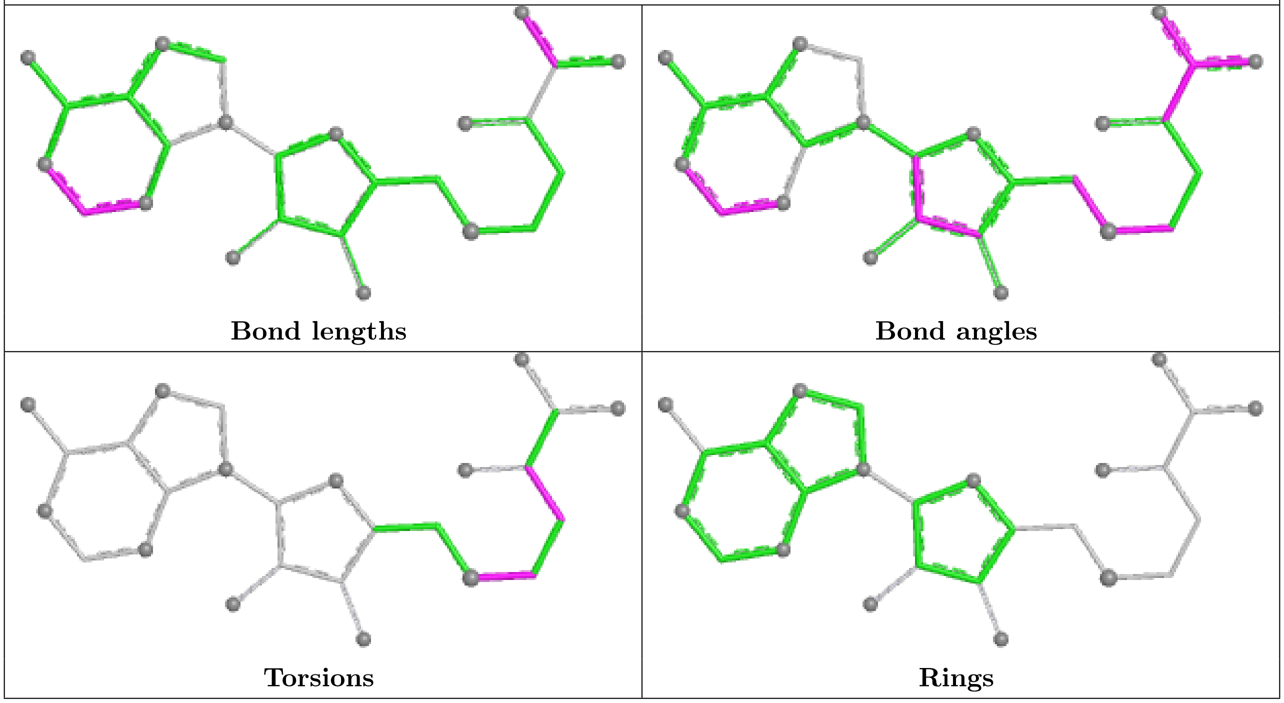
Bond angles



Torsions

Rings

Ligand SAH F1 1102



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

All 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Uh	88:UNK	C	98:UNK	N	42.20
1	UY	338:UNK	C	339:UNK	N	40.51
1	Uh	124:UNK	C	125:UNK	N	38.95
1	Uh	199:UNK	C	200:UNK	N	38.08
1	Ug	129:UNK	C	130:UNK	N	36.01
1	Uh	145:UNK	C	184:UNK	N	35.40
1	UY	411:UNK	C	412:UNK	N	35.07
1	Ug	102:UNK	C	103:UNK	N	29.64
1	UB	110:UNK	C	201:UNK	N	25.53
1	Uh	39:UNK	C	40:UNK	N	25.18
1	Ug	83:UNK	C	84:UNK	N	24.10
1	Uh	68:UNK	C	69:UNK	N	21.48
1	UY	455:UNK	C	456:UNK	N	20.24
1	Uh	134:UNK	C	135:UNK	N	17.12
1	Uh	280:UNK	C	281:UNK	N	15.79
1	UY	394:UNK	C	395:UNK	N	15.52
1	Ux	15:UNK	C	28:UNK	N	14.65
1	Ug	52:UNK	C	53:UNK	N	12.65
1	Ug	70:UNK	C	71:UNK	N	12.57
1	Ux	66:UNK	C	74:UNK	N	12.41
1	Ux	47:UNK	C	49:UNK	N	12.23
