Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

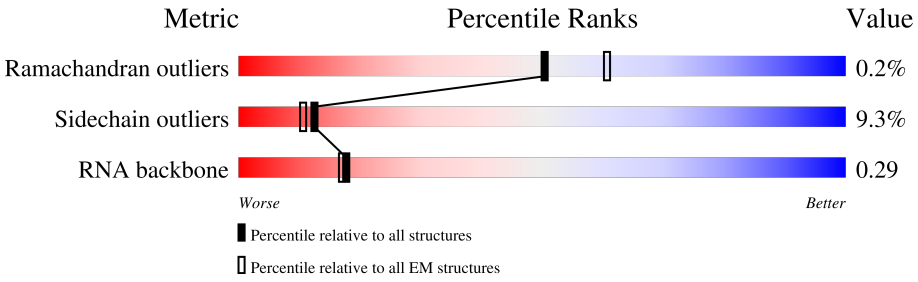
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

Continued on next page...

Continued from previous page...

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%

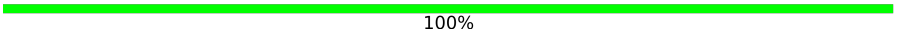
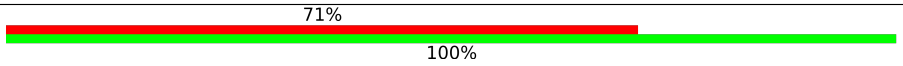
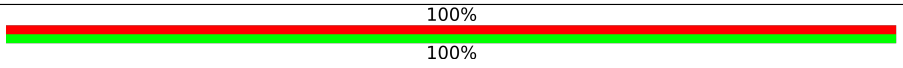
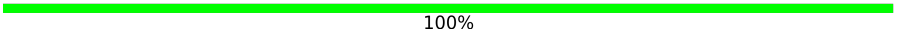
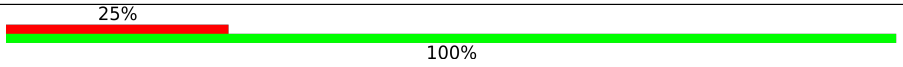
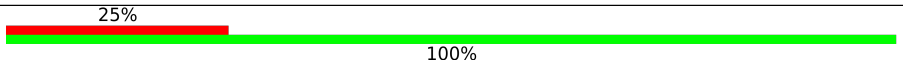
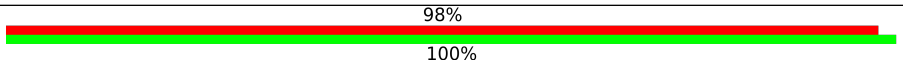
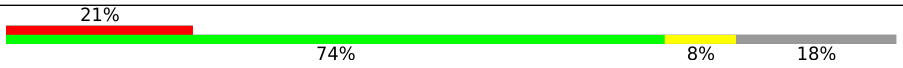
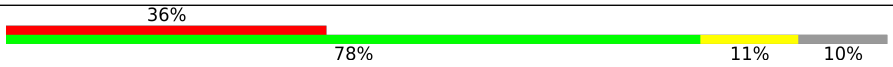
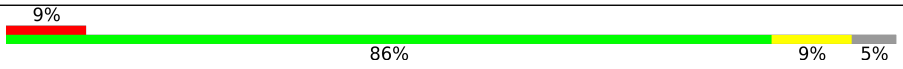
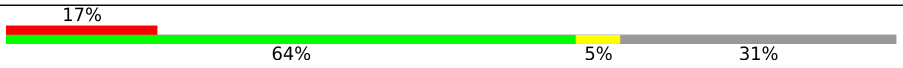
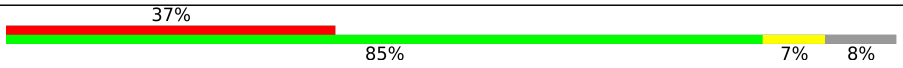
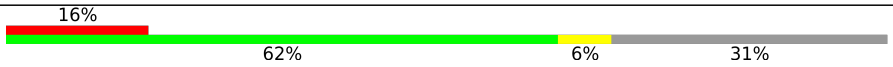
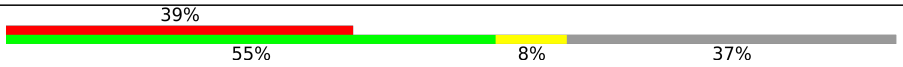
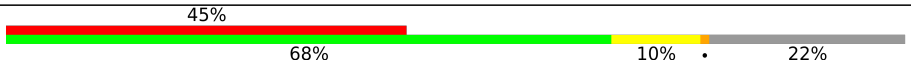
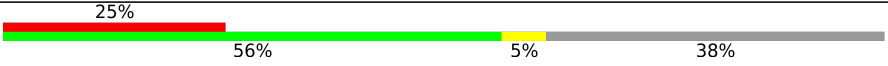
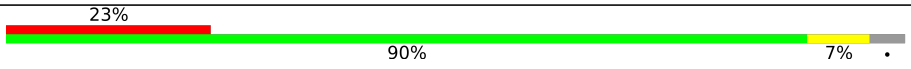
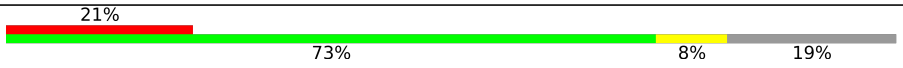
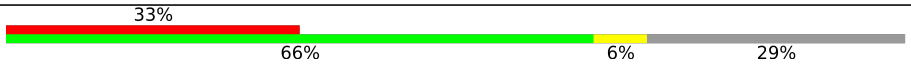
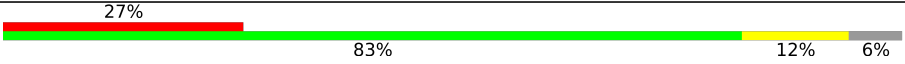
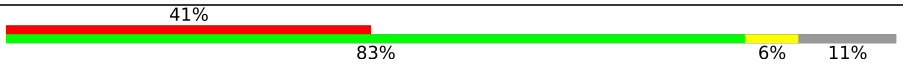
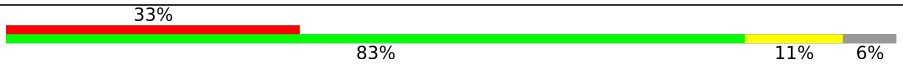
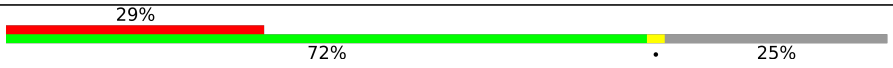
Continued on next page...

Continued from previous page...

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%

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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%

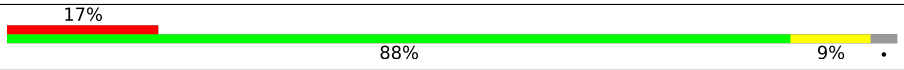
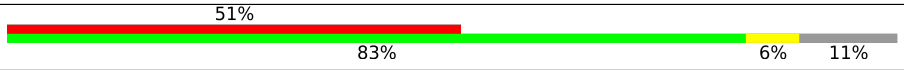
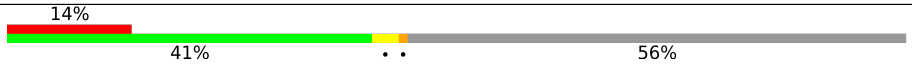
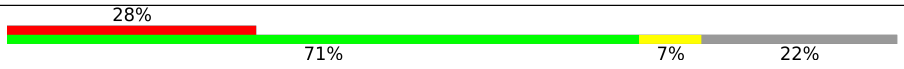
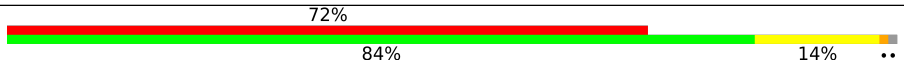
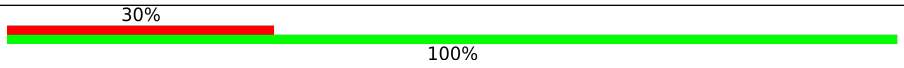
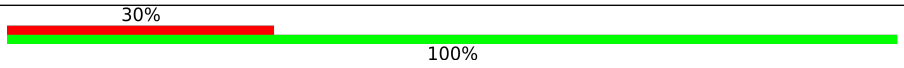
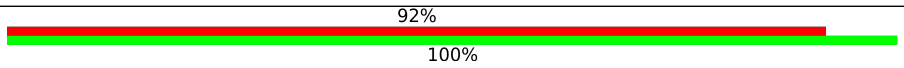
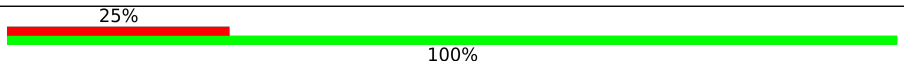
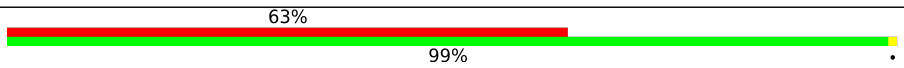
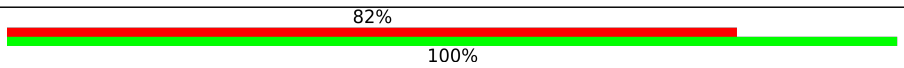
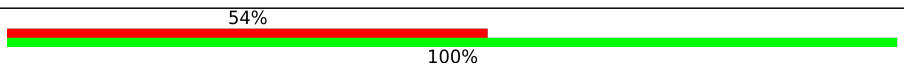
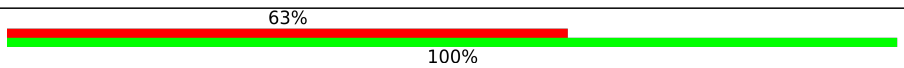
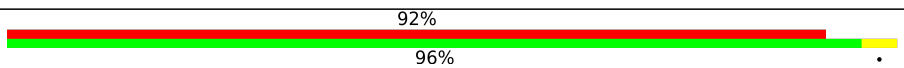
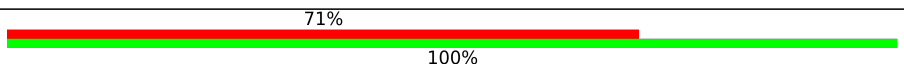
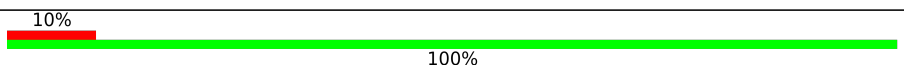
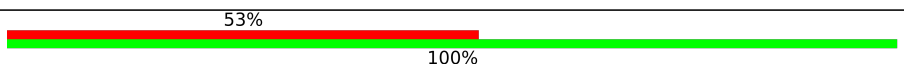
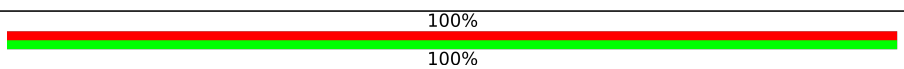
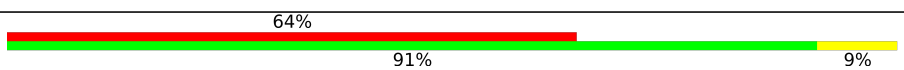
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
105	BC	523	16% 82% 9% 9%
106	BD	547	34% 72% 24%
107	BE	449	21% 81% 6% 13%
108	BF	426	16% 73% 7% 19%
109	BG	378	12% 78% 6% 16%
110	BH	349	16% 54% 7% 40%
111	BI	343	34% 86% 7% 7%
112	BJ	333	15% 46% 50%
113	BK	386	38% 63% 33%
114	BL	312	22% 69% 6% 25%
115	BM	283	21% 79% 7% 13%
116	BN	302	28% 67% 29%
117	BO	262	19% 51% 5% 44%
118	BP	266	28% 68% 8% 24%
119	BQ	231	18% 87% 7% 6%
120	BR	205	25% 84% 11% 5%
121	BS	160	21% 56% 5% 39%
122	BT	191	11% 81% 7% 12%
123	BU	185	6% 41% 56%
124	BV	190	29% 77% 5% 18%
125	BW	188	9% 92% 7%
126	BX	190	45% 50% 6% 44%
127	BY	172	23% 54% 5% 41%
128	BZ	190	24% 96%
129	Ba	139	17% 88% 12%

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 1792	C 1138	N 310	O 340	S 4	0	0

- Molecule 50 is a protein called mS35.

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

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 51 is a protein called mS37.

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

- Molecule 52 is a protein called mS38.

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

- Molecule 53 is a protein called ms34.

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

- Molecule 54 is a protein called ms42.

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

- 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

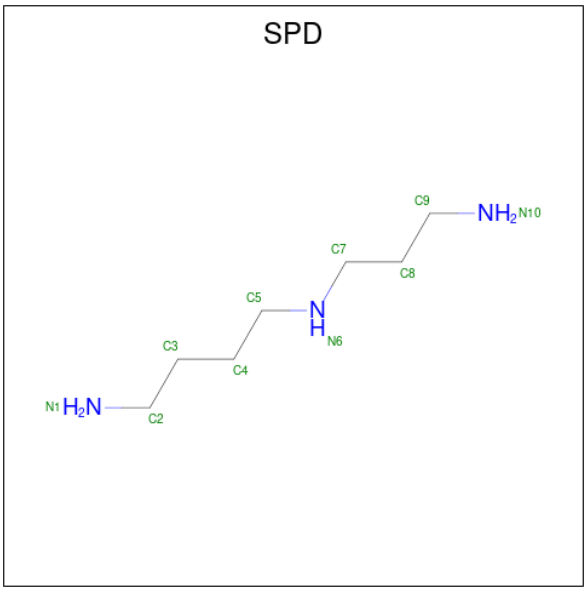
- Molecule 147 is a protein called UNK.

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: $C_7H_{19}N_3$).



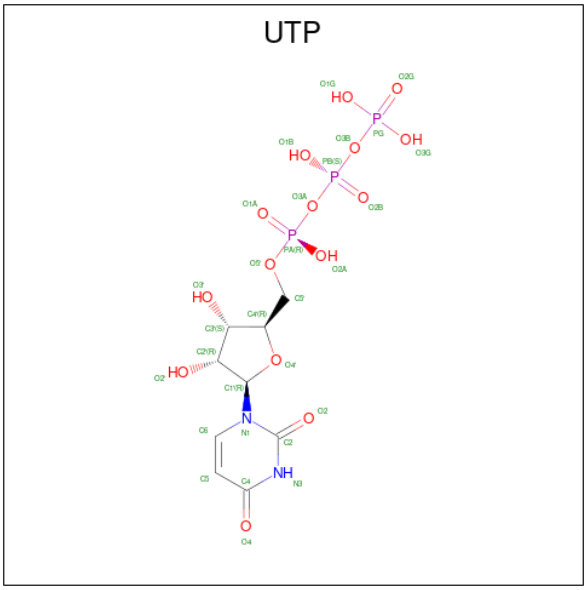
Mol	Chain	Residues	Atoms	AltConf
149	DL	1	Total C N 10 7 3	0
149	CA	1	Total C N 30 21 9	0
149	CA	1	Total C N 30 21 9	0

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: $C_9H_{15}N_2O_{15}P_3$).

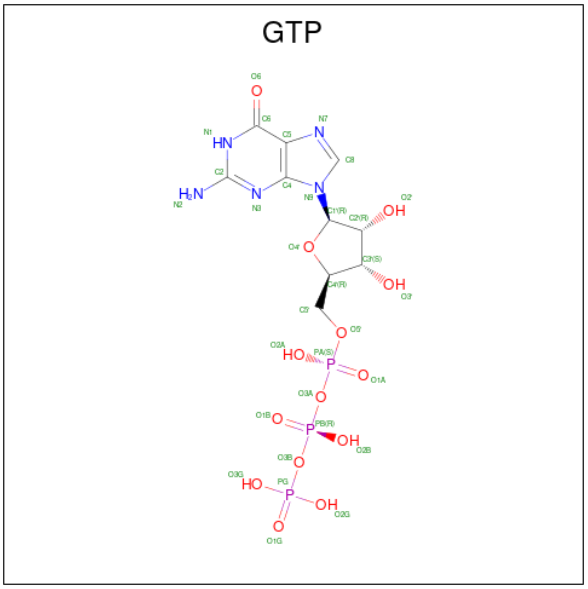


Mol	Chain	Residues	Atoms					AltConf
150	DJ	1	Total 29	C 9	N 2	O 15	P 3	0

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

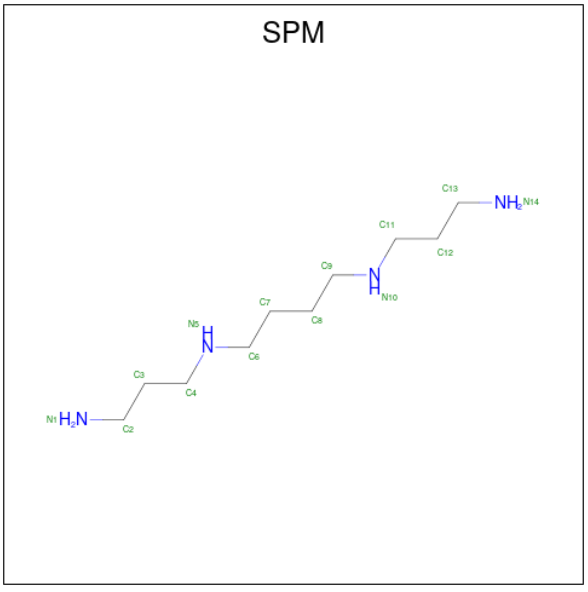
Mol	Chain	Residues	Atoms		AltConf
151	CO	1	Total 1	Mg 1	0
151	CQ	1	Total 1	Mg 1	0
151	Ca	1	Total 1	Mg 1	0
151	Cg	1	Total 1	Mg 1	0
151	Cv	1	Total 1	Mg 1	0
151	CA	34	Total 34	Mg 34	0
151	AA	7	Total 7	Mg 7	0

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



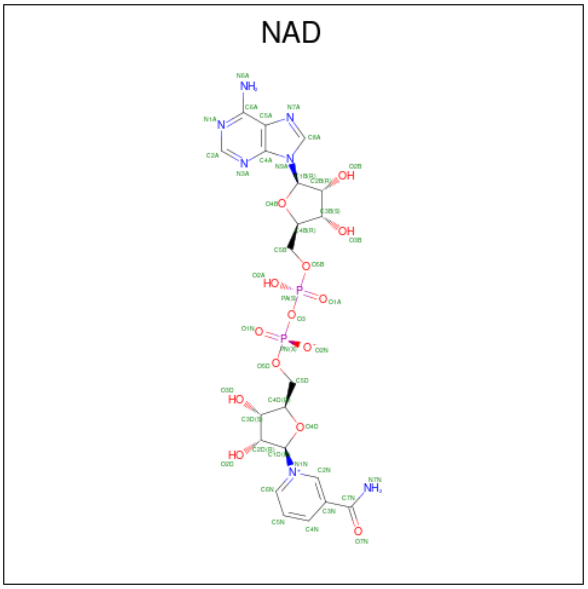
Mol	Chain	Residues	Atoms					AltConf
152	Cg	1	Total	C	N	O	P	0
			32	10	5	14	3	

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



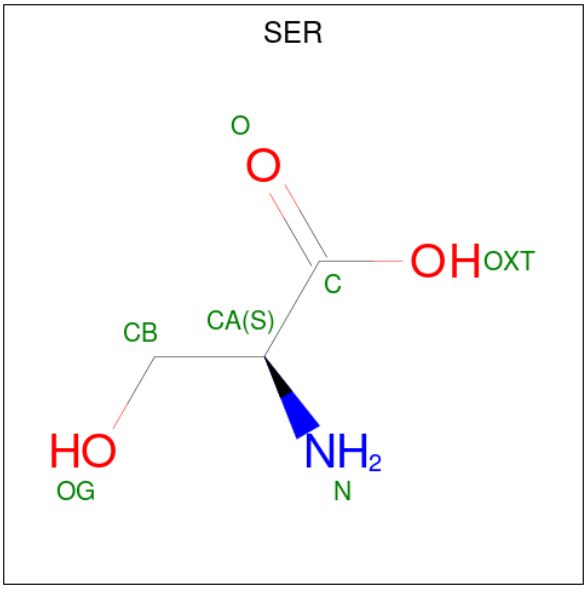
Mol	Chain	Residues	Atoms			AltConf
153	CA	1	Total	C	N	0
			14	10	4	

- 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.

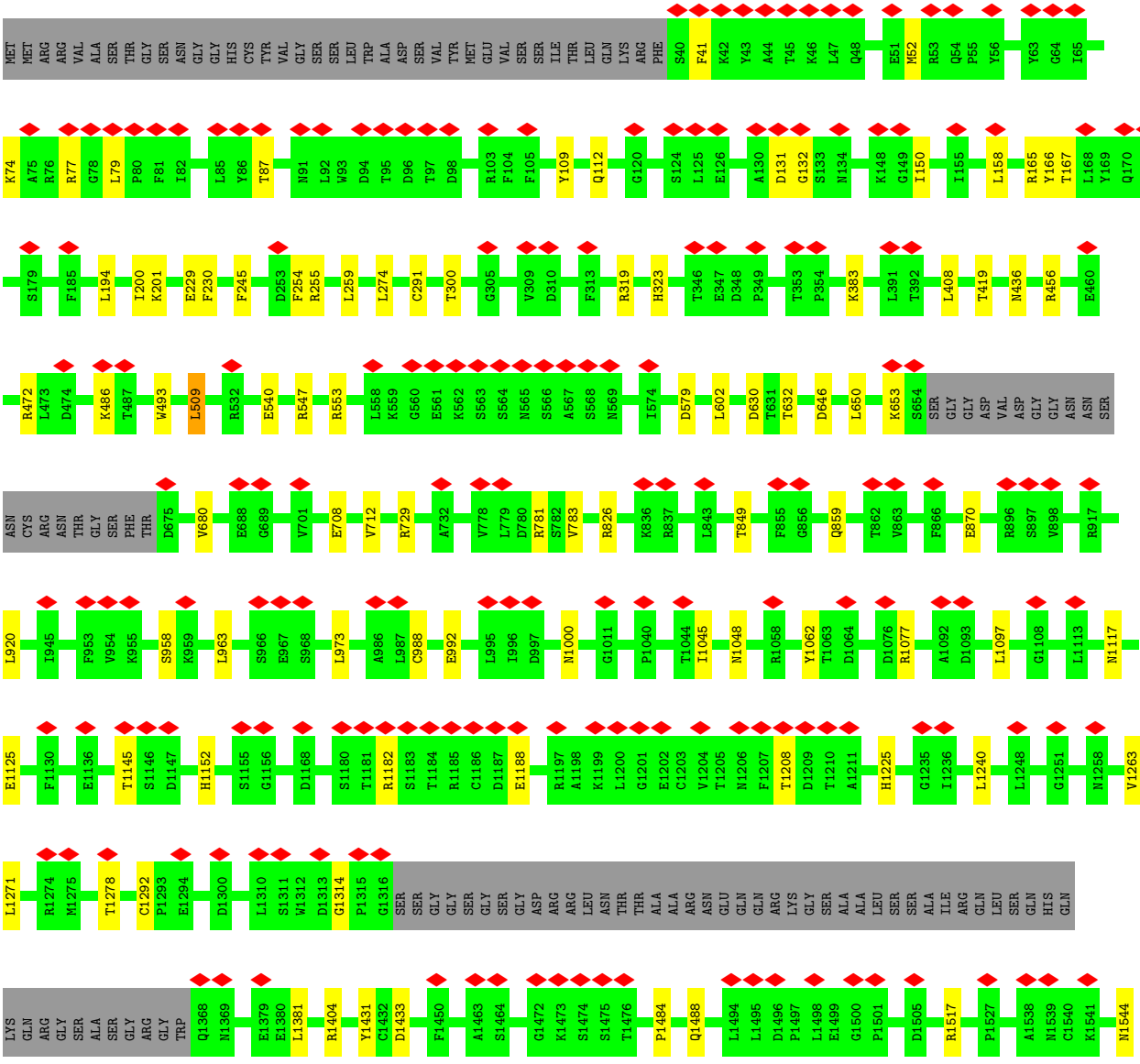
Mol	Chain	Residues	Atoms		AltConf
156	Cg	3	Total	O	0
			3	3	

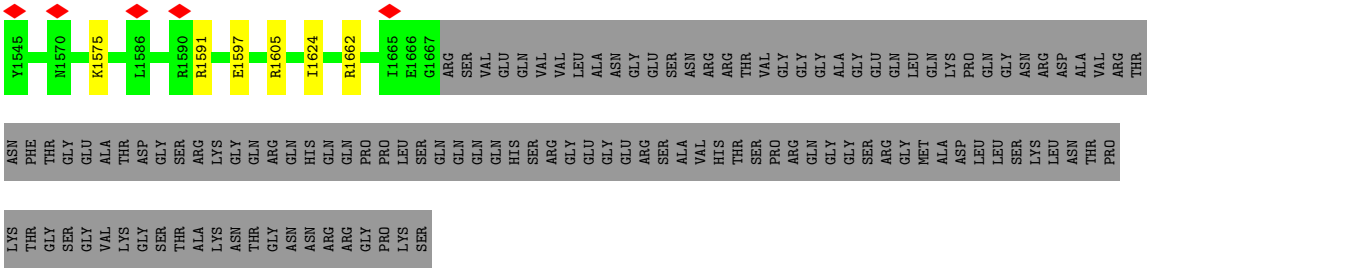
3 Residue-property plots (i)

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

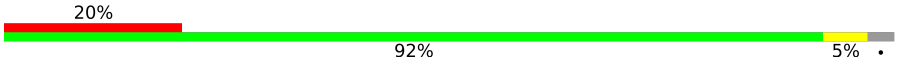
Chain DA:

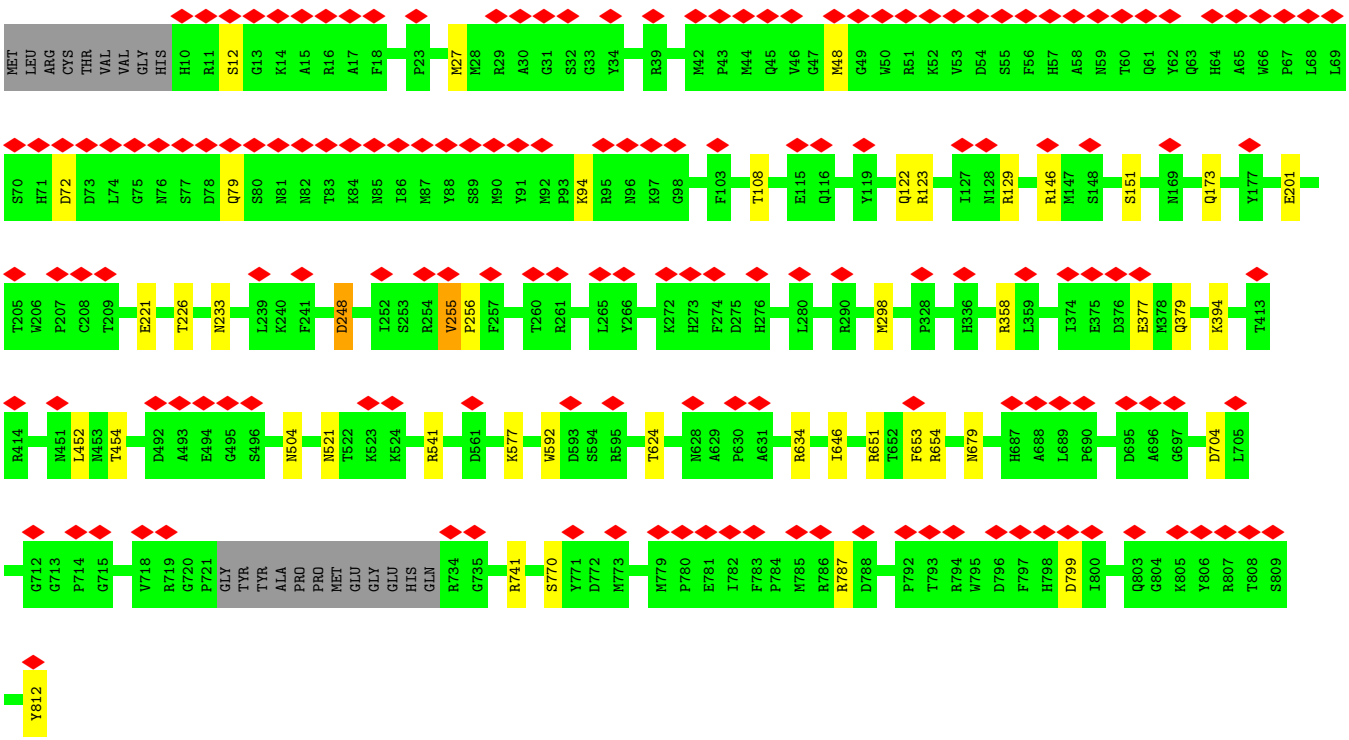




• Molecule 2: ms51

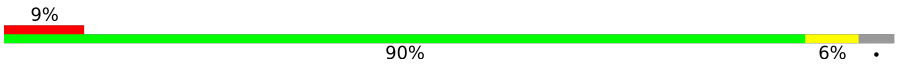
Chain DD:

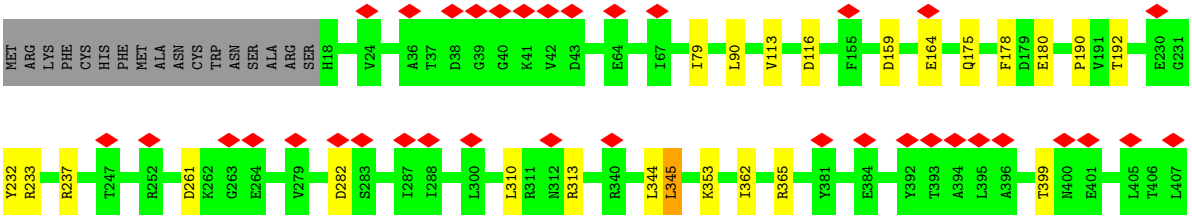




• Molecule 3: ms56

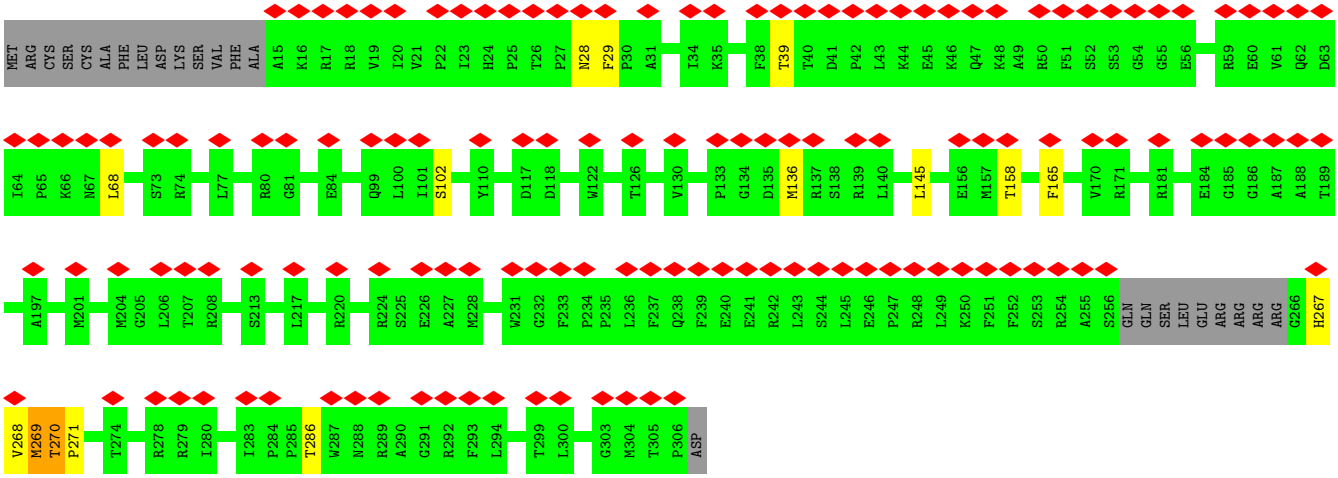
Chain DI:



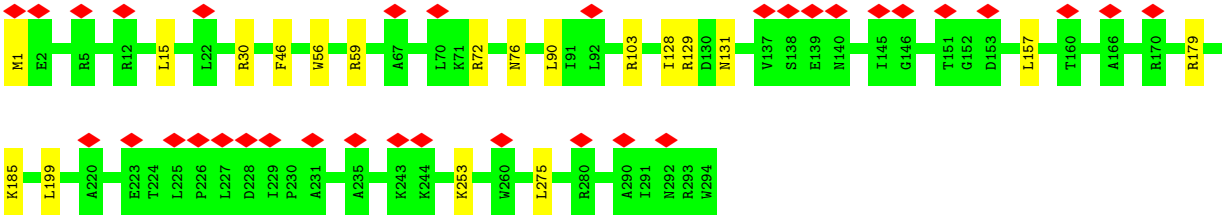


• Molecule 4: ms59

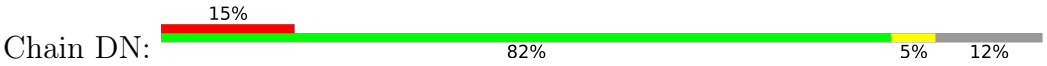
Chain DL:

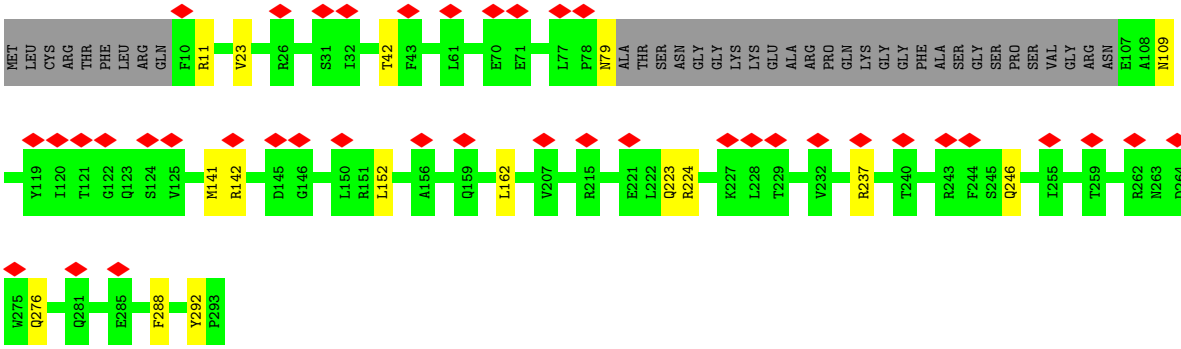


• Molecule 5: ms60

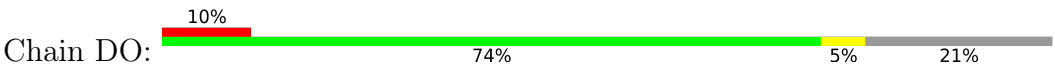


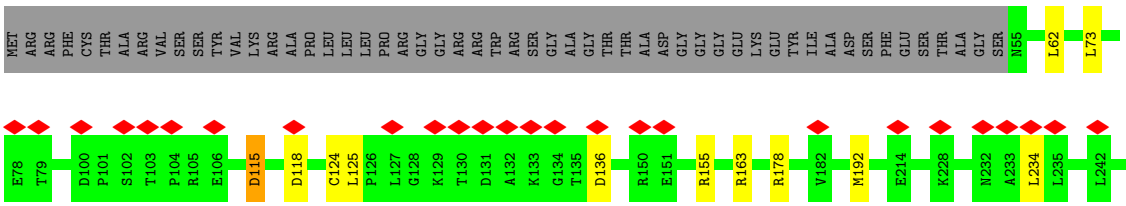
• Molecule 6: ms61





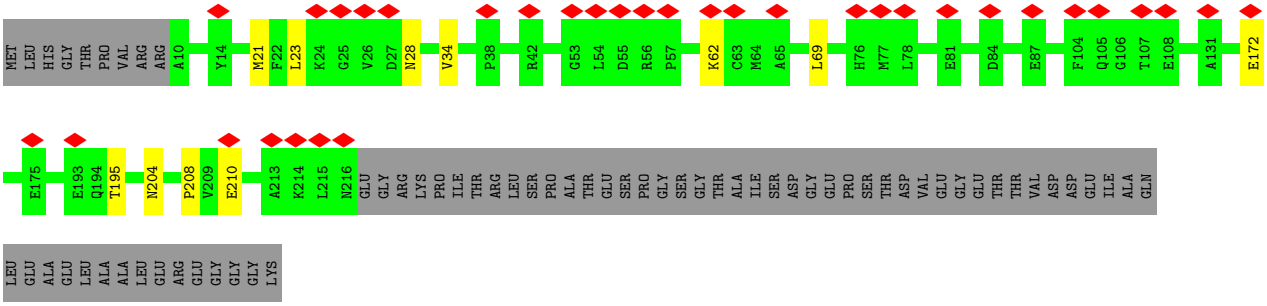
• Molecule 7: ms62





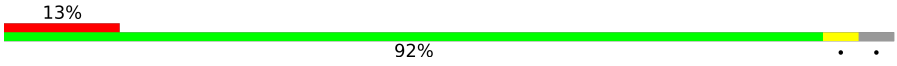
• Molecule 8: ms63

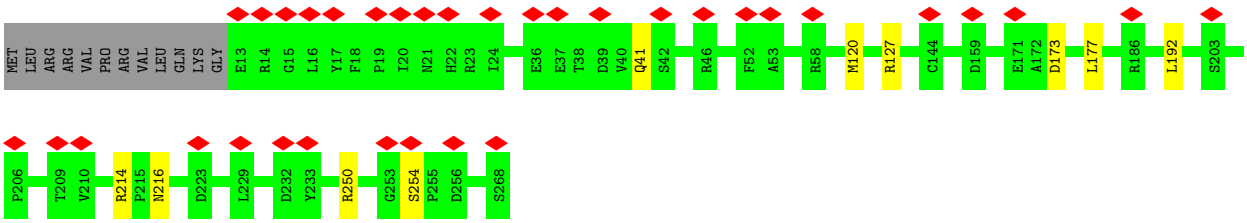
Chain DP:



• Molecule 9: ms64

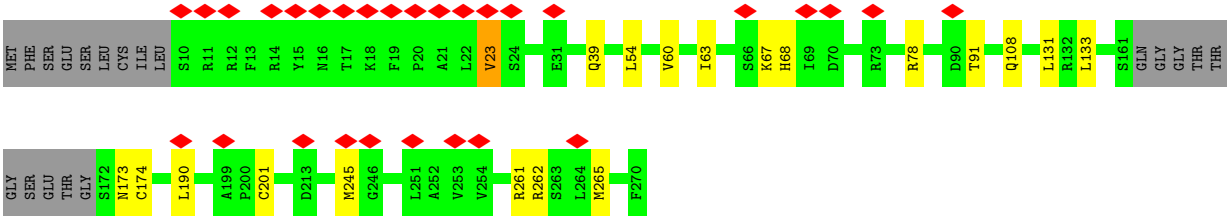
Chain DQ:





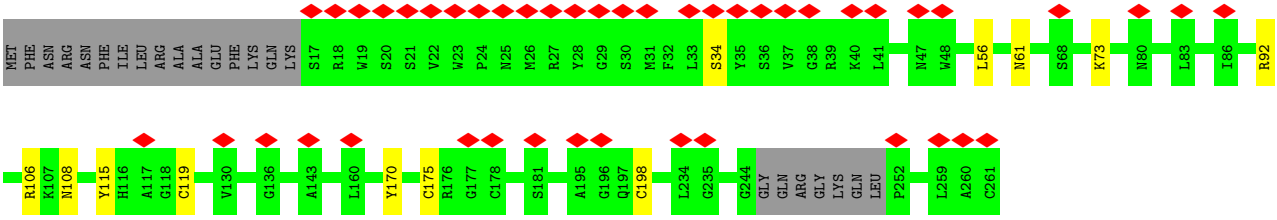
• Molecule 10: ms65

Chain DR:



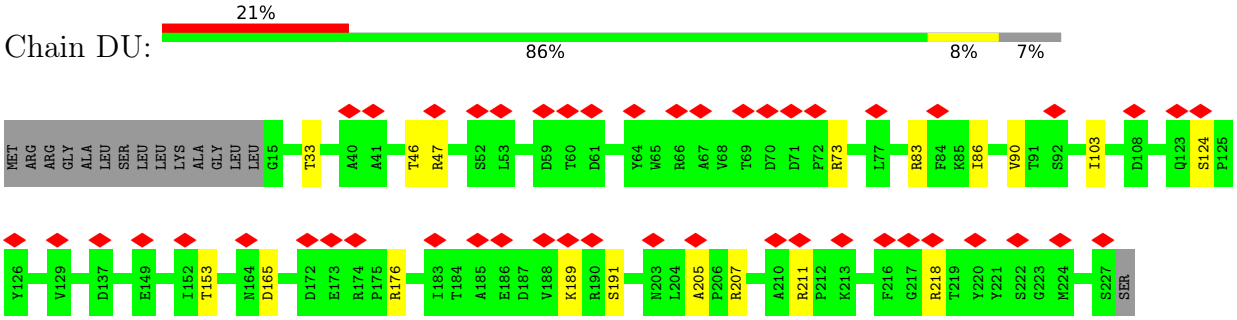
• Molecule 11: ms66

Chain DS:



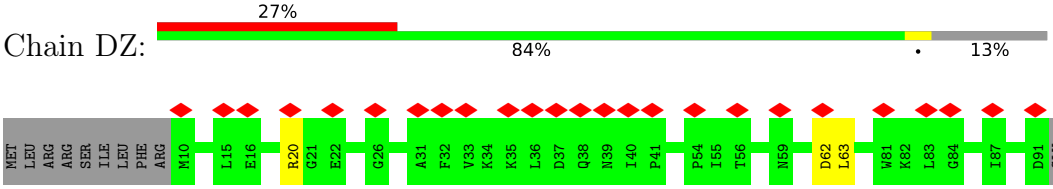
• Molecule 12: ms68

Chain DU:



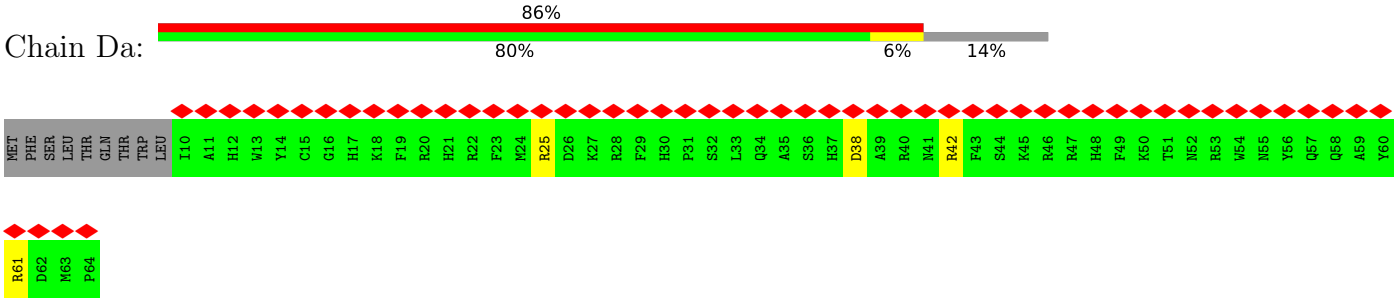
• Molecule 13: ms73

Chain DZ:



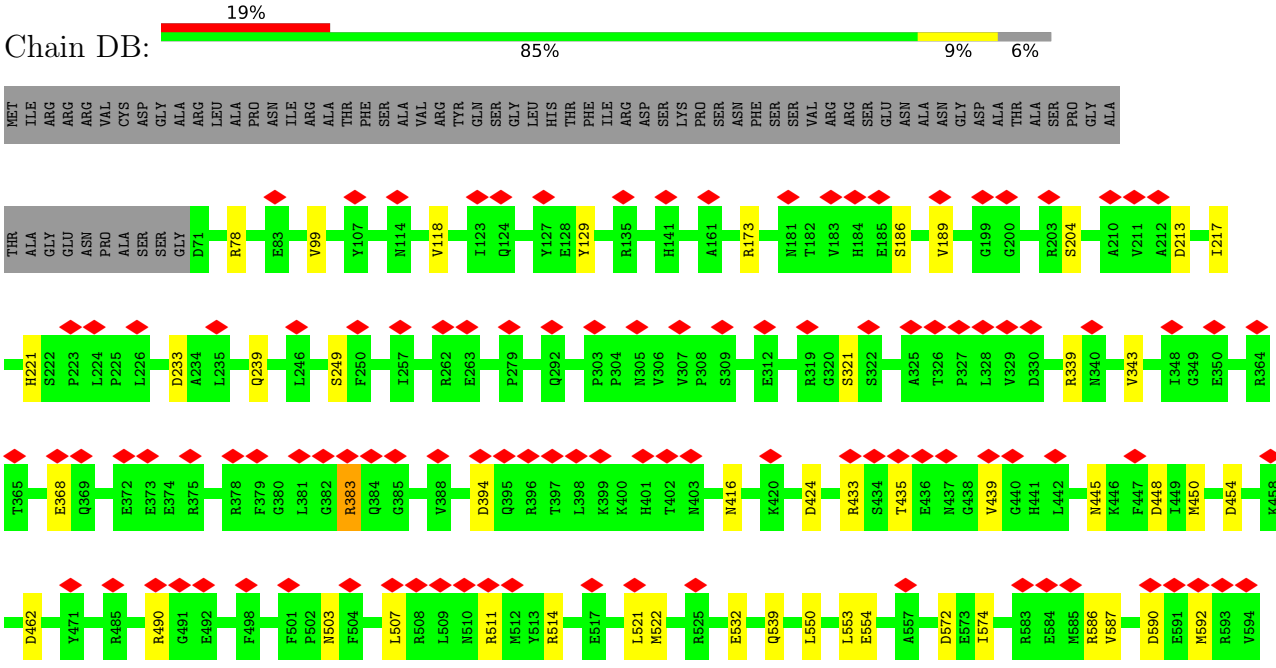
• Molecule 14: ms74

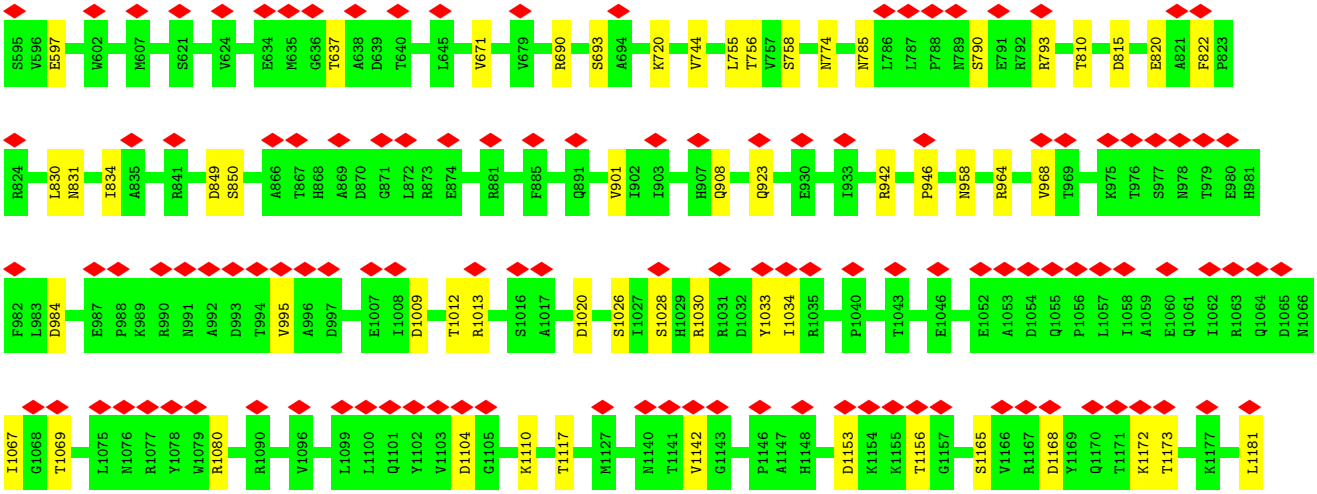
Chain Da:



• Molecule 15: ms49

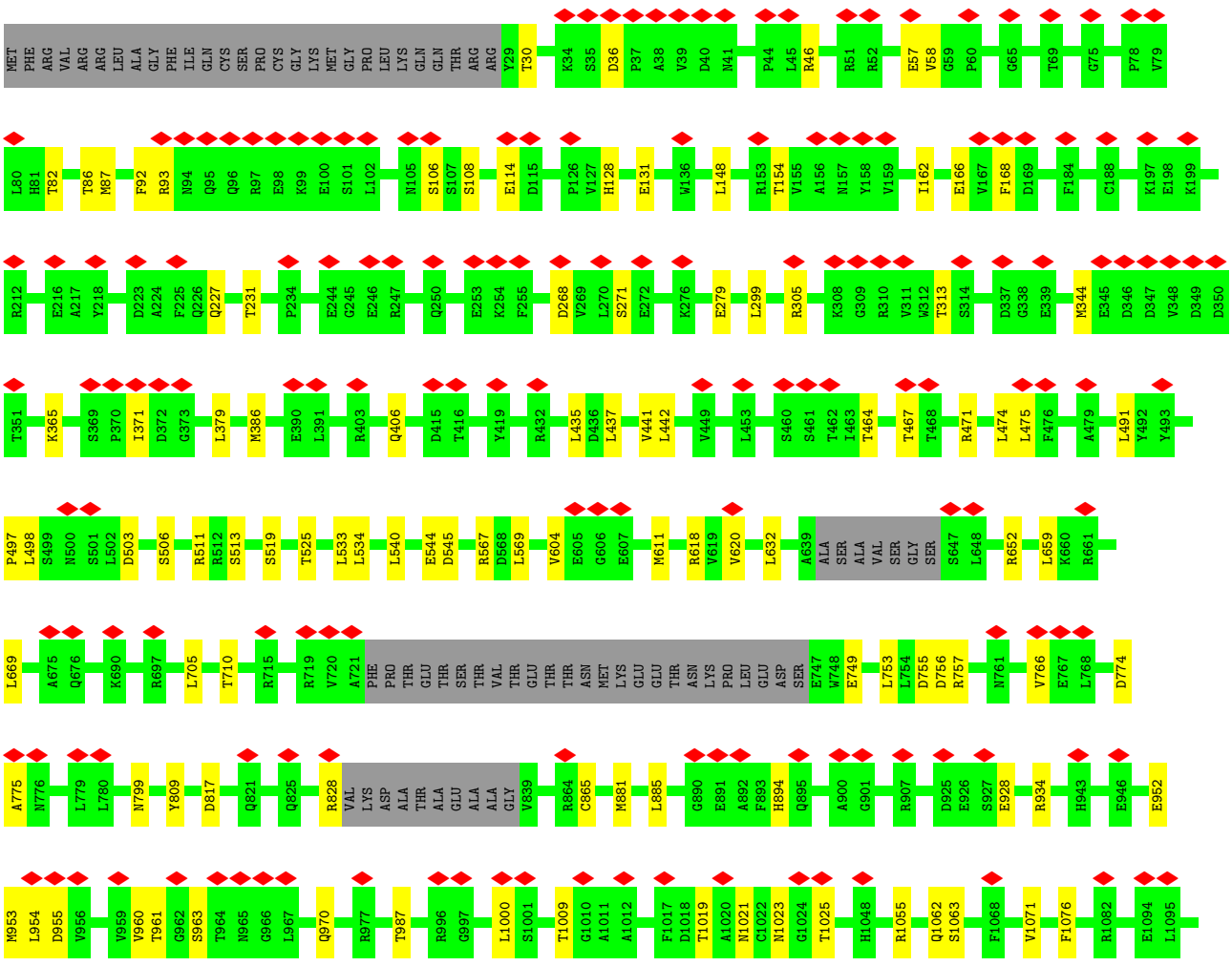
Chain DB:

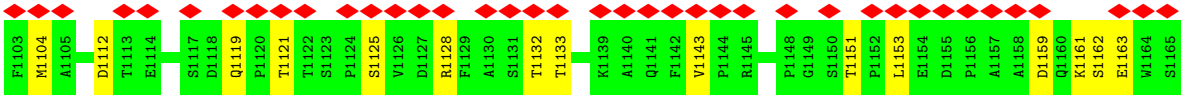




• Molecule 16: ms50

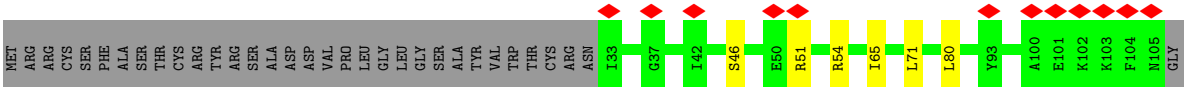
Chain DC:

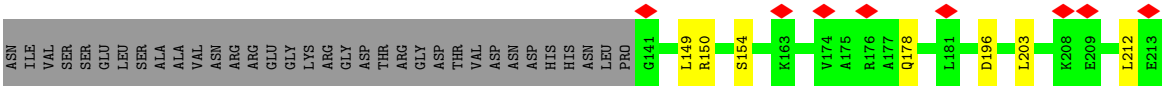


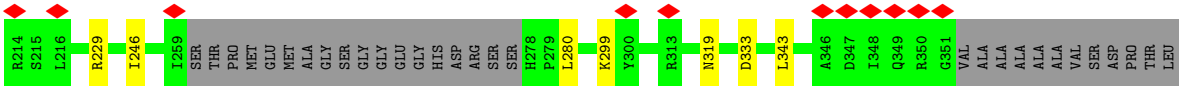


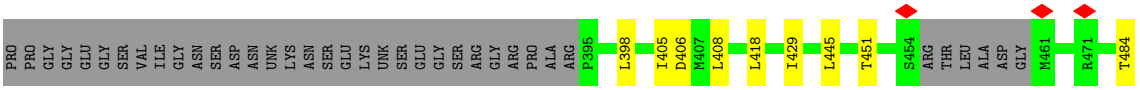
• Molecule 17: mS52

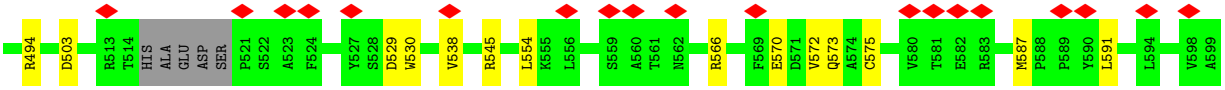
Chain DE:

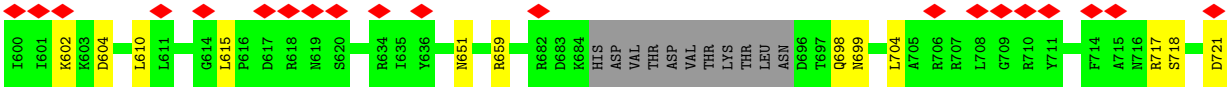


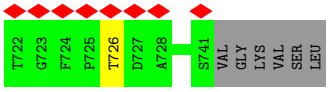






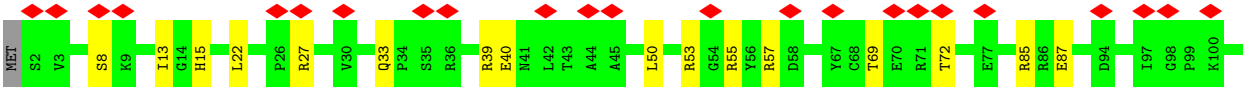


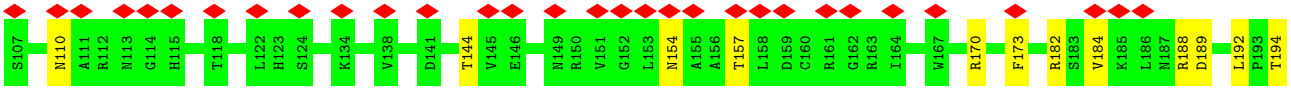


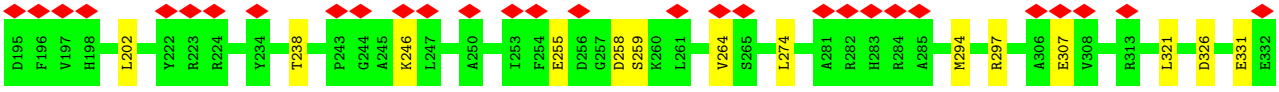


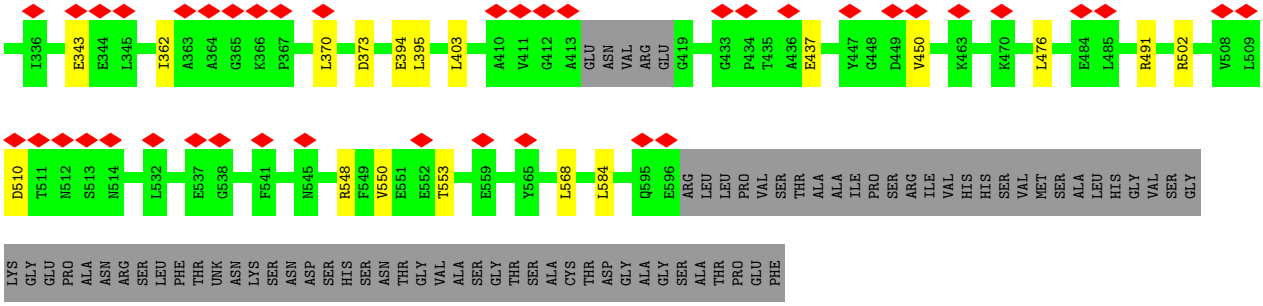
• Molecule 18: ms53

Chain DF:



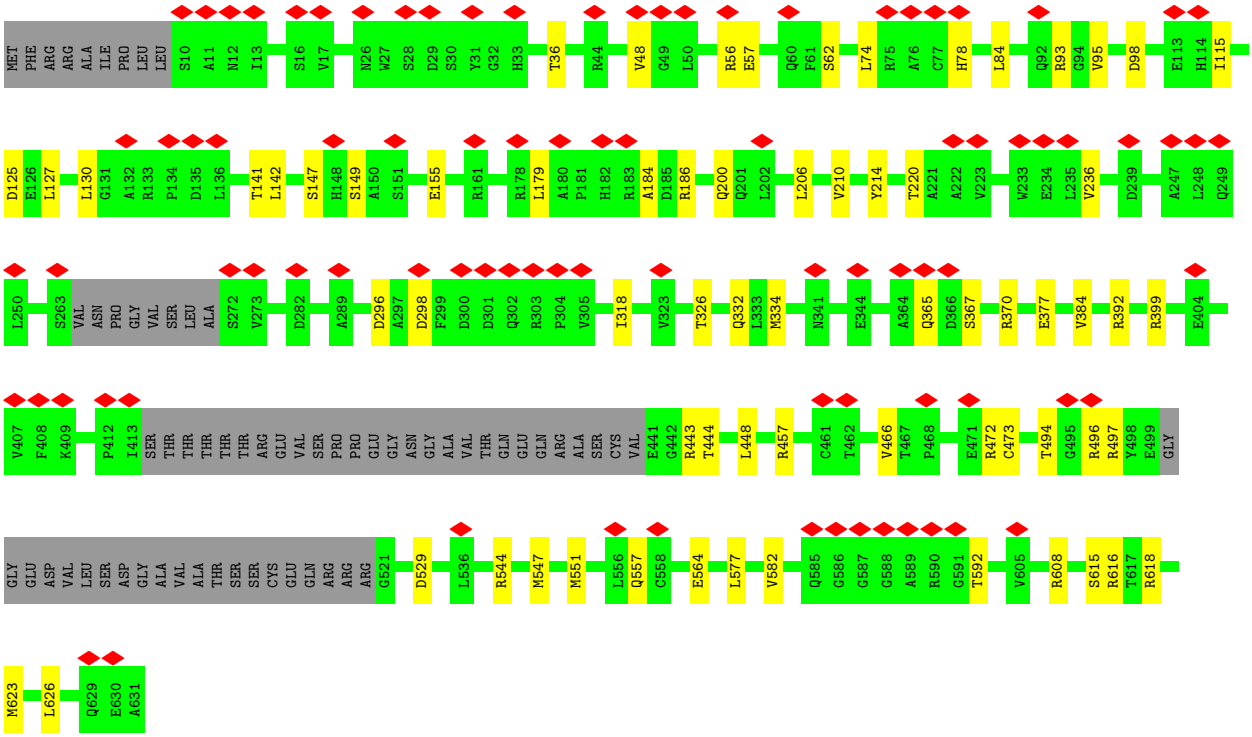






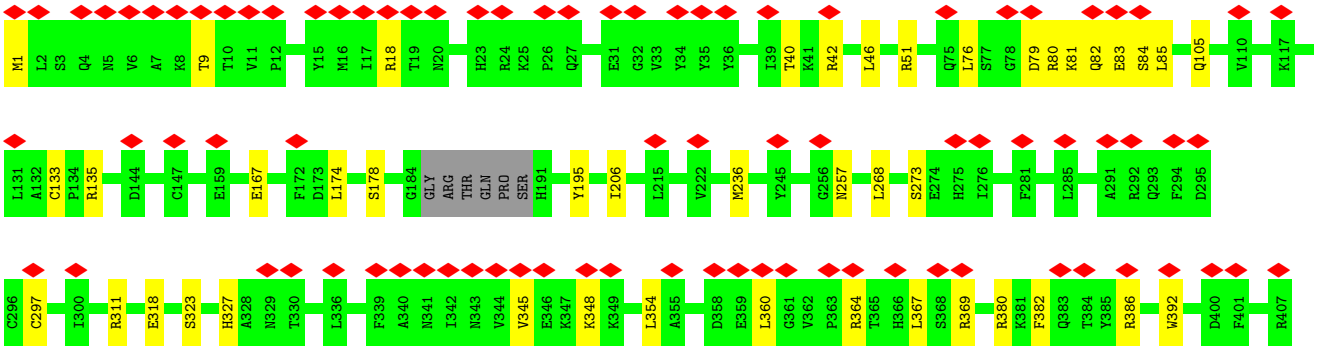
• Molecule 19: ms54

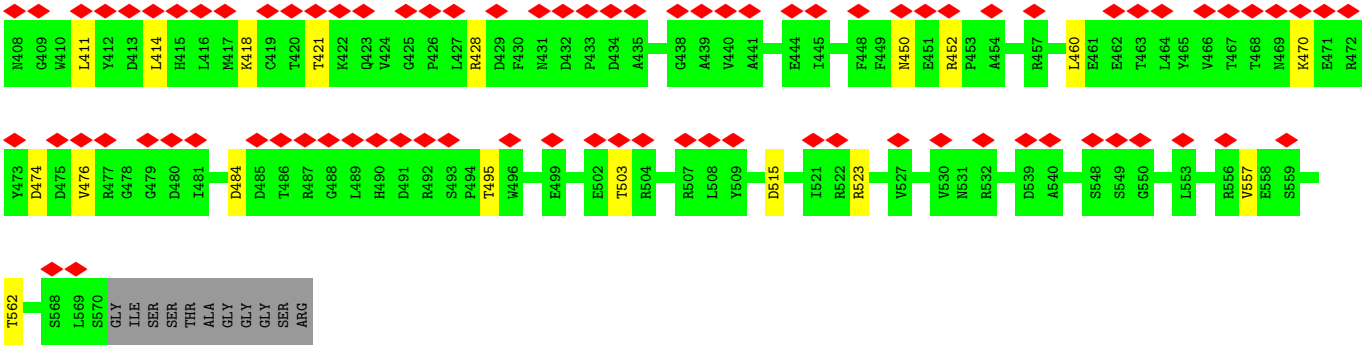
Chain DG:



• Molecule 20: ms55

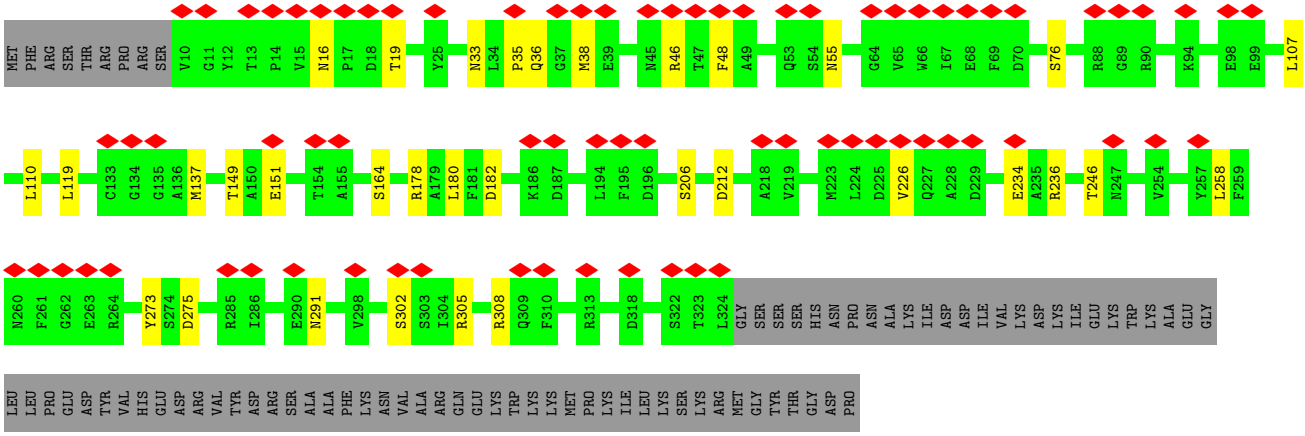
Chain DH:





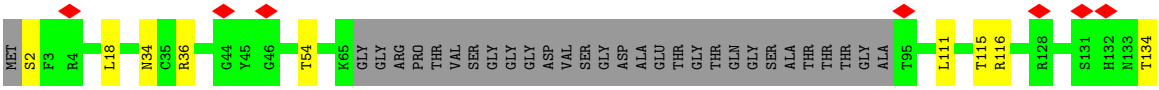
• Molecule 21: ms57

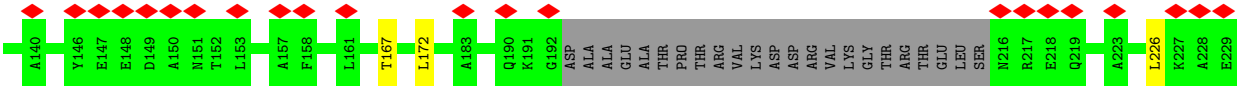
Chain DJ:

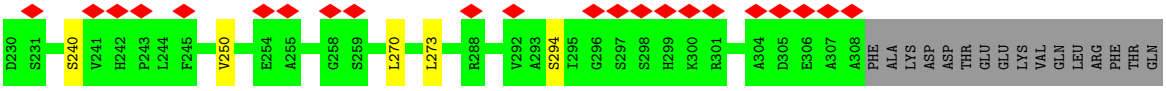


• Molecule 22: ms58

Chain DK:

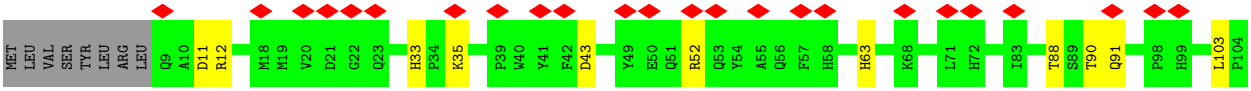


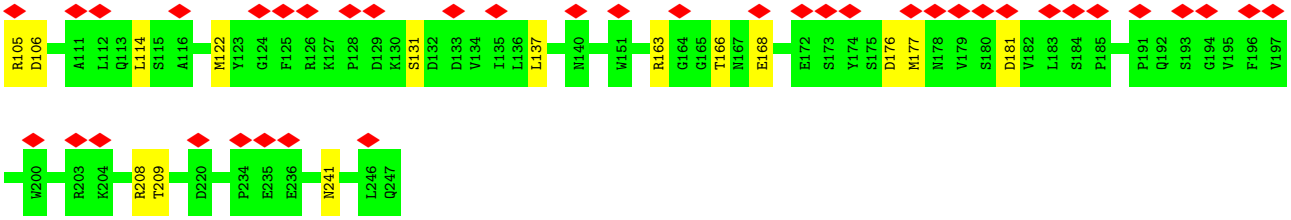




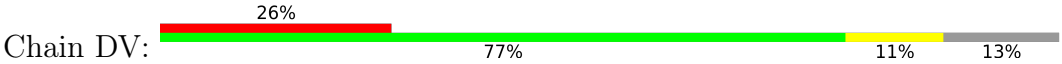
• Molecule 23: ms67

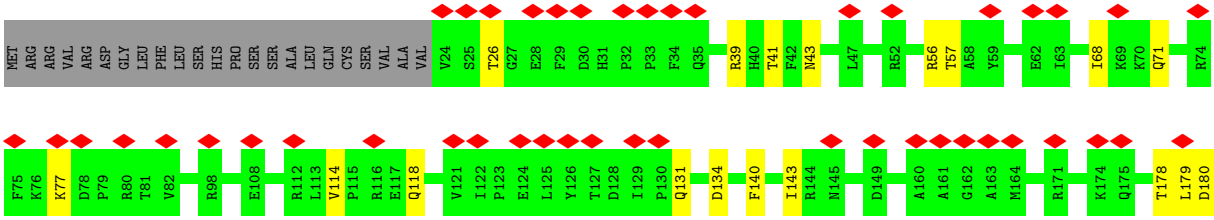
Chain DT:



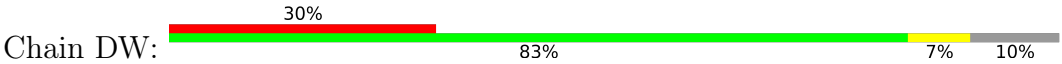


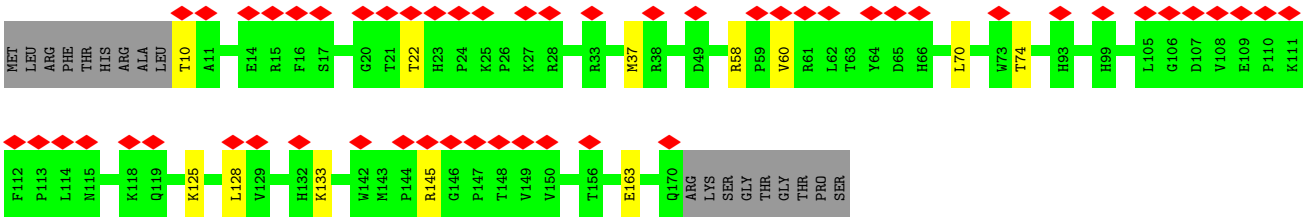
• Molecule 24: ms69



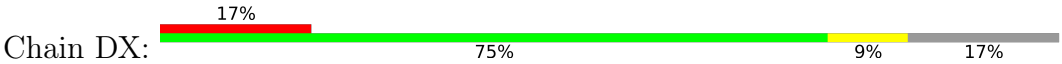


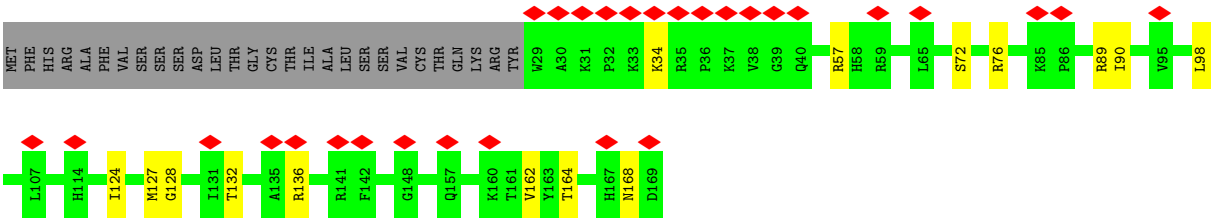
• Molecule 25: ms70



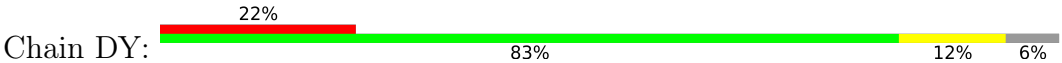


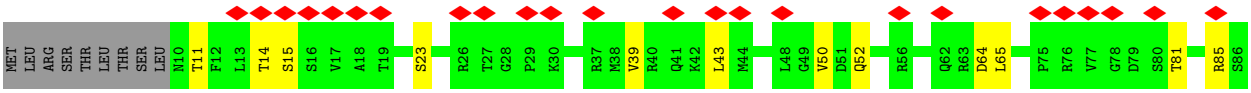
• Molecule 26: ms71

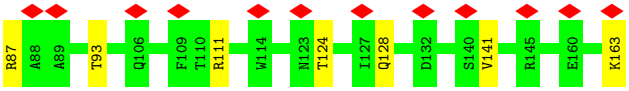




• Molecule 27: ms72

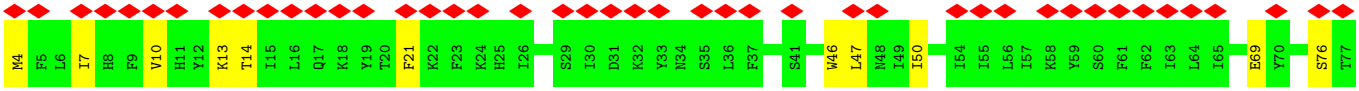






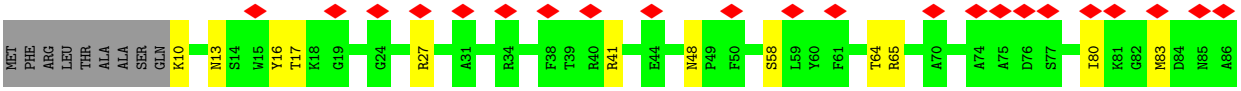
• Molecule 28: uS3m

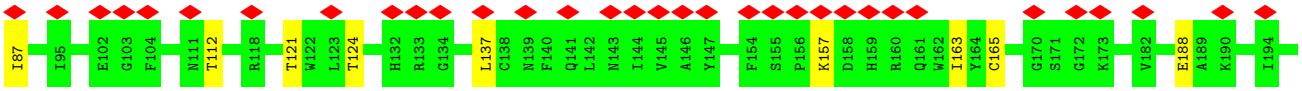
Chain CC:

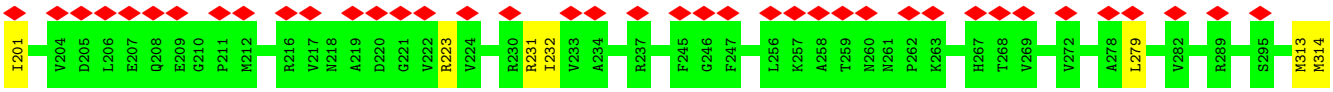


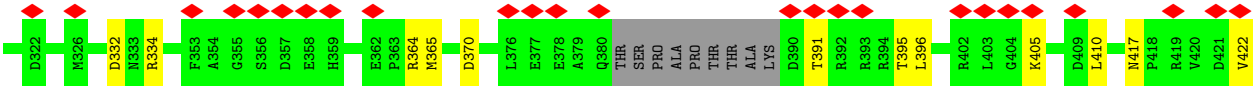
• Molecule 29: uS55m

Chain CE:



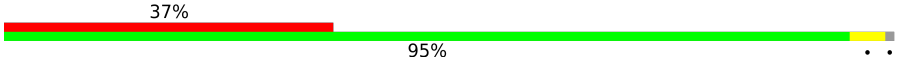


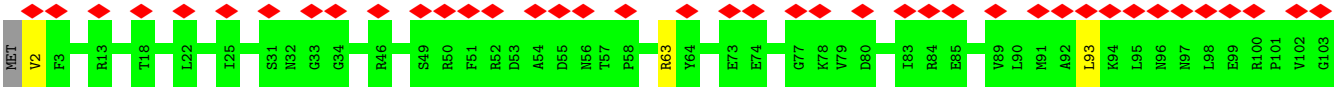




• Molecule 30: bS6m

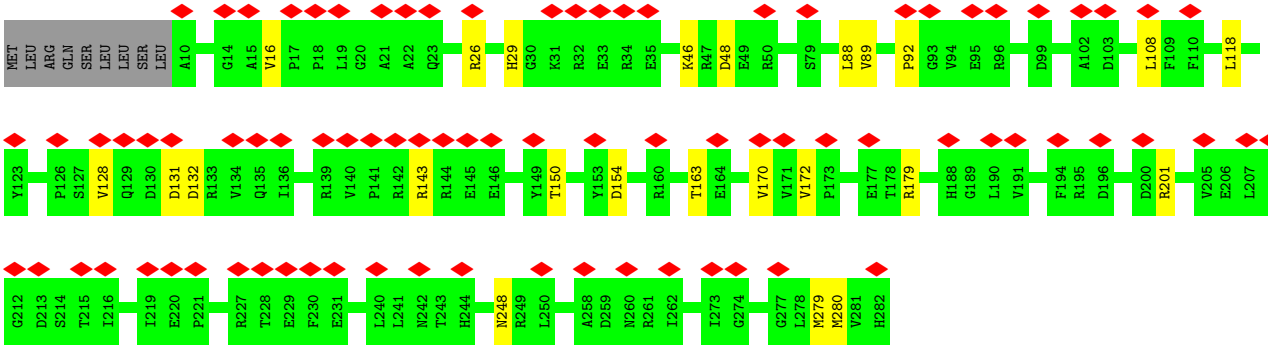
Chain CF:



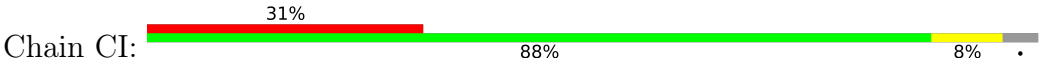


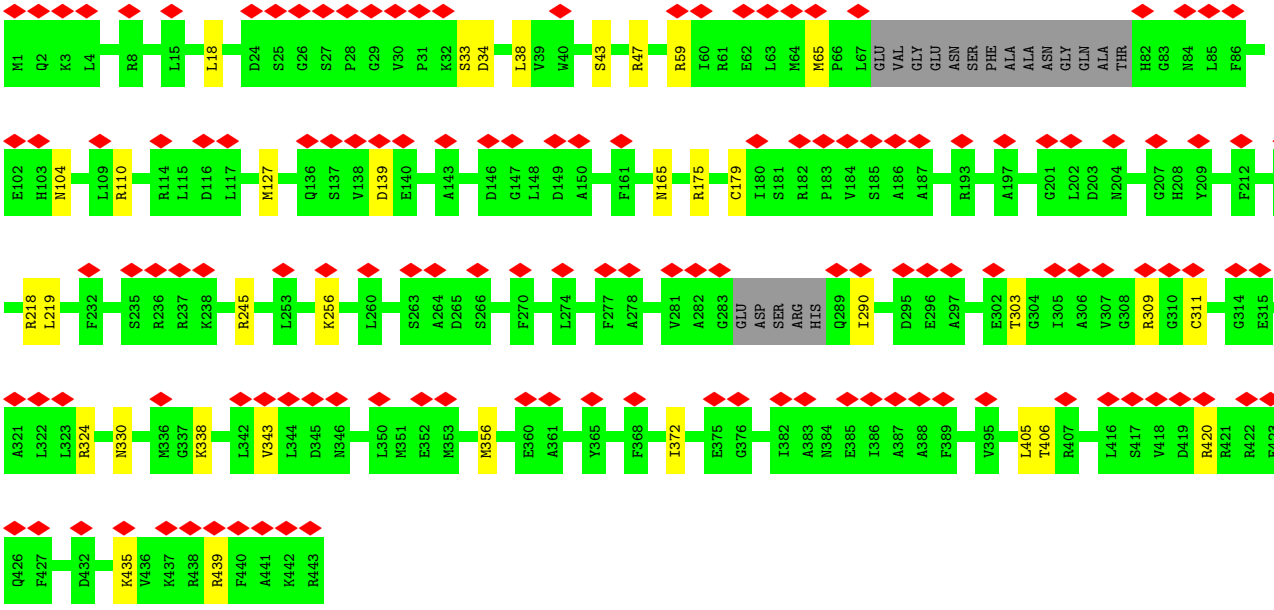
• Molecule 31: uS8m

Chain CH:

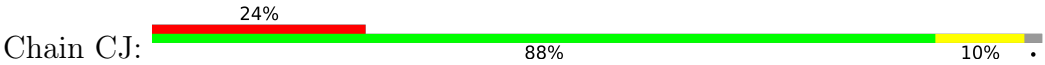


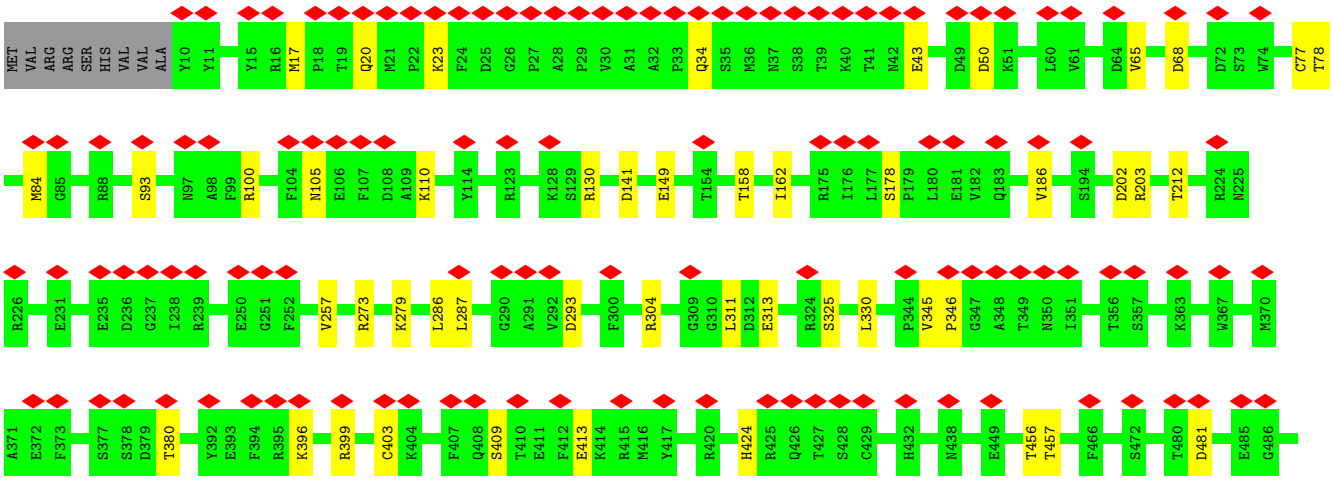
• Molecule 32: uS9m

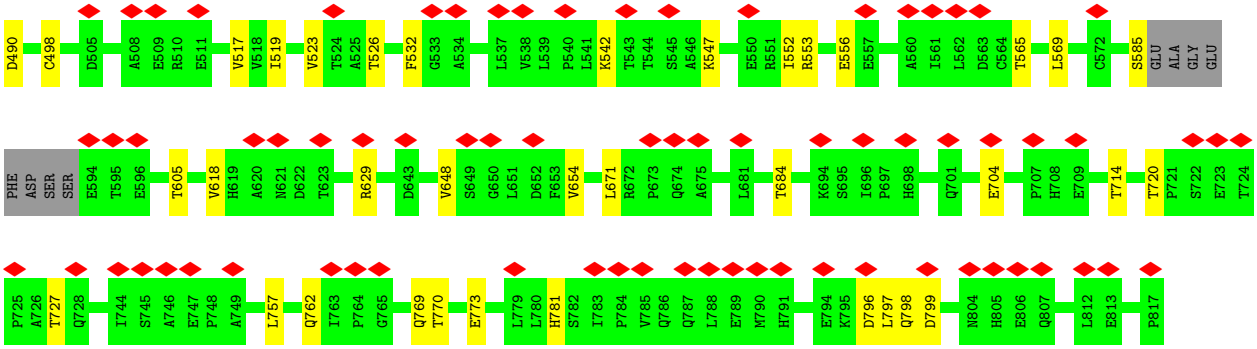




• Molecule 33: uS10m

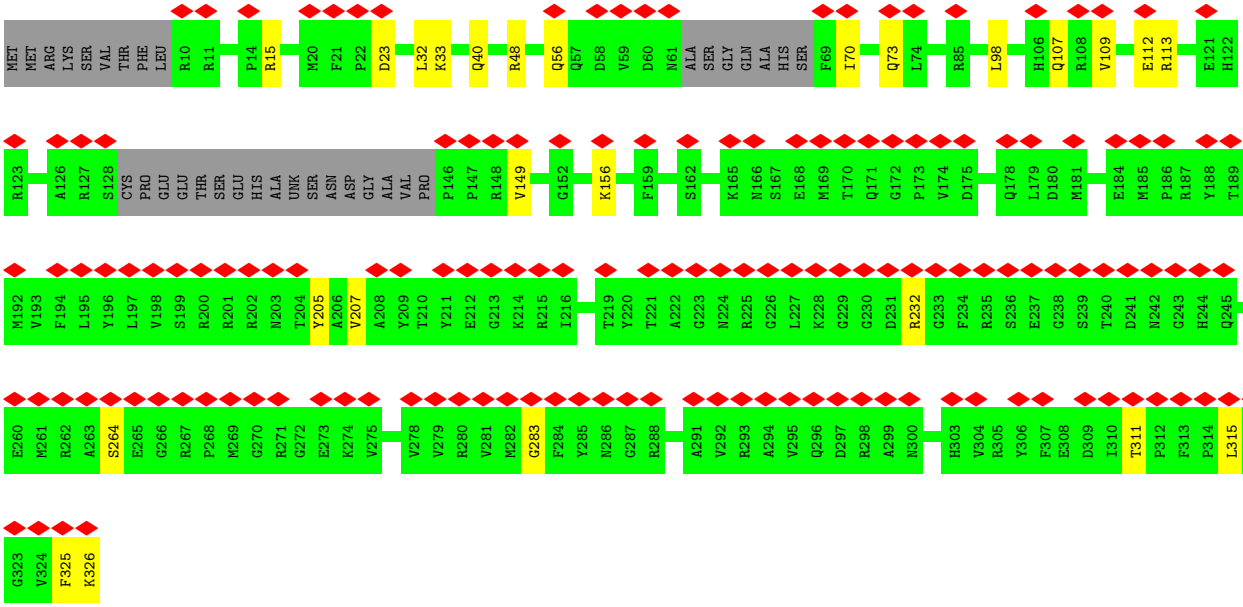






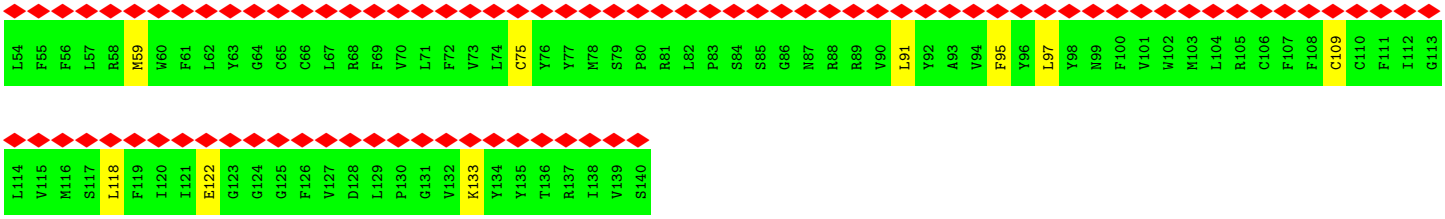
• Molecule 34: uS11m

Chain CK:



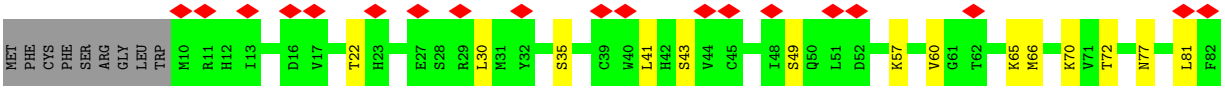
• Molecule 35: uS12

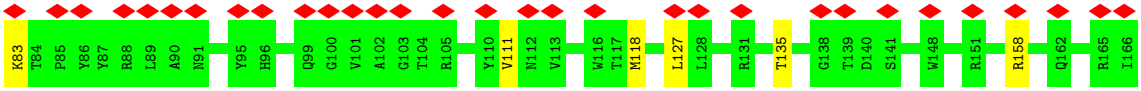
Chain CL:



• Molecule 36: uS14m

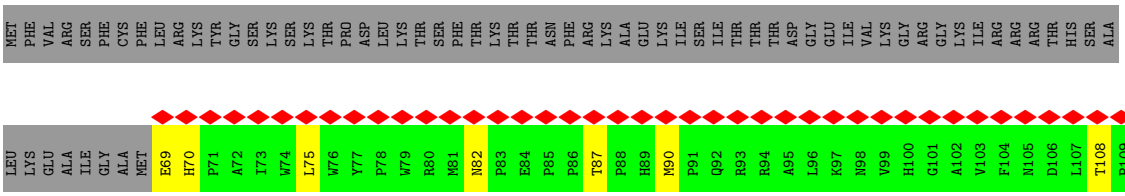
Chain CN:





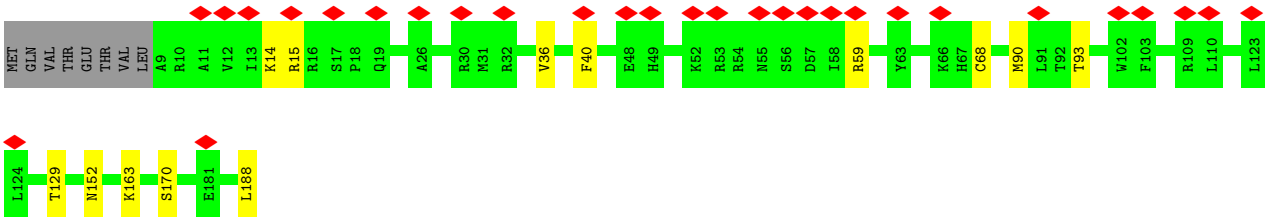
• Molecule 37: uS15m

Chain CO:



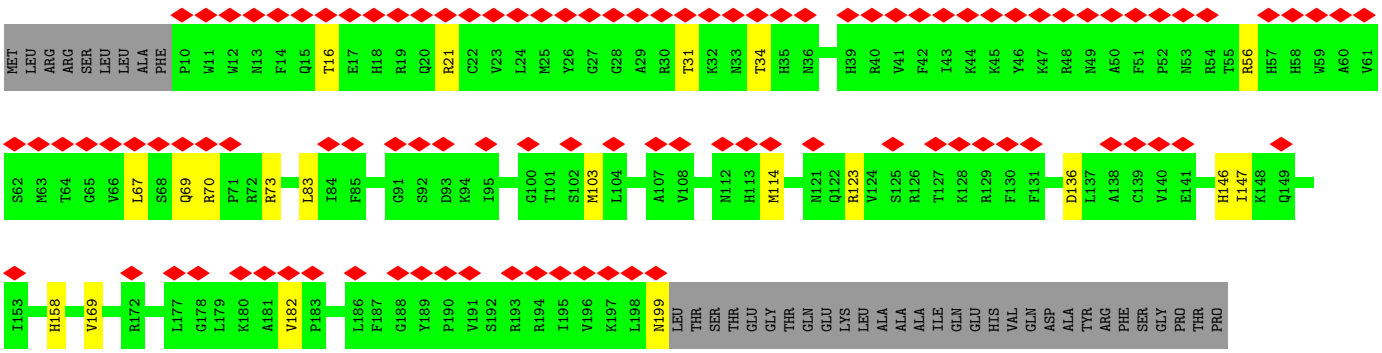
• Molecule 38: bS16m

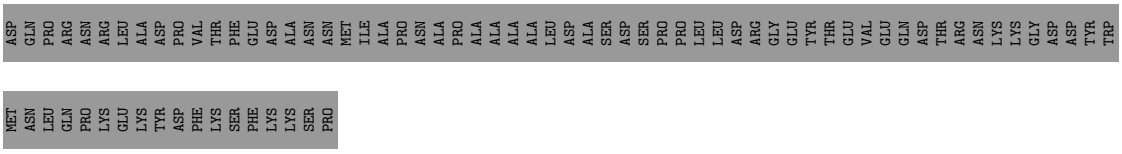
Chain CP:



• Molecule 39: uS17m

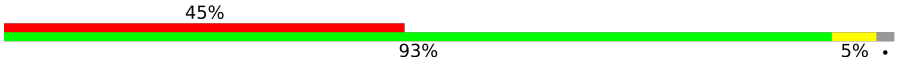
Chain CQ:

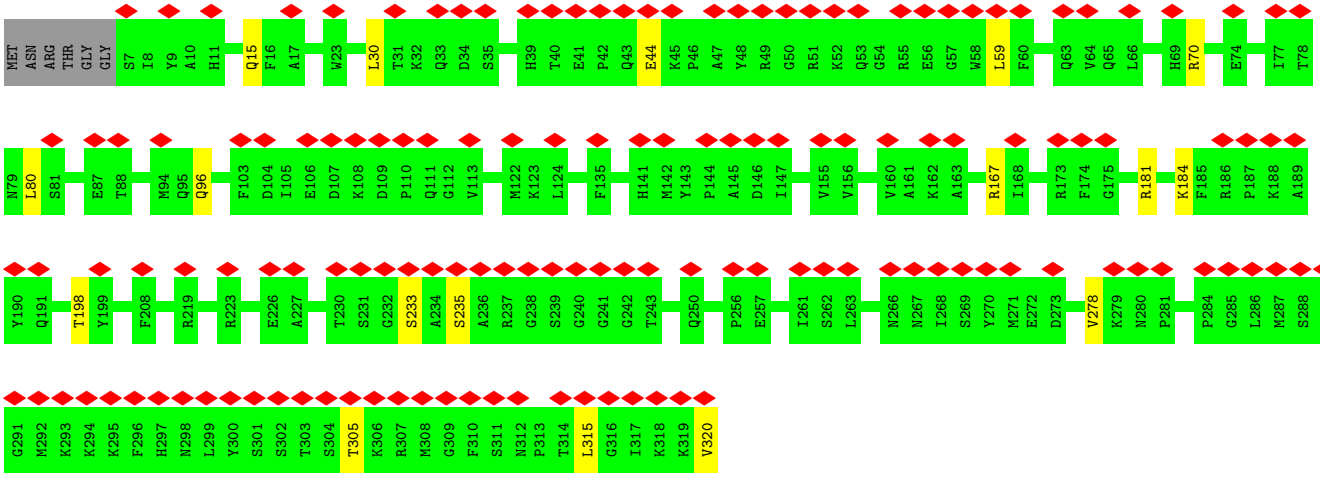




• Molecule 40: bS18m

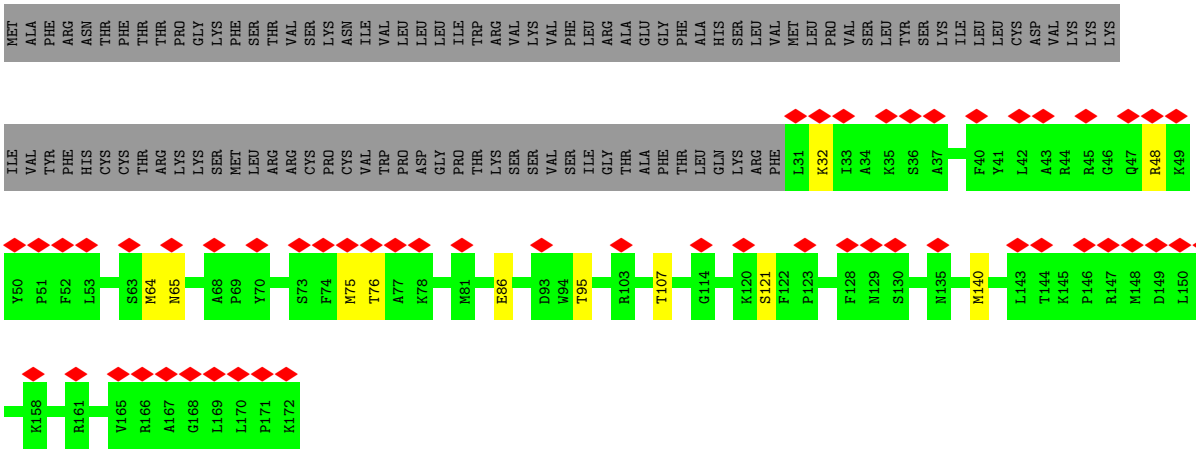
Chain CR:





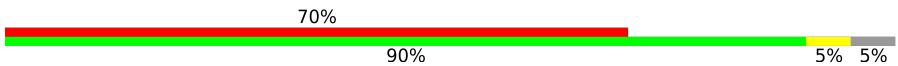
• Molecule 41: uS19m

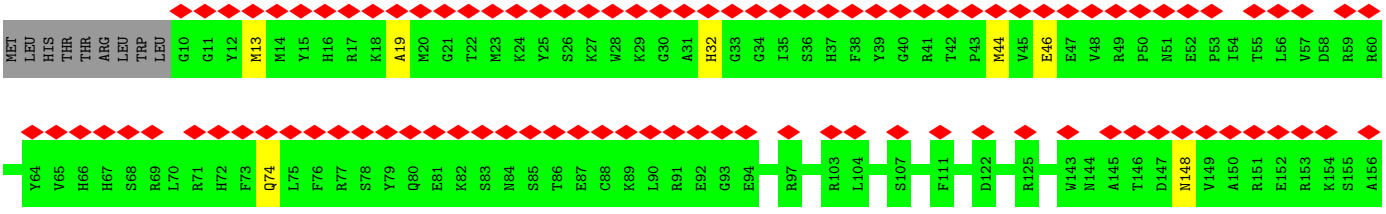
Chain CS:

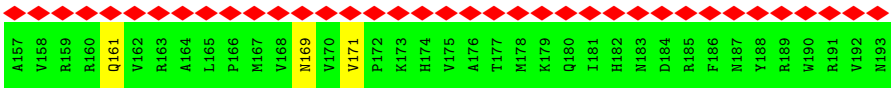


• Molecule 42: bS12m

Chain CU:

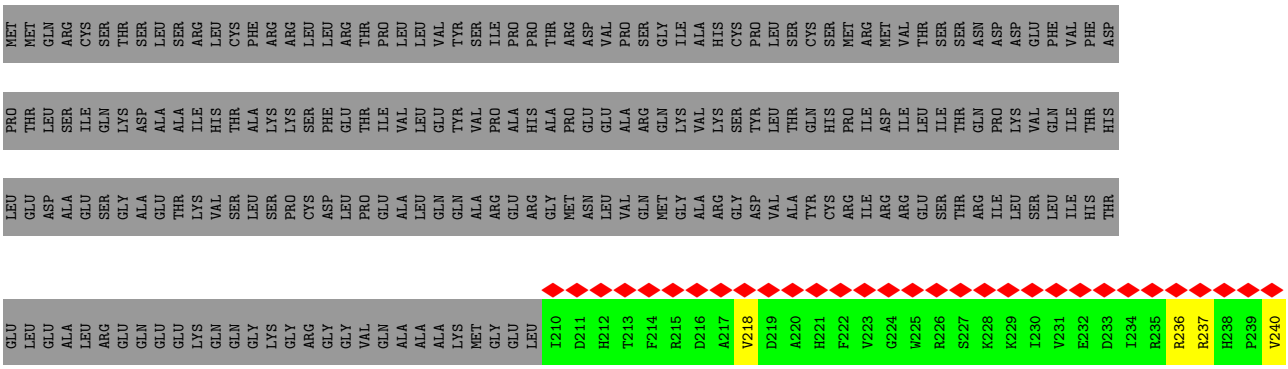






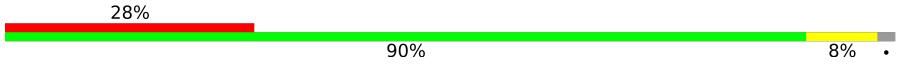
• Molecule 43: mt-IF-3

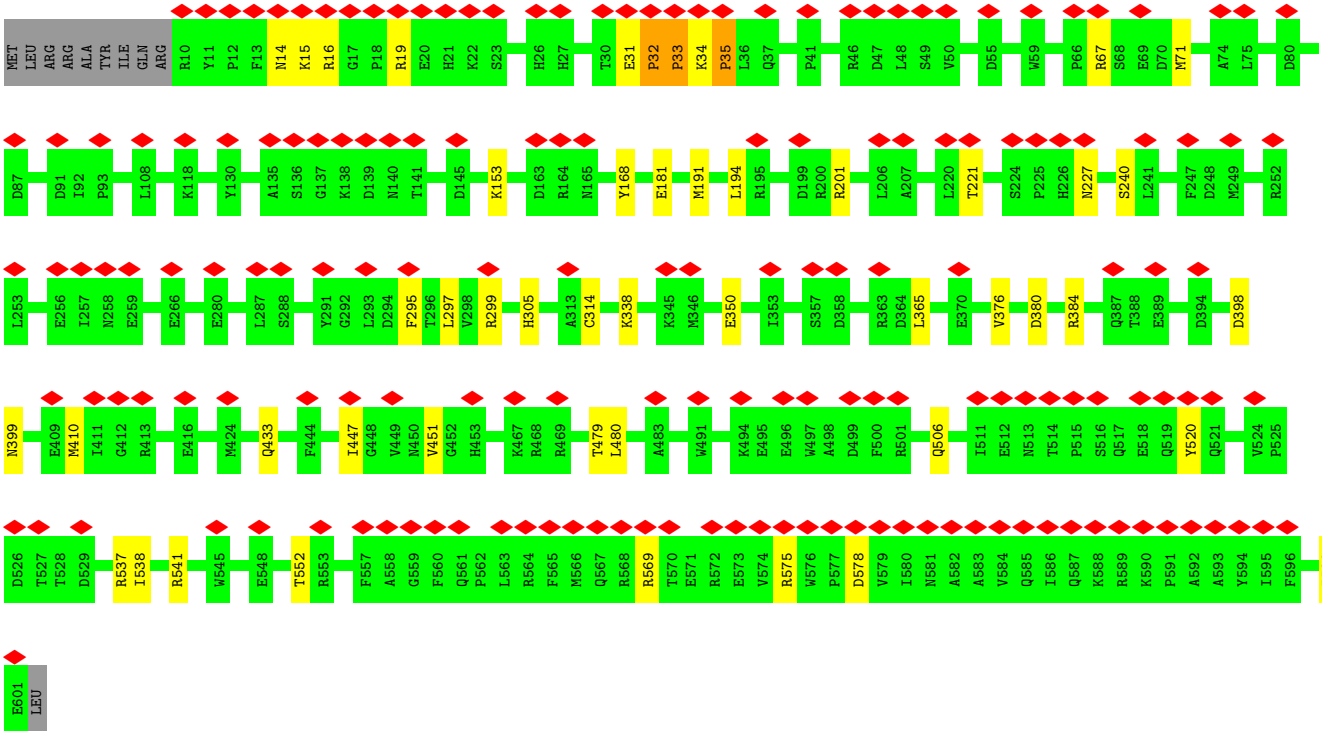
Chain CZ:



• Molecule 44: mS22

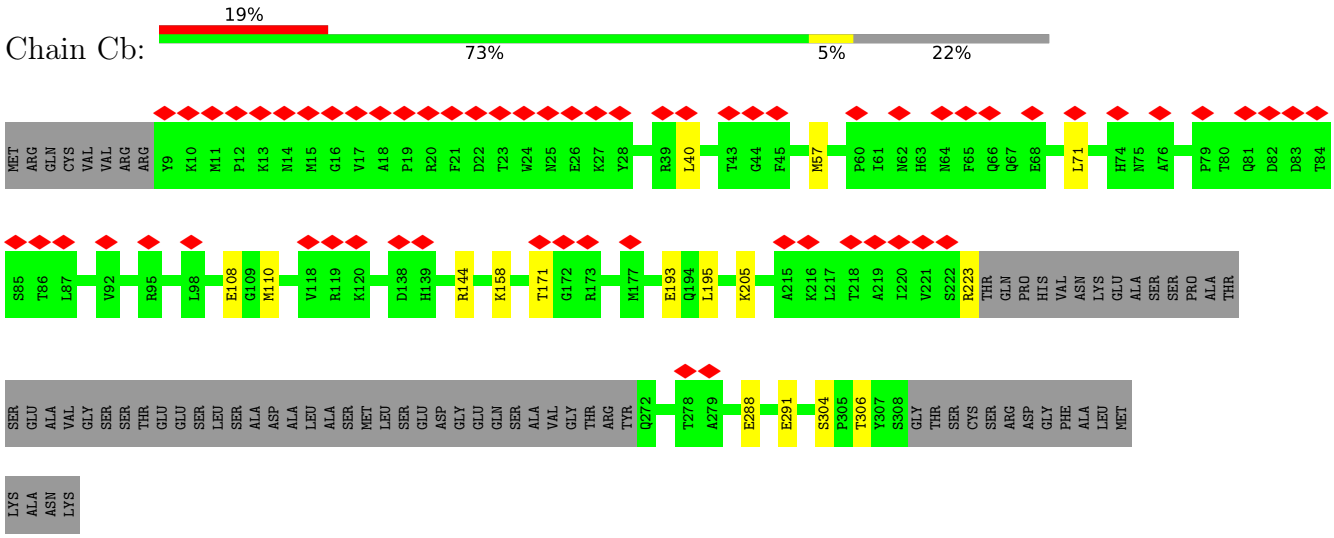
Chain Ca:





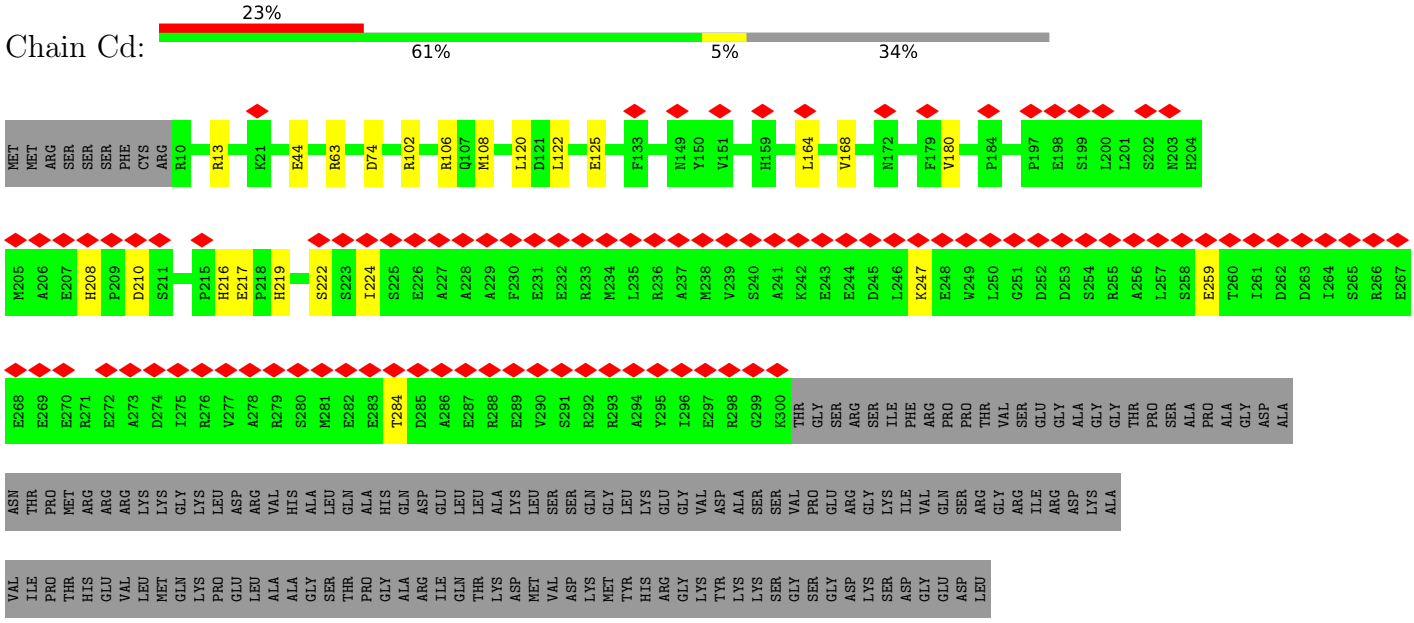
- Molecule 45: mS23

Chain Cb:



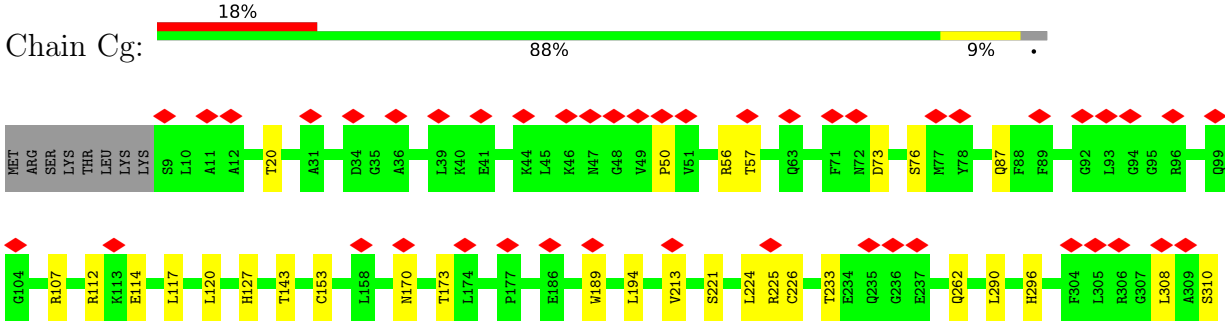
- Molecule 46: mS26

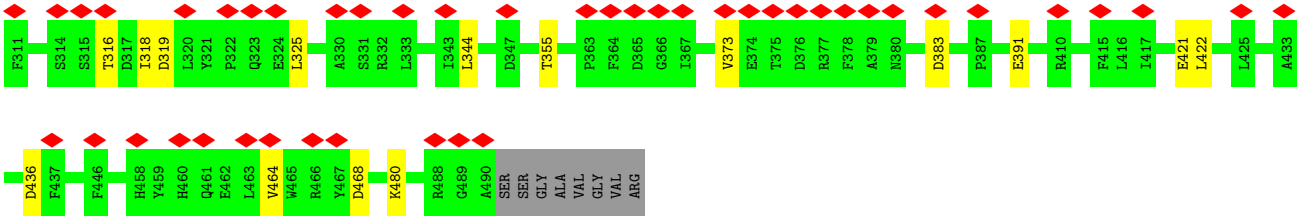
Chain Cd:



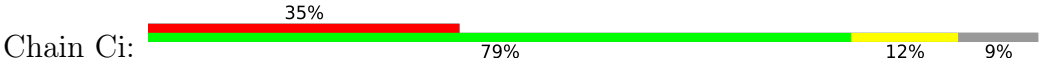
- Molecule 47: mS29

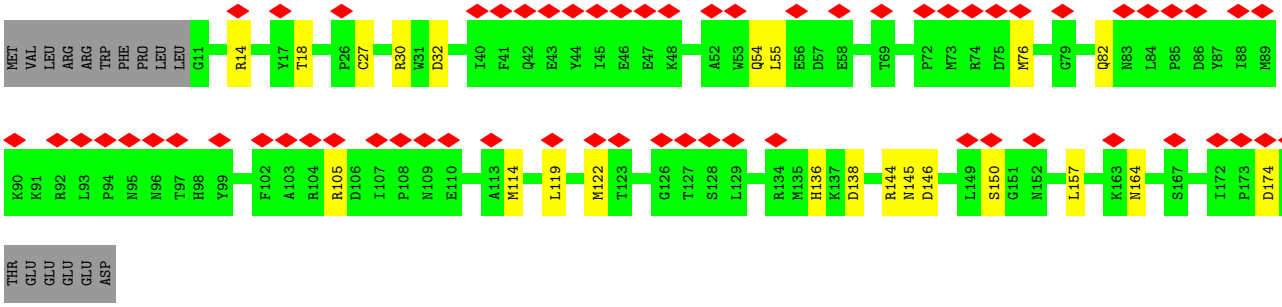
Chain Cg:



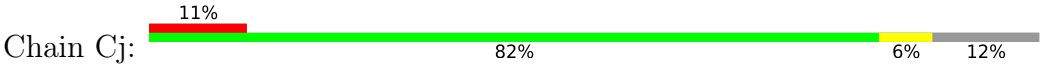


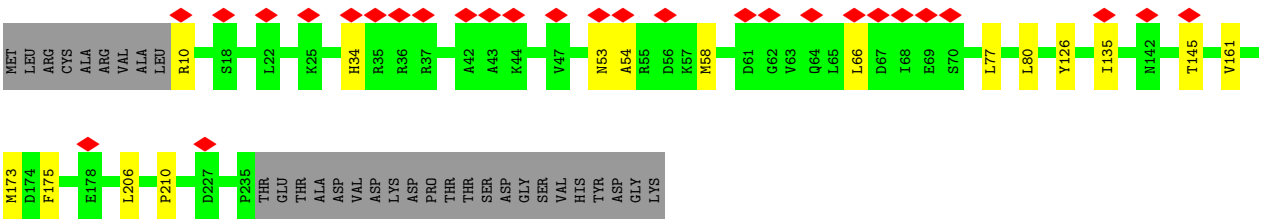
• Molecule 48: mS33



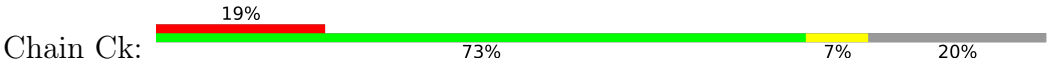


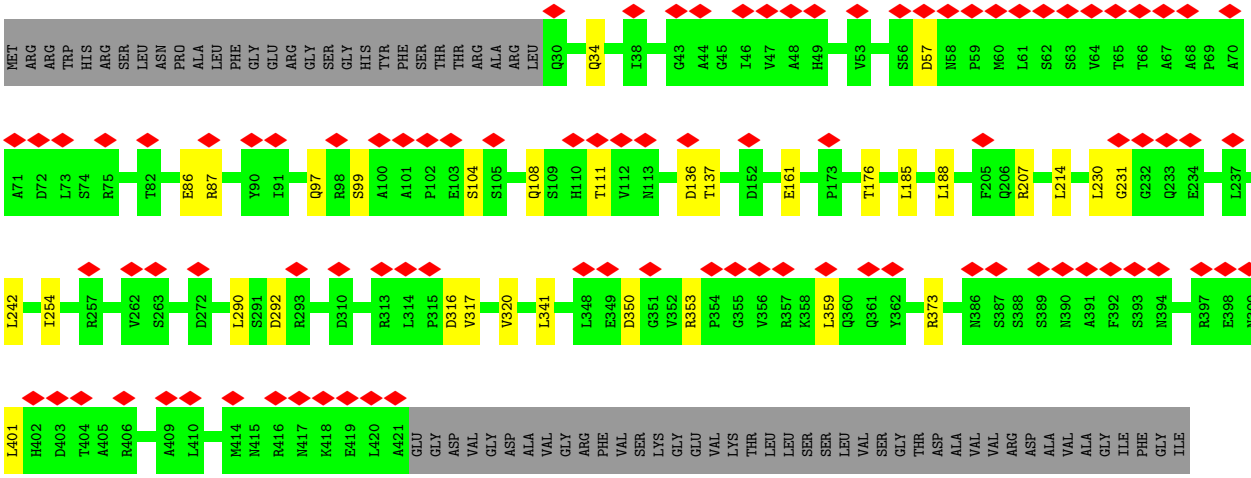
• Molecule 49: mS34

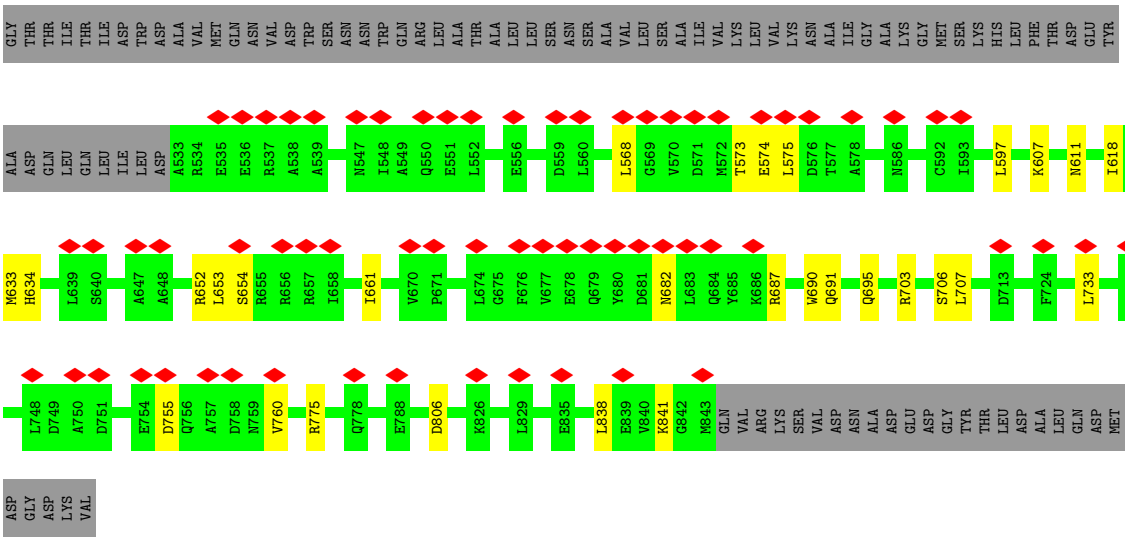


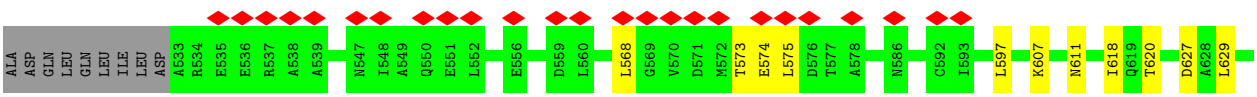


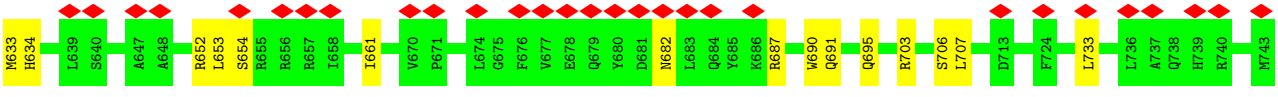
• Molecule 50: mS35





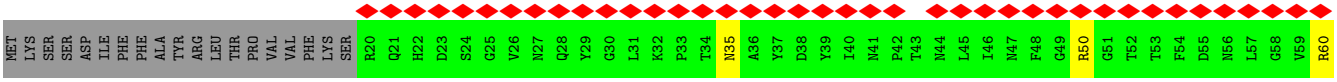


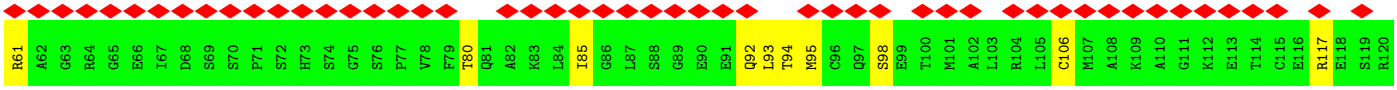


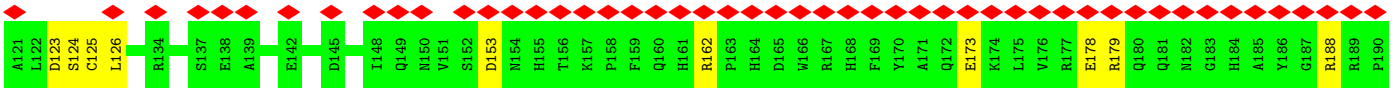


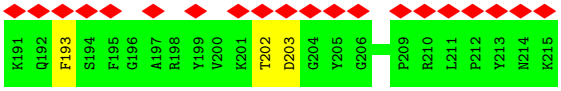
• Molecule 51: mS37

Chain Cm:



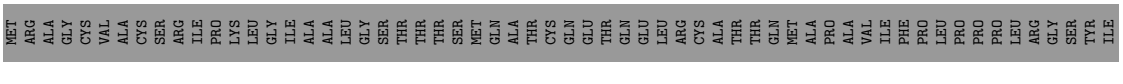


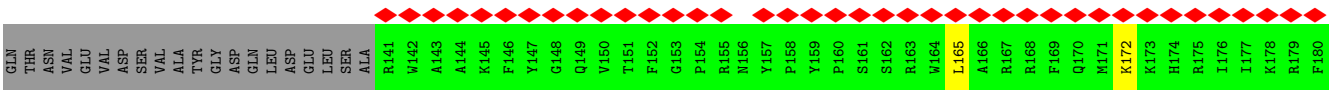


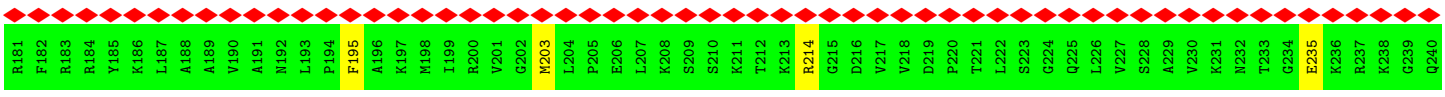


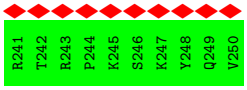
• Molecule 52: mS38

Chain Cn:



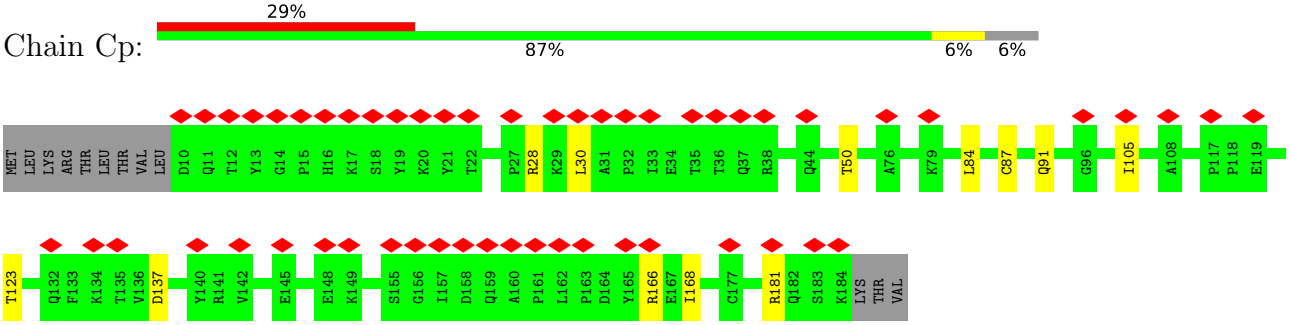






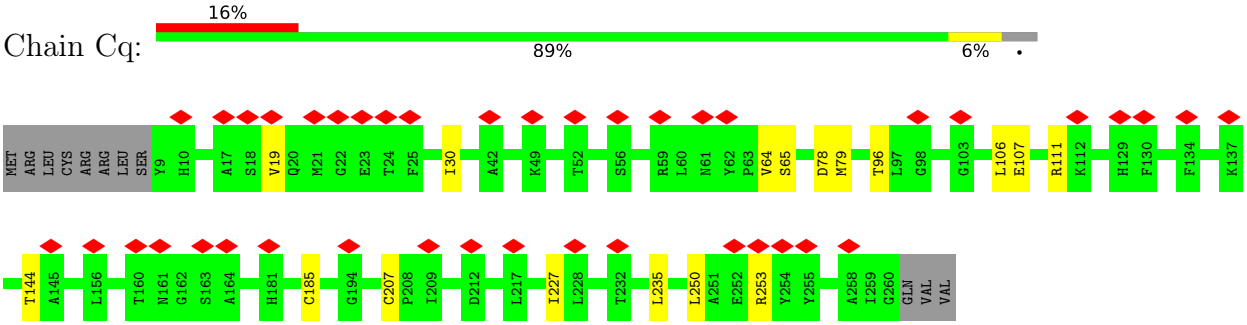
- Molecule 53: ms34

Chain Cp:



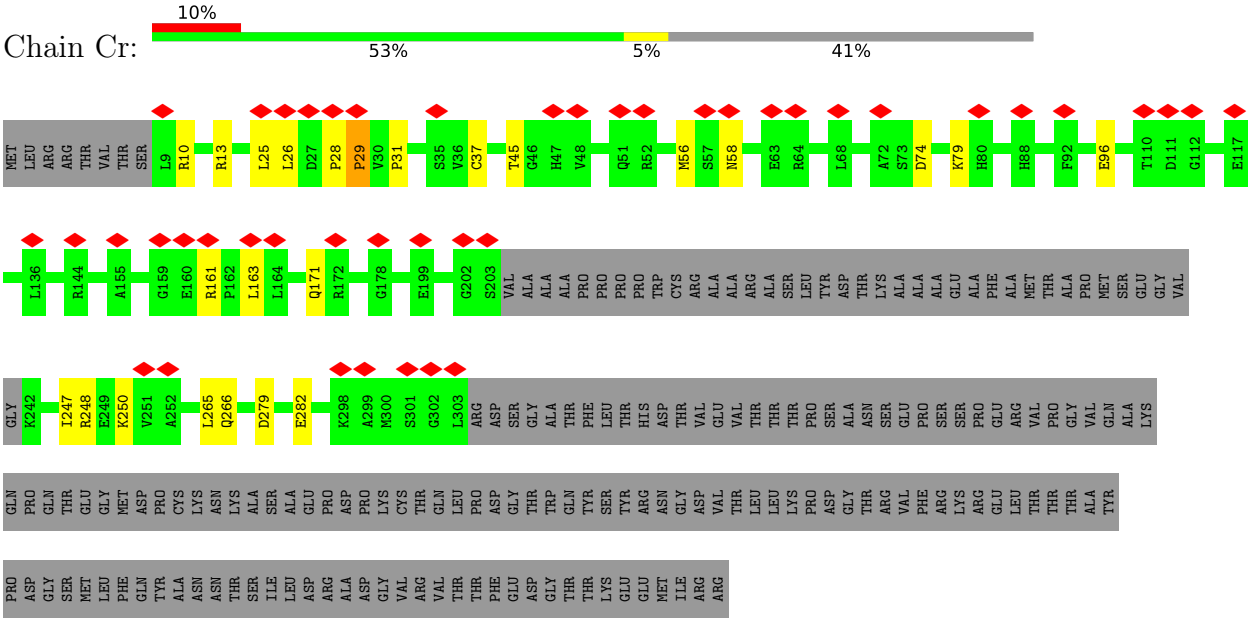
- Molecule 54: ms42

Chain Cq:



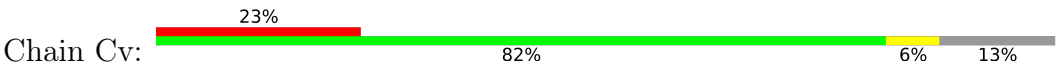
- Molecule 55: mS43

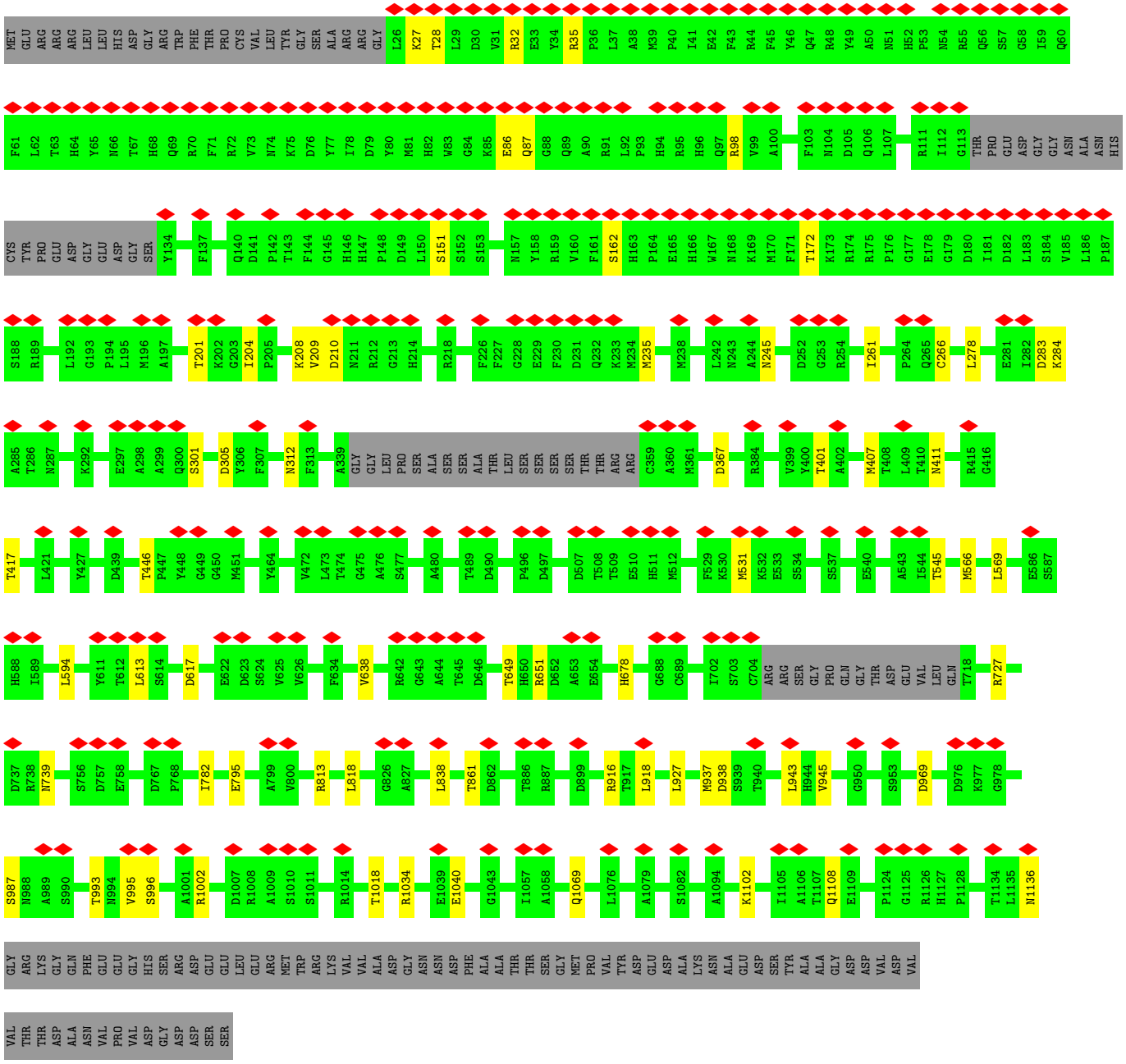
Chain Cr:



- Molecule 56: mS47

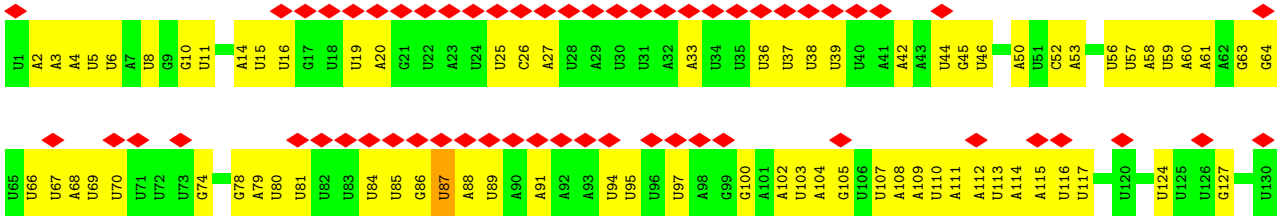
Chain Cv:

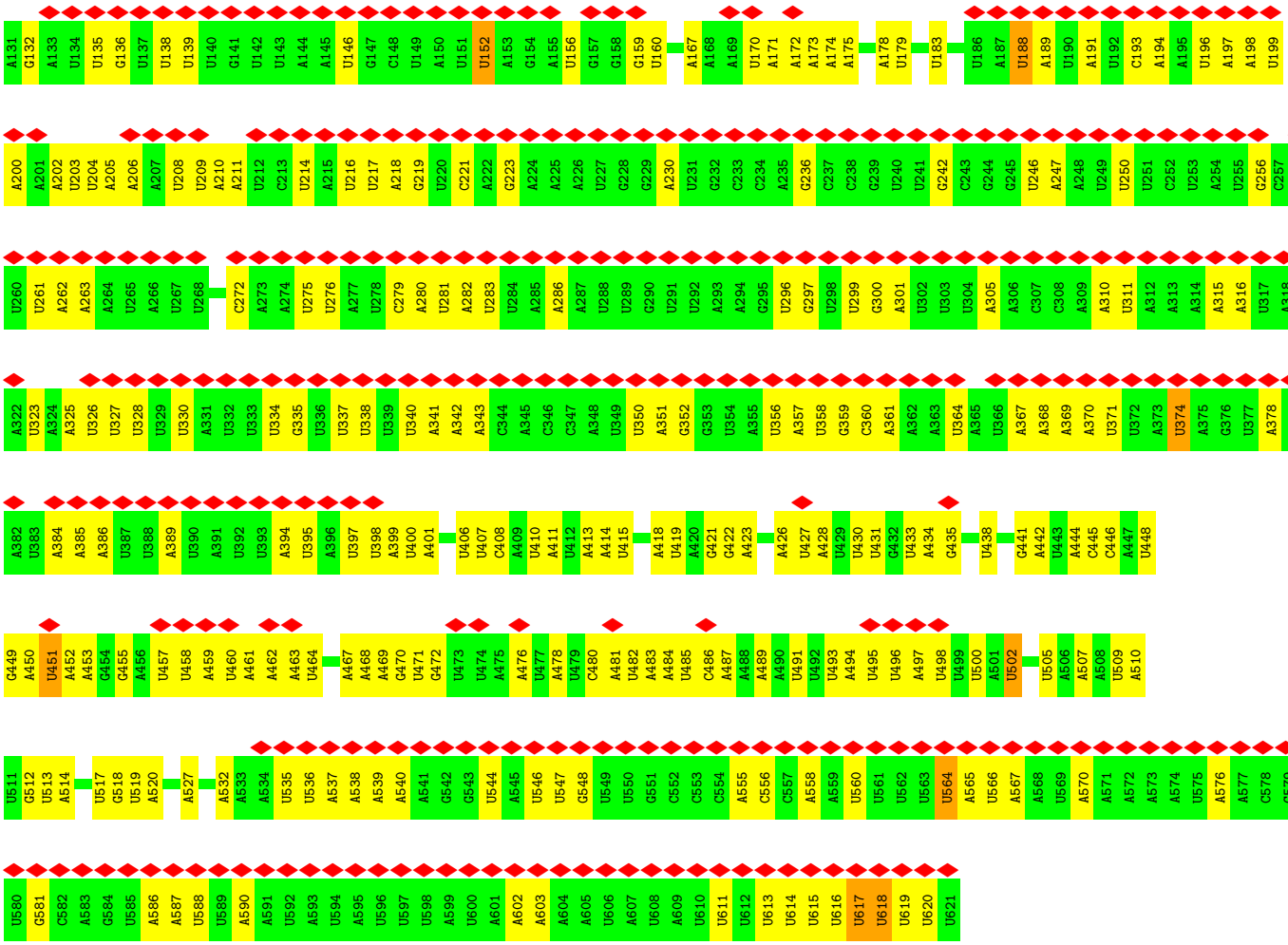




• Molecule 57: 9s rRNA

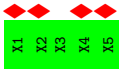
Chain CA:





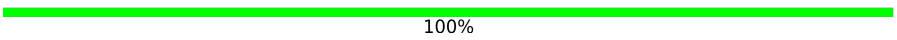
• Molecule 58: UNK

Chain UO:



• Molecule 59: UNK

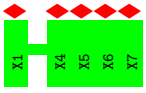
Chain UP:



There are no outlier residues recorded for this chain.

