wwPDB EM Validation Summary Report

Nov 20, 2022 – 12:54 pm GMT

PDB ID	:	6HIV
EMDB ID	:	EMD-0229
Title	:	Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the complete mitoribosome
Authors	:	Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boerhringer, D.; Schneider, A.; Ban, N.
Deposited on	:	2018-08-31
Resolution	:	7.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

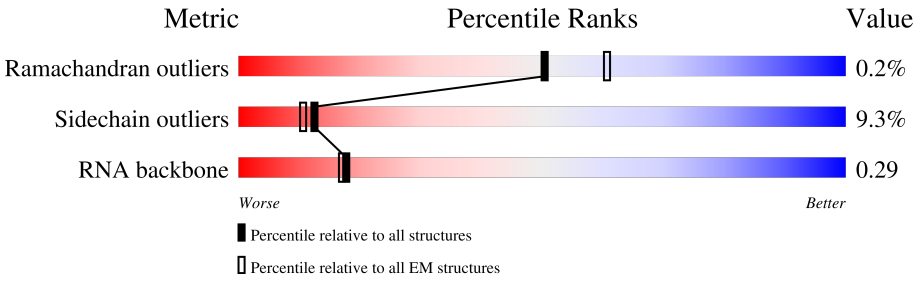
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.80 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	DA	1788	11% 81% 6% 13%
2	DD	812	20% 92% 5% •
3	DI	407	9% 90% 6% •
4	DL	307	45% 87% • • 8%
5	DM	294	12% 94% 6%
6	DN	293	15% 82% 5% 12%
7	DO	282	10% 74% 5% 21%
8	DP	274	12% 72% • 24%

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Mol	Chain	Length	Quality of chain
9	DQ	268	13% 92%
10	DR	270	11% 86% 7% 7%
11	DS	261	17% 87% 5% 9%
12	DU	228	21% 86% 8% 7%
13	DZ	94	27% 84% 13%
14	Da	64	86% 80% 6% 14%
15	DB	1181	19% 85% 9% 6%
16	DC	1165	18% 84% 10% 6%
17	DE	746	11% 72% 8% 21%
18	DF	666	19% 80% 9% 11%
19	DG	631	14% 79% 11% 10%
20	DH	581	29% 87% 10%
21	DJ	396	19% 71% 8% 20%
22	DK	324	16% 73% 5% 21%
23	DT	247	26% 86% 11%
24	DV	183	26% 77% 11% 13%
25	DW	179	30% 83% 7% 10%
26	DX	169	17% 75% 9% 17%
27	DY	163	22% 83% 12% 6%
28	CC	74	59% 85% 15%
29	CE	435	28% 86% 9%
30	CF	160	37% 95%
31	CH	282	29% 88% 9%
32	CI	443	31% 88% 8%
33	CJ	817	24% 88% 10%

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Mol	Chain	Length	Quality of chain
34	CK	326	50% 82% 8% 10%
35	CL	87	100% 90% 10%
36	CN	166	30% 83% 12% 5%
37	CO	429	31% 78% 6% 16%
38	CP	188	15% 89% 7%
39	CQ	307	34% 55% 7% 38%
40	CR	320	45% 93% 5%
41	CS	244	24% 53% 5% 42%
42	CU	193	70% 90% 5% 5%
43	CZ	360	42% 39% 58%
44	Ca	602	28% 90% 8%
45	Cb	324	19% 73% 5% 22%
46	Cd	440	23% 61% 5% 34%
47	Cg	498	18% 88% 9%
48	Ci	181	35% 79% 12% 9%
49	Cj	257	11% 82% 6% 12%
50	Ck	874	19% 73% 7% 20%
51	Cm	215	75% 79% 12% 9%
52	Cn	250	44% 42% 56%
53	Cp	187	29% 87% 6% 6%
54	Cq	263	16% 89% 6%
55	Cr	439	10% 53% 5% 41%
56	Cv	1211	23% 82% 6% 13%
57	CA	621	63% 50% 49%
58	UO	5	80% 100%

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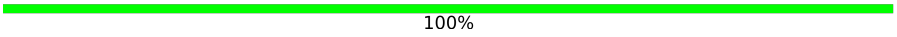
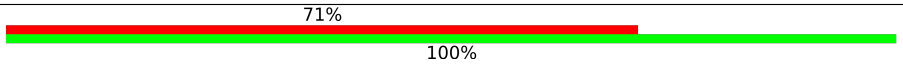
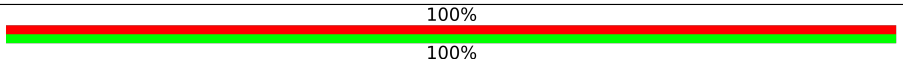
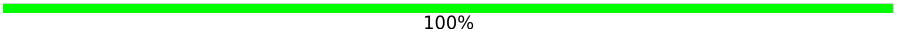
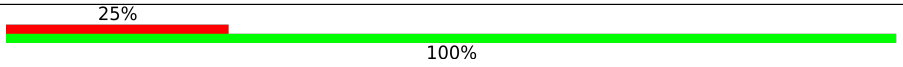
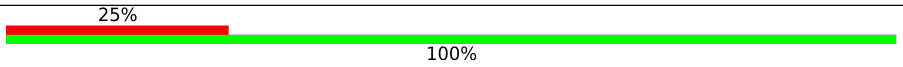
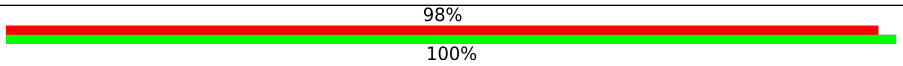
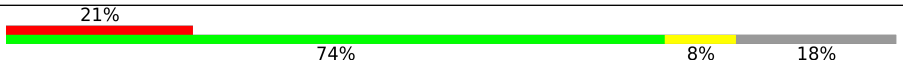
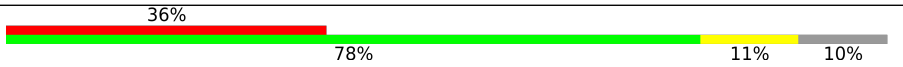
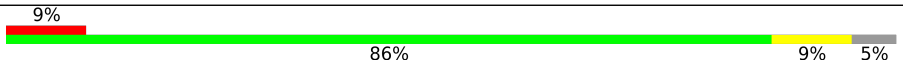
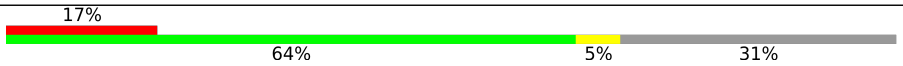
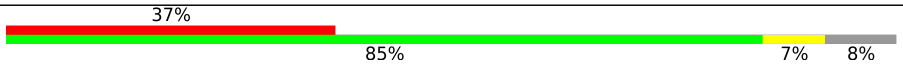
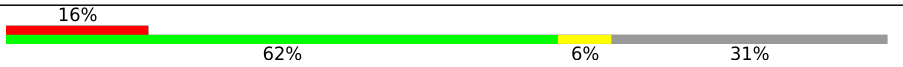
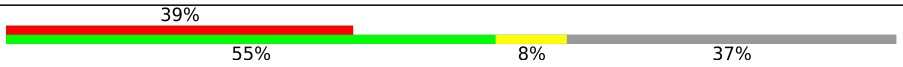
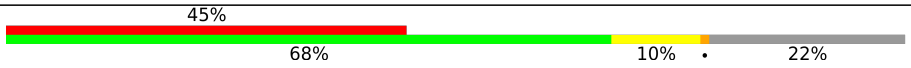
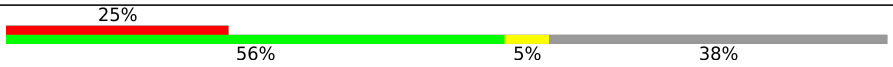
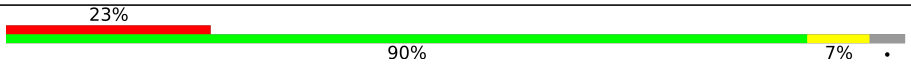
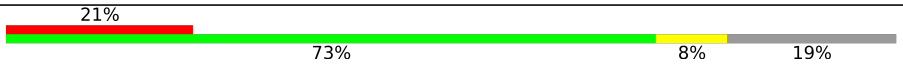
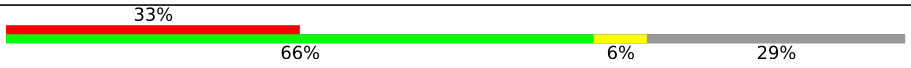
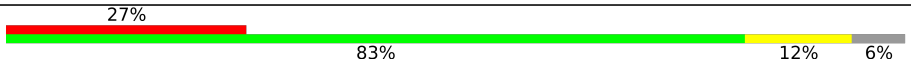
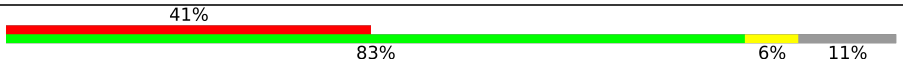
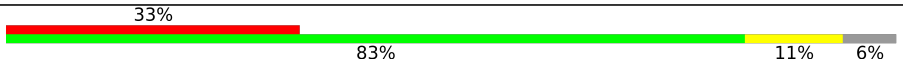
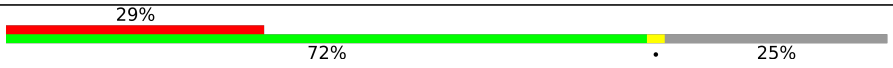
Mol	Chain	Length	Quality of chain
59	UP	7	
59	UW	7	
60	UQ	32	
61	UR	8	
61	UV	8	
61	UX	8	
62	US	54	
63	UT	44	
64	A0	185	
65	A1	241	
66	A2	471	
67	A3	218	
68	A4	183	
69	A5	80	
70	A6	114	
71	A8	181	
72	A9	184	
73	AE	473	
74	AF	459	
75	AI	263	
76	AJ	177	
77	AK	342	
78	AN	202	
79	AP	374	
80	AQ	167	

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Mol	Chain	Length	Quality of chain
81	AR	301	21% 70% 5% 25%
82	AT	144	14% 22% 76%
83	AU	213	25% 74% 8% 18%
84	AV	188	28% 87% 9%
85	AW	278	29% 88% 11%
86	AX	246	15% 65% 32%
87	AY	378	21% 81% 8% 10%
88	Ab	507	20% 83% 6% 11%
89	Ad	289	21% 80% 9% 11%
90	Ae	197	14% 54% 5% 41%
91	Af	189	20% 60% 7% 33%
92	Ag	260	26% 93% 7%
93	Aj	296	14% 91% 6%
94	Al	218	33% 88% 8%
95	Ao	259	28% 64% 7% 29%
96	Ap	309	35% 77% 8% 16%
97	At	154	32% 79% 10% 10%
98	Av	242	22% 79% 9% 12%
99	AB	56	82% 100%
100	AC	28	79% 100%
100	AD	28	96% 100%
101	AG	27	100% 100%
102	AA	1179	11% 25% 25% 50%
103	BA	831	24% 75% 7% 18%
104	BB	541	16% 66% 6% 28%

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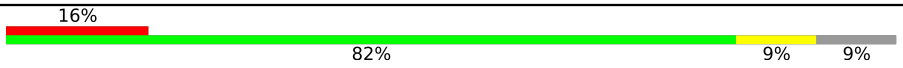
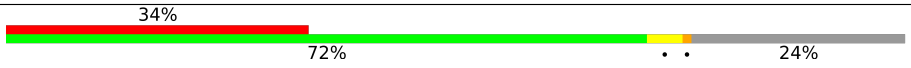
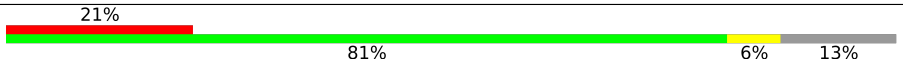
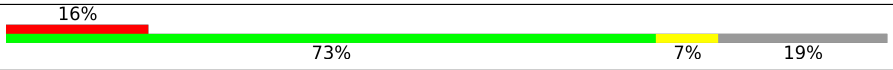
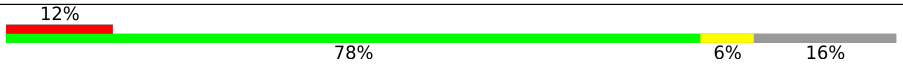
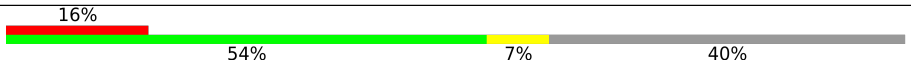
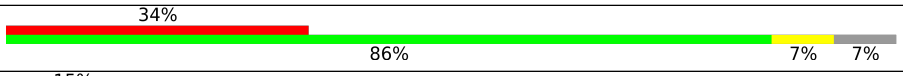
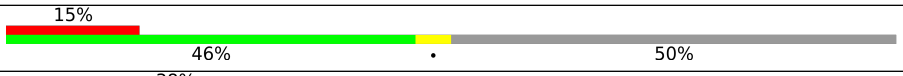
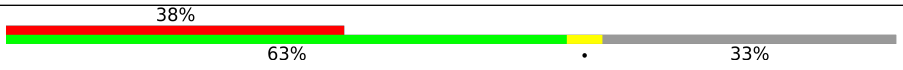
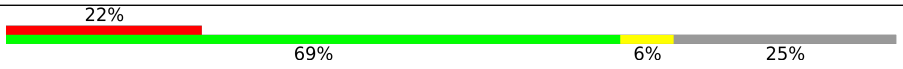
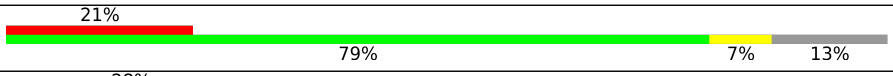
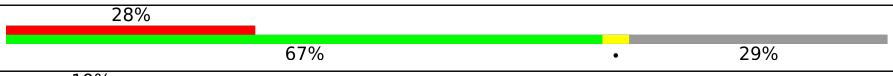
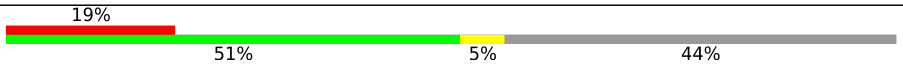
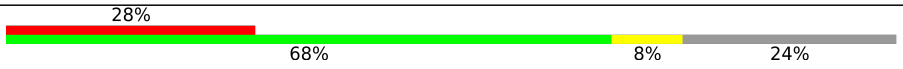
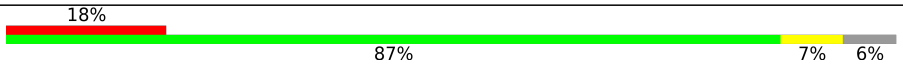
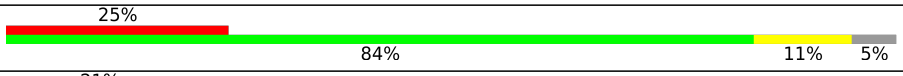
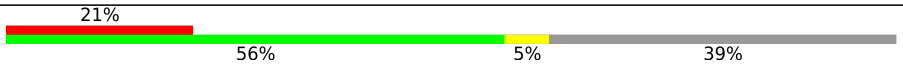
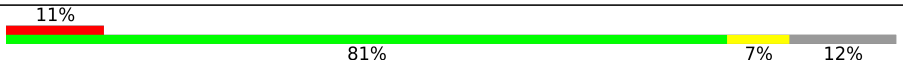
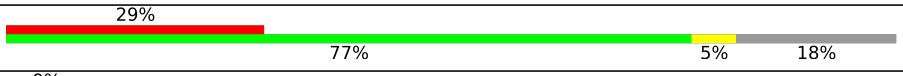
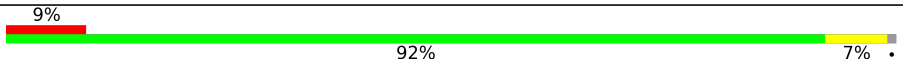
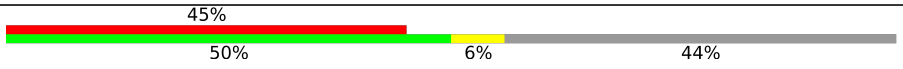
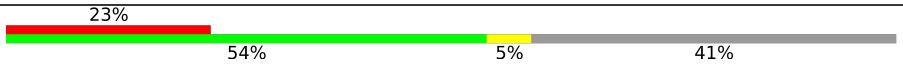
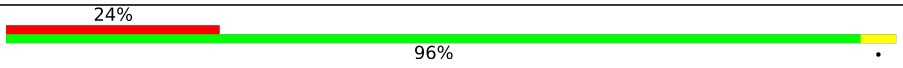
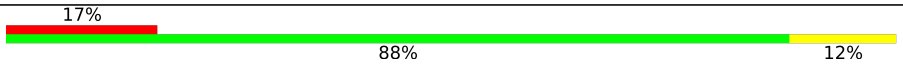
Mol	Chain	Length	Quality of chain
105	BC	523	
106	BD	547	
107	BE	449	
108	BF	426	
109	BG	378	
110	BH	349	
111	BI	343	
112	BJ	333	
113	BK	386	
114	BL	312	
115	BM	283	
116	BN	302	
117	BO	262	
118	BP	266	
119	BQ	231	
120	BR	205	
121	BS	160	
122	BT	191	
123	BU	185	
124	BV	190	
125	BW	188	
126	BX	190	
127	BY	172	
128	BZ	190	
129	Ba	139	

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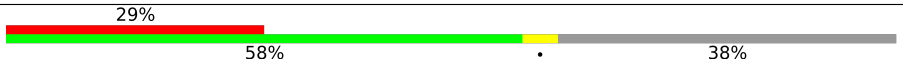
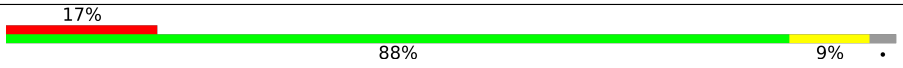
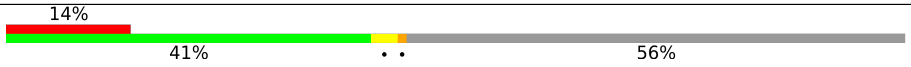
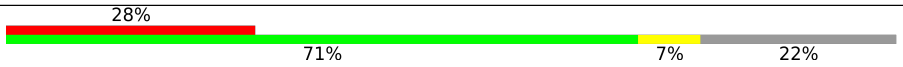
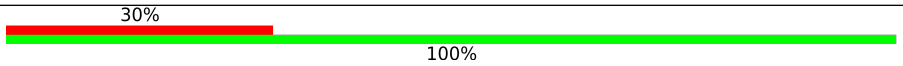
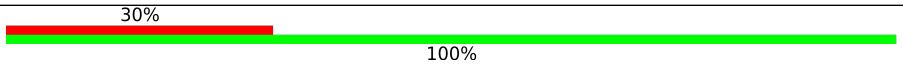
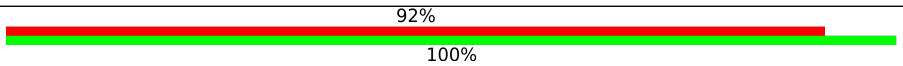
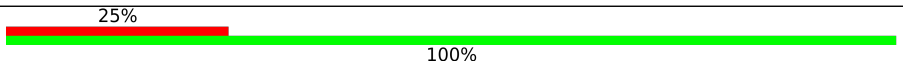
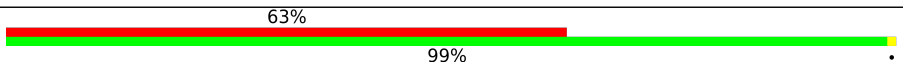
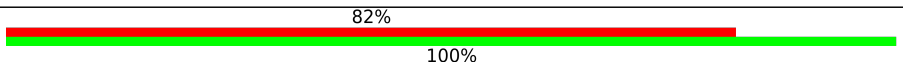
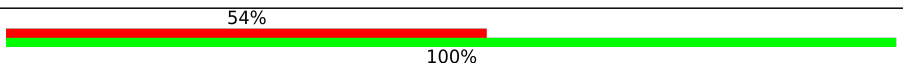
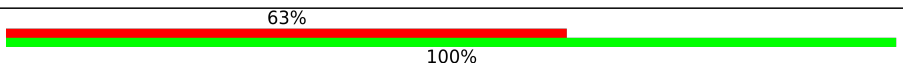
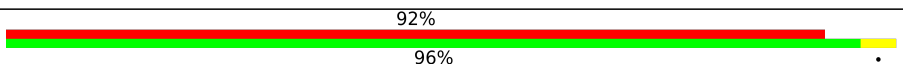
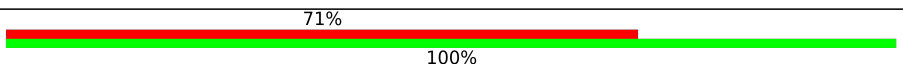
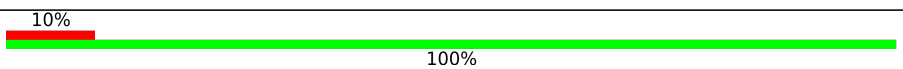
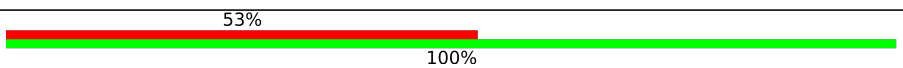
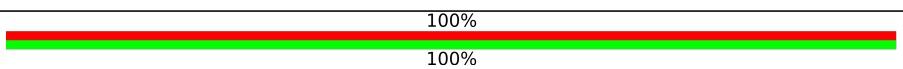
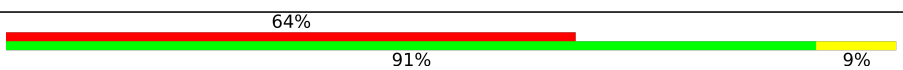
Mol	Chain	Length	Quality of chain
130	Bb	162	
131	Bc	146	
132	Bd	144	
133	Be	113	
134	Bf	113	
135	Bg	105	
136	Bh	92	
137	UA	46	
138	UB	40	
139	UC	12	
139	UH	12	
140	UD	177	
141	UE	22	
142	UF	24	
142	UG	24	
142	UN	24	
143	UI	17	
144	UK	10	
145	UL	15	
146	UM	6	
147	UU	11	

2 Entry composition (i)

There are 156 unique types of molecules in this entry. The entry contains 311240 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 ms48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DA	1557	12482	7881	2226	2337	38	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

- Molecule 2 is a protein called ms51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DD	791	6523	4127	1184	1171	41	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	371	PRO	SER	conflict	UNP Q385L8
DD	599	ALA	VAL	conflict	UNP Q385L8

- Molecule 3 is a protein called ms56.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	92	GLU	GLY	conflict	UNP Q587C2
DI	116	ASP	GLU	conflict	UNP Q587C2

- Molecule 4 is a protein called ms59.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DL	283	Total	C	N	O	S	0	0
			2287	1451	423	401	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

- Molecule 5 is a protein called ms60.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DM	294	Total	C	N	O	S	0	0
			2430	1533	459	426	12		

- Molecule 6 is a protein called ms61.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DN	257	Total	C	N	O	S	0	0
			2091	1331	379	371	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DN	51	GLY	SER	conflict	UNP Q38D60

- Molecule 7 is a protein called ms62.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DO	222	Total	C	N	O	S	0	0
			1804	1127	327	340	10		

- Molecule 8 is a protein called ms63.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DP	207	Total	C	N	O	S	0	0
			1760	1132	312	307	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DP	3	HIS	ARG	conflict	UNP Q38F25

- Molecule 9 is a protein called ms64.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DQ	256	Total	C	N	O	S	0	0
			2061	1293	389	370	9		

- Molecule 10 is a protein called ms65.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DR	251	Total	C	N	O	S	0	0
			2025	1304	369	342	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DR	128	PRO	SER	conflict	UNP C9ZPP1

- Molecule 11 is a protein called ms66.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	DS	238	Total	C	N	O	S	0	0
			1904	1185	356	348	15		

- Molecule 12 is a protein called ms68.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	DU	213	Total	C	N	O	S	0	0
			1754	1103	310	335	6		

- Molecule 13 is a protein called ms73.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	DZ	82	Total	C	N	O	S	0	0
			697	457	113	123	4		

- Molecule 14 is a protein called ms74.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Da	55	Total	C	N	O	S	0	0
			501	315	109	74	3		

- Molecule 15 is a protein called ms49.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DB	1111	Total	C	N	O	S	0	0
			9148	5691	1717	1711	29		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	359	ILE	THR	conflict	UNP C9ZJE4

- Molecule 16 is a protein called ms50.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	DC	1095	Total	C	N	O	S	0	0
			8748	5519	1544	1654	31		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	373	GLY	GLU	conflict	UNP C9ZSK8
DC	671	ARG	CYS	conflict	UNP C9ZSK8
DC	696	VAL	ALA	conflict	UNP C9ZSK8

- Molecule 17 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	DE	590	Total	C	N	O	S	0	0
			4831	3075	874	863	19		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	378	UNK	LYS	conflict	UNP Q386Q7
DE	384	UNK	THR	conflict	UNP Q386Q7
DE	?	-	SER	deletion	UNP Q386Q7

- Molecule 18 is a protein called ms53.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DF	590	Total	C	N	O	S	0	0
			4747	2979	896	847	25		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	conflict	UNP Q38ET1
DF	258	ASP	ASN	conflict	UNP Q38ET1
DF	372	ASN	ASP	conflict	UNP Q38ET1
DF	406	ASN	SER	conflict	UNP Q38ET1
DF	510	ASP	GLY	conflict	UNP Q38ET1
DF	577	ALA	VAL	conflict	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	conflict	UNP Q38ET1

- Molecule 19 is a protein called ms54.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	conflict	UNP Q57ZP8
DG	429	GLY	SER	conflict	UNP Q57ZP8

- Molecule 20 is a protein called ms55.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DH	564	Total	C	N	O	S	0	0
			4578	2872	850	834	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	conflict	UNP Q580V1
DH	194	PRO	ARG	conflict	UNP Q580V1
DH	488	GLY	SER	conflict	UNP Q580V1

- Molecule 21 is a protein called ms57.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DJ	315	Total	C	N	O	S	0	0
			2572	1646	452	460	14		

- Molecule 22 is a protein called ms58.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DK	255	Total	C	N	O	S	0	0
			2007	1260	365	377	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	conflict	UNP Q38BP1
DK	257	GLY	SER	conflict	UNP Q38BP1

- Molecule 23 is a protein called ms67.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DT	239	Total	C	N	O	S	0	0
			2058	1321	364	362	11		

- Molecule 24 is a protein called ms69.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DV	160	Total	C	N	O	S	0	0
			1346	855	252	235	4		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a protein called ms70.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DW	161	Total	C	N	O	S	0	0
			1359	866	260	228	5		

- Molecule 26 is a protein called ms71.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DX	141	Total	C	N	O	S	0	0
			1196	762	226	201	7		

- Molecule 27 is a protein called ms72.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DY	154	Total	C	N	O	S	0	0
			1293	827	245	216	5		

- Molecule 28 is a protein called uS3m.

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

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	4	MET	-	initiating methionine	UNP E0A3K1
CC	5	PHE	-	expression tag	UNP E0A3K1
CC	6	LEU	-	expression tag	UNP E0A3K1
CC	7	ILE	-	expression tag	UNP E0A3K1
CC	8	HIS	-	expression tag	UNP E0A3K1
CC	9	PHE	-	expression tag	UNP E0A3K1
CC	10	VAL	-	expression tag	UNP E0A3K1
CC	11	HIS	-	expression tag	UNP E0A3K1
CC	12	TYR	-	expression tag	UNP E0A3K1
CC	13	LYS	-	expression tag	UNP E0A3K1
CC	14	THR	-	expression tag	UNP E0A3K1
CC	15	ILE	-	expression tag	UNP E0A3K1
CC	16	LEU	-	expression tag	UNP E0A3K1
CC	17	GLN	-	expression tag	UNP E0A3K1
CC	18	LYS	-	expression tag	UNP E0A3K1
CC	20	THR	LYS	conflict	UNP E0A3K1
CC	21	PHE	ILE	conflict	UNP E0A3K1
CC	24	LYS	ILE	conflict	UNP E0A3K1
CC	25	HIS	PHE	conflict	UNP E0A3K1
CC	26	ILE	ASN	conflict	UNP E0A3K1
CC	27	PHE	LEU	conflict	UNP E0A3K1
CC	28	LEU	TYR	conflict	UNP E0A3K1
CC	29	SER	CYS	conflict	UNP E0A3K1
CC	32	LYS	ASN	conflict	UNP E0A3K1
CC	36	LEU	ILE	conflict	UNP E0A3K1

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	37	PHE	TYR	conflict	UNP E0A3K1
CC	40	ILE	LEU	conflict	UNP E0A3K1
CC	41	SER	ASN	conflict	UNP E0A3K1
CC	45	ILE	LEU	conflict	UNP E0A3K1
CC	50	ILE	LEU	conflict	UNP E0A3K1
CC	57	ILE	VAL	conflict	UNP E0A3K1
CC	62	PHE	LEU	conflict	UNP E0A3K1
CC	65	ILE	LEU	conflict	UNP E0A3K1
CC	68	PHE	LEU	conflict	UNP E0A3K1
CC	74	LEU	-	expression tag	UNP E0A3K1
CC	75	ILE	-	expression tag	UNP E0A3K1
CC	76	SER	-	expression tag	UNP E0A3K1
CC	77	THR	-	expression tag	UNP E0A3K1

- Molecule 29 is a protein called uS55m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CE	417	Total	C	N	O	S	0	0
			3399	2151	632	600	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	341	ARG	LYS	conflict	UNP Q38AX6

- Molecule 30 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CF	159	Total	C	N	O	S	0	0
			1292	821	228	237	6		

- Molecule 31 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CH	273	Total	C	N	O	S	0	0
			2228	1387	432	398	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CH	74	ASN	SER	conflict	UNP Q388R7

- Molecule 32 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CI	424	Total	C	N	O	S	0	0
			3386	2136	611	622	17		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 33 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CJ	800	Total	C	N	O	S	0	0
			6516	4119	1151	1216	30		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	conflict	UNP Q57Z45
CJ	484	HIS	ARG	conflict	UNP Q57Z45
CJ	488	SER	ASN	conflict	UNP Q57Z45
CJ	594	GLU	VAL	conflict	UNP Q57Z45
CJ	629	ARG	LYS	conflict	UNP Q57Z45

- Molecule 34 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CK	293	Total	C	N	O	S	0	0
			2418	1506	458	437	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 35 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CL	87	Total	C	N	O	S	0	0
			733	503	113	107	10		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	54	LEU	-	expression tag	UNP A0A0E3J9R6
CL	55	PHE	-	expression tag	UNP A0A0E3J9R6
CL	56	PHE	-	expression tag	UNP A0A0E3J9R6
CL	57	LEU	-	expression tag	UNP A0A0E3J9R6
CL	58	ARG	-	expression tag	UNP A0A0E3J9R6
CL	103	MET	LEU	conflict	UNP A0A0E3J9R6
CL	?	-	VAL	deletion	UNP A0A0E3J9R6
CL	112	ILE	PHE	conflict	UNP A0A0E3J9R6
CL	115	VAL	HIS	conflict	UNP A0A0E3J9R6
CL	116	MET	LEU	conflict	UNP A0A0E3J9R6
CL	132	VAL	ILE	conflict	UNP A0A0E3J9R6
CL	138	ILE	MET	conflict	UNP A0A0E3J9R6
CL	139	VAL	-	expression tag	UNP A0A0E3J9R6
CL	140	SER	-	expression tag	UNP A0A0E3J9R6

- Molecule 36 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	CN	157	Total	C	N	O	S	0	0
			1322	843	251	220	8		

- Molecule 37 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CO	361	Total	C	N	O	S	0	0
			3003	1907	560	520	16		

- Molecule 38 is a protein called bS16m.

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

- Molecule 39 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	CQ	190	Total	C	N	O	S	0	0
			1584	1015	302	259	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CQ	138	ALA	VAL	conflict	UNP Q38DP8

- Molecule 40 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CR	314	Total	C	N	O	S	0	0
			2567	1623	471	465	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

- Molecule 41 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	CS	142	Total	C	N	O	S	0	0
			1175	761	210	198	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CS	-71	MET	-	initiating methionine	UNP Q584T8
CS	-70	ALA	-	expression tag	UNP Q584T8
CS	-69	PHE	-	expression tag	UNP Q584T8
CS	-68	ARG	-	expression tag	UNP Q584T8
CS	-67	ASN	-	expression tag	UNP Q584T8
CS	-66	THR	-	expression tag	UNP Q584T8
CS	-65	PHE	-	expression tag	UNP Q584T8
CS	-64	THR	-	expression tag	UNP Q584T8
CS	-63	THR	-	expression tag	UNP Q584T8
CS	-62	PRO	-	expression tag	UNP Q584T8
CS	-61	GLY	-	expression tag	UNP Q584T8
CS	-60	LYS	-	expression tag	UNP Q584T8
CS	-59	PHE	-	expression tag	UNP Q584T8
CS	-58	SER	-	expression tag	UNP Q584T8
CS	-57	THR	-	expression tag	UNP Q584T8
CS	-56	VAL	-	expression tag	UNP Q584T8
CS	-55	SER	-	expression tag	UNP Q584T8
CS	-54	LYS	-	expression tag	UNP Q584T8
CS	-53	ASN	-	expression tag	UNP Q584T8
CS	-52	ILE	-	expression tag	UNP Q584T8
CS	-51	VAL	-	expression tag	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-50	LEU	-	expression tag	UNP Q584T8
CS	-49	LEU	-	expression tag	UNP Q584T8
CS	-48	LEU	-	expression tag	UNP Q584T8
CS	-47	ILE	-	expression tag	UNP Q584T8
CS	-46	TRP	-	expression tag	UNP Q584T8
CS	-45	ARG	-	expression tag	UNP Q584T8
CS	-44	VAL	-	expression tag	UNP Q584T8
CS	-43	LYS	-	expression tag	UNP Q584T8
CS	-42	VAL	-	expression tag	UNP Q584T8
CS	-41	PHE	-	expression tag	UNP Q584T8
CS	-40	LEU	-	expression tag	UNP Q584T8
CS	-39	ARG	-	expression tag	UNP Q584T8
CS	-38	ALA	-	expression tag	UNP Q584T8
CS	-37	GLU	-	expression tag	UNP Q584T8
CS	-36	GLY	-	expression tag	UNP Q584T8
CS	-35	PHE	-	expression tag	UNP Q584T8
CS	-34	ALA	-	expression tag	UNP Q584T8
CS	-33	HIS	-	expression tag	UNP Q584T8
CS	-32	SER	-	expression tag	UNP Q584T8
CS	-31	LEU	-	expression tag	UNP Q584T8
CS	-30	VAL	-	expression tag	UNP Q584T8
CS	-29	MET	-	expression tag	UNP Q584T8
CS	-28	LEU	-	expression tag	UNP Q584T8
CS	-27	PRO	-	expression tag	UNP Q584T8
CS	-26	VAL	-	expression tag	UNP Q584T8
CS	-25	SER	-	expression tag	UNP Q584T8
CS	-24	LEU	-	expression tag	UNP Q584T8
CS	-23	TYR	-	expression tag	UNP Q584T8
CS	-22	SER	-	expression tag	UNP Q584T8
CS	-21	LYS	-	expression tag	UNP Q584T8
CS	-20	ILE	-	expression tag	UNP Q584T8
CS	-19	LEU	-	expression tag	UNP Q584T8
CS	-18	LEU	-	expression tag	UNP Q584T8
CS	-17	CYS	-	expression tag	UNP Q584T8
CS	-16	ASP	-	expression tag	UNP Q584T8
CS	-15	VAL	-	expression tag	UNP Q584T8
CS	-14	LYS	-	expression tag	UNP Q584T8
CS	-13	LYS	-	expression tag	UNP Q584T8
CS	-12	LYS	-	expression tag	UNP Q584T8
CS	-11	ILE	-	expression tag	UNP Q584T8
CS	-10	VAL	-	expression tag	UNP Q584T8
CS	-9	TYR	-	expression tag	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-8	PHE	-	expression tag	UNP Q584T8
CS	-7	HIS	-	expression tag	UNP Q584T8
CS	-6	CYS	-	expression tag	UNP Q584T8
CS	-5	CYS	-	expression tag	UNP Q584T8
CS	-4	THR	-	expression tag	UNP Q584T8
CS	-3	ARG	-	expression tag	UNP Q584T8
CS	-2	LYS	-	expression tag	UNP Q584T8
CS	-1	LYS	-	expression tag	UNP Q584T8
CS	0	SER	-	expression tag	UNP Q584T8

- Molecule 42 is a protein called bS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	CU	184	Total	C	N	O	S	0	0
			1538	965	307	254	12		

- Molecule 43 is a protein called mt-IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CZ	151	Total	C	N	O	S	0	0
			1212	759	231	215	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CZ	30	THR	ILE	conflict	UNP C9ZRZ4

- Molecule 44 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ca	592	Total	C	N	O	S	0	0
			5004	3201	898	882	23		

- Molecule 45 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cb	252	Total	C	N	O	S	0	0
			2056	1300	368	380	8		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cb	244	SER	ASN	conflict	UNP Q57VB2
Cb	?	-	GLU	deletion	UNP Q57VB2
Cb	312	CYS	-	expression tag	UNP Q57VB2
Cb	313	SER	-	expression tag	UNP Q57VB2
Cb	314	ARG	-	expression tag	UNP Q57VB2
Cb	315	ASP	-	expression tag	UNP Q57VB2
Cb	316	GLY	-	expression tag	UNP Q57VB2
Cb	317	PHE	-	expression tag	UNP Q57VB2
Cb	318	ALA	-	expression tag	UNP Q57VB2
Cb	319	LEU	-	expression tag	UNP Q57VB2
Cb	320	MET	-	expression tag	UNP Q57VB2
Cb	321	LYS	-	expression tag	UNP Q57VB2
Cb	322	ALA	-	expression tag	UNP Q57VB2
Cb	323	ASN	-	expression tag	UNP Q57VB2
Cb	324	LYS	-	expression tag	UNP Q57VB2

- Molecule 46 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Cd	291	Total	C	N	O	S	0	0
			2389	1491	442	446	10		

- Molecule 47 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Cg	482	Total	C	N	O	S	0	0
			3904	2499	684	701	20		

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	-	expression tag	UNP Q585C2

- Molecule 48 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ci	165	Total	C	N	O	S	0	0
			1348	848	247	244	9		

- Molecule 49 is a protein called mS34.

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

- Molecule 50 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ck	703	Total	C	N	O	S	0	0
			5596	3503	1017	1050	26		

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 51 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Cm	196	Total	C	N	O	S	0	0
			1577	975	304	289	9		

- Molecule 52 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Cn	110	Total	C	N	O	S	0	0
			912	585	181	143	3		

- Molecule 53 is a protein called ms34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Cp	175	Total	C	N	O	S	0	0
			1483	937	268	273	5		

- Molecule 54 is a protein called ms42.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Cq	252	Total	C	N	O	S	0	0
			2005	1285	342	369	9		

- Molecule 55 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Cr	257	Total	C	N	O	S	0	0
			1999	1261	368	356	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cr	351	LYS	GLU	conflict	UNP Q585I1

- Molecule 56 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Cv	1059	Total	C	N	O	S	0	0
			8557	5387	1535	1596	39		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	16	CYS	PRO	conflict	UNP Q383R4
Cv	718	THR	ALA	conflict	UNP Q383R4
Cv	1179	GLU	GLY	conflict	UNP Q383R4

- Molecule 57 is a RNA chain called 9s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CA	621	Total	C	N	O	P	0	0
			13122	5906	2227	4368	621		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	298	U	C	conflict	GB 343546
CA	473	U	G	conflict	GB 343546
CA	614	U	-	expression tag	GB 343546
CA	615	U	-	expression tag	GB 343546
CA	616	U	-	expression tag	GB 343546
CA	617	U	-	expression tag	GB 343546
CA	618	U	-	expression tag	GB 343546
CA	619	U	-	expression tag	GB 343546
CA	620	U	-	expression tag	GB 343546
CA	621	U	-	expression tag	GB 343546

- Molecule 58 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	UO	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 59 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UP	7	Total	C	N	O	0	0
			42	28	7	7		
59	UW	7	Total	C	N	O	0	0
			42	28	7	7		

- Molecule 60 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	UQ	32	Total	C	N	O	0	0
			192	128	32	32		

- Molecule 61 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UR	8	Total	C	N	O	0	0
			48	32	8	8		
61	UV	8	Total	C	N	O	0	0
			48	32	8	8		
61	UX	8	Total	C	N	O	0	0
			48	32	8	8		

- Molecule 62 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	US	54	Total	C	N	O	0	0
			324	216	54	54		

- Molecule 63 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	UT	44	Total	C	N	O	0	0
			264	176	44	44		

- Molecule 64 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	A0	151	Total	C	N	O	S	0	0
			1269	801	236	227	5		

- Molecule 65 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	A1	217	Total	C	N	O	S	0	0
			1788	1138	324	317	9		

- Molecule 66 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	A2	449	Total	C	N	O	S	0	0
			3638	2324	631	670	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	238	GLY	ALA	conflict	UNP Q38EM7

- Molecule 67 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	A3	150	Total	C	N	O	S	0	0
			1215	776	234	199	6		

- Molecule 68 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A4	168	Total	C	N	O	S	0	0
			1387	880	262	240	5		

- Molecule 69 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	A5	55	Total	C	N	O	S	0	0
			483	311	90	76	6		

- Molecule 70 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	A6	72	Total	C	N	O	S	0	0
			568	361	102	101	4		

- Molecule 71 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	A8	142	Total	C	N	O	S	0	0
			1203	753	243	198	9		

- Molecule 72 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	A9	53	Total	C	N	O	S	0	0
			459	288	85	78	8		

- Molecule 73 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AE	293	Total	C	N	O	S	0	0
			2390	1543	395	440	12		

- Molecule 74 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AF	442	Total	C	N	O	S	0	0
			3597	2294	624	654	25		

- Molecule 75 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AI	212	Total	C	N	O	S	0	0
			1790	1153	316	312	9		

- Molecule 76 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AJ	126	Total	C	N	O	S	0	0
			965	606	191	165	3		

- Molecule 77 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AK	323	Total	C	N	O	S	0	0
			2676	1703	485	469	19		

- Molecule 78 is a protein called 50S ribosomal protein L13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AN	179	Total	C	N	O	S	0	0
			1508	973	275	251	9		

- Molecule 79 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AP	352	Total	C	N	O	S	0	0
			2904	1846	538	507	13		

- Molecule 80 is a protein called 50S ribosomal protein L16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AQ	125	Total	C	N	O	S	0	0
			1020	658	183	175	4		

- Molecule 81 is a protein called 50S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AR	227	Total	C	N	O	S	0	0
			1912	1211	356	332	13		

- Molecule 82 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AT	35	Total	C	N	O	S	0	0
			287	180	61	45	1		

- Molecule 83 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	AU	175	Total	C	N	O	S	0	0
			1423	895	280	243	5		

- Molecule 84 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	AV	181	Total	C	N	O	S	0	0
			1424	909	257	252	6		

- Molecule 85 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AW	276	Total	C	N	O	S	0	0
			2235	1416	415	391	13		

- Molecule 86 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	AX	168	Total	C	N	O	S	0	0
			1416	913	253	245	5		

- Molecule 87 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	AY	340	Total	C	N	O	S	0	0
			2712	1689	493	517	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	345	GLU	VAL	conflict	UNP C9ZK52

- Molecule 88 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ab	453	Total	C	N	O	S	0	0
			3545	2252	621	657	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	290	SER	PHE	conflict	UNP Q381T7
Ab	299	GLU	LYS	conflict	UNP Q381T7
Ab	471	ASN	ILE	conflict	UNP Q381T7

- Molecule 89 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Ad	257	Total	C	N	O	S	0	0
			2122	1319	386	405	12		

- Molecule 90 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Ae	116	Total	C	N	O	S	0	0
			927	594	170	158	5		

- Molecule 91 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Af	126	Total	C	N	O	S	0	0
			1013	630	196	183	4		

- Molecule 92 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	Ag	259	Total	C	N	O	S	0	0
			2193	1368	422	392	11		

- Molecule 93 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	Aj	279	Total	C	N	O	S	0	0
			2246	1408	414	416	8		

- Molecule 94 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	Al	209	Total	C	N	O	S	0	0
			1618	1051	281	279	7		

- Molecule 95 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	Ao	183	Total	C	N	O	S	0	0
			1475	936	272	264	3		

- Molecule 96 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	Ap	261	Total	C	N	O	S	0	0
			2143	1391	372	368	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ap	2	LEU	SER	conflict	UNP Q57YA9

- Molecule 97 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	At	138	Total	C	N	O	S	0	0
			1100	690	210	196	4		

- Molecule 98 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	Av	213	Total	C	N	O	S	0	0
			1792	1138	333	308	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Av	164	ARG	GLN	conflict	UNP Q383B7

- Molecule 99 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
99	AB	56	Total	C	N	O	0	0
			280	168	56	56		

- Molecule 100 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
100	AC	28	Total	C	N	O	0	0
			140	84	28	28		
100	AD	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 101 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
101	AG	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 102 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	AA	591	Total	C	N	O	P	0	0
			12491	5628	2125	4147	591		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	448	A	U	conflict	GB 343546
AA	454	U	G	conflict	GB 343546
AA	455	U	G	conflict	GB 343546
AA	622	A	U	conflict	GB 343546
AA	636	A	G	conflict	GB 343546
AA	702	G	A	conflict	GB 343546
AA	706	C	U	conflict	GB 343546
AA	743	C	G	conflict	GB 343546
AA	752	G	A	conflict	GB 343546
AA	757	U	A	conflict	GB 343546
AA	760	U	G	conflict	GB 343546
AA	762	U	G	conflict	GB 343546
AA	789	G	C	conflict	GB 343546
AA	793	G	U	conflict	GB 343546
AA	877	A	UNK	conflict	GB 343546

- Molecule 103 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	BA	679	Total	C	N	O	S	0	0
			5384	3422	948	981	33		

- Molecule 104 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	BB	389	Total	C	N	O	S	0	0
			3050	1883	535	619	13		

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	264	SER	ALA	conflict	UNP Q38CI0
BB	265	SER	PRO	conflict	UNP Q38CI0
BB	267	SER	HIS	conflict	UNP Q38CI0
BB	268	SER	GLY	conflict	UNP Q38CI0
BB	269	SER	ALA	conflict	UNP Q38CI0
BB	270	SER	LEU	conflict	UNP Q38CI0
BB	271	SER	THR	conflict	UNP Q38CI0
BB	272	SER	LEU	conflict	UNP Q38CI0
BB	273	SER	ASP	conflict	UNP Q38CI0
BB	274	SER	ASP	conflict	UNP Q38CI0
BB	275	SER	VAL	conflict	UNP Q38CI0
BB	276	SER	PRO	conflict	UNP Q38CI0
BB	277	SER	HIS	conflict	UNP Q38CI0
BB	278	SER	GLN	conflict	UNP Q38CI0
BB	279	SER	GLU	conflict	UNP Q38CI0
BB	280	SER	ALA	conflict	UNP Q38CI0
BB	281	SER	VAL	conflict	UNP Q38CI0
BB	282	SER	ARG	conflict	UNP Q38CI0
BB	283	SER	LEU	conflict	UNP Q38CI0
BB	284	SER	TYR	conflict	UNP Q38CI0
BB	285	SER	ARG	conflict	UNP Q38CI0
BB	286	SER	ASP	conflict	UNP Q38CI0
BB	287	SER	LEU	conflict	UNP Q38CI0
BB	288	SER	MET	conflict	UNP Q38CI0
BB	289	SER	GLU	conflict	UNP Q38CI0
BB	290	SER	LYS	conflict	UNP Q38CI0
BB	291	SER	ALA	conflict	UNP Q38CI0
BB	292	SER	ASP	conflict	UNP Q38CI0
BB	293	SER	MET	conflict	UNP Q38CI0
BB	294	SER	PRO	conflict	UNP Q38CI0
BB	295	SER	VAL	conflict	UNP Q38CI0
BB	296	SER	MET	conflict	UNP Q38CI0
BB	297	SER	LEU	conflict	UNP Q38CI0
BB	298	SER	GLY	conflict	UNP Q38CI0
BB	299	SER	ASN	conflict	UNP Q38CI0
BB	300	SER	GLY	conflict	UNP Q38CI0
BB	301	SER	ALA	conflict	UNP Q38CI0
BB	302	SER	GLU	conflict	UNP Q38CI0
BB	303	SER	ILE	conflict	UNP Q38CI0
BB	304	SER	PRO	conflict	UNP Q38CI0
BB	305	SER	PRO	conflict	UNP Q38CI0
BB	306	SER	MET	conflict	UNP Q38CI0
BB	307	SER	ASP	conflict	UNP Q38CI0

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	308	SER	LEU	conflict	UNP Q38CI0
BB	309	SER	ARG	conflict	UNP Q38CI0
BB	310	SER	ALA	conflict	UNP Q38CI0
BB	311	SER	LEU	conflict	UNP Q38CI0
BB	312	SER	PHE	conflict	UNP Q38CI0
BB	313	SER	HIS	conflict	UNP Q38CI0
BB	314	SER	LEU	conflict	UNP Q38CI0
BB	316	SER	ALA	conflict	UNP Q38CI0
BB	317	SER	ASN	conflict	UNP Q38CI0
BB	318	SER	PRO	conflict	UNP Q38CI0
BB	319	SER	GLU	conflict	UNP Q38CI0
BB	320	SER	ARG	conflict	UNP Q38CI0
BB	321	SER	MET	conflict	UNP Q38CI0
BB	322	SER	LYS	conflict	UNP Q38CI0
BB	323	SER	ALA	conflict	UNP Q38CI0
BB	324	SER	ALA	conflict	UNP Q38CI0
BB	326	SER	GLU	conflict	UNP Q38CI0
BB	327	SER	LEU	conflict	UNP Q38CI0
BB	330	SER	TRP	conflict	UNP Q38CI0
BB	331	SER	ARG	conflict	UNP Q38CI0
BB	332	SER	GLU	conflict	UNP Q38CI0
BB	333	SER	VAL	conflict	UNP Q38CI0
BB	334	SER	ARG	conflict	UNP Q38CI0
BB	335	SER	GLY	conflict	UNP Q38CI0
BB	336	SER	MET	conflict	UNP Q38CI0
BB	337	SER	LEU	conflict	UNP Q38CI0
BB	338	SER	ALA	conflict	UNP Q38CI0
BB	339	SER	PRO	conflict	UNP Q38CI0
BB	340	SER	VAL	conflict	UNP Q38CI0
BB	341	SER	GLN	conflict	UNP Q38CI0
BB	342	SER	GLU	conflict	UNP Q38CI0
BB	343	SER	VAL	conflict	UNP Q38CI0
BB	361	ALA	VAL	conflict	UNP Q38CI0
BB	403	THR	ARG	conflict	UNP Q38CI0

- Molecule 105 is a protein called mL69.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	BC	478	Total	C	N	O	S	0	0
			3821	2451	670	680	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	29	PRO	SER	conflict	UNP Q584V5
BC	42	GLY	SER	conflict	UNP Q584V5

- Molecule 106 is a protein called mL70.