1	UY	430:UNK	C	431:UNK	N	11.78
1	Ug	39:UNK	C	40:UNK	N	11.09
1	Ug	26:UNK	C	27:UNK	N	8.34
1	Uh	323:UNK	C	324:UNK	N	7.01
1	UY	245:UNK	C	246:UNK	N	6.90
1	Ug	46:UNK	C	47:UNK	N	6.90
1	UY	403:UNK	C	405:UNK	N	6.75
1	UY	125:UNK	C	126:UNK	N	5.67
1	UY	117:UNK	C	118:UNK	N	5.53
1	Ug	33:UNK	C	34:UNK	N	4.79
1	Ug	145:UNK	C	146:UNK	N	4.56
1	UY	426:UNK	C	427:UNK	N	4.10
1	UY	56:UNK	C	57:UNK	N	3.43
1	CA	529:A	O3'	530:A	P	3.34

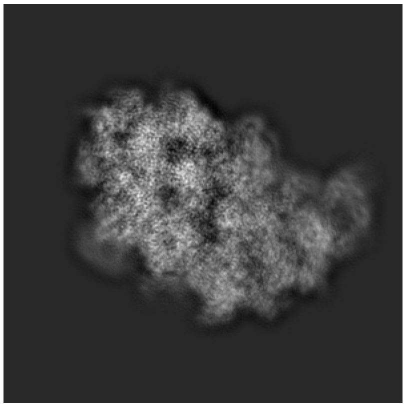
6 Map visualisation

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.

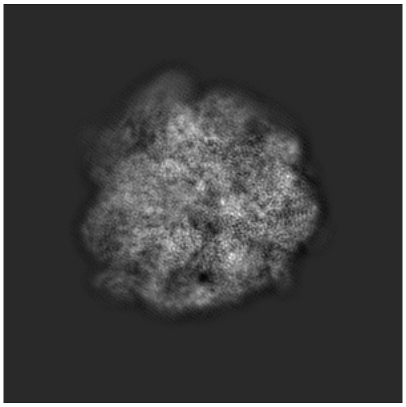
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

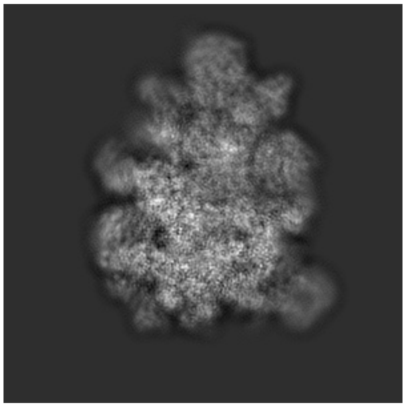
6.1.1 Primary map



X



Y

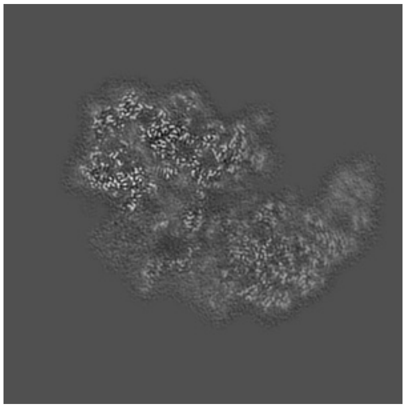


Z

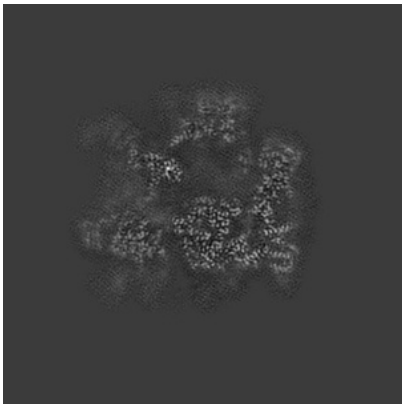
The images above show the map projected in three orthogonal directions.