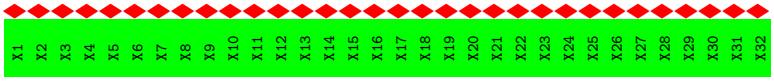
• Molecule 59: UNK

Chain UW:



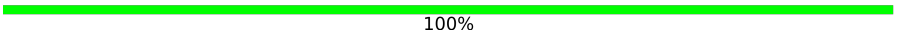
• Molecule 60: UNK

Chain UQ:



• Molecule 61: UNK

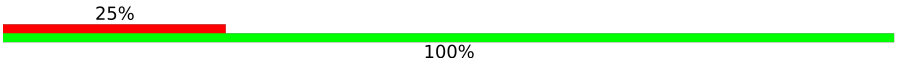
Chain UR:

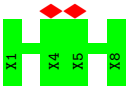


There are no outlier residues recorded for this chain.

• Molecule 61: UNK

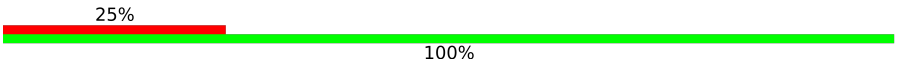
Chain UV:

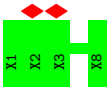




• Molecule 61: UNK

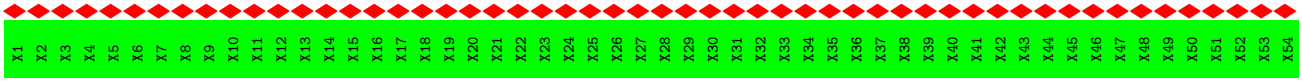
Chain UX:





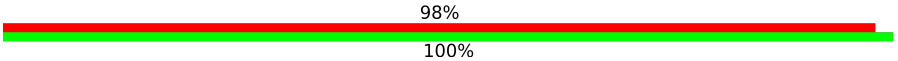
• Molecule 62: UNK

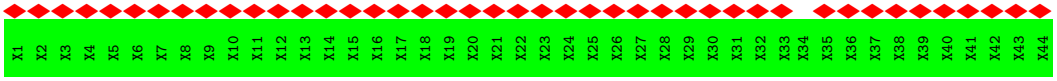
Chain US:



• Molecule 63: UNK

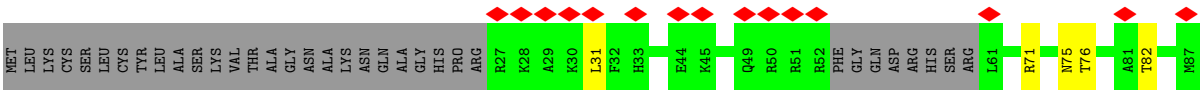
Chain UT:

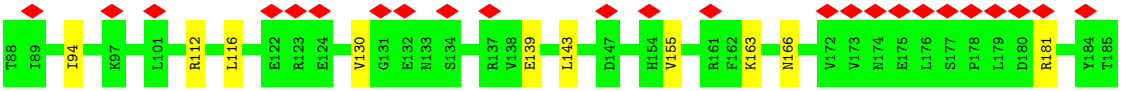




• Molecule 64: bL27m

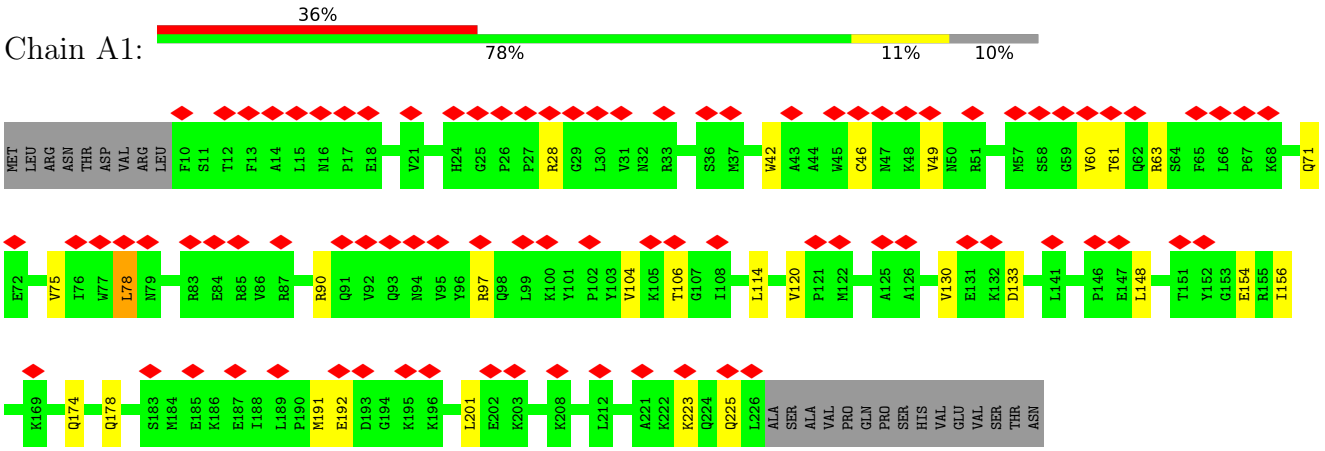
Chain A0:





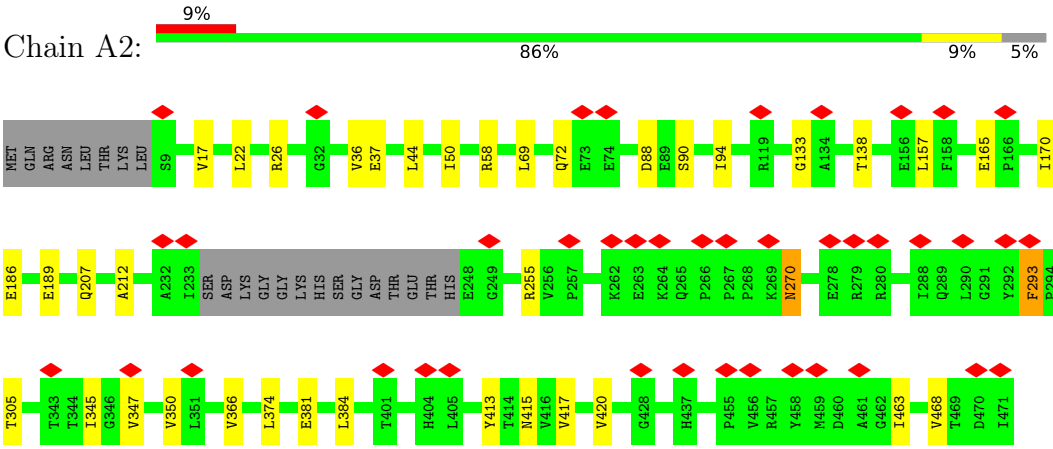
• Molecule 65: bL28m

Chain A1:



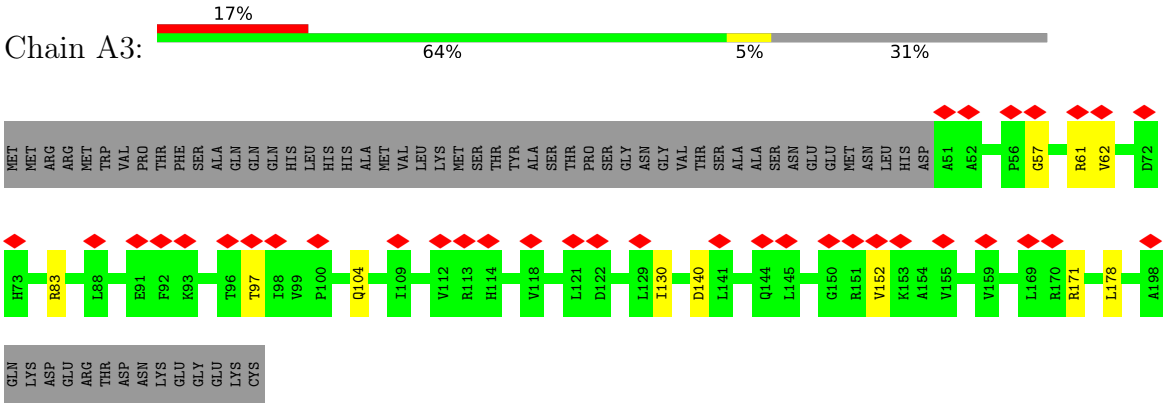
• Molecule 66: uL29m

Chain A2:



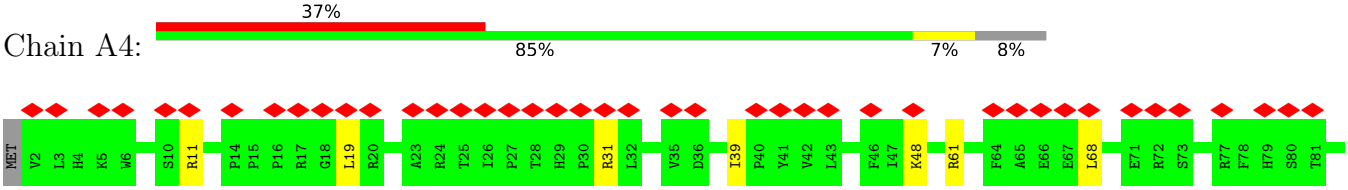
• Molecule 67: uL30m

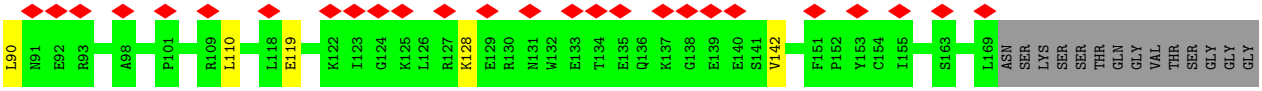
Chain A3:



• Molecule 68: bL31m

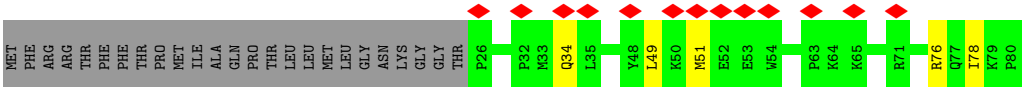
Chain A4:





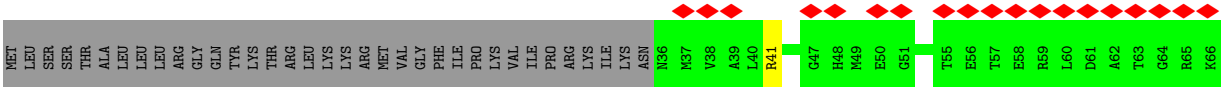
• Molecule 69: bL32m

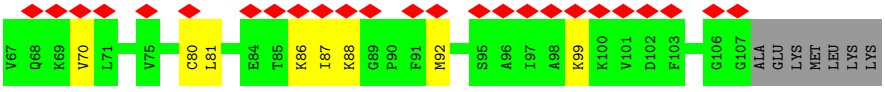
Chain A5:



• Molecule 70: bL33m

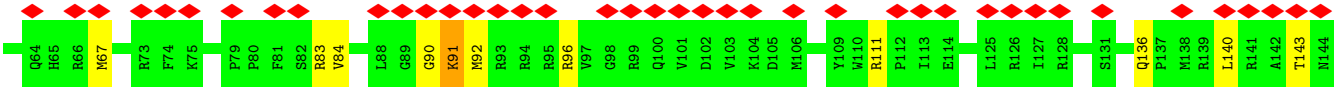
Chain A6:

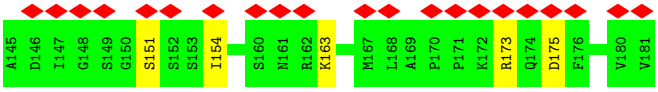




• Molecule 71: bL35m

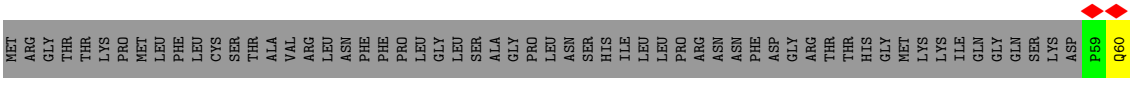
Chain A8:

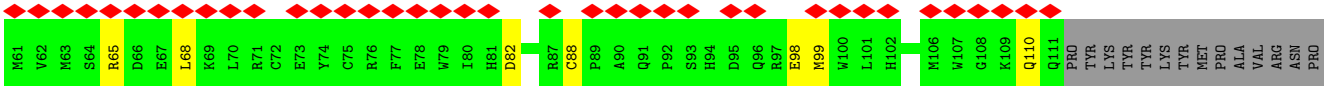


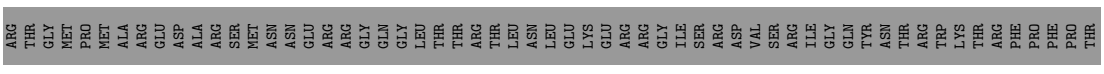


• Molecule 72: bL36m

Chain A9:

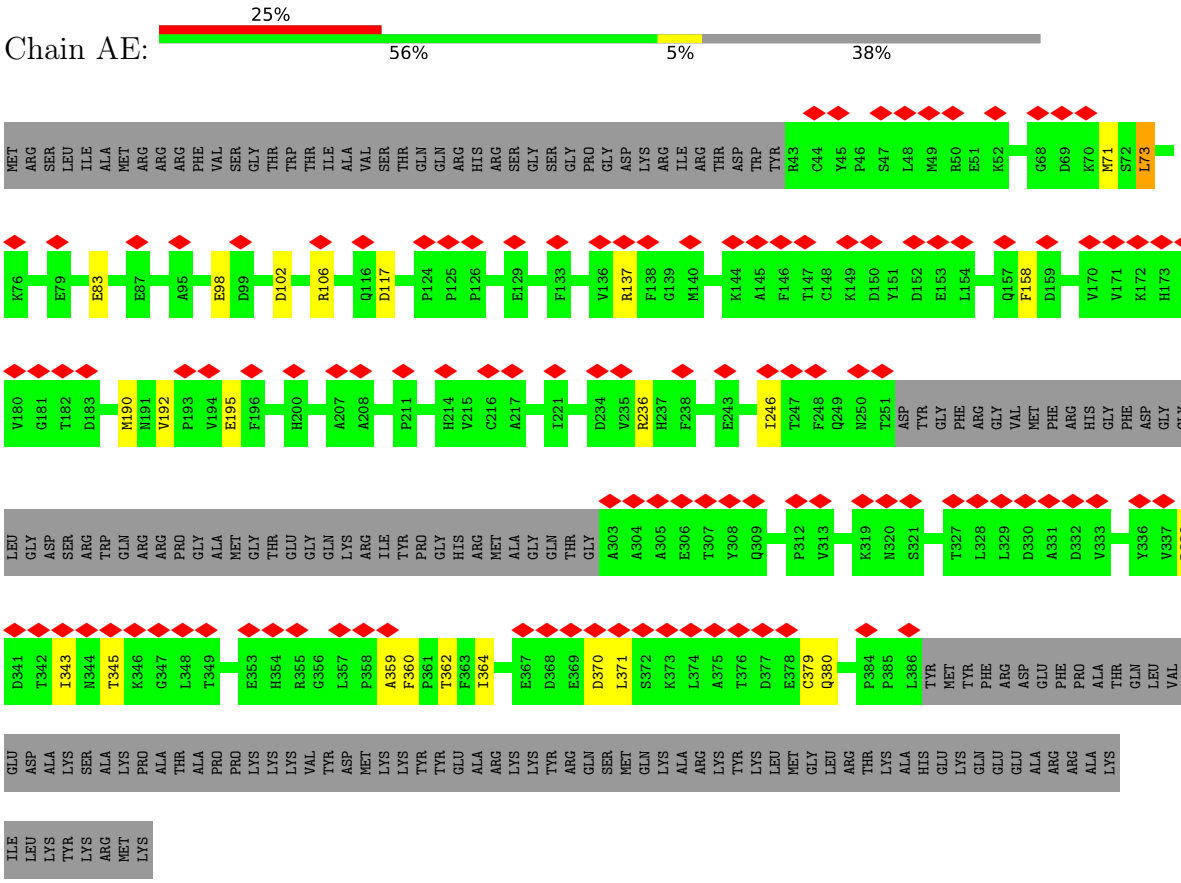






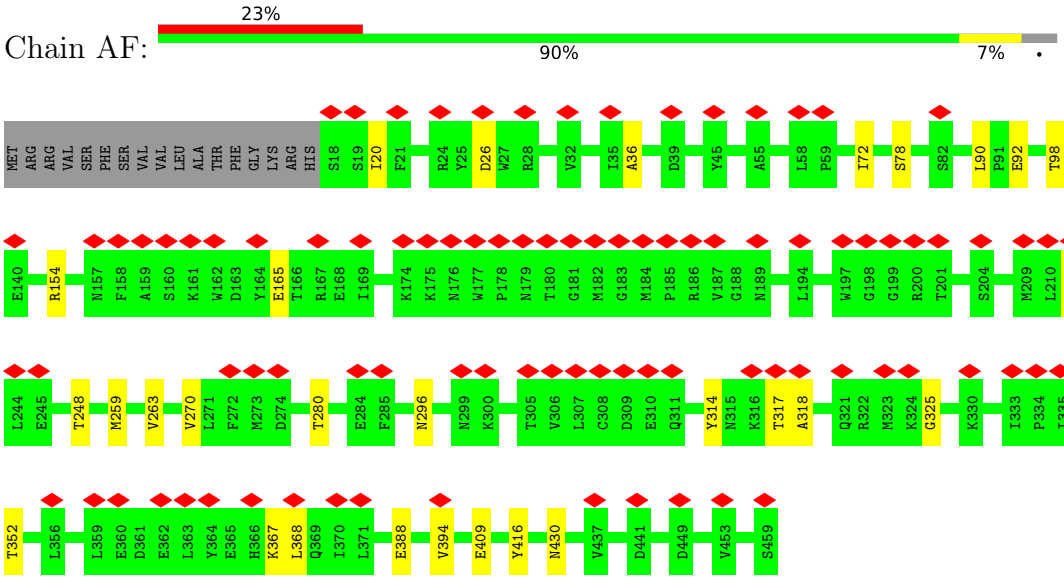
• Molecule 73: uL3m

Chain AE:



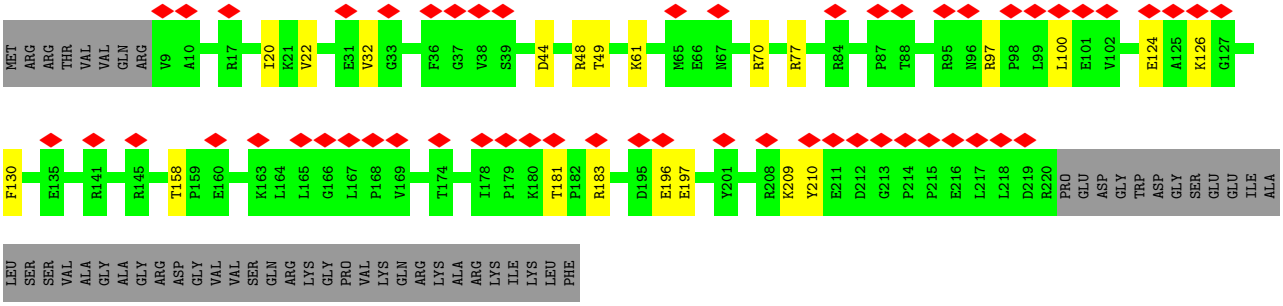
• Molecule 74: uL4m

Chain AF:



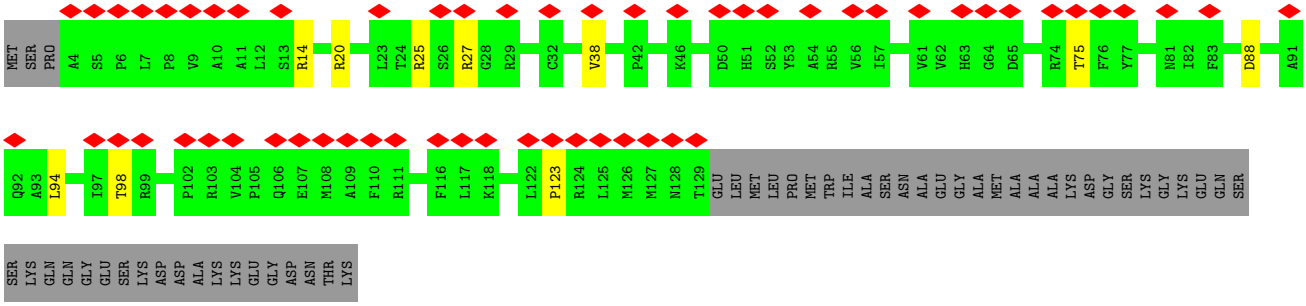
• Molecule 75: bL9m

Chain AI:



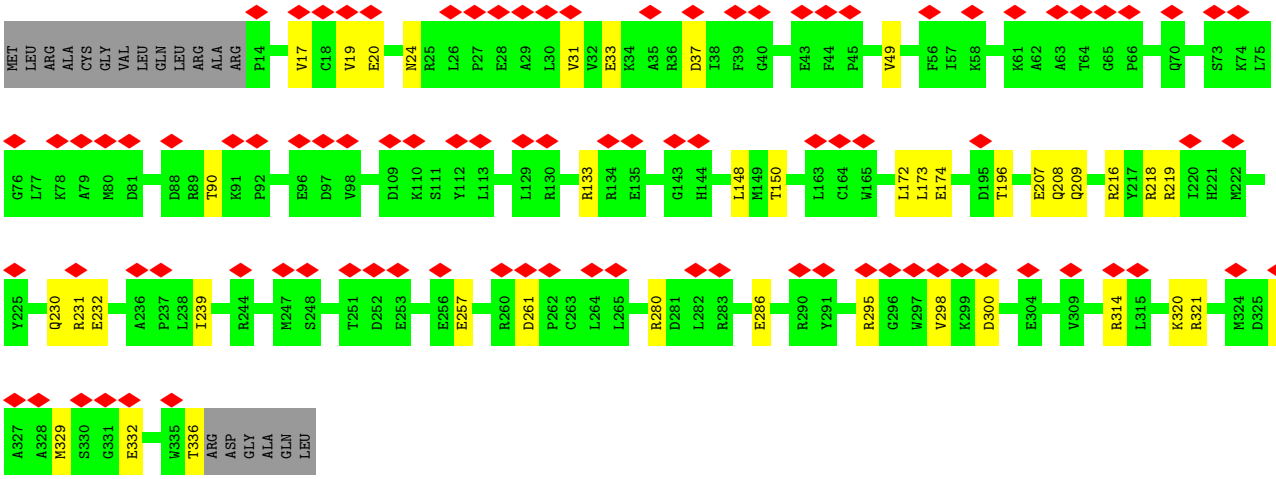
• Molecule 76: uL10m

Chain AJ:



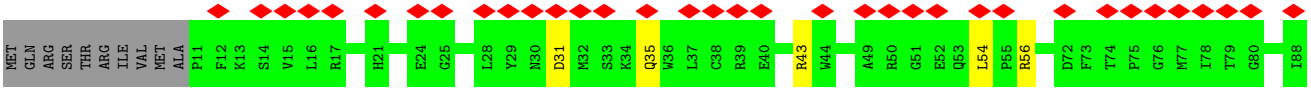
• Molecule 77: uL11m

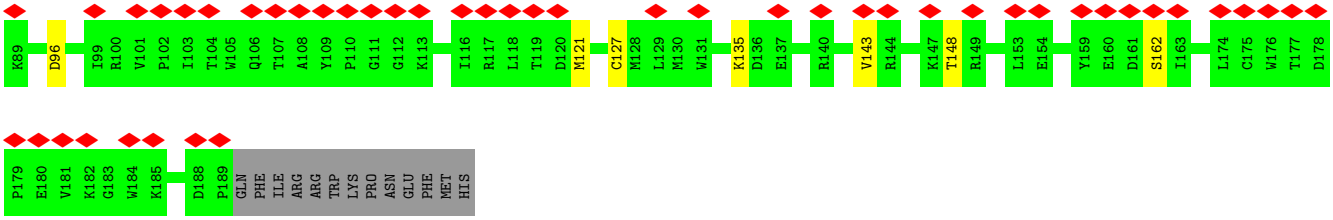
Chain AK:



• Molecule 78: 50S ribosomal protein L13, putative

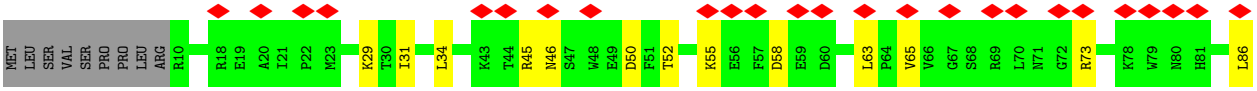
Chain AN:





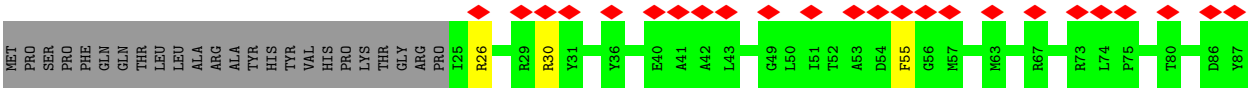
• Molecule 79: uL15m

Chain AP:



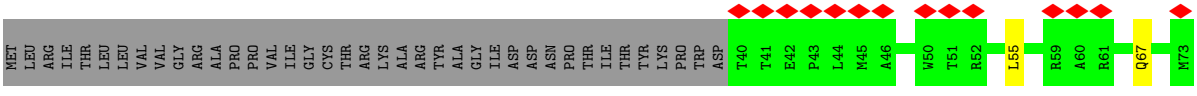
• Molecule 80: 50S ribosomal protein L16, putative

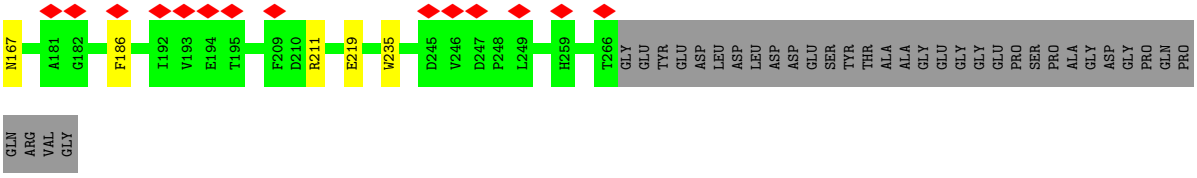
Chain AQ:



• Molecule 81: 50S ribosomal protein L17, putative

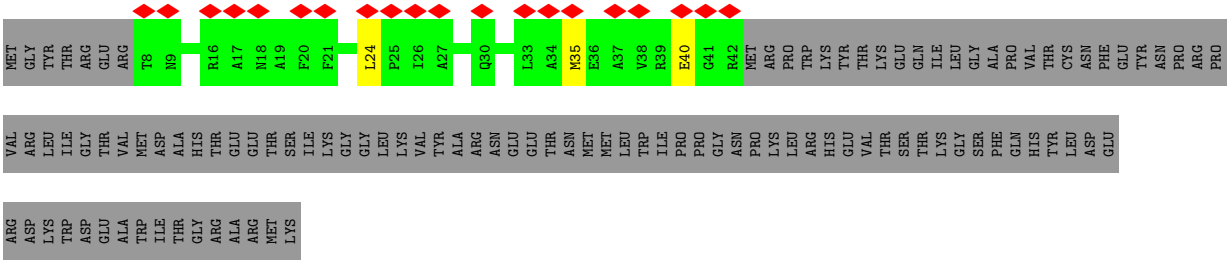
Chain AR:





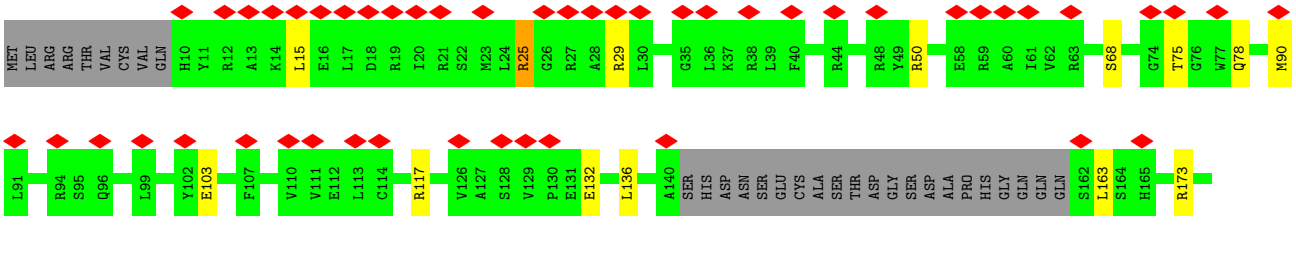
• Molecule 82: bL19m

Chain AT:



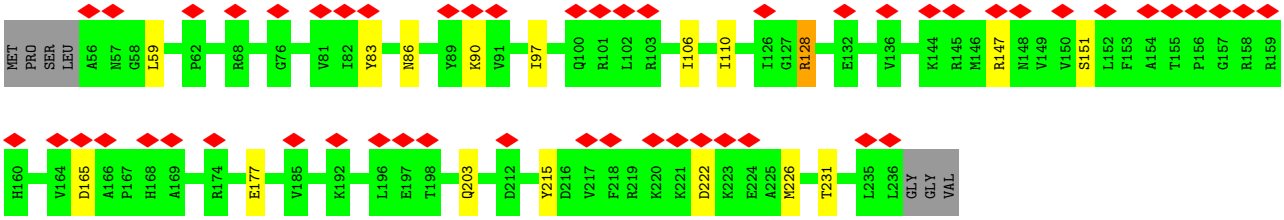
• Molecule 83: bL20m

Chain AU:



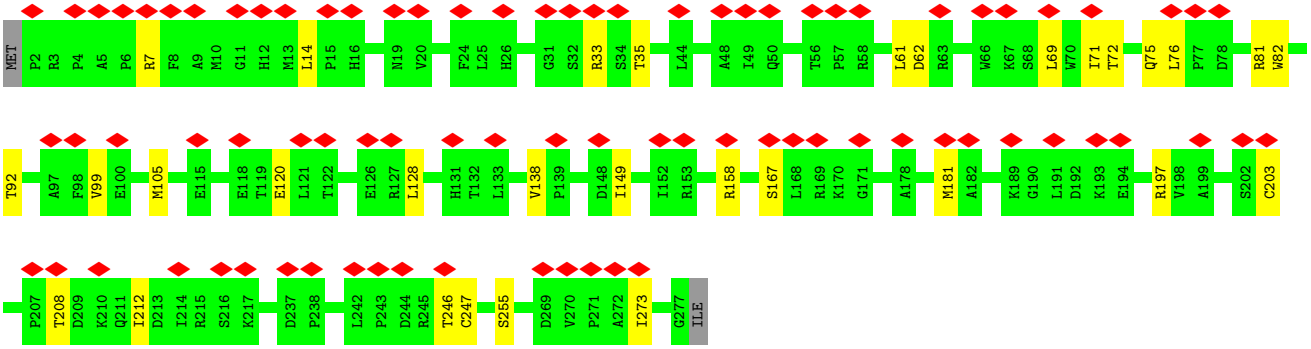
• Molecule 84: bL21m

Chain AV:

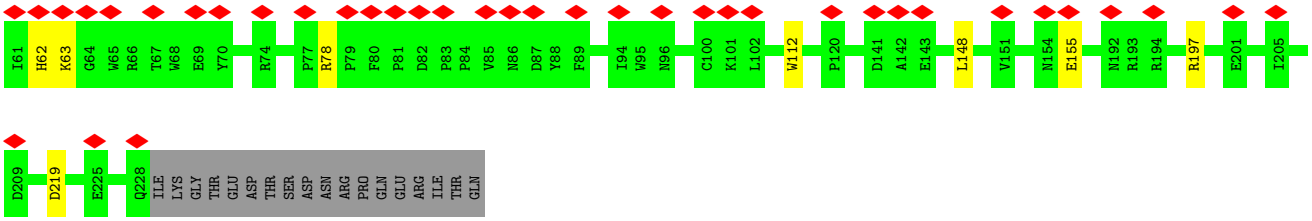


• Molecule 85: uL22m

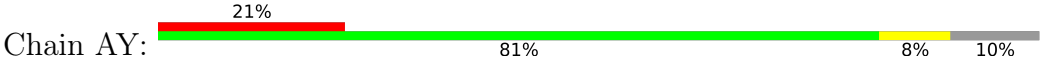
Chain AW:

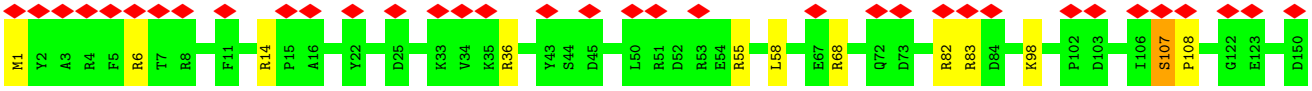


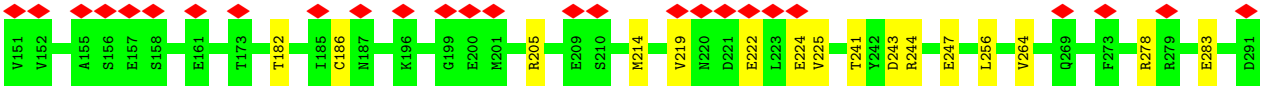
• Molecule 86: uL23m

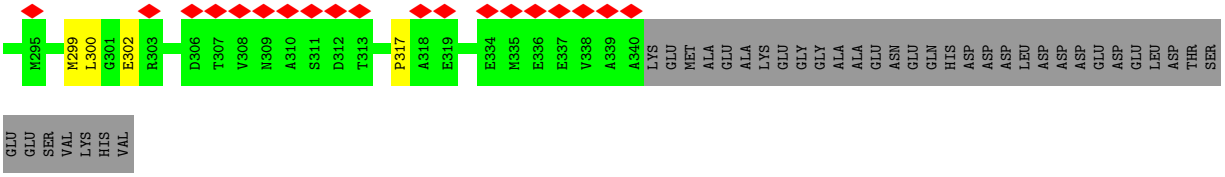


• Molecule 87: uL24m

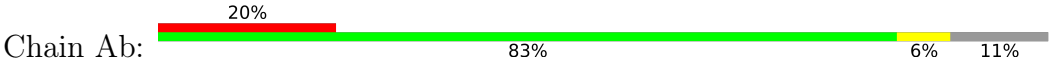


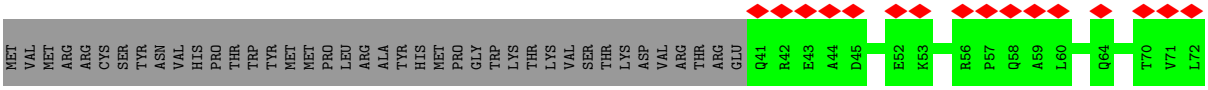


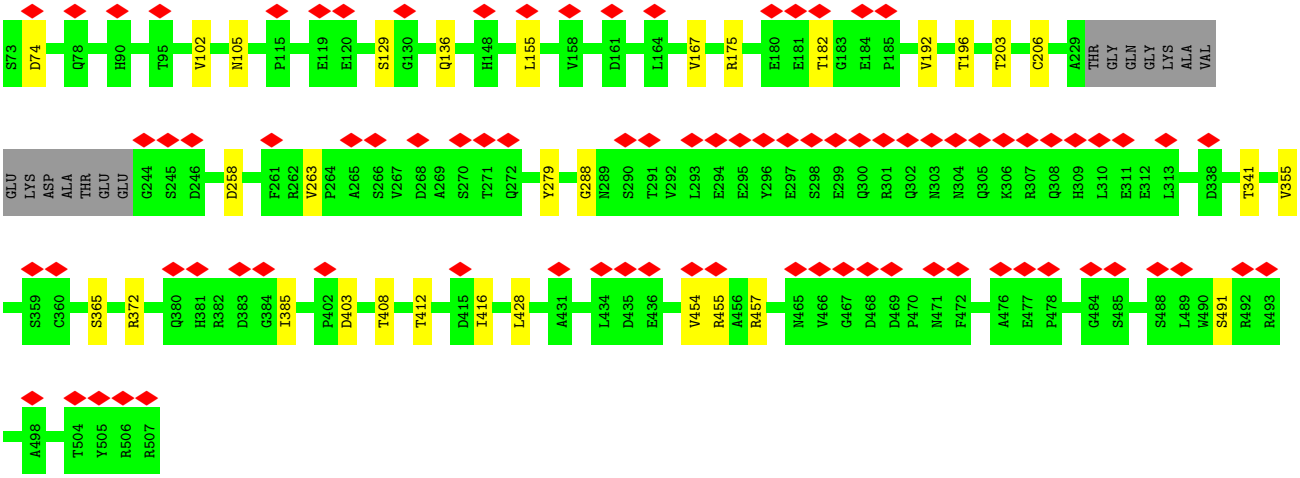




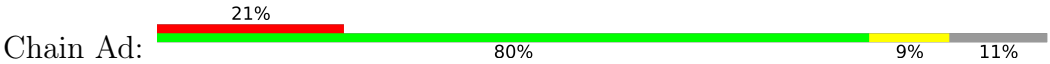
• Molecule 88: mL38

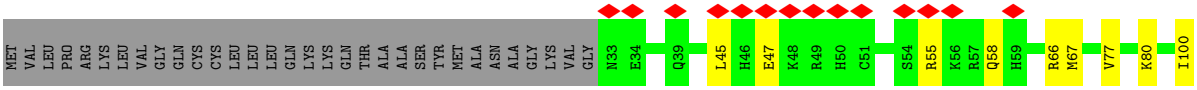


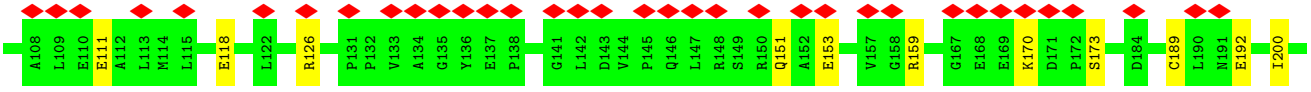


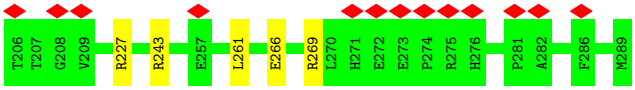


• Molecule 89: mL40

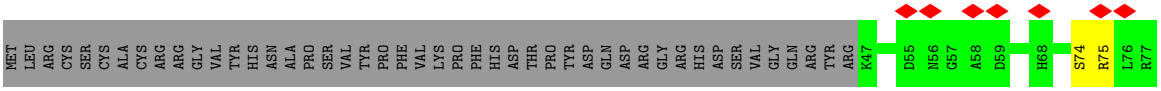


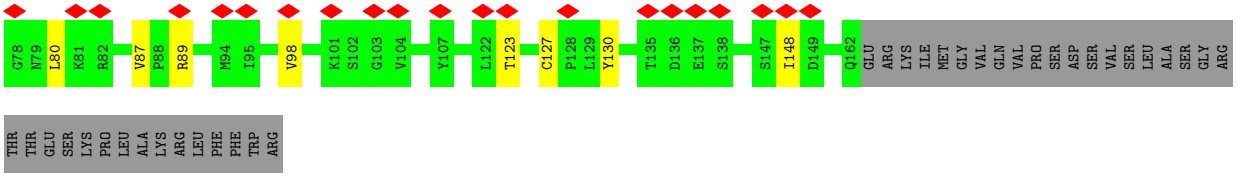




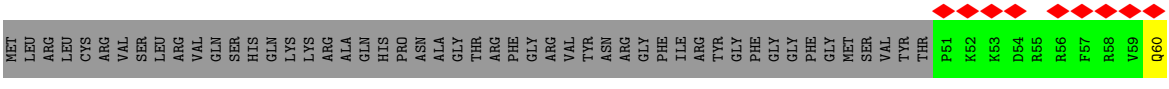


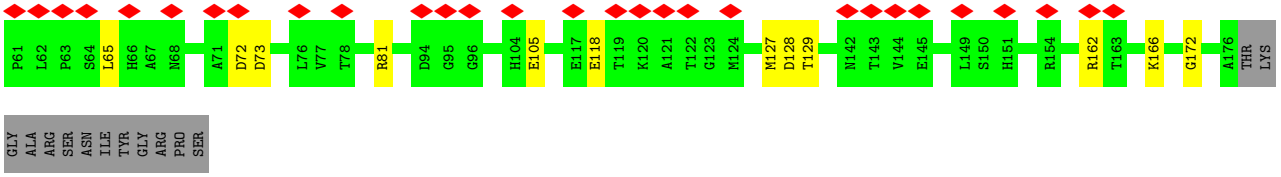
• Molecule 90: mL41





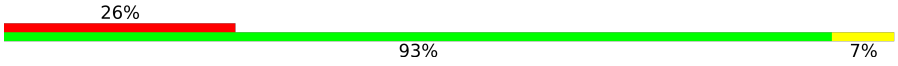
• Molecule 91: mL42

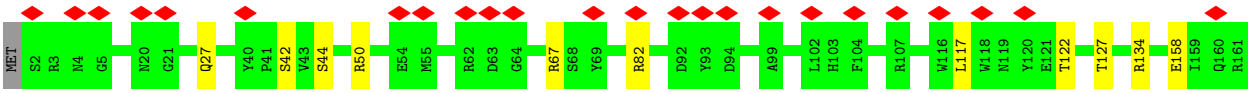


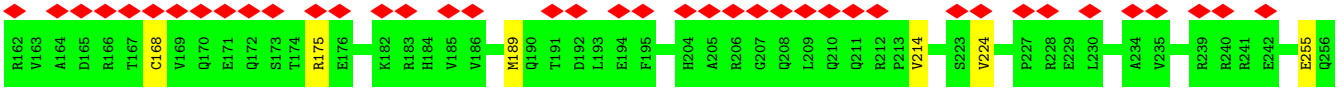


• Molecule 92: mL43

Chain Ag:

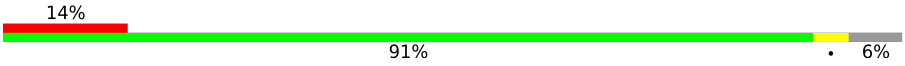


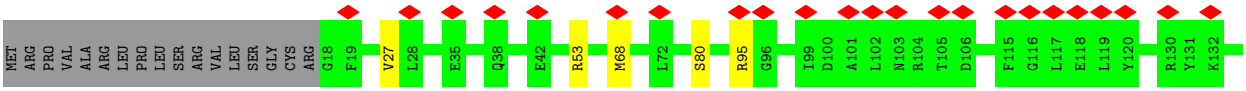




• Molecule 93: mL46

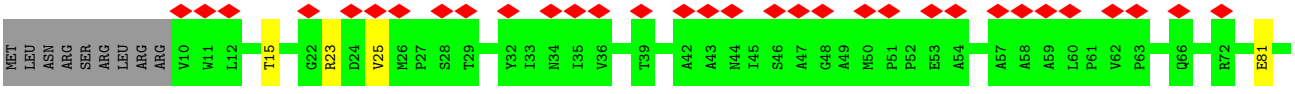
Chain Aj:

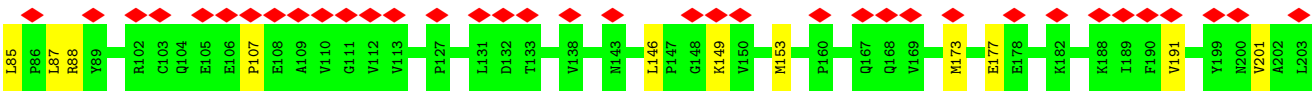


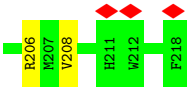


• Molecule 94: mL49

Chain Al:

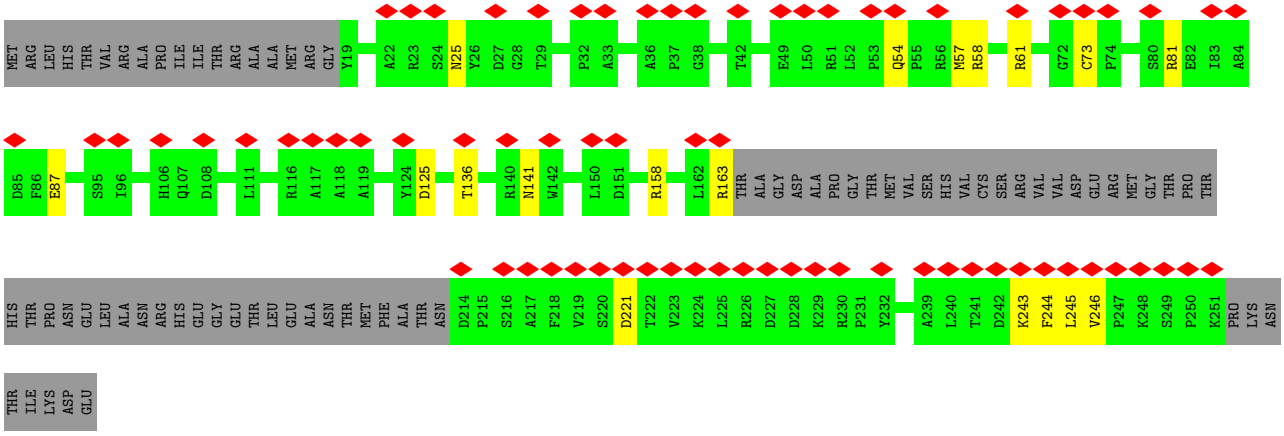






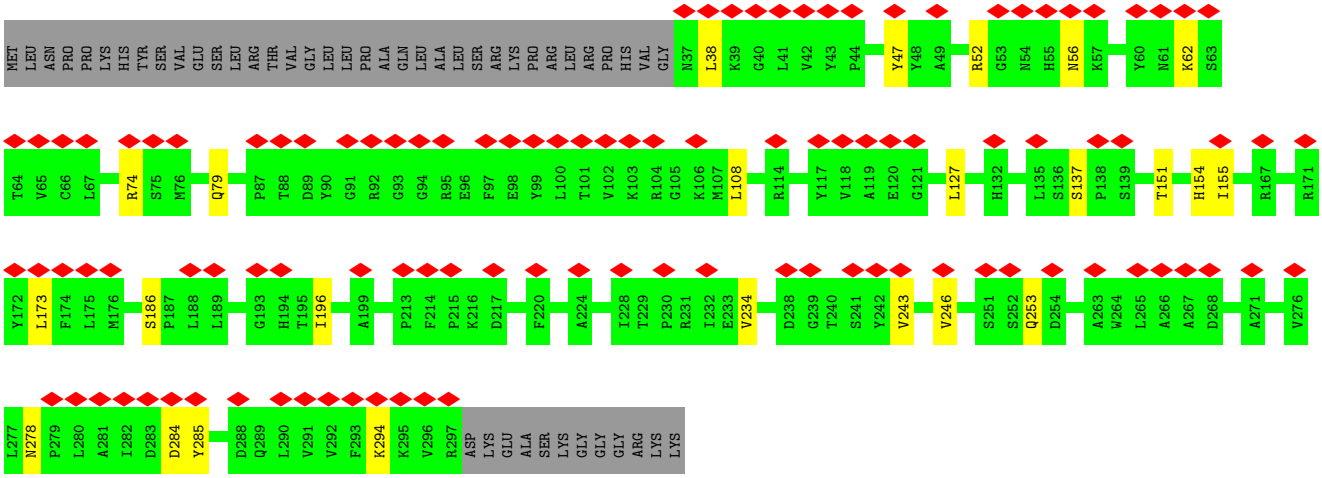
• Molecule 95: mL52

Chain Ao:



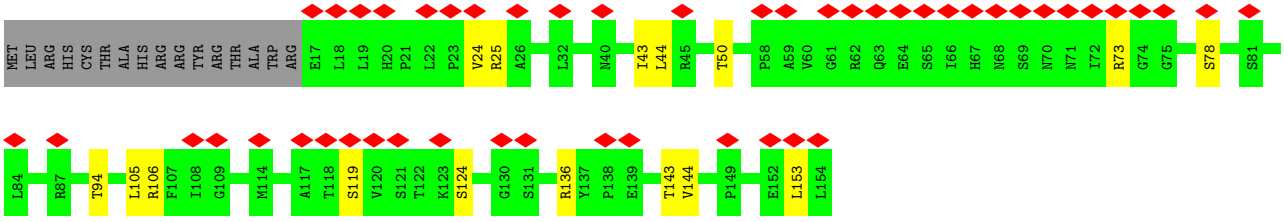
• Molecule 96: mL53

Chain Ap:



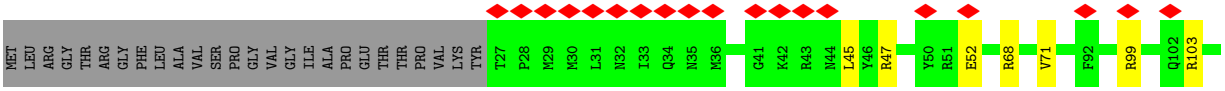
• Molecule 97: mL63

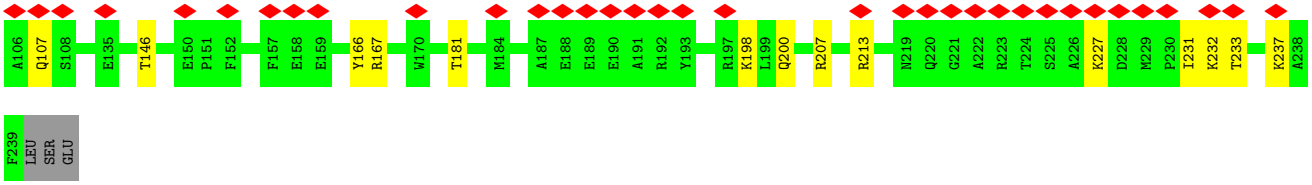
Chain At:



• Molecule 98: mL68

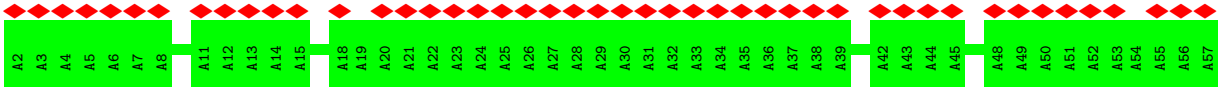
Chain Av:





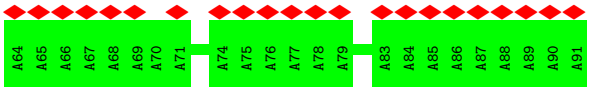
• Molecule 99: bL12m

Chain AB:



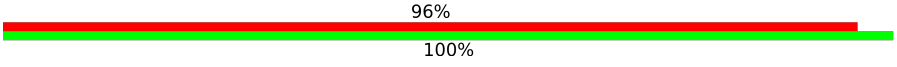
• Molecule 100: bL12m

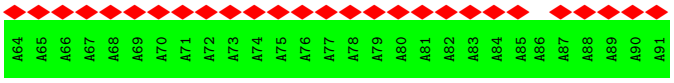
Chain AC:



• Molecule 100: bL12m

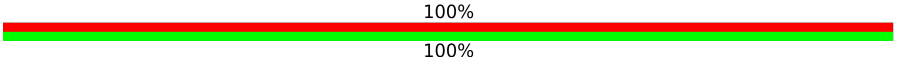
Chain AD:

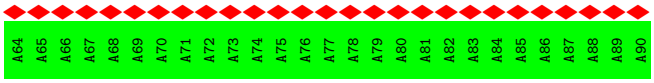




• Molecule 101: bL12m

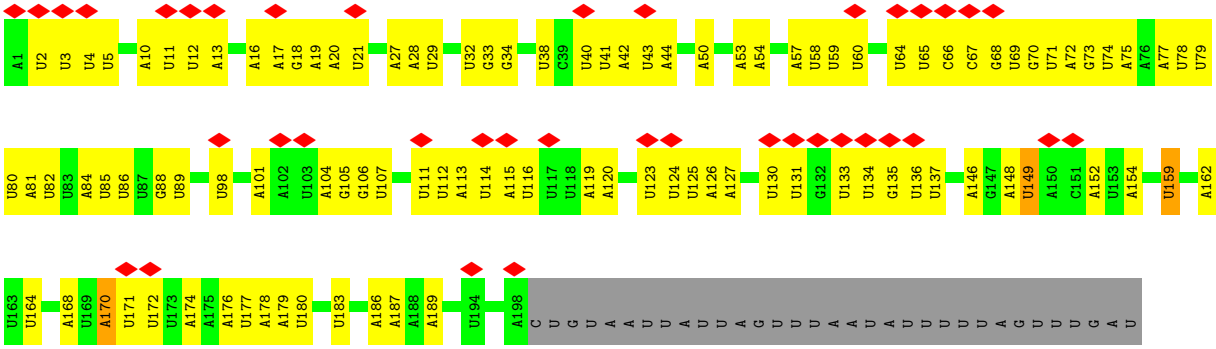
Chain AG:

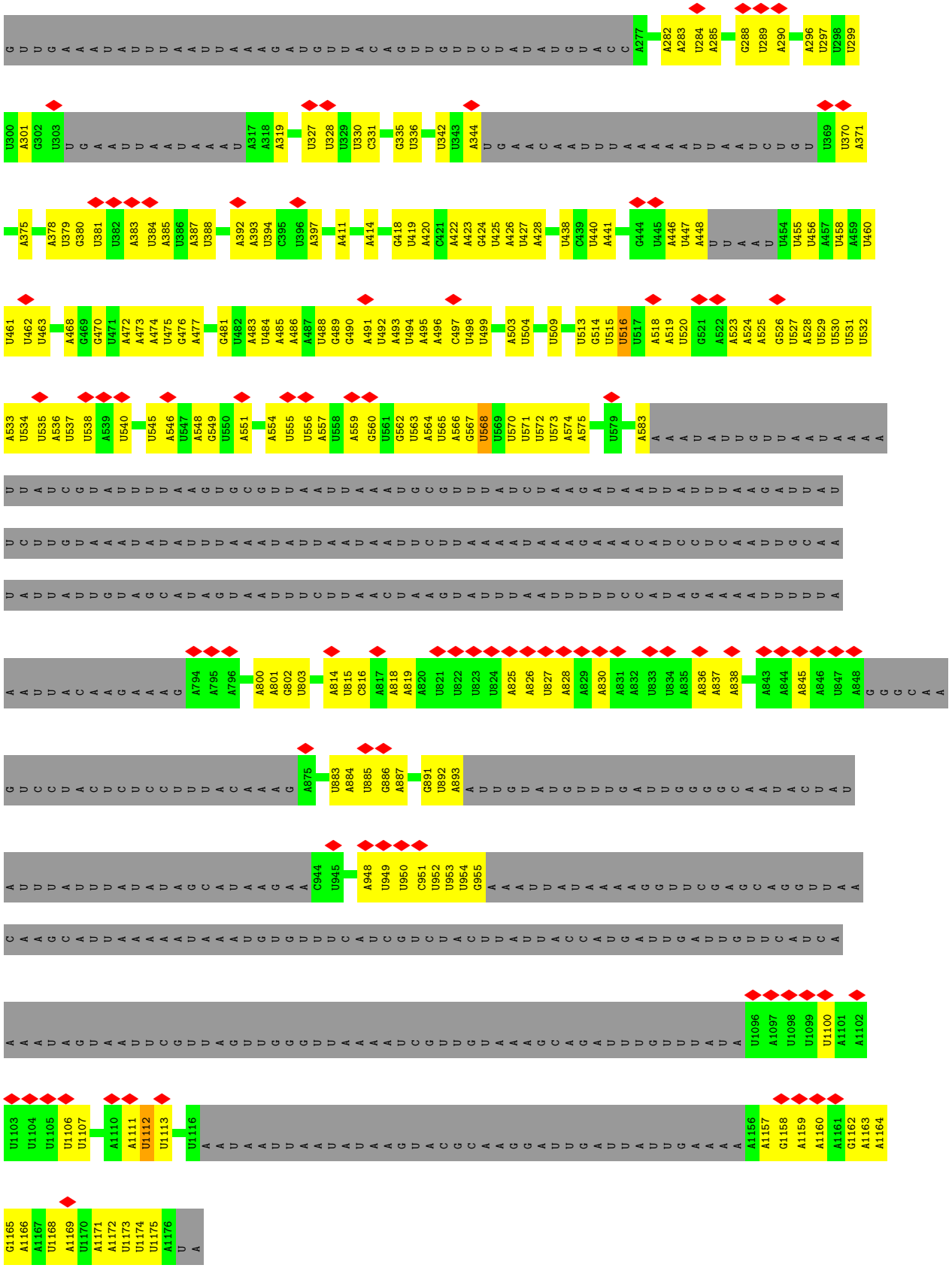




• Molecule 102: 12S rRNA

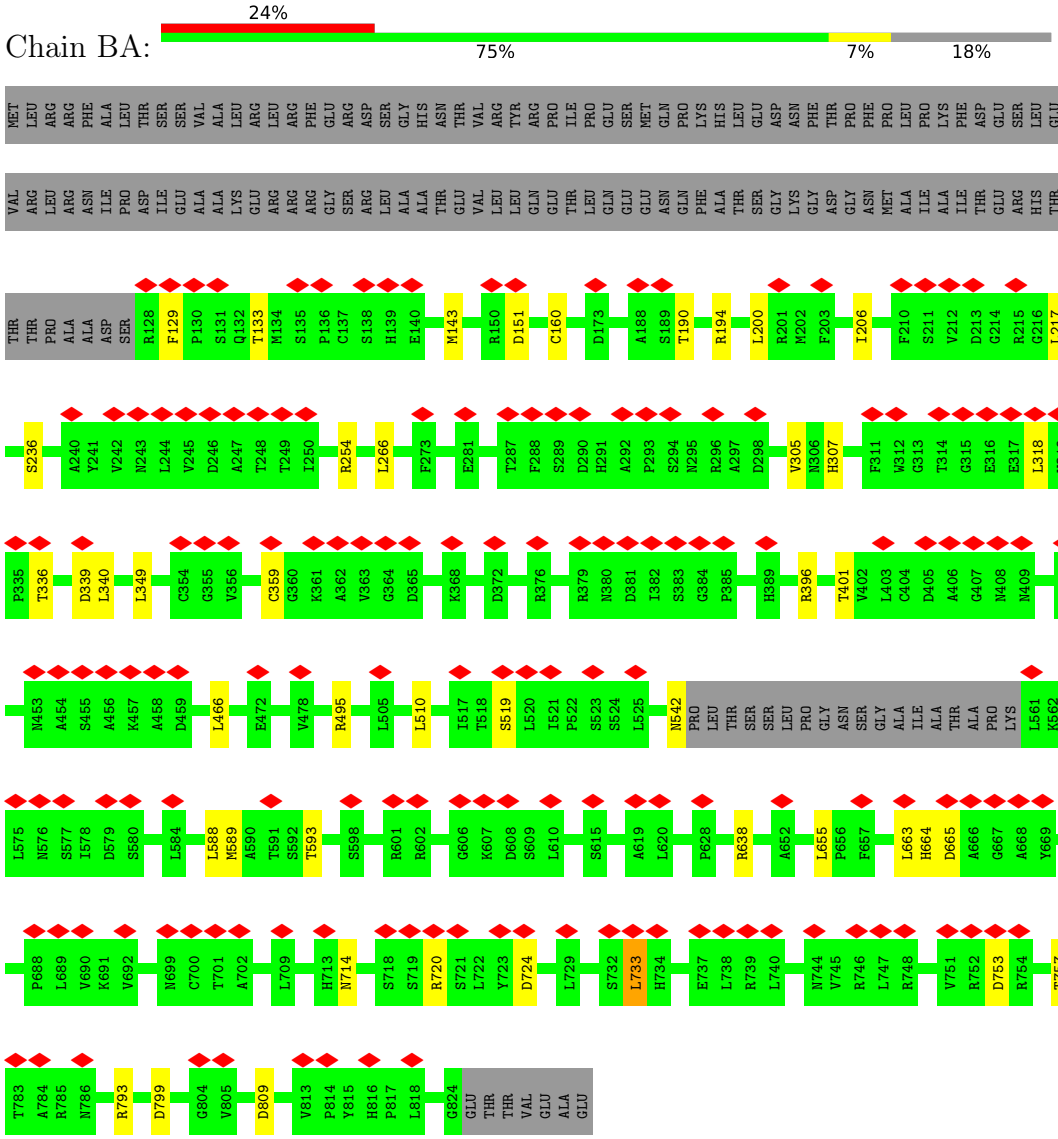
Chain AA:





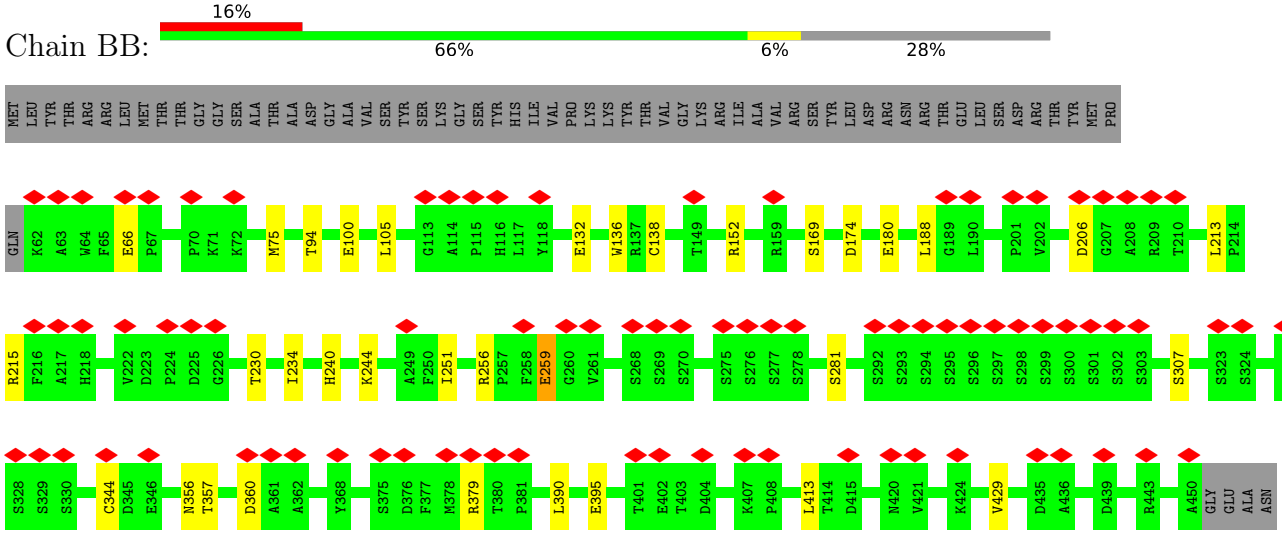
• Molecule 103: mL67

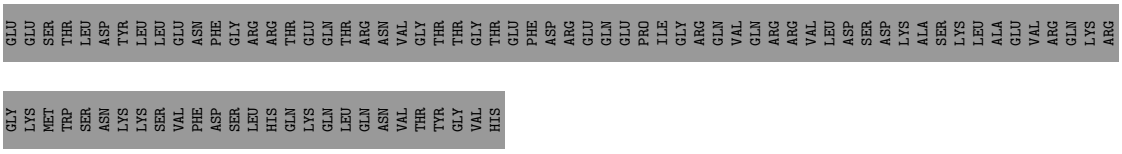
Chain BA:



- Molecule 104: mL68

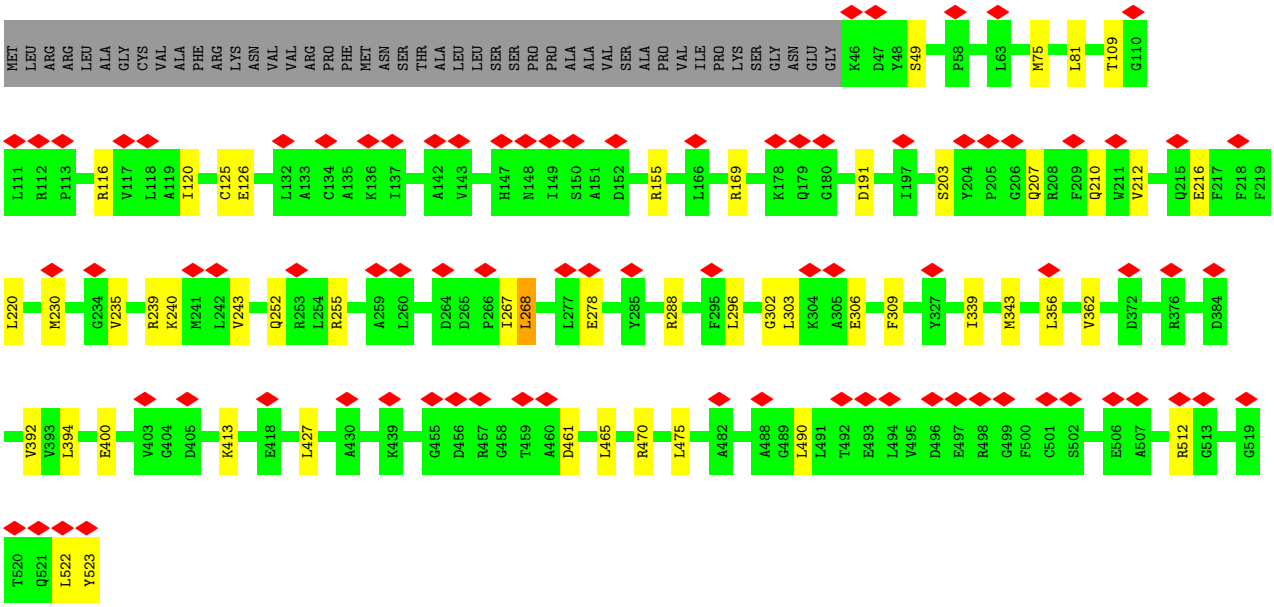
Chain BB:





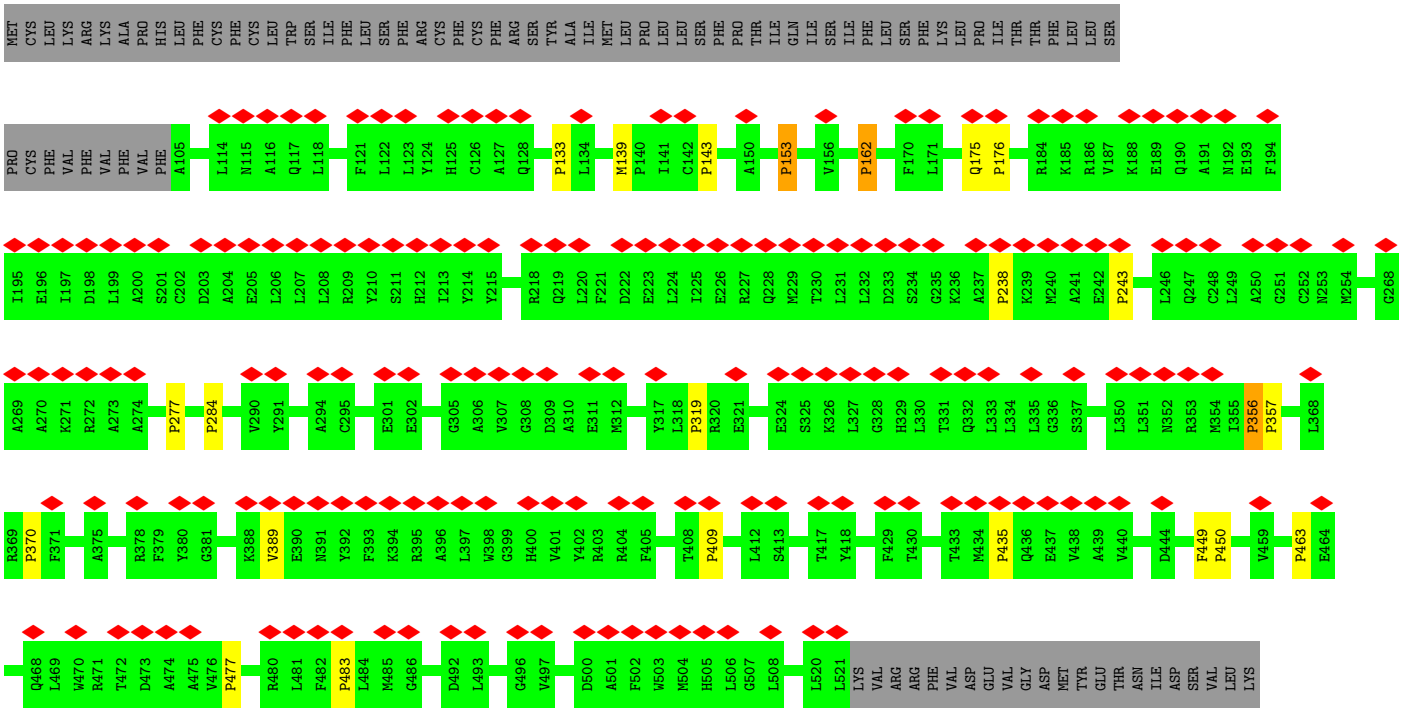
• Molecule 105: mL69

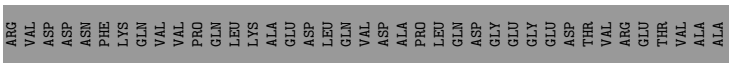
Chain BC:



• Molecule 106: mL70

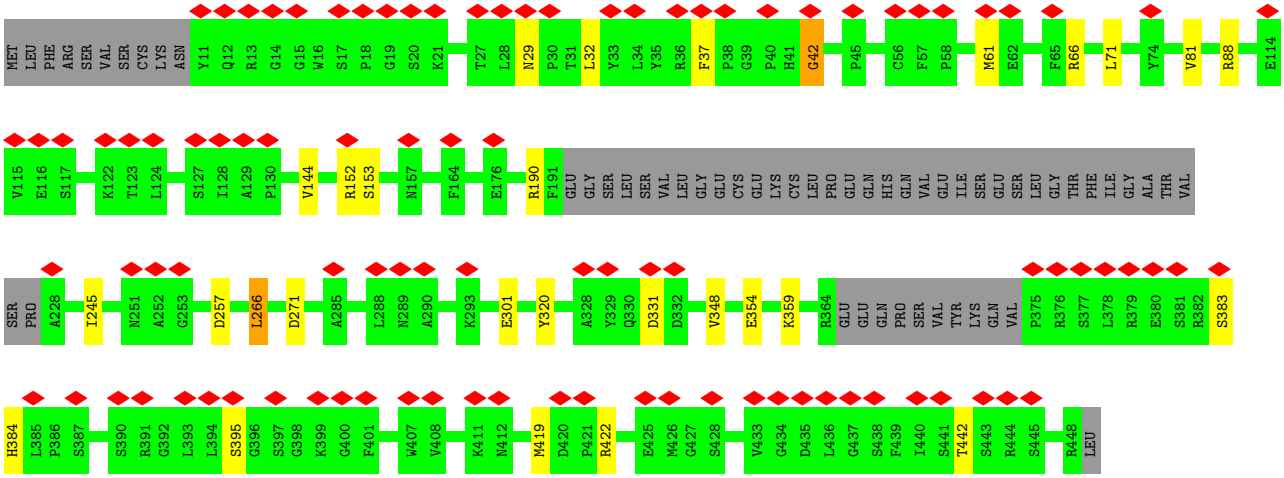
Chain BD:





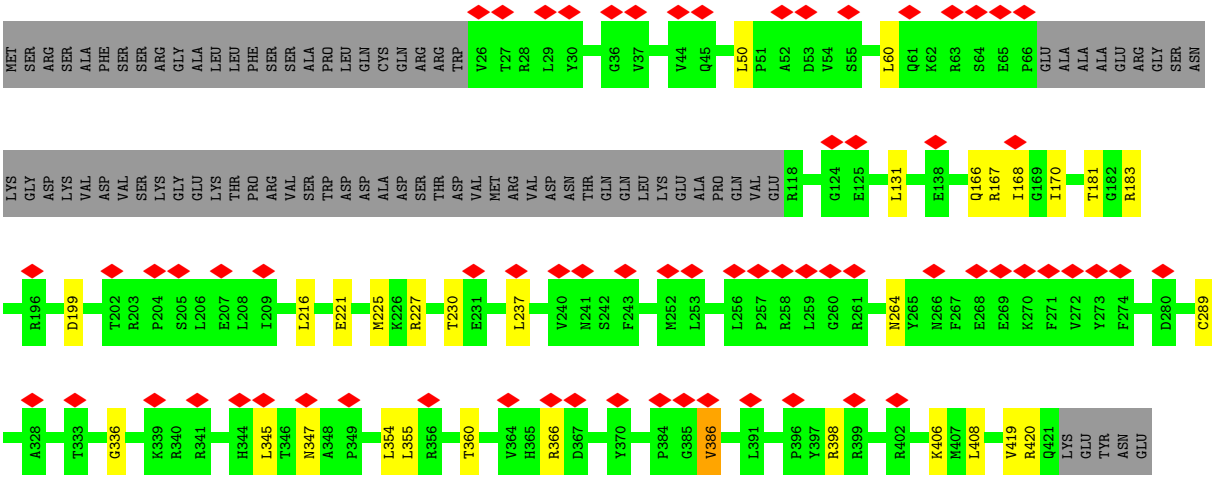
• Molecule 107: mL71

Chain BE:



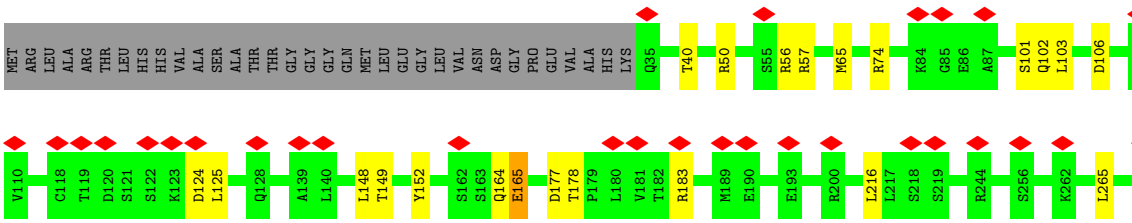
• Molecule 108: mL72

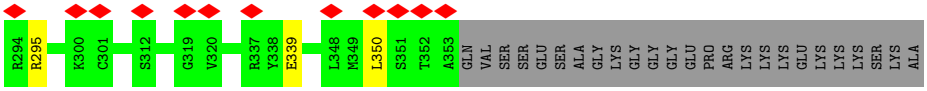
Chain BF:



• Molecule 109: mL73

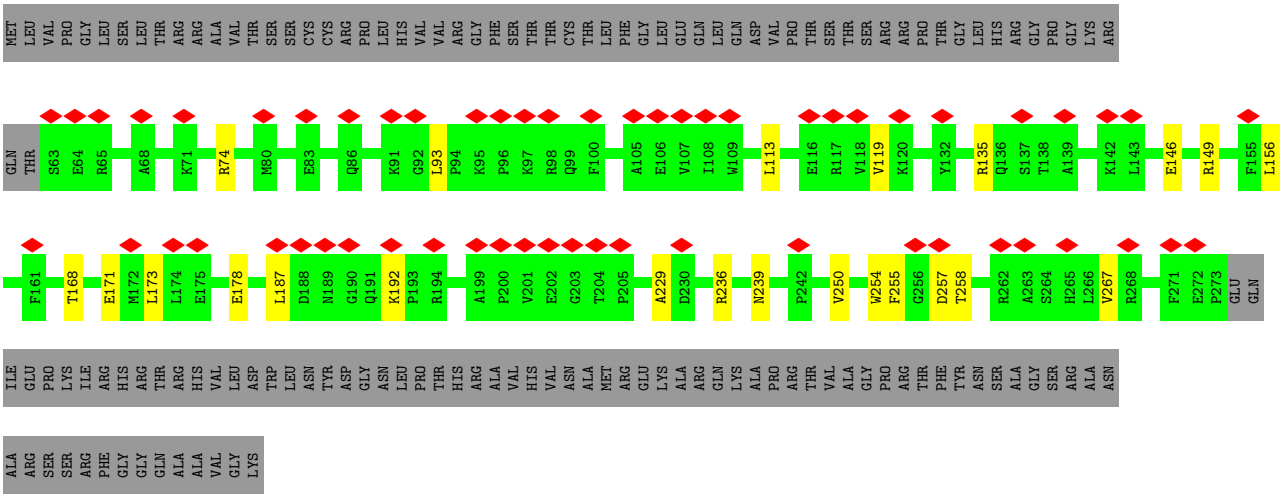
Chain BG:





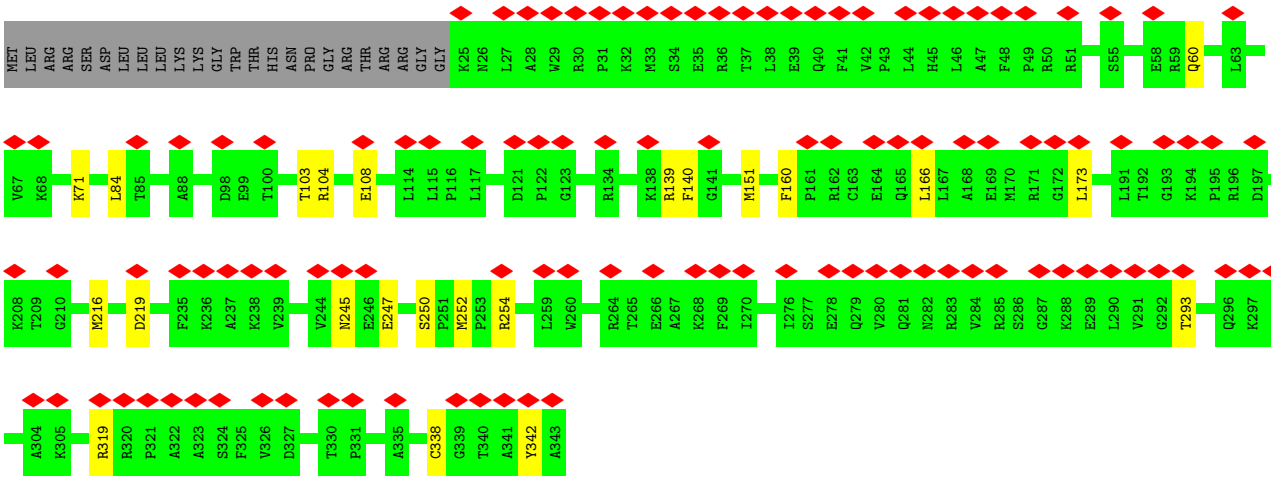
• Molecule 110: mL74

Chain BH:



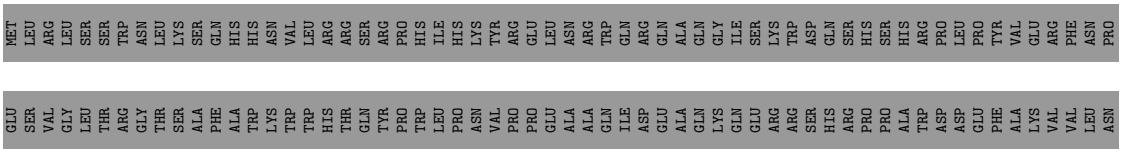
• Molecule 111: mL75

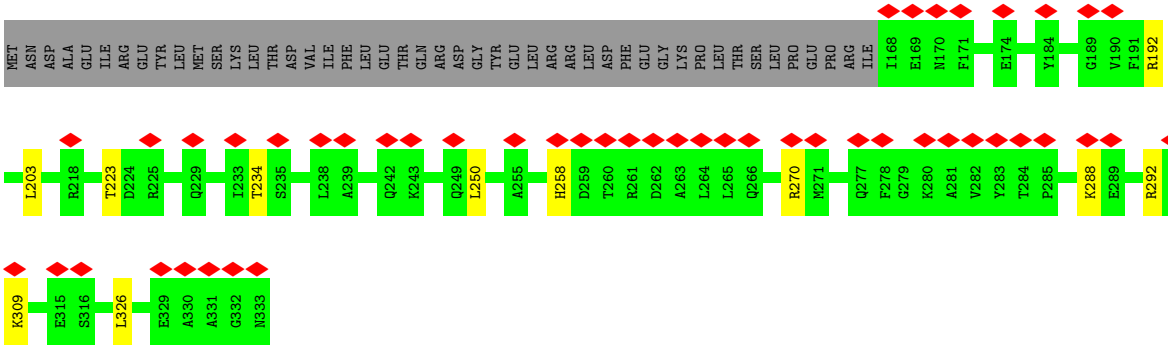
Chain BI:



• Molecule 112: mL76

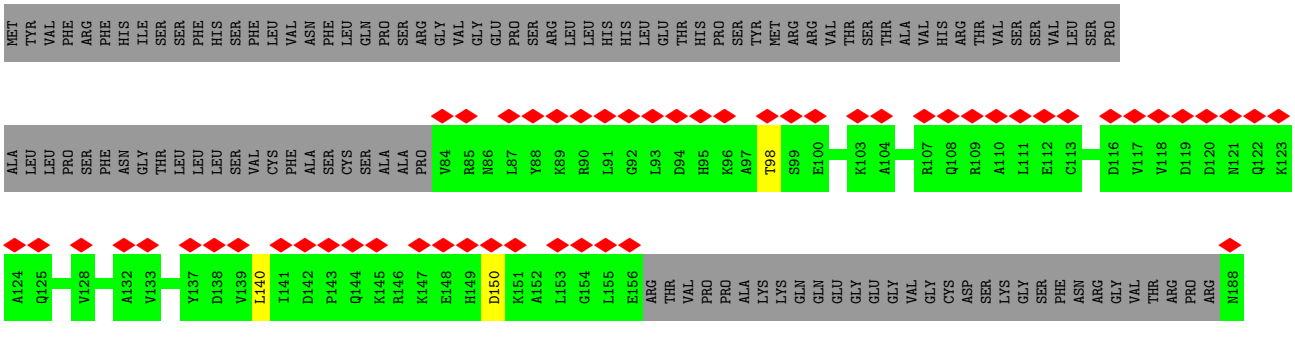
Chain BJ:





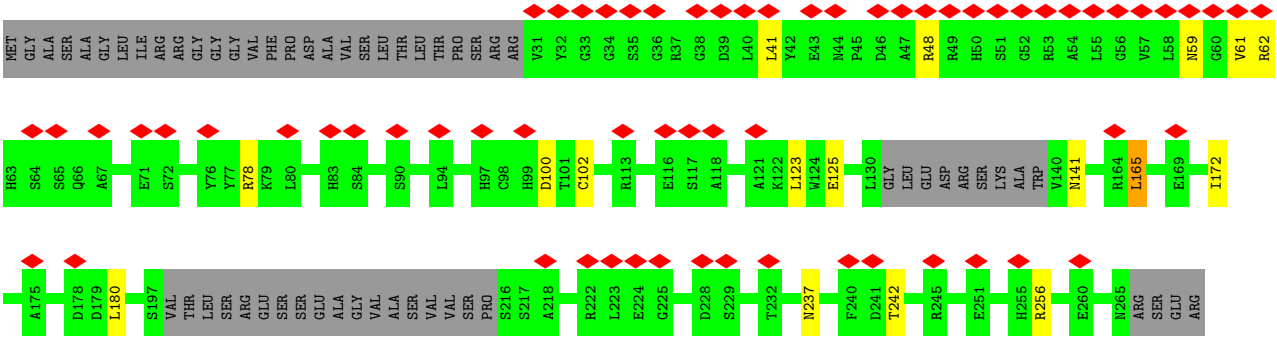
• Molecule 113: mL77

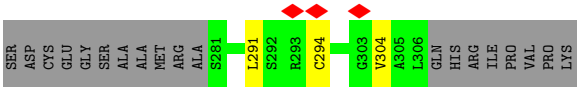
Chain BK:



• Molecule 114: mL78

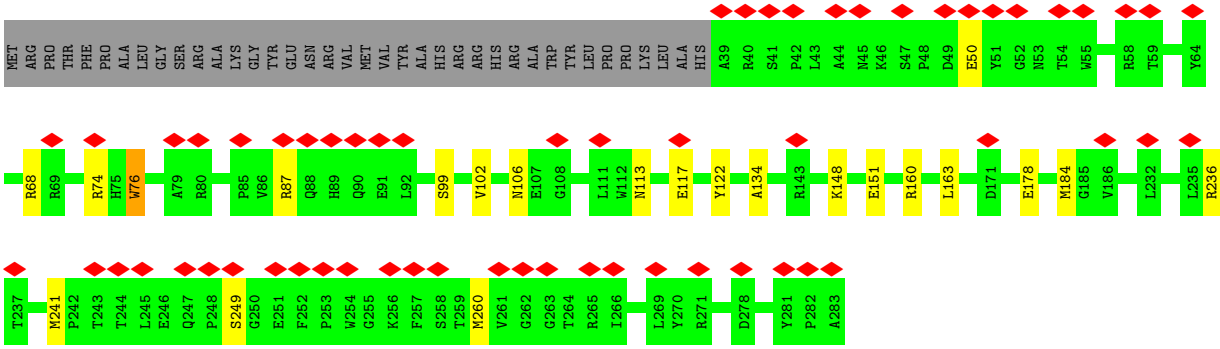
Chain BL:





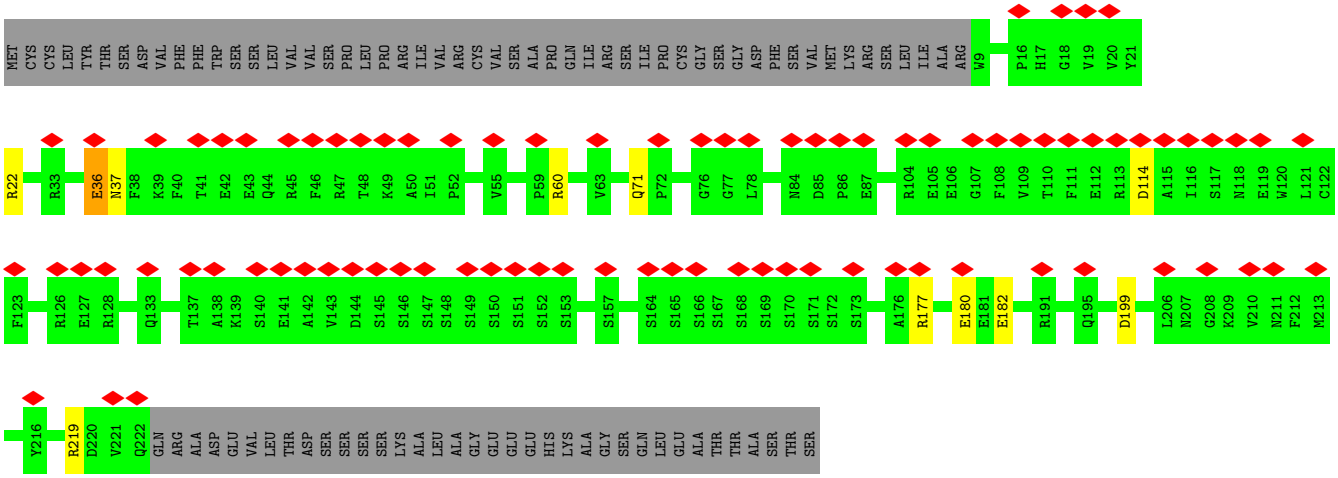
• Molecule 115: mL79

Chain BM:



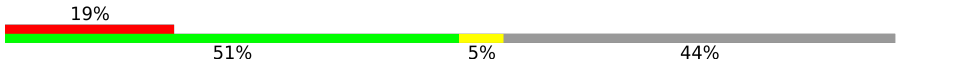
• Molecule 116: mL80

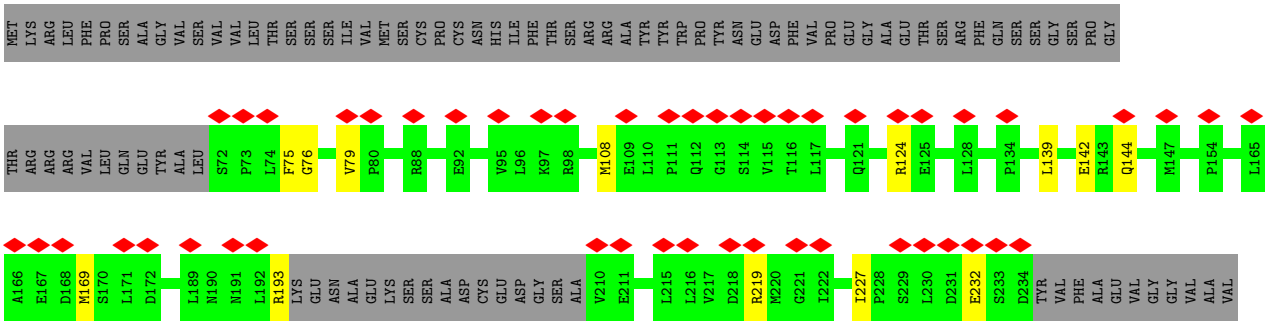
Chain BN:

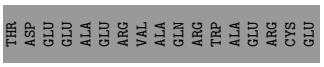


• Molecule 117: mL81

Chain BO:

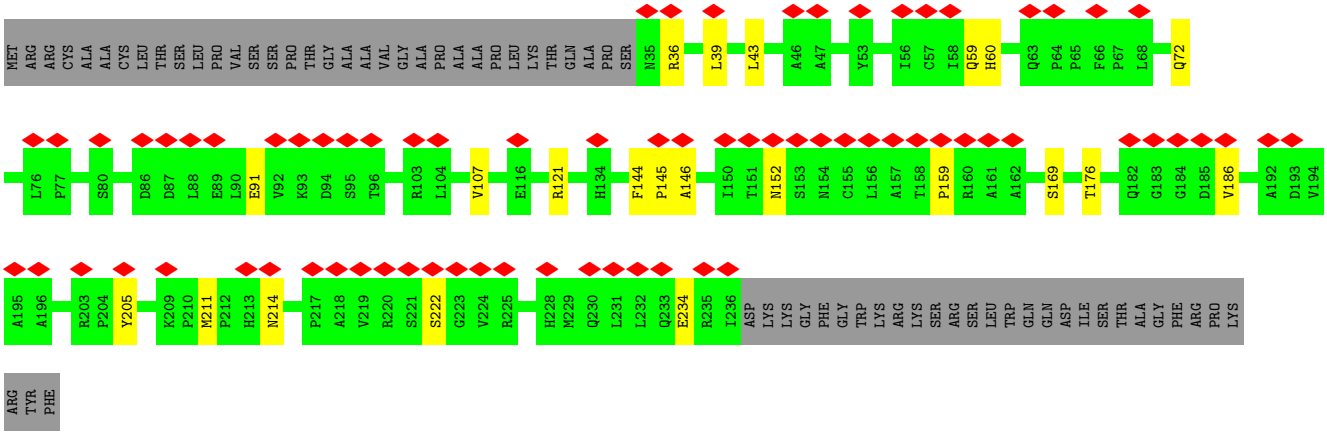






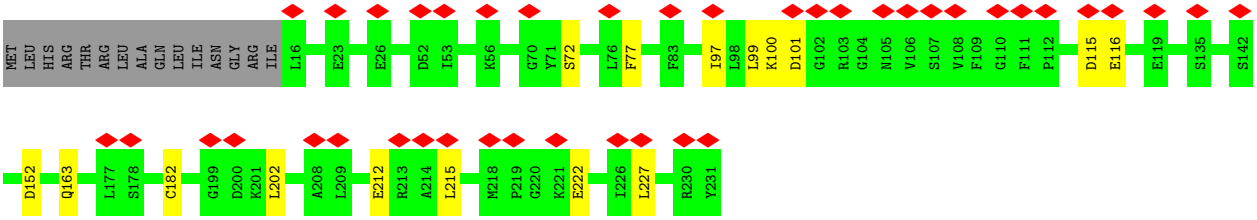
• Molecule 118: mL82

Chain BP:



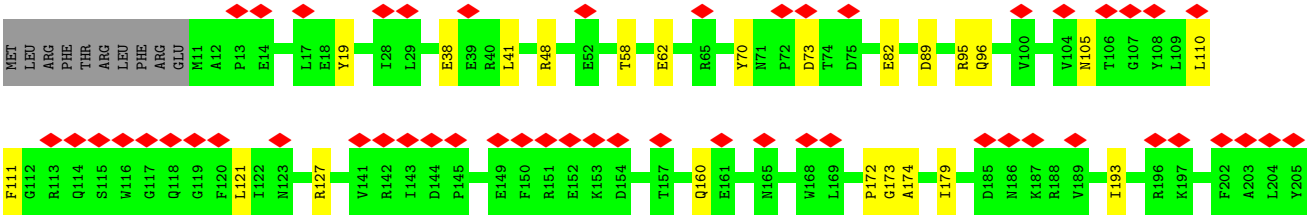
• Molecule 119: mL83

Chain BQ:



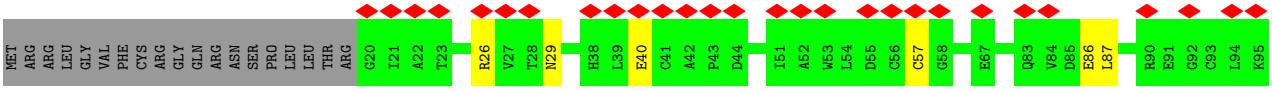
• Molecule 120: mL84

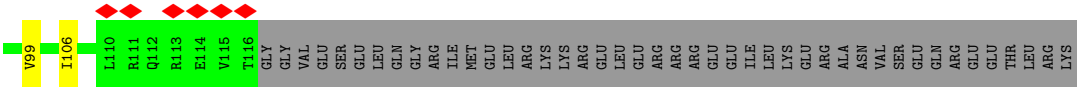
Chain BR:



• Molecule 121: mL85

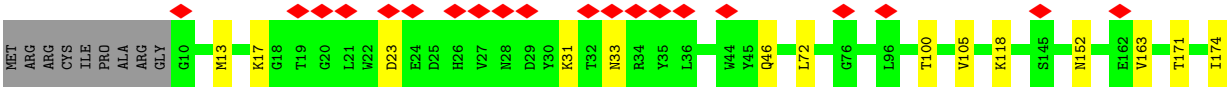
Chain BS:

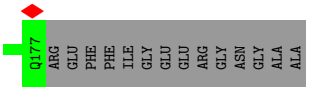




• Molecule 122: mL86

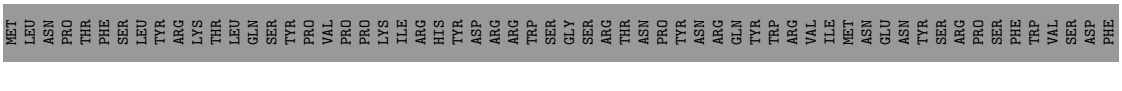
Chain BT:

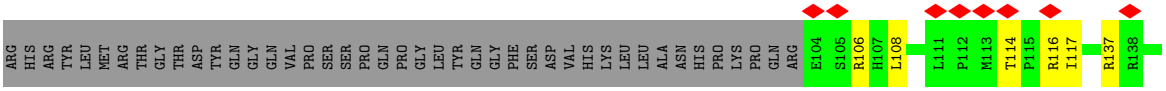


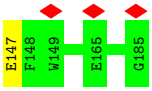


• Molecule 123: mL87

Chain BU:

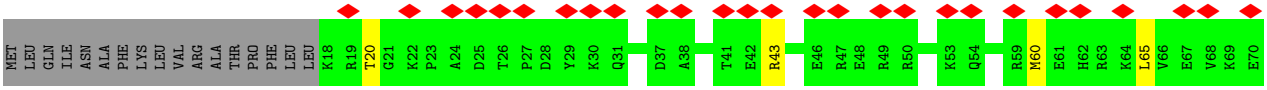


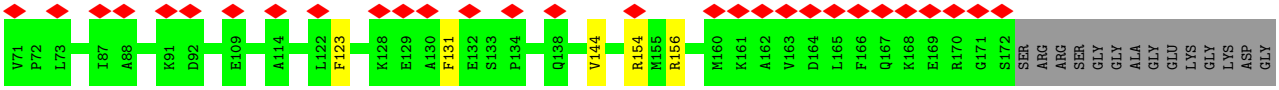




• Molecule 124: mL88

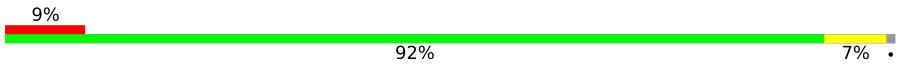
Chain BV:

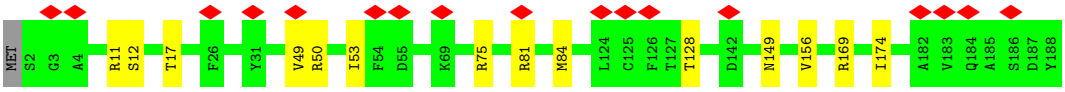




• Molecule 125: mL89

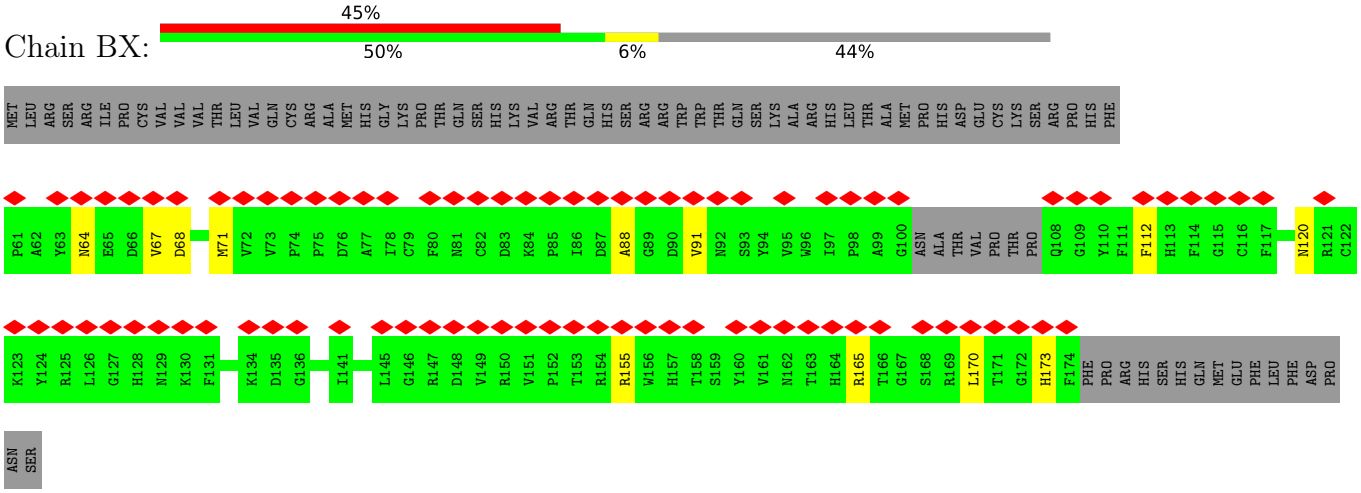
Chain BW:





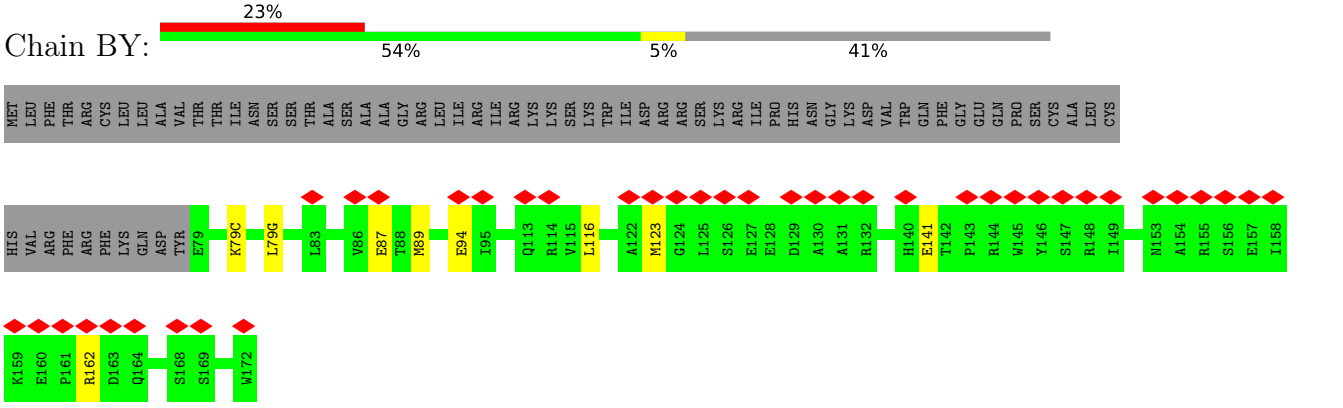
• Molecule 126: mL90

Chain BX:



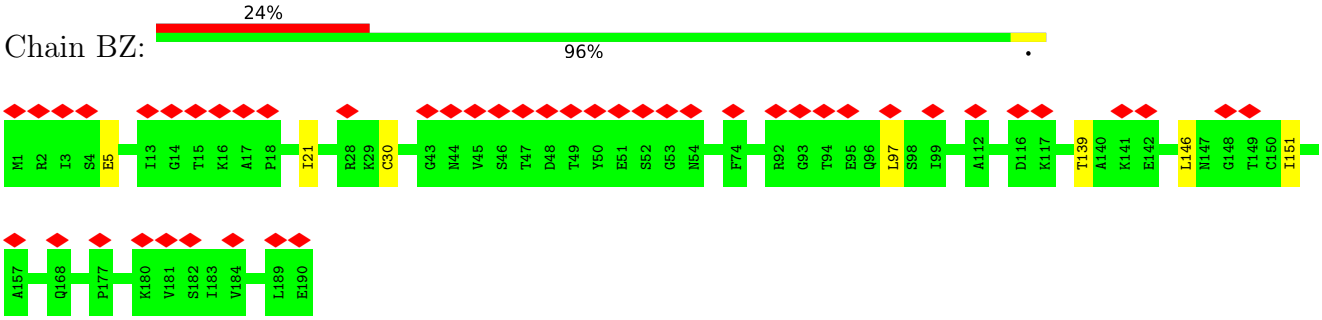
• Molecule 127: mS91

Chain BY:



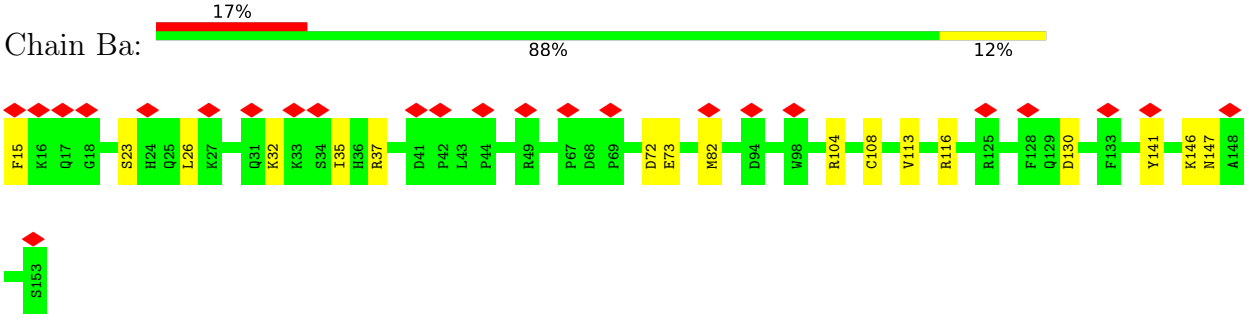
• Molecule 128: mL92

Chain BZ:



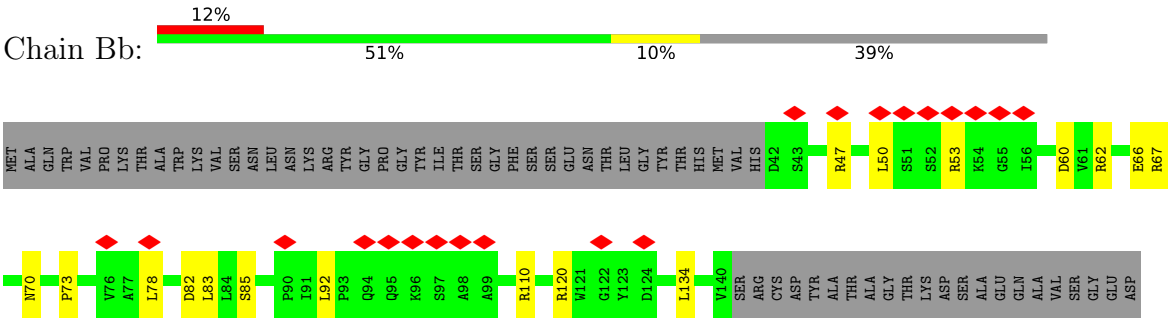
• Molecule 129: mL93

Chain Ba:



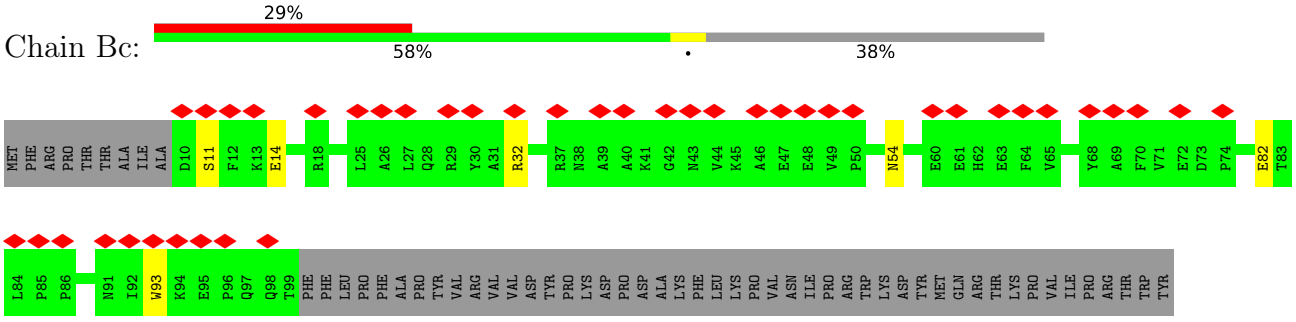
• Molecule 130: mL94

Chain Bb:



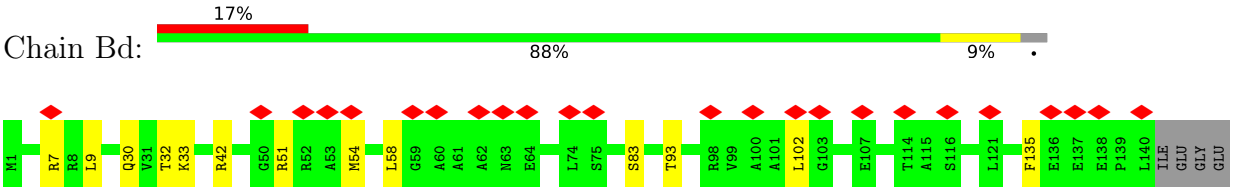
• Molecule 131: mL95

Chain Bc:



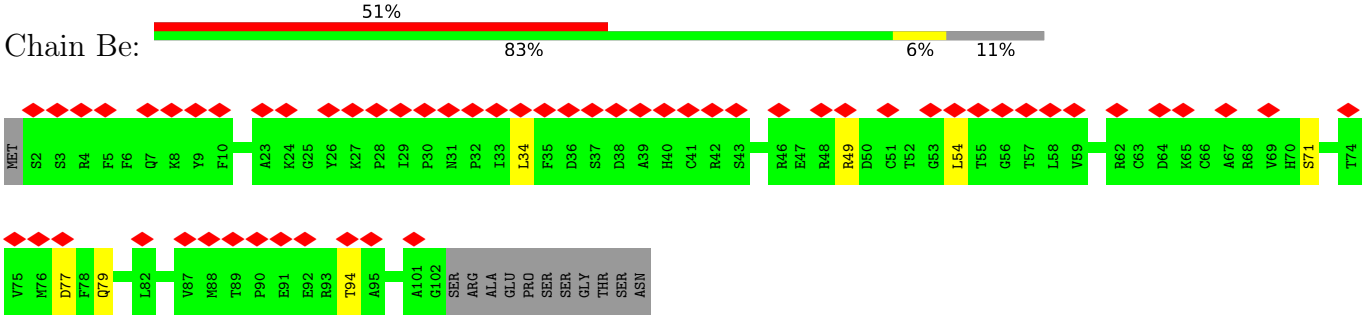
• Molecule 132: mL96

Chain Bd:



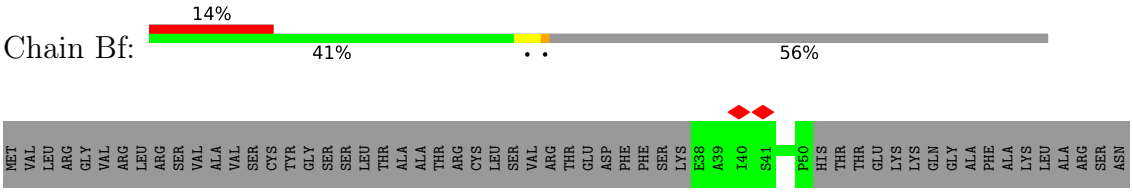
• Molecule 133: mL97

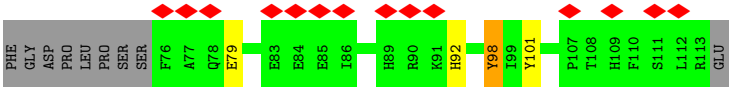
Chain Be:



• Molecule 134: mL98

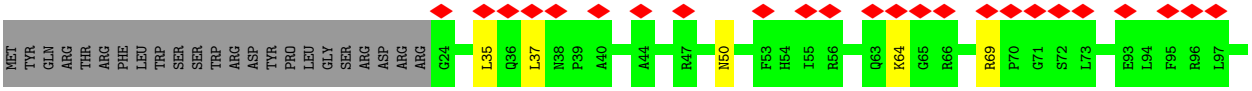
Chain Bf:

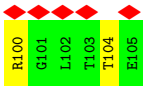




• Molecule 135: mL99

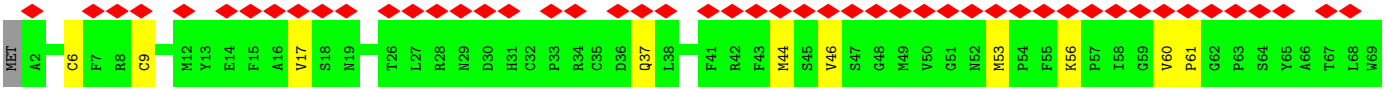
Chain Bg:

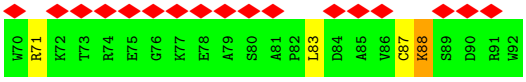




• Molecule 136: mL100

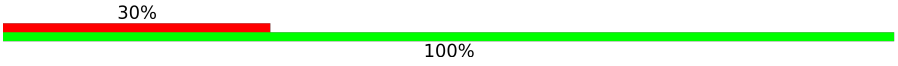
Chain Bh:

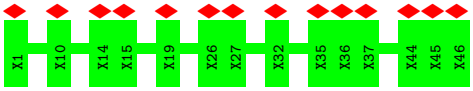




• Molecule 137: UNK

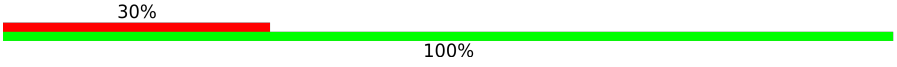
Chain UA:

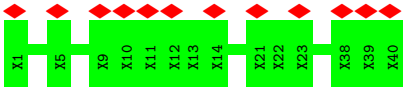




• Molecule 138: UNK

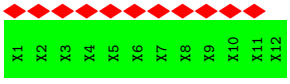
Chain UB:





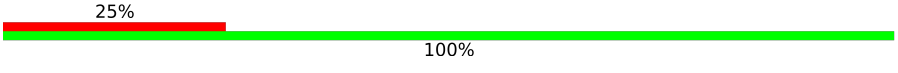
• Molecule 139: UNK

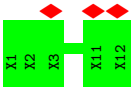
Chain UC:



• Molecule 139: UNK

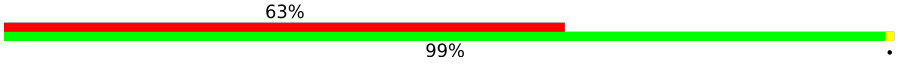
Chain UH:

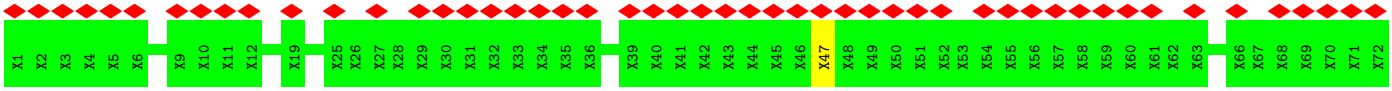


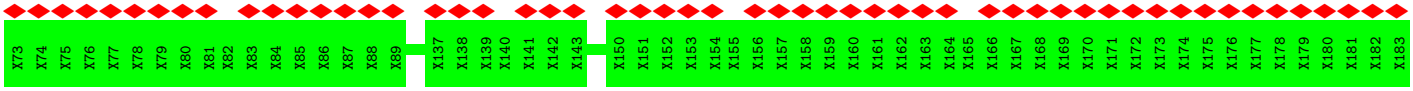


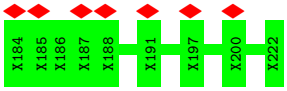
• Molecule 140: UNK

Chain UD:



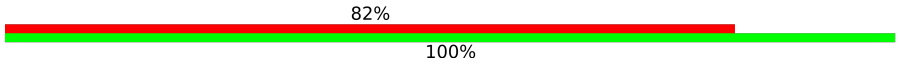


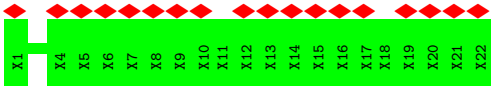




• Molecule 141: UNK

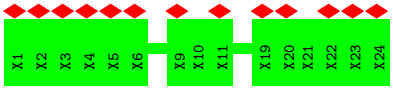
Chain UE:





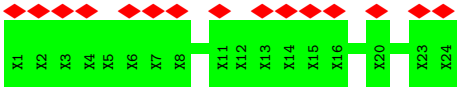
• Molecule 142: UNK

Chain UF:



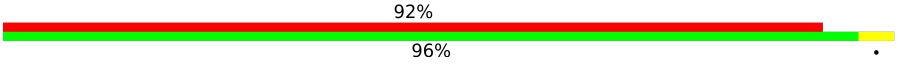
• Molecule 142: UNK

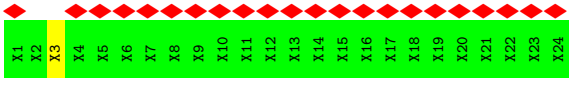
Chain UG:



• Molecule 142: UNK

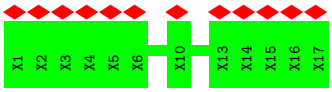
Chain UN:





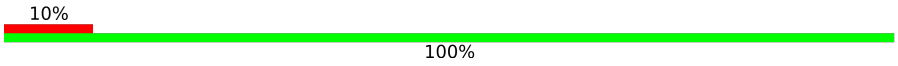
• Molecule 143: UNK

Chain UI:



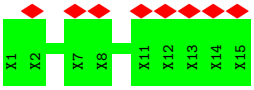
• Molecule 144: UNK

Chain UK:



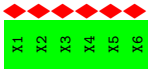
• Molecule 145: UNK

Chain UL:



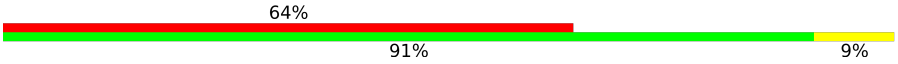
• Molecule 146: UNK

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

Continued on next page...

Continued from previous page...

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

All (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
102	AA	1112	U	N1-C2-O2	7.32	127.92	122.80
102	AA	149	U	C2-N1-C1'	7.09	126.21	117.70
57	CA	188	U	C2-N1-C1'	7.05	126.16	117.70
106	BD	356	PRO	N-CA-CB	7.00	111.70	103.30
57	CA	502	U	C5-C6-N1	-6.92	119.24	122.70
102	AA	1112	U	C2-N1-C1'	6.87	125.94	117.70
102	AA	149	U	N1-C2-O2	6.70	127.49	122.80
102	AA	149	U	N3-C2-O2	-6.58	117.59	122.20
44	Ca	35	PRO	N-CA-CB	6.56	111.17	103.30
103	BA	733	LEU	CA-CB-CG	6.54	130.34	115.30
106	BD	143	PRO	N-CA-CB	6.49	111.08	103.30
44	Ca	33	PRO	N-CA-CB	6.39	110.97	103.30
44	Ca	32	PRO	N-CA-CB	6.39	110.97	103.30
87	AY	317	PRO	N-CA-CB	6.38	110.96	103.30
57	CA	422	G	N3-C4-C5	6.33	131.76	128.60
73	AE	73	LEU	CA-CB-CG	6.32	129.84	115.30
102	AA	180	U	N3-C2-O2	-6.31	117.78	122.20
57	CA	63	G	N3-C4-C5	6.29	131.75	128.60
57	CA	617	U	C2-N1-C1'	6.27	125.23	117.70
57	CA	451	U	N1-C2-O2	6.27	127.19	122.80
3	DI	345	LEU	CA-CB-CG	6.23	129.63	115.30
106	BD	370	PRO	N-CA-CB	6.22	110.76	103.30
102	AA	180	U	N1-C2-O2	6.20	127.14	122.80
106	BD	435	PRO	N-CA-CB	6.18	110.71	103.30
57	CA	451	U	N3-C2-O2	-6.17	117.88	122.20
65	A1	78	LEU	CA-CB-CG	6.17	129.49	115.30
57	CA	493	U	C2-N1-C1'	6.15	125.08	117.70
57	CA	618	U	O5'-P-OP2	-6.12	100.19	105.70
57	CA	152	U	C5-C6-N1	6.11	125.76	122.70
55	Cr	28	PRO	N-CA-CB	6.08	110.59	103.30
102	AA	159	U	N1-C2-O2	6.06	127.04	122.80
102	AA	67	C	C2-N1-C1'	6.04	125.44	118.80
20	DH	133	CYS	C-N-CD	6.02	141.04	128.40
106	BD	409	PRO	N-CA-CB	5.97	110.47	103.30
57	CA	617	U	N1-C2-O2	5.94	126.96	122.80
55	Cr	31	PRO	N-CA-CB	5.94	110.43	103.30
102	AA	159	U	N3-C2-O2	-5.93	118.05	122.20
102	AA	170	A	C4-C5-C6	5.91	119.95	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
106	BD	176	PRO	N-CA-CB	5.88	110.35	103.30
32	CI	405	LEU	CA-CB-CG	-5.87	101.79	115.30
57	CA	617	U	N3-C2-O2	-5.87	118.09	122.20
57	CA	69	U	N3-C2-O2	-5.87	118.09	122.20
106	BD	238	PRO	N-CA-CB	5.86	110.33	103.30
106	BD	319	PRO	N-CA-CB	5.85	110.32	103.30
108	BF	408	LEU	CA-CB-CG	5.85	128.75	115.30
57	CA	310	A	C2-N3-C4	5.84	113.52	110.60
107	BE	42	GLY	N-CA-C	5.84	127.70	113.10
48	Ci	55	LEU	CA-CB-CG	5.82	128.68	115.30
94	Al	107	PRO	N-CA-CB	5.80	110.27	103.30
106	BD	162	PRO	N-CA-CB	5.80	110.26	103.30
106	BD	133	PRO	N-CA-CB	5.80	110.26	103.30
76	AJ	123	PRO	N-CA-CB	5.77	110.22	103.30
106	BD	284	PRO	N-CA-CB	5.75	110.20	103.30
106	BD	477	PRO	N-CA-CB	5.74	110.19	103.30
106	BD	483	PRO	N-CA-CB	5.74	110.19	103.30
57	CA	196	U	N1-C2-O2	5.72	126.81	122.80
57	CA	196	U	C2-N1-C1'	5.71	124.55	117.70
43	CZ	296	PRO	N-CA-CB	5.65	110.08	103.30
106	BD	277	PRO	N-CA-CB	5.64	110.07	103.30
20	DH	367	LEU	N-CA-C	-5.63	95.81	111.00
26	DX	128	GLY	N-CA-C	5.62	127.15	113.10
18	DF	55	ARG	NE-CZ-NH1	-5.62	117.49	120.30
57	CA	451	U	C6-N1-C1'	-5.62	113.34	121.20
102	AA	516	U	C6-N1-C1'	-5.60	113.36	121.20
106	BD	153	PRO	N-CA-CB	5.60	110.02	103.30
79	AP	347	LEU	CA-CB-CG	-5.59	102.43	115.30
118	BP	159	PRO	N-CA-CB	5.59	110.01	103.30
57	CA	374	U	C2-N1-C1'	5.58	124.40	117.70
2	DD	255	VAL	C-N-CD	-5.56	108.36	120.60
57	CA	370	A	O4'-C1'-N9	5.56	112.65	108.20
50	Ck	687	ARG	N-CA-C	5.56	126.01	111.00
102	AA	568	U	C2-N1-C1'	5.55	124.36	117.70
1	DA	1314	GLY	N-CA-C	5.54	126.94	113.10
57	CA	493	U	N1-C2-O2	5.51	126.66	122.80
1	DA	1484	PRO	N-CA-CB	5.51	109.91	103.30
106	BD	463	PRO	N-CA-CB	5.48	109.87	103.30
57	CA	87	U	N3-C2-O2	-5.41	118.41	122.20
50	Ck	359	LEU	CA-CB-CG	5.40	127.73	115.30
57	CA	188	U	N1-C2-O2	5.40	126.58	122.80
107	BE	266	LEU	CA-CB-CG	5.40	127.73	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
102	AA	568	U	N1-C2-O2	5.36	126.55	122.80
102	AA	568	U	N3-C2-O2	-5.35	118.45	122.20
91	Af	172	GLY	N-CA-C	-5.35	99.72	113.10
65	A1	148	LEU	CA-CB-CG	5.33	127.56	115.30
106	BD	357	PRO	N-CA-CB	5.32	109.69	103.30
114	BL	165	LEU	CA-CB-CG	5.32	127.54	115.30
102	AA	67	C	N1-C2-O2	5.32	122.09	118.90
102	AA	516	U	N1-C2-O2	5.30	126.51	122.80
57	CA	493	U	N3-C2-O2	-5.28	118.51	122.20
1	DA	509	LEU	CA-CB-CG	5.27	127.42	115.30
55	Cr	29	PRO	N-CA-CB	5.25	109.61	103.30
57	CA	564	U	C5-C6-N1	5.24	125.32	122.70
18	DF	510	ASP	CB-CG-OD2	5.19	122.97	118.30
51	Cm	203	ASP	CB-CG-OD2	5.19	122.97	118.30
106	BD	243	PRO	N-CA-CB	5.16	109.49	103.30
73	AE	360	PHE	C-N-CD	5.14	139.20	128.40
102	AA	149	U	C6-N1-C1'	-5.14	114.01	121.20
3	DI	116	ASP	CB-CG-OD2	5.11	122.90	118.30
57	CA	66	U	C2-N1-C1'	5.10	123.82	117.70
68	A4	68	LEU	CA-CB-CG	5.10	127.02	115.30
57	CA	87	U	N1-C2-O2	5.04	126.33	122.80
24	DV	183	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	A2	133	GLY	Peptide
66	A2	293	PHE	Peptide
67	A3	57	GLY	Peptide
71	A8	90	GLY	Peptide
71	A8	91	LYS	Peptide
73	AE	359	ALA	Peptide
74	AF	314	TYR	Peptide
74	AF	318	ALA	Peptide
74	AF	325	GLY	Peptide
81	AR	140	ASN	Peptide
81	AR	166	LYS	Peptide
81	AR	235	TRP	Peptide
83	AU	25	ARG	Peptide
84	AV	128	ARG	Peptide
85	AW	71	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
87	AY	107	SER	Peptide
87	AY	243	ASP	Peptide
88	Ab	288	GLY	Peptide
98	Av	231	ILE	Peptide
104	BB	259	GLU	Peptide
105	BC	400	GLU	Peptide
107	BE	383	SER	Peptide
107	BE	42	GLY	Peptide
108	BF	336	GLY	Peptide
109	BG	165	GLU	Peptide
110	BH	229	ALA	Peptide
113	BK	311	GLU	Peptide
113	BK	324	LYS	Peptide
115	BM	134	ALA	Peptide
115	BM	76	TRP	Peptide
116	BN	114	ASP	Peptide
116	BN	36	GLU	Peptide
116	BN	37	ASN	Peptide
117	BO	75	PHE	Peptide
118	BP	144	PHE	Peptide
118	BP	59	GLN	Peptide
120	BR	173	GLY	Peptide
120	BR	174	ALA	Peptide
130	Bb	70	ASN	Peptide
130	Bb	73	PRO	Peptide
134	Bf	92	HIS	Peptide
134	Bf	98	TYR	Peptide
136	Bh	60	VAL	Peptide
136	Bh	88	LYS	Peptide
31	CH	92	PRO	Peptide
33	CJ	100	ARG	Peptide
44	Ca	599	ILE	Peptide
47	Cg	50	PRO	Peptide
48	Ci	150	SER	Peptide
49	Cj	53	ASN	Peptide
50	Ck	230	LEU	Peptide
56	Cv	545	THR	Peptide
56	Cv	943	LEU	Peptide
1	DA	166	TYR	Peptide
15	DB	383	ARG	Sidechain
15	DB	586	ARG	Sidechain
16	DC	497	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
16	DC	775	ALA	Peptide
2	DD	248	ASP	Peptide
2	DD	255	VAL	Peptide
19	DG	184	ALA	Peptide
19	DG	592	THR	Peptide
21	DJ	35	PRO	Peptide
4	DL	269	MET	Peptide
4	DL	270	THR	Peptide
6	DN	142	ARG	Peptide
6	DN	292	TYR	Peptide
7	DO	124	CYS	Peptide
7	DO	251	ASN	Peptide
10	DR	23	VAL	Peptide
23	DT	43	ASP	Peptide
26	DX	127	MET	Peptide
140	UD	47	UNK	Peptide
142	UN	3	UNK	Peptide
147	UU	7	UNK	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	AI	210/263 (80%)	199 (95%)	11 (5%)	0	100	100
76	AJ	124/177 (70%)	117 (94%)	7 (6%)	0	100	100
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	34481/41413 (83%)	33099 (96%)	1303 (4%)	79 (0%)	50 81