Mol	Chain	Residues	Atoms				AltConf	Trace
106	BD	417	Total	C	N	O	0	0
			2063	1229	417	417		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	47	CYS	LEU	conflict	UNP C9ZR91
BD	49	CYS	LEU	conflict	UNP C9ZR91
BD	50	LEU	SER	conflict	UNP C9ZR91
BD	51	TRP	LEU	conflict	UNP C9ZR91
BD	52	SER	VAL	conflict	UNP C9ZR91
BD	53	ILE	HIS	conflict	UNP C9ZR91
BD	55	LEU	PRO	conflict	UNP C9ZR91
BD	56	SER	GLN	conflict	UNP C9ZR91
BD	57	PHE	LEU	conflict	UNP C9ZR91
BD	58	ARG	PRO	conflict	UNP C9ZR91
BD	59	CYS	VAL	conflict	UNP C9ZR91
BD	60	PHE	LEU	conflict	UNP C9ZR91
BD	61	CYS	LEU	conflict	UNP C9ZR91
BD	63	ARG	SER	conflict	UNP C9ZR91
BD	64	SER	PHE	conflict	UNP C9ZR91
BD	65	TYR	LEU	conflict	UNP C9ZR91
BD	66	ALA	CYS	conflict	UNP C9ZR91
BD	67	ILE	ASP	conflict	UNP C9ZR91
BD	68	MET	HIS	conflict	UNP C9ZR91
BD	69	LEU	ALA	conflict	UNP C9ZR91
BD	?	-	THR	deletion	UNP C9ZR91
BD	?	-	THR	deletion	UNP C9ZR91
BD	?	-	PHE	deletion	UNP C9ZR91
BD	?	-	PHE	deletion	UNP C9ZR91
BD	?	-	SER	deletion	UNP C9ZR91
BD	?	-	ASP	deletion	UNP C9ZR91
BD	?	-	ASN	deletion	UNP C9ZR91
BD	?	-	SER	deletion	UNP C9ZR91
BD	71	LEU	ASP	conflict	UNP C9ZR91
BD	73	SER	HIS	conflict	UNP C9ZR91
BD	76	THR	PHE	conflict	UNP C9ZR91

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Chain	Residue	Modelled	Actual	Comment	Reference
BD	80	SER	ALA	conflict	UNP C9ZR91
BD	81	ILE	ASN	conflict	UNP C9ZR91
BD	82	PHE	TYR	conflict	UNP C9ZR91
BD	83	LEU	TYR	conflict	UNP C9ZR91
BD	84	SER	LEU	conflict	UNP C9ZR91
BD	86	LYS	-	insertion	UNP C9ZR91
BD	87	LEU	-	insertion	UNP C9ZR91
BD	88	PRO	-	insertion	UNP C9ZR91
BD	89	ILE	-	insertion	UNP C9ZR91
BD	90	THR	-	insertion	UNP C9ZR91
BD	93	LEU	SER	conflict	UNP C9ZR91
BD	95	SER	-	insertion	UNP C9ZR91
BD	96	PRO	PHE	conflict	UNP C9ZR91
BD	99	VAL	CYS	conflict	UNP C9ZR91
BD	100	PHE	VAL	conflict	UNP C9ZR91
BD	101	VAL	CYS	conflict	UNP C9ZR91
BD	102	PHE	LEU	conflict	UNP C9ZR91
BD	103	VAL	ARG	conflict	UNP C9ZR91
BD	104	PHE	TYR	conflict	UNP C9ZR91
BD	105	ALA	SER	conflict	UNP C9ZR91
BD	106	ILE	LEU	conflict	UNP C9ZR91
BD	107	ARG	LEU	conflict	UNP C9ZR91
BD	108	TYR	TRP	conflict	UNP C9ZR91
BD	109	CYS	VAL	conflict	UNP C9ZR91
BD	110	GLY	THR	conflict	UNP C9ZR91

- Molecule 107 is a protein called mL71.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	BE	392	Total	C	N	O	S	0	0
			3105	1970	540	582	13		

- Molecule 108 is a protein called mL72.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	BF	345	Total	C	N	O	S	0	0
			2838	1797	517	511	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	296	ILE	THR	conflict	UNP C9ZR63

- Molecule 109 is a protein called mL73.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	BG	319	Total	C	N	O	S	0	0
			2503	1578	449	459	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	185	PHE	LEU	conflict	UNP Q57Y49

- Molecule 110 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	BH	211	Total	C	N	O	S	0	0
			1729	1110	301	315	3		

- Molecule 111 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	BI	319	Total	C	N	O	S	0	0
			2609	1664	473	456	16		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	227	ASN	ASP	conflict	UNP Q38CK0
BI	319	ARG	GLN	conflict	UNP Q38CK0
BI	343	ALA	-	expression tag	UNP Q38CK0

- Molecule 112 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	BJ	166	Total	C	N	O	S	0	0
			1339	832	262	239	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	329	GLU	ALA	conflict	UNP Q383M2

- Molecule 113 is a protein called mL77.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	BK	258	Total	C	N	O	S	0	0
			1998	1239	383	368	8		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	234	SER	GLU	conflict	UNP C9ZQR6
BK	235	SER	GLY	conflict	UNP C9ZQR6
BK	236	SER	ASP	conflict	UNP C9ZQR6
BK	237	SER	ASP	conflict	UNP C9ZQR6
BK	238	SER	GLY	conflict	UNP C9ZQR6
BK	240	SER	PRO	conflict	UNP C9ZQR6
BK	241	SER	ALA	conflict	UNP C9ZQR6
BK	242	SER	GLY	conflict	UNP C9ZQR6
BK	243	SER	ARG	conflict	UNP C9ZQR6
BK	244	SER	GLU	conflict	UNP C9ZQR6
BK	245	SER	GLU	conflict	UNP C9ZQR6
BK	247	SER	ILE	conflict	UNP C9ZQR6
BK	248	SER	ARG	conflict	UNP C9ZQR6
BK	249	SER	ARG	conflict	UNP C9ZQR6
BK	250	SER	VAL	conflict	UNP C9ZQR6
BK	251	SER	ALA	conflict	UNP C9ZQR6
BK	252	SER	ALA	conflict	UNP C9ZQR6
BK	253	SER	ALA	conflict	UNP C9ZQR6
BK	254	SER	ALA	conflict	UNP C9ZQR6
BK	255	SER	ALA	conflict	UNP C9ZQR6
BK	256	SER	GLU	conflict	UNP C9ZQR6
BK	257	SER	ARG	conflict	UNP C9ZQR6
BK	258	SER	PHE	conflict	UNP C9ZQR6
BK	259	SER	ALA	conflict	UNP C9ZQR6
BK	260	SER	GLU	conflict	UNP C9ZQR6
BK	261	SER	LYS	conflict	UNP C9ZQR6
BK	262	SER	VAL	conflict	UNP C9ZQR6
BK	263	SER	ARG	conflict	UNP C9ZQR6
BK	264	SER	ARG	conflict	UNP C9ZQR6
BK	265	SER	GLN	conflict	UNP C9ZQR6
BK	266	SER	TYR	conflict	UNP C9ZQR6
BK	267	SER	GLY	conflict	UNP C9ZQR6
BK	268	SER	PRO	conflict	UNP C9ZQR6
BK	269	SER	GLY	conflict	UNP C9ZQR6
BK	270	SER	MET	conflict	UNP C9ZQR6
BK	271	SER	LEU	conflict	UNP C9ZQR6
BK	272	SER	ARG	conflict	UNP C9ZQR6

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Chain	Residue	Modelled	Actual	Comment	Reference
BK	273	SER	HIS	conflict	UNP C9ZQR6
BK	274	SER	ALA	conflict	UNP C9ZQR6
BK	275	SER	ARG	conflict	UNP C9ZQR6
BK	276	SER	VAL	conflict	UNP C9ZQR6
BK	277	SER	TYR	conflict	UNP C9ZQR6
BK	278	SER	THR	conflict	UNP C9ZQR6
BK	280	SER	LEU	conflict	UNP C9ZQR6
BK	348	VAL	LEU	conflict	UNP C9ZQR6

- Molecule 114 is a protein called mL78.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	BL	234	Total	C	N	O	S	0	0
			1887	1158	370	349	10		

- Molecule 115 is a protein called mL79.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	BM	245	Total	C	N	O	S	0	0
			2015	1280	370	356	9		

- Molecule 116 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	BN	214	Total	C	N	O	S	0	0
			1746	1079	320	342	5		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	145	SER	ALA	conflict	UNP Q585A3
BN	146	SER	HIS	conflict	UNP Q585A3
BN	148	SER	GLY	conflict	UNP Q585A3
BN	149	SER	LEU	conflict	UNP Q585A3
BN	150	SER	ARG	conflict	UNP Q585A3
BN	151	SER	GLY	conflict	UNP Q585A3
BN	152	SER	ALA	conflict	UNP Q585A3
BN	153	SER	ALA	conflict	UNP Q585A3
BN	154	SER	ALA	conflict	UNP Q585A3
BN	155	SER	THR	conflict	UNP Q585A3
BN	156	SER	GLU	conflict	UNP Q585A3
BN	157	SER	THR	conflict	UNP Q585A3

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Chain	Residue	Modelled	Actual	Comment	Reference
BN	159	SER	THR	conflict	UNP Q585A3
BN	160	SER	TYR	conflict	UNP Q585A3
BN	161	SER	ALA	conflict	UNP Q585A3
BN	162	SER	GLU	conflict	UNP Q585A3
BN	163	SER	LYS	conflict	UNP Q585A3
BN	164	SER	PHE	conflict	UNP Q585A3
BN	165	SER	ARG	conflict	UNP Q585A3
BN	166	SER	GLU	conflict	UNP Q585A3
BN	167	SER	MET	conflict	UNP Q585A3
BN	168	SER	ASN	conflict	UNP Q585A3
BN	169	SER	VAL	conflict	UNP Q585A3
BN	170	SER	GLU	conflict	UNP Q585A3
BN	171	SER	ALA	conflict	UNP Q585A3
BN	172	SER	LYS	conflict	UNP Q585A3
BN	173	SER	GLU	conflict	UNP Q585A3
BN	174	SER	ALA	conflict	UNP Q585A3

- Molecule 117 is a protein called mL81.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	BO	147	Total	C	N	O	S	0	0
			1146	719	202	213	12		

- Molecule 118 is a protein called mL82.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	BP	202	Total	C	N	O	S	0	0
			1550	973	292	276	9		

- Molecule 119 is a protein called mL83.

Mol	Chain	Residues	Atoms					AltConf	Trace
119	BQ	216	Total	C	N	O	S	0	0
			1675	1061	291	315	8		

- Molecule 120 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	BR	195	Total	C	N	O	S	0	0
			1650	1059	298	284	9		

- Molecule 121 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
121	BS	97	Total	C	N	O	S	0	0
			784	493	141	144	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	45	ILE	VAL	conflict	UNP Q38FG8

- Molecule 122 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
122	BT	168	Total	C	N	O	S	0	0
			1389	853	270	260	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	70	ARG	GLN	conflict	UNP C9ZPU8

- Molecule 123 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
123	BU	82	Total	C	N	O	S	0	0
			694	436	139	115	4		

- Molecule 124 is a protein called mL88.

Mol	Chain	Residues	Atoms					AltConf	Trace
124	BV	155	Total	C	N	O	S	0	0
			1307	832	233	236	6		

- Molecule 125 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
125	BW	187	Total	C	N	O	S	0	0
			1557	987	298	264	8		

- Molecule 126 is a protein called mL90.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	BX	107	Total	C	N	O	S	0	0
			867	552	160	147	8		

- Molecule 127 is a protein called mS91.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	BY	102	Total	C	N	O	S	0	0
			877	549	171	154	3		

- Molecule 128 is a protein called mL92.

Mol	Chain	Residues	Atoms					AltConf	Trace
128	BZ	190	Total	C	N	O	S	0	0
			1390	878	242	263	7		

- Molecule 129 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
129	Ba	139	Total	C	N	O	S	0	0
			1224	785	223	209	7		

- Molecule 130 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
130	Bb	99	Total	C	N	O	S	0	0
			770	482	144	143	1		

- Molecule 131 is a protein called mL95.

Mol	Chain	Residues	Atoms				AltConf	Trace
131	Bc	90	Total	C	N	O	0	0
			781	495	148	138		

- Molecule 132 is a protein called mL96.

Mol	Chain	Residues	Atoms					AltConf	Trace
132	Bd	140	Total	C	N	O	S	0	0
			1113	689	209	204	11		

- Molecule 133 is a protein called mL97.

Mol	Chain	Residues	Atoms					AltConf	Trace
133	Be	101	Total	C	N	O	S	0	0
			822	517	152	144	9		

- Molecule 134 is a protein called mL98.

Mol	Chain	Residues	Atoms				AltConf	Trace
134	Bf	50	Total 434	C 279	N 80	O 75	0	0

- Molecule 135 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
135	Bg	82	Total 656	C 412	N 126	O 116	S 2	0	0

- Molecule 136 is a protein called mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
136	Bh	91	Total 730	C 466	N 129	O 125	S 10	0	0

- Molecule 137 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
137	UA	46	Total 276	C 184	N 46	O 46	0	0

- Molecule 138 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
138	UB	40	Total 240	C 160	N 40	O 40	0	0

- Molecule 139 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
139	UC	12	Total 72	C 48	N 12	O 12	0	0
139	UH	12	Total 72	C 48	N 12	O 12	0	0

- Molecule 140 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
140	UD	177	Total 1062	C 708	N 177	O 177	0	0

- Molecule 141 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
141	UE	22	Total 132	C 88	N 22	O 22	0	0

- Molecule 142 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
142	UF	24	Total 144	C 96	N 24	O 24	0	0
142	UG	24	Total 144	C 96	N 24	O 24	0	0
142	UN	24	Total 144	C 96	N 24	O 24	0	0

- Molecule 143 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
143	UI	17	Total 102	C 68	N 17	O 17	0	0

- Molecule 144 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
144	UK	10	Total 60	C 40	N 10	O 10	0	0

- Molecule 145 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
145	UL	15	Total 90	C 60	N 15	O 15	0	0

- Molecule 146 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
146	UM	6	Total 36	C 24	N 6	O 6	0	0

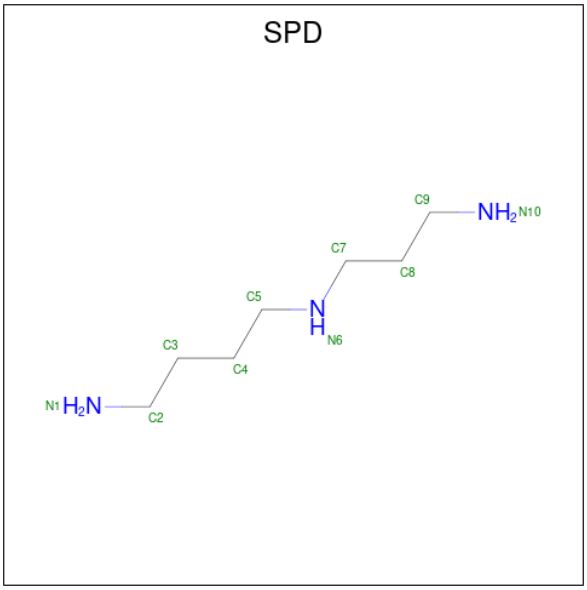
- Molecule 147 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
147	UU	11	Total 66	C 44	N 11	O 11	0	0

- Molecule 148 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
148	DA	1	Total Zn 1 1	0
148	DS	2	Total Zn 2 2	0
148	Cr	1	Total Zn 1 1	0
148	A5	1	Total Zn 1 1	0
148	A9	1	Total Zn 1 1	0
148	BX	2	Total Zn 2 2	0
148	Be	1	Total Zn 1 1	0
148	Bh	1	Total Zn 1 1	0

- Molecule 149 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



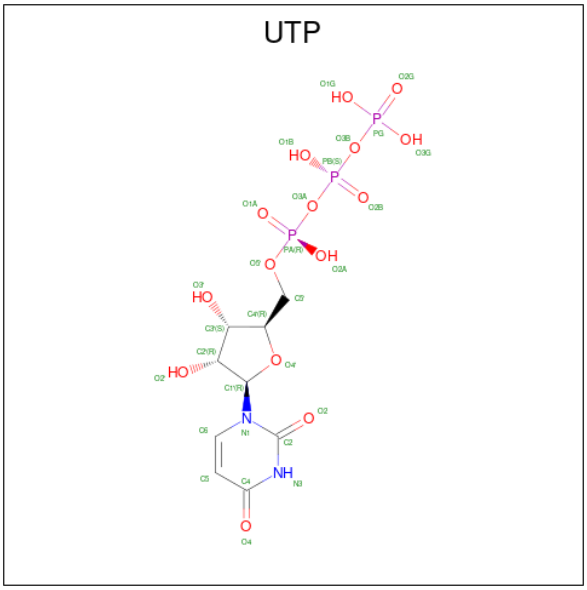
Mol	Chain	Residues	Atoms	AltConf
149	DL	1	Total C N 10 7 3	0
149	CA	1	Total C N 30 21 9	0
149	CA	1	Total C N 30 21 9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
149	CA	1	Total 30	C 21	N 9	0

- Molecule 150 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).

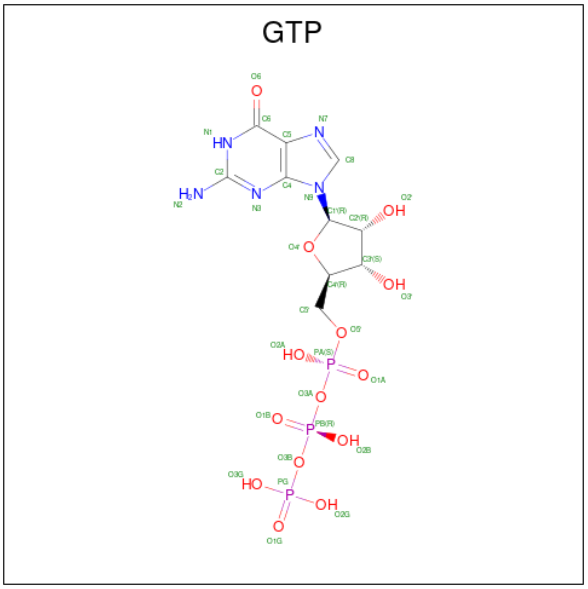


Mol	Chain	Residues	Atoms					AltConf
150	DJ	1	Total 29	C 9	N 2	O 15	P 3	0

- Molecule 151 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

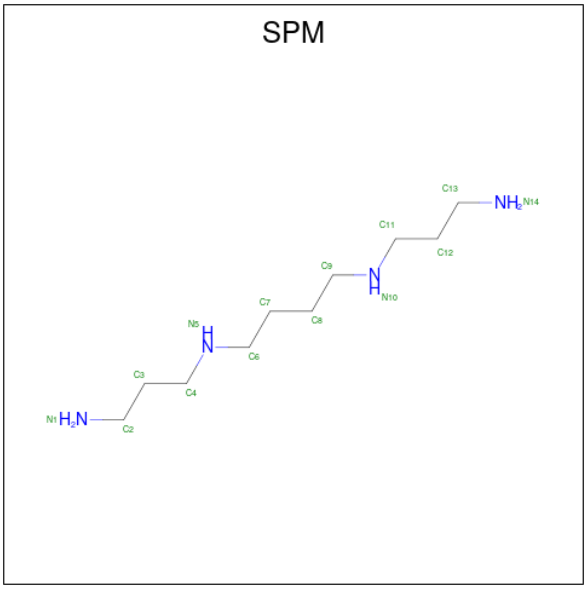
Mol	Chain	Residues	Atoms		AltConf
151	CO	1	Total 1	Mg 1	0
151	CQ	1	Total 1	Mg 1	0
151	Ca	1	Total 1	Mg 1	0
151	Cg	1	Total 1	Mg 1	0
151	Cv	1	Total 1	Mg 1	0
151	CA	34	Total 34	Mg 34	0
151	AA	7	Total 7	Mg 7	0

- Molecule 152 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



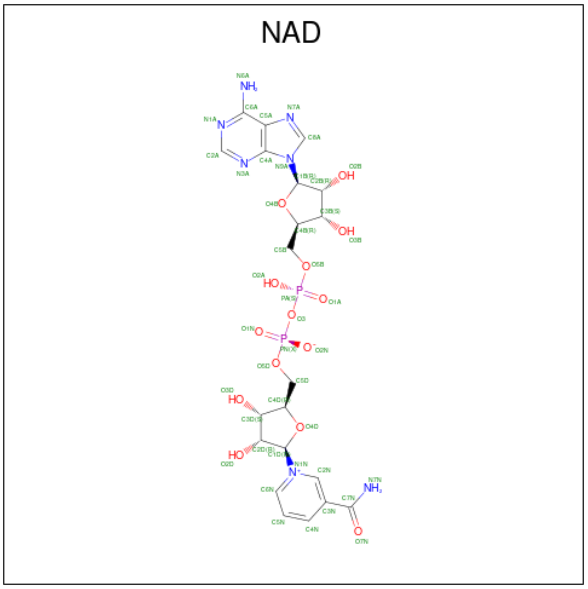
Mol	Chain	Residues	Atoms					AltConf
152	Cg	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 153 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



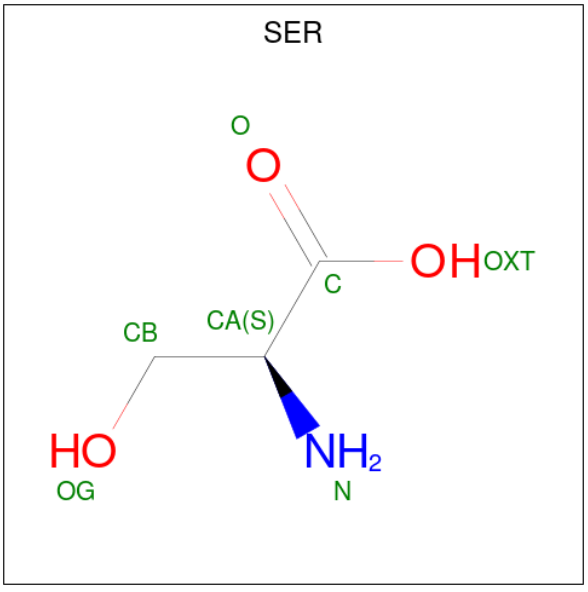
Mol	Chain	Residues	Atoms			AltConf
153	CA	1	Total	C	N	0
			14	10	4	

- Molecule 154 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
154	Av	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 155 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms		AltConf
155	UB	1	Total	O	0
			1	1	

- Molecule 156 is water.

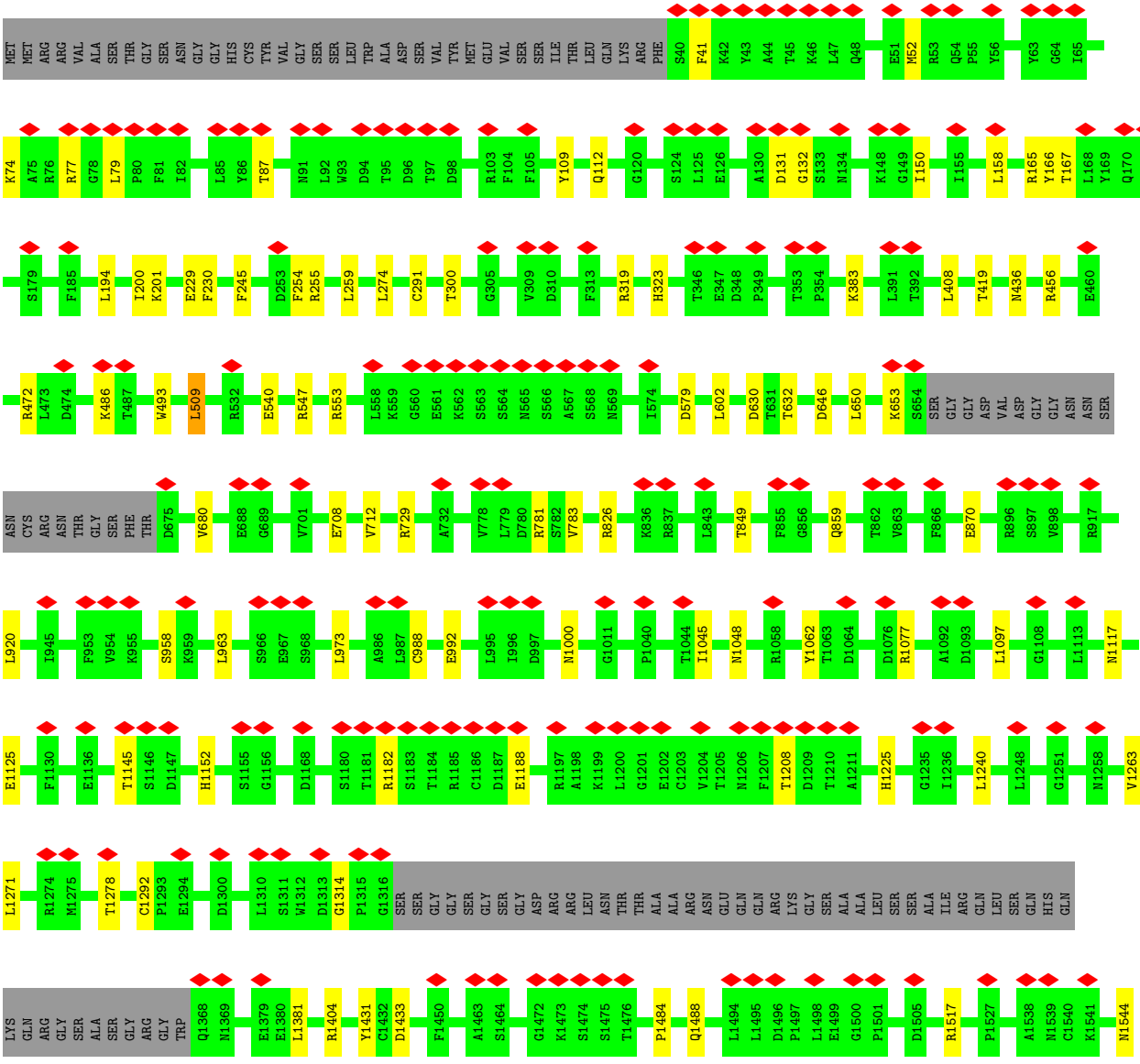
Mol	Chain	Residues	Atoms		AltConf
156	Cg	3	Total	O	0
			3	3	

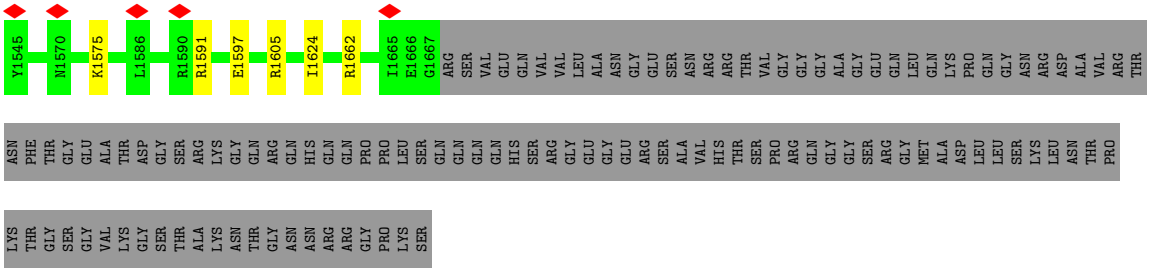
3 Residue-property plots (i)

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

- Molecule 1: ms48

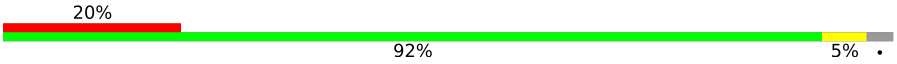
Chain DA:

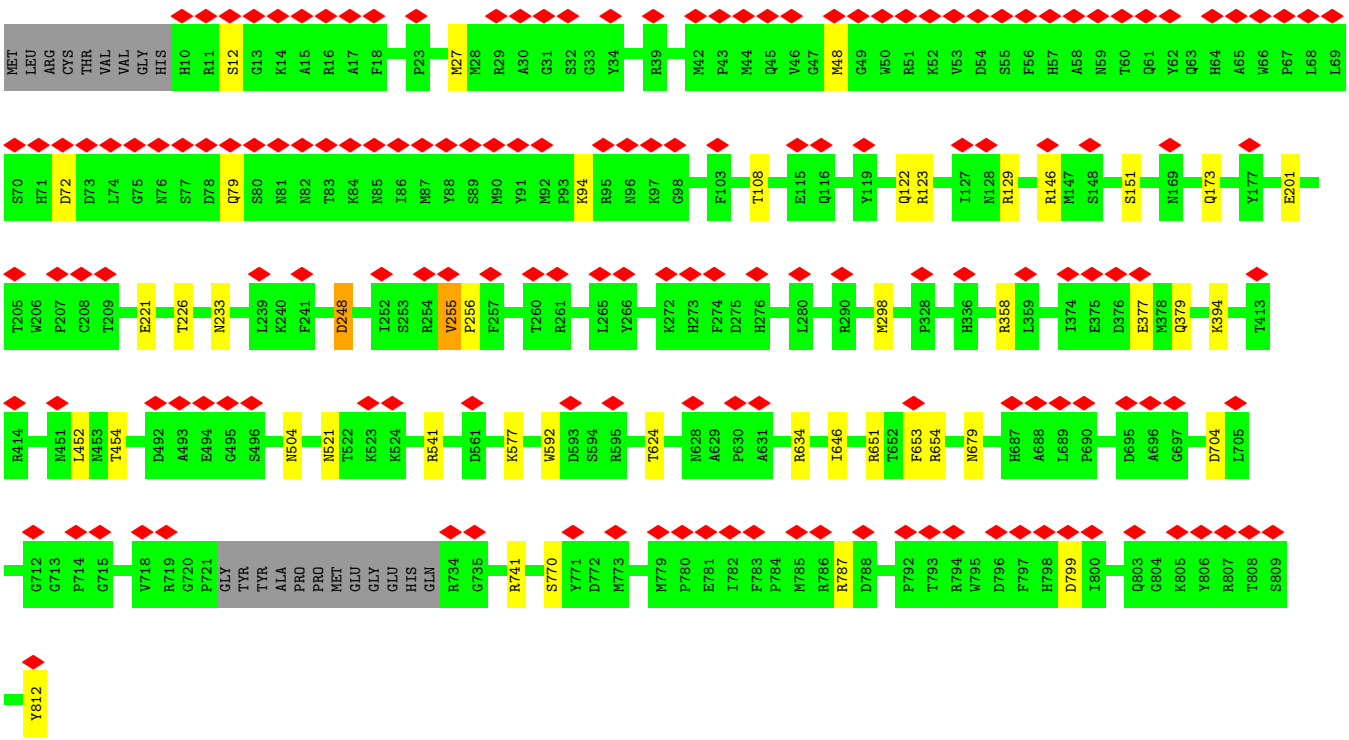




• Molecule 2: ms51

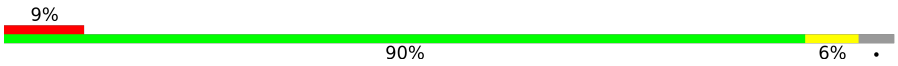
Chain DD:

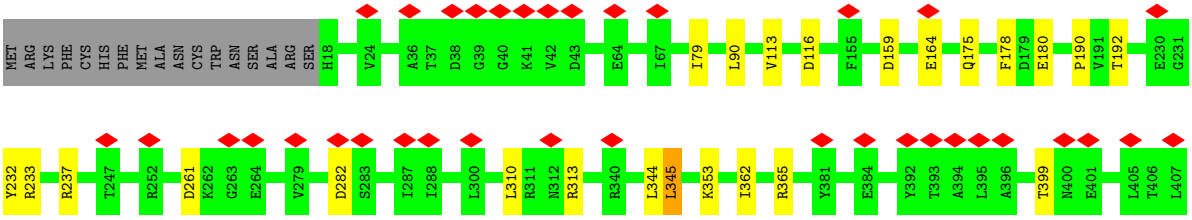




• Molecule 3: ms56

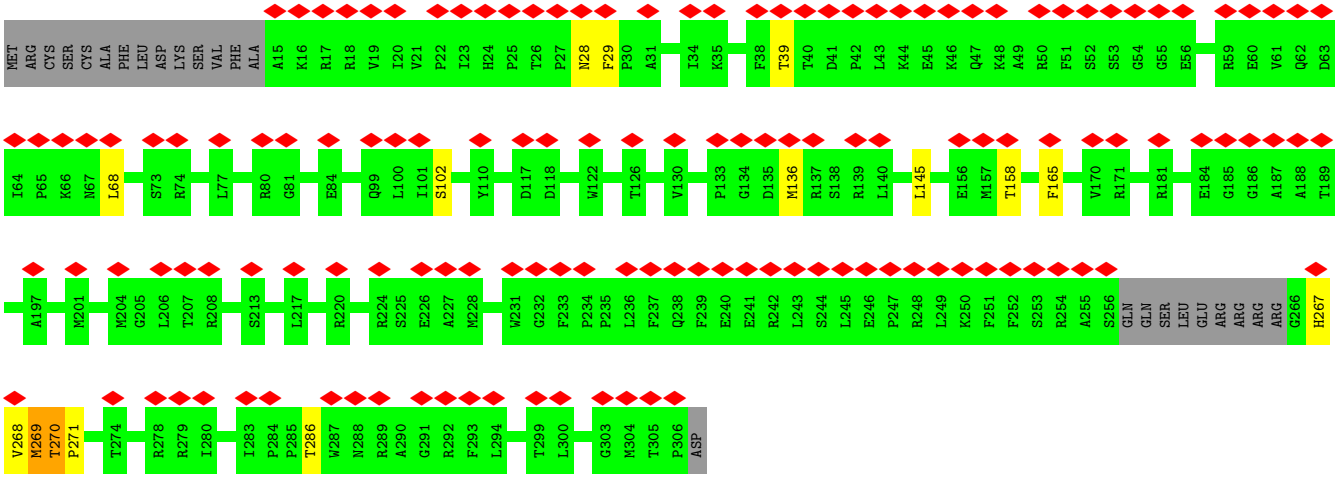
Chain DI:



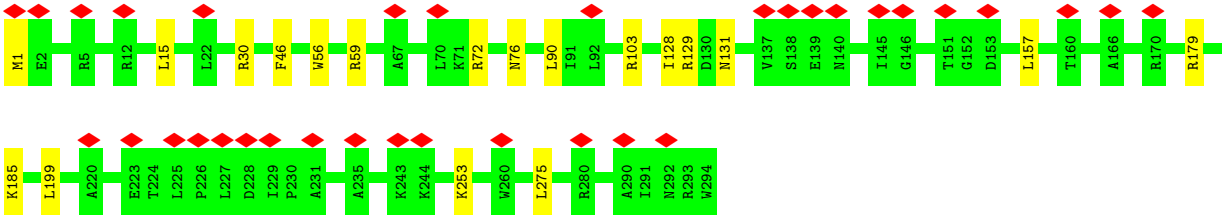


• Molecule 4: ms59

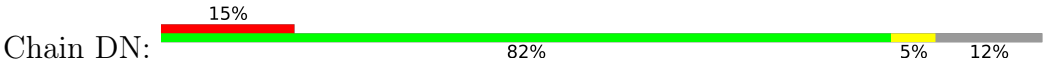
Chain DL:

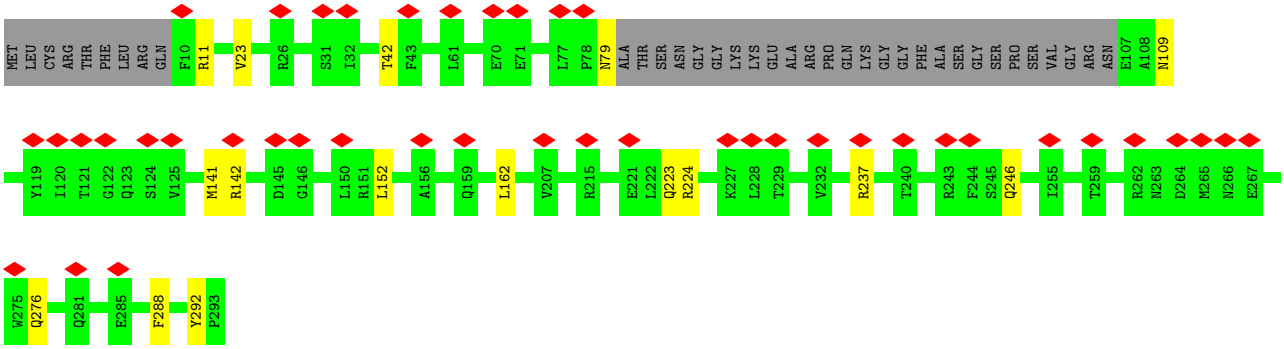


• Molecule 5: ms60

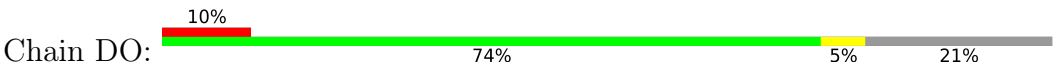


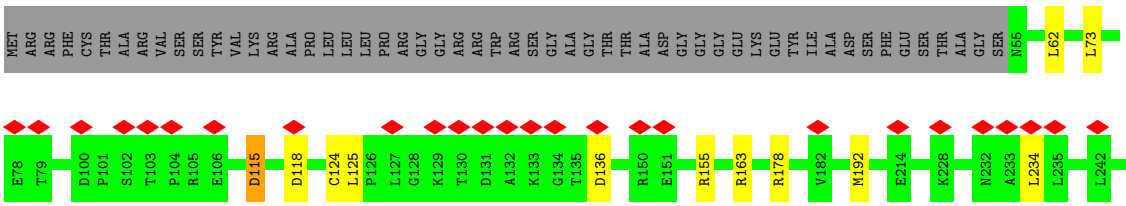
• Molecule 6: ms61





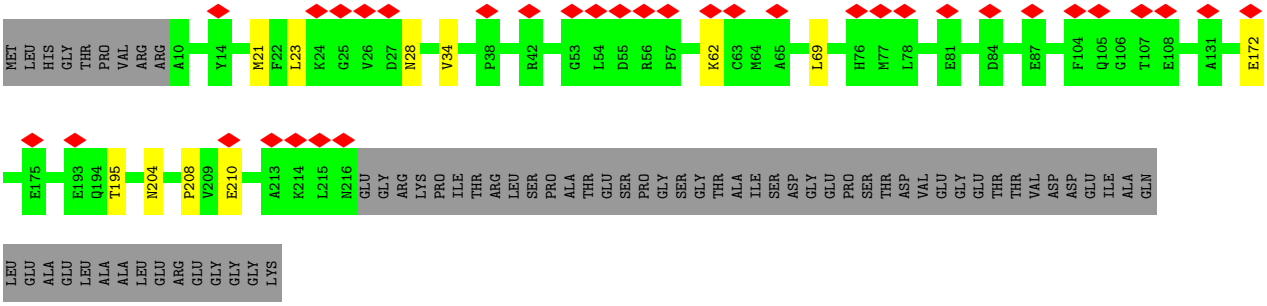
• Molecule 7: ms62





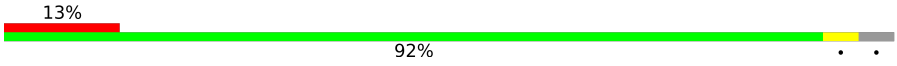
• Molecule 8: ms63

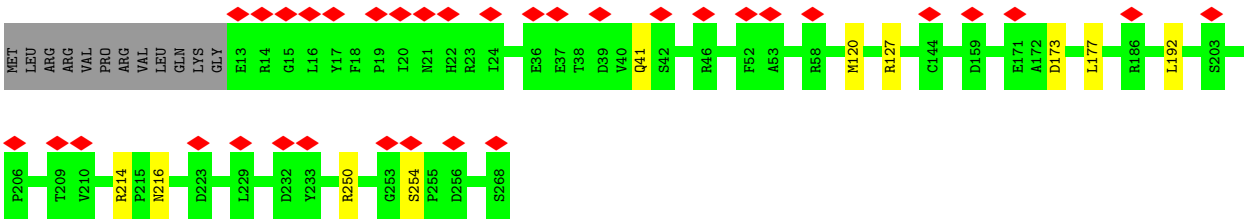
Chain DP:



• Molecule 9: ms64

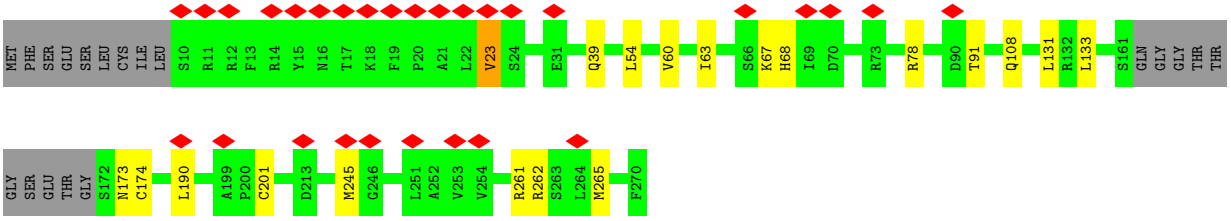
Chain DQ:





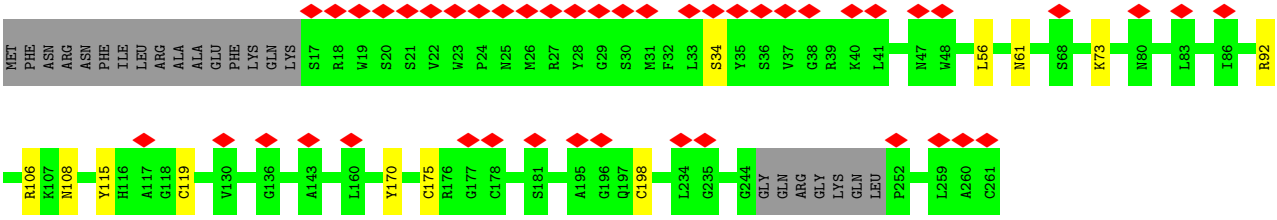
• Molecule 10: ms65

Chain DR:



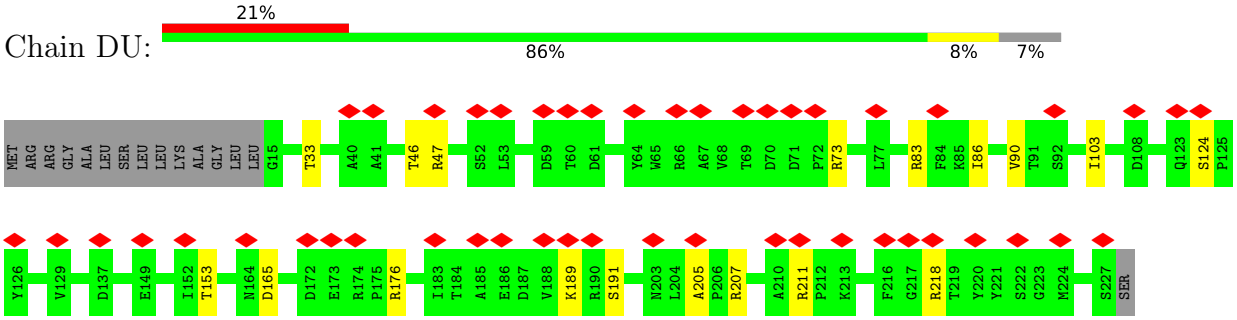
• Molecule 11: ms66

Chain DS:



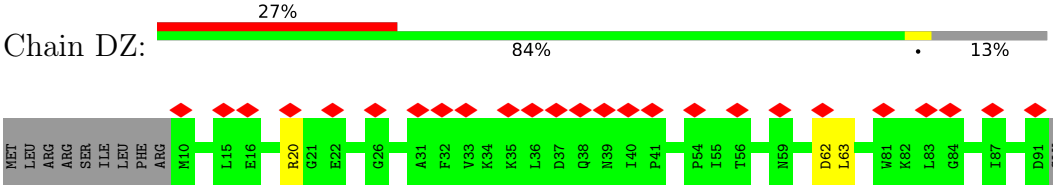
• Molecule 12: ms68

Chain DU:



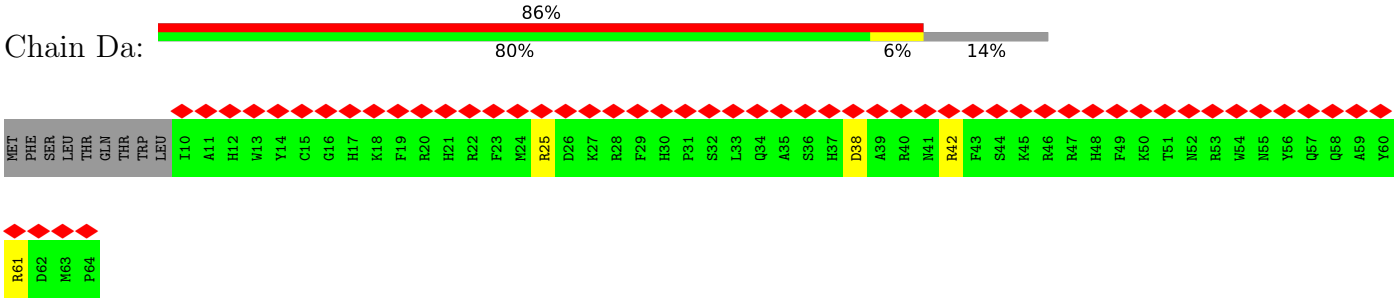
• Molecule 13: ms73

Chain DZ:



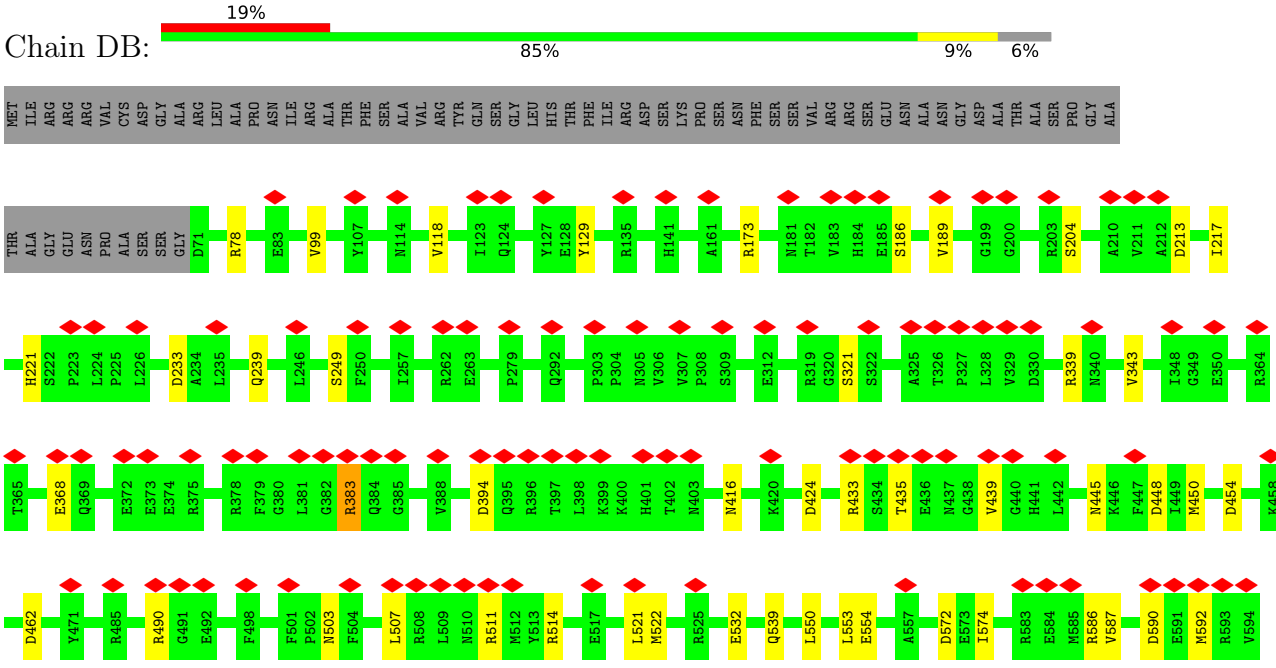
• Molecule 14: ms74

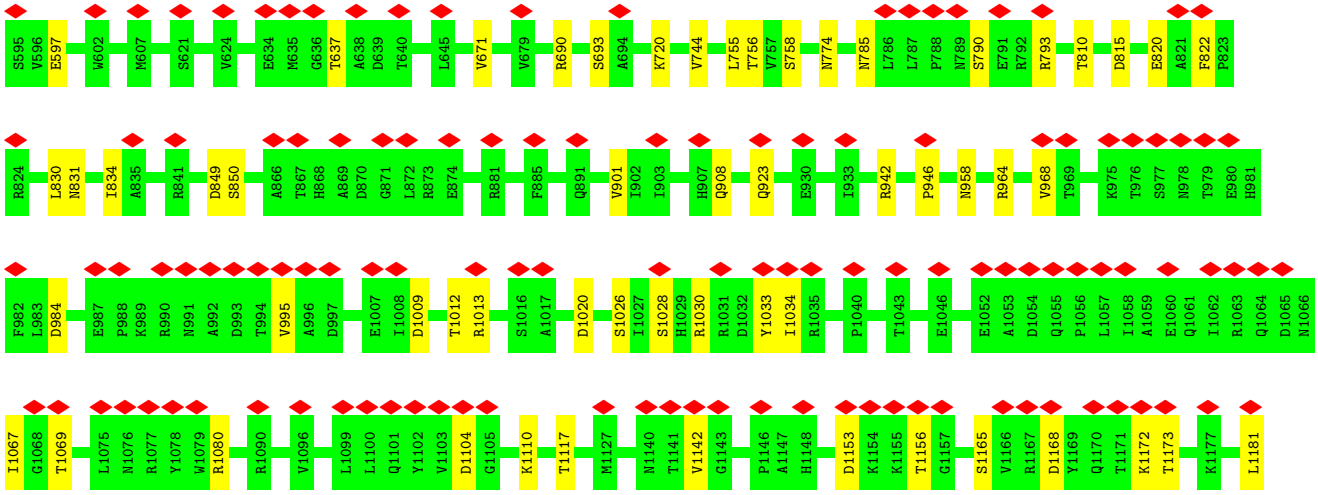
Chain Da:



• Molecule 15: ms49

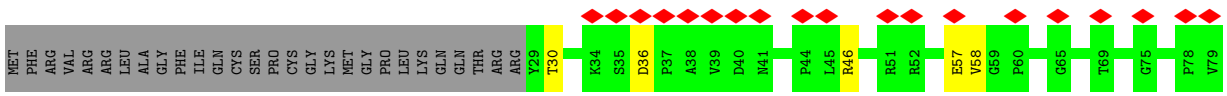
Chain DB:

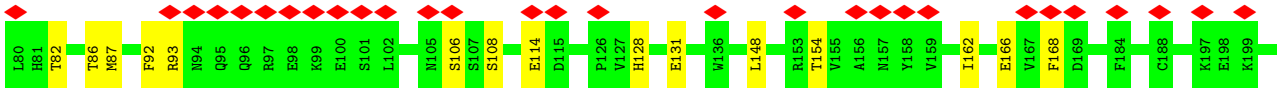


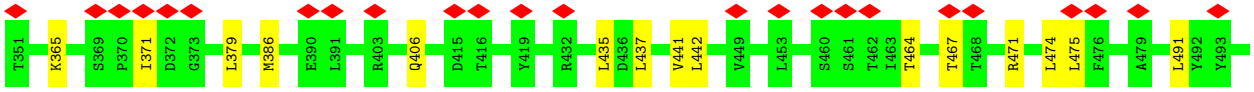


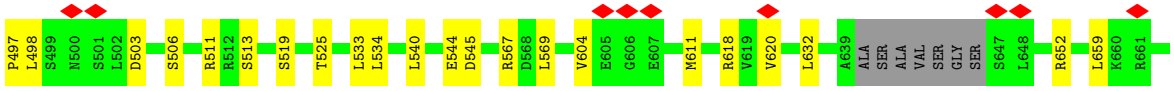
- Molecule 16: ms50

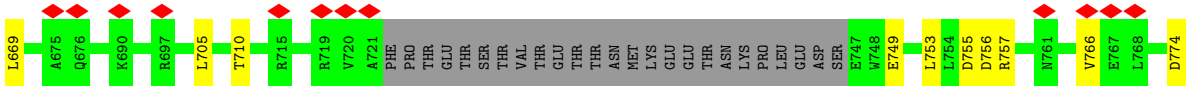
Chain DC:

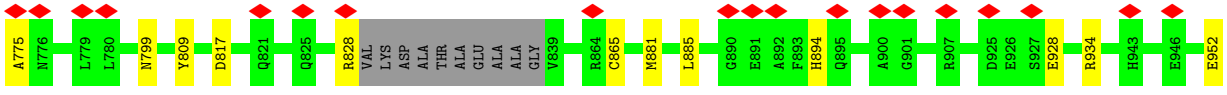


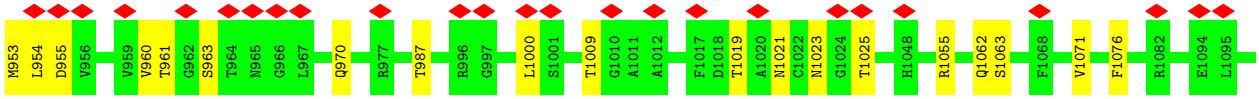


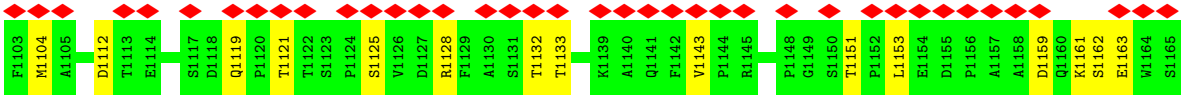






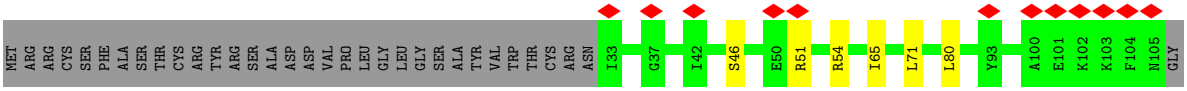


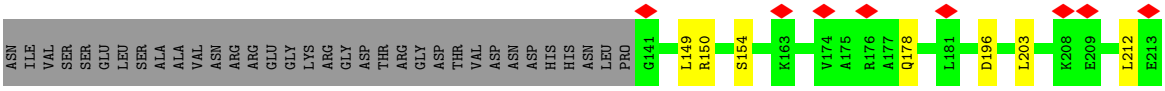


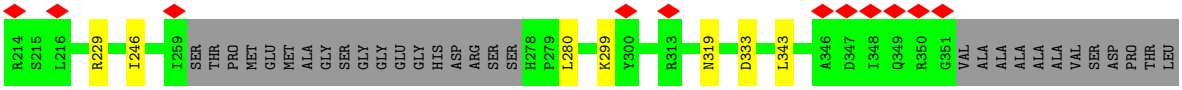


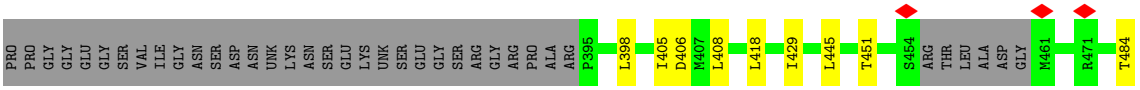
• Molecule 17: mS52

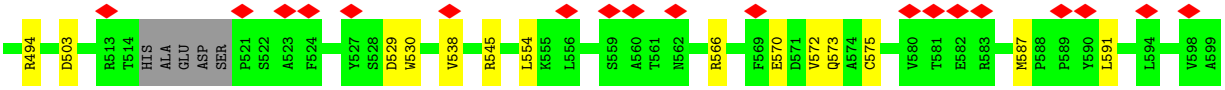
Chain DE:

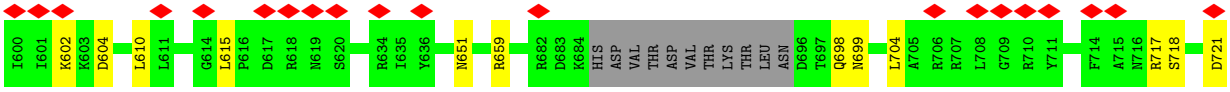


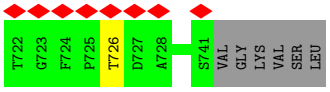






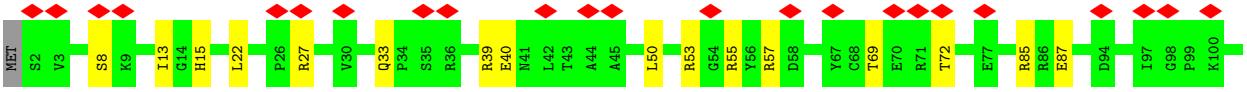


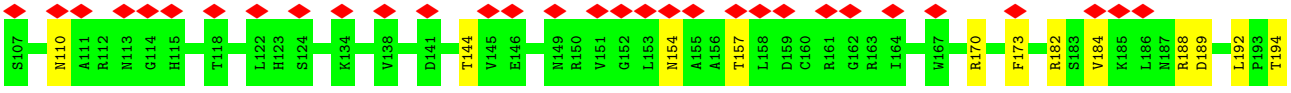


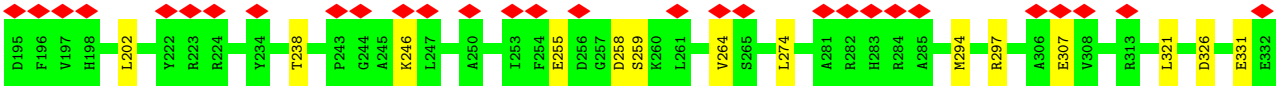


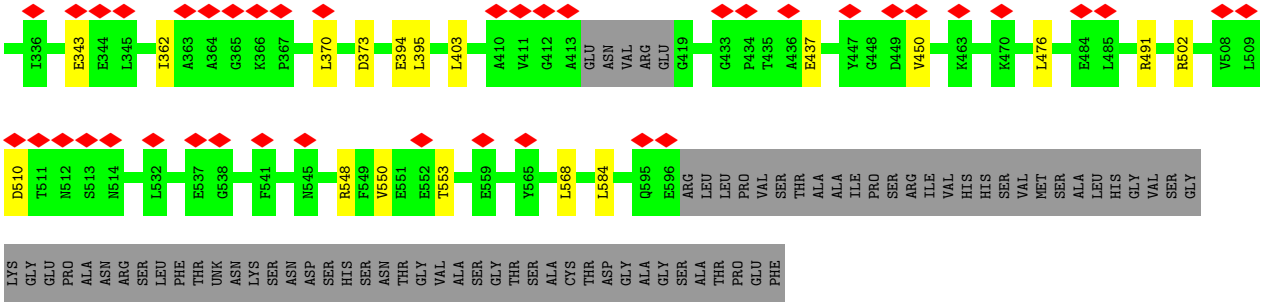
• Molecule 18: ms53

Chain DF:



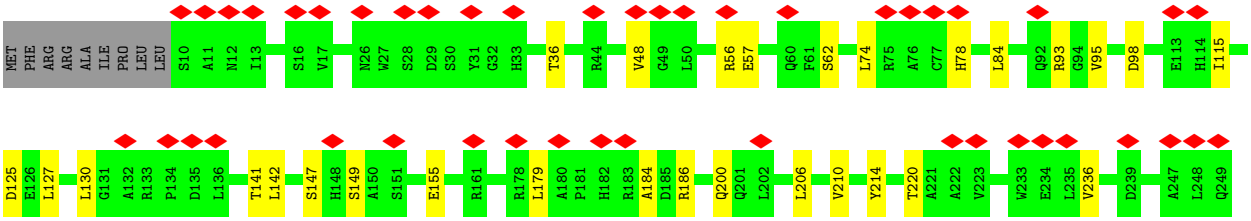






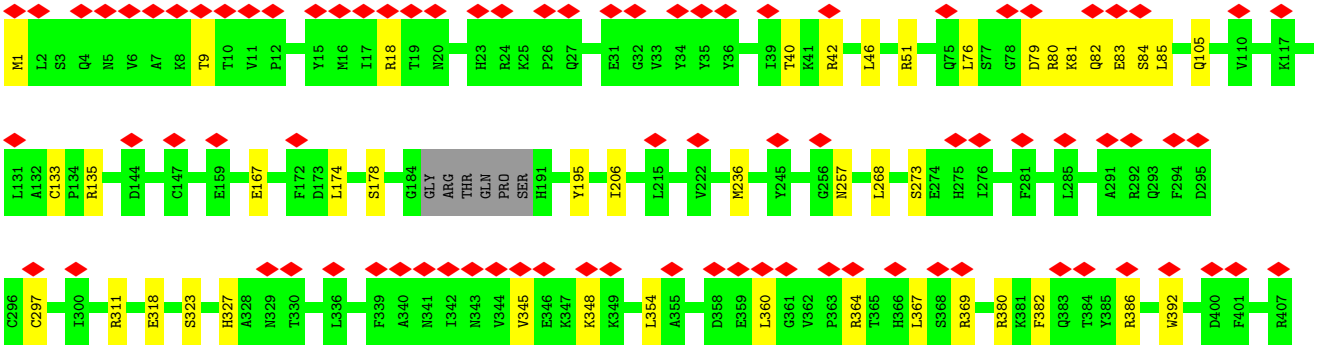
- Molecule 19: ms54

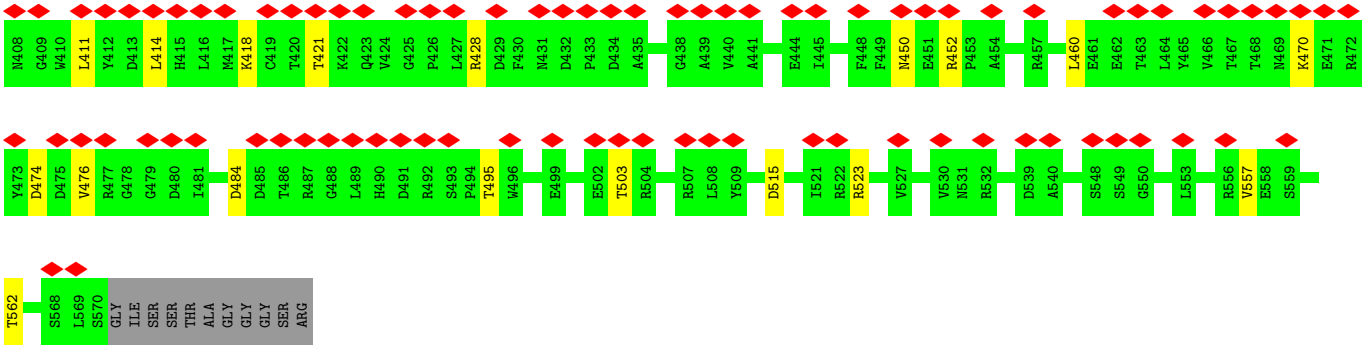
Chain DG:



- Molecule 20: ms55

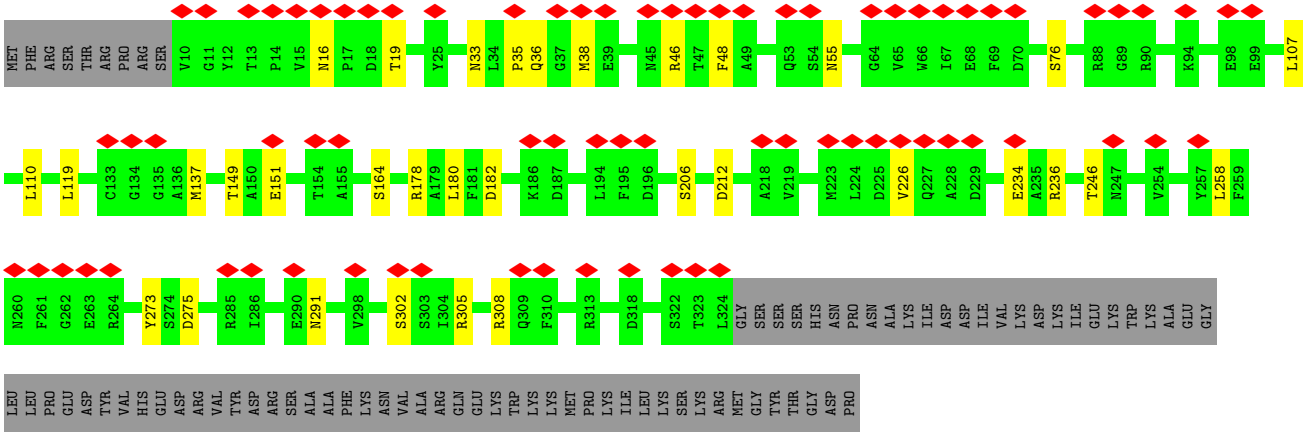
Chain DH:





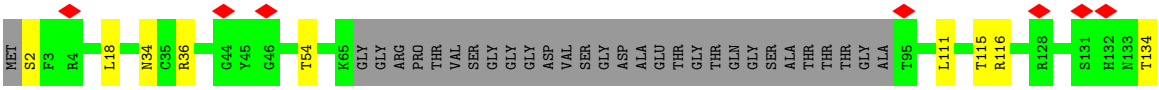
• Molecule 21: ms57

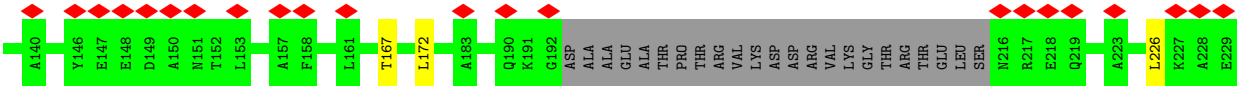
Chain DJ:

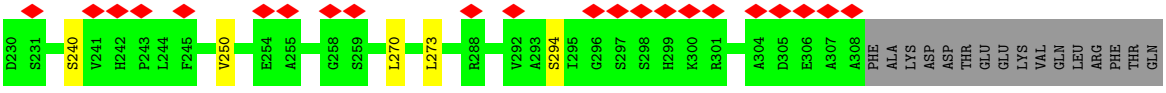


• Molecule 22: ms58

Chain DK:

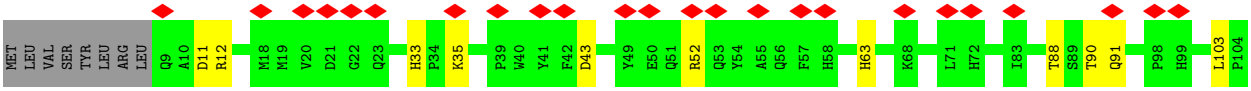


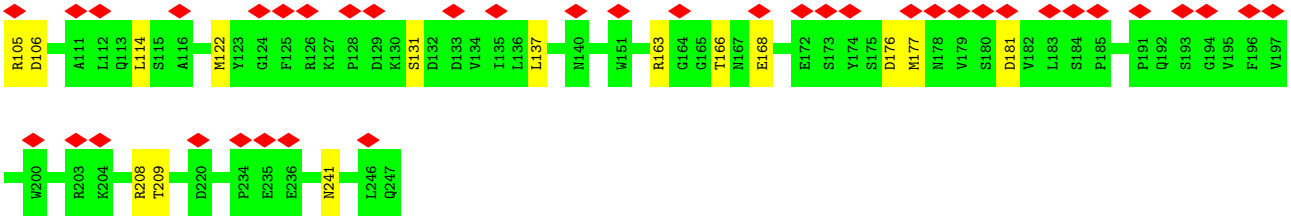




• Molecule 23: ms67

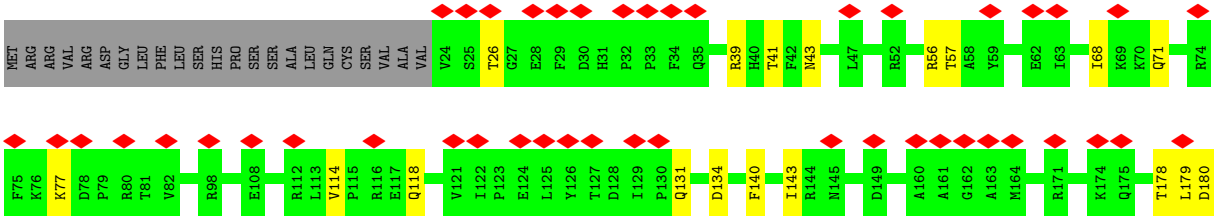
Chain DT:





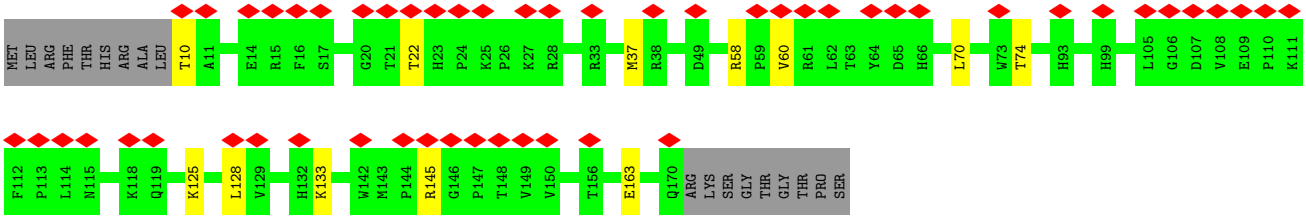
• Molecule 24: ms69

Chain DV:



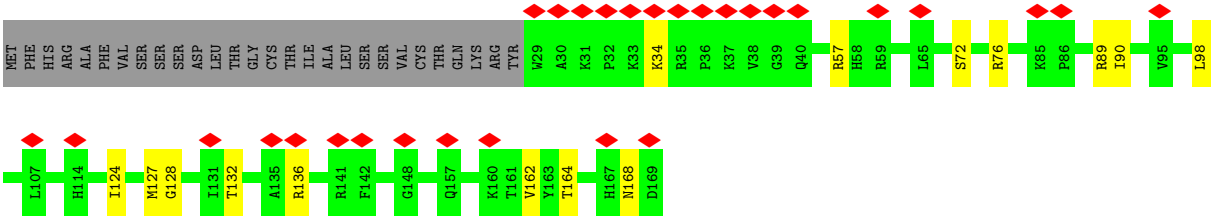
• Molecule 25: ms70

Chain DW:



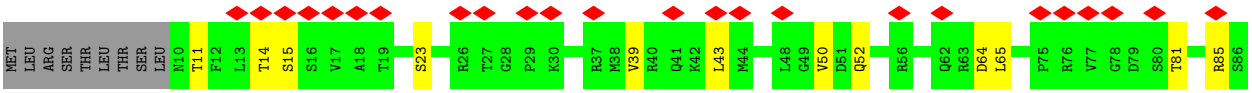
• Molecule 26: ms71

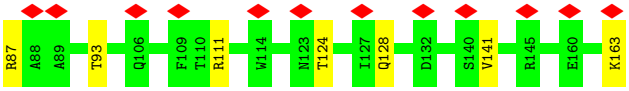
Chain DX:



• Molecule 27: ms72

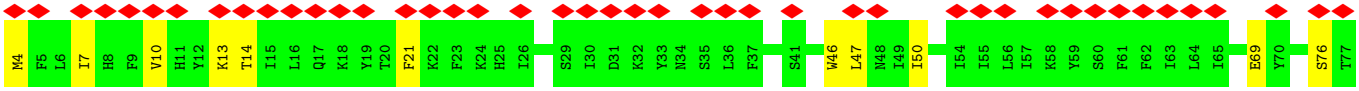
Chain DY:





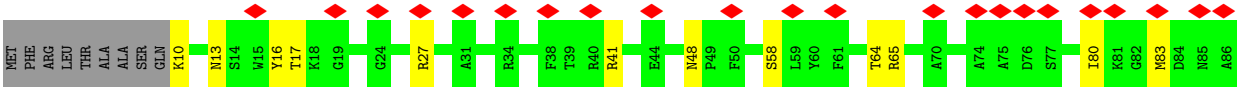
• Molecule 28: uS3m

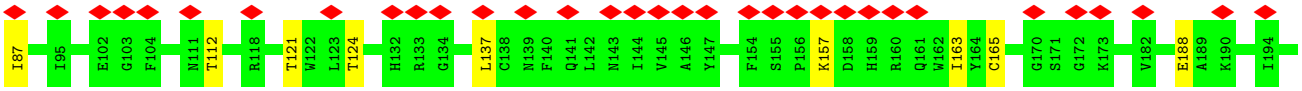
Chain CC:

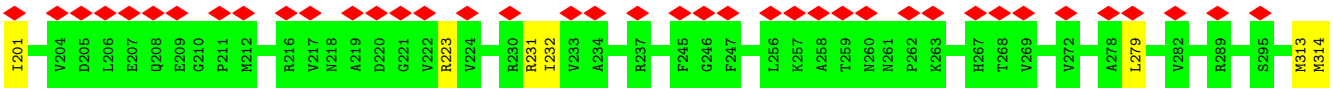


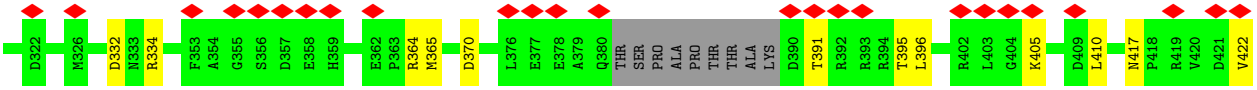
• Molecule 29: uS55m

Chain CE:



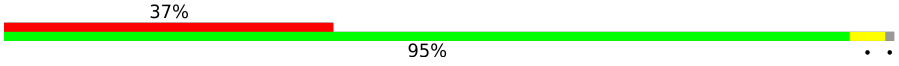


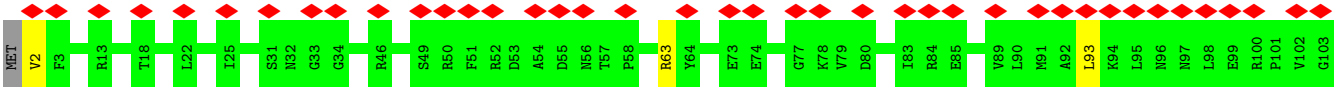




• Molecule 30: bS6m

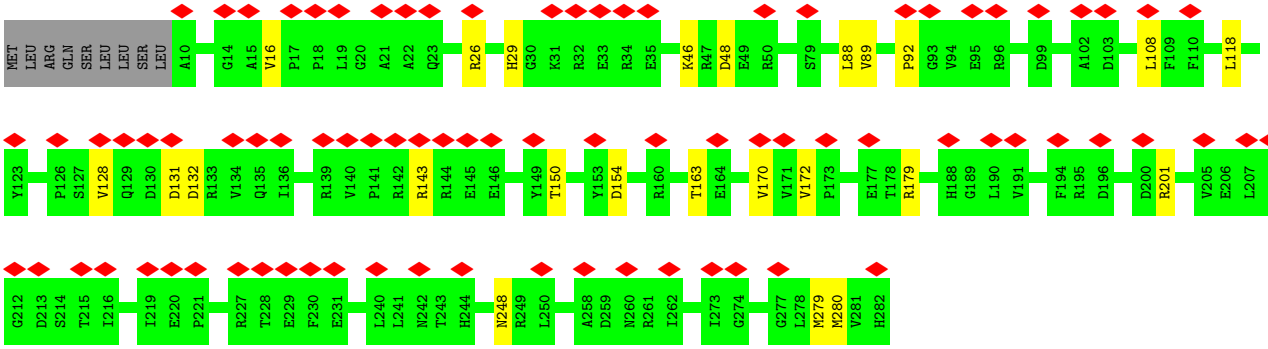
Chain CF:





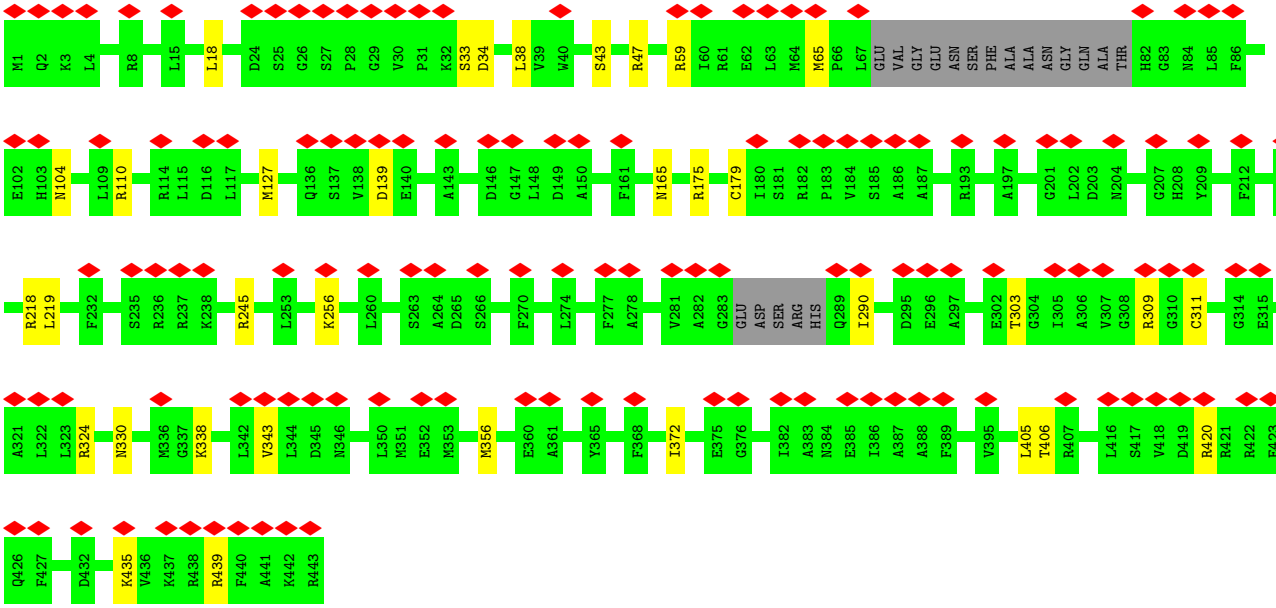
• Molecule 31: uS8m

Chain CH:



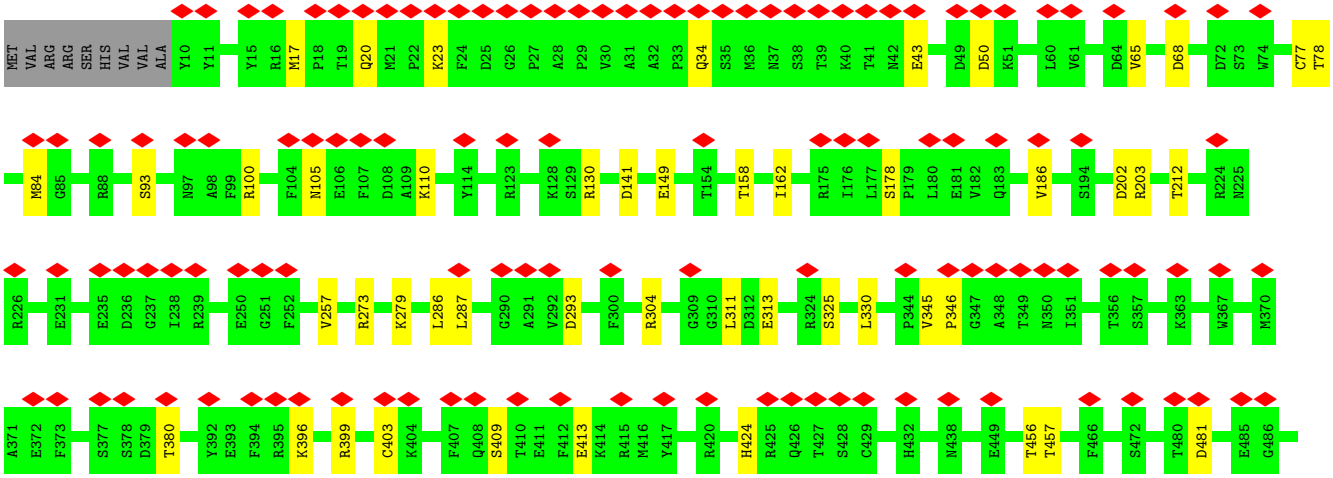
• Molecule 32: uS9m

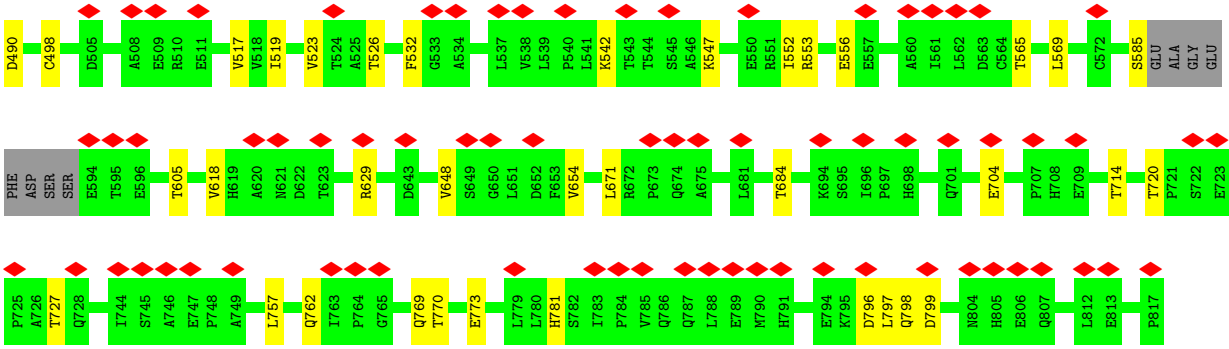
Chain CI:



• Molecule 33: uS10m

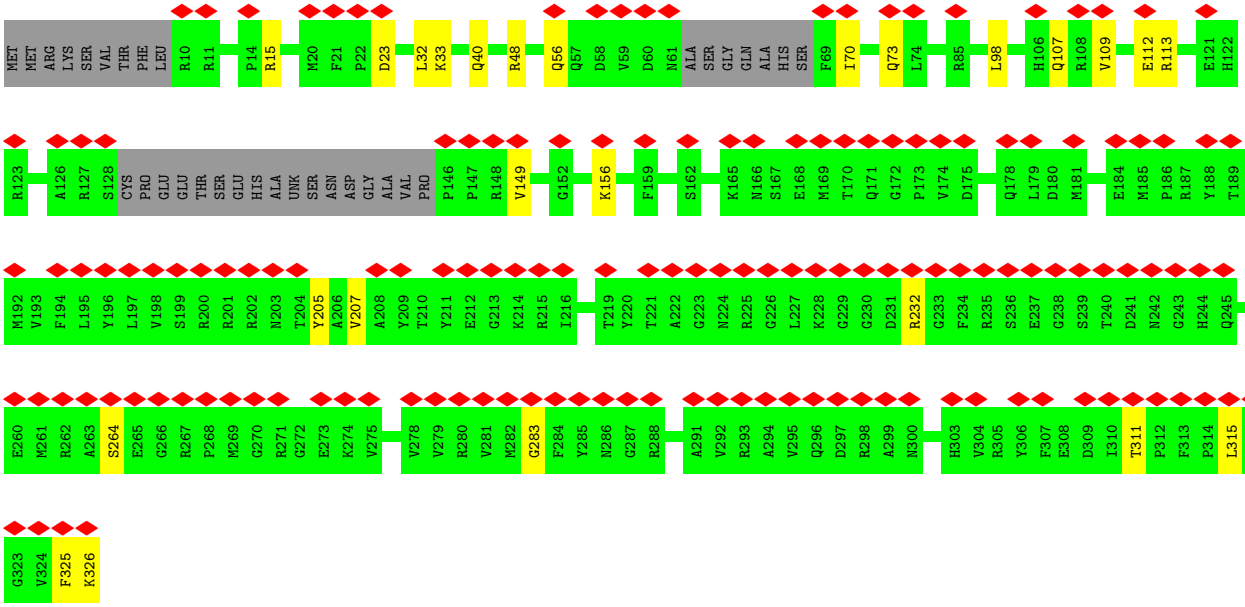
Chain CJ:





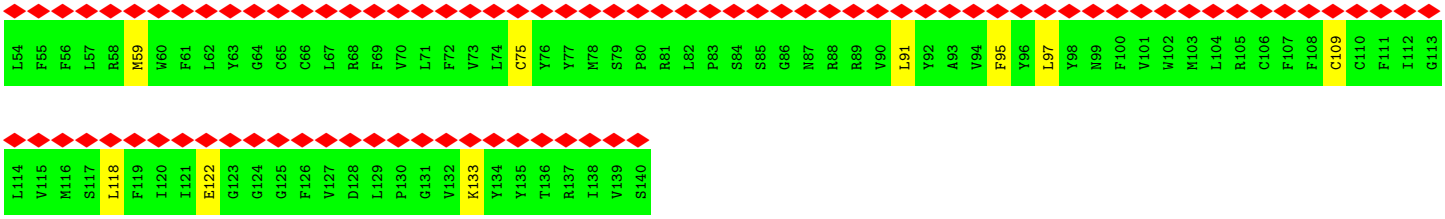
• Molecule 34: uS11m

Chain CK:



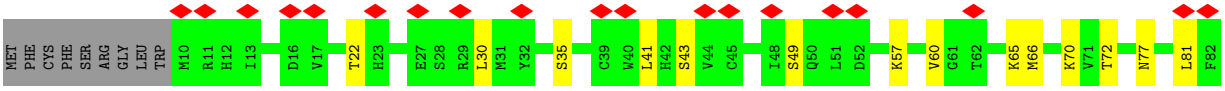
• Molecule 35: uS12

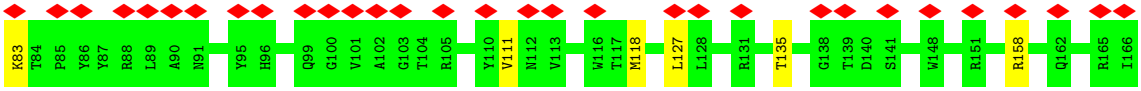
Chain CL:



• Molecule 36: uS14m

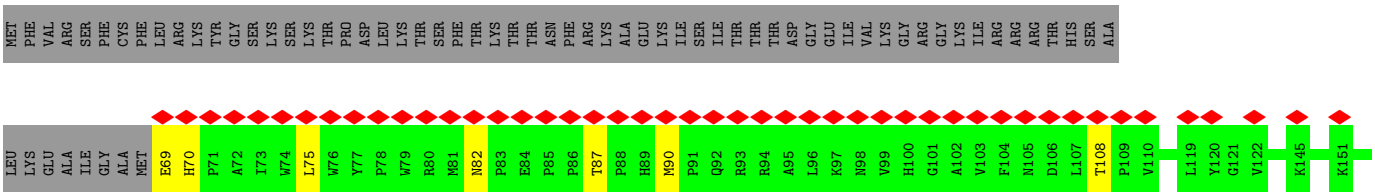
Chain CN:





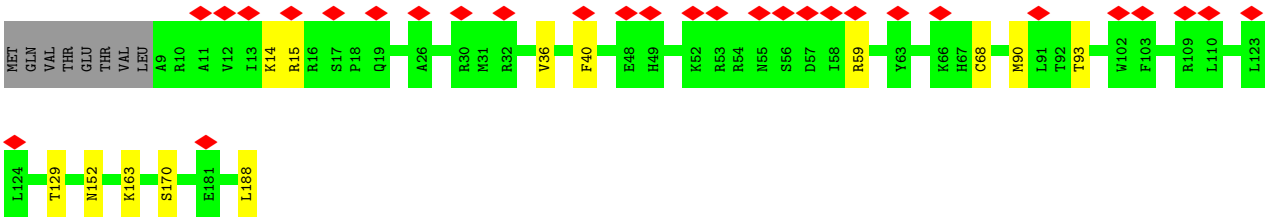
• Molecule 37: uS15m

Chain CO:



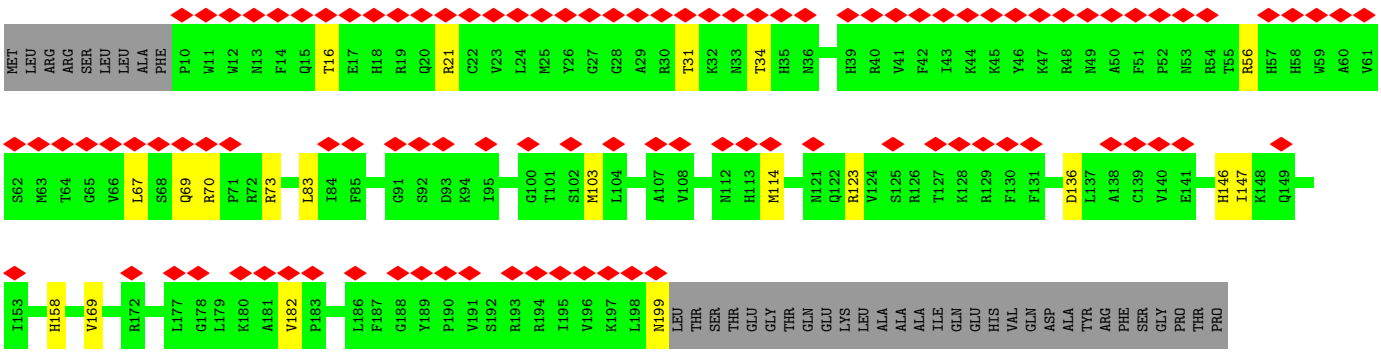
• Molecule 38: bS16m

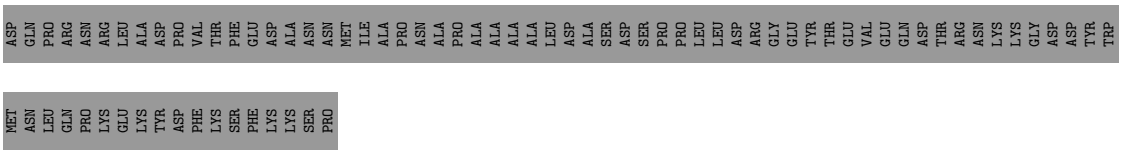
Chain CP:



• Molecule 39: uS17m

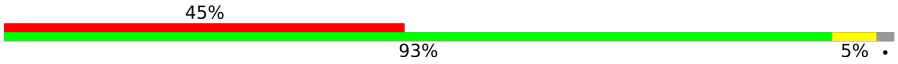
Chain CQ:

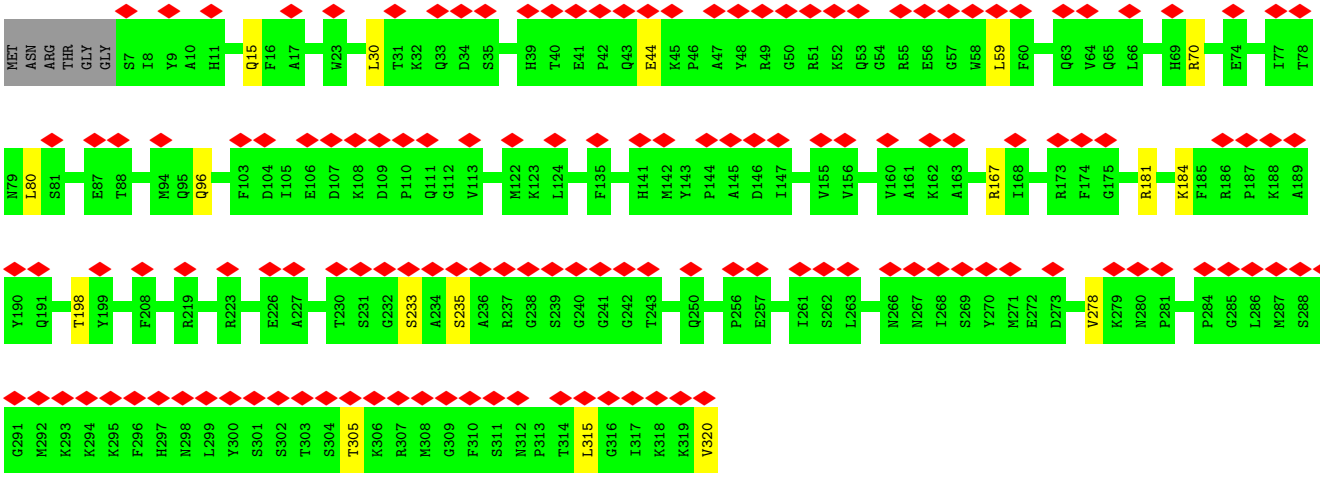




• Molecule 40: bS18m

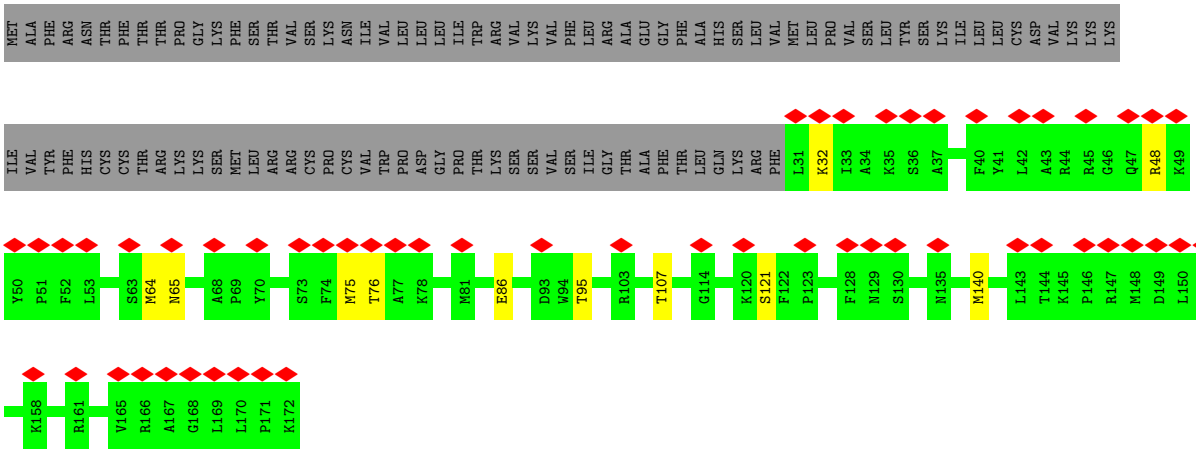
Chain CR:





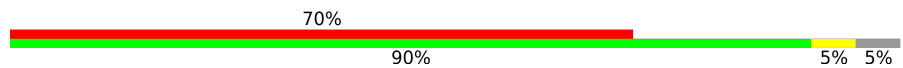
• Molecule 41: uS19m

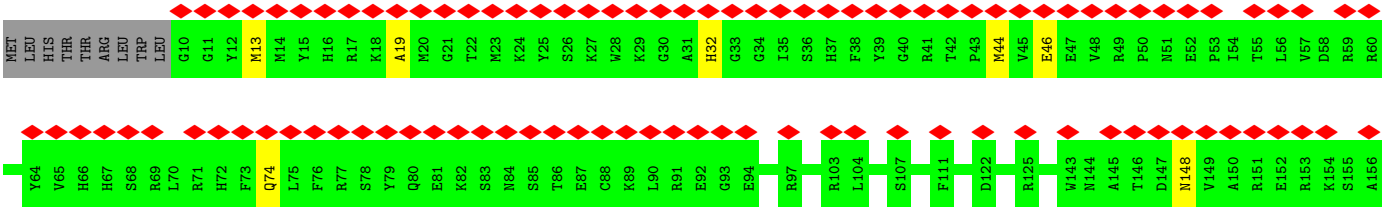
Chain CS:

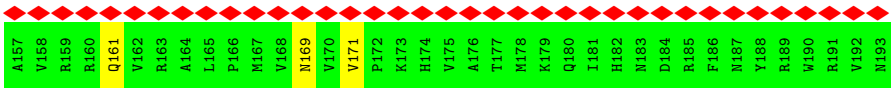


• Molecule 42: bS12m

Chain CU:

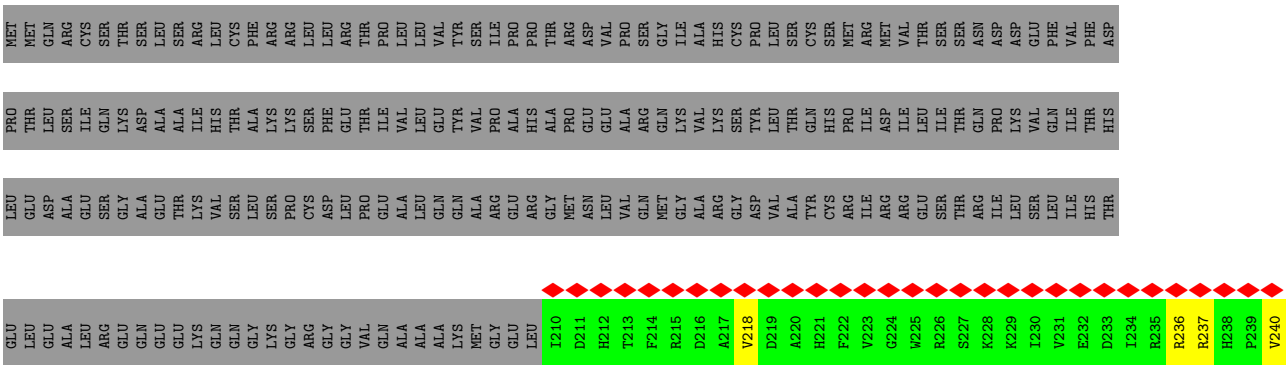






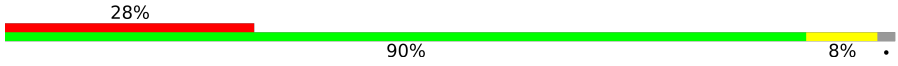
• Molecule 43: mt-IF-3

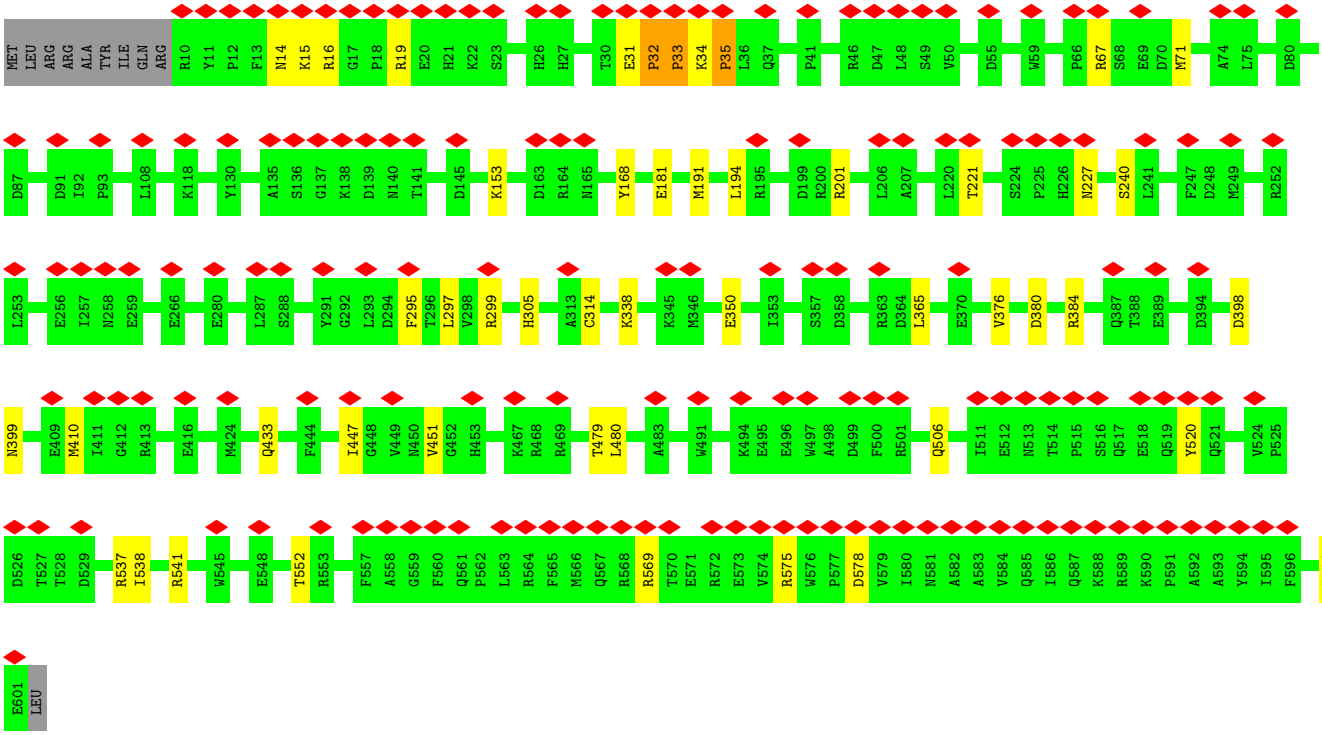
Chain CZ:



• Molecule 44: mS22

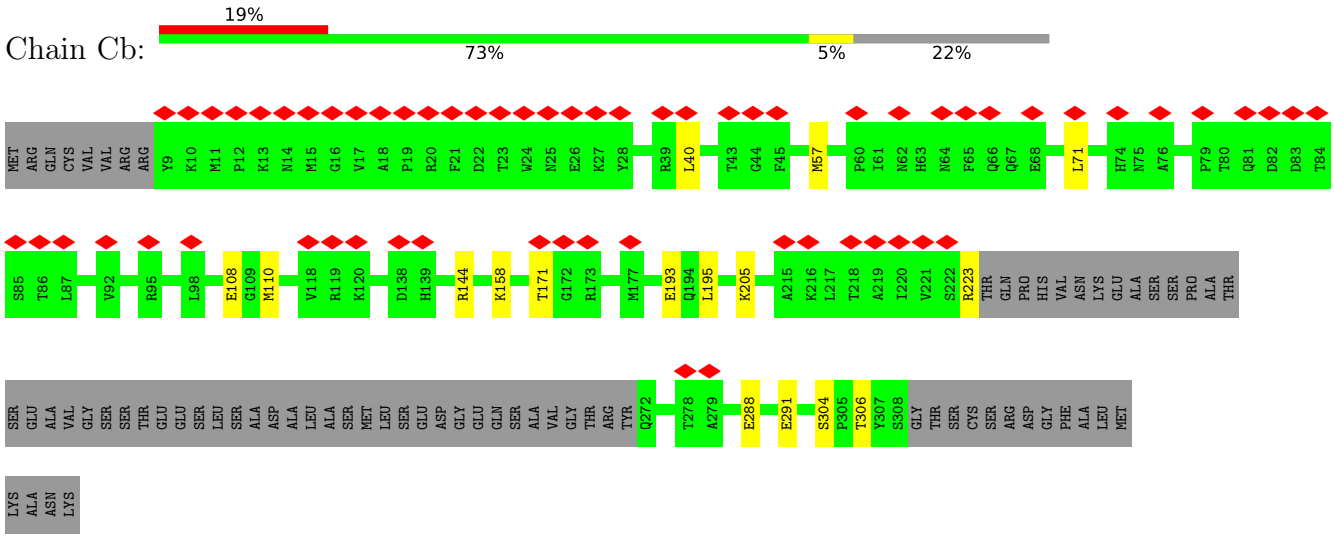
Chain Ca:





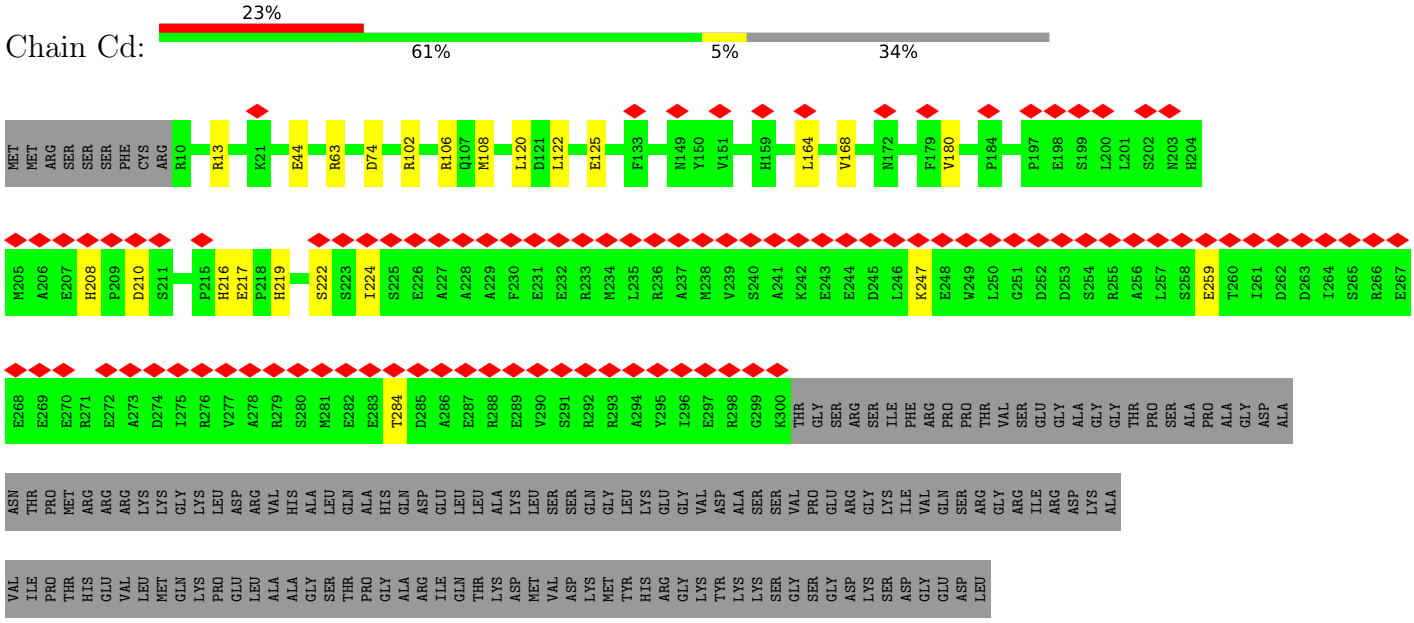
- Molecule 45: mS23

Chain Cb:



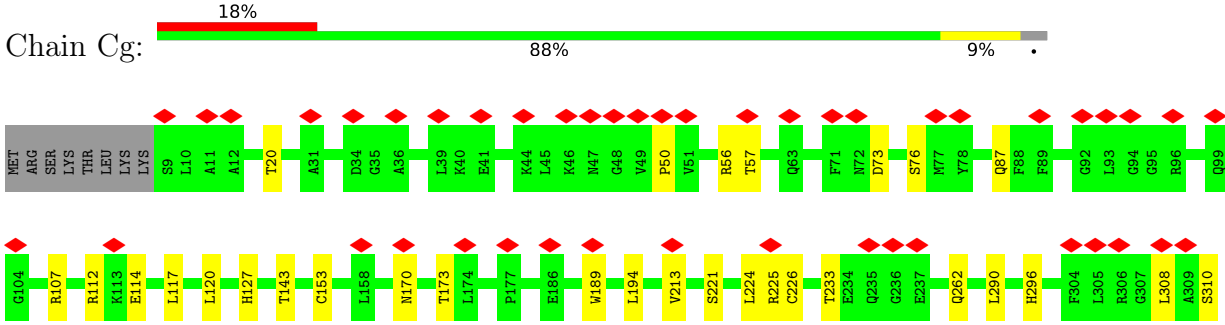
- Molecule 46: mS26

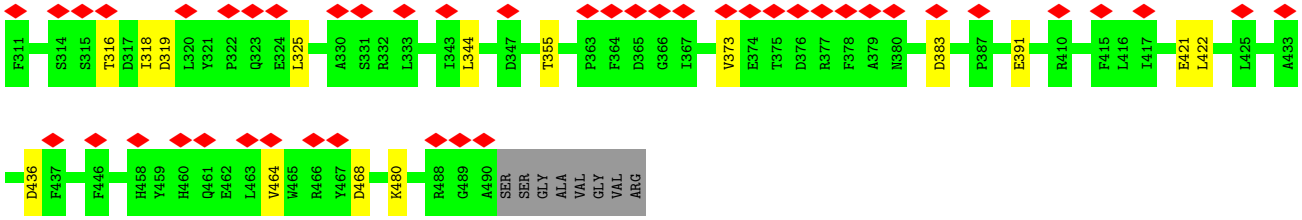
Chain Cd:



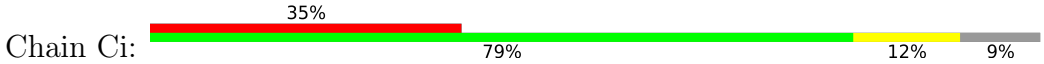
- Molecule 47: mS29

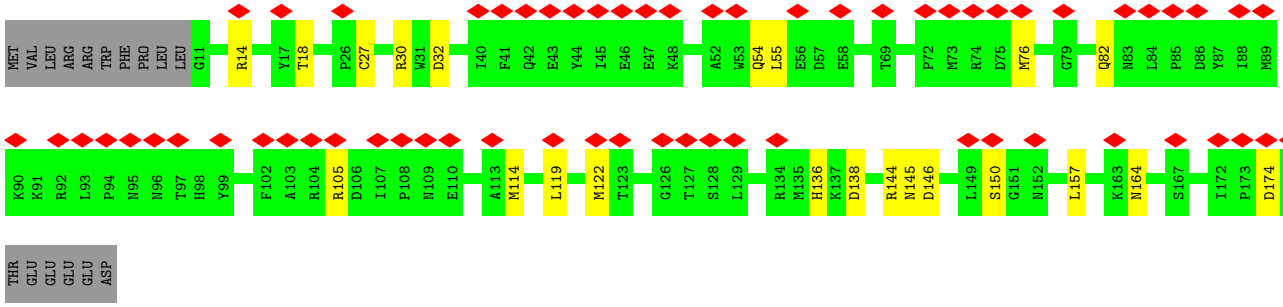
Chain Cg:



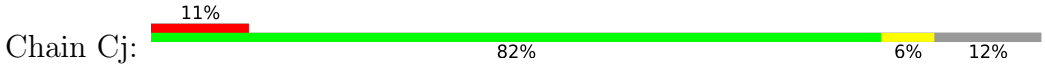


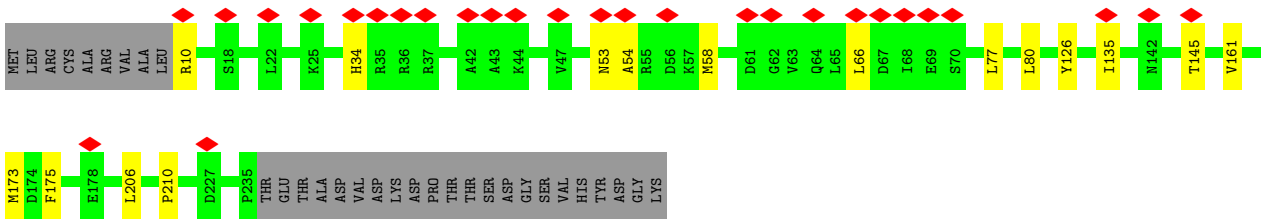
• Molecule 48: mS33



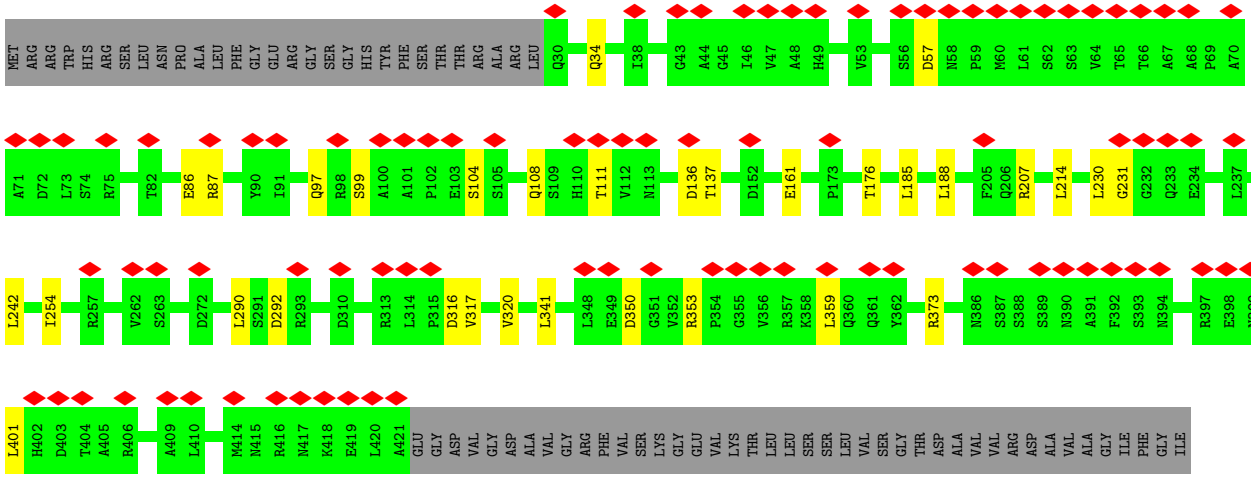


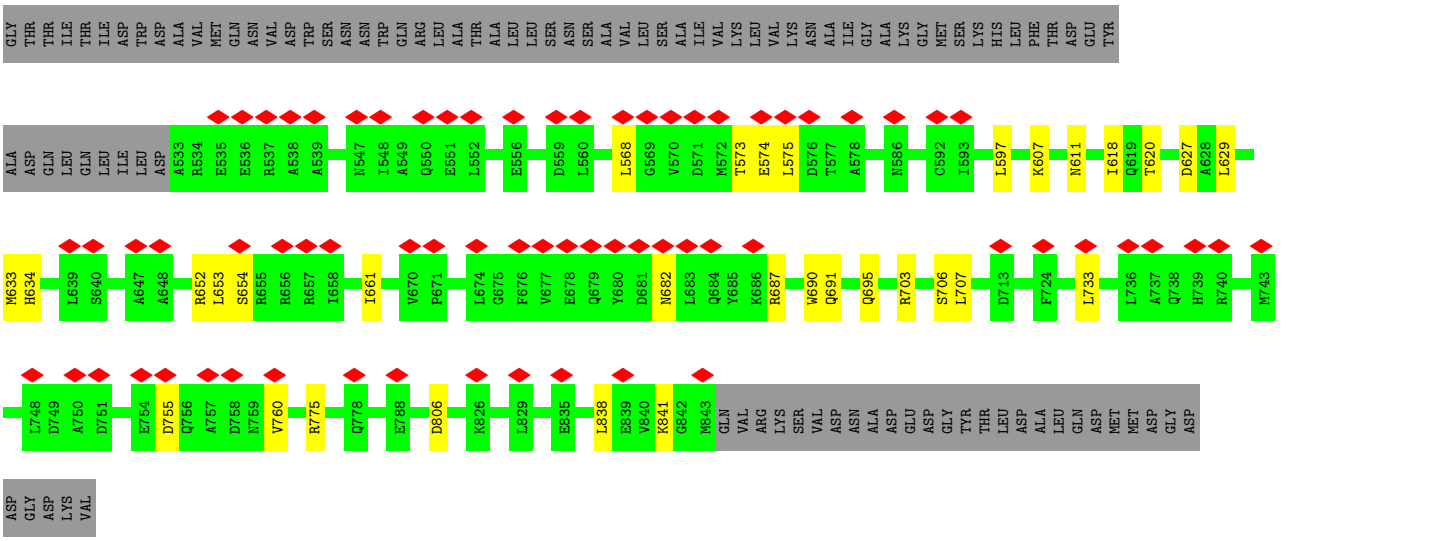
• Molecule 49: mS34





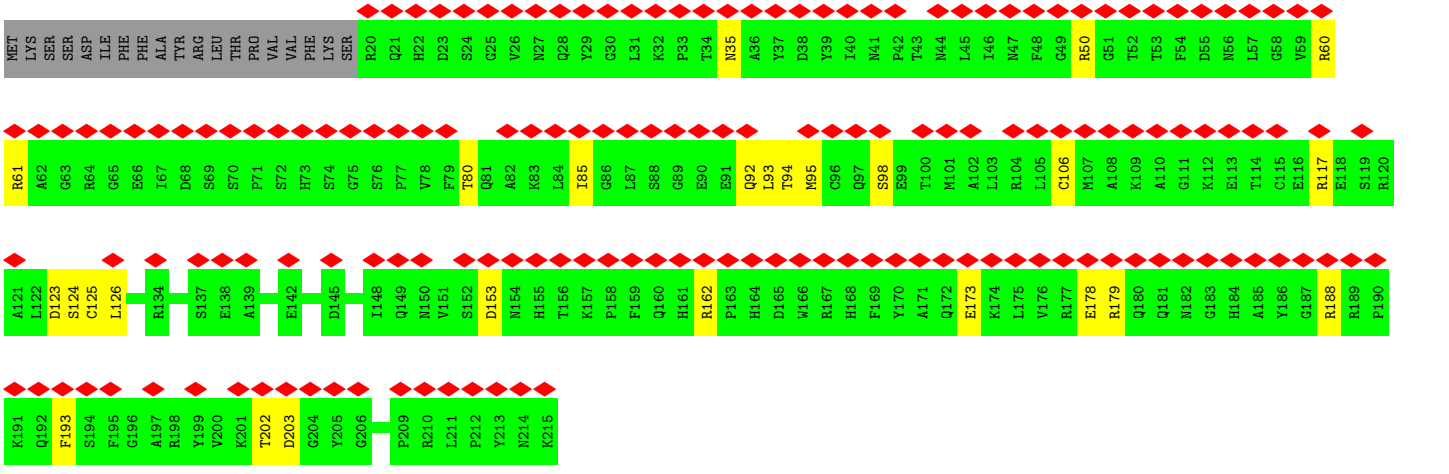
• Molecule 50: mS35





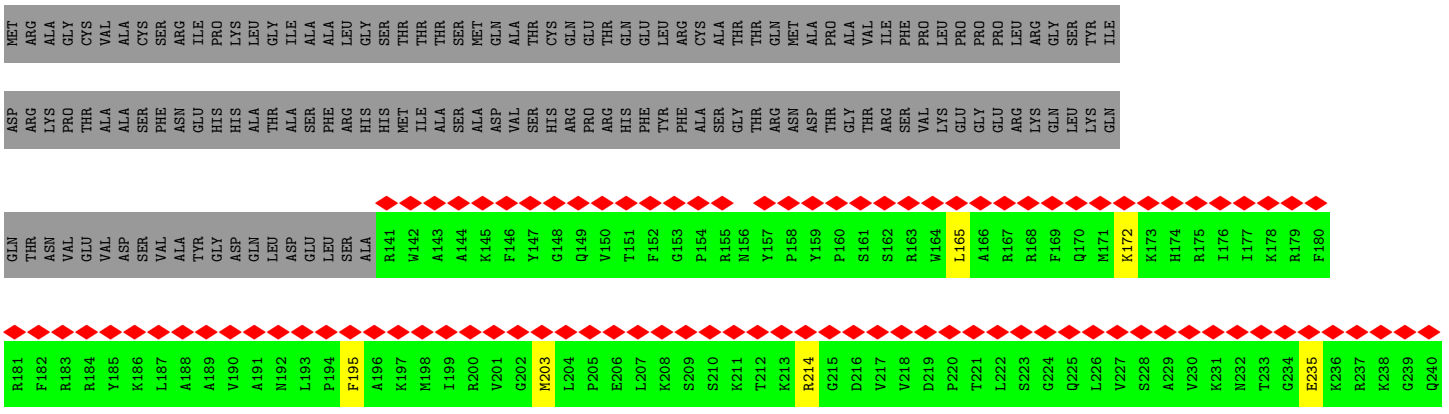
• Molecule 51: mS37

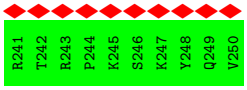
Chain Cm:



• Molecule 52: mS38

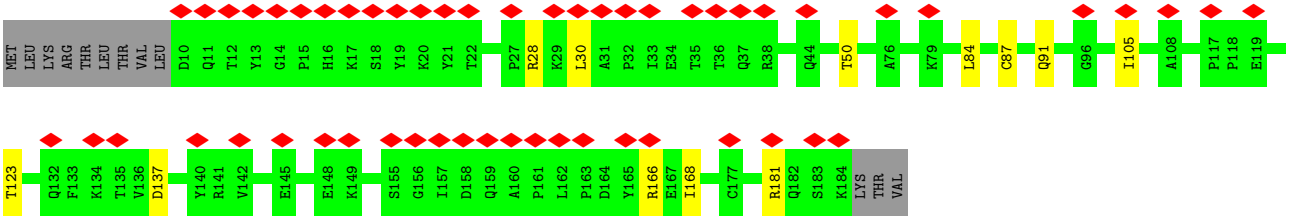
Chain Cn:





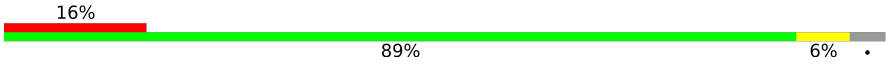
• Molecule 53: ms34

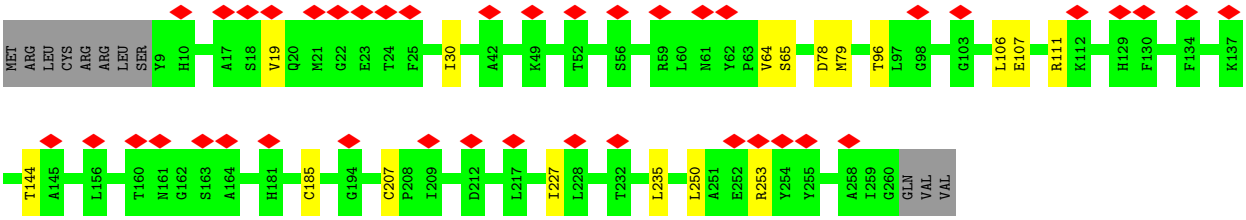
Chain Cp:



• Molecule 54: ms42

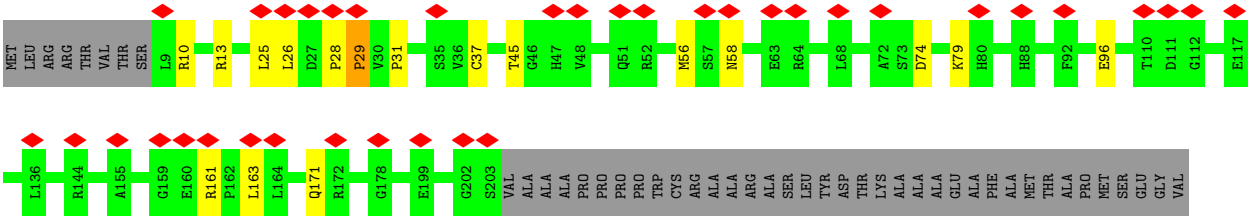
Chain Cq:





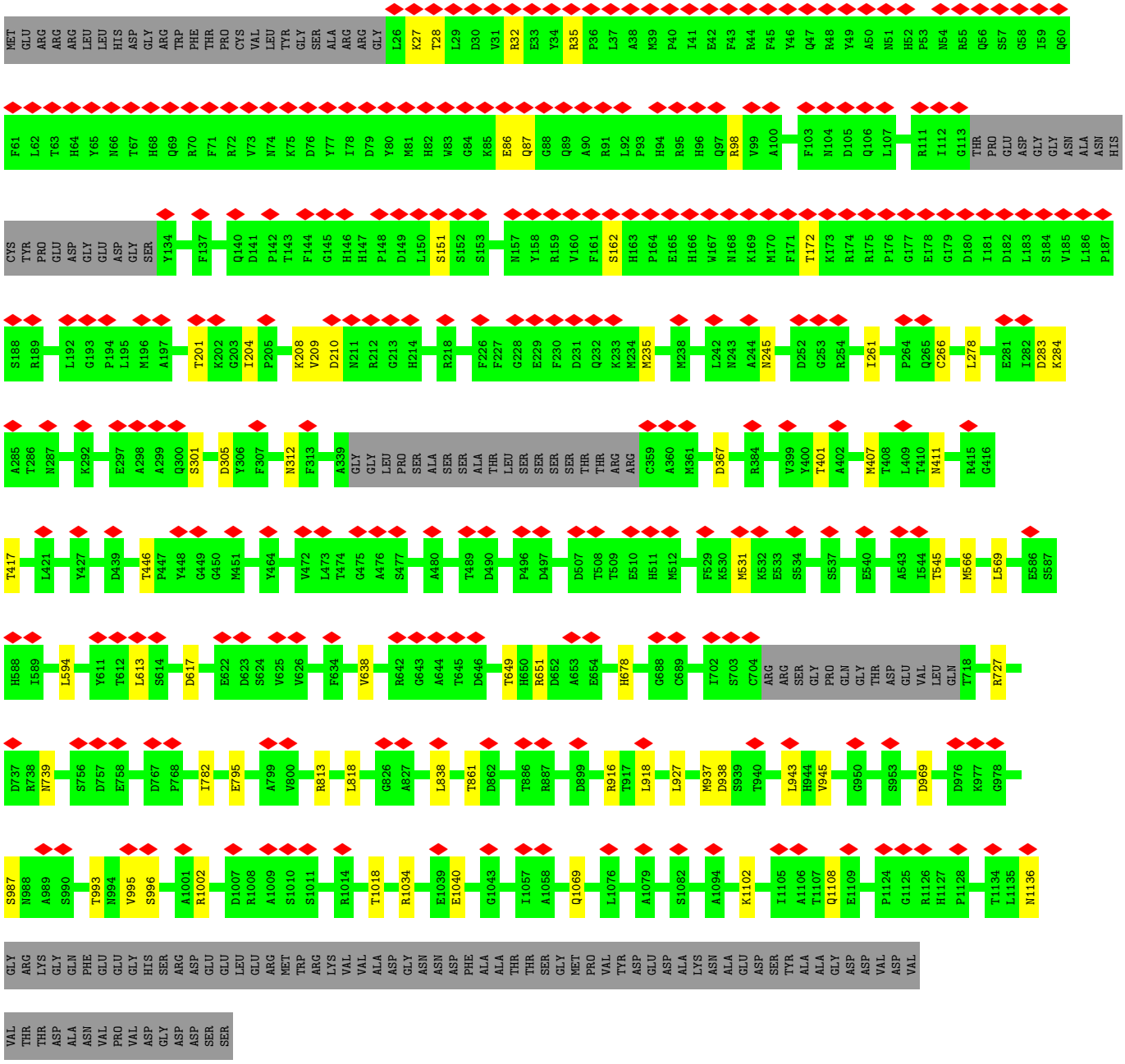
• Molecule 55: mS43

Chain Cr:



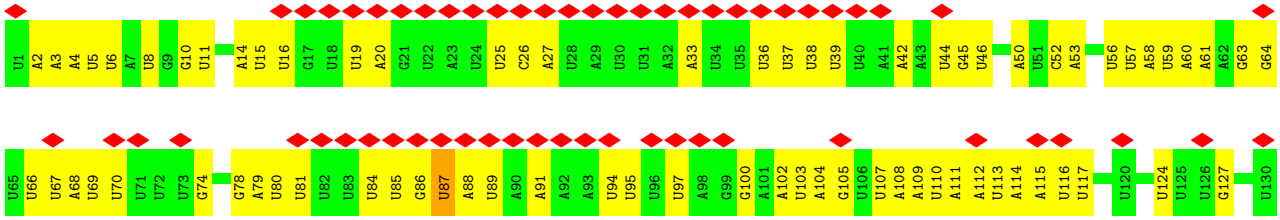
• Molecule 56: mS47

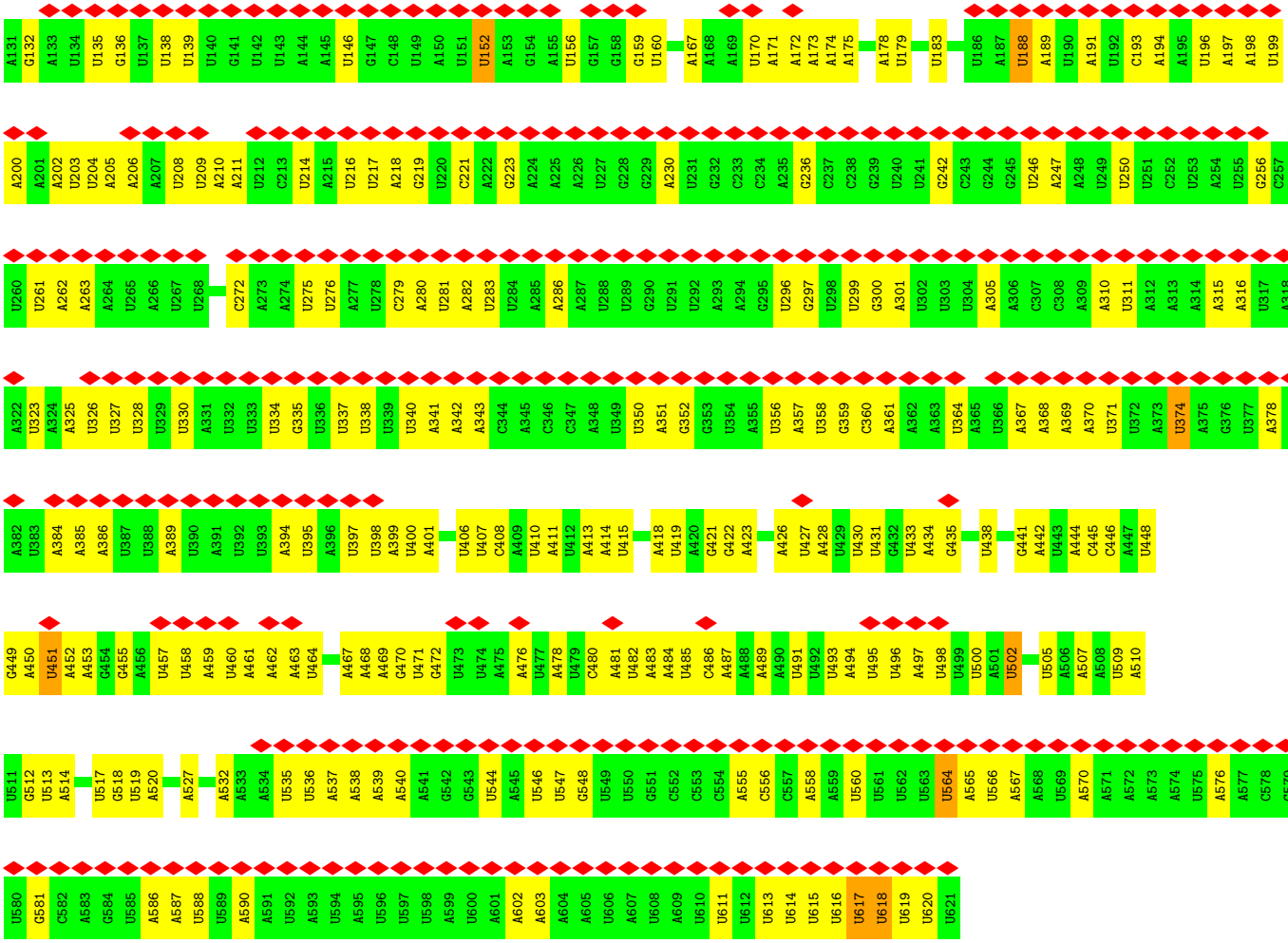
Chain Cv:



• Molecule 57: 9s rRNA

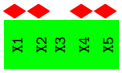
Chain CA:





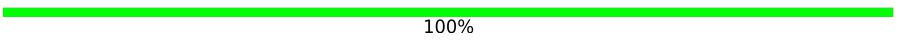
• Molecule 58: UNK

Chain UO:



• Molecule 59: UNK

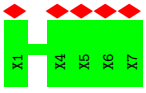
Chain UP:



There are no outlier residues recorded for this chain.

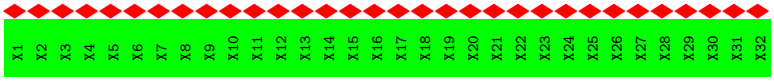
• Molecule 59: UNK

Chain UW:



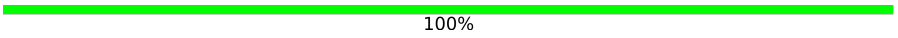
• Molecule 60: UNK

Chain UQ:



• Molecule 61: UNK

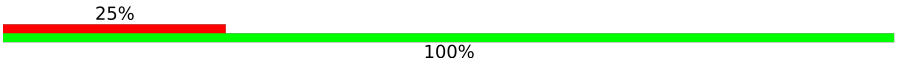
Chain UR:

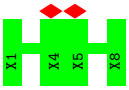


There are no outlier residues recorded for this chain.

• Molecule 61: UNK

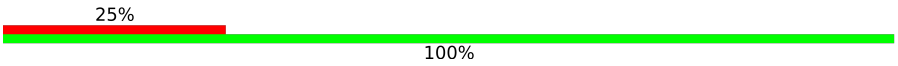
Chain UV:

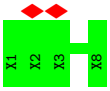




• Molecule 61: UNK

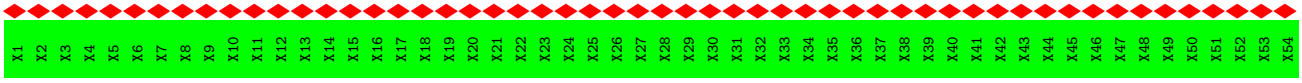
Chain UX:





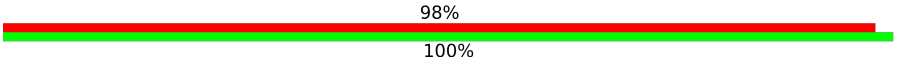
• Molecule 62: UNK

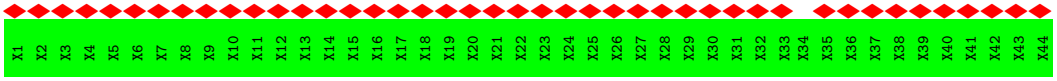
Chain US:



• Molecule 63: UNK

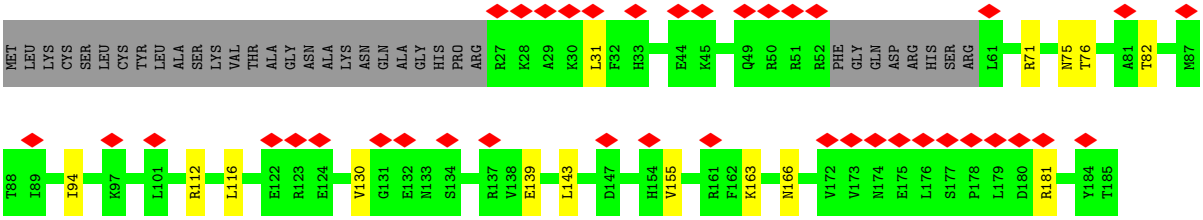
Chain UT:





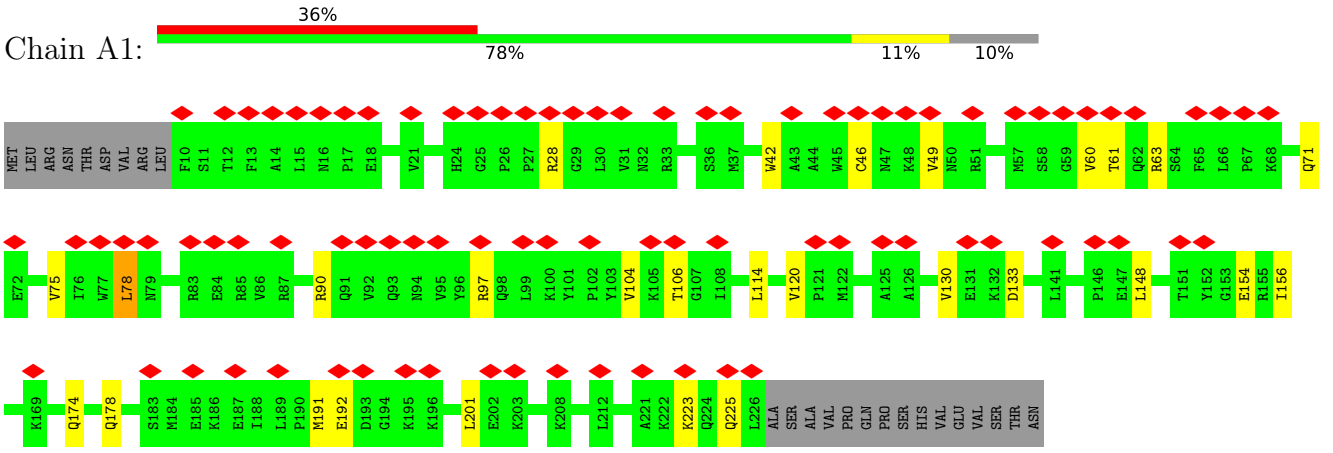
• Molecule 64: bL27m

Chain A0:



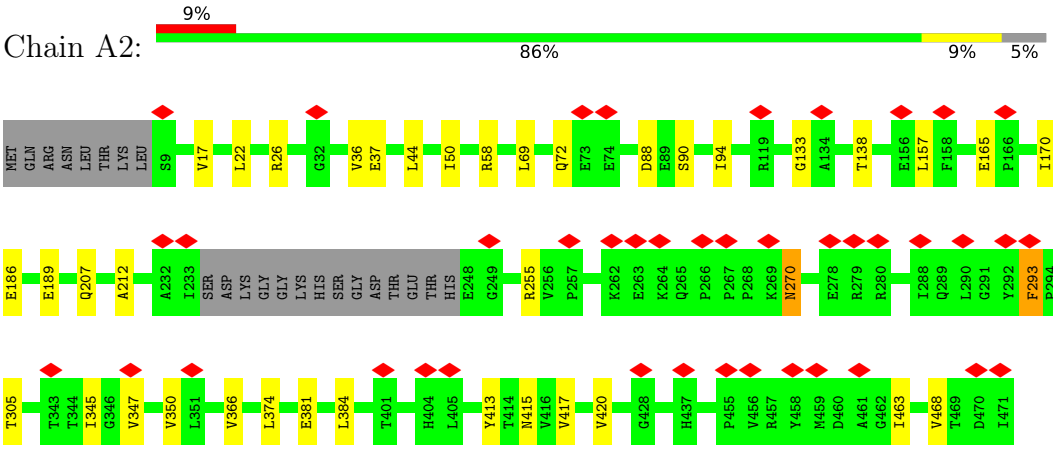
• Molecule 65: bL28m

Chain A1:



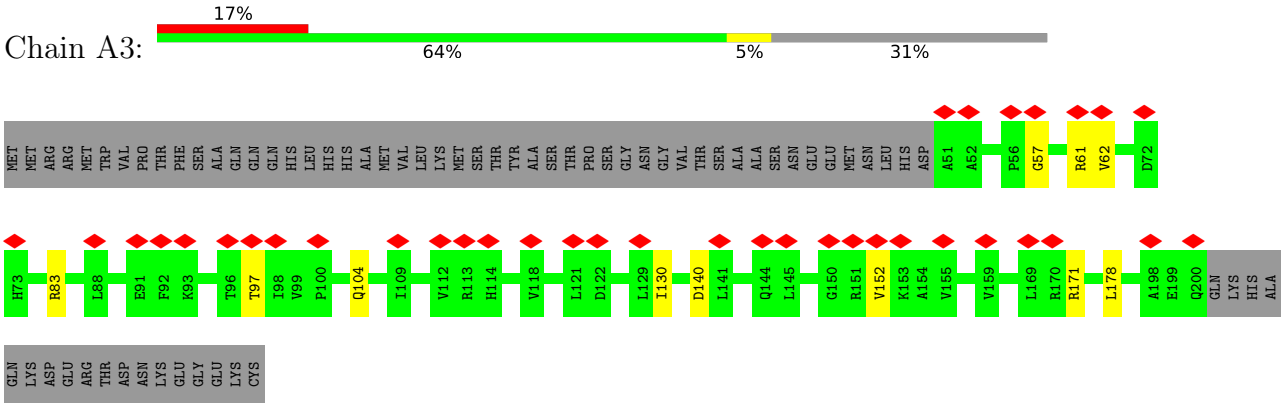
• Molecule 66: uL29m

Chain A2:



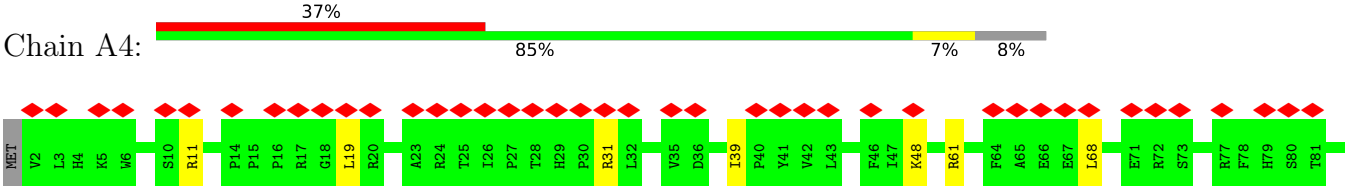
• Molecule 67: uL30m

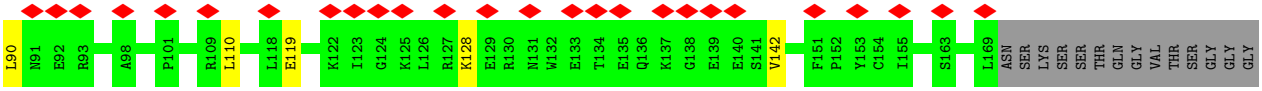
Chain A3:



• Molecule 68: bL31m

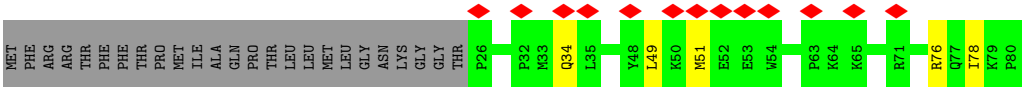
Chain A4:





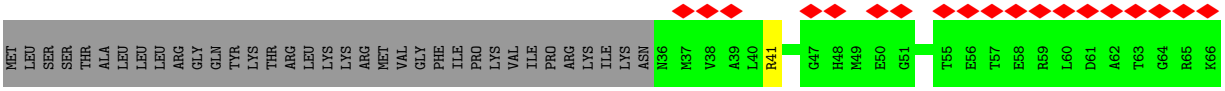
• Molecule 69: bL32m

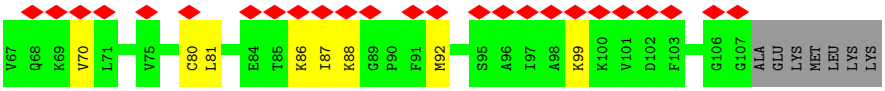
Chain A5:



• Molecule 70: bL33m

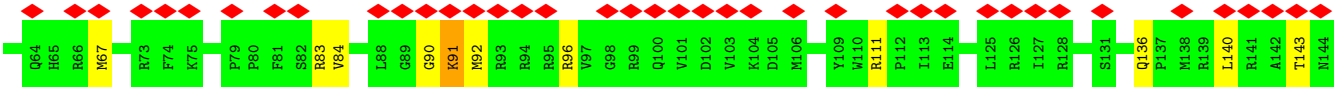
Chain A6:

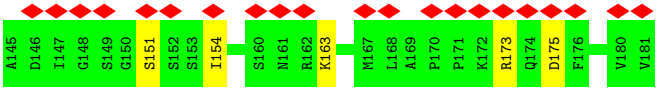




• Molecule 71: bL35m

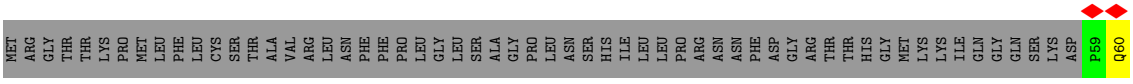
Chain A8:

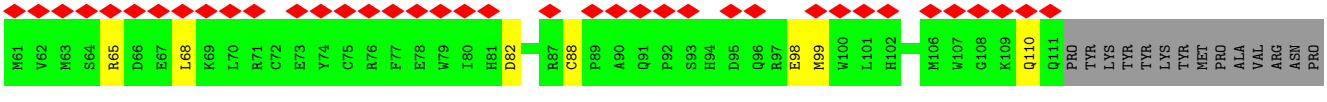


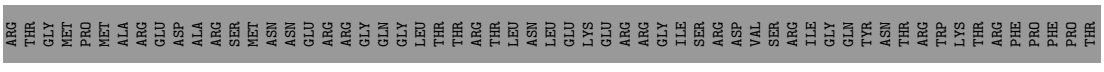


• Molecule 72: bL36m

Chain A9:

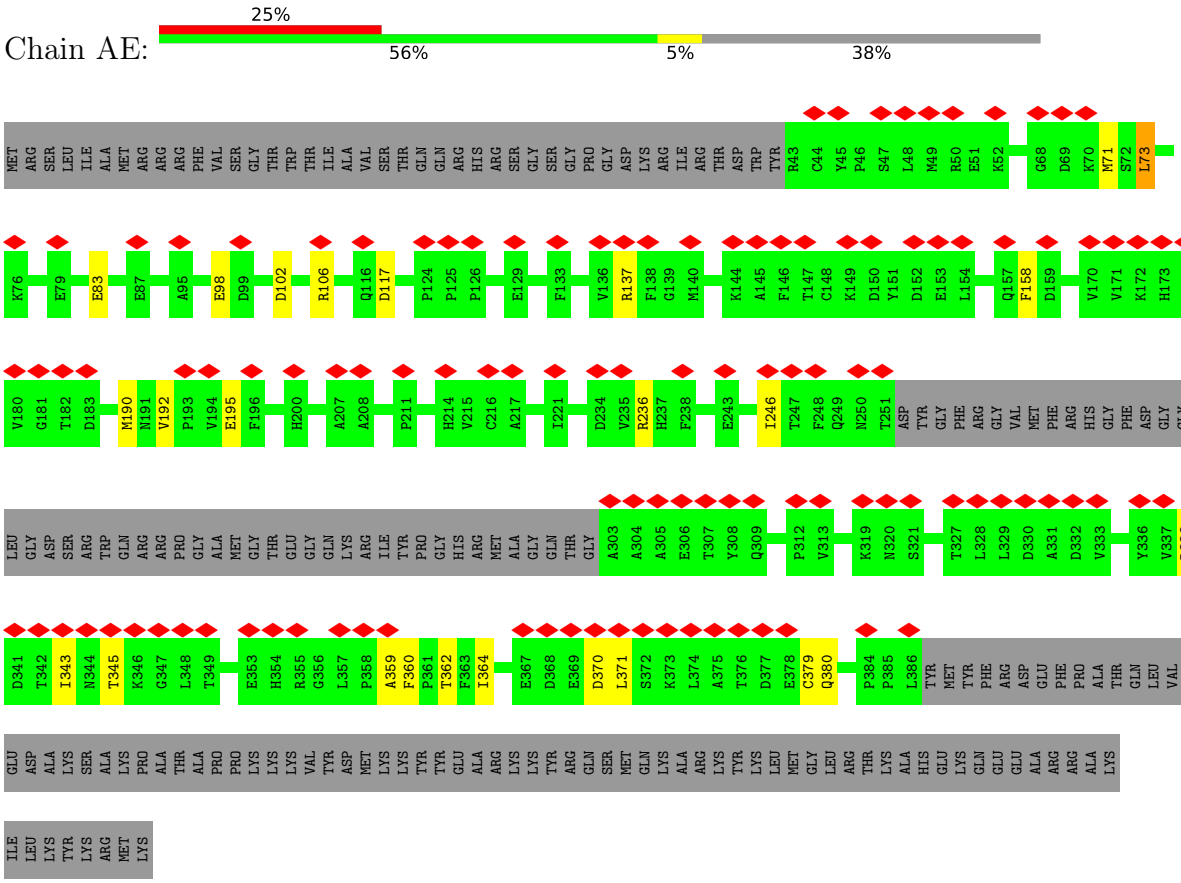






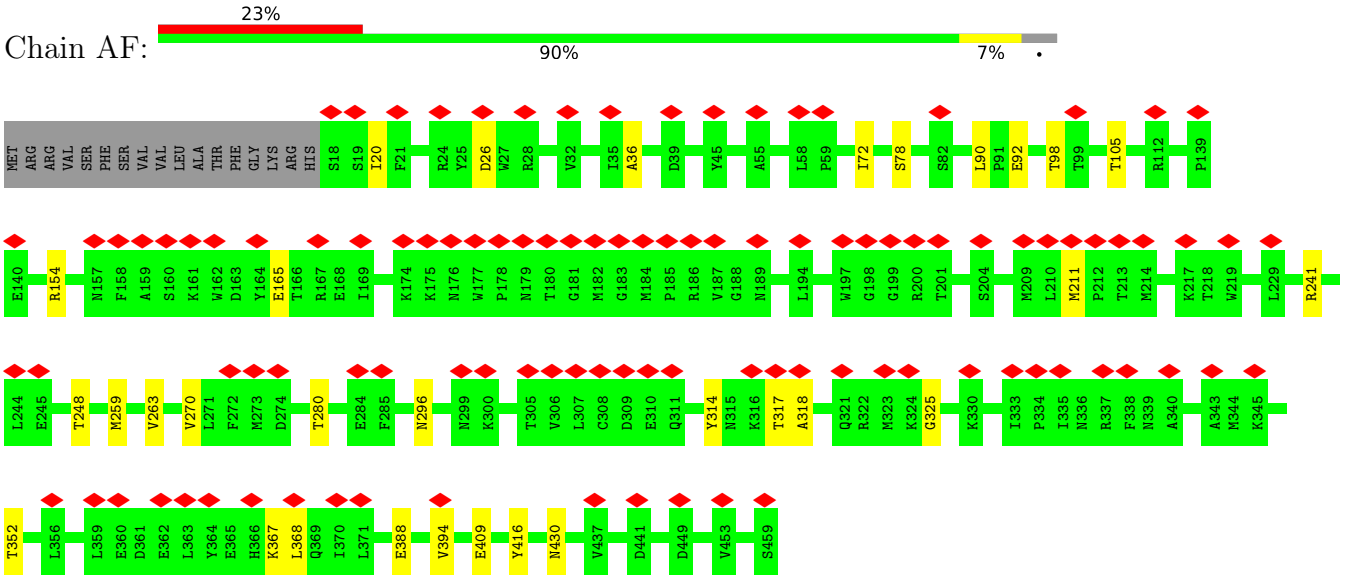
• Molecule 73: uL3m

Chain AE:



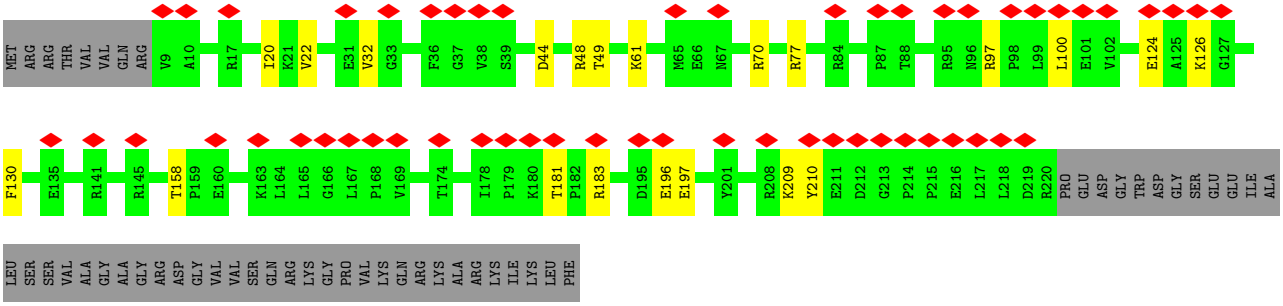
• Molecule 74: uL4m

Chain AF:



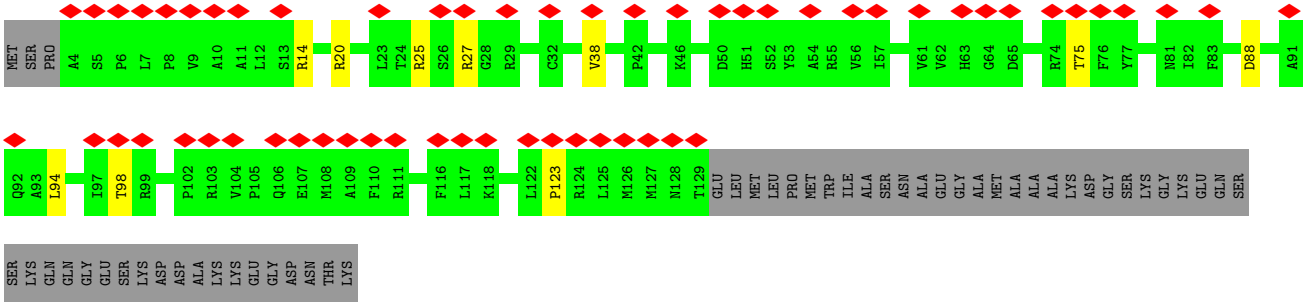
• Molecule 75: bL9m

Chain AI:



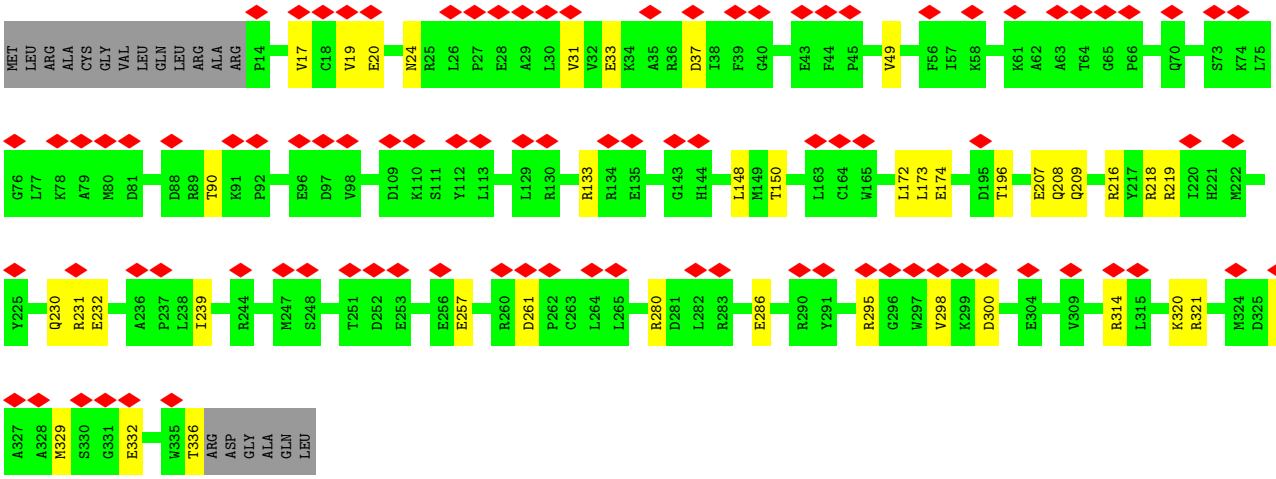
• Molecule 76: uL10m

Chain AJ:



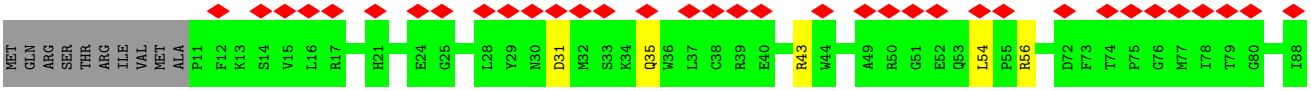
• Molecule 77: uL11m

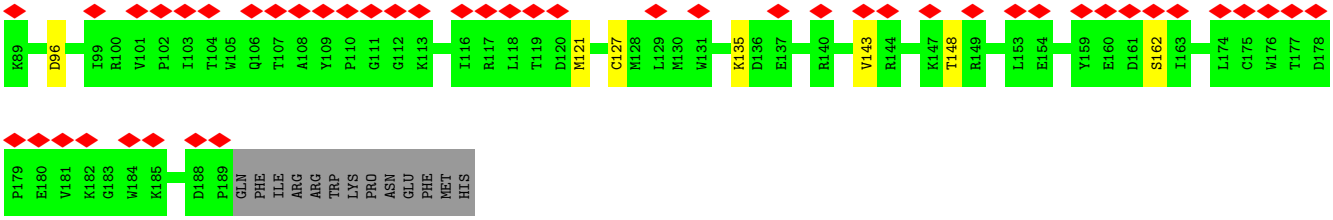
Chain AK:



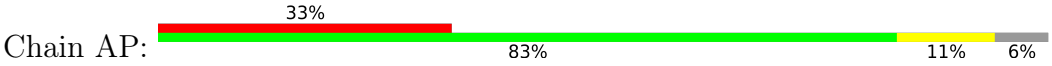
• Molecule 78: 50S ribosomal protein L13, putative

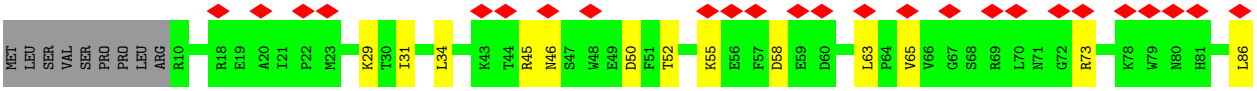
Chain AN:

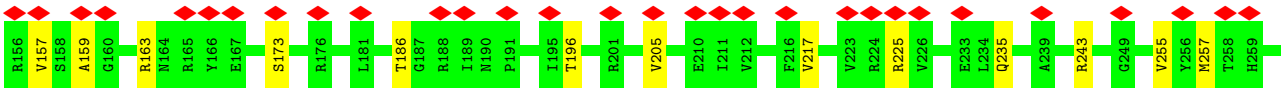




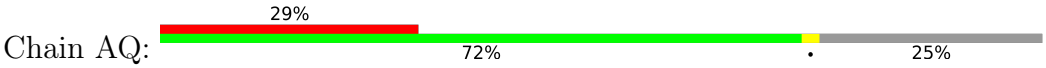
• Molecule 79: uL15m

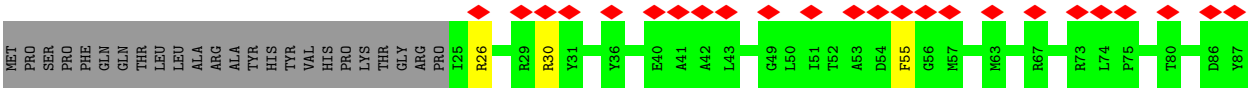




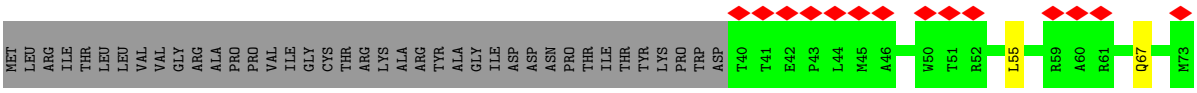


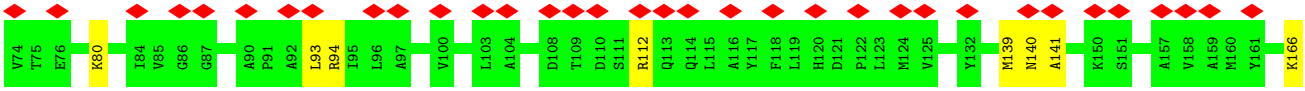
• Molecule 80: 50S ribosomal protein L16, putative

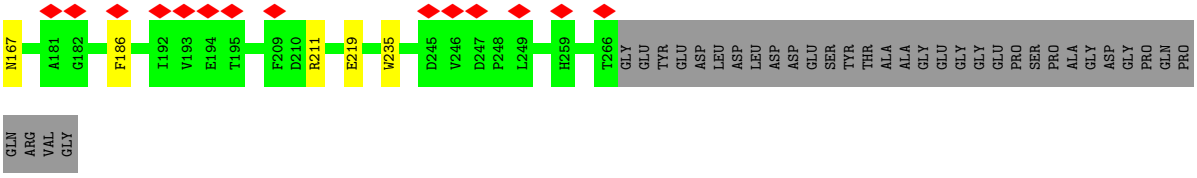




• Molecule 81: 50S ribosomal protein L17, putative

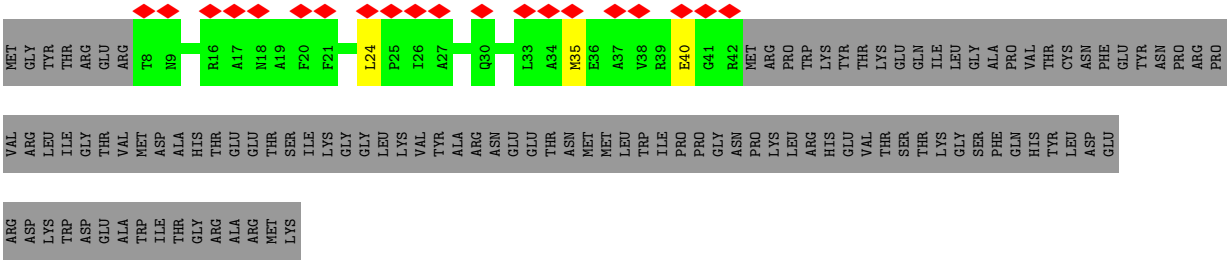






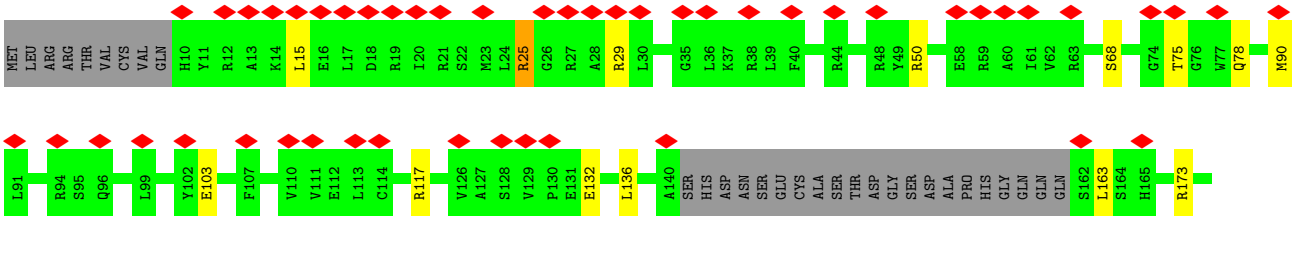
• Molecule 82: bL19m

Chain AT:



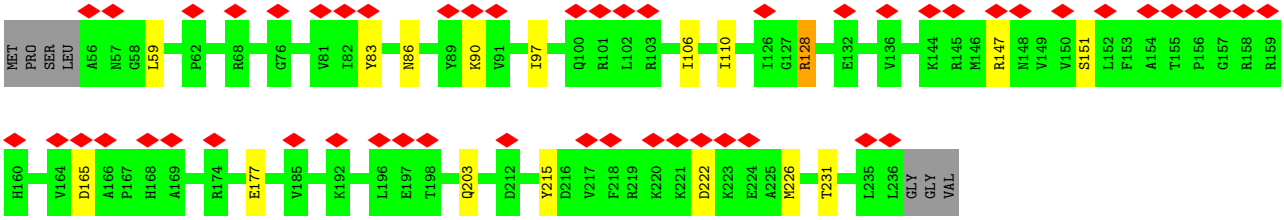
• Molecule 83: bL20m

Chain AU:



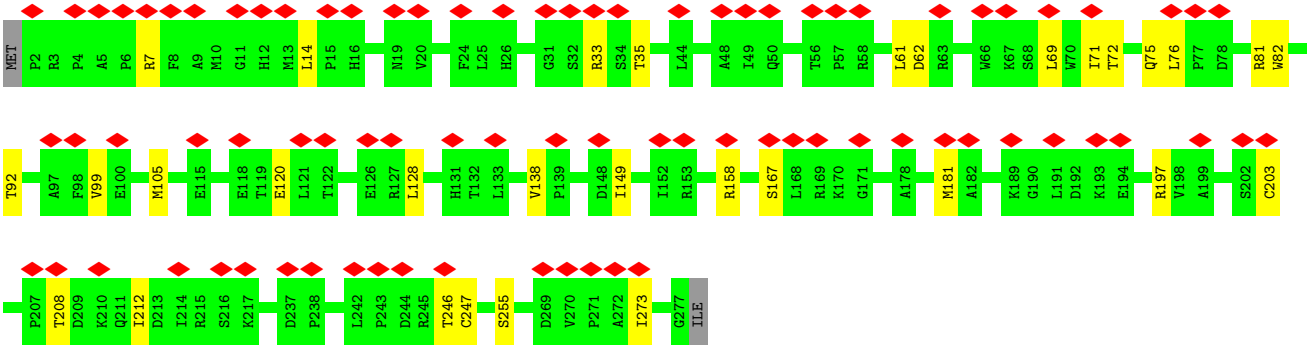
• Molecule 84: bL21m

Chain AV:

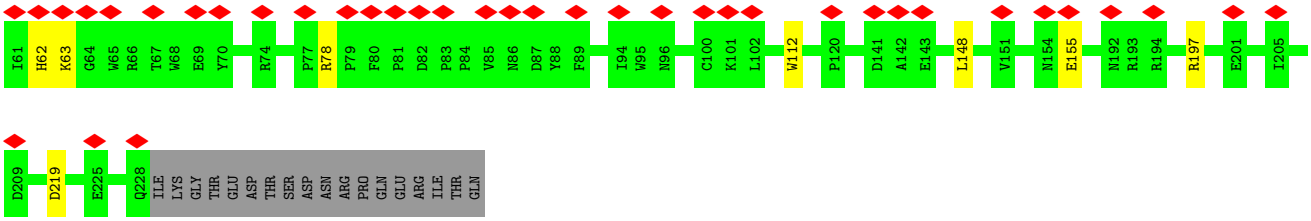


• Molecule 85: uL22m

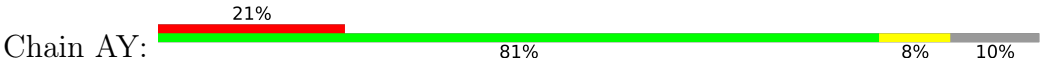
Chain AW:

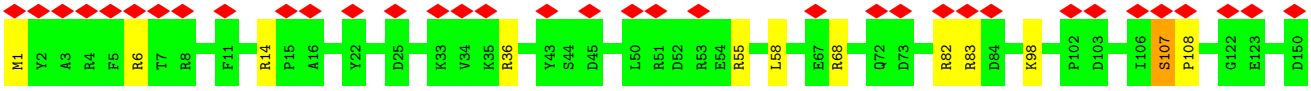


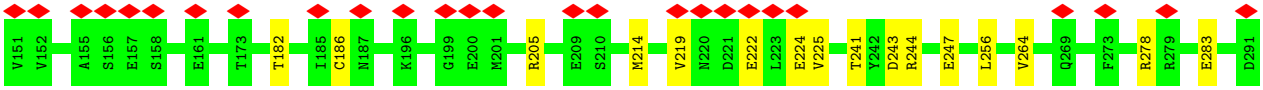
• Molecule 86: uL23m

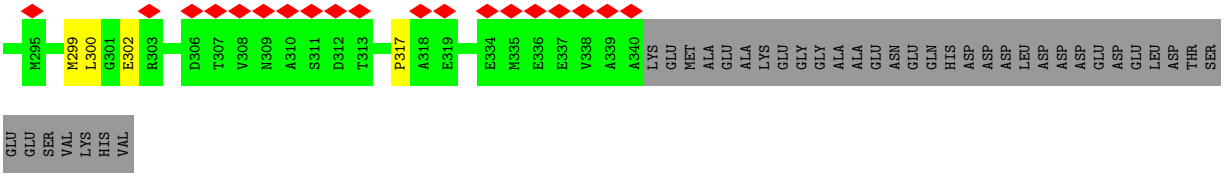


• Molecule 87: uL24m

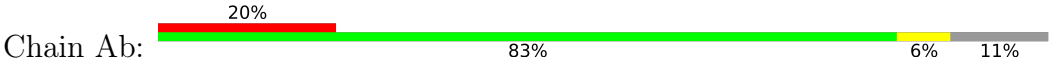


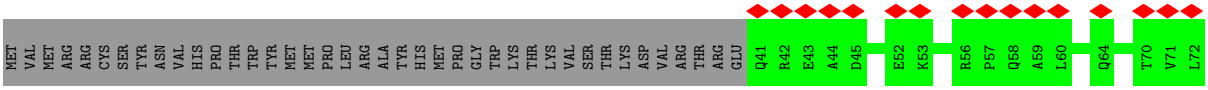


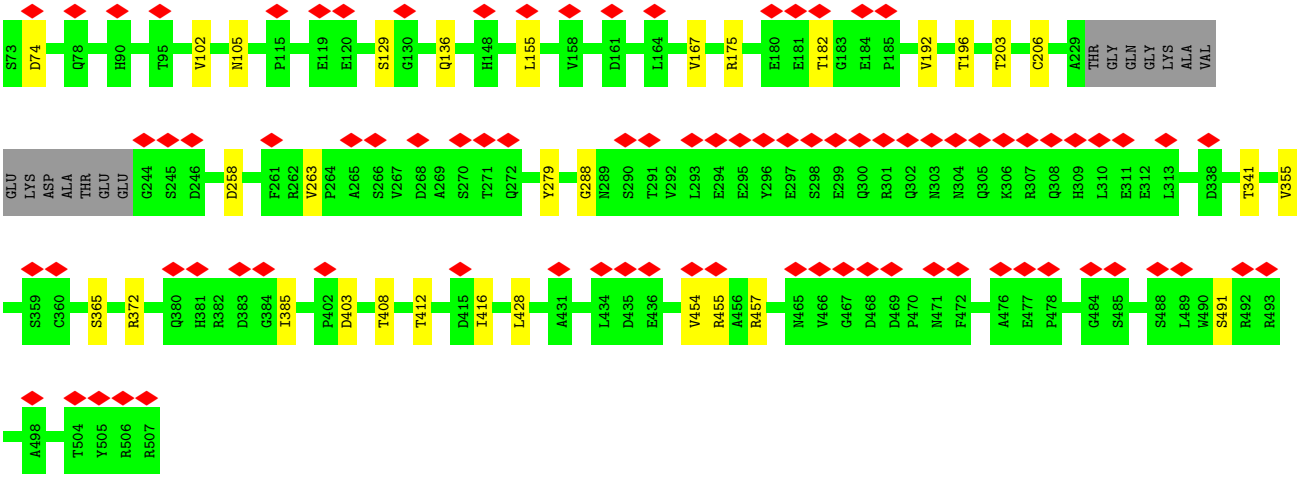




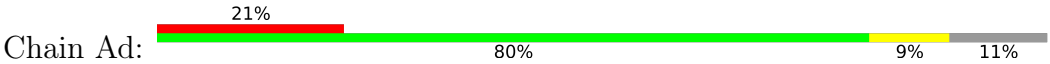
• Molecule 88: mL38

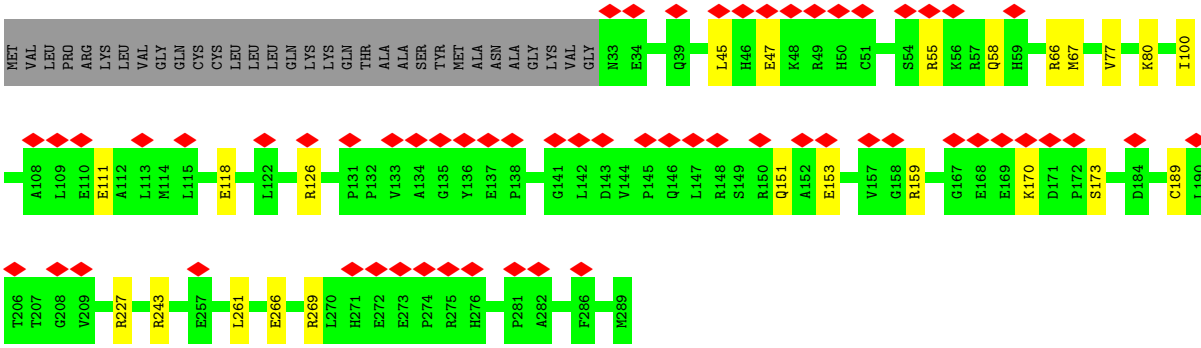




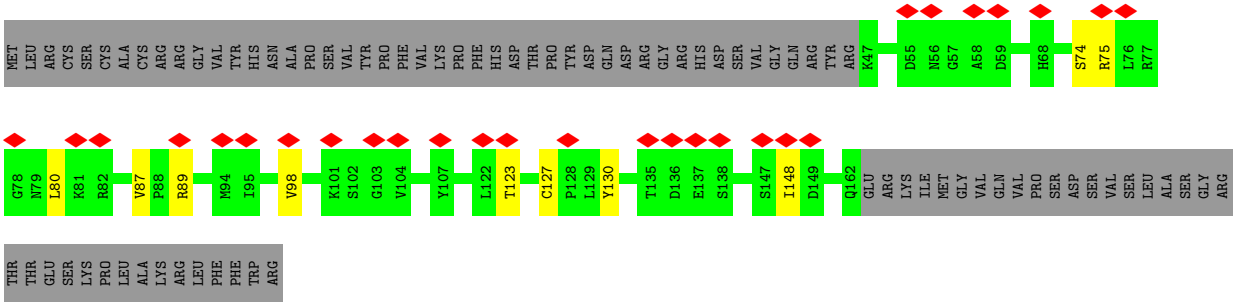


• Molecule 89: mL40

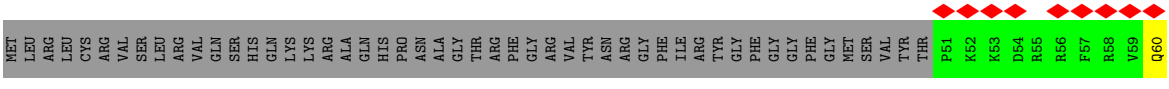


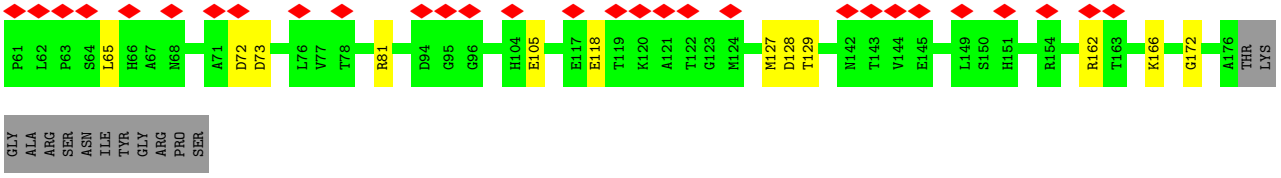


• Molecule 90: mL41



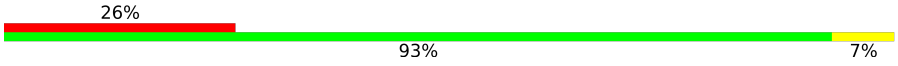
• Molecule 91: mL42

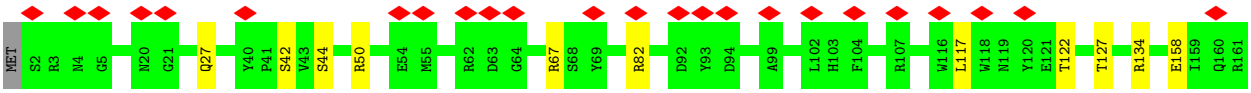


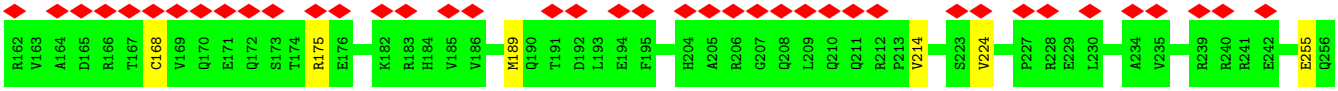


• Molecule 92: mL43

Chain Ag:

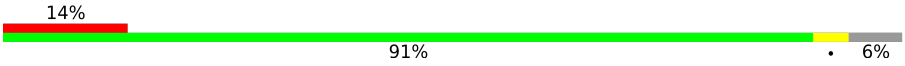


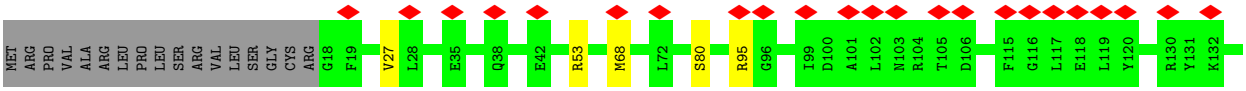




• Molecule 93: mL46

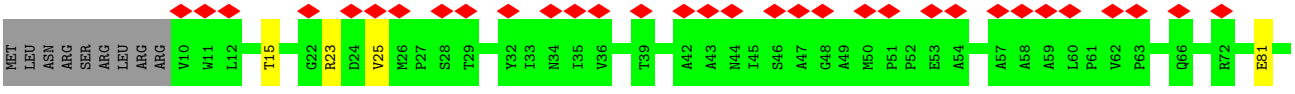
Chain Aj:

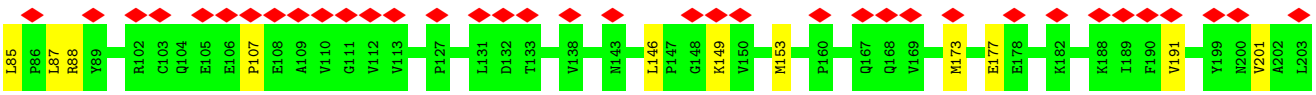


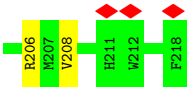


• Molecule 94: mL49

Chain Al:

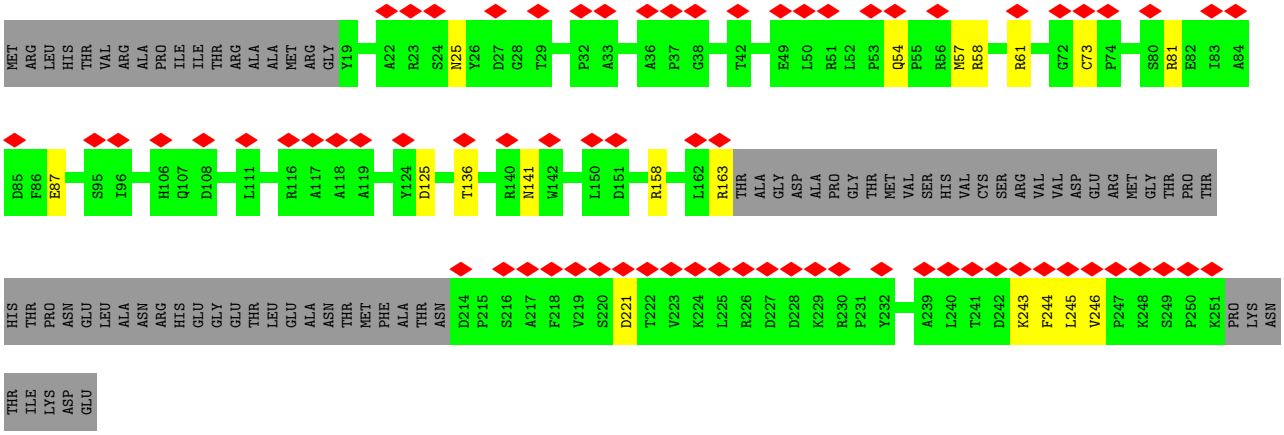






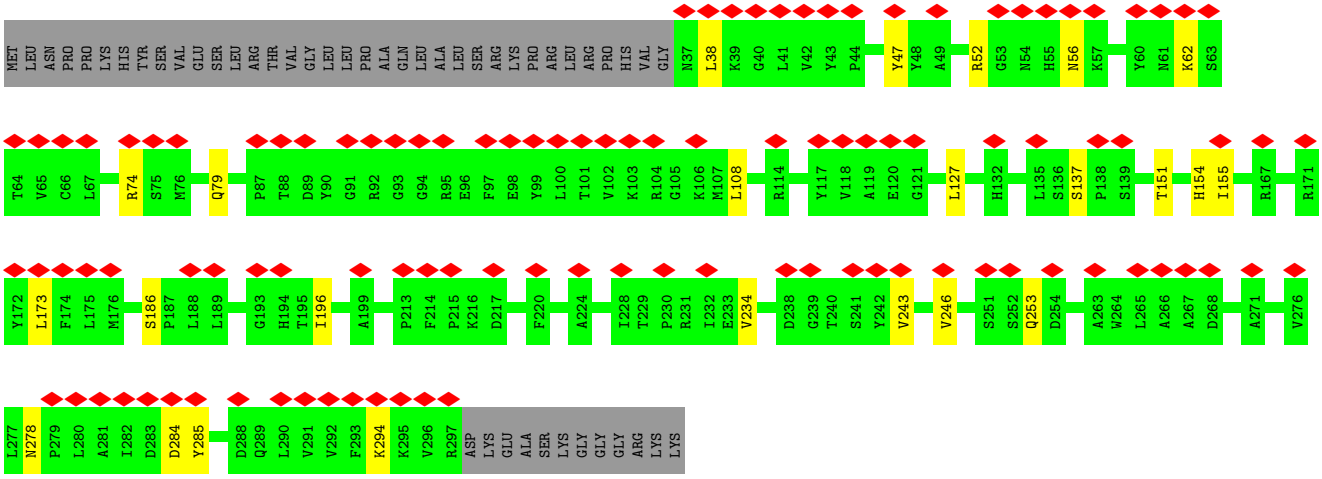
• Molecule 95: mL52

Chain Ao:



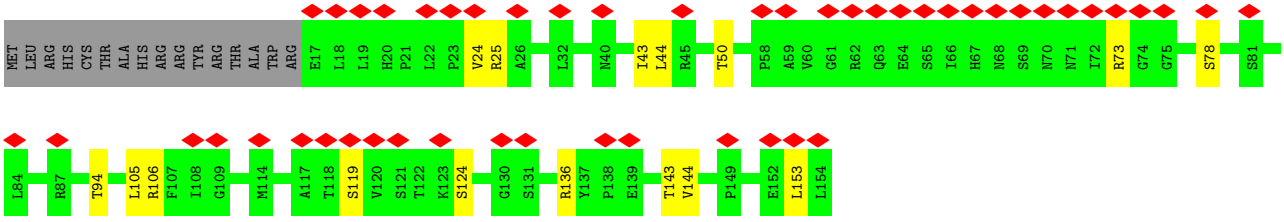
• Molecule 96: mL53

Chain Ap:



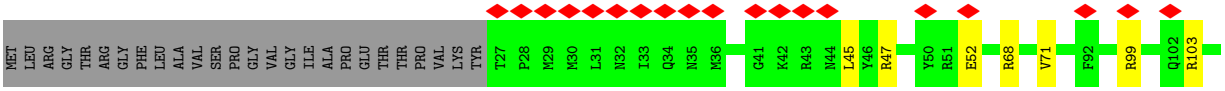
• Molecule 97: mL63

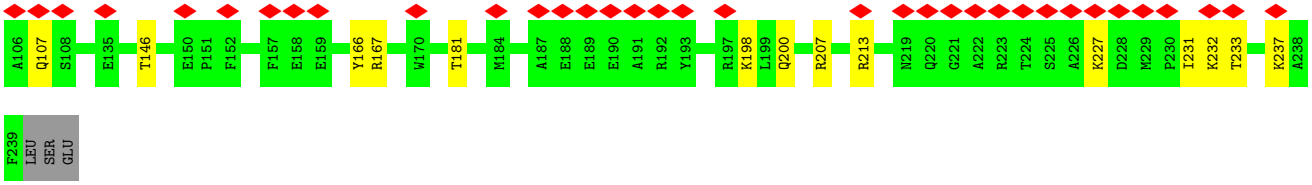
Chain At:



• Molecule 98: mL68

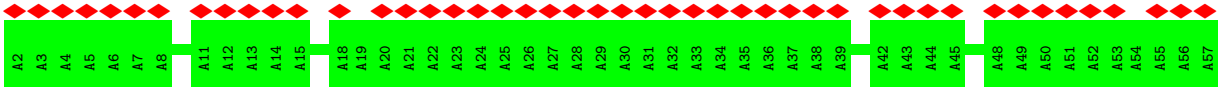
Chain Av:





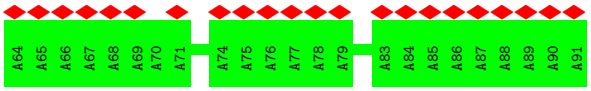
• Molecule 99: bL12m

Chain AB:



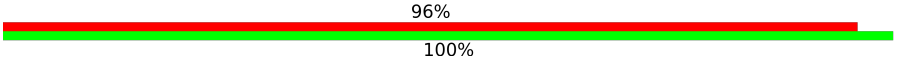
• Molecule 100: bL12m

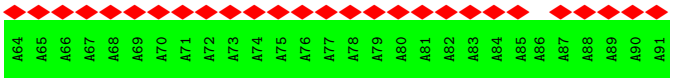
Chain AC:



• Molecule 100: bL12m

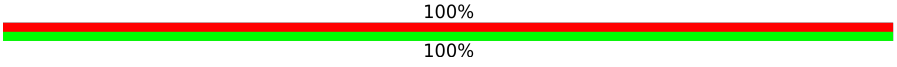
Chain AD:

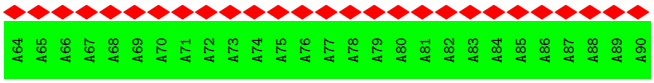




• Molecule 101: bL12m

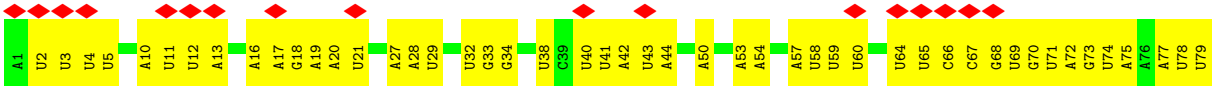
Chain AG:

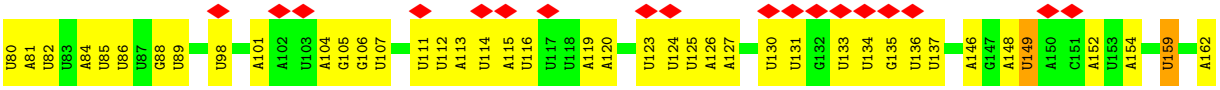


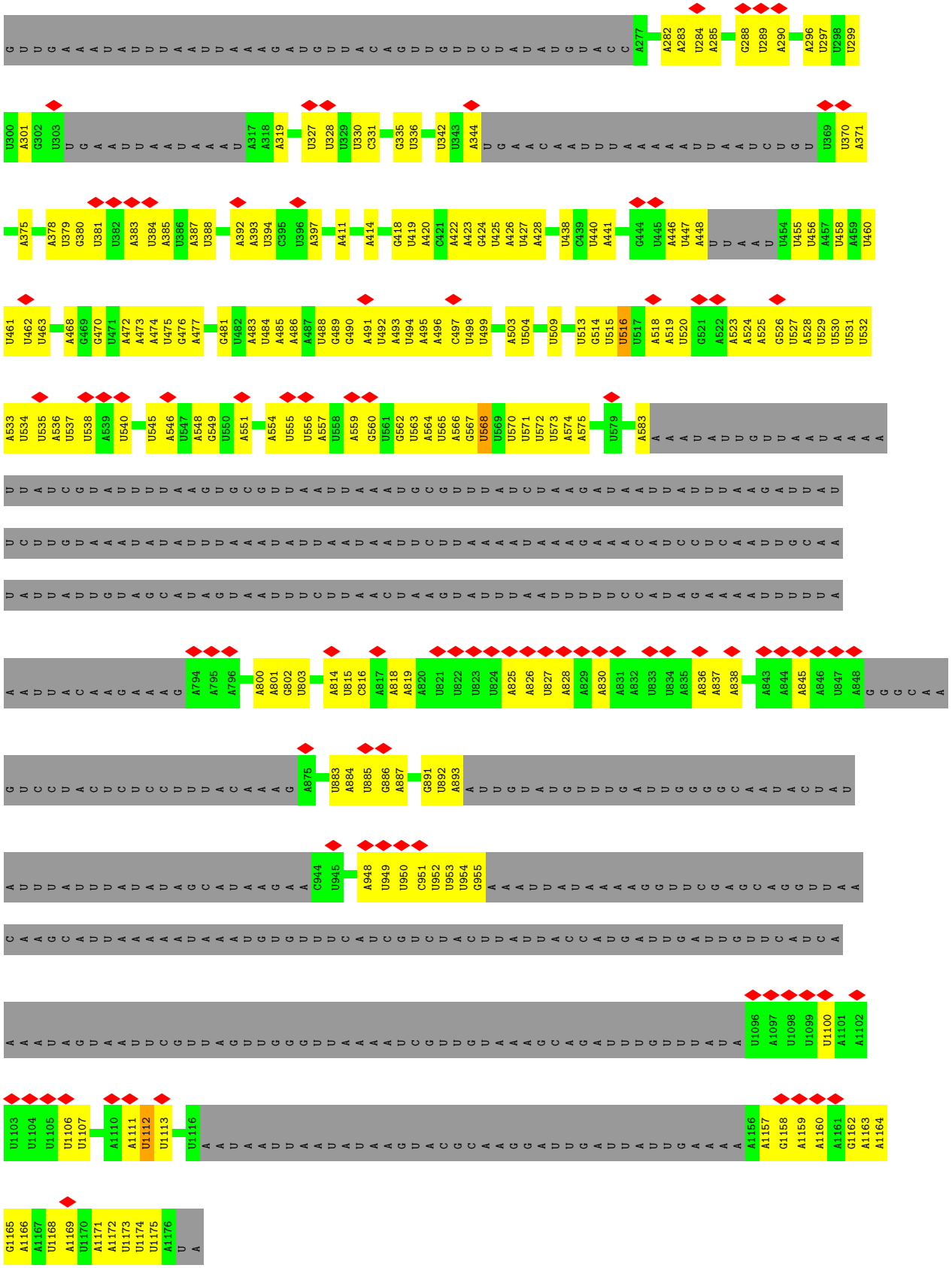


• Molecule 102: 12S rRNA

Chain AA:

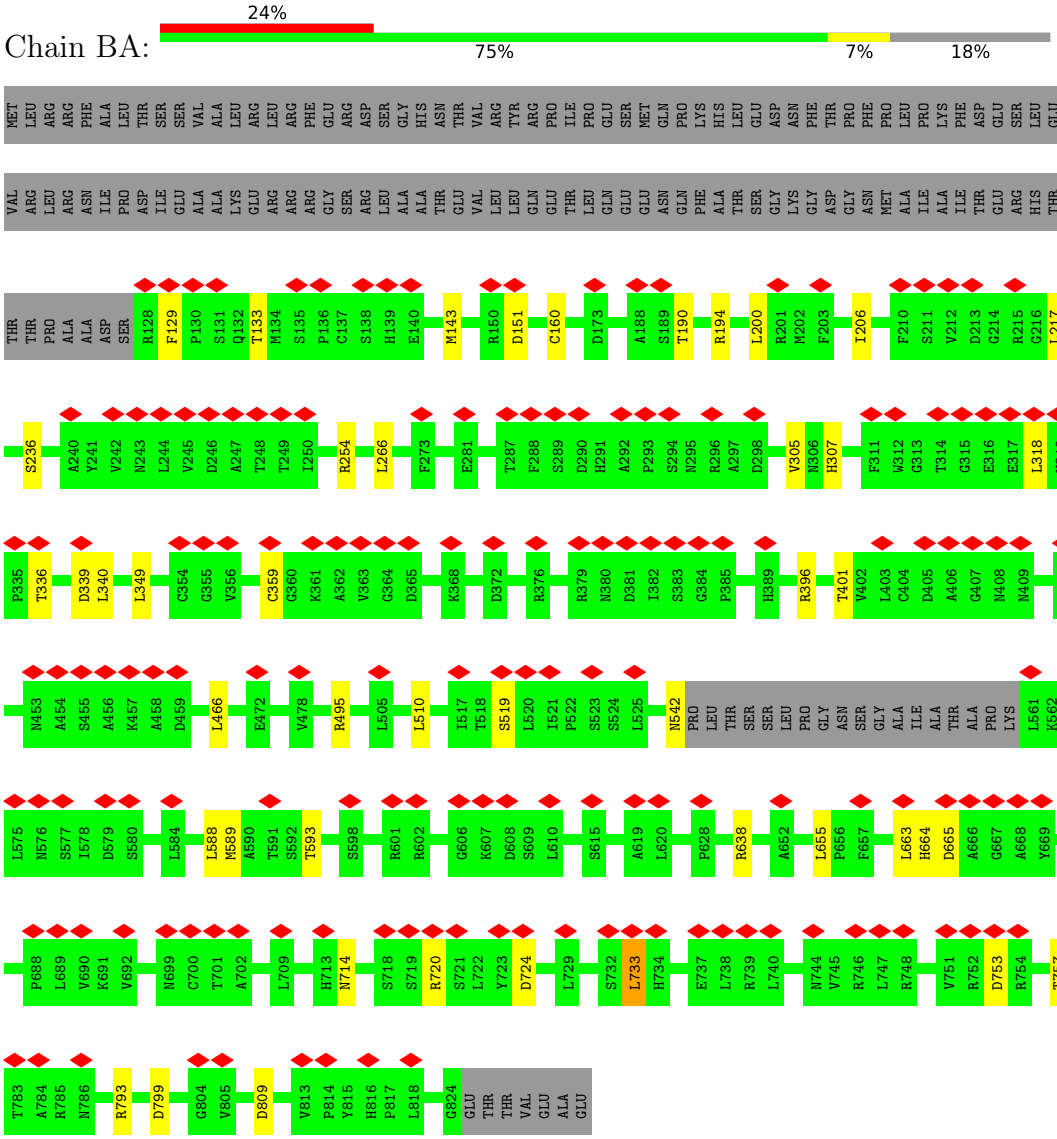






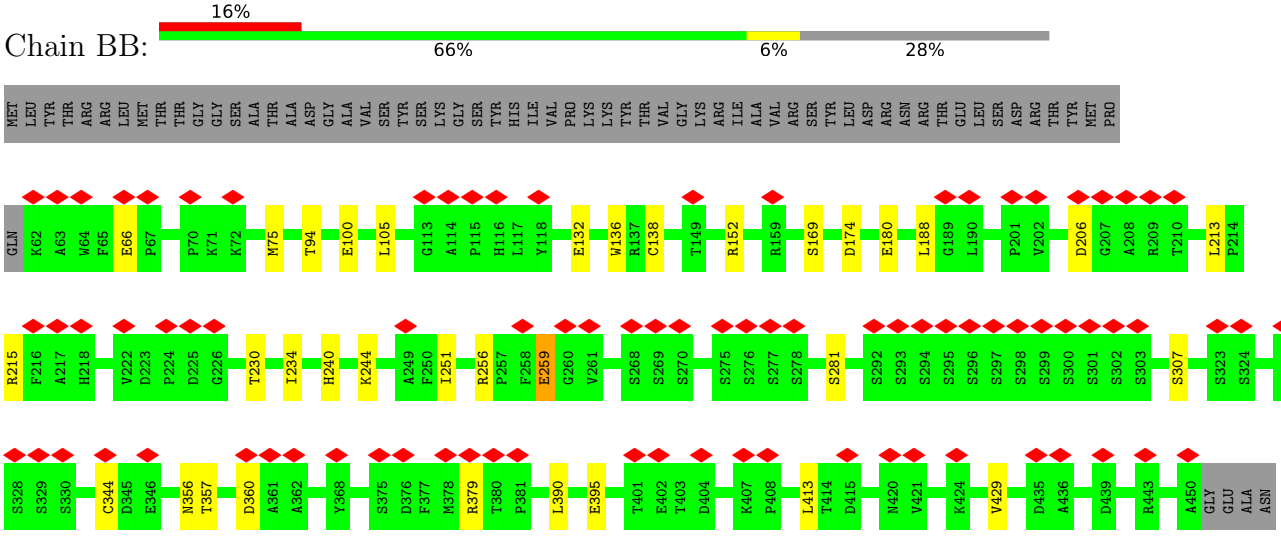
• Molecule 103: mL67

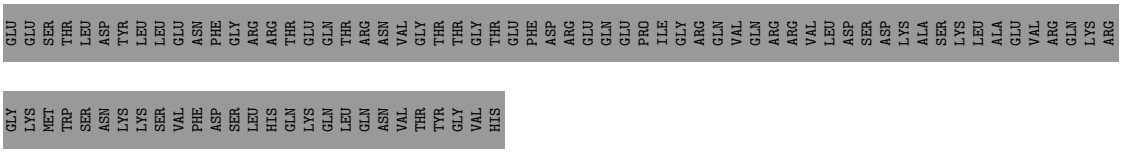
Chain BA:



- Molecule 104: mL68

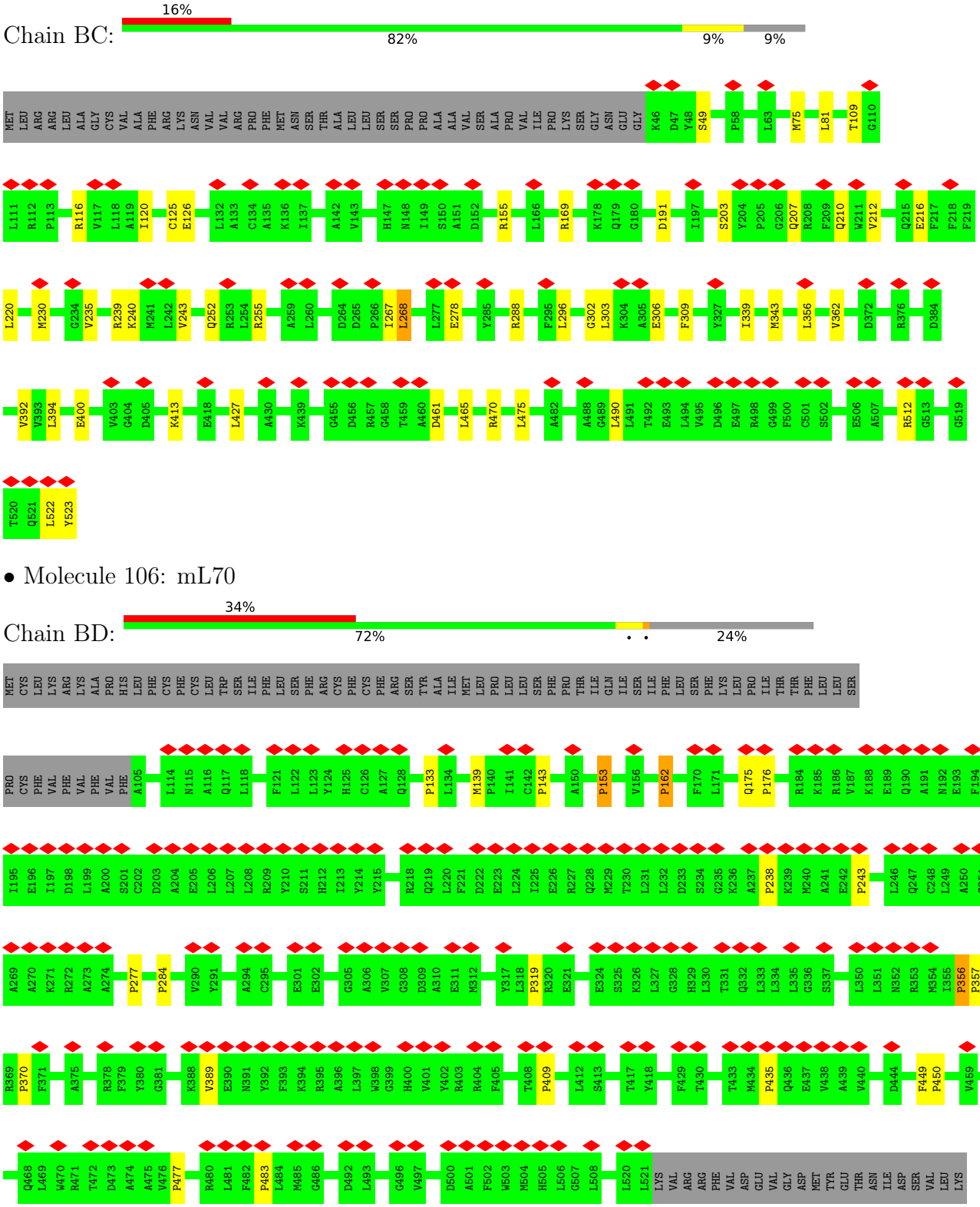
Chain BB:





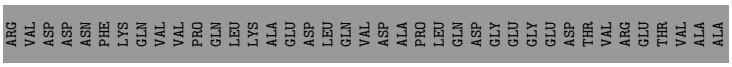
• Molecule 105: mL69

Chain BC:



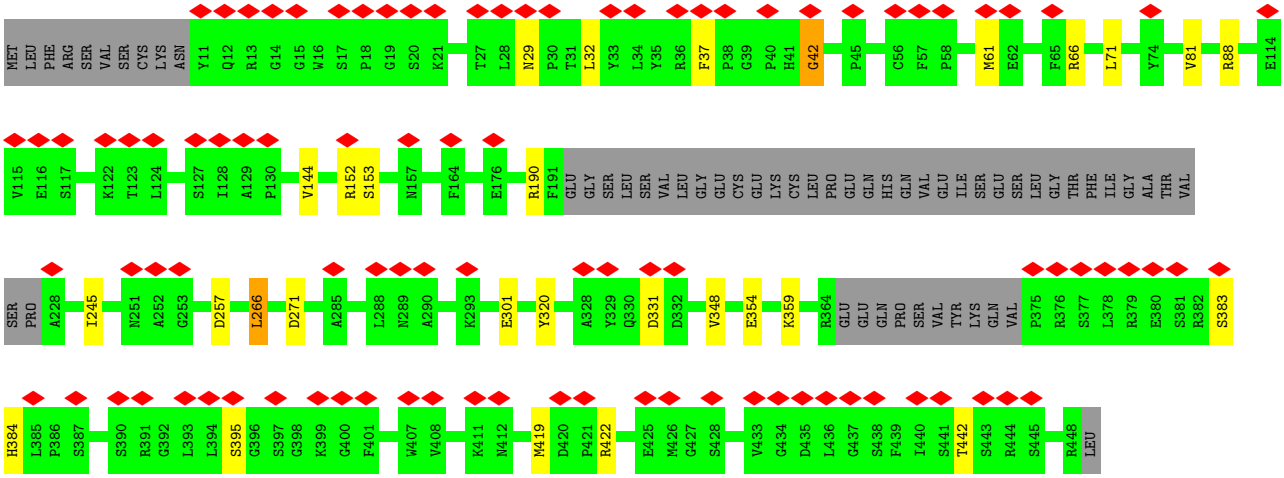
• Molecule 106: mL70

Chain BD:



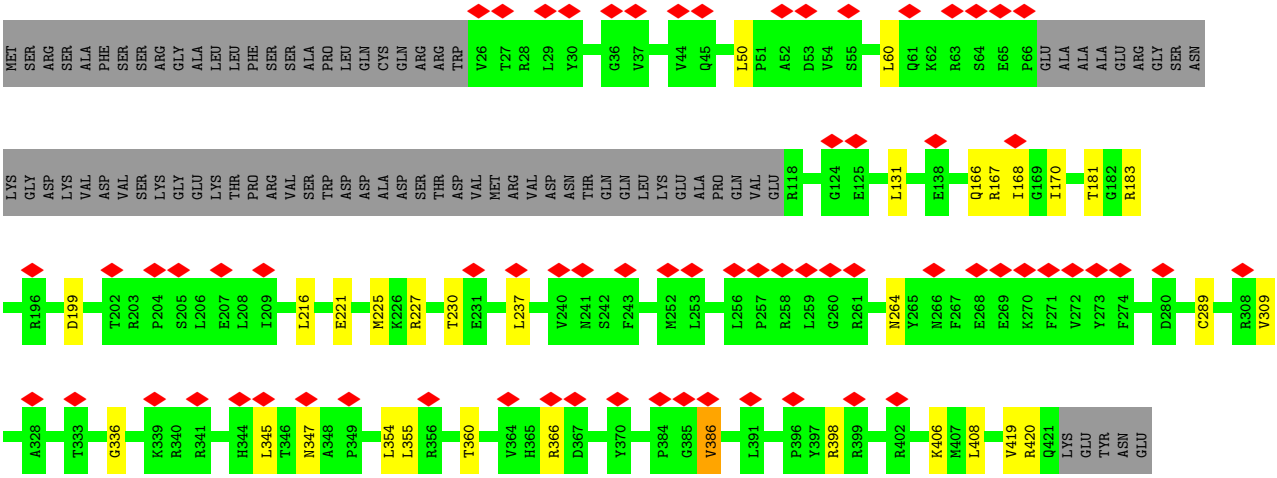
- Molecule 107: mL71

Chain BE:



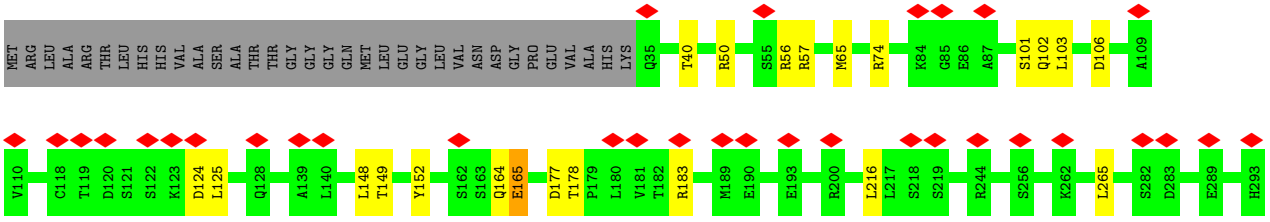
- Molecule 108: mL72

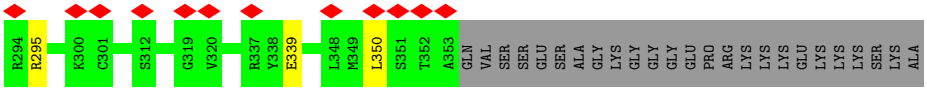
Chain BF:



- Molecule 109: mL73

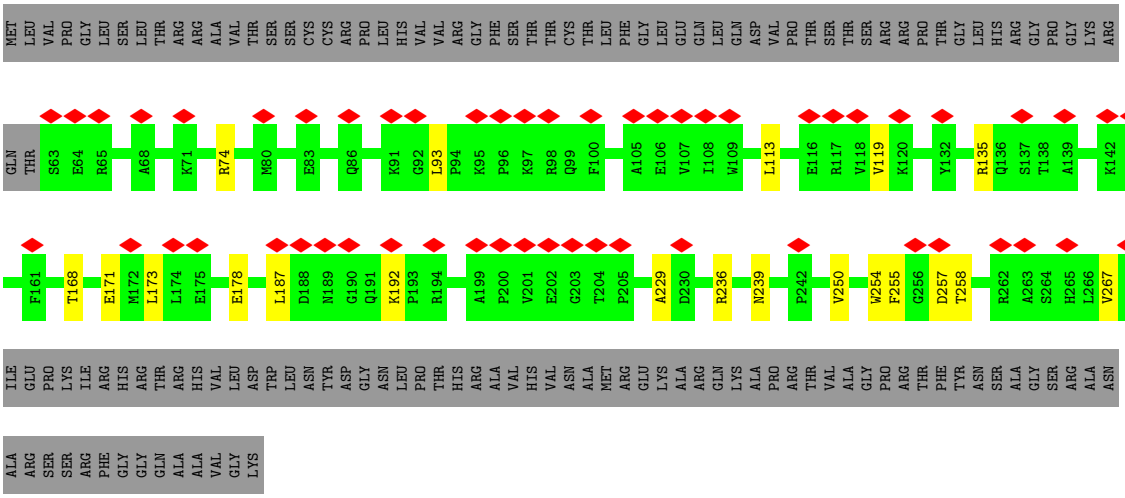
Chain BG:





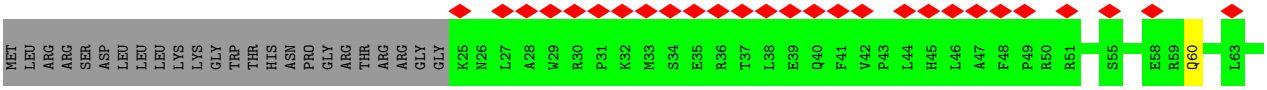
• Molecule 110: mL74

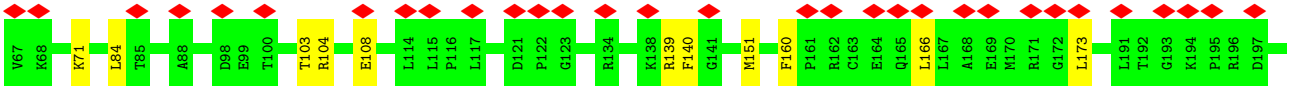
Chain BH:

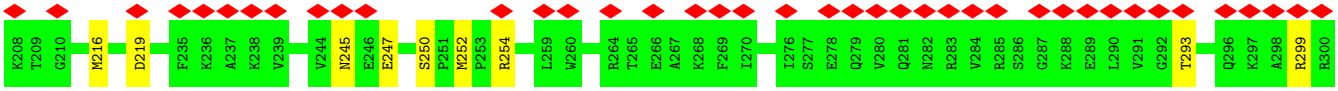


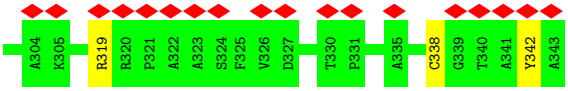
• Molecule 111: mL75

Chain BI:



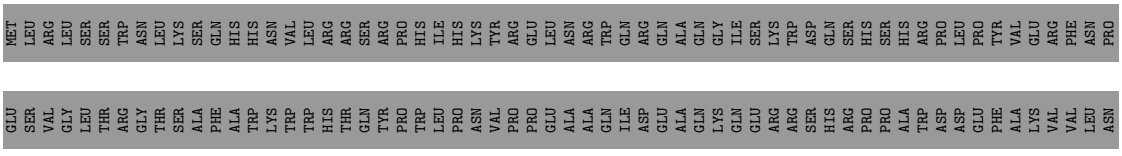


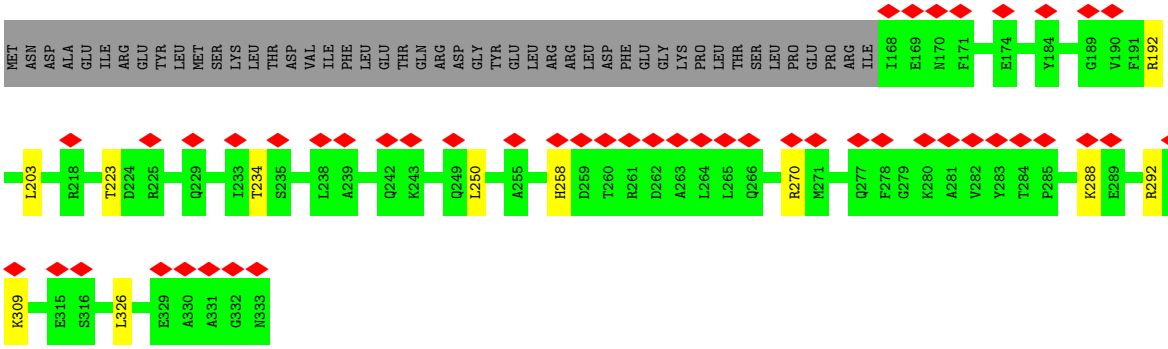




• Molecule 112: mL76

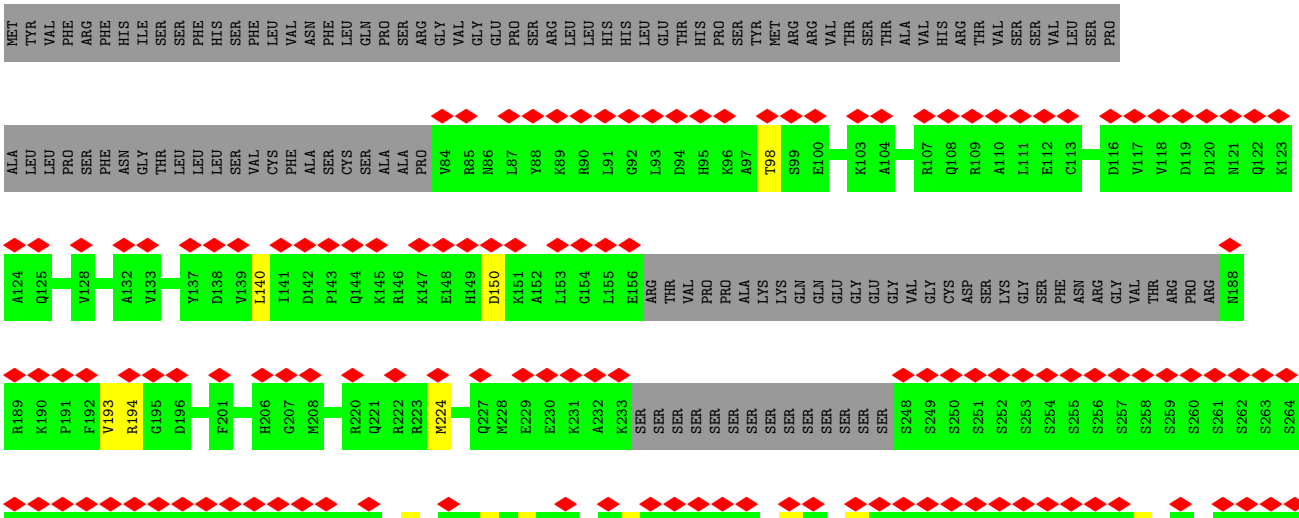
Chain BJ:





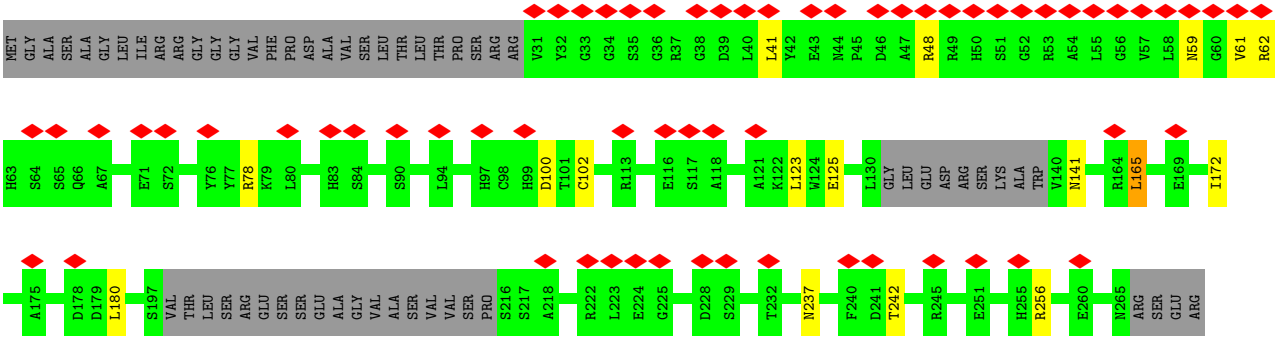
• Molecule 113: mL77

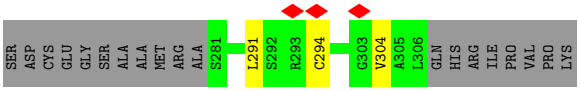
Chain BK:



• Molecule 114: mL78

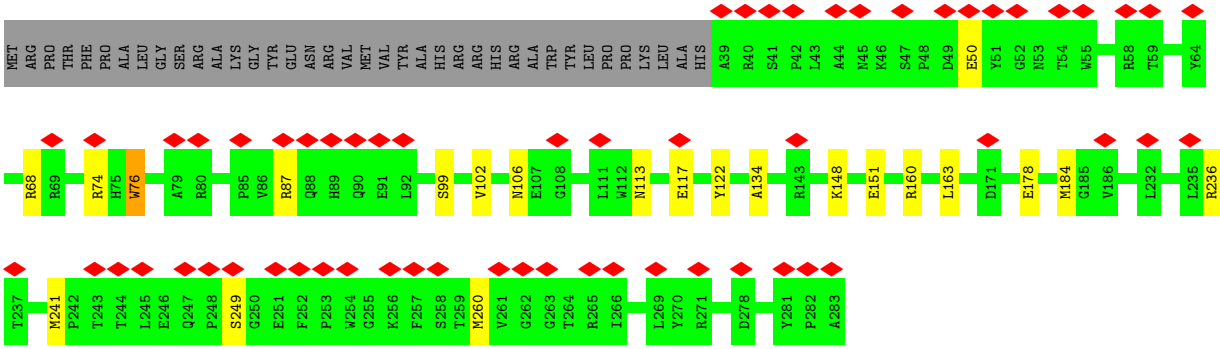
Chain BL:





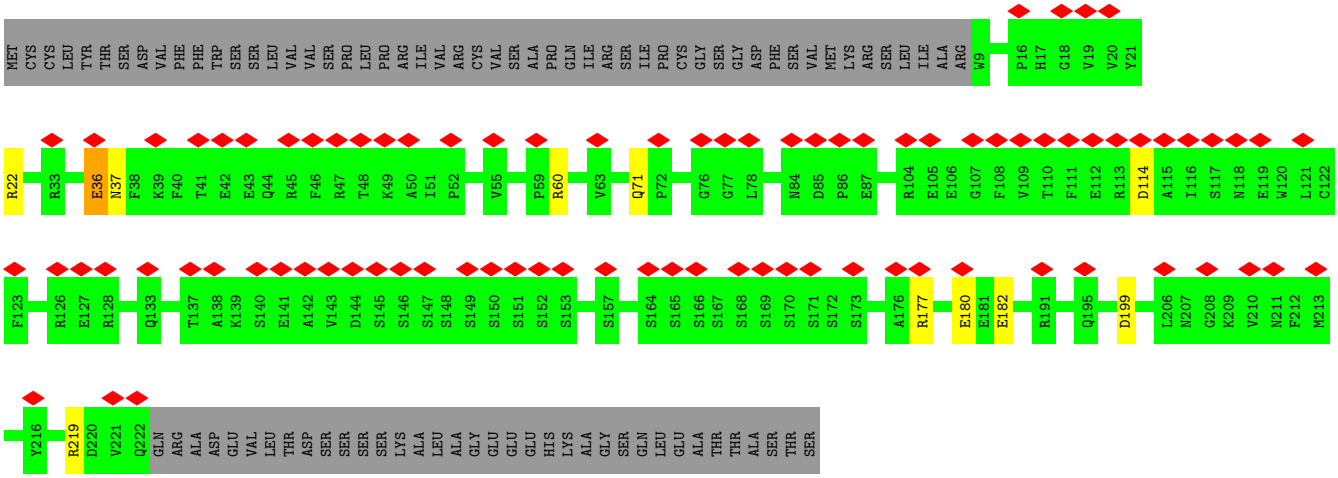
- Molecule 115: mL79

Chain BM:



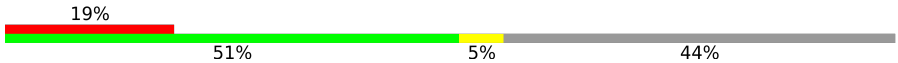
- Molecule 116: mL80

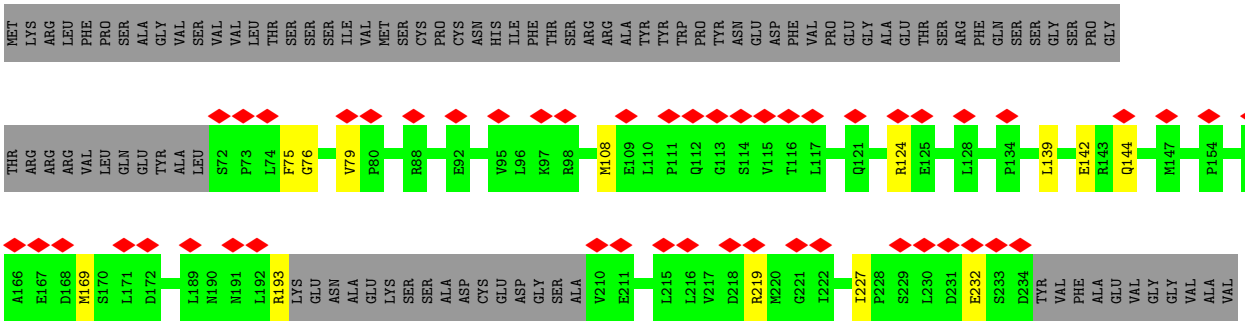
Chain BN:

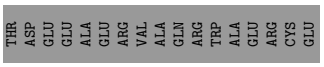


- Molecule 117: mL81

Chain BO:

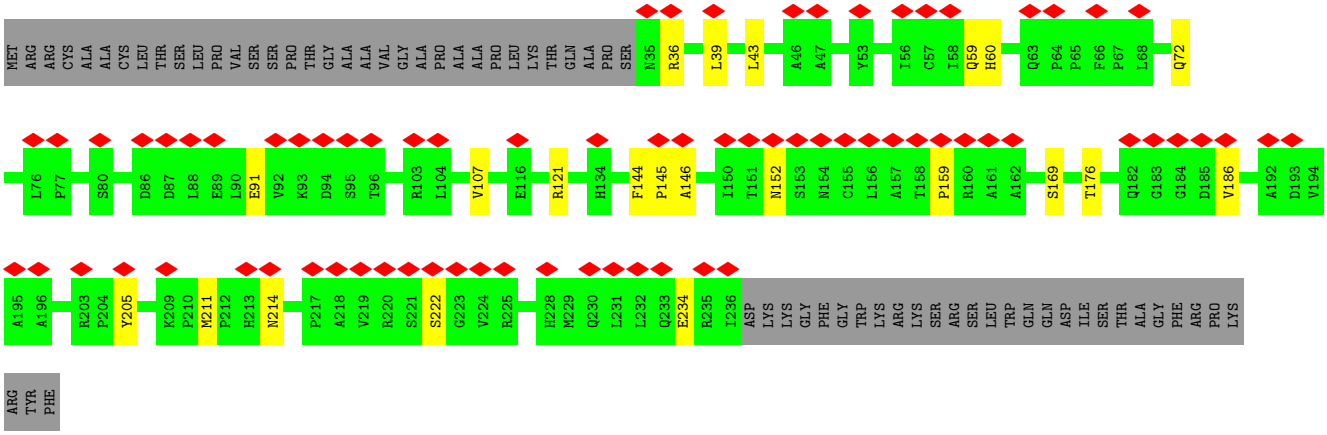






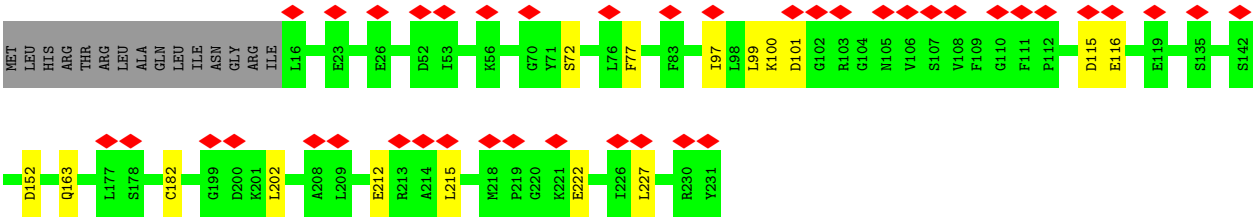
• Molecule 118: mL82

Chain BP:



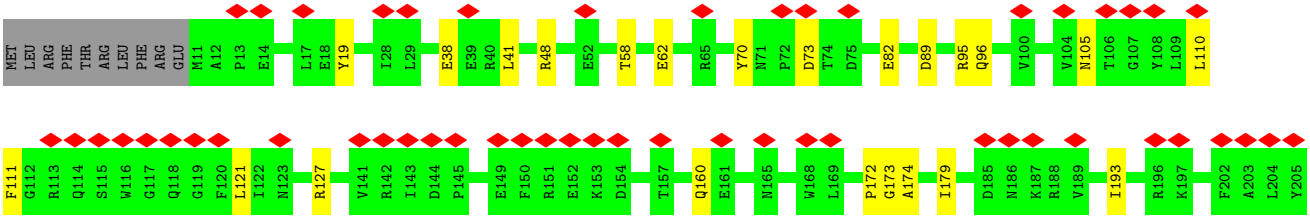
• Molecule 119: mL83

Chain BQ:



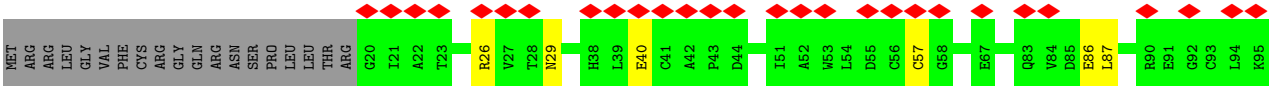
• Molecule 120: mL84

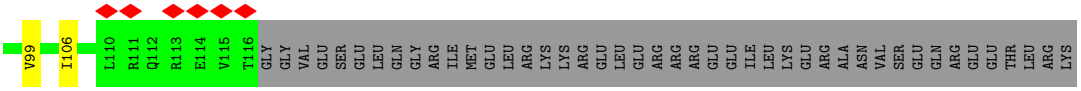
Chain BR:



• Molecule 121: mL85

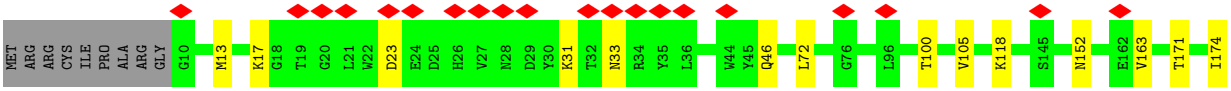
Chain BS:

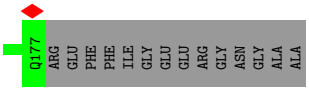




• Molecule 122: mL86

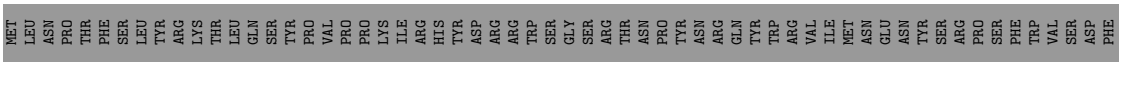
Chain BT:

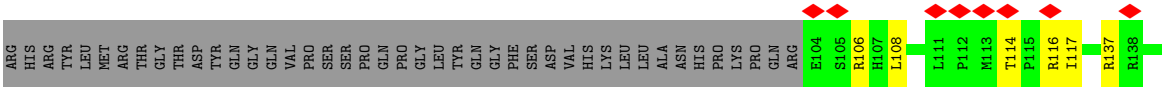


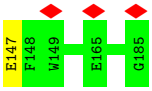


• Molecule 123: mL87

Chain BU:

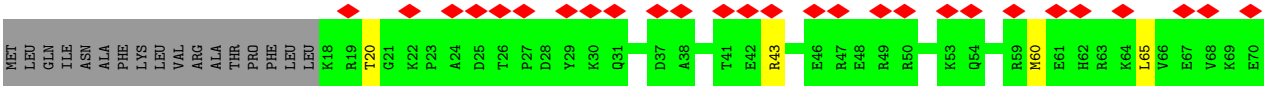


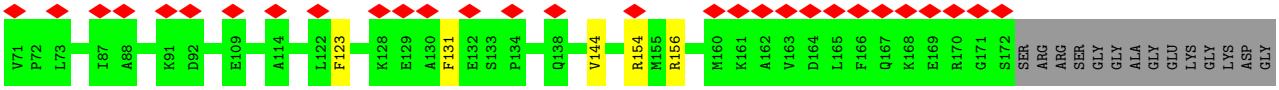




• Molecule 124: mL88

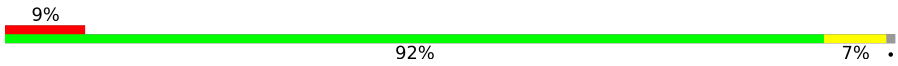
Chain BV:

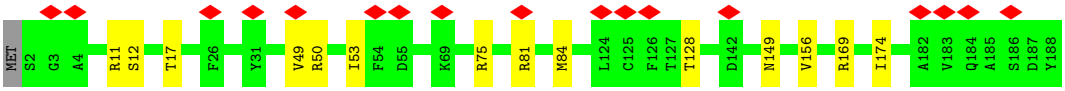




• Molecule 125: mL89

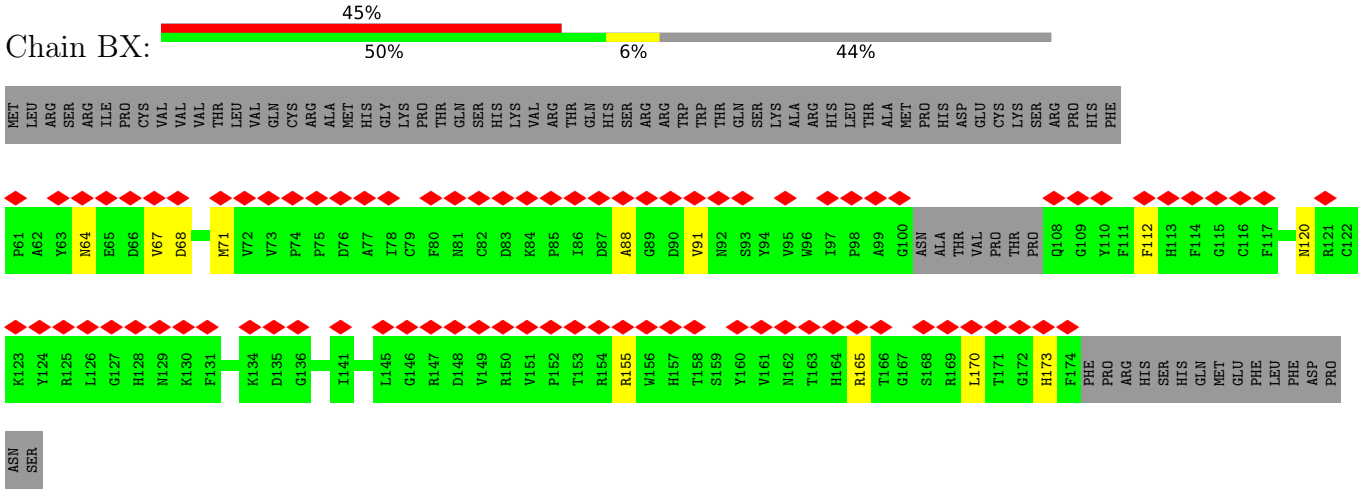
Chain BW:





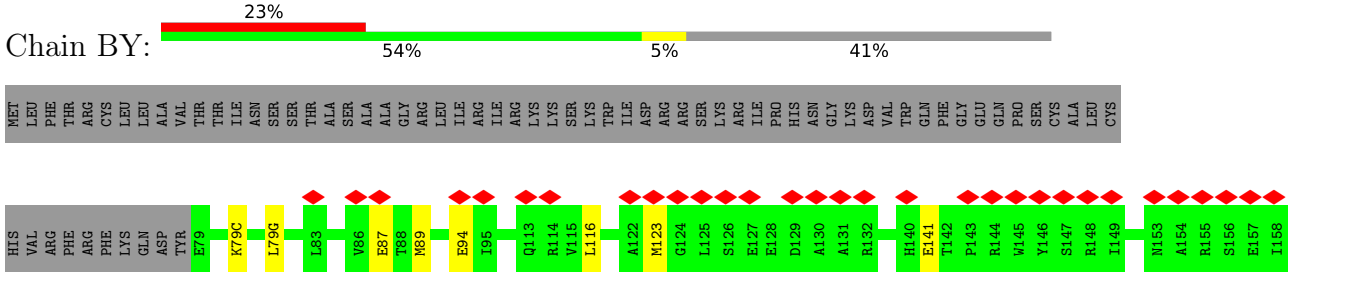
• Molecule 126: mL90

Chain BX:



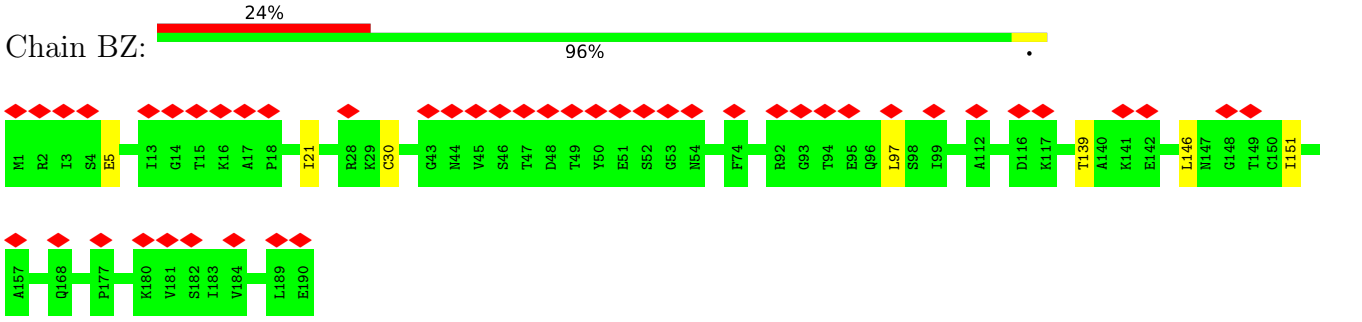
• Molecule 127: mS91

Chain BY:



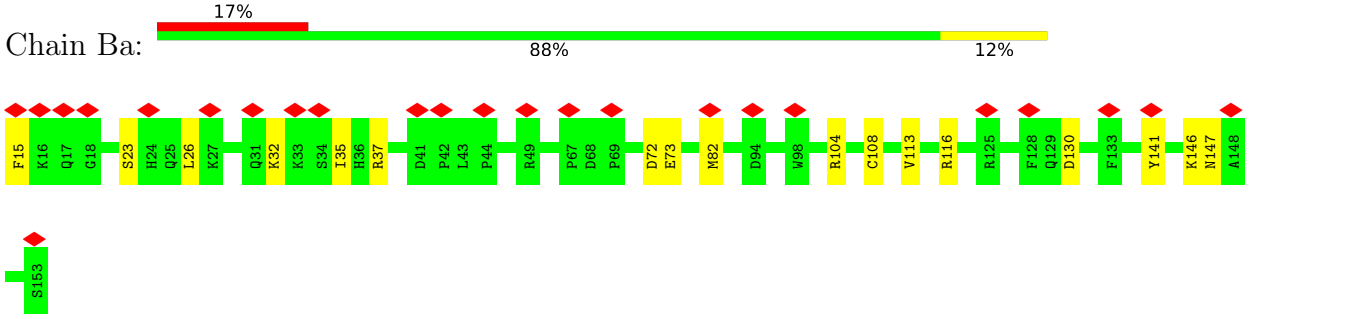
• Molecule 128: mL92

Chain BZ:



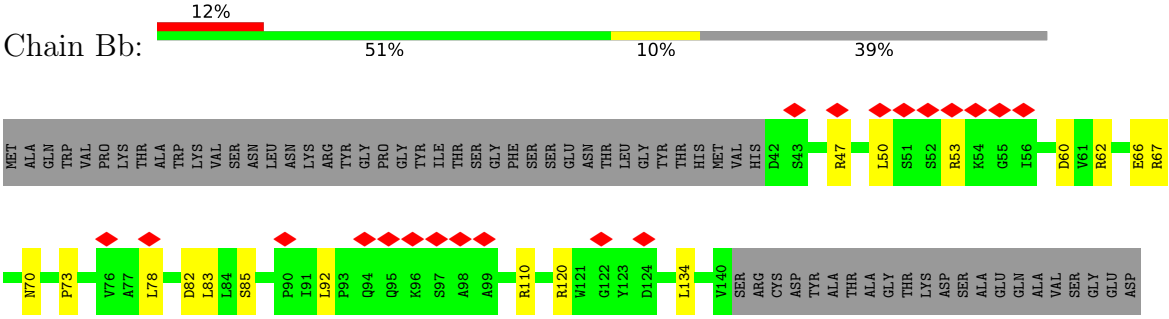
• Molecule 129: mL93

Chain Ba:



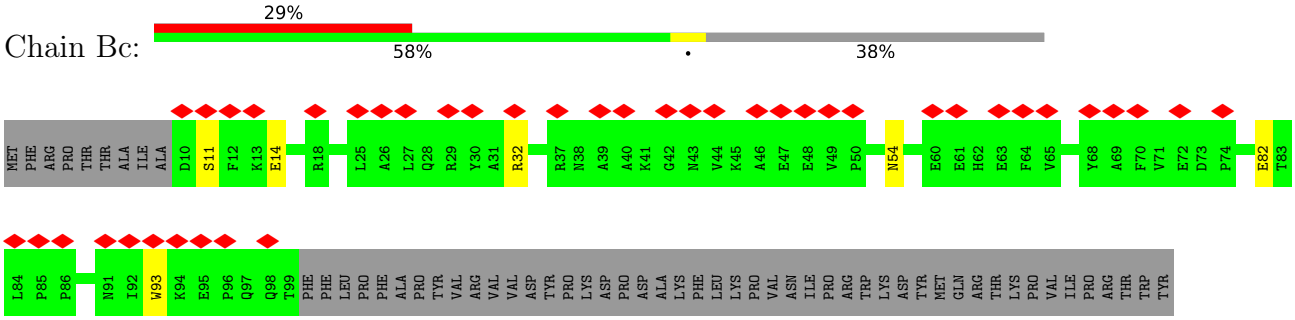
• Molecule 130: mL94

Chain Bb:



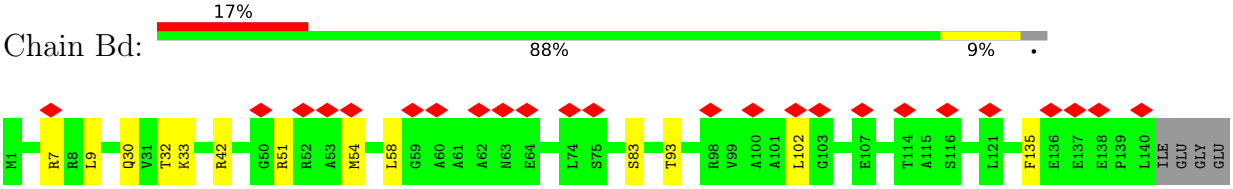
• Molecule 131: mL95

Chain Bc:



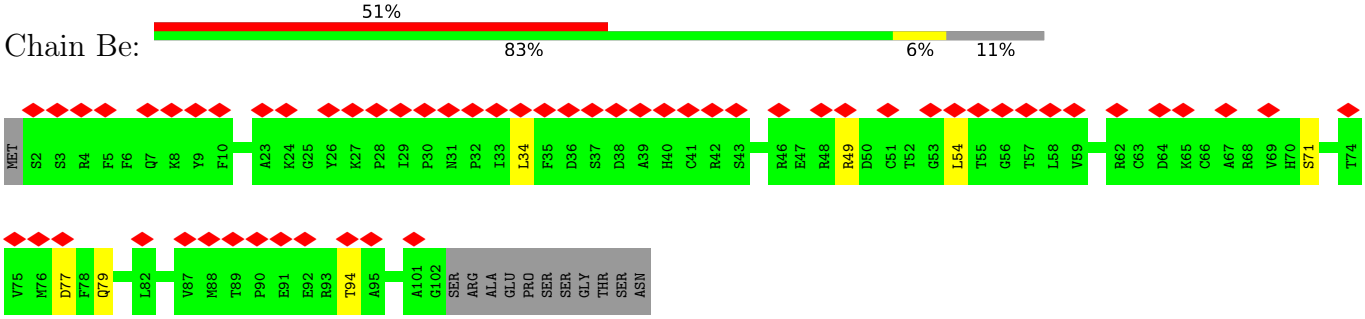
• Molecule 132: mL96

Chain Bd:



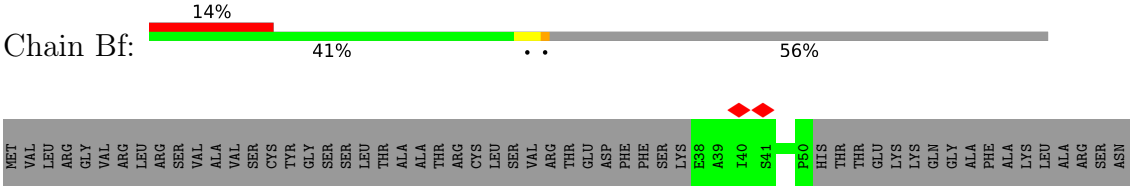
• Molecule 133: mL97

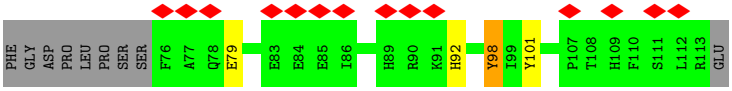
Chain Be:



• Molecule 134: mL98

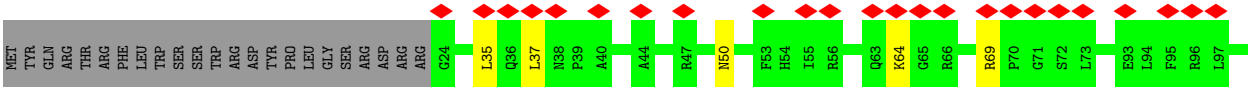
Chain Bf:

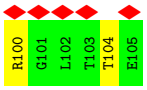




• Molecule 135: mL99

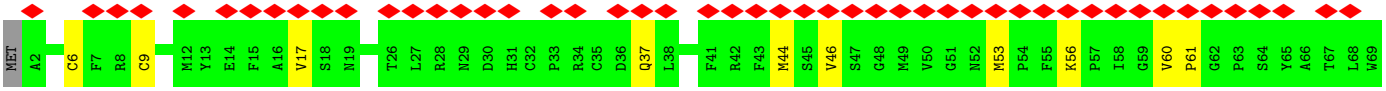
Chain Bg:

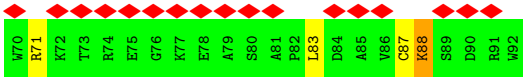




• Molecule 136: mL100

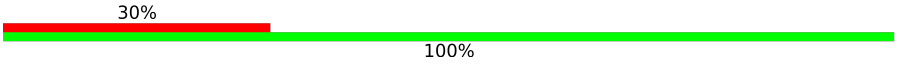
Chain Bh:

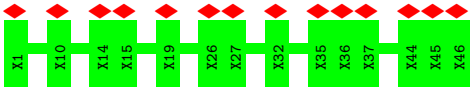




• Molecule 137: UNK

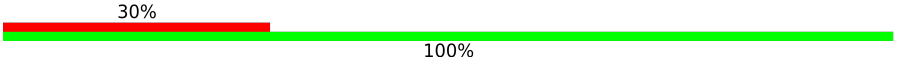
Chain UA:

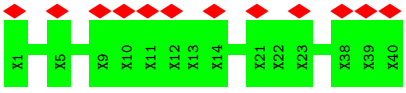




• Molecule 138: UNK

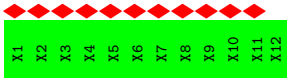
Chain UB:





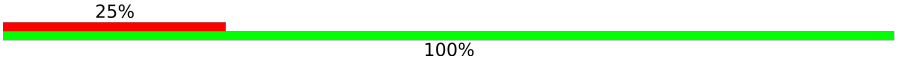
• Molecule 139: UNK

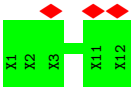
Chain UC:



• Molecule 139: UNK

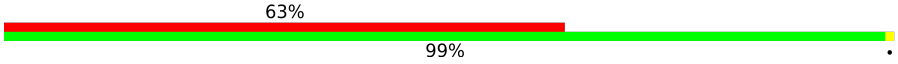
Chain UH:

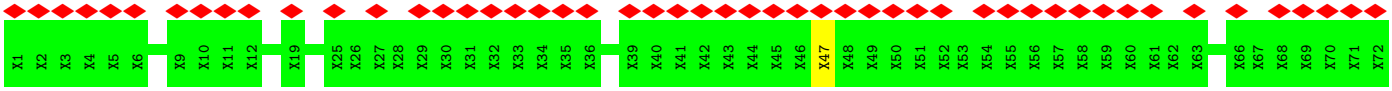


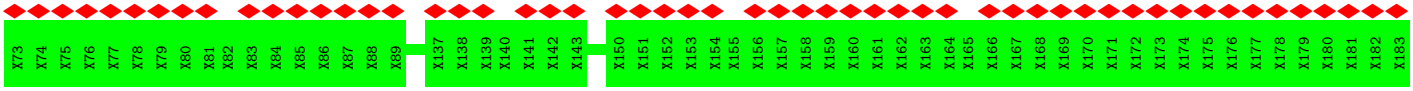


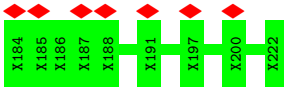
• Molecule 140: UNK

Chain UD:



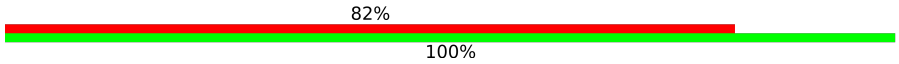


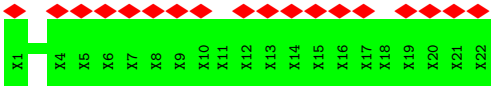




• Molecule 141: UNK

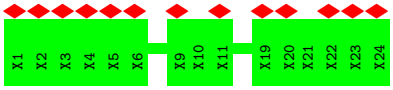
Chain UE:





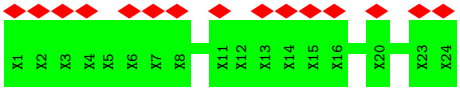
• Molecule 142: UNK

Chain UF:



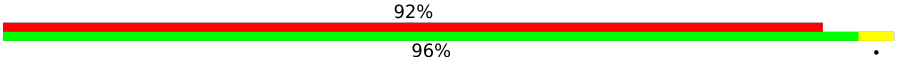
• Molecule 142: UNK

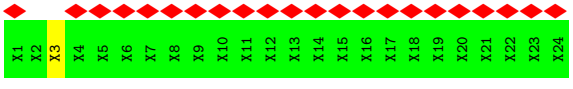
Chain UG:



• Molecule 142: UNK

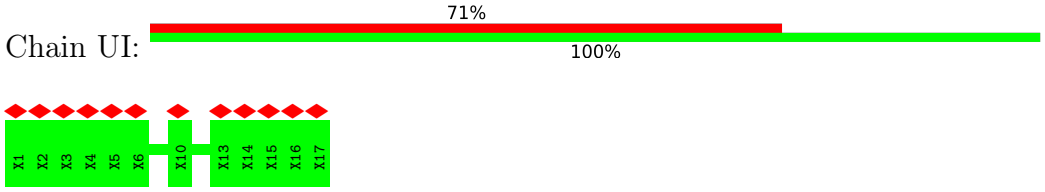
Chain UN:





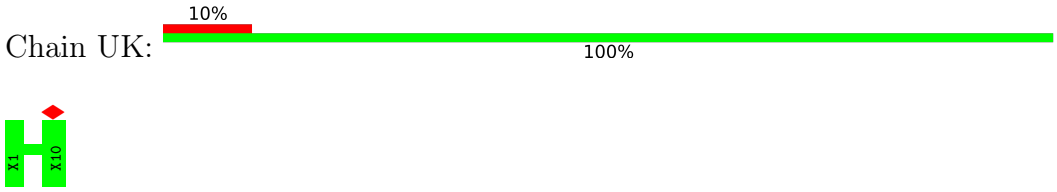
• Molecule 143: UNK

Chain UI:



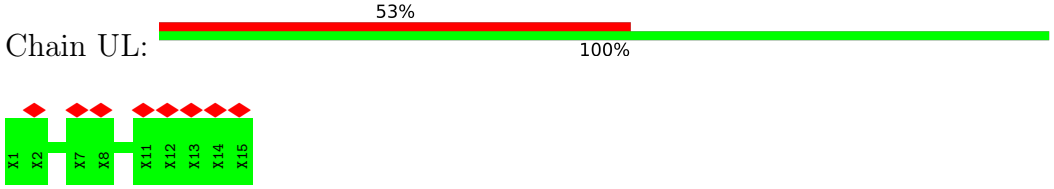
• Molecule 144: UNK

Chain UK:



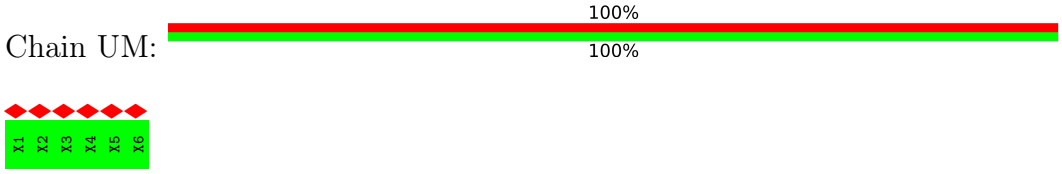
• Molecule 145: UNK

Chain UL:



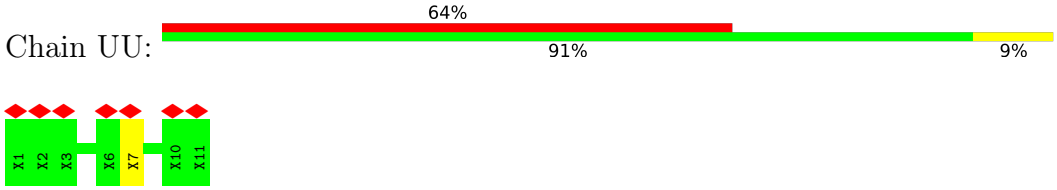
• Molecule 146: UNK

Chain UM:



• Molecule 147: UNK

Chain UU:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.054	Depositor
Map size (Å)	556.0, 556.0, 556.0	wwPDB
Map dimensions	400, 400, 400	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: SPM, MG, ZN, NAD, SPD, GTP, UTP

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	DA	0.38	1/12780 (0.0%)	0.55	3/17297 (0.0%)
2	DD	0.38	0/6710	0.56	1/9087 (0.0%)
3	DI	0.37	0/3248	0.57	2/4401 (0.0%)
4	DL	0.43	0/2346	0.59	0/3164
5	DM	0.39	0/2488	0.55	0/3362
6	DN	0.40	0/2148	0.59	0/2916
7	DO	0.38	0/1840	0.56	0/2482
8	DP	0.52	1/1813 (0.1%)	0.56	0/2457
9	DQ	0.37	0/2111	0.56	0/2863
10	DR	0.36	0/2090	0.56	0/2849
11	DS	0.36	0/1950	0.52	0/2633
12	DU	0.37	0/1799	0.54	0/2438
13	DZ	0.38	0/725	0.55	0/984
14	Da	0.40	0/520	0.54	0/694
15	DB	0.44	0/9369	0.62	0/12692
16	DC	0.41	0/8952	0.57	0/12145
17	DE	0.41	0/4955	0.59	0/6708
18	DF	0.43	0/4856	0.62	2/6581 (0.0%)
19	DG	0.40	0/4674	0.58	0/6333
20	DH	0.46	0/4684	0.62	2/6347 (0.0%)
21	DJ	0.46	0/2649	0.65	0/3598
22	DK	0.45	0/2045	0.59	0/2759
23	DT	0.50	0/2133	0.66	0/2889
24	DV	0.47	0/1382	0.66	1/1871 (0.1%)
25	DW	0.41	0/1407	0.55	0/1916
26	DX	0.45	0/1231	0.66	1/1654 (0.1%)
27	DY	0.50	0/1334	0.63	0/1810
28	CC	0.50	0/666	0.72	0/900
29	CE	0.41	0/3484	0.56	0/4708
30	CF	0.38	0/1319	0.54	0/1783
31	CH	0.42	0/2276	0.55	0/3071
32	CI	0.42	0/3453	0.59	1/4655 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	CJ	0.52	1/6705 (0.0%)	0.65	0/9124
34	CK	0.38	0/2472	0.57	1/3315 (0.0%)
35	CL	0.42	0/759	0.55	0/1026
36	CN	0.50	0/1361	0.67	0/1840
37	CO	0.38	0/3085	0.54	0/4165
38	CP	0.42	0/1533	0.57	0/2074
39	CQ	0.46	0/1631	0.59	0/2203
40	CR	0.39	0/2640	0.55	0/3572
41	CS	0.45	0/1209	0.64	0/1626
42	CU	0.38	0/1576	0.52	0/2115
43	CZ	0.39	0/1237	0.54	1/1659 (0.1%)
44	Ca	0.40	0/5159	0.55	3/6980 (0.0%)
45	Cb	0.40	0/2105	0.54	0/2842
46	Cd	0.40	0/2446	0.51	0/3299
47	Cg	0.46	0/4025	0.63	0/5467
48	Ci	0.49	0/1388	0.73	1/1878 (0.1%)
49	Cj	0.35	0/1842	0.55	0/2511
50	Ck	0.42	0/5696	0.61	2/7705 (0.0%)
51	Cm	0.42	0/1616	0.60	1/2175 (0.0%)
52	Cn	0.41	0/934	0.57	0/1248
53	Cp	0.36	0/1528	0.51	0/2072
54	Cq	0.40	0/2066	0.54	0/2815
55	Cr	0.36	0/2038	0.56	3/2759 (0.1%)
56	Cv	0.37	0/8780	0.55	0/11901
57	CA	0.54	1/14680 (0.0%)	1.00	27/22831 (0.1%)
64	A0	0.34	0/1297	0.52	0/1750
65	A1	0.39	0/1828	0.60	2/2466 (0.1%)
66	A2	0.36	0/3740	0.56	0/5094
67	A3	0.41	0/1241	0.58	0/1674
68	A4	0.33	0/1423	0.55	1/1924 (0.1%)
69	A5	0.38	0/498	0.54	0/663
70	A6	0.36	0/578	0.52	0/774
71	A8	0.41	0/1230	0.62	0/1645
72	A9	0.36	0/474	0.52	0/639
73	AE	0.41	0/2469	0.57	2/3364 (0.1%)
74	AF	0.41	0/3706	0.58	0/5029
75	AI	0.36	0/1850	0.59	0/2515
76	AJ	0.33	0/986	0.52	1/1339 (0.1%)
77	AK	0.33	0/2745	0.55	0/3705
78	AN	0.42	0/1561	0.55	0/2123
79	AP	0.39	0/2993	0.60	1/4060 (0.0%)
80	AQ	0.35	0/1046	0.51	0/1415
81	AR	0.39	0/1969	0.58	0/2656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
82	AT	0.35	0/292	0.51	0/390
83	AU	0.38	0/1456	0.54	0/1971
84	AV	0.41	0/1453	0.59	0/1970
85	AW	0.40	0/2291	0.58	0/3097
86	AX	0.37	0/1462	0.55	0/1986
87	AY	0.35	0/2763	0.55	1/3739 (0.0%)
88	Ab	0.36	0/3651	0.55	0/4988
89	Ad	0.33	0/2171	0.50	0/2930
90	Ae	0.36	0/960	0.58	0/1304
91	Af	0.35	0/1037	0.57	1/1406 (0.1%)
92	Ag	0.37	0/2253	0.55	0/3046
93	Aj	0.30	0/2306	0.50	0/3136
94	Al	0.40	0/1665	0.58	1/2270 (0.0%)
95	Ao	0.37	0/1523	0.55	0/2070
96	Ap	0.34	0/2213	0.55	0/3007
97	At	0.36	0/1128	0.54	0/1532
98	Av	0.37	0/1839	0.53	0/2478
99	AB	0.30	0/279	0.42	0/389
100	AC	0.30	0/139	0.31	0/193
100	AD	0.38	0/139	0.29	0/193
101	AG	0.35	0/134	0.30	0/186
102	AA	0.46	0/13972	0.93	20/21705 (0.1%)
103	BA	0.36	0/5501	0.57	1/7463 (0.0%)
104	BB	0.33	0/3122	0.51	0/4222
105	BC	0.39	0/3919	0.60	1/5318 (0.0%)
106	BD	0.34	0/2062	0.66	18/2872 (0.6%)
107	BE	0.36	0/3184	0.56	2/4308 (0.0%)
108	BF	0.40	0/2900	0.58	1/3909 (0.0%)
109	BG	0.31	0/2561	0.53	0/3469
110	BH	0.34	0/1778	0.51	0/2423
111	BI	0.36	0/2685	0.57	0/3633
112	BJ	0.31	0/1366	0.53	0/1846
113	BK	0.33	0/2040	0.50	0/2757
114	BL	0.36	0/1924	0.56	1/2596 (0.0%)
115	BM	0.35	0/2082	0.59	0/2830
116	BN	0.33	0/1787	0.51	0/2415
117	BO	0.32	0/1160	0.51	0/1565
118	BP	0.34	0/1593	0.59	1/2166 (0.0%)
119	BQ	0.40	0/1716	0.62	0/2324
120	BR	0.38	0/1693	0.63	0/2284
121	BS	0.32	0/801	0.52	0/1090
122	BT	0.36	0/1417	0.58	0/1907
123	BU	0.33	0/711	0.50	0/955

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
124	BV	0.33	0/1340	0.49	0/1802
125	BW	0.42	0/1604	0.57	0/2167
126	BX	0.29	0/897	0.52	0/1215
127	BY	0.31	0/908	0.51	0/1231
128	BZ	0.34	0/1416	0.53	0/1919
129	Ba	0.45	1/1267 (0.1%)	0.58	0/1711
130	Bb	0.33	0/785	0.60	0/1063
131	Bc	0.36	0/805	0.50	0/1091
132	Bd	0.33	0/1133	0.53	0/1528
133	Be	0.33	0/844	0.55	0/1139
134	Bf	0.38	0/450	0.64	0/609
135	Bg	0.34	0/671	0.56	0/905
136	Bh	0.33	0/752	0.55	0/1015
All	All	0.41	5/317582 (0.0%)	0.62	107/435817 (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
1	DA	0	1
2	DD	0	2
4	DL	0	2
6	DN	0	2
7	DO	0	2
10	DR	0	1
15	DB	0	2
16	DC	0	2
19	DG	0	2
21	DJ	0	1
23	DT	0	1
26	DX	0	1
31	CH	0	1
33	CJ	0	1
44	Ca	0	1
47	Cg	0	1
48	Ci	0	1
49	Cj	0	1
50	Ck	0	1
56	Cv	0	2
66	A2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	A3	0	1
71	A8	0	2
73	AE	0	1
74	AF	0	3
81	AR	0	3
83	AU	0	1
84	AV	0	1
85	AW	0	1
87	AY	0	2
88	Ab	0	1
98	Av	0	1
104	BB	0	1
105	BC	0	1
107	BE	0	2
108	BF	0	1
109	BG	0	1
110	BH	0	1
113	BK	0	2
115	BM	0	2
116	BN	0	3
117	BO	0	1
118	BP	0	2
120	BR	0	2
130	Bb	0	2
134	Bf	0	2
136	Bh	0	2
140	UD	0	1
142	UN	0	1
147	UU	0	1
All	All	0	75

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	CJ	424	HIS	CG-CD2	-8.17	1.21	1.35
1	DA	323	HIS	CG-CD2	6.74	1.47	1.35
57	CA	310	A	N9-C4	5.67	1.41	1.37
129	Ba	108	CYS	CB-SG	-5.53	1.72	1.81
8	DP	210	GLU	CD-OE2	5.46	1.31	1.25

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
105	BC	302	GLY	N-CA-C	-8.48	91.90	113.10
34	CK	283	GLY	N-CA-C	7.77	132.53	113.10
57	CA	451	U	C2-N1-C1'	7.44	126.63	117.70
102	AA	1112	U	N3-C2-O2	-7.42	117.01	122.20
102	AA	516	U	C2-N1-C1'	7.37	126.54	117.70

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DA	166	TYR	Peptide
2	DD	248	ASP	Peptide
2	DD	255	VAL	Peptide
4	DL	269	MET	Peptide
4	DL	270	THR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	DA	1551/1788 (87%)	1498 (97%)	50 (3%)	3 (0%)	47 81
2	DD	787/812 (97%)	747 (95%)	38 (5%)	2 (0%)	41 77
3	DI	388/407 (95%)	366 (94%)	21 (5%)	1 (0%)	41 77
4	DL	279/307 (91%)	263 (94%)	16 (6%)	0	100 100
5	DM	292/294 (99%)	283 (97%)	9 (3%)	0	100 100
6	DN	253/293 (86%)	242 (96%)	11 (4%)	0	100 100
7	DO	220/282 (78%)	213 (97%)	6 (3%)	1 (0%)	29 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	DP	205/274 (75%)	195 (95%)	9 (4%)	1 (0%)	29	69
9	DQ	254/268 (95%)	246 (97%)	6 (2%)	2 (1%)	19	60
10	DR	247/270 (92%)	239 (97%)	8 (3%)	0	100	100
11	DS	234/261 (90%)	227 (97%)	7 (3%)	0	100	100
12	DU	211/228 (92%)	202 (96%)	7 (3%)	2 (1%)	17	57
13	DZ	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
14	Da	53/64 (83%)	52 (98%)	1 (2%)	0	100	100
15	DB	1109/1181 (94%)	1078 (97%)	29 (3%)	2 (0%)	47	81
16	DC	1087/1165 (93%)	1052 (97%)	34 (3%)	1 (0%)	51	86
17	DE	576/746 (77%)	564 (98%)	11 (2%)	1 (0%)	47	81
18	DF	586/666 (88%)	569 (97%)	16 (3%)	1 (0%)	47	81
19	DG	558/631 (88%)	543 (97%)	14 (2%)	1 (0%)	47	81
20	DH	560/581 (96%)	540 (96%)	20 (4%)	0	100	100
21	DJ	313/396 (79%)	304 (97%)	8 (3%)	1 (0%)	41	77
22	DK	249/324 (77%)	240 (96%)	9 (4%)	0	100	100
23	DT	237/247 (96%)	233 (98%)	4 (2%)	0	100	100
24	DV	158/183 (86%)	151 (96%)	6 (4%)	1 (1%)	25	66
25	DW	159/179 (89%)	153 (96%)	6 (4%)	0	100	100
26	DX	139/169 (82%)	133 (96%)	6 (4%)	0	100	100
27	DY	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
28	CC	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
29	CE	413/435 (95%)	395 (96%)	18 (4%)	0	100	100
30	CF	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
31	CH	271/282 (96%)	265 (98%)	5 (2%)	1 (0%)	34	72
32	CI	418/443 (94%)	406 (97%)	12 (3%)	0	100	100
33	CJ	796/817 (97%)	765 (96%)	30 (4%)	1 (0%)	51	86
34	CK	287/326 (88%)	272 (95%)	15 (5%)	0	100	100
35	CL	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
36	CN	155/166 (93%)	150 (97%)	5 (3%)	0	100	100
37	CO	359/429 (84%)	343 (96%)	14 (4%)	2 (1%)	25	66
38	CP	178/188 (95%)	171 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CQ	188/307 (61%)	182 (97%)	6 (3%)	0	100	100
40	CR	312/320 (98%)	301 (96%)	11 (4%)	0	100	100
41	CS	140/244 (57%)	135 (96%)	5 (4%)	0	100	100
42	CU	182/193 (94%)	177 (97%)	4 (2%)	1 (0%)	29	69
43	CZ	149/360 (41%)	142 (95%)	6 (4%)	1 (1%)	22	63
44	Ca	590/602 (98%)	556 (94%)	29 (5%)	5 (1%)	19	60
45	Cb	248/324 (76%)	242 (98%)	6 (2%)	0	100	100
46	Cd	289/440 (66%)	281 (97%)	6 (2%)	2 (1%)	22	63
47	Cg	480/498 (96%)	461 (96%)	19 (4%)	0	100	100
48	Ci	163/181 (90%)	155 (95%)	8 (5%)	0	100	100
49	Cj	224/257 (87%)	216 (96%)	7 (3%)	1 (0%)	34	72
50	Ck	699/874 (80%)	671 (96%)	26 (4%)	2 (0%)	41	77
51	Cm	194/215 (90%)	184 (95%)	10 (5%)	0	100	100
52	Cn	108/250 (43%)	103 (95%)	5 (5%)	0	100	100
53	Cp	173/187 (92%)	169 (98%)	4 (2%)	0	100	100
54	Cq	250/263 (95%)	243 (97%)	7 (3%)	0	100	100
55	Cr	253/439 (58%)	243 (96%)	9 (4%)	1 (0%)	34	72
56	Cv	1051/1211 (87%)	1011 (96%)	40 (4%)	0	100	100
64	A0	147/185 (80%)	142 (97%)	4 (3%)	1 (1%)	22	63
65	A1	215/241 (89%)	209 (97%)	6 (3%)	0	100	100
66	A2	445/471 (94%)	433 (97%)	9 (2%)	3 (1%)	22	63
67	A3	148/218 (68%)	145 (98%)	3 (2%)	0	100	100
68	A4	166/183 (91%)	156 (94%)	10 (6%)	0	100	100
69	A5	53/80 (66%)	51 (96%)	2 (4%)	0	100	100
70	A6	70/114 (61%)	70 (100%)	0	0	100	100
71	A8	139/181 (77%)	128 (92%)	11 (8%)	0	100	100
72	A9	51/184 (28%)	48 (94%)	3 (6%)	0	100	100
73	AE	289/473 (61%)	278 (96%)	11 (4%)	0	100	100
74	AF	440/459 (96%)	417 (95%)	22 (5%)	1 (0%)	47	81
75	AI	210/263 (80%)	199 (95%)	11 (5%)	0	100	100
76	AJ	124/177 (70%)	117 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
77	AK	319/342 (93%)	307 (96%)	11 (3%)	1 (0%)	41 77
78	AN	177/202 (88%)	172 (97%)	5 (3%)	0	100 100
79	AP	348/374 (93%)	332 (95%)	14 (4%)	2 (1%)	25 66
80	AQ	121/167 (72%)	118 (98%)	3 (2%)	0	100 100
81	AR	225/301 (75%)	212 (94%)	12 (5%)	1 (0%)	34 72
82	AT	33/144 (23%)	32 (97%)	1 (3%)	0	100 100
83	AU	171/213 (80%)	168 (98%)	3 (2%)	0	100 100
84	AV	178/188 (95%)	174 (98%)	4 (2%)	0	100 100
85	AW	274/278 (99%)	267 (97%)	6 (2%)	1 (0%)	34 72
86	AX	166/246 (68%)	163 (98%)	3 (2%)	0	100 100
87	AY	338/378 (89%)	326 (96%)	8 (2%)	4 (1%)	13 50
88	Ab	449/507 (89%)	425 (95%)	24 (5%)	0	100 100
89	Ad	255/289 (88%)	251 (98%)	4 (2%)	0	100 100
90	Ae	114/197 (58%)	109 (96%)	5 (4%)	0	100 100
91	Af	124/189 (66%)	119 (96%)	5 (4%)	0	100 100
92	Ag	257/260 (99%)	249 (97%)	8 (3%)	0	100 100
93	Aj	277/296 (94%)	260 (94%)	17 (6%)	0	100 100
94	Al	207/218 (95%)	196 (95%)	11 (5%)	0	100 100
95	Ao	179/259 (69%)	170 (95%)	9 (5%)	0	100 100
96	Ap	259/309 (84%)	248 (96%)	11 (4%)	0	100 100
97	At	136/154 (88%)	129 (95%)	6 (4%)	1 (1%)	22 63
98	Av	211/242 (87%)	203 (96%)	6 (3%)	2 (1%)	17 57
99	AB	54/56 (96%)	48 (89%)	6 (11%)	0	100 100
100	AC	26/28 (93%)	26 (100%)	0	0	100 100
100	AD	26/28 (93%)	25 (96%)	1 (4%)	0	100 100
101	AG	25/27 (93%)	25 (100%)	0	0	100 100
103	BA	675/831 (81%)	654 (97%)	21 (3%)	0	100 100
104	BB	387/541 (72%)	369 (95%)	17 (4%)	1 (0%)	41 77
105	BC	476/523 (91%)	451 (95%)	23 (5%)	2 (0%)	34 72
106	BD	415/547 (76%)	385 (93%)	22 (5%)	8 (2%)	8 38
107	BE	386/449 (86%)	362 (94%)	22 (6%)	2 (0%)	29 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
108	BF	341/426 (80%)	330 (97%)	10 (3%)	1 (0%)	41 77
109	BG	317/378 (84%)	292 (92%)	25 (8%)	0	100 100
110	BH	209/349 (60%)	203 (97%)	6 (3%)	0	100 100
111	BI	317/343 (92%)	302 (95%)	14 (4%)	1 (0%)	41 77
112	BJ	164/333 (49%)	157 (96%)	7 (4%)	0	100 100
113	BK	252/386 (65%)	241 (96%)	11 (4%)	0	100 100
114	BL	226/312 (72%)	221 (98%)	5 (2%)	0	100 100
115	BM	243/283 (86%)	227 (93%)	15 (6%)	1 (0%)	34 72
116	BN	212/302 (70%)	203 (96%)	9 (4%)	0	100 100
117	BO	143/262 (55%)	135 (94%)	7 (5%)	1 (1%)	22 63
118	BP	200/266 (75%)	190 (95%)	8 (4%)	2 (1%)	15 55
119	BQ	214/231 (93%)	201 (94%)	13 (6%)	0	100 100
120	BR	193/205 (94%)	181 (94%)	11 (6%)	1 (0%)	29 69
121	BS	95/160 (59%)	92 (97%)	3 (3%)	0	100 100
122	BT	166/191 (87%)	160 (96%)	6 (4%)	0	100 100
123	BU	80/185 (43%)	79 (99%)	1 (1%)	0	100 100
124	BV	153/190 (80%)	145 (95%)	7 (5%)	1 (1%)	22 63
125	BW	185/188 (98%)	177 (96%)	8 (4%)	0	100 100
126	BX	103/190 (54%)	93 (90%)	9 (9%)	1 (1%)	15 55
127	BY	100/172 (58%)	91 (91%)	8 (8%)	1 (1%)	15 55
128	BZ	188/190 (99%)	180 (96%)	8 (4%)	0	100 100
129	Ba	137/139 (99%)	132 (96%)	5 (4%)	0	100 100
130	Bb	97/162 (60%)	90 (93%)	7 (7%)	0	100 100
131	Bc	88/146 (60%)	85 (97%)	3 (3%)	0	100 100
132	Bd	138/144 (96%)	133 (96%)	5 (4%)	0	100 100
133	Be	99/113 (88%)	99 (100%)	0	0	100 100
134	Bf	46/113 (41%)	42 (91%)	3 (6%)	1 (2%)	6 35
135	Bg	80/105 (76%)	71 (89%)	9 (11%)	0	100 100
136	Bh	89/92 (97%)	84 (94%)	4 (4%)	1 (1%)	14 52
All	All	34481/41413 (83%)	33099 (96%)	1303 (4%)	79 (0%)	50 81

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DA	1188	GLU
21	DJ	36	GLN
43	CZ	296	PRO
44	Ca	32	PRO
44	Ca	33	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	1322/1514 (87%)	1229 (93%)	93 (7%)	15	40
2	DD	694/711 (98%)	652 (94%)	42 (6%)	18	44
3	DI	350/365 (96%)	328 (94%)	22 (6%)	18	43
4	DL	241/263 (92%)	226 (94%)	15 (6%)	18	43
5	DM	252/252 (100%)	233 (92%)	19 (8%)	13	38
6	DN	229/256 (90%)	215 (94%)	14 (6%)	18	44
7	DO	186/229 (81%)	174 (94%)	12 (6%)	17	42
8	DP	187/239 (78%)	178 (95%)	9 (5%)	25	51
9	DQ	228/239 (95%)	220 (96%)	8 (4%)	36	59
10	DR	220/235 (94%)	200 (91%)	20 (9%)	9	29
11	DS	209/228 (92%)	197 (94%)	12 (6%)	20	45
12	DU	190/201 (94%)	174 (92%)	16 (8%)	11	33
13	DZ	72/84 (86%)	69 (96%)	3 (4%)	30	54
14	Da	50/59 (85%)	46 (92%)	4 (8%)	12	35
15	DB	976/1030 (95%)	875 (90%)	101 (10%)	7	25
16	DC	927/985 (94%)	808 (87%)	119 (13%)	4	18
17	DE	519/641 (81%)	464 (89%)	55 (11%)	6	24
18	DF	500/560 (89%)	443 (89%)	57 (11%)	5	21
19	DG	490/543 (90%)	426 (87%)	64 (13%)	4	18
20	DH	493/504 (98%)	434 (88%)	59 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	DJ	275/347 (79%)	244 (89%)	31 (11%)	6 21
22	DK	209/261 (80%)	192 (92%)	17 (8%)	11 35
23	DT	220/228 (96%)	195 (89%)	25 (11%)	5 21
24	DV	145/165 (88%)	127 (88%)	18 (12%)	4 19
25	DW	148/163 (91%)	136 (92%)	12 (8%)	11 35
26	DX	124/149 (83%)	111 (90%)	13 (10%)	7 24
27	DY	137/146 (94%)	118 (86%)	19 (14%)	3 17
28	CC	73/73 (100%)	62 (85%)	11 (15%)	3 14
29	CE	358/372 (96%)	317 (88%)	41 (12%)	5 21
30	CF	136/144 (94%)	129 (95%)	7 (5%)	24 48
31	CH	237/246 (96%)	215 (91%)	22 (9%)	9 28
32	CI	357/371 (96%)	324 (91%)	33 (9%)	9 29
33	CJ	709/723 (98%)	628 (89%)	81 (11%)	5 21
34	CK	257/283 (91%)	233 (91%)	24 (9%)	9 28
35	CL	79/79 (100%)	70 (89%)	9 (11%)	5 21
36	CN	142/150 (95%)	122 (86%)	20 (14%)	3 16
37	CO	318/377 (84%)	293 (92%)	25 (8%)	12 35
38	CP	160/168 (95%)	147 (92%)	13 (8%)	11 35
39	CQ	171/270 (63%)	151 (88%)	20 (12%)	5 21
40	CR	275/279 (99%)	258 (94%)	17 (6%)	18 43
41	CS	126/220 (57%)	114 (90%)	12 (10%)	8 27
42	CU	160/169 (95%)	151 (94%)	9 (6%)	21 46
43	CZ	121/313 (39%)	111 (92%)	10 (8%)	11 34
44	Ca	516/543 (95%)	473 (92%)	43 (8%)	11 34
45	Cb	219/277 (79%)	203 (93%)	16 (7%)	14 39
46	Cd	240/381 (63%)	219 (91%)	21 (9%)	10 31
47	Cg	424/437 (97%)	380 (90%)	44 (10%)	7 24
48	Ci	144/160 (90%)	124 (86%)	20 (14%)	3 17
49	Cj	193/219 (88%)	179 (93%)	14 (7%)	14 39
50	Ck	608/747 (81%)	549 (90%)	59 (10%)	8 27
51	Cm	165/184 (90%)	140 (85%)	25 (15%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	Cn	95/210 (45%)	89 (94%)	6 (6%)	18	43
53	Cp	163/175 (93%)	151 (93%)	12 (7%)	13	38
54	Cq	210/221 (95%)	193 (92%)	17 (8%)	11	35
55	Cr	211/369 (57%)	190 (90%)	21 (10%)	7	26
56	Cv	912/1034 (88%)	844 (92%)	68 (8%)	13	38
64	A0	140/167 (84%)	126 (90%)	14 (10%)	7	26
65	A1	195/217 (90%)	168 (86%)	27 (14%)	3	17
66	A2	394/413 (95%)	353 (90%)	41 (10%)	7	24
67	A3	131/193 (68%)	121 (92%)	10 (8%)	13	37
68	A4	153/164 (93%)	142 (93%)	11 (7%)	14	39
69	A5	52/73 (71%)	47 (90%)	5 (10%)	8	27
70	A6	61/99 (62%)	52 (85%)	9 (15%)	3	15
71	A8	126/161 (78%)	108 (86%)	18 (14%)	3	16
72	A9	51/166 (31%)	43 (84%)	8 (16%)	2	14
73	AE	258/406 (64%)	233 (90%)	25 (10%)	8	27
74	AF	394/409 (96%)	367 (93%)	27 (7%)	15	40
75	AI	192/233 (82%)	171 (89%)	21 (11%)	6	23
76	AJ	90/151 (60%)	81 (90%)	9 (10%)	7	26
77	AK	287/301 (95%)	248 (86%)	39 (14%)	3	17
78	AN	160/182 (88%)	148 (92%)	12 (8%)	13	38
79	AP	310/330 (94%)	272 (88%)	38 (12%)	4	19
80	AQ	106/141 (75%)	102 (96%)	4 (4%)	33	57
81	AR	198/256 (77%)	187 (94%)	11 (6%)	21	46
82	AT	28/124 (23%)	25 (89%)	3 (11%)	6	23
83	AU	151/184 (82%)	134 (89%)	17 (11%)	6	21
84	AV	153/158 (97%)	136 (89%)	17 (11%)	6	22
85	AW	244/246 (99%)	215 (88%)	29 (12%)	5	20
86	AX	156/221 (71%)	148 (95%)	8 (5%)	24	48
87	AY	283/337 (84%)	257 (91%)	26 (9%)	9	29
88	Ab	373/451 (83%)	343 (92%)	30 (8%)	12	35
89	Ad	225/250 (90%)	200 (89%)	25 (11%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
90	Ae	100/172 (58%)	90 (90%)	10 (10%)	7	26
91	Af	111/162 (68%)	99 (89%)	12 (11%)	6	23
92	Ag	238/239 (100%)	221 (93%)	17 (7%)	14	39
93	Aj	237/260 (91%)	226 (95%)	11 (5%)	27	52
94	Al	170/186 (91%)	154 (91%)	16 (9%)	8	28
95	Ao	153/216 (71%)	135 (88%)	18 (12%)	5	20
96	Ap	227/267 (85%)	203 (89%)	24 (11%)	6	24
97	At	116/140 (83%)	101 (87%)	15 (13%)	4	18
98	Av	187/210 (89%)	169 (90%)	18 (10%)	8	27
103	BA	598/727 (82%)	542 (91%)	56 (9%)	8	28
104	BB	351/484 (72%)	318 (91%)	33 (9%)	8	28
105	BC	406/443 (92%)	359 (88%)	47 (12%)	5	21
107	BE	334/386 (86%)	309 (92%)	25 (8%)	13	38
108	BF	299/368 (81%)	269 (90%)	30 (10%)	7	26
109	BG	266/310 (86%)	241 (91%)	25 (9%)	8	28
110	BH	182/297 (61%)	160 (88%)	22 (12%)	5	20
111	BI	268/288 (93%)	245 (91%)	23 (9%)	10	32
112	BJ	136/298 (46%)	122 (90%)	14 (10%)	7	25
113	BK	196/344 (57%)	184 (94%)	12 (6%)	18	44
114	BL	201/262 (77%)	181 (90%)	20 (10%)	7	26
115	BM	209/240 (87%)	189 (90%)	20 (10%)	8	27
116	BN	197/273 (72%)	188 (95%)	9 (5%)	27	52
117	BO	129/225 (57%)	118 (92%)	11 (8%)	10	33
118	BP	162/219 (74%)	145 (90%)	17 (10%)	7	24
119	BQ	182/195 (93%)	166 (91%)	16 (9%)	10	31
120	BR	171/181 (94%)	151 (88%)	20 (12%)	5	21
121	BS	85/142 (60%)	77 (91%)	8 (9%)	8	28
122	BT	147/163 (90%)	133 (90%)	14 (10%)	8	27
123	BU	71/168 (42%)	64 (90%)	7 (10%)	8	26
124	BV	138/163 (85%)	130 (94%)	8 (6%)	20	45
125	BW	163/164 (99%)	149 (91%)	14 (9%)	10	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
126	BX	92/170 (54%)	81 (88%)	11 (12%)	5 20
127	BY	89/151 (59%)	81 (91%)	8 (9%)	9 30
128	BZ	143/160 (89%)	136 (95%)	7 (5%)	25 50
129	Ba	131/131 (100%)	115 (88%)	16 (12%)	5 20
130	Bb	84/135 (62%)	69 (82%)	15 (18%)	2 10
131	Bc	82/134 (61%)	76 (93%)	6 (7%)	14 39
132	Bd	117/120 (98%)	104 (89%)	13 (11%)	6 22
133	Be	89/99 (90%)	82 (92%)	7 (8%)	12 35
134	Bf	45/98 (46%)	43 (96%)	2 (4%)	28 53
135	Bg	65/87 (75%)	58 (89%)	7 (11%)	6 23
136	Bh	79/80 (99%)	67 (85%)	12 (15%)	3 14
All	All	29729/35381 (84%)	26950 (91%)	2779 (9%)	12 28

5 of 2779 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
77	AK	286	GLU
104	BB	188	LEU
79	AP	281	GLU
77	AK	261	ASP
89	Ad	261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 652 such sidechains are listed below:

Mol	Chain	Res	Type
84	AV	206	ASN
108	BF	362	HIS
88	Ab	157	HIS
84	AV	168	HIS
96	Ap	253	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
102	AA	581/1179 (49%)	289 (49%)	17 (2%)
57	CA	620/621 (99%)	300 (48%)	8 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1201/1800 (66%)	589 (49%)	25 (2%)

5 of 589 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
57	CA	2	A
57	CA	3	A
57	CA	4	A
57	CA	5	U
57	CA	6	U

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
102	AA	387	A
102	AA	422	A
102	AA	1164	A
102	AA	418	G
102	AA	425	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 56 are monoatomic and 1 is modelled with single atom - leaving 8 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	$\#\|Z\|>2$
154	NAD	Av	301	-	42,48,48	1.96	8 (19%)	50,73,73	1.83	9 (18%)
152	GTP	Cg	501	151	26,34,34	1.26	3 (11%)	32,54,54	1.87	10 (31%)
149	SPD	DL	401	-	9,9,9	0.40	0	8,8,8	1.03	0
149	SPD	CA	736	-	9,9,9	0.49	0	8,8,8	0.49	0
153	SPM	CA	738	-	13,13,13	0.34	0	12,12,12	0.85	0
149	SPD	CA	737	-	9,9,9	0.35	0	8,8,8	0.68	0
150	UTP	DJ	401	-	22,30,30	1.84	6 (27%)	27,47,47	1.25	3 (11%)
149	SPD	CA	735	-	9,9,9	0.40	0	8,8,8	0.58	0

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
154	NAD	Av	301	-	-	7/26/62/62	0/5/5/5
152	GTP	Cg	501	151	-	5/18/38/38	0/3/3/3
149	SPD	DL	401	-	-	2/7/7/7	-
149	SPD	CA	736	-	-	5/7/7/7	-
153	SPM	CA	738	-	-	8/11/11/11	-
149	SPD	CA	737	-	-	3/7/7/7	-
150	UTP	DJ	401	-	-	8/20/38/38	0/2/2/2
149	SPD	CA	735	-	-	5/7/7/7	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
154	Av	301	NAD	C3N-C7N	-7.58	1.39	1.50
154	Av	301	NAD	C2A-N3A	4.54	1.39	1.32
154	Av	301	NAD	C2N-N1N	4.07	1.39	1.35
150	DJ	401	UTP	C6-N1	4.06	1.40	1.35
152	Cg	501	GTP	C5-C6	-3.71	1.39	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
154	Av	301	NAD	N3A-C2A-N1A	-6.53	118.48	128.68
152	Cg	501	GTP	O2G-PG-O3B	4.60	120.05	104.64
154	Av	301	NAD	O4D-C1D-C2D	-4.50	100.35	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
154	Av	301	NAD	C3D-C2D-C1D	-4.31	94.49	100.98
152	Cg	501	GTP	C2-N1-C6	-4.24	117.29	125.10

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

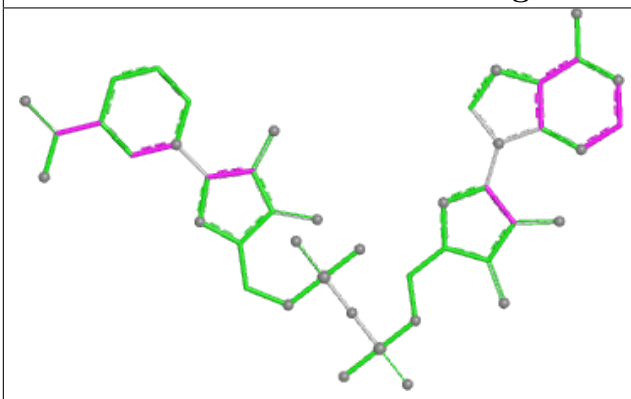
Mol	Chain	Res	Type	Atoms
150	DJ	401	UTP	C5'-O5'-PA-O1A
150	DJ	401	UTP	C5'-O5'-PA-O2A
150	DJ	401	UTP	C5'-O5'-PA-O3A
150	DJ	401	UTP	O4'-C4'-C5'-O5'
150	DJ	401	UTP	O4'-C1'-N1-C6

There are no ring outliers.

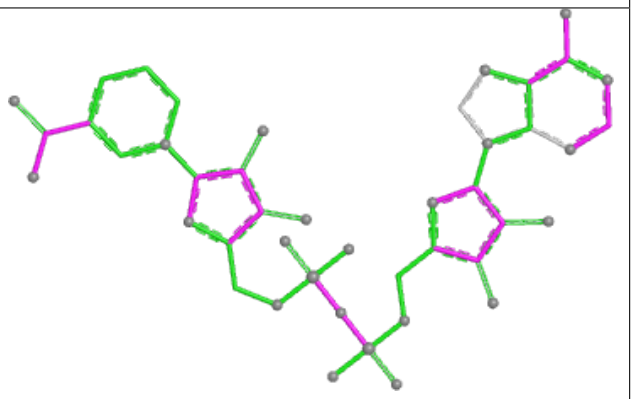
No monomer is involved in short contacts.

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.