6.2 Central slices

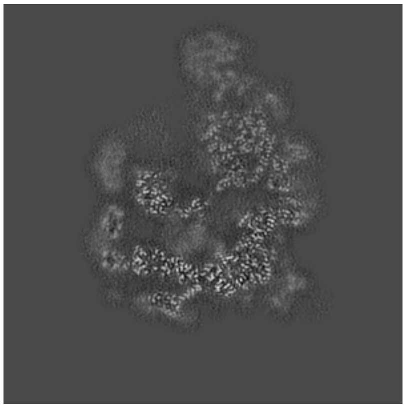
6.2.1 Primary map



X Index: 160



Y Index: 160

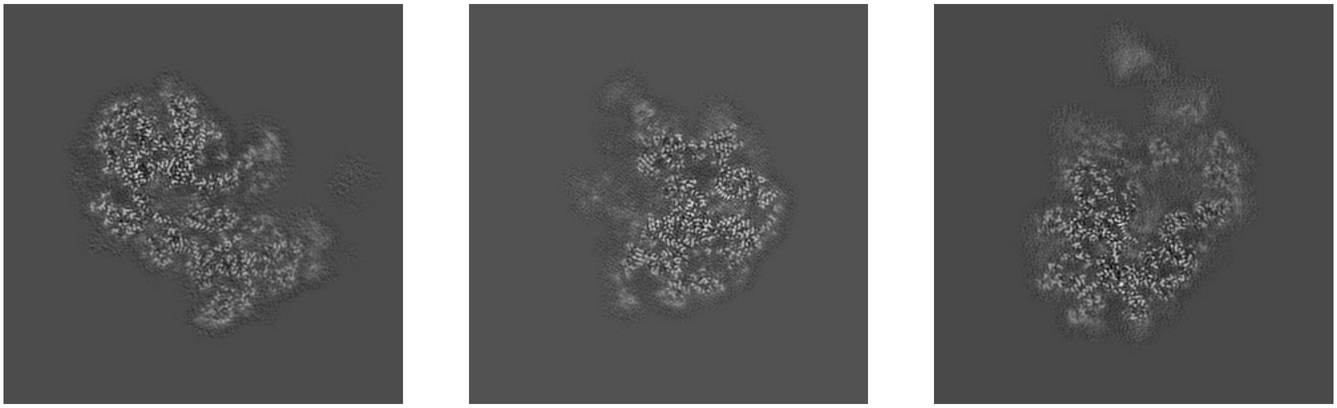


Z Index: 160

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

6.3 Largest variance slices

6.3.1 Primary map

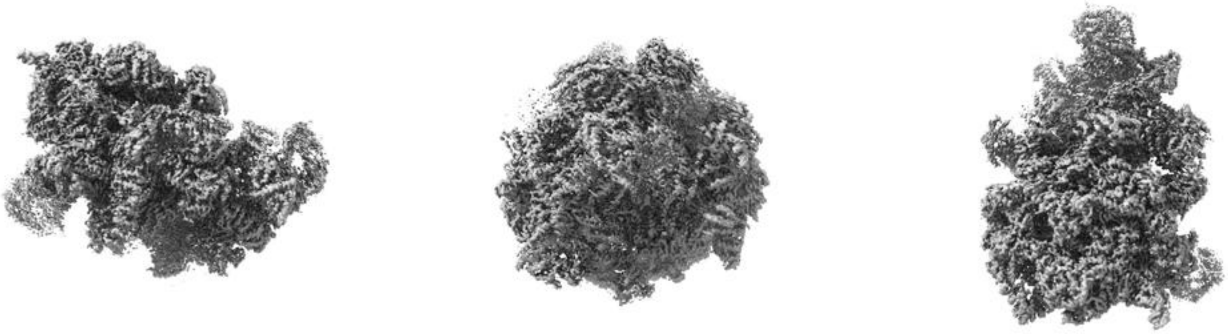


X Index: 137 Y Index: 109 Z Index: 181

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

6.4 Orthogonal surface views

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.

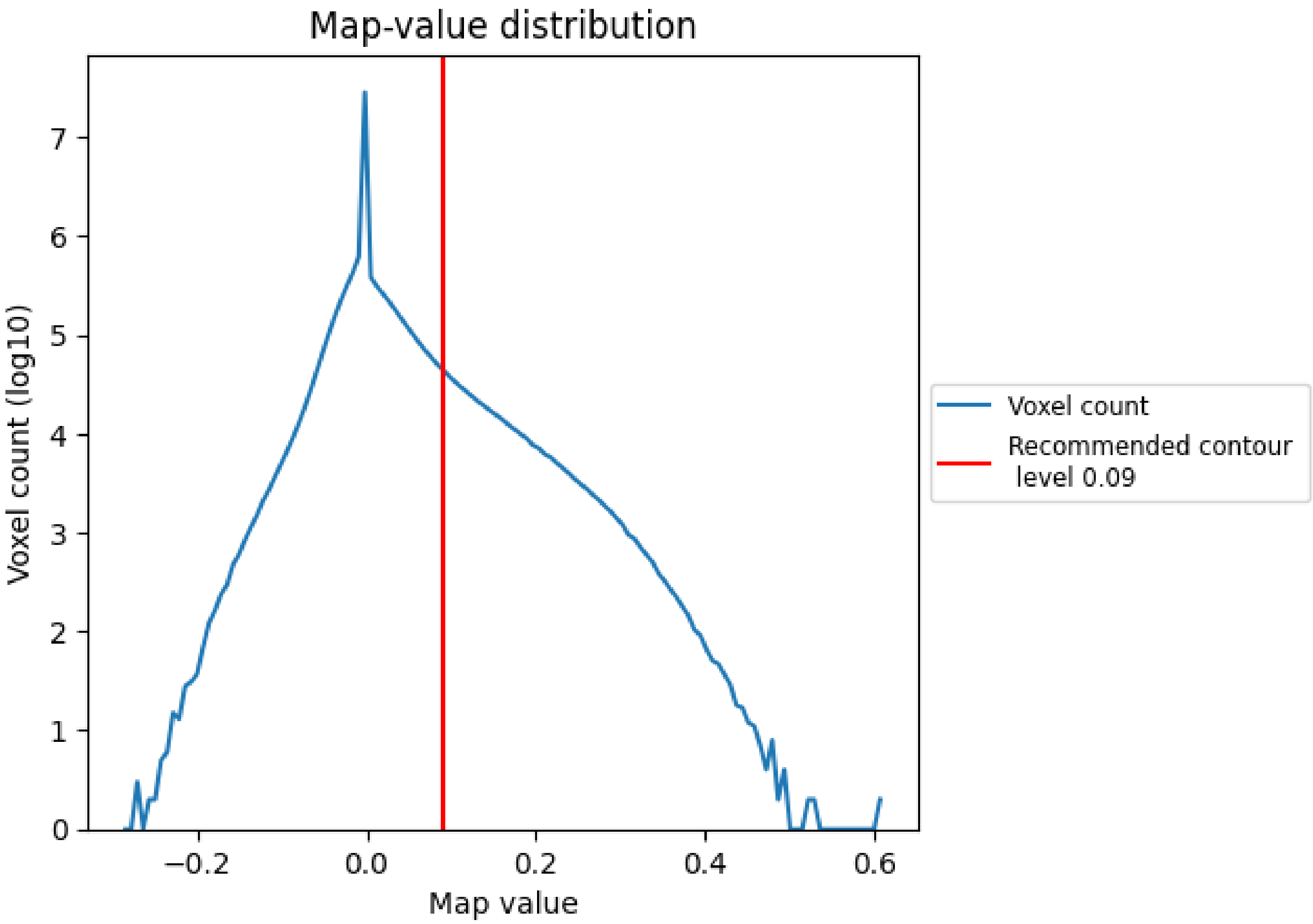
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