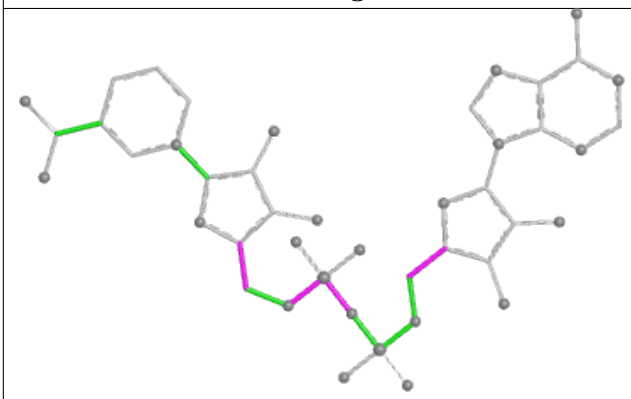
Ligand NAD Av 301



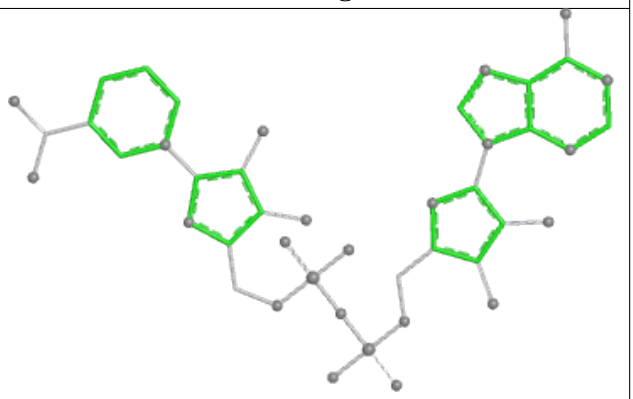
Bond lengths



Bond angles

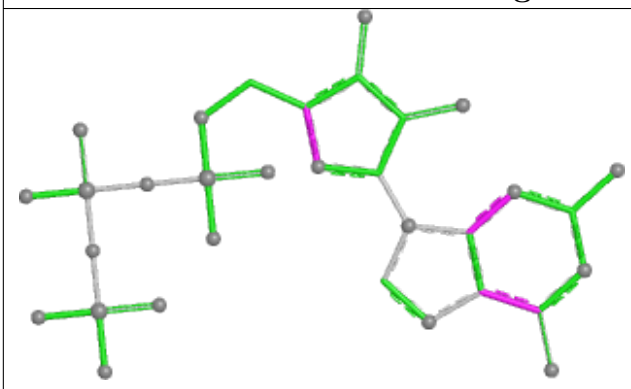


Torsions

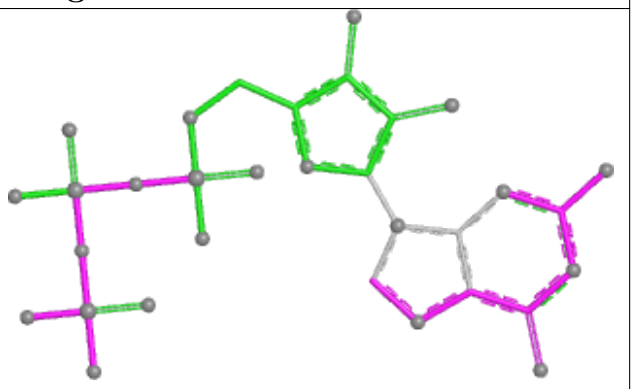


Rings

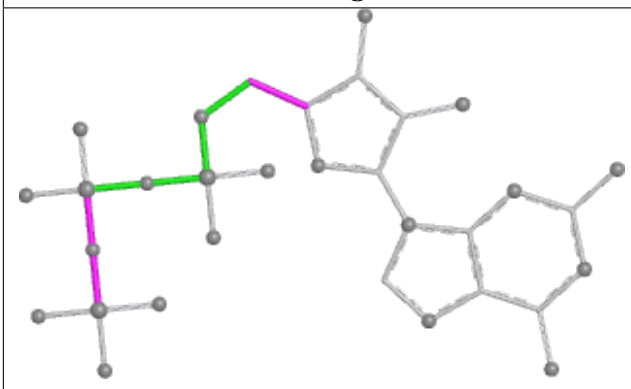
Ligand GTP Cg 501



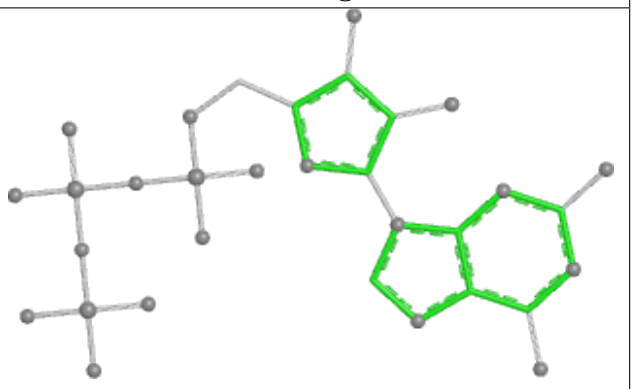
Bond lengths



Bond angles

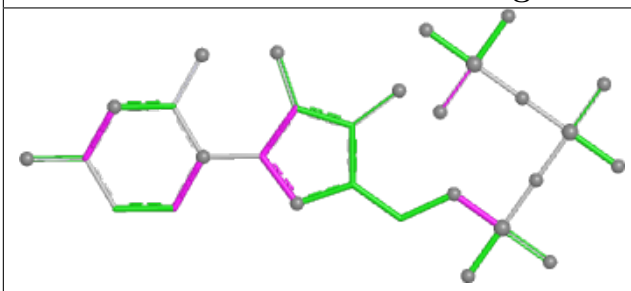


Torsions

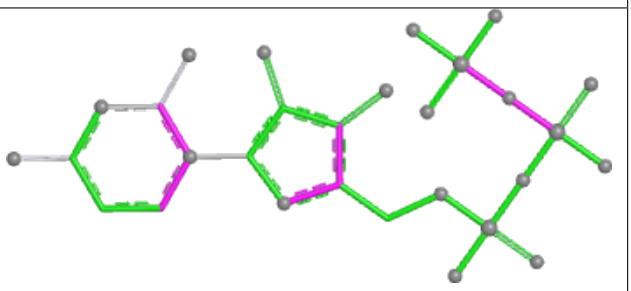


Rings

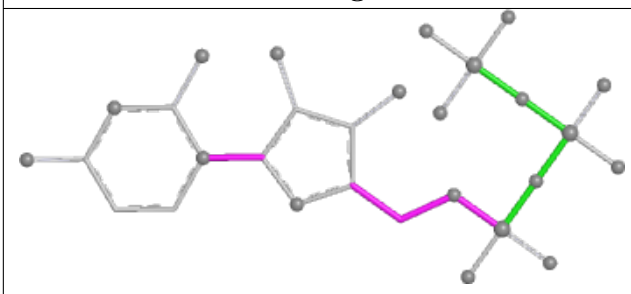
Ligand UTP DJ 401



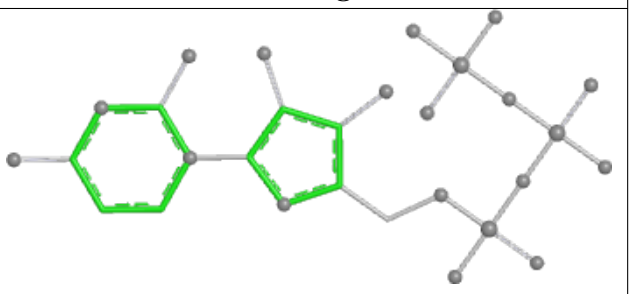
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
140	UD	3
77	AK	1
71	A8	1
84	AV	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UD	90:UNK	C	136:UNK	N	14.38
1	UD	158:UNK	C	159:UNK	N	11.27
1	UD	68:UNK	C	69:UNK	N	10.02
1	AK	250:LEU	C	251:THR	N	5.50
1	A8	40:PRO	C	41:LYS	N	5.26

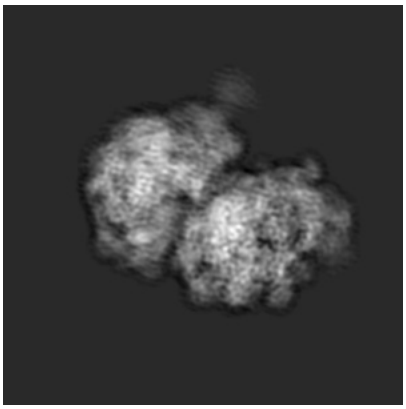
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0229. These allow visual inspection of the internal detail of the map and identification of artifacts.

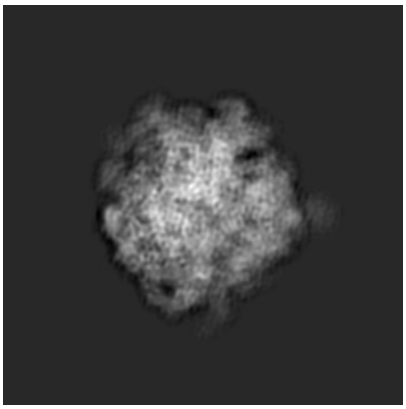
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

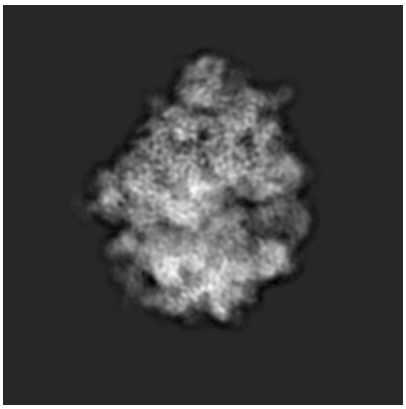
6.1.1 Primary map



X

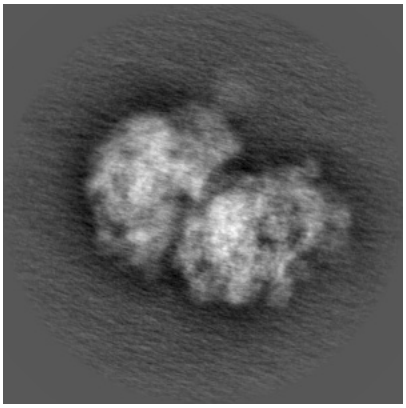


Y

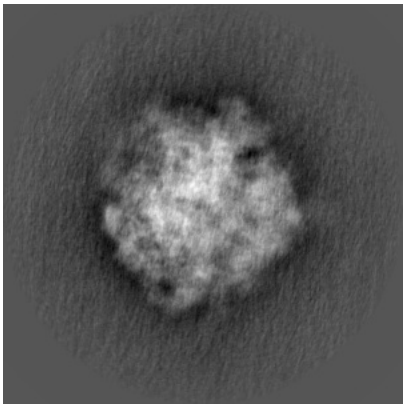


Z

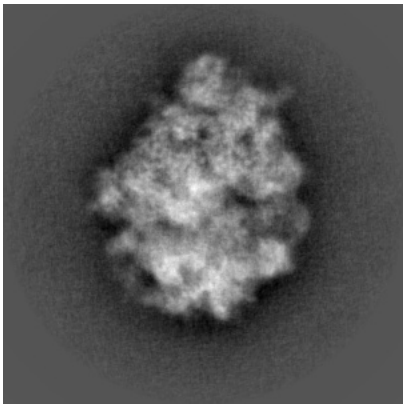
6.1.2 Raw map



X



Y

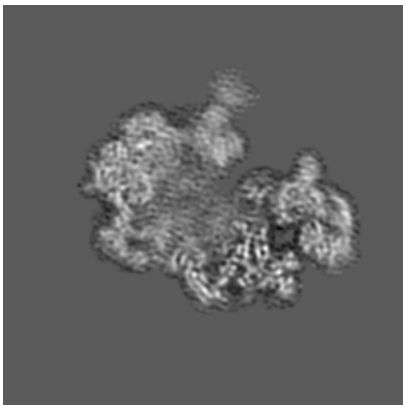


Z

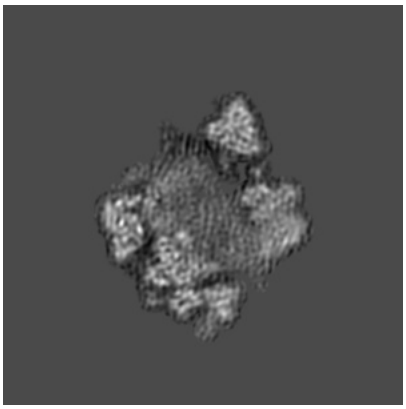
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

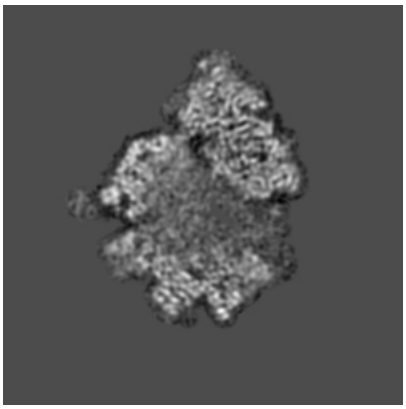
6.2.1 Primary map



X Index: 200

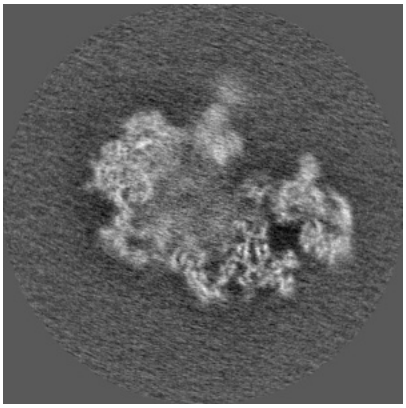


Y Index: 200

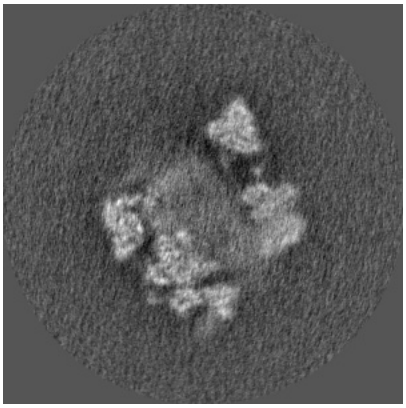


Z Index: 200

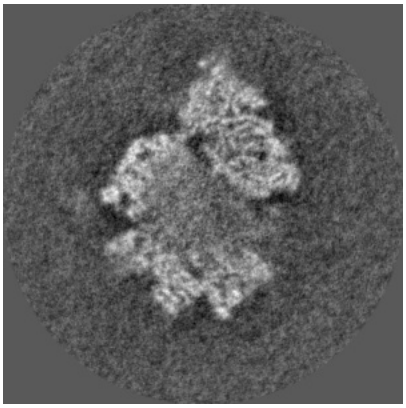
6.2.2 Raw map



X Index: 200



Y Index: 200

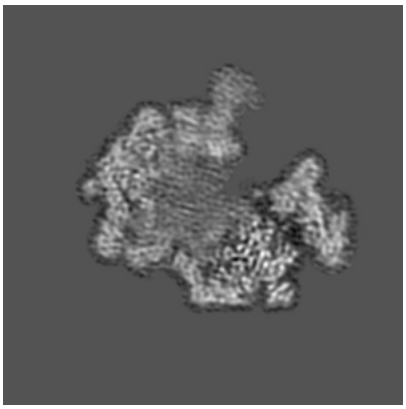


Z Index: 200

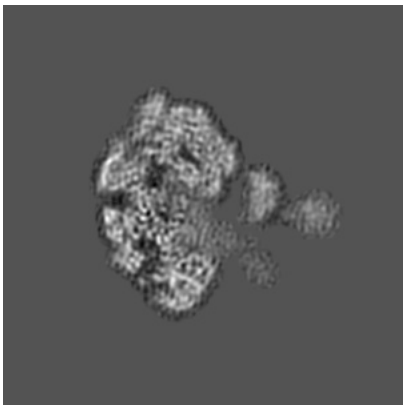
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

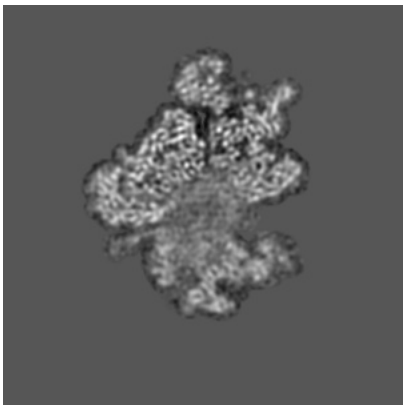
6.3.1 Primary map



X Index: 192

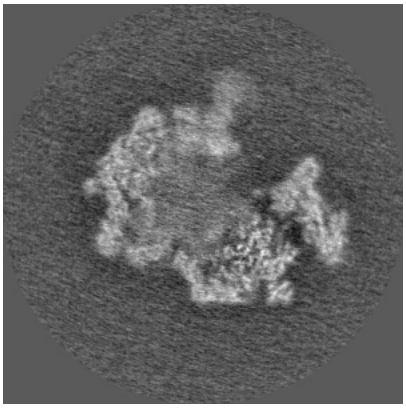


Y Index: 231

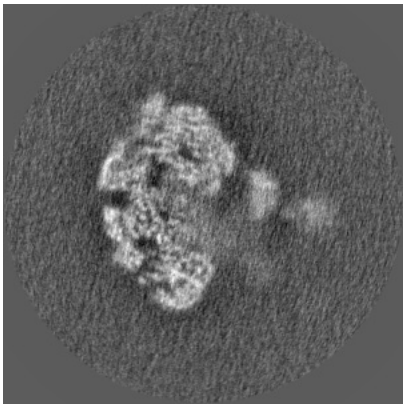


Z Index: 174

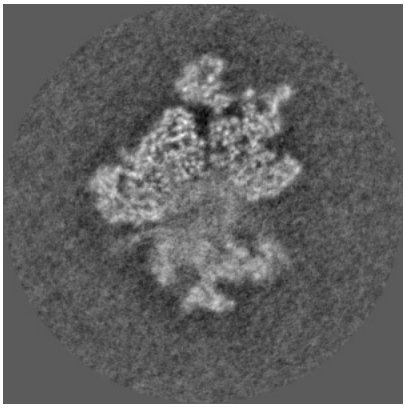
6.3.2 Raw map



X Index: 192



Y Index: 230

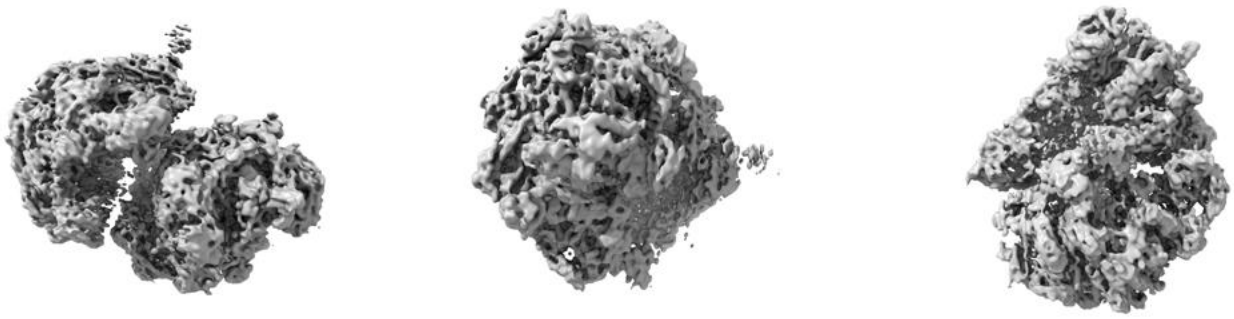


Z Index: 173

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

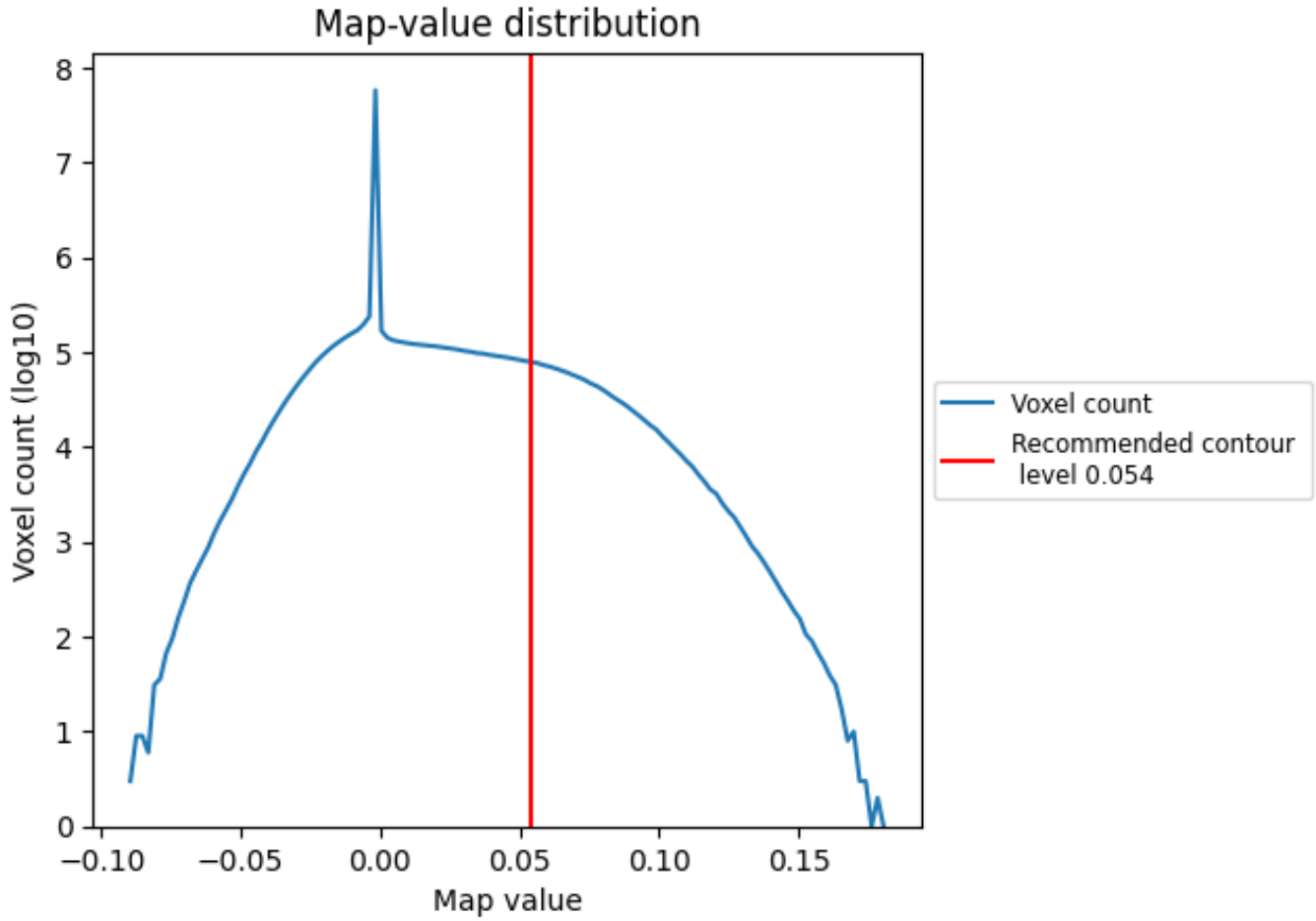
6.5 Mask visualisation (i)

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

7 Map analysis

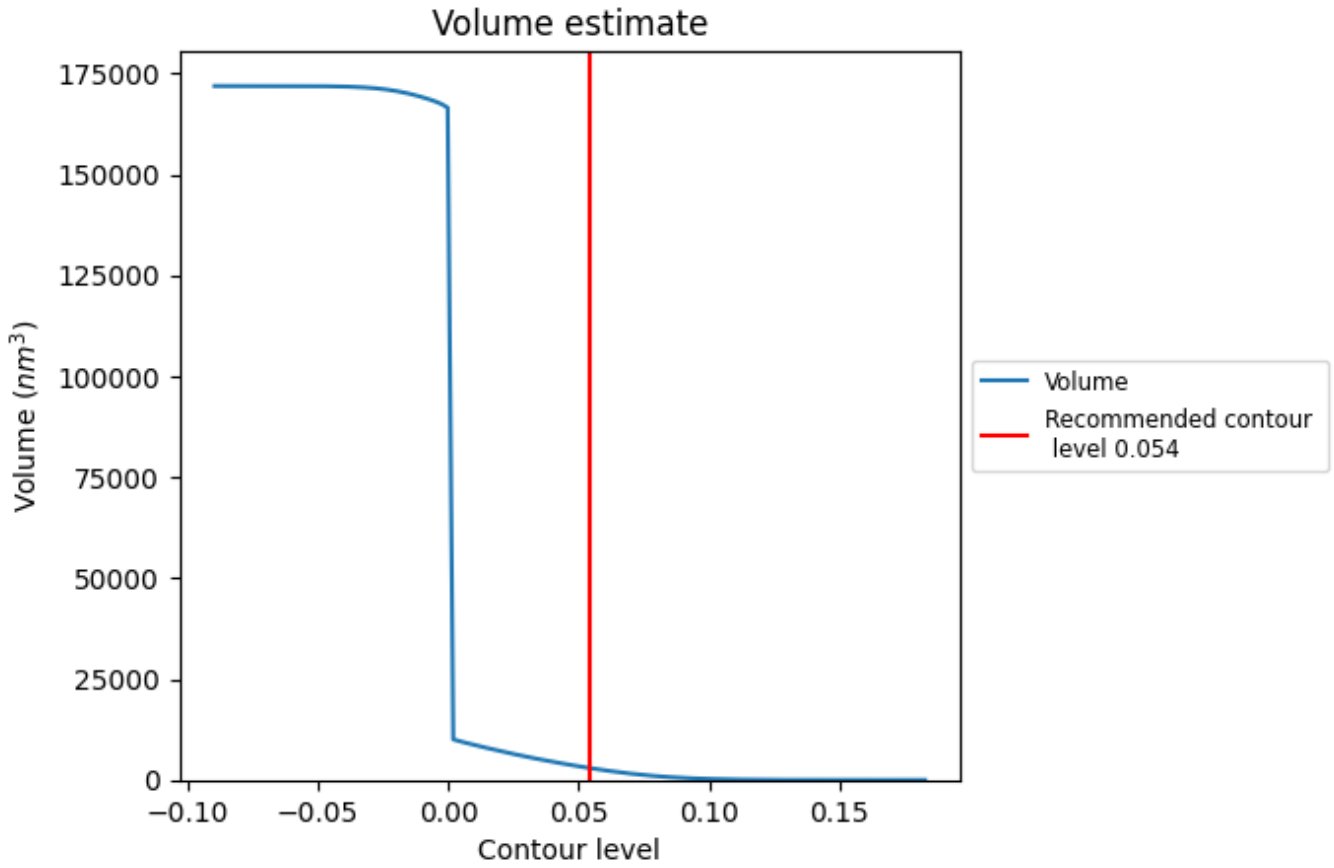
This section contains the results of statistical analysis of the map.

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.

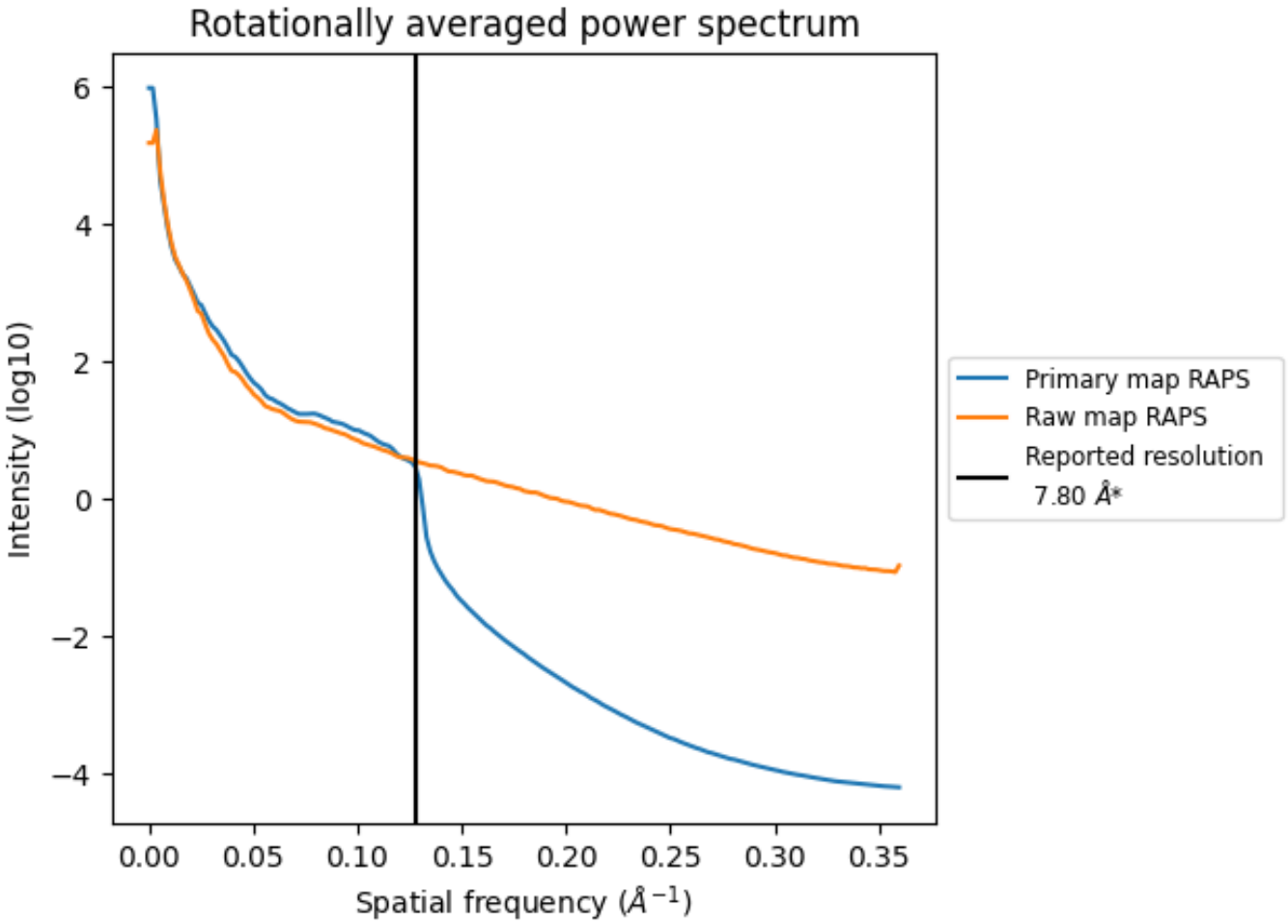
7.2 Volume estimate (i)



The volume at the recommended contour level is 2967 nm^3; this corresponds to an approximate mass of 2680 kDa.

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

7.3 Rotationally averaged power spectrum (i)

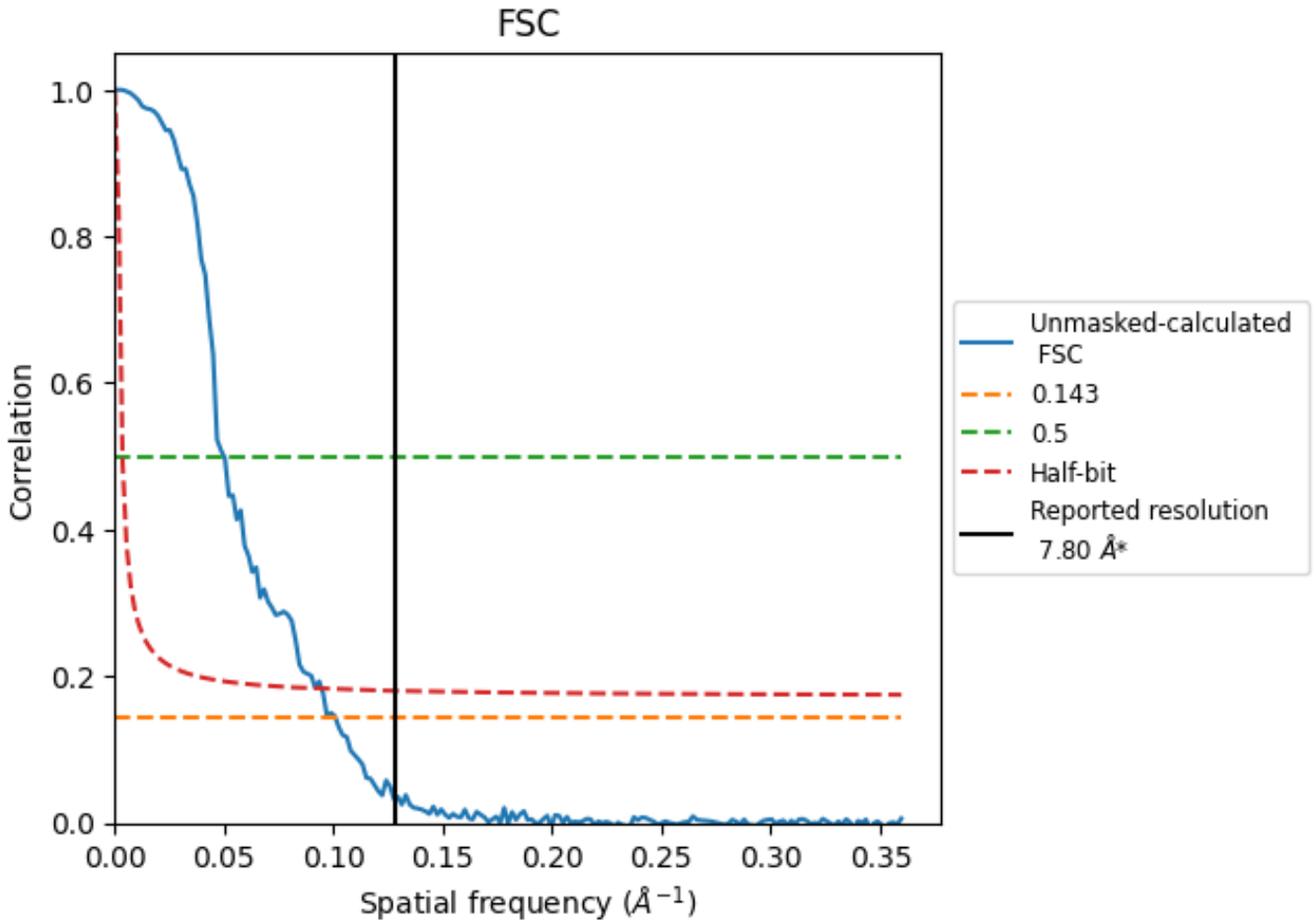


*Reported resolution corresponds to spatial frequency of 0.128 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.128 Å^{-1}

8.2 Resolution estimates (i)

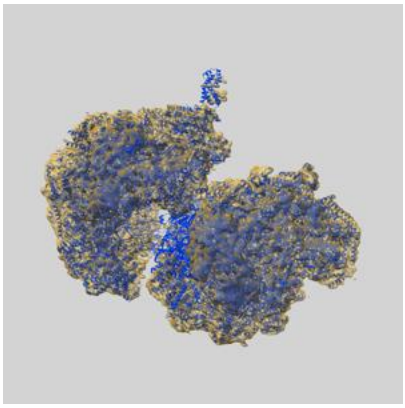
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.90	20.04	10.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.90 differs from the reported value 7.8 by more than 10 %

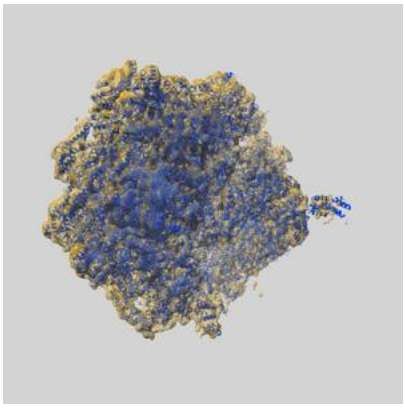
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0229 and PDB model 6HIV. Per-residue inclusion information can be found in section 3 on page 50.

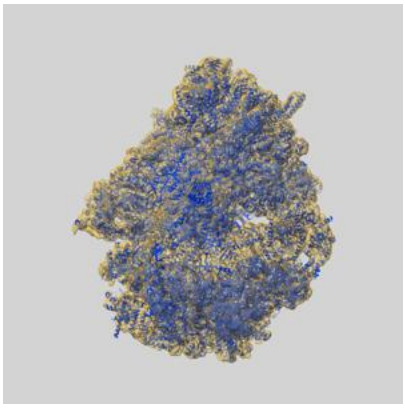
9.1 Map-model overlay



X



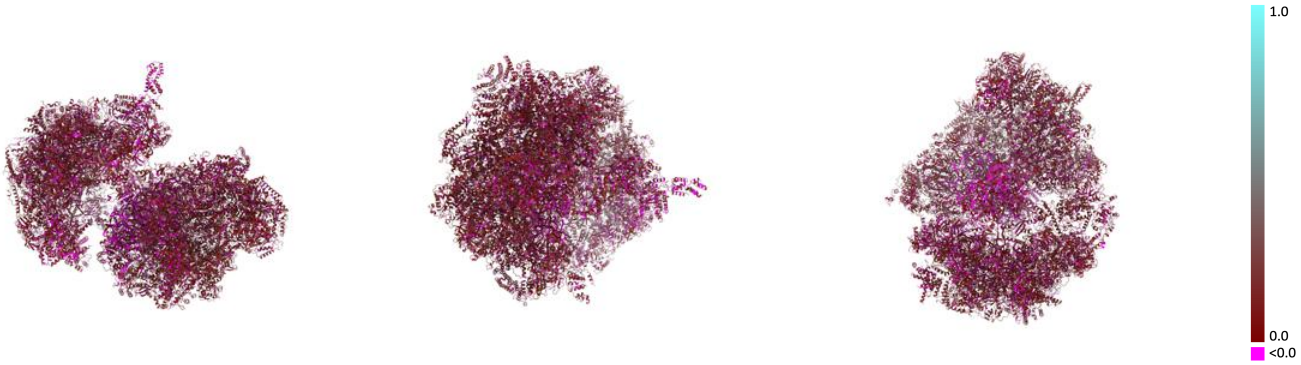
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.054 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.

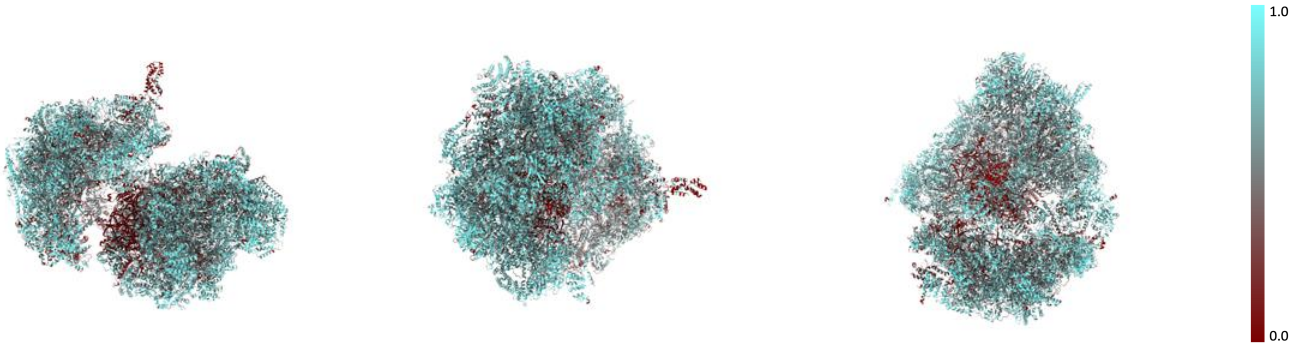
9.2 Q-score mapped to coordinate model



X Y Z

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

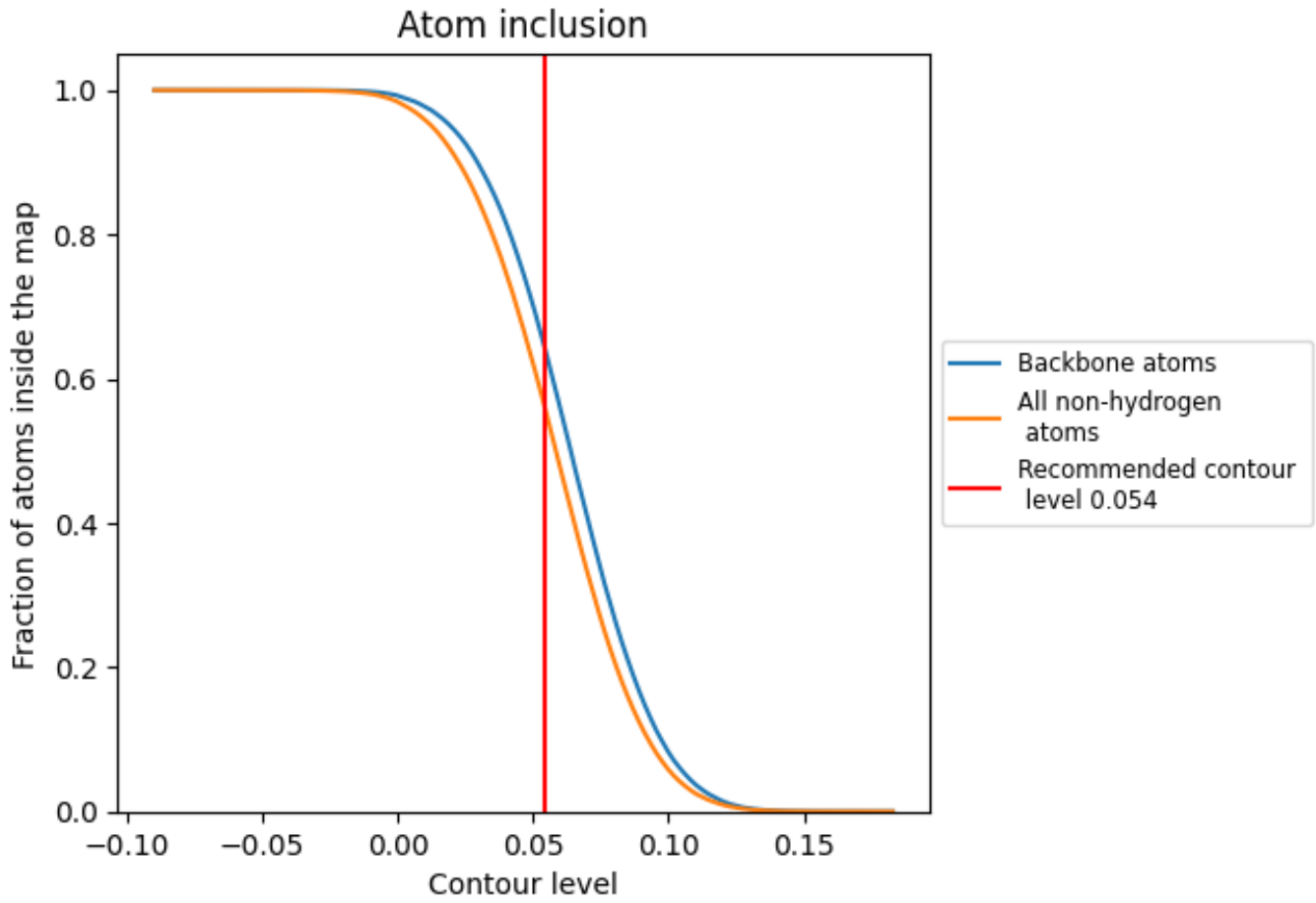
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.054).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (0.054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5655	0.1160
A0	0.5422	0.1260
A1	0.4980	0.1090
A2	0.7340	0.1440
A3	0.5536	0.1270
A4	0.4821	0.1320
A5	0.5622	0.0700
A6	0.3136	0.1280
A8	0.3563	0.1060
A9	0.2449	0.0770
AA	0.6588	0.1450
AB	0.2036	0.0370
AC	0.2143	0.1210
AD	0.0643	0.0040
AE	0.5216	0.0880
AF	0.6061	0.1060
AG	0.0370	0.0440
AI	0.6171	0.1130
AJ	0.4957	0.0700
AK	0.6035	0.0940
AN	0.4236	0.0880
AP	0.5235	0.0920
AQ	0.4833	0.1010
AR	0.5569	0.1100
AT	0.3663	0.0830
AU	0.5735	0.1090
AV	0.5839	0.0980
AW	0.5428	0.1180
AX	0.5901	0.1150
AY	0.5999	0.1320
Ab	0.6637	0.1270
Ad	0.6077	0.1340
Ae	0.6082	0.1130
Af	0.5990	0.1290
Ag	0.5791	0.1100

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Chain	Atom inclusion	Q-score
Aj	0.7354	0.1160
Al	0.5231	0.1230
Ao	0.5200	0.1080
Ap	0.5034	0.0730
At	0.5652	0.1310
Av	0.5982	0.1430
BA	0.5787	0.1110
BB	0.6648	0.1170
BC	0.6656	0.1150
BD	0.5603	0.1170
BE	0.6098	0.1310
BF	0.6476	0.1140
BG	0.7314	0.1240
BH	0.6260	0.1080
BI	0.5806	0.0910
BJ	0.6029	0.1280
BK	0.3893	0.1030
BL	0.5741	0.1290
BM	0.6191	0.1250
BN	0.5287	0.1070
BO	0.5533	0.1050
BP	0.5206	0.1280
BQ	0.6596	0.1280
BR	0.5915	0.1280
BS	0.5656	0.1060
BT	0.7237	0.1300
BU	0.6409	0.1230
BV	0.5611	0.0840
BW	0.7219	0.1420
BX	0.2221	0.0500
BY	0.4917	0.1180
BZ	0.6761	0.1050
Ba	0.6571	0.1170
Bb	0.6707	0.1280
Bc	0.4768	0.1130
Bd	0.6385	0.1270
Be	0.4141	0.1240
Bf	0.5704	0.0380
Bg	0.5531	0.1120
Bh	0.2684	0.0620
CA	0.3198	0.0570
CC	0.3484	0.0990

Continued on next page...

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Chain	Atom inclusion	Q-score
CE	0.5333	0.1260
CF	0.5463	0.1060
CH	0.5316	0.1480
CI	0.5217	0.1190
CJ	0.5827	0.1300
CK	0.3836	0.0780
CL	0.0042	0.0000
CN	0.5188	0.1030
CO	0.4830	0.1020
CP	0.6343	0.1170
CQ	0.3601	0.0700
CR	0.4341	0.1130
CS	0.5009	0.0870
CU	0.2203	0.0410
CZ	0.0000	0.0060
Ca	0.5430	0.1220
Cb	0.5639	0.1400
Cd	0.5259	0.0810
Cg	0.6681	0.1090
Ci	0.5280	0.1080
Cj	0.7423	0.1290
Ck	0.6128	0.1340
Cm	0.1545	0.0260
Cn	0.0091	-0.0110
Cp	0.6071	0.1290
Cq	0.6403	0.1420
Cr	0.7045	0.1400
Cv	0.5837	0.1210
DA	0.6834	0.1390
DB	0.6112	0.1430
DC	0.6736	0.1160
DD	0.6325	0.1340
DE	0.6964	0.1280
DF	0.6429	0.1270
DG	0.6743	0.1300
DH	0.5388	0.1280
DI	0.7135	0.1380
DJ	0.6638	0.1200
DK	0.6238	0.1310
DL	0.3870	0.1200
DM	0.6532	0.1280
DN	0.6360	0.1350

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Chain	Atom inclusion	Q-score
DO	0.7247	0.1350
DP	0.7296	0.1320
DQ	0.6987	0.1410
DR	0.7137	0.1300
DS	0.7076	0.1260
DT	0.5892	0.1170
DU	0.5924	0.1340
DV	0.5522	0.1030
DW	0.5562	0.1060
DX	0.6308	0.1080
DY	0.6293	0.1110
DZ	0.5344	0.1430
Da	0.0126	-0.0220
UA	0.6304	0.1420
UB	0.6432	0.1370
UC	0.1806	0.0290
UD	0.3371	0.1450
UE	0.1515	0.0250
UF	0.4722	0.1480
UG	0.3681	0.1280
UH	0.5694	0.2180
UI	0.2157	0.1470
UK	0.7500	0.2190
UL	0.3667	0.1000
UM	0.0556	0.0120
UN	0.0764	0.0010
UO	0.2667	0.1750
UP	0.9048	0.2410
UQ	0.0000	-0.0030
UR	0.9792	0.2030
US	0.0000	-0.0250
UT	0.0227	0.0160
UU	0.2879	0.0830
UV	0.5417	0.1600
UW	0.2619	0.0490
UX	0.6667	0.2630