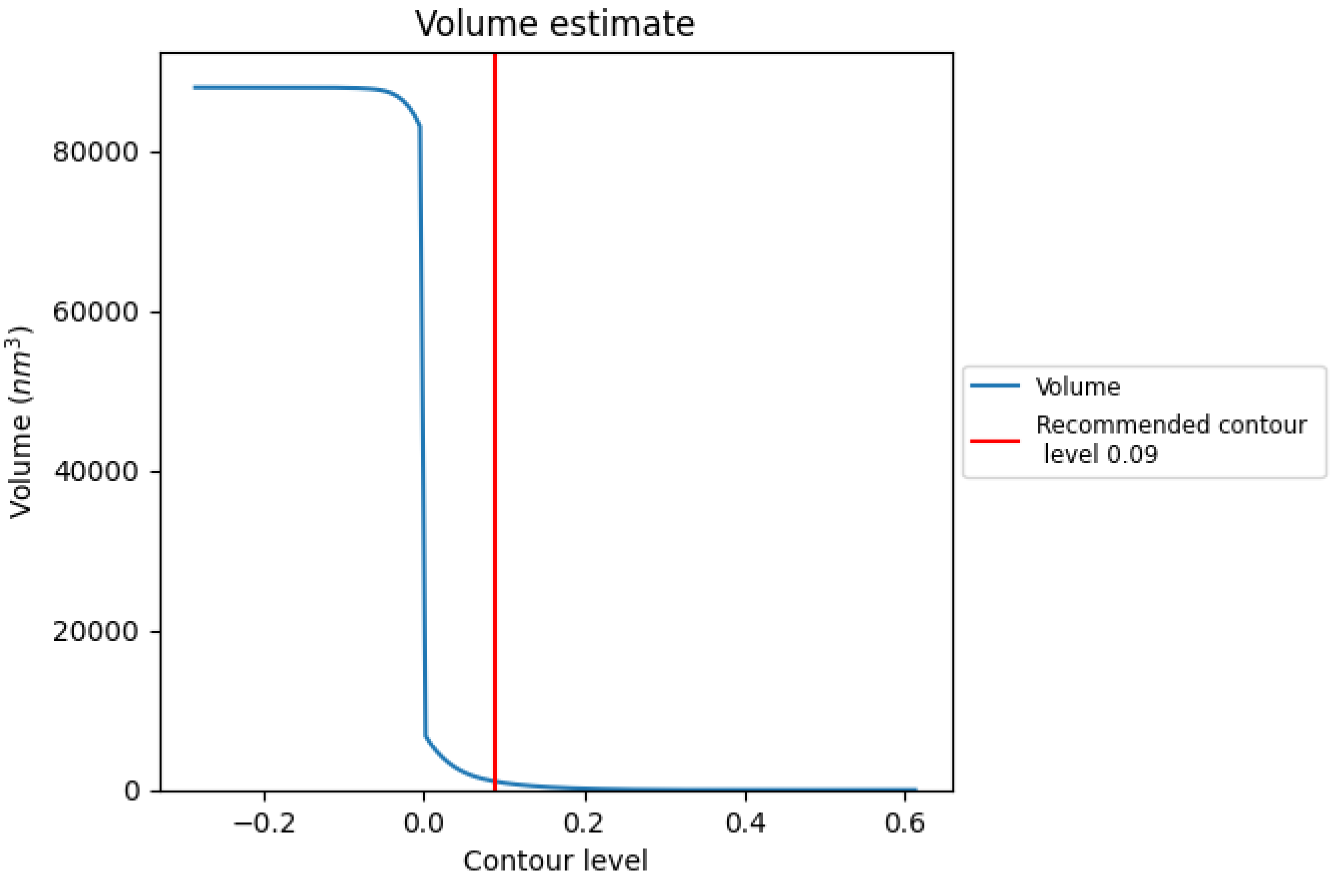
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

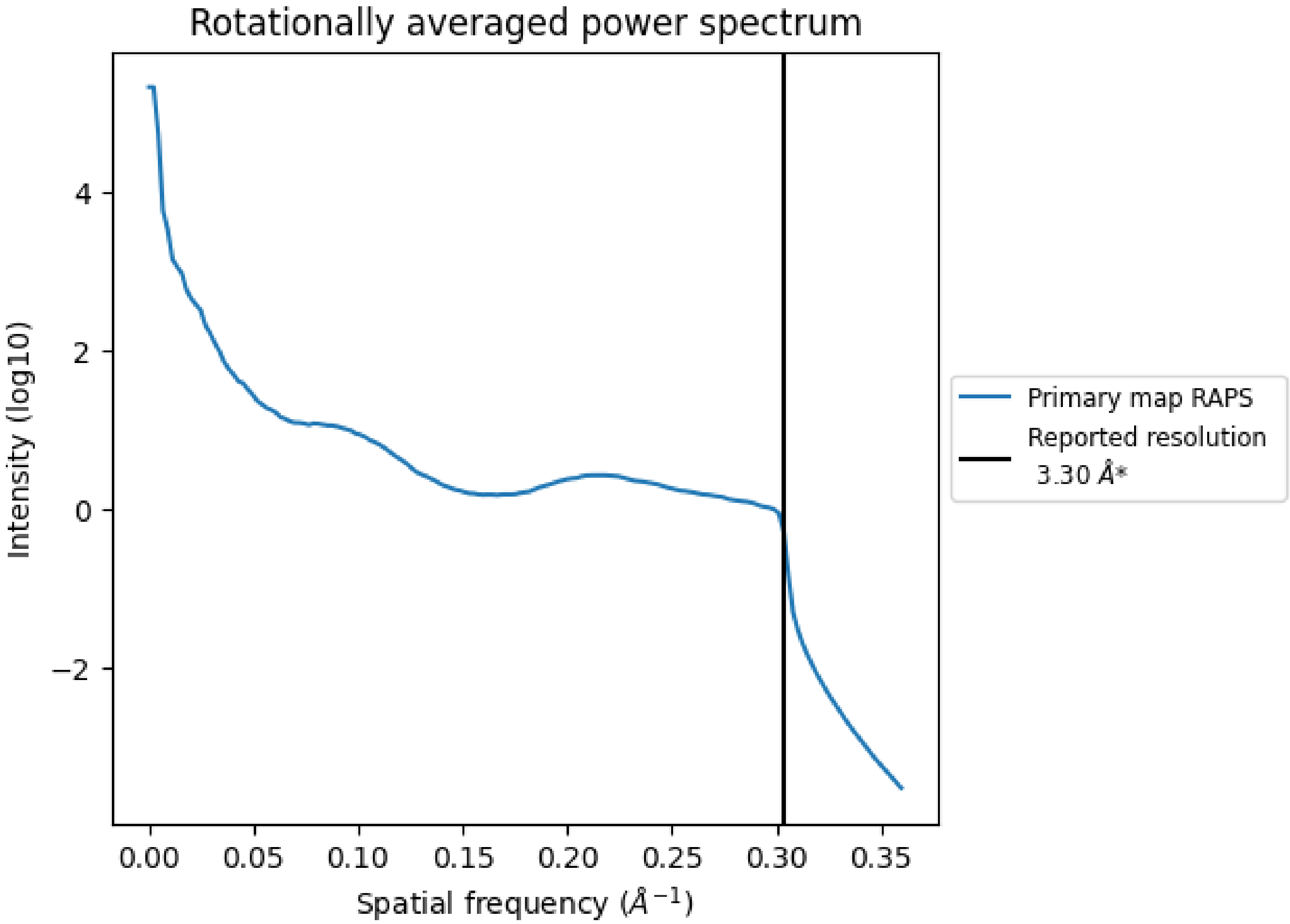
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1051 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

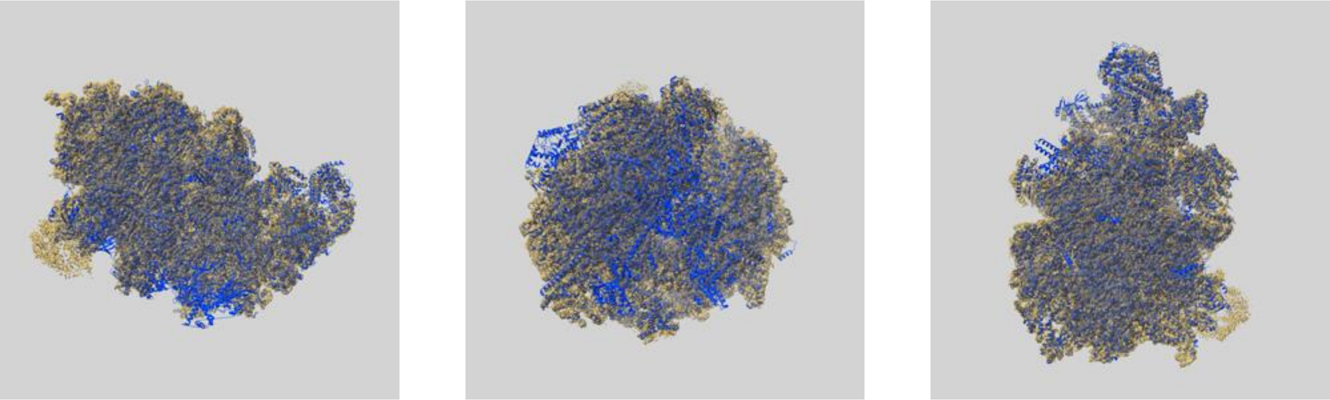
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

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.

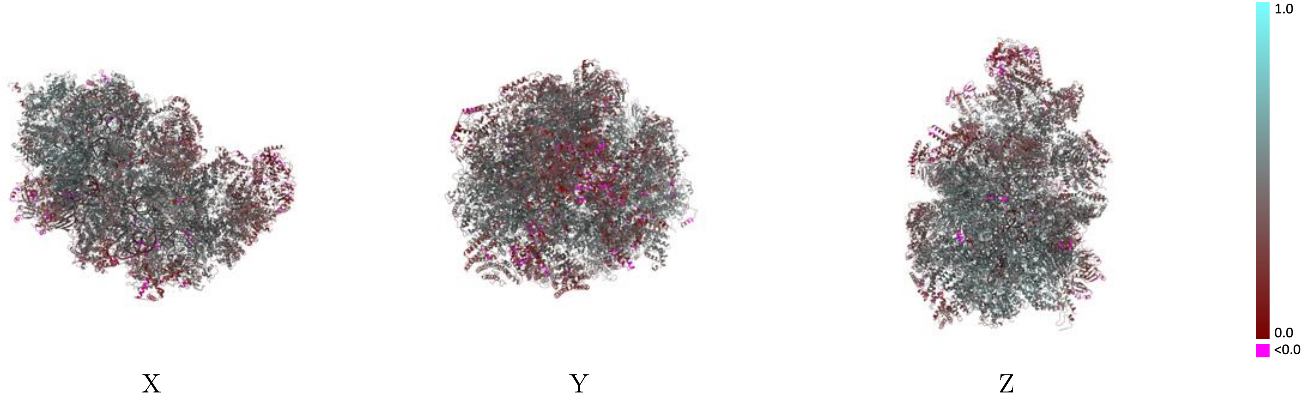
9.1 Map-model overlay



X Y Z

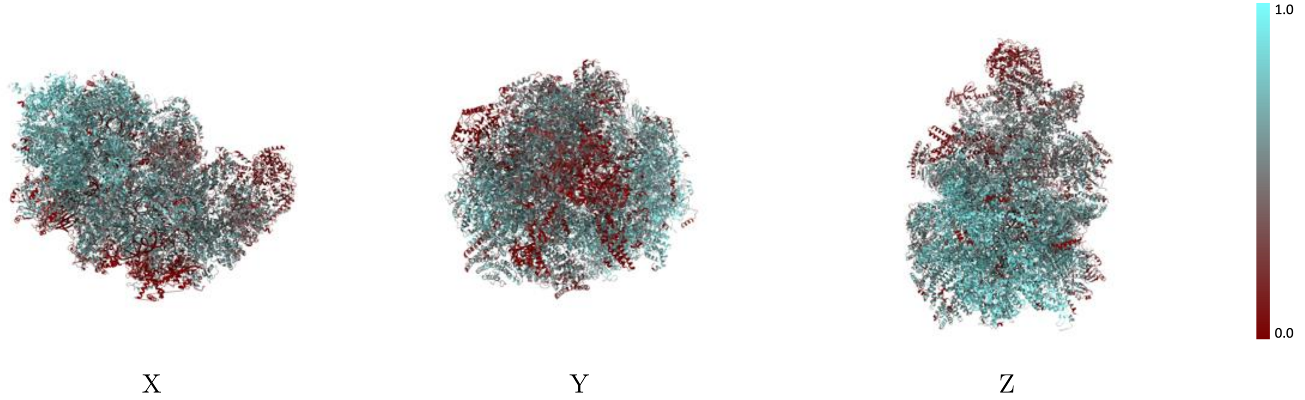
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



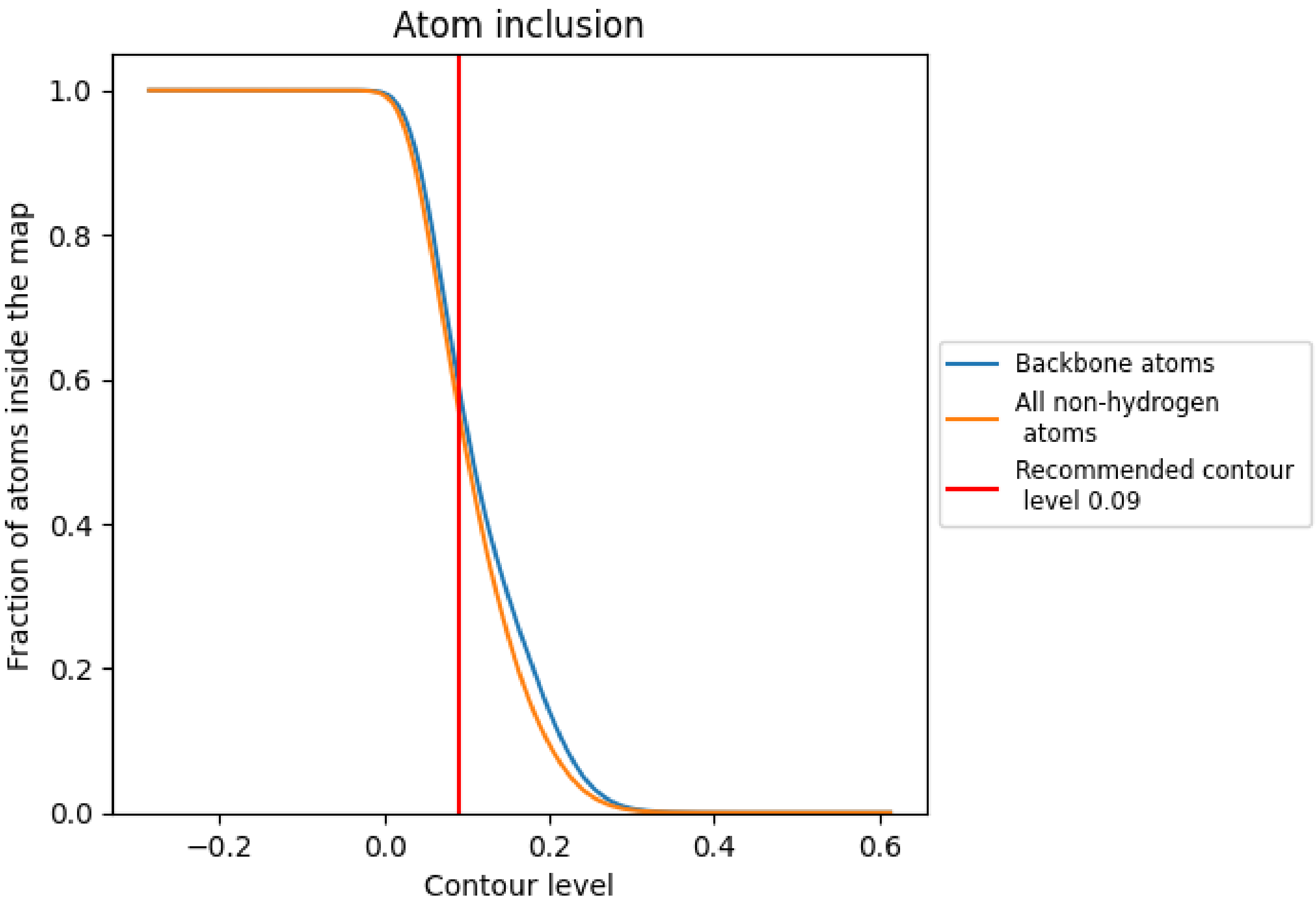
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 ⓘ



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

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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