All (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
44	Ca	35	PRO
85	AW	72	THR
106	BD	356	PRO
106	BD	389	VAL
134	Bf	101	TYR
24	DV	57	THR
44	Ca	34	LYS
87	AY	244	ARG
98	Av	232	LYS
2	DD	256	PRO
12	DU	191	SER
31	CH	16	VAL
33	CJ	799	ASP
49	Cj	54	ALA
79	AP	159	ALA
81	AR	141	ALA
87	AY	98	LYS
87	AY	107	SER
105	BC	268	LEU
111	BI	216	MET
115	BM	76	TRP
124	BV	60	MET
1	DA	132	GLY
3	DI	190	PRO
8	DP	62	LYS
15	DB	1033	TYR
42	CU	19	ALA
46	Cd	224	ILE
46	Cd	247	LYS
50	Ck	231	GLY
50	Ck	653	LEU
66	A2	293	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	AP	359	HIS
87	AY	108	PRO
98	Av	68	ARG
106	BD	153	PRO
107	BE	348	VAL
117	BO	76	GLY
118	BP	145	PRO
126	BX	88	ALA
127	BY	162	ARG
2	DD	248	ASP
7	DO	115	ASP
9	DQ	173	ASP
12	DU	205	ALA
17	DE	71	LEU
37	CO	70	HIS
66	A2	270	ASN
97	At	73	ARG
106	BD	162	PRO
107	BE	384	HIS
118	BP	146	ALA
120	BR	172	PRO
1	DA	229	GLU
16	DC	441	VAL
106	BD	449	PHE
136	Bh	61	PRO
44	Ca	31	GLU
64	A0	94	ILE
77	AK	17	VAL
105	BC	339	ILE
106	BD	139	MET
55	Cr	29	PRO
74	AF	36	ALA
104	BB	429	VAL
106	BD	450	PRO
108	BF	386	VAL
9	DQ	254	SER
19	DG	48	VAL
37	CO	90	MET
18	DF	184	VAL
66	A2	212	ALA
106	BD	175	GLN
15	DB	946	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (2779) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DA	41	PHE
1	DA	52	MET
1	DA	74	LYS
1	DA	77	ARG
1	DA	79	LEU
1	DA	87	THR
1	DA	109	TYR
1	DA	112	GLN
1	DA	131	ASP
1	DA	150	ILE
1	DA	158	LEU
1	DA	165	ARG
1	DA	167	THR
1	DA	174	HIS
1	DA	194	LEU
1	DA	200	ILE
1	DA	201	LYS
1	DA	230	PHE
1	DA	245	PHE
1	DA	254	PHE
1	DA	255	ARG
1	DA	259	LEU
1	DA	274	LEU
1	DA	291	CYS
1	DA	300	THR
1	DA	319	ARG
1	DA	383	LYS
1	DA	408	LEU
1	DA	419	THR
1	DA	436	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DA	456	ARG
1	DA	472	ARG
1	DA	486	LYS
1	DA	493	TRP
1	DA	509	LEU
1	DA	540	GLU
1	DA	547	ARG
1	DA	553	ARG
1	DA	579	ASP
1	DA	602	LEU
1	DA	630	ASP
1	DA	632	THR
1	DA	646	ASP
1	DA	650	LEU
1	DA	653	LYS
1	DA	680	VAL
1	DA	708	GLU
1	DA	712	VAL
1	DA	729	ARG
1	DA	781	ARG
1	DA	783	VAL
1	DA	826	ARG
1	DA	849	THR
1	DA	859	GLN
1	DA	870	GLU
1	DA	920	LEU
1	DA	958	SER
1	DA	963	LEU
1	DA	973	LEU
1	DA	988	CYS
1	DA	992	GLU
1	DA	1000	ASN
1	DA	1045	ILE
1	DA	1048	ASN
1	DA	1062	TYR
1	DA	1077	ARG
1	DA	1097	LEU
1	DA	1117	ASN
1	DA	1125	GLU
1	DA	1145	THR
1	DA	1152	HIS
1	DA	1182	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DA	1208	THR
1	DA	1225	HIS
1	DA	1240	LEU
1	DA	1263	VAL
1	DA	1268	LEU
1	DA	1271	LEU
1	DA	1278	THR
1	DA	1292	CYS
1	DA	1381	LEU
1	DA	1404	ARG
1	DA	1431	TYR
1	DA	1433	ASP
1	DA	1488	GLN
1	DA	1517	ARG
1	DA	1544	ASN
1	DA	1575	LYS
1	DA	1591	ARG
1	DA	1597	GLU
1	DA	1605	ARG
1	DA	1624	ILE
1	DA	1662	ARG
2	DD	12	SER
2	DD	27	MET
2	DD	48	MET
2	DD	72	ASP
2	DD	79	GLN
2	DD	94	LYS
2	DD	108	THR
2	DD	122	GLN
2	DD	123	ARG
2	DD	129	ARG
2	DD	146	ARG
2	DD	151	SER
2	DD	173	GLN
2	DD	201	GLU
2	DD	221	GLU
2	DD	226	THR
2	DD	233	ASN
2	DD	298	MET
2	DD	358	ARG
2	DD	377	GLU
2	DD	379	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	DD	394	LYS
2	DD	452	LEU
2	DD	454	THR
2	DD	504	ASN
2	DD	521	ASN
2	DD	541	ARG
2	DD	577	LYS
2	DD	592	TRP
2	DD	624	THR
2	DD	634	ARG
2	DD	646	ILE
2	DD	651	ARG
2	DD	653	PHE
2	DD	654	ARG
2	DD	679	ASN
2	DD	704	ASP
2	DD	741	ARG
2	DD	770	SER
2	DD	787	ARG
2	DD	799	ASP
2	DD	812	TYR
3	DI	79	ILE
3	DI	90	LEU
3	DI	113	VAL
3	DI	159	ASP
3	DI	164	GLU
3	DI	175	GLN
3	DI	178	PHE
3	DI	180	GLU
3	DI	192	THR
3	DI	232	TYR
3	DI	233	ARG
3	DI	237	ARG
3	DI	261	ASP
3	DI	282	ASP
3	DI	310	LEU
3	DI	313	ARG
3	DI	344	LEU
3	DI	345	LEU
3	DI	353	LYS
3	DI	362	ILE
3	DI	365	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	DI	399	THR
4	DL	28	ASN
4	DL	29	PHE
4	DL	39	THR
4	DL	68	LEU
4	DL	102	SER
4	DL	136	MET
4	DL	145	LEU
4	DL	158	THR
4	DL	165	PHE
4	DL	267	HIS
4	DL	268	VAL
4	DL	269	MET
4	DL	270	THR
4	DL	271	PRO
4	DL	286	THR
5	DM	1	MET
5	DM	15	LEU
5	DM	30	ARG
5	DM	46	PHE
5	DM	56	TRP
5	DM	59	ARG
5	DM	72	ARG
5	DM	76	ASN
5	DM	90	LEU
5	DM	103	ARG
5	DM	128	ILE
5	DM	129	ARG
5	DM	131	ASN
5	DM	157	LEU
5	DM	179	ARG
5	DM	185	LYS
5	DM	199	LEU
5	DM	253	LYS
5	DM	275	LEU
6	DN	11	ARG
6	DN	23	VAL
6	DN	42	THR
6	DN	79	ASN
6	DN	109	ASN
6	DN	141	MET
6	DN	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DN	162	LEU
6	DN	223	GLN
6	DN	224	ARG
6	DN	237	ARG
6	DN	246	GLN
6	DN	276	GLN
6	DN	288	PHE
7	DO	62	LEU
7	DO	73	LEU
7	DO	115	ASP
7	DO	118	ASP
7	DO	125	LEU
7	DO	136	ASP
7	DO	155	ARG
7	DO	163	ARG
7	DO	178	ARG
7	DO	192	MET
7	DO	234	LEU
7	DO	255	ARG
8	DP	21	MET
8	DP	23	LEU
8	DP	28	ASN
8	DP	34	VAL
8	DP	69	LEU
8	DP	172	GLU
8	DP	195	THR
8	DP	204	ASN
8	DP	208	PRO
9	DQ	41	GLN
9	DQ	120	MET
9	DQ	127	ARG
9	DQ	177	LEU
9	DQ	192	LEU
9	DQ	214	ARG
9	DQ	216	ASN
9	DQ	250	ARG
10	DR	23	VAL
10	DR	39	GLN
10	DR	54	LEU
10	DR	60	VAL
10	DR	63	ILE
10	DR	67	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	DR	68	HIS
10	DR	78	ARG
10	DR	91	THR
10	DR	108	GLN
10	DR	131	LEU
10	DR	133	LEU
10	DR	173	ASN
10	DR	174	CYS
10	DR	190	LEU
10	DR	201	CYS
10	DR	245	MET
10	DR	261	ARG
10	DR	262	ARG
10	DR	265	MET
11	DS	34	SER
11	DS	56	LEU
11	DS	61	ASN
11	DS	73	LYS
11	DS	92	ARG
11	DS	106	ARG
11	DS	108	ASN
11	DS	115	TYR
11	DS	119	CYS
11	DS	170	TYR
11	DS	175	CYS
11	DS	198	CYS
12	DU	33	THR
12	DU	46	THR
12	DU	47	ARG
12	DU	73	ARG
12	DU	83	ARG
12	DU	86	ILE
12	DU	90	VAL
12	DU	103	ILE
12	DU	124	SER
12	DU	153	THR
12	DU	165	ASP
12	DU	176	ARG
12	DU	189	LYS
12	DU	207	ARG
12	DU	211	ARG
12	DU	218	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	DZ	20	ARG
13	DZ	62	ASP
13	DZ	63	LEU
14	Da	25	ARG
14	Da	38	ASP
14	Da	42	ARG
14	Da	61	ARG
15	DB	78	ARG
15	DB	99	VAL
15	DB	118	VAL
15	DB	129	TYR
15	DB	173	ARG
15	DB	186	SER
15	DB	189	VAL
15	DB	204	SER
15	DB	213	ASP
15	DB	217	ILE
15	DB	221	HIS
15	DB	233	ASP
15	DB	239	GLN
15	DB	249	SER
15	DB	321	SER
15	DB	339	ARG
15	DB	343	VAL
15	DB	368	GLU
15	DB	383	ARG
15	DB	394	ASP
15	DB	416	ASN
15	DB	424	ASP
15	DB	433	ARG
15	DB	435	THR
15	DB	439	VAL
15	DB	445	ASN
15	DB	448	ASP
15	DB	450	MET
15	DB	454	ASP
15	DB	462	ASP
15	DB	490	ARG
15	DB	503	ASN
15	DB	507	LEU
15	DB	511	ARG
15	DB	514	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	DB	521	LEU
15	DB	522	MET
15	DB	532	GLU
15	DB	539	GLN
15	DB	550	LEU
15	DB	553	LEU
15	DB	554	GLU
15	DB	572	ASP
15	DB	574	ILE
15	DB	587	VAL
15	DB	590	ASP
15	DB	592	MET
15	DB	597	GLU
15	DB	637	THR
15	DB	671	VAL
15	DB	690	ARG
15	DB	693	SER
15	DB	720	LYS
15	DB	744	VAL
15	DB	755	LEU
15	DB	756	THR
15	DB	758	SER
15	DB	774	ASN
15	DB	785	ASN
15	DB	790	SER
15	DB	793	ARG
15	DB	810	THR
15	DB	815	ASP
15	DB	820	GLU
15	DB	822	PHE
15	DB	830	LEU
15	DB	831	ASN
15	DB	834	ILE
15	DB	849	ASP
15	DB	850	SER
15	DB	901	VAL
15	DB	908	GLN
15	DB	923	GLN
15	DB	942	ARG
15	DB	958	ASN
15	DB	964	ARG
15	DB	968	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	DB	984	ASP
15	DB	995	VAL
15	DB	1009	ASP
15	DB	1012	THR
15	DB	1013	ARG
15	DB	1020	ASP
15	DB	1026	SER
15	DB	1028	SER
15	DB	1030	ARG
15	DB	1034	ILE
15	DB	1067	ILE
15	DB	1069	THR
15	DB	1080	ARG
15	DB	1104	ASP
15	DB	1110	LYS
15	DB	1117	THR
15	DB	1142	VAL
15	DB	1153	ASP
15	DB	1156	THR
15	DB	1165	SER
15	DB	1168	ASP
15	DB	1172	LYS
15	DB	1173	THR
15	DB	1181	LEU
16	DC	30	THR
16	DC	36	ASP
16	DC	46	ARG
16	DC	57	GLU
16	DC	58	VAL
16	DC	82	THR
16	DC	86	THR
16	DC	87	MET
16	DC	92	PHE
16	DC	93	ARG
16	DC	106	SER
16	DC	108	SER
16	DC	114	GLU
16	DC	128	HIS
16	DC	131	GLU
16	DC	148	LEU
16	DC	154	THR
16	DC	162	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	DC	166	GLU
16	DC	168	PHE
16	DC	227	GLN
16	DC	231	THR
16	DC	268	ASP
16	DC	271	SER
16	DC	279	GLU
16	DC	299	LEU
16	DC	305	ARG
16	DC	313	THR
16	DC	344	MET
16	DC	365	LYS
16	DC	371	ILE
16	DC	379	LEU
16	DC	386	MET
16	DC	406	GLN
16	DC	435	LEU
16	DC	437	LEU
16	DC	442	LEU
16	DC	464	THR
16	DC	467	THR
16	DC	471	ARG
16	DC	474	LEU
16	DC	475	LEU
16	DC	491	LEU
16	DC	498	LEU
16	DC	503	ASP
16	DC	506	SER
16	DC	511	ARG
16	DC	513	SER
16	DC	519	SER
16	DC	525	THR
16	DC	533	LEU
16	DC	534	LEU
16	DC	540	LEU
16	DC	544	GLU
16	DC	545	ASP
16	DC	567	ARG
16	DC	569	LEU
16	DC	604	VAL
16	DC	611	MET
16	DC	618	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	DC	620	VAL
16	DC	632	LEU
16	DC	652	ARG
16	DC	659	LEU
16	DC	669	LEU
16	DC	705	LEU
16	DC	710	THR
16	DC	749	GLU
16	DC	753	LEU
16	DC	755	ASP
16	DC	756	ASP
16	DC	757	ARG
16	DC	766	VAL
16	DC	774	ASP
16	DC	799	ASN
16	DC	809	TYR
16	DC	817	ASP
16	DC	828	ARG
16	DC	865	CYS
16	DC	881	MET
16	DC	885	LEU
16	DC	894	HIS
16	DC	928	GLU
16	DC	934	ARG
16	DC	952	GLU
16	DC	953	MET
16	DC	954	LEU
16	DC	955	ASP
16	DC	960	VAL
16	DC	961	THR
16	DC	963	SER
16	DC	970	GLN
16	DC	987	THR
16	DC	1000	LEU
16	DC	1009	THR
16	DC	1019	THR
16	DC	1021	ASN
16	DC	1023	ASN
16	DC	1025	THR
16	DC	1055	ARG
16	DC	1062	GLN
16	DC	1063	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	DC	1071	VAL
16	DC	1076	PHE
16	DC	1104	MET
16	DC	1112	ASP
16	DC	1119	GLN
16	DC	1121	THR
16	DC	1125	SER
16	DC	1128	ARG
16	DC	1132	THR
16	DC	1133	THR
16	DC	1143	VAL
16	DC	1151	THR
16	DC	1153	LEU
16	DC	1159	ASP
16	DC	1161	LYS
16	DC	1162	SER
16	DC	1163	GLU
17	DE	46	SER
17	DE	51	ARG
17	DE	54	ARG
17	DE	65	ILE
17	DE	80	LEU
17	DE	149	LEU
17	DE	150	ARG
17	DE	154	SER
17	DE	178	GLN
17	DE	196	ASP
17	DE	203	LEU
17	DE	212	LEU
17	DE	229	ARG
17	DE	246	ILE
17	DE	280	LEU
17	DE	299	LYS
17	DE	319	ASN
17	DE	333	ASP
17	DE	343	LEU
17	DE	398	LEU
17	DE	405	ILE
17	DE	406	ASP
17	DE	408	LEU
17	DE	418	LEU
17	DE	429	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	DE	445	LEU
17	DE	451	THR
17	DE	484	THR
17	DE	494	ARG
17	DE	503	ASP
17	DE	529	ASP
17	DE	530	TRP
17	DE	538	VAL
17	DE	545	ARG
17	DE	554	LEU
17	DE	566	ARG
17	DE	570	GLU
17	DE	572	VAL
17	DE	573	GLN
17	DE	575	CYS
17	DE	587	MET
17	DE	591	LEU
17	DE	602	LYS
17	DE	604	ASP
17	DE	610	LEU
17	DE	615	LEU
17	DE	651	ASN
17	DE	659	ARG
17	DE	698	GLN
17	DE	699	ASN
17	DE	704	LEU
17	DE	717	ARG
17	DE	718	SER
17	DE	721	ASP
17	DE	726	THR
18	DF	8	SER
18	DF	13	ILE
18	DF	15	HIS
18	DF	22	LEU
18	DF	27	ARG
18	DF	33	GLN
18	DF	39	ARG
18	DF	40	GLU
18	DF	50	LEU
18	DF	53	ARG
18	DF	57	ARG
18	DF	69	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	DF	72	THR
18	DF	85	ARG
18	DF	87	GLU
18	DF	110	ASN
18	DF	144	THR
18	DF	154	ASN
18	DF	157	THR
18	DF	170	ARG
18	DF	173	PHE
18	DF	182	ARG
18	DF	188	ARG
18	DF	189	ASP
18	DF	192	LEU
18	DF	194	THR
18	DF	202	LEU
18	DF	238	THR
18	DF	246	LYS
18	DF	255	GLU
18	DF	258	ASP
18	DF	259	SER
18	DF	264	VAL
18	DF	274	LEU
18	DF	294	MET
18	DF	297	ARG
18	DF	307	GLU
18	DF	321	LEU
18	DF	326	ASP
18	DF	331	GLU
18	DF	343	GLU
18	DF	362	ILE
18	DF	370	LEU
18	DF	373	ASP
18	DF	394	GLU
18	DF	395	LEU
18	DF	403	LEU
18	DF	437	GLU
18	DF	450	VAL
18	DF	476	LEU
18	DF	491	ARG
18	DF	502	ARG
18	DF	548	ARG
18	DF	550	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	DF	553	THR
18	DF	568	LEU
18	DF	584	LEU
19	DG	36	THR
19	DG	56	ARG
19	DG	57	GLU
19	DG	62	SER
19	DG	74	LEU
19	DG	78	HIS
19	DG	84	LEU
19	DG	93	ARG
19	DG	95	VAL
19	DG	98	ASP
19	DG	115	ILE
19	DG	125	ASP
19	DG	127	LEU
19	DG	130	LEU
19	DG	141	THR
19	DG	142	LEU
19	DG	147	SER
19	DG	149	SER
19	DG	155	GLU
19	DG	179	LEU
19	DG	186	ARG
19	DG	200	GLN
19	DG	206	LEU
19	DG	210	VAL
19	DG	214	TYR
19	DG	220	THR
19	DG	236	VAL
19	DG	296	ASP
19	DG	298	ASP
19	DG	318	ILE
19	DG	326	THR
19	DG	332	GLN
19	DG	334	MET
19	DG	365	GLN
19	DG	367	SER
19	DG	370	ARG
19	DG	377	GLU
19	DG	384	VAL
19	DG	392	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	DG	399	ARG
19	DG	443	ARG
19	DG	444	THR
19	DG	448	LEU
19	DG	457	ARG
19	DG	466	VAL
19	DG	472	ARG
19	DG	473	CYS
19	DG	494	THR
19	DG	496	ARG
19	DG	497	ARG
19	DG	529	ASP
19	DG	544	ARG
19	DG	547	MET
19	DG	551	MET
19	DG	557	GLN
19	DG	564	GLU
19	DG	577	LEU
19	DG	582	VAL
19	DG	608	ARG
19	DG	615	SER
19	DG	616	ARG
19	DG	618	ARG
19	DG	623	MET
19	DG	626	LEU
20	DH	1	MET
20	DH	9	THR
20	DH	18	ARG
20	DH	40	THR
20	DH	42	ARG
20	DH	46	LEU
20	DH	51	ARG
20	DH	76	LEU
20	DH	79	ASP
20	DH	80	ARG
20	DH	81	LYS
20	DH	82	GLN
20	DH	83	GLU
20	DH	84	SER
20	DH	85	LEU
20	DH	105	GLN
20	DH	135	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	DH	167	GLU
20	DH	174	LEU
20	DH	178	SER
20	DH	195	TYR
20	DH	206	ILE
20	DH	236	MET
20	DH	257	ASN
20	DH	268	LEU
20	DH	273	SER
20	DH	297	CYS
20	DH	311	ARG
20	DH	318	GLU
20	DH	323	SER
20	DH	327	HIS
20	DH	345	VAL
20	DH	348	LYS
20	DH	354	LEU
20	DH	360	LEU
20	DH	364	ARG
20	DH	369	ARG
20	DH	380	ARG
20	DH	382	PHE
20	DH	386	ARG
20	DH	392	TRP
20	DH	411	LEU
20	DH	414	LEU
20	DH	418	LYS
20	DH	421	THR
20	DH	428	ARG
20	DH	450	ASN
20	DH	452	ARG
20	DH	460	LEU
20	DH	470	LYS
20	DH	474	ASP
20	DH	476	VAL
20	DH	484	ASP
20	DH	495	THR
20	DH	503	THR
20	DH	515	ASP
20	DH	523	ARG
20	DH	557	VAL
20	DH	562	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	DJ	16	ASN
21	DJ	19	THR
21	DJ	33	ASN
21	DJ	38	MET
21	DJ	46	ARG
21	DJ	48	PHE
21	DJ	55	ASN
21	DJ	76	SER
21	DJ	107	LEU
21	DJ	110	LEU
21	DJ	119	LEU
21	DJ	137	MET
21	DJ	149	THR
21	DJ	151	GLU
21	DJ	164	SER
21	DJ	178	ARG
21	DJ	180	LEU
21	DJ	182	ASP
21	DJ	206	SER
21	DJ	212	ASP
21	DJ	226	VAL
21	DJ	234	GLU
21	DJ	236	ARG
21	DJ	246	THR
21	DJ	258	LEU
21	DJ	273	TYR
21	DJ	275	ASP
21	DJ	291	ASN
21	DJ	302	SER
21	DJ	305	ARG
21	DJ	308	ARG
22	DK	2	SER
22	DK	18	LEU
22	DK	34	ASN
22	DK	36	ARG
22	DK	54	THR
22	DK	111	LEU
22	DK	115	THR
22	DK	116	ARG
22	DK	134	THR
22	DK	167	THR
22	DK	172	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	DK	226	LEU
22	DK	240	SER
22	DK	250	VAL
22	DK	270	LEU
22	DK	273	LEU
22	DK	294	SER
23	DT	11	ASP
23	DT	12	ARG
23	DT	33	HIS
23	DT	35	LYS
23	DT	52	ARG
23	DT	63	HIS
23	DT	88	THR
23	DT	90	THR
23	DT	91	GLN
23	DT	103	LEU
23	DT	105	ARG
23	DT	106	ASP
23	DT	114	LEU
23	DT	122	MET
23	DT	131	SER
23	DT	137	LEU
23	DT	163	ARG
23	DT	166	THR
23	DT	168	GLU
23	DT	176	ASP
23	DT	177	MET
23	DT	181	ASP
23	DT	208	ARG
23	DT	209	THR
23	DT	241	ASN
24	DV	26	THR
24	DV	39	ARG
24	DV	41	THR
24	DV	43	ASN
24	DV	56	ARG
24	DV	68	ILE
24	DV	71	GLN
24	DV	77	LYS
24	DV	114	VAL
24	DV	118	GLN
24	DV	131	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	DV	134	ASP
24	DV	140	PHE
24	DV	143	ILE
24	DV	178	THR
24	DV	179	LEU
24	DV	180	ASP
24	DV	182	TYR
25	DW	10	THR
25	DW	22	THR
25	DW	37	MET
25	DW	58	ARG
25	DW	60	VAL
25	DW	70	LEU
25	DW	74	THR
25	DW	125	LYS
25	DW	128	LEU
25	DW	133	LYS
25	DW	145	ARG
25	DW	163	GLU
26	DX	34	LYS
26	DX	57	ARG
26	DX	72	SER
26	DX	76	ARG
26	DX	89	ARG
26	DX	90	ILE
26	DX	98	LEU
26	DX	124	ILE
26	DX	132	THR
26	DX	136	ARG
26	DX	162	VAL
26	DX	164	THR
26	DX	168	ASN
27	DY	11	THR
27	DY	14	THR
27	DY	15	SER
27	DY	23	SER
27	DY	39	VAL
27	DY	43	LEU
27	DY	50	VAL
27	DY	52	GLN
27	DY	64	ASP
27	DY	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	DY	81	THR
27	DY	85	ARG
27	DY	87	ARG
27	DY	93	THR
27	DY	111	ARG
27	DY	124	THR
27	DY	128	GLN
27	DY	141	VAL
27	DY	163	LYS
28	CC	4	MET
28	CC	7	ILE
28	CC	10	VAL
28	CC	13	LYS
28	CC	14	THR
28	CC	21	PHE
28	CC	46	TRP
28	CC	47	LEU
28	CC	50	ILE
28	CC	69	GLU
28	CC	76	SER
29	CE	10	LYS
29	CE	13	ASN
29	CE	16	TYR
29	CE	17	THR
29	CE	27	ARG
29	CE	41	ARG
29	CE	48	ASN
29	CE	58	SER
29	CE	64	THR
29	CE	65	ARG
29	CE	80	ILE
29	CE	83	MET
29	CE	87	ILE
29	CE	112	THR
29	CE	121	THR
29	CE	124	THR
29	CE	137	LEU
29	CE	157	LYS
29	CE	163	ILE
29	CE	165	CYS
29	CE	188	GLU
29	CE	201	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	CE	223	ARG
29	CE	231	ARG
29	CE	232	ILE
29	CE	279	LEU
29	CE	313	MET
29	CE	314	MET
29	CE	332	ASP
29	CE	334	ARG
29	CE	364	ARG
29	CE	365	MET
29	CE	370	ASP
29	CE	391	THR
29	CE	395	THR
29	CE	396	LEU
29	CE	405	LYS
29	CE	410	LEU
29	CE	417	ASN
29	CE	422	VAL
29	CE	424	LEU
30	CF	2	VAL
30	CF	63	ARG
30	CF	93	LEU
30	CF	123	ARG
30	CF	133	GLN
30	CF	141	GLN
30	CF	152	THR
31	CH	26	ARG
31	CH	29	HIS
31	CH	46	LYS
31	CH	48	ASP
31	CH	88	LEU
31	CH	89	VAL
31	CH	108	LEU
31	CH	118	LEU
31	CH	128	VAL
31	CH	131	ASP
31	CH	132	ASP
31	CH	143	ARG
31	CH	150	THR
31	CH	154	ASP
31	CH	163	THR
31	CH	170	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CH	172	VAL
31	CH	179	ARG
31	CH	201	ARG
31	CH	248	ASN
31	CH	279	MET
31	CH	280	MET
32	CI	18	LEU
32	CI	33	SER
32	CI	34	ASP
32	CI	38	LEU
32	CI	43	SER
32	CI	47	ARG
32	CI	59	ARG
32	CI	65	MET
32	CI	104	ASN
32	CI	110	ARG
32	CI	127	MET
32	CI	139	ASP
32	CI	165	ASN
32	CI	175	ARG
32	CI	179	CYS
32	CI	218	ARG
32	CI	219	LEU
32	CI	245	ARG
32	CI	256	LYS
32	CI	290	ILE
32	CI	303	THR
32	CI	309	ARG
32	CI	311	CYS
32	CI	324	ARG
32	CI	330	ASN
32	CI	338	LYS
32	CI	343	VAL
32	CI	356	MET
32	CI	372	ILE
32	CI	406	THR
32	CI	420	ARG
32	CI	435	LYS
32	CI	439	ARG
33	CJ	17	MET
33	CJ	20	GLN
33	CJ	23	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	CJ	34	GLN
33	CJ	43	GLU
33	CJ	50	ASP
33	CJ	65	VAL
33	CJ	68	ASP
33	CJ	77	CYS
33	CJ	78	THR
33	CJ	84	MET
33	CJ	93	SER
33	CJ	105	ASN
33	CJ	110	LYS
33	CJ	130	ARG
33	CJ	141	ASP
33	CJ	149	GLU
33	CJ	158	THR
33	CJ	162	ILE
33	CJ	178	SER
33	CJ	186	VAL
33	CJ	202	ASP
33	CJ	203	ARG
33	CJ	212	THR
33	CJ	257	VAL
33	CJ	273	ARG
33	CJ	279	LYS
33	CJ	286	LEU
33	CJ	287	LEU
33	CJ	293	ASP
33	CJ	304	ARG
33	CJ	311	LEU
33	CJ	313	GLU
33	CJ	325	SER
33	CJ	330	LEU
33	CJ	345	VAL
33	CJ	346	PRO
33	CJ	380	THR
33	CJ	396	LYS
33	CJ	399	ARG
33	CJ	403	CYS
33	CJ	409	SER
33	CJ	413	GLU
33	CJ	456	THR
33	CJ	457	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	CJ	481	ASP
33	CJ	490	ASP
33	CJ	498	CYS
33	CJ	517	VAL
33	CJ	519	ILE
33	CJ	523	VAL
33	CJ	526	THR
33	CJ	532	PHE
33	CJ	542	LYS
33	CJ	547	LYS
33	CJ	552	ILE
33	CJ	553	ARG
33	CJ	556	GLU
33	CJ	565	THR
33	CJ	569	LEU
33	CJ	585	SER
33	CJ	605	THR
33	CJ	618	VAL
33	CJ	629	ARG
33	CJ	648	VAL
33	CJ	654	VAL
33	CJ	671	LEU
33	CJ	684	THR
33	CJ	704	GLU
33	CJ	714	THR
33	CJ	720	THR
33	CJ	727	THR
33	CJ	757	LEU
33	CJ	762	GLN
33	CJ	769	GLN
33	CJ	770	THR
33	CJ	773	GLU
33	CJ	781	HIS
33	CJ	796	ASP
33	CJ	797	LEU
33	CJ	798	GLN
34	CK	15	ARG
34	CK	23	ASP
34	CK	32	LEU
34	CK	33	LYS
34	CK	40	GLN
34	CK	48	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	CK	56	GLN
34	CK	70	ILE
34	CK	73	GLN
34	CK	98	LEU
34	CK	107	GLN
34	CK	109	VAL
34	CK	112	GLU
34	CK	113	ARG
34	CK	149	VAL
34	CK	156	LYS
34	CK	205	TYR
34	CK	207	VAL
34	CK	232	ARG
34	CK	264	SER
34	CK	311	THR
34	CK	315	LEU
34	CK	325	PHE
34	CK	326	LYS
35	CL	59	MET
35	CL	75	CYS
35	CL	91	LEU
35	CL	95	PHE
35	CL	97	LEU
35	CL	109	CYS
35	CL	118	LEU
35	CL	122	GLU
35	CL	133	LYS
36	CN	22	THR
36	CN	30	LEU
36	CN	35	SER
36	CN	41	LEU
36	CN	43	SER
36	CN	49	SER
36	CN	57	LYS
36	CN	60	VAL
36	CN	65	LYS
36	CN	66	MET
36	CN	70	LYS
36	CN	72	THR
36	CN	77	ASN
36	CN	81	LEU
36	CN	83	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	CN	111	VAL
36	CN	118	MET
36	CN	127	LEU
36	CN	135	THR
36	CN	158	ARG
37	CO	69	GLU
37	CO	75	LEU
37	CO	82	ASN
37	CO	87	THR
37	CO	108	THR
37	CO	190	SER
37	CO	209	GLU
37	CO	210	ARG
37	CO	220	SER
37	CO	224	LEU
37	CO	237	ASN
37	CO	242	ASN
37	CO	244	HIS
37	CO	245	ASN
37	CO	266	LEU
37	CO	285	ASP
37	CO	304	ASP
37	CO	329	GLU
37	CO	336	GLU
37	CO	353	GLU
37	CO	362	VAL
37	CO	395	VAL
37	CO	400	ARG
37	CO	412	ARG
37	CO	419	VAL
38	CP	14	LYS
38	CP	15	ARG
38	CP	36	VAL
38	CP	40	PHE
38	CP	59	ARG
38	CP	68	CYS
38	CP	90	MET
38	CP	93	THR
38	CP	129	THR
38	CP	152	ASN
38	CP	163	LYS
38	CP	170	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	CP	188	LEU
39	CQ	16	THR
39	CQ	21	ARG
39	CQ	31	THR
39	CQ	34	THR
39	CQ	56	ARG
39	CQ	67	LEU
39	CQ	69	GLN
39	CQ	70	ARG
39	CQ	73	ARG
39	CQ	83	LEU
39	CQ	103	MET
39	CQ	114	MET
39	CQ	123	ARG
39	CQ	136	ASP
39	CQ	146	HIS
39	CQ	147	ILE
39	CQ	158	HIS
39	CQ	169	VAL
39	CQ	182	VAL
39	CQ	199	ASN
40	CR	15	GLN
40	CR	30	LEU
40	CR	44	GLU
40	CR	59	LEU
40	CR	70	ARG
40	CR	80	LEU
40	CR	96	GLN
40	CR	167	ARG
40	CR	181	ARG
40	CR	184	LYS
40	CR	198	THR
40	CR	233	SER
40	CR	235	SER
40	CR	278	VAL
40	CR	305	THR
40	CR	315	LEU
40	CR	320	VAL
41	CS	32	LYS
41	CS	48	ARG
41	CS	64	MET
41	CS	65	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	CS	75	MET
41	CS	76	THR
41	CS	86	GLU
41	CS	95	THR
41	CS	107	THR
41	CS	121	SER
41	CS	140	MET
41	CS	152	ASP
42	CU	13	MET
42	CU	32	HIS
42	CU	44	MET
42	CU	46	GLU
42	CU	74	GLN
42	CU	148	ASN
42	CU	161	GLN
42	CU	169	ASN
42	CU	171	VAL
43	CZ	218	VAL
43	CZ	236	ARG
43	CZ	237	ARG
43	CZ	240	VAL
43	CZ	260	MET
43	CZ	265	GLN
43	CZ	277	PHE
43	CZ	318	LEU
43	CZ	321	MET
43	CZ	360	ASP
44	Ca	14	ASN
44	Ca	15	LYS
44	Ca	16	ARG
44	Ca	19	ARG
44	Ca	67	ARG
44	Ca	71	MET
44	Ca	153	LYS
44	Ca	168	TYR
44	Ca	181	GLU
44	Ca	191	MET
44	Ca	194	LEU
44	Ca	201	ARG
44	Ca	221	THR
44	Ca	227	ASN
44	Ca	240	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	Ca	295	PHE
44	Ca	297	LEU
44	Ca	299	ARG
44	Ca	305	HIS
44	Ca	314	CYS
44	Ca	338	LYS
44	Ca	350	GLU
44	Ca	365	LEU
44	Ca	376	VAL
44	Ca	380	ASP
44	Ca	384	ARG
44	Ca	398	ASP
44	Ca	399	ASN
44	Ca	410	MET
44	Ca	433	GLN
44	Ca	447	ILE
44	Ca	451	VAL
44	Ca	479	THR
44	Ca	480	LEU
44	Ca	506	GLN
44	Ca	520	TYR
44	Ca	537	ARG
44	Ca	538	ILE
44	Ca	541	ARG
44	Ca	552	THR
44	Ca	569	ARG
44	Ca	575	ARG
44	Ca	578	ASP
45	Cb	40	LEU
45	Cb	57	MET
45	Cb	71	LEU
45	Cb	108	GLU
45	Cb	110	MET
45	Cb	144	ARG
45	Cb	158	LYS
45	Cb	171	THR
45	Cb	193	GLU
45	Cb	195	LEU
45	Cb	205	LYS
45	Cb	223	ARG
45	Cb	288	GLU
45	Cb	291	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	Cb	304	SER
45	Cb	306	THR
46	Cd	13	ARG
46	Cd	44	GLU
46	Cd	63	ARG
46	Cd	74	ASP
46	Cd	102	ARG
46	Cd	106	ARG
46	Cd	108	MET
46	Cd	120	LEU
46	Cd	122	LEU
46	Cd	125	GLU
46	Cd	164	LEU
46	Cd	168	VAL
46	Cd	180	VAL
46	Cd	208	HIS
46	Cd	210	ASP
46	Cd	216	HIS
46	Cd	217	GLU
46	Cd	219	HIS
46	Cd	222	SER
46	Cd	259	GLU
46	Cd	284	THR
47	Cg	20	THR
47	Cg	56	ARG
47	Cg	57	THR
47	Cg	73	ASP
47	Cg	76	SER
47	Cg	87	GLN
47	Cg	107	ARG
47	Cg	112	ARG
47	Cg	114	GLU
47	Cg	117	LEU
47	Cg	120	LEU
47	Cg	127	HIS
47	Cg	143	THR
47	Cg	153	CYS
47	Cg	170	ASN
47	Cg	173	THR
47	Cg	189	TRP
47	Cg	194	LEU
47	Cg	213	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	Cg	221	SER
47	Cg	224	LEU
47	Cg	225	ARG
47	Cg	226	CYS
47	Cg	233	THR
47	Cg	262	GLN
47	Cg	290	LEU
47	Cg	296	HIS
47	Cg	308	LEU
47	Cg	310	SER
47	Cg	316	THR
47	Cg	318	ILE
47	Cg	319	ASP
47	Cg	325	LEU
47	Cg	344	LEU
47	Cg	355	THR
47	Cg	373	VAL
47	Cg	383	ASP
47	Cg	391	GLU
47	Cg	421	GLU
47	Cg	422	LEU
47	Cg	436	ASP
47	Cg	464	VAL
47	Cg	468	ASP
47	Cg	480	LYS
48	Ci	14	ARG
48	Ci	18	THR
48	Ci	27	CYS
48	Ci	30	ARG
48	Ci	32	ASP
48	Ci	54	GLN
48	Ci	76	MET
48	Ci	82	GLN
48	Ci	105	ARG
48	Ci	114	MET
48	Ci	119	LEU
48	Ci	122	MET
48	Ci	136	HIS
48	Ci	138	ASP
48	Ci	144	ARG
48	Ci	145	ASN
48	Ci	146	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	Ci	157	LEU
48	Ci	164	ASN
48	Ci	174	ASP
49	Cj	10	ARG
49	Cj	34	HIS
49	Cj	58	MET
49	Cj	66	LEU
49	Cj	77	LEU
49	Cj	80	LEU
49	Cj	126	TYR
49	Cj	135	ILE
49	Cj	145	THR
49	Cj	161	VAL
49	Cj	173	MET
49	Cj	175	PHE
49	Cj	206	LEU
49	Cj	210	PRO
50	Ck	34	GLN
50	Ck	57	ASP
50	Ck	86	GLU
50	Ck	87	ARG
50	Ck	97	GLN
50	Ck	99	SER
50	Ck	104	SER
50	Ck	108	GLN
50	Ck	111	THR
50	Ck	136	ASP
50	Ck	137	THR
50	Ck	161	GLU
50	Ck	176	THR
50	Ck	185	LEU
50	Ck	188	LEU
50	Ck	207	ARG
50	Ck	214	LEU
50	Ck	242	LEU
50	Ck	254	ILE
50	Ck	290	LEU
50	Ck	292	ASP
50	Ck	316	ASP
50	Ck	317	VAL
50	Ck	320	VAL
50	Ck	341	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	Ck	350	ASP
50	Ck	353	ARG
50	Ck	373	ARG
50	Ck	401	LEU
50	Ck	568	LEU
50	Ck	573	THR
50	Ck	574	GLU
50	Ck	575	LEU
50	Ck	597	LEU
50	Ck	607	LYS
50	Ck	611	ASN
50	Ck	618	ILE
50	Ck	620	THR
50	Ck	627	ASP
50	Ck	629	LEU
50	Ck	633	MET
50	Ck	634	HIS
50	Ck	652	ARG
50	Ck	654	SER
50	Ck	661	ILE
50	Ck	682	ASN
50	Ck	690	TRP
50	Ck	691	GLN
50	Ck	695	GLN
50	Ck	703	ARG
50	Ck	706	SER
50	Ck	707	LEU
50	Ck	733	LEU
50	Ck	755	ASP
50	Ck	760	VAL
50	Ck	775	ARG
50	Ck	806	ASP
50	Ck	838	LEU
50	Ck	841	LYS
51	Cm	35	ASN
51	Cm	50	ARG
51	Cm	60	ARG
51	Cm	61	ARG
51	Cm	80	THR
51	Cm	85	ILE
51	Cm	92	GLN
51	Cm	93	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	Cm	94	THR
51	Cm	95	MET
51	Cm	98	SER
51	Cm	106	CYS
51	Cm	117	ARG
51	Cm	123	ASP
51	Cm	124	SER
51	Cm	125	CYS
51	Cm	126	LEU
51	Cm	153	ASP
51	Cm	162	ARG
51	Cm	173	GLU
51	Cm	178	GLU
51	Cm	179	ARG
51	Cm	188	ARG
51	Cm	193	PHE
51	Cm	202	THR
52	Cn	165	LEU
52	Cn	172	LYS
52	Cn	195	PHE
52	Cn	203	MET
52	Cn	214	ARG
52	Cn	235	GLU
53	Cp	28	ARG
53	Cp	30	LEU
53	Cp	50	THR
53	Cp	84	LEU
53	Cp	87	CYS
53	Cp	91	GLN
53	Cp	105	ILE
53	Cp	123	THR
53	Cp	137	ASP
53	Cp	166	ARG
53	Cp	168	ILE
53	Cp	181	ARG
54	Cq	19	VAL
54	Cq	30	ILE
54	Cq	64	VAL
54	Cq	65	SER
54	Cq	78	ASP
54	Cq	79	MET
54	Cq	96	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	Cq	106	LEU
54	Cq	107	GLU
54	Cq	111	ARG
54	Cq	144	THR
54	Cq	185	CYS
54	Cq	207	CYS
54	Cq	227	ILE
54	Cq	235	LEU
54	Cq	250	LEU
54	Cq	253	ARG
55	Cr	10	ARG
55	Cr	13	ARG
55	Cr	25	LEU
55	Cr	26	LEU
55	Cr	37	CYS
55	Cr	45	THR
55	Cr	56	MET
55	Cr	58	ASN
55	Cr	74	ASP
55	Cr	79	LYS
55	Cr	96	GLU
55	Cr	161	ARG
55	Cr	163	LEU
55	Cr	171	GLN
55	Cr	247	ILE
55	Cr	248	ARG
55	Cr	250	LYS
55	Cr	265	LEU
55	Cr	266	GLN
55	Cr	279	ASP
55	Cr	282	GLU
56	Cv	27	LYS
56	Cv	28	THR
56	Cv	32	ARG
56	Cv	35	ARG
56	Cv	86	GLU
56	Cv	87	GLN
56	Cv	98	ARG
56	Cv	151	SER
56	Cv	162	SER
56	Cv	172	THR
56	Cv	201	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	Cv	204	ILE
56	Cv	208	LYS
56	Cv	209	VAL
56	Cv	210	ASP
56	Cv	235	MET
56	Cv	245	ASN
56	Cv	261	ILE
56	Cv	266	CYS
56	Cv	278	LEU
56	Cv	283	ASP
56	Cv	284	LYS
56	Cv	301	SER
56	Cv	305	ASP
56	Cv	312	ASN
56	Cv	367	ASP
56	Cv	401	THR
56	Cv	407	MET
56	Cv	411	ASN
56	Cv	417	THR
56	Cv	446	THR
56	Cv	531	MET
56	Cv	566	MET
56	Cv	569	LEU
56	Cv	594	LEU
56	Cv	613	LEU
56	Cv	617	ASP
56	Cv	638	VAL
56	Cv	649	THR
56	Cv	651	ARG
56	Cv	678	HIS
56	Cv	727	ARG
56	Cv	739	ASN
56	Cv	782	ILE
56	Cv	795	GLU
56	Cv	813	ARG
56	Cv	818	LEU
56	Cv	838	LEU
56	Cv	861	THR
56	Cv	916	ARG
56	Cv	918	LEU
56	Cv	927	LEU
56	Cv	937	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	Cv	938	ASP
56	Cv	945	VAL
56	Cv	969	ASP
56	Cv	987	SER
56	Cv	993	THR
56	Cv	995	VAL
56	Cv	996	SER
56	Cv	1002	ARG
56	Cv	1018	THR
56	Cv	1034	ARG
56	Cv	1040	GLU
56	Cv	1069	GLN
56	Cv	1102	LYS
56	Cv	1108	GLN
56	Cv	1136	ASN
64	A0	31	LEU
64	A0	71	ARG
64	A0	75	ASN
64	A0	76	THR
64	A0	82	THR
64	A0	112	ARG
64	A0	116	LEU
64	A0	130	VAL
64	A0	139	GLU
64	A0	143	LEU
64	A0	155	VAL
64	A0	163	LYS
64	A0	166	ASN
64	A0	181	ARG
65	A1	28	ARG
65	A1	42	TRP
65	A1	46	CYS
65	A1	49	VAL
65	A1	60	VAL
65	A1	61	THR
65	A1	63	ARG
65	A1	71	GLN
65	A1	75	VAL
65	A1	78	LEU
65	A1	90	ARG
65	A1	97	ARG
65	A1	104	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
65	A1	106	THR
65	A1	114	LEU
65	A1	120	VAL
65	A1	130	VAL
65	A1	133	ASP
65	A1	154	GLU
65	A1	156	ILE
65	A1	174	GLN
65	A1	178	GLN
65	A1	191	MET
65	A1	192	GLU
65	A1	201	LEU
65	A1	223	LYS
65	A1	225	GLN
66	A2	17	VAL
66	A2	22	LEU
66	A2	26	ARG
66	A2	36	VAL
66	A2	37	GLU
66	A2	44	LEU
66	A2	50	ILE
66	A2	58	ARG
66	A2	69	LEU
66	A2	72	GLN
66	A2	88	ASP
66	A2	90	SER
66	A2	94	ILE
66	A2	138	THR
66	A2	157	LEU
66	A2	165	GLU
66	A2	170	ILE
66	A2	182	LEU
66	A2	183	LYS
66	A2	186	GLU
66	A2	189	GLU
66	A2	207	GLN
66	A2	255	ARG
66	A2	270	ASN
66	A2	295	ASN
66	A2	296	VAL
66	A2	298	LEU
66	A2	305	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	A2	345	ILE
66	A2	347	VAL
66	A2	350	VAL
66	A2	366	VAL
66	A2	374	LEU
66	A2	381	GLU
66	A2	384	LEU
66	A2	413	TYR
66	A2	415	ASN
66	A2	417	VAL
66	A2	420	VAL
66	A2	463	ILE
66	A2	468	VAL
67	A3	61	ARG
67	A3	62	VAL
67	A3	83	ARG
67	A3	97	THR
67	A3	104	GLN
67	A3	130	ILE
67	A3	140	ASP
67	A3	152	VAL
67	A3	171	ARG
67	A3	178	LEU
68	A4	11	ARG
68	A4	19	LEU
68	A4	31	ARG
68	A4	39	ILE
68	A4	48	LYS
68	A4	61	ARG
68	A4	90	LEU
68	A4	110	LEU
68	A4	119	GLU
68	A4	128	LYS
68	A4	142	VAL
69	A5	34	GLN
69	A5	49	LEU
69	A5	51	MET
69	A5	76	ARG
69	A5	78	ILE
70	A6	41	ARG
70	A6	70	VAL
70	A6	80	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
70	A6	81	LEU
70	A6	86	LYS
70	A6	87	ILE
70	A6	88	LYS
70	A6	92	MET
70	A6	99	LYS
71	A8	42	MET
71	A8	44	CYS
71	A8	54	VAL
71	A8	67	MET
71	A8	83	ARG
71	A8	84	VAL
71	A8	91	LYS
71	A8	92	MET
71	A8	96	ARG
71	A8	111	ARG
71	A8	136	GLN
71	A8	140	LEU
71	A8	143	THR
71	A8	151	SER
71	A8	154	ILE
71	A8	163	LYS
71	A8	173	ARG
71	A8	175	ASP
72	A9	60	GLN
72	A9	65	ARG
72	A9	68	LEU
72	A9	82	ASP
72	A9	88	CYS
72	A9	98	GLU
72	A9	99	MET
72	A9	110	GLN
73	AE	71	MET
73	AE	73	LEU
73	AE	83	GLU
73	AE	98	GLU
73	AE	102	ASP
73	AE	106	ARG
73	AE	117	ASP
73	AE	137	ARG
73	AE	158	PHE
73	AE	175	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
73	AE	190	MET
73	AE	192	VAL
73	AE	195	GLU
73	AE	236	ARG
73	AE	246	ILE
73	AE	338	ARG
73	AE	340	SER
73	AE	343	ILE
73	AE	345	THR
73	AE	362	THR
73	AE	364	ILE
73	AE	370	ASP
73	AE	371	LEU
73	AE	379	CYS
73	AE	380	GLN
74	AF	20	ILE
74	AF	26	ASP
74	AF	72	ILE
74	AF	78	SER
74	AF	90	LEU
74	AF	92	GLU
74	AF	98	THR
74	AF	105	THR
74	AF	154	ARG
74	AF	165	GLU
74	AF	211	MET
74	AF	241	ARG
74	AF	248	THR
74	AF	259	MET
74	AF	263	VAL
74	AF	270	VAL
74	AF	280	THR
74	AF	296	ASN
74	AF	317	THR
74	AF	352	THR
74	AF	367	LYS
74	AF	368	LEU
74	AF	388	GLU
74	AF	394	VAL
74	AF	409	GLU
74	AF	416	TYR
74	AF	430	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	AI	20	ILE
75	AI	22	VAL
75	AI	32	VAL
75	AI	44	ASP
75	AI	48	ARG
75	AI	49	THR
75	AI	61	LYS
75	AI	70	ARG
75	AI	77	ARG
75	AI	97	ARG
75	AI	100	LEU
75	AI	124	GLU
75	AI	126	LYS
75	AI	130	PHE
75	AI	158	THR
75	AI	181	THR
75	AI	183	ARG
75	AI	196	GLU
75	AI	197	GLU
75	AI	209	LYS
75	AI	210	TYR
76	AJ	14	ARG
76	AJ	20	ARG
76	AJ	25	ARG
76	AJ	27	ARG
76	AJ	38	VAL
76	AJ	75	THR
76	AJ	88	ASP
76	AJ	94	LEU
76	AJ	98	THR
77	AK	19	VAL
77	AK	20	GLU
77	AK	24	ASN
77	AK	31	VAL
77	AK	33	GLU
77	AK	37	ASP
77	AK	49	VAL
77	AK	90	THR
77	AK	133	ARG
77	AK	148	LEU
77	AK	150	THR
77	AK	172	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
77	AK	173	LEU
77	AK	174	GLU
77	AK	196	THR
77	AK	207	GLU
77	AK	208	GLN
77	AK	209	GLN
77	AK	216	ARG
77	AK	218	ARG
77	AK	219	ARG
77	AK	230	GLN
77	AK	231	ARG
77	AK	232	GLU
77	AK	239	ILE
77	AK	257	GLU
77	AK	261	ASP
77	AK	280	ARG
77	AK	286	GLU
77	AK	295	ARG
77	AK	298	VAL
77	AK	300	ASP
77	AK	314	ARG
77	AK	320	LYS
77	AK	321	ARG
77	AK	326	GLU
77	AK	329	MET
77	AK	332	GLU
77	AK	336	THR
78	AN	31	ASP
78	AN	35	GLN
78	AN	43	ARG
78	AN	54	LEU
78	AN	56	ARG
78	AN	96	ASP
78	AN	121	MET
78	AN	127	CYS
78	AN	135	LYS
78	AN	143	VAL
78	AN	148	THR
78	AN	162	SER
79	AP	29	LYS
79	AP	31	ILE
79	AP	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	AP	45	ARG
79	AP	46	ASN
79	AP	50	ASP
79	AP	52	THR
79	AP	55	LYS
79	AP	58	ASP
79	AP	63	LEU
79	AP	65	VAL
79	AP	73	ARG
79	AP	86	LEU
79	AP	93	SER
79	AP	98	THR
79	AP	100	THR
79	AP	111	ASN
79	AP	133	ARG
79	AP	136	VAL
79	AP	157	VAL
79	AP	163	ARG
79	AP	173	SER
79	AP	186	THR
79	AP	196	THR
79	AP	205	VAL
79	AP	217	VAL
79	AP	225	ARG
79	AP	235	GLN
79	AP	243	ARG
79	AP	255	VAL
79	AP	257	MET
79	AP	262	LEU
79	AP	281	GLU
79	AP	283	ARG
79	AP	315	ARG
79	AP	322	LYS
79	AP	358	TRP
79	AP	373	ARG
80	AQ	26	ARG
80	AQ	30	ARG
80	AQ	55	PHE
80	AQ	138	GLU
81	AR	55	LEU
81	AR	67	GLN
81	AR	80	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	AR	93	LEU
81	AR	94	ARG
81	AR	112	ARG
81	AR	139	MET
81	AR	167	ASN
81	AR	186	PHE
81	AR	211	ARG
81	AR	219	GLU
82	AT	24	LEU
82	AT	35	MET
82	AT	40	GLU
83	AU	15	LEU
83	AU	25	ARG
83	AU	29	ARG
83	AU	50	ARG
83	AU	68	SER
83	AU	75	THR
83	AU	78	GLN
83	AU	90	MET
83	AU	103	GLU
83	AU	117	ARG
83	AU	132	GLU
83	AU	136	LEU
83	AU	163	LEU
83	AU	173	ARG
83	AU	178	ARG
83	AU	185	SER
83	AU	189	ASN
84	AV	59	LEU
84	AV	83	TYR
84	AV	86	ASN
84	AV	90	LYS
84	AV	97	ILE
84	AV	106	ILE
84	AV	110	ILE
84	AV	128	ARG
84	AV	147	ARG
84	AV	151	SER
84	AV	165	ASP
84	AV	177	GLU
84	AV	203	GLN
84	AV	215	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
84	AV	222	ASP
84	AV	226	MET
84	AV	231	THR
85	AW	7	ARG
85	AW	14	LEU
85	AW	33	ARG
85	AW	35	THR
85	AW	61	LEU
85	AW	62	ASP
85	AW	69	LEU
85	AW	75	GLN
85	AW	76	LEU
85	AW	81	ARG
85	AW	82	TRP
85	AW	92	THR
85	AW	99	VAL
85	AW	105	MET
85	AW	120	GLU
85	AW	128	LEU
85	AW	138	VAL
85	AW	149	ILE
85	AW	158	ARG
85	AW	167	SER
85	AW	181	MET
85	AW	197	ARG
85	AW	203	CYS
85	AW	208	THR
85	AW	212	ILE
85	AW	246	THR
85	AW	247	CYS
85	AW	255	SER
85	AW	273	ILE
86	AX	62	HIS
86	AX	63	LYS
86	AX	78	ARG
86	AX	112	TRP
86	AX	148	LEU
86	AX	155	GLU
86	AX	197	ARG
86	AX	219	ASP
87	AY	1	MET
87	AY	6	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	AY	14	ARG
87	AY	36	ARG
87	AY	55	ARG
87	AY	58	LEU
87	AY	68	ARG
87	AY	82	ARG
87	AY	83	ARG
87	AY	182	THR
87	AY	186	CYS
87	AY	205	ARG
87	AY	214	MET
87	AY	219	VAL
87	AY	222	GLU
87	AY	224	GLU
87	AY	225	VAL
87	AY	241	THR
87	AY	247	GLU
87	AY	256	LEU
87	AY	264	VAL
87	AY	278	ARG
87	AY	283	GLU
87	AY	299	MET
87	AY	300	LEU
87	AY	302	GLU
88	Ab	74	ASP
88	Ab	102	VAL
88	Ab	105	ASN
88	Ab	129	SER
88	Ab	136	GLN
88	Ab	155	LEU
88	Ab	167	VAL
88	Ab	175	ARG
88	Ab	182	THR
88	Ab	192	VAL
88	Ab	196	THR
88	Ab	203	THR
88	Ab	206	CYS
88	Ab	258	ASP
88	Ab	263	VAL
88	Ab	279	TYR
88	Ab	341	THR
88	Ab	355	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
88	Ab	365	SER
88	Ab	372	ARG
88	Ab	385	ILE
88	Ab	403	ASP
88	Ab	408	THR
88	Ab	412	THR
88	Ab	416	ILE
88	Ab	428	LEU
88	Ab	454	VAL
88	Ab	455	ARG
88	Ab	457	ARG
88	Ab	491	SER
89	Ad	45	LEU
89	Ad	47	GLU
89	Ad	55	ARG
89	Ad	58	GLN
89	Ad	66	ARG
89	Ad	67	MET
89	Ad	77	VAL
89	Ad	80	LYS
89	Ad	100	ILE
89	Ad	111	GLU
89	Ad	118	GLU
89	Ad	126	ARG
89	Ad	151	GLN
89	Ad	153	GLU
89	Ad	159	ARG
89	Ad	170	LYS
89	Ad	173	SER
89	Ad	189	CYS
89	Ad	192	GLU
89	Ad	200	ILE
89	Ad	227	ARG
89	Ad	243	ARG
89	Ad	261	LEU
89	Ad	266	GLU
89	Ad	269	ARG
90	Ae	74	SER
90	Ae	75	ARG
90	Ae	80	LEU
90	Ae	87	VAL
90	Ae	89	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
90	Ae	98	VAL
90	Ae	123	THR
90	Ae	127	CYS
90	Ae	130	TYR
90	Ae	148	ILE
91	Af	60	GLN
91	Af	65	LEU
91	Af	72	ASP
91	Af	73	ASP
91	Af	81	ARG
91	Af	105	GLU
91	Af	118	GLU
91	Af	127	MET
91	Af	128	ASP
91	Af	129	THR
91	Af	162	ARG
91	Af	166	LYS
92	Ag	27	GLN
92	Ag	42	SER
92	Ag	44	SER
92	Ag	50	ARG
92	Ag	67	ARG
92	Ag	82	ARG
92	Ag	117	LEU
92	Ag	122	THR
92	Ag	127	THR
92	Ag	134	ARG
92	Ag	158	GLU
92	Ag	168	CYS
92	Ag	175	ARG
92	Ag	189	MET
92	Ag	214	VAL
92	Ag	224	VAL
92	Ag	255	GLU
93	Aj	27	VAL
93	Aj	53	ARG
93	Aj	68	MET
93	Aj	80	SER
93	Aj	95	ARG
93	Aj	137	VAL
93	Aj	168	ARG
93	Aj	180	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
93	Aj	205	ARG
93	Aj	217	CYS
93	Aj	276	PHE
94	Al	15	THR
94	Al	23	ARG
94	Al	25	VAL
94	Al	81	GLU
94	Al	85	LEU
94	Al	87	LEU
94	Al	88	ARG
94	Al	146	LEU
94	Al	149	LYS
94	Al	153	MET
94	Al	173	MET
94	Al	177	GLU
94	Al	191	VAL
94	Al	201	VAL
94	Al	206	ARG
94	Al	208	VAL
95	Ao	25	ASN
95	Ao	54	GLN
95	Ao	57	MET
95	Ao	58	ARG
95	Ao	61	ARG
95	Ao	73	CYS
95	Ao	81	ARG
95	Ao	87	GLU
95	Ao	125	ASP
95	Ao	136	THR
95	Ao	141	ASN
95	Ao	158	ARG
95	Ao	163	ARG
95	Ao	221	ASP
95	Ao	243	LYS
95	Ao	244	PHE
95	Ao	245	LEU
95	Ao	246	VAL
96	Ap	38	LEU
96	Ap	47	TYR
96	Ap	52	ARG
96	Ap	56	ASN
96	Ap	62	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
96	Ap	74	ARG
96	Ap	79	GLN
96	Ap	108	LEU
96	Ap	127	LEU
96	Ap	137	SER
96	Ap	151	THR
96	Ap	154	HIS
96	Ap	155	ILE
96	Ap	173	LEU
96	Ap	186	SER
96	Ap	196	ILE
96	Ap	234	VAL
96	Ap	243	VAL
96	Ap	246	VAL
96	Ap	253	GLN
96	Ap	278	ASN
96	Ap	284	ASP
96	Ap	285	TYR
96	Ap	294	LYS
97	At	24	VAL
97	At	25	ARG
97	At	43	ILE
97	At	44	LEU
97	At	50	THR
97	At	78	SER
97	At	94	THR
97	At	105	LEU
97	At	106	ARG
97	At	119	SER
97	At	124	SER
97	At	136	ARG
97	At	143	THR
97	At	144	VAL
97	At	153	LEU
98	Av	45	LEU
98	Av	47	ARG
98	Av	52	GLU
98	Av	71	VAL
98	Av	99	ARG
98	Av	103	ARG
98	Av	107	GLN
98	Av	146	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
98	Av	166	TYR
98	Av	167	ARG
98	Av	181	THR
98	Av	198	LYS
98	Av	200	GLN
98	Av	207	ARG
98	Av	213	ARG
98	Av	227	LYS
98	Av	233	THR
98	Av	237	LYS
103	BA	129	PHE
103	BA	133	THR
103	BA	143	MET
103	BA	151	ASP
103	BA	160	CYS
103	BA	190	THR
103	BA	194	ARG
103	BA	200	LEU
103	BA	206	ILE
103	BA	217	LEU
103	BA	221	THR
103	BA	236	SER
103	BA	254	ARG
103	BA	266	LEU
103	BA	305	VAL
103	BA	307	HIS
103	BA	318	LEU
103	BA	327	ARG
103	BA	328	VAL
103	BA	336	THR
103	BA	339	ASP
103	BA	340	LEU
103	BA	349	LEU
103	BA	359	CYS
103	BA	396	ARG
103	BA	401	THR
103	BA	419	THR
103	BA	466	LEU
103	BA	495	ARG
103	BA	510	LEU
103	BA	519	SER
103	BA	542	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
103	BA	563	ARG
103	BA	567	THR
103	BA	569	LEU
103	BA	573	GLU
103	BA	588	LEU
103	BA	589	MET
103	BA	593	THR
103	BA	638	ARG
103	BA	655	LEU
103	BA	663	LEU
103	BA	664	HIS
103	BA	665	ASP
103	BA	672	GLU
103	BA	714	ASN
103	BA	720	ARG
103	BA	724	ASP
103	BA	733	LEU
103	BA	753	ASP
103	BA	757	THR
103	BA	767	ARG
103	BA	779	LYS
103	BA	793	ARG
103	BA	799	ASP
103	BA	809	ASP
104	BB	66	GLU
104	BB	75	MET
104	BB	94	THR
104	BB	100	GLU
104	BB	105	LEU
104	BB	132	GLU
104	BB	136	TRP
104	BB	138	CYS
104	BB	152	ARG
104	BB	169	SER
104	BB	174	ASP
104	BB	180	GLU
104	BB	188	LEU
104	BB	206	ASP
104	BB	213	LEU
104	BB	215	ARG
104	BB	230	THR
104	BB	234	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
104	BB	240	HIS
104	BB	244	LYS
104	BB	251	ILE
104	BB	256	ARG
104	BB	259	GLU
104	BB	281	SER
104	BB	307	SER
104	BB	344	CYS
104	BB	356	ASN
104	BB	357	THR
104	BB	360	ASP
104	BB	379	ARG
104	BB	390	LEU
104	BB	395	GLU
104	BB	413	LEU
105	BC	49	SER
105	BC	75	MET
105	BC	81	LEU
105	BC	109	THR
105	BC	116	ARG
105	BC	120	ILE
105	BC	125	CYS
105	BC	126	GLU
105	BC	155	ARG
105	BC	169	ARG
105	BC	191	ASP
105	BC	203	SER
105	BC	207	GLN
105	BC	210	GLN
105	BC	212	VAL
105	BC	216	GLU
105	BC	220	LEU
105	BC	230	MET
105	BC	235	VAL
105	BC	239	ARG
105	BC	240	LYS
105	BC	243	VAL
105	BC	252	GLN
105	BC	255	ARG
105	BC	267	ILE
105	BC	268	LEU
105	BC	278	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
105	BC	288	ARG
105	BC	296	LEU
105	BC	303	LEU
105	BC	306	GLU
105	BC	309	PHE
105	BC	343	MET
105	BC	356	LEU
105	BC	362	VAL
105	BC	392	VAL
105	BC	394	LEU
105	BC	413	LYS
105	BC	427	LEU
105	BC	461	ASP
105	BC	465	LEU
105	BC	470	ARG
105	BC	475	LEU
105	BC	490	LEU
105	BC	512	ARG
105	BC	522	LEU
105	BC	523	TYR
107	BE	29	ASN
107	BE	32	LEU
107	BE	37	PHE
107	BE	61	MET
107	BE	66	ARG
107	BE	71	LEU
107	BE	81	VAL
107	BE	88	ARG
107	BE	144	VAL
107	BE	152	ARG
107	BE	153	SER
107	BE	190	ARG
107	BE	245	ILE
107	BE	257	ASP
107	BE	266	LEU
107	BE	271	ASP
107	BE	301	GLU
107	BE	320	TYR
107	BE	331	ASP
107	BE	354	GLU
107	BE	359	LYS
107	BE	395	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
107	BE	419	MET
107	BE	422	ARG
107	BE	442	THR
108	BF	50	LEU
108	BF	60	LEU
108	BF	131	LEU
108	BF	166	GLN
108	BF	167	ARG
108	BF	168	ILE
108	BF	170	ILE
108	BF	181	THR
108	BF	183	ARG
108	BF	199	ASP
108	BF	216	LEU
108	BF	221	GLU
108	BF	225	MET
108	BF	227	ARG
108	BF	230	THR
108	BF	237	LEU
108	BF	264	ASN
108	BF	289	CYS
108	BF	309	VAL
108	BF	345	LEU
108	BF	347	ASN
108	BF	354	LEU
108	BF	355	LEU
108	BF	360	THR
108	BF	366	ARG
108	BF	386	VAL
108	BF	398	ARG
108	BF	406	LYS
108	BF	419	VAL
108	BF	420	ARG
109	BG	40	THR
109	BG	50	ARG
109	BG	56	ARG
109	BG	57	ARG
109	BG	65	MET
109	BG	74	ARG
109	BG	101	SER
109	BG	102	GLN
109	BG	103	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
109	BG	106	ASP
109	BG	124	ASP
109	BG	125	LEU
109	BG	148	LEU
109	BG	149	THR
109	BG	152	TYR
109	BG	164	GLN
109	BG	165	GLU
109	BG	177	ASP
109	BG	178	THR
109	BG	183	ARG
109	BG	216	LEU
109	BG	265	LEU
109	BG	295	ARG
109	BG	339	GLU
109	BG	350	LEU
110	BH	74	ARG
110	BH	93	LEU
110	BH	113	LEU
110	BH	119	VAL
110	BH	135	ARG
110	BH	146	GLU
110	BH	149	ARG
110	BH	156	LEU
110	BH	168	THR
110	BH	171	GLU
110	BH	173	LEU
110	BH	178	GLU
110	BH	187	LEU
110	BH	192	LYS
110	BH	236	ARG
110	BH	239	ASN
110	BH	250	VAL
110	BH	254	TRP
110	BH	255	PHE
110	BH	257	ASP
110	BH	258	THR
110	BH	267	VAL
111	BI	60	GLN
111	BI	71	LYS
111	BI	84	LEU
111	BI	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
111	BI	104	ARG
111	BI	108	GLU
111	BI	139	ARG
111	BI	140	PHE
111	BI	151	MET
111	BI	160	PHE
111	BI	166	LEU
111	BI	173	LEU
111	BI	219	ASP
111	BI	245	ASN
111	BI	247	GLU
111	BI	250	SER
111	BI	252	MET
111	BI	254	ARG
111	BI	293	THR
111	BI	299	ARG
111	BI	319	ARG
111	BI	338	CYS
111	BI	342	TYR
112	BJ	192	ARG
112	BJ	203	LEU
112	BJ	223	THR
112	BJ	234	THR
112	BJ	250	LEU
112	BJ	258	HIS
112	BJ	270	ARG
112	BJ	288	LYS
112	BJ	292	ARG
112	BJ	300	GLU
112	BJ	301	ASP
112	BJ	307	ARG
112	BJ	309	LYS
112	BJ	326	LEU
113	BK	98	THR
113	BK	140	LEU
113	BK	150	ASP
113	BK	193	VAL
113	BK	194	ARG
113	BK	224	MET
113	BK	285	GLN
113	BK	300	TRP
113	BK	302	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
113	BK	328	LEU
113	BK	340	ARG
113	BK	379	LEU
114	BL	41	LEU
114	BL	48	ARG
114	BL	59	ASN
114	BL	61	VAL
114	BL	62	ARG
114	BL	78	ARG
114	BL	100	ASP
114	BL	102	CYS
114	BL	123	LEU
114	BL	125	GLU
114	BL	141	ASN
114	BL	165	LEU
114	BL	172	ILE
114	BL	180	LEU
114	BL	237	ASN
114	BL	242	THR
114	BL	256	ARG
114	BL	291	LEU
114	BL	294	CYS
114	BL	304	VAL
115	BM	50	GLU
115	BM	68	ARG
115	BM	74	ARG
115	BM	87	ARG
115	BM	99	SER
115	BM	102	VAL
115	BM	106	ASN
115	BM	113	ASN
115	BM	117	GLU
115	BM	122	TYR
115	BM	148	LYS
115	BM	151	GLU
115	BM	160	ARG
115	BM	163	LEU
115	BM	178	GLU
115	BM	184	MET
115	BM	236	ARG
115	BM	241	MET
115	BM	249	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
115	BM	260	MET
116	BN	22	ARG
116	BN	36	GLU
116	BN	60	ARG
116	BN	71	GLN
116	BN	177	ARG
116	BN	180	GLU
116	BN	182	GLU
116	BN	199	ASP
116	BN	219	ARG
117	BO	79	VAL
117	BO	108	MET
117	BO	124	ARG
117	BO	139	LEU
117	BO	142	GLU
117	BO	144	GLN
117	BO	169	MET
117	BO	193	ARG
117	BO	219	ARG
117	BO	227	ILE
117	BO	232	GLU
118	BP	36	ARG
118	BP	39	LEU
118	BP	43	LEU
118	BP	60	HIS
118	BP	72	GLN
118	BP	91	GLU
118	BP	107	VAL
118	BP	121	ARG
118	BP	152	ASN
118	BP	169	SER
118	BP	176	THR
118	BP	186	VAL
118	BP	205	TYR
118	BP	211	MET
118	BP	214	ASN
118	BP	222	SER
118	BP	234	GLU
119	BQ	72	SER
119	BQ	77	PHE
119	BQ	97	ILE
119	BQ	99	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
119	BQ	100	LYS
119	BQ	101	ASP
119	BQ	115	ASP
119	BQ	116	GLU
119	BQ	152	ASP
119	BQ	163	GLN
119	BQ	182	CYS
119	BQ	202	LEU
119	BQ	212	GLU
119	BQ	215	LEU
119	BQ	222	GLU
119	BQ	227	LEU
120	BR	19	TYR
120	BR	38	GLU
120	BR	41	LEU
120	BR	48	ARG
120	BR	58	THR
120	BR	62	GLU
120	BR	70	TYR
120	BR	73	ASP
120	BR	82	GLU
120	BR	89	ASP
120	BR	95	ARG
120	BR	96	GLN
120	BR	105	ASN
120	BR	110	LEU
120	BR	111	PHE
120	BR	121	LEU
120	BR	127	ARG
120	BR	160	GLN
120	BR	179	ILE
120	BR	193	ILE
121	BS	26	ARG
121	BS	29	ASN
121	BS	40	GLU
121	BS	57	CYS
121	BS	86	GLU
121	BS	87	LEU
121	BS	99	VAL
121	BS	106	ILE
122	BT	13	MET
122	BT	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
122	BT	23	ASP
122	BT	31	LYS
122	BT	33	ASN
122	BT	46	GLN
122	BT	72	LEU
122	BT	100	THR
122	BT	105	VAL
122	BT	118	LYS
122	BT	152	ASN
122	BT	163	VAL
122	BT	171	THR
122	BT	174	ILE
123	BU	106	ARG
123	BU	108	LEU
123	BU	114	THR
123	BU	116	ARG
123	BU	117	ILE
123	BU	137	ARG
123	BU	147	GLU
124	BV	20	THR
124	BV	43	ARG
124	BV	65	LEU
124	BV	123	PHE
124	BV	131	PHE
124	BV	144	VAL
124	BV	154	ARG
124	BV	156	ARG
125	BW	11	ARG
125	BW	12	SER
125	BW	17	THR
125	BW	49	VAL
125	BW	50	ARG
125	BW	53	ILE
125	BW	75	ARG
125	BW	81	ARG
125	BW	84	MET
125	BW	128	THR
125	BW	149	ASN
125	BW	156	VAL
125	BW	169	ARG
125	BW	174	ILE
126	BX	64	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
126	BX	67	VAL
126	BX	68	ASP
126	BX	71	MET
126	BX	91	VAL
126	BX	112	PHE
126	BX	120	ASN
126	BX	155	ARG
126	BX	165	ARG
126	BX	170	LEU
126	BX	173	HIS
127	BY	79(C)	LYS
127	BY	79(G)	LEU
127	BY	87	GLU
127	BY	89	MET
127	BY	94	GLU
127	BY	116	LEU
127	BY	123	MET
127	BY	141	GLU
128	BZ	5	GLU
128	BZ	21	ILE
128	BZ	30	CYS
128	BZ	97	LEU
128	BZ	139	THR
128	BZ	146	LEU
128	BZ	151	ILE
129	Ba	15	PHE
129	Ba	23	SER
129	Ba	26	LEU
129	Ba	32	LYS
129	Ba	35	ILE
129	Ba	37	ARG
129	Ba	72	ASP
129	Ba	73	GLU
129	Ba	82	MET
129	Ba	104	ARG
129	Ba	113	VAL
129	Ba	116	ARG
129	Ba	130	ASP
129	Ba	141	TYR
129	Ba	146	LYS
129	Ba	147	ASN
130	Bb	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
130	Bb	50	LEU
130	Bb	53	ARG
130	Bb	60	ASP
130	Bb	62	ARG
130	Bb	66	GLU
130	Bb	67	ARG
130	Bb	78	LEU
130	Bb	82	ASP
130	Bb	83	LEU
130	Bb	85	SER
130	Bb	92	LEU
130	Bb	110	ARG
130	Bb	120	ARG
130	Bb	134	LEU
131	Bc	11	SER
131	Bc	14	GLU
131	Bc	32	ARG
131	Bc	54	ASN
131	Bc	82	GLU
131	Bc	93	TRP
132	Bd	7	ARG
132	Bd	9	LEU
132	Bd	30	GLN
132	Bd	32	THR
132	Bd	33	LYS
132	Bd	42	ARG
132	Bd	51	ARG
132	Bd	54	MET
132	Bd	58	LEU
132	Bd	83	SER
132	Bd	93	THR
132	Bd	102	LEU
132	Bd	135	PHE
133	Be	34	LEU
133	Be	49	ARG
133	Be	54	LEU
133	Be	71	SER
133	Be	77	ASP
133	Be	79	GLN
133	Be	94	THR
134	Bf	79	GLU
134	Bf	98	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
135	Bg	35	LEU
135	Bg	37	LEU
135	Bg	50	ASN
135	Bg	64	LYS
135	Bg	69	ARG
135	Bg	100	ARG
135	Bg	104	THR
136	Bh	6	CYS
136	Bh	9	CYS
136	Bh	17	VAL
136	Bh	37	GLN
136	Bh	44	MET
136	Bh	46	VAL
136	Bh	53	MET
136	Bh	56	LYS
136	Bh	71	ARG
136	Bh	83	LEU
136	Bh	87	CYS
136	Bh	88	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (652) such sidechains are listed below:

Mol	Chain	Res	Type
1	DA	49	HIS
1	DA	59	HIS
1	DA	91	ASN
1	DA	112	GLN
1	DA	123	HIS
1	DA	196	GLN
1	DA	237	HIS
1	DA	287	HIS
1	DA	414	HIS
1	DA	436	ASN
1	DA	457	GLN
1	DA	746	GLN
1	DA	882	GLN
1	DA	907	GLN
1	DA	910	HIS
1	DA	979	GLN
1	DA	984	GLN
1	DA	1038	HIS
1	DA	1048	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DA	1081	GLN
1	DA	1117	ASN
1	DA	1175	HIS
1	DA	1179	GLN
1	DA	1225	HIS
1	DA	1258	ASN
1	DA	1399	ASN
1	DA	1488	GLN
1	DA	1513	GLN
1	DA	1562	GLN
1	DA	1570	ASN
1	DA	1629	GLN
2	DD	76	ASN
2	DD	137	HIS
2	DD	156	GLN
2	DD	174	HIS
2	DD	176	HIS
2	DD	203	GLN
2	DD	300	GLN
2	DD	312	GLN
2	DD	313	HIS
2	DD	348	HIS
2	DD	353	HIS
2	DD	379	GLN
2	DD	387	GLN
2	DD	404	HIS
2	DD	408	HIS
2	DD	453	ASN
2	DD	499	ASN
2	DD	507	GLN
2	DD	521	ASN
2	DD	542	HIS
2	DD	669	HIS
2	DD	679	ASN
2	DD	687	HIS
3	DI	30	GLN
3	DI	61	ASN
3	DI	317	HIS
3	DI	320	GLN
3	DI	370	GLN
4	DL	125	HIS
5	DM	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	DM	43	GLN
5	DM	76	ASN
5	DM	193	GLN
5	DM	208	HIS
6	DN	28	HIS
6	DN	79	ASN
6	DN	223	GLN
6	DN	234	HIS
6	DN	235	ASN
6	DN	238	ASN
6	DN	246	GLN
7	DO	71	HIS
7	DO	181	HIS
8	DP	28	ASN
8	DP	98	HIS
8	DP	116	HIS
8	DP	186	HIS
8	DP	194	GLN
8	DP	204	ASN
9	DQ	41	GLN
9	DQ	73	HIS
9	DQ	95	HIS
9	DQ	235	HIS
10	DR	26	ASN
10	DR	108	GLN
10	DR	145	HIS
10	DR	191	GLN
11	DS	134	GLN
11	DS	150	GLN
11	DS	201	HIS
12	DU	63	HIS
12	DU	96	GLN
13	DZ	25	HIS
15	DB	92	HIS
15	DB	114	ASN
15	DB	122	HIS
15	DB	134	HIS
15	DB	153	HIS
15	DB	190	HIS
15	DB	194	GLN
15	DB	209	GLN
15	DB	221	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	DB	300	GLN
15	DB	414	GLN
15	DB	445	ASN
15	DB	461	GLN
15	DB	486	HIS
15	DB	551	HIS
15	DB	562	GLN
15	DB	569	HIS
15	DB	686	GLN
15	DB	703	HIS
15	DB	729	GLN
15	DB	748	HIS
15	DB	774	ASN
15	DB	785	ASN
15	DB	828	HIS
15	DB	908	GLN
15	DB	923	GLN
15	DB	958	ASN
15	DB	981	HIS
15	DB	1004	GLN
15	DB	1051	GLN
15	DB	1055	GLN
15	DB	1124	HIS
16	DC	81	HIS
16	DC	128	HIS
16	DC	242	HIS
16	DC	445	HIS
16	DC	530	GLN
16	DC	574	GLN
16	DC	841	HIS
16	DC	943	HIS
16	DC	970	GLN
16	DC	1110	HIS
16	DC	1134	HIS
16	DC	1141	GLN
16	DC	1160	GLN
17	DE	67	ASN
17	DE	105	ASN
17	DE	194	HIS
17	DE	202	HIS
17	DE	414	ASN
17	DE	442	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	DE	465	ASN
17	DE	501	HIS
17	DE	567	HIS
17	DE	628	HIS
17	DE	658	ASN
17	DE	671	ASN
17	DE	698	GLN
18	DF	41	ASN
18	DF	115	HIS
18	DF	140	HIS
18	DF	154	ASN
18	DF	175	GLN
18	DF	187	ASN
18	DF	198	HIS
18	DF	214	HIS
18	DF	283	HIS
18	DF	327	HIS
18	DF	474	GLN
18	DF	543	HIS
18	DF	572	HIS
19	DG	65	ASN
19	DG	71	ASN
19	DG	92	GLN
19	DG	112	HIS
19	DG	170	ASN
19	DG	191	GLN
19	DG	200	GLN
19	DG	229	HIS
19	DG	230	ASN
19	DG	365	GLN
19	DG	405	GLN
19	DG	476	GLN
19	DG	477	GLN
19	DG	545	HIS
20	DH	4	GLN
20	DH	45	HIS
20	DH	100	HIS
20	DH	123	HIS
20	DH	146	GLN
20	DH	257	ASN
20	DH	302	GLN
20	DH	469	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	DH	490	HIS
20	DH	498	ASN
20	DH	526	ASN
21	DJ	27	GLN
21	DJ	31	HIS
21	DJ	33	ASN
21	DJ	42	HIS
21	DJ	247	ASN
21	DJ	291	ASN
21	DJ	293	ASN
21	DJ	301	HIS
21	DJ	314	GLN
22	DK	171	GLN
22	DK	175	HIS
23	DT	16	HIS
23	DT	45	HIS
23	DT	58	HIS
23	DT	72	HIS
23	DT	82	HIS
23	DT	139	HIS
23	DT	140	ASN
23	DT	158	HIS
23	DT	161	ASN
23	DT	219	GLN
24	DV	31	HIS
24	DV	40	HIS
24	DV	48	HIS
24	DV	71	GLN
24	DV	83	GLN
24	DV	131	GLN
25	DW	66	HIS
25	DW	87	ASN
25	DW	99	HIS
25	DW	121	HIS
25	DW	154	HIS
26	DX	58	HIS
26	DX	130	GLN
26	DX	167	HIS
26	DX	168	ASN
27	DY	10	ASN
27	DY	99	GLN
27	DY	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	CC	25	HIS
28	CC	48	ASN
29	CE	85	ASN
29	CE	105	GLN
29	CE	108	HIS
29	CE	132	HIS
29	CE	235	ASN
29	CE	260	ASN
29	CE	317	HIS
29	CE	417	ASN
31	CH	80	HIS
31	CH	116	HIS
31	CH	186	HIS
31	CH	247	HIS
31	CH	260	ASN
31	CH	267	HIS
31	CH	282	HIS
32	CI	12	HIS
32	CI	104	ASN
32	CI	165	ASN
32	CI	174	GLN
32	CI	211	ASN
32	CI	269	HIS
33	CJ	82	HIS
33	CJ	134	GLN
33	CJ	151	ASN
33	CJ	441	HIS
33	CJ	450	HIS
33	CJ	460	HIS
33	CJ	476	ASN
33	CJ	484	HIS
33	CJ	621	ASN
33	CJ	755	ASN
33	CJ	761	GLN
33	CJ	769	GLN
33	CJ	781	HIS
33	CJ	792	HIS
33	CJ	793	HIS
34	CK	73	GLN
34	CK	107	GLN
34	CK	111	ASN
34	CK	244	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	CL	87	ASN
36	CN	133	HIS
36	CN	150	HIS
36	CN	153	ASN
37	CO	82	ASN
37	CO	111	GLN
37	CO	129	GLN
37	CO	214	HIS
37	CO	359	HIS
37	CO	426	HIS
38	CP	84	GLN
38	CP	87	HIS
38	CP	169	ASN
39	CQ	13	ASN
39	CQ	69	GLN
40	CR	24	ASN
40	CR	249	GLN
40	CR	250	GLN
41	CS	110	HIS
42	CU	16	HIS
42	CU	72	HIS
42	CU	123	GLN
42	CU	148	ASN
42	CU	174	HIS
43	CZ	305	HIS
44	Ca	14	ASN
44	Ca	76	GLN
44	Ca	177	GLN
44	Ca	227	ASN
44	Ca	423	GLN
44	Ca	506	GLN
44	Ca	519	GLN
44	Ca	585	GLN
45	Cb	64	ASN
45	Cb	67	GLN
45	Cb	191	HIS
45	Cb	280	ASN
46	Cd	48	ASN
46	Cd	72	ASN
46	Cd	87	GLN
46	Cd	155	GLN
46	Cd	159	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	Cd	182	GLN
47	Cg	164	HIS
47	Cg	170	ASN
47	Cg	184	HIS
47	Cg	239	GLN
47	Cg	289	ASN
47	Cg	301	HIS
47	Cg	350	ASN
47	Cg	460	HIS
48	Ci	19	HIS
48	Ci	29	GLN
48	Ci	83	ASN
48	Ci	95	ASN
48	Ci	96	ASN
48	Ci	112	ASN
48	Ci	125	HIS
48	Ci	136	HIS
48	Ci	145	ASN
49	Cj	34	HIS
49	Cj	153	HIS
50	Ck	95	HIS
50	Ck	97	GLN
50	Ck	110	HIS
50	Ck	134	HIS
50	Ck	264	ASN
50	Ck	589	GLN
50	Ck	611	ASN
50	Ck	634	HIS
50	Ck	644	HIS
50	Ck	666	HIS
50	Ck	679	GLN
50	Ck	682	ASN
50	Ck	691	GLN
50	Ck	728	GLN
51	Cm	28	GLN
51	Cm	56	ASN
51	Cm	73	HIS
51	Cm	155	HIS
51	Cm	168	HIS
51	Cm	184	HIS
52	Cn	149	GLN
52	Cn	192	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	Cp	91	GLN
53	Cp	154	GLN
54	Cq	20	GLN
54	Cq	29	ASN
54	Cq	93	ASN
54	Cq	104	HIS
54	Cq	129	HIS
54	Cq	155	GLN
54	Cq	196	HIS
55	Cr	58	ASN
55	Cr	80	HIS
55	Cr	125	GLN
55	Cr	157	GLN
55	Cr	287	HIS
56	Cv	147	HIS
56	Cv	166	HIS
56	Cv	198	HIS
56	Cv	245	ASN
56	Cv	312	ASN
56	Cv	321	HIS
56	Cv	392	HIS
56	Cv	411	ASN
56	Cv	511	HIS
56	Cv	523	HIS
56	Cv	535	HIS
56	Cv	559	GLN
56	Cv	678	HIS
56	Cv	739	ASN
56	Cv	755	HIS
56	Cv	830	ASN
56	Cv	878	ASN
56	Cv	948	HIS
56	Cv	960	GLN
56	Cv	1066	GLN
56	Cv	1108	GLN
56	Cv	1129	ASN
65	A1	16	ASN
65	A1	116	HIS
66	A2	59	ASN
66	A2	167	HIS
66	A2	206	HIS
66	A2	207	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	A2	270	ASN
66	A2	295	ASN
66	A2	314	HIS
66	A2	389	HIS
66	A2	440	HIS
67	A3	95	GLN
67	A3	104	GLN
68	A4	29	HIS
68	A4	56	GLN
68	A4	85	GLN
69	A5	77	GLN
70	A6	77	GLN
71	A8	71	GLN
71	A8	116	GLN
72	A9	102	HIS
73	AE	168	ASN
73	AE	169	GLN
73	AE	191	ASN
73	AE	214	HIS
74	AF	33	HIS
74	AF	56	HIS
74	AF	64	HIS
74	AF	80	GLN
74	AF	83	HIS
74	AF	176	ASN
74	AF	193	HIS
74	AF	223	ASN
74	AF	321	GLN
74	AF	331	ASN
74	AF	346	HIS
74	AF	430	ASN
75	AI	76	HIS
75	AI	120	ASN
76	AJ	81	ASN
77	AK	24	ASN
77	AK	52	ASN
77	AK	144	HIS
77	AK	230	GLN
78	AN	19	HIS
78	AN	30	ASN
78	AN	82	HIS
78	AN	141	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	AN	164	HIS
78	AN	166	HIS
79	AP	89	GLN
79	AP	111	ASN
79	AP	199	HIS
79	AP	259	HIS
79	AP	310	HIS
79	AP	346	HIS
79	AP	348	ASN
80	AQ	47	GLN
80	AQ	164	HIS
81	AR	65	HIS
81	AR	99	HIS
81	AR	113	GLN
81	AR	223	HIS
81	AR	229	HIS
81	AR	242	HIS
83	AU	65	ASN
83	AU	165	HIS
83	AU	192	ASN
84	AV	75	ASN
84	AV	87	HIS
84	AV	100	GLN
84	AV	168	HIS
84	AV	206	ASN
85	AW	30	HIS
85	AW	40	HIS
85	AW	109	ASN
85	AW	172	HIS
86	AX	72	HIS
87	AY	64	HIS
87	AY	72	GLN
87	AY	168	HIS
88	Ab	61	HIS
88	Ab	84	ASN
88	Ab	93	ASN
88	Ab	122	HIS
88	Ab	157	HIS
88	Ab	199	ASN
88	Ab	205	HIS
88	Ab	351	GLN
88	Ab	419	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
89	Ad	78	ASN
89	Ad	146	GLN
89	Ad	151	GLN
89	Ad	221	GLN
89	Ad	276	HIS
89	Ad	279	GLN
89	Ad	284	HIS
90	Ae	100	HIS
90	Ae	115	ASN
91	Af	101	HIS
91	Af	146	ASN
91	Af	156	HIS
91	Af	164	HIS
92	Ag	27	GLN
92	Ag	73	ASN
92	Ag	84	ASN
92	Ag	101	HIS
92	Ag	114	ASN
92	Ag	170	GLN
92	Ag	204	HIS
92	Ag	244	HIS
93	Aj	22	GLN
93	Aj	37	GLN
93	Aj	54	GLN
93	Aj	90	HIS
93	Aj	121	GLN
93	Aj	211	ASN
93	Aj	225	GLN
93	Aj	267	HIS
94	Al	34	ASN
95	Ao	25	ASN
95	Ao	54	GLN
95	Ao	141	ASN
96	Ap	55	HIS
96	Ap	78	HIS
96	Ap	83	HIS
96	Ap	150	HIS
96	Ap	154	HIS
96	Ap	194	HIS
96	Ap	253	GLN
97	At	63	GLN
97	At	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
97	At	147	HIS
97	At	148	GLN
98	Av	34	GLN
98	Av	44	ASN
98	Av	206	ASN
98	Av	212	ASN
103	BA	272	GLN
103	BA	301	HIS
103	BA	307	HIS
103	BA	408	ASN
103	BA	490	ASN
103	BA	502	HIS
103	BA	585	HIS
103	BA	693	HIS
103	BA	699	ASN
103	BA	734	HIS
103	BA	798	HIS
104	BB	82	HIS
104	BB	162	GLN
104	BB	170	GLN
104	BB	218	HIS
104	BB	240	HIS
104	BB	242	GLN
104	BB	356	ASN
104	BB	359	HIS
104	BB	420	ASN
104	BB	432	HIS
105	BC	71	GLN
105	BC	108	GLN
105	BC	165	HIS
105	BC	282	HIS
105	BC	289	ASN
105	BC	292	ASN
105	BC	340	HIS
105	BC	351	ASN
107	BE	23	GLN
107	BE	25	HIS
107	BE	29	ASN
107	BE	41	HIS
107	BE	76	GLN
107	BE	350	ASN
107	BE	352	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
108	BF	132	GLN
108	BF	143	GLN
108	BF	148	HIS
108	BF	164	HIS
108	BF	180	GLN
108	BF	250	HIS
108	BF	311	GLN
108	BF	347	ASN
108	BF	362	HIS
108	BF	413	HIS
109	BG	81	HIS
109	BG	269	HIS
109	BG	287	HIS
109	BG	340	GLN
110	BH	122	HIS
110	BH	134	GLN
110	BH	239	ASN
111	BI	45	HIS
111	BI	60	GLN
111	BI	144	HIS
111	BI	148	ASN
111	BI	152	GLN
111	BI	184	ASN
111	BI	223	GLN
111	BI	228	GLN
111	BI	263	HIS
111	BI	307	ASN
112	BJ	333	ASN
113	BK	200	ASN
113	BK	212	GLN
113	BK	227	GLN
113	BK	285	GLN
114	BL	83	HIS
114	BL	99	HIS
114	BL	141	ASN
114	BL	226	HIS
114	BL	238	GLN
115	BM	88	GLN
115	BM	89	HIS
115	BM	138	HIS
115	BM	189	HIS
115	BM	193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
115	BM	279	ASN
116	BN	14	HIS
116	BN	28	ASN
117	BO	101	GLN
118	BP	152	ASN
118	BP	213	HIS
119	BQ	147	ASN
119	BQ	163	GLN
120	BR	96	GLN
120	BR	138	GLN
120	BR	164	HIS
122	BT	66	HIS
122	BT	135	ASN
122	BT	152	ASN
123	BU	156	GLN
124	BV	74	ASN
124	BV	110	ASN
125	BW	35	GLN
125	BW	46	HIS
125	BW	65	ASN
125	BW	95	HIS
125	BW	168	HIS
127	BY	150	GLN
128	BZ	96	GLN
128	BZ	129	ASN
129	Ba	36	HIS
129	Ba	147	ASN
130	Bb	79	HIS
130	Bb	128	GLN
131	Bc	17	HIS
131	Bc	33	GLN
131	Bc	34	GLN
131	Bc	38	ASN
131	Bc	66	HIS
132	Bd	30	GLN
132	Bd	77	HIS
132	Bd	90	GLN
132	Bd	97	GLN
133	Be	70	HIS
133	Be	72	HIS
134	Bf	104	ASN
135	Bg	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
135	Bg	77	GLN
135	Bg	85	GLN
136	Bh	29	ASN

5.3.3 RNA

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%)
All	All	1201/1800 (66%)	589 (49%)	25 (2%)

All (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
57	CA	8	U
57	CA	10	G
57	CA	11	U
57	CA	15	U
57	CA	16	U
57	CA	19	U
57	CA	20	A
57	CA	25	U
57	CA	26	C
57	CA	27	A
57	CA	33	A
57	CA	36	U
57	CA	37	U
57	CA	38	U
57	CA	39	U
57	CA	42	A
57	CA	44	U
57	CA	45	G
57	CA	46	U
57	CA	50	A
57	CA	52	C
57	CA	53	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	56	U
57	CA	57	U
57	CA	58	A
57	CA	59	U
57	CA	60	A
57	CA	61	A
57	CA	64	G
57	CA	67	U
57	CA	68	A
57	CA	70	U
57	CA	74	G
57	CA	78	G
57	CA	79	A
57	CA	81	U
57	CA	84	U
57	CA	85	U
57	CA	86	G
57	CA	87	U
57	CA	88	A
57	CA	89	U
57	CA	91	A
57	CA	94	U
57	CA	95	U
57	CA	97	U
57	CA	100	G
57	CA	102	A
57	CA	103	U
57	CA	104	A
57	CA	105	G
57	CA	107	U
57	CA	108	A
57	CA	109	A
57	CA	110	U
57	CA	111	A
57	CA	112	A
57	CA	113	U
57	CA	114	A
57	CA	115	A
57	CA	116	U
57	CA	117	U
57	CA	124	U
57	CA	127	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	132	G
57	CA	135	U
57	CA	136	G
57	CA	138	U
57	CA	139	U
57	CA	146	U
57	CA	152	U
57	CA	156	U
57	CA	159	G
57	CA	160	U
57	CA	167	A
57	CA	170	U
57	CA	171	A
57	CA	172	A
57	CA	173	A
57	CA	174	A
57	CA	175	A
57	CA	178	A
57	CA	179	U
57	CA	183	U
57	CA	188	U
57	CA	189	A
57	CA	191	A
57	CA	193	C
57	CA	194	A
57	CA	197	A
57	CA	198	A
57	CA	199	U
57	CA	200	A
57	CA	202	A
57	CA	203	U
57	CA	204	U
57	CA	205	A
57	CA	206	A
57	CA	208	U
57	CA	209	U
57	CA	210	A
57	CA	211	A
57	CA	214	U
57	CA	216	U
57	CA	217	U
57	CA	218	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	219	G
57	CA	221	C
57	CA	223	G
57	CA	230	A
57	CA	236	G
57	CA	242	G
57	CA	246	U
57	CA	247	A
57	CA	250	U
57	CA	256	G
57	CA	258	U
57	CA	259	U
57	CA	261	U
57	CA	262	A
57	CA	263	A
57	CA	272	C
57	CA	275	U
57	CA	276	U
57	CA	279	C
57	CA	280	A
57	CA	281	U
57	CA	282	A
57	CA	283	U
57	CA	286	A
57	CA	296	U
57	CA	297	G
57	CA	299	U
57	CA	300	G
57	CA	301	A
57	CA	305	A
57	CA	311	U
57	CA	315	A
57	CA	316	A
57	CA	321	A
57	CA	323	U
57	CA	325	A
57	CA	326	U
57	CA	327	U
57	CA	328	U
57	CA	330	U
57	CA	334	U
57	CA	335	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	337	U
57	CA	338	U
57	CA	340	U
57	CA	341	A
57	CA	342	A
57	CA	343	A
57	CA	350	U
57	CA	351	A
57	CA	352	G
57	CA	356	U
57	CA	357	A
57	CA	358	U
57	CA	359	G
57	CA	360	C
57	CA	361	A
57	CA	364	U
57	CA	367	A
57	CA	368	A
57	CA	369	A
57	CA	371	U
57	CA	374	U
57	CA	378	A
57	CA	380	U
57	CA	384	A
57	CA	385	A
57	CA	386	A
57	CA	389	A
57	CA	394	A
57	CA	395	U
57	CA	397	U
57	CA	398	U
57	CA	399	A
57	CA	400	U
57	CA	401	A
57	CA	406	U
57	CA	407	U
57	CA	408	C
57	CA	410	U
57	CA	411	A
57	CA	413	A
57	CA	414	A
57	CA	415	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	418	A
57	CA	419	U
57	CA	421	G
57	CA	423	A
57	CA	426	A
57	CA	427	U
57	CA	428	A
57	CA	430	U
57	CA	431	U
57	CA	433	U
57	CA	434	A
57	CA	435	G
57	CA	438	U
57	CA	441	G
57	CA	442	A
57	CA	444	A
57	CA	445	C
57	CA	446	C
57	CA	448	U
57	CA	449	G
57	CA	450	A
57	CA	451	U
57	CA	452	A
57	CA	453	A
57	CA	455	G
57	CA	457	U
57	CA	458	U
57	CA	459	A
57	CA	460	U
57	CA	461	A
57	CA	462	A
57	CA	463	A
57	CA	464	U
57	CA	467	A
57	CA	468	A
57	CA	469	A
57	CA	470	G
57	CA	471	U
57	CA	472	G
57	CA	476	A
57	CA	478	A
57	CA	480	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	481	A
57	CA	482	U
57	CA	483	A
57	CA	484	A
57	CA	485	U
57	CA	486	C
57	CA	487	A
57	CA	489	A
57	CA	491	U
57	CA	494	A
57	CA	495	U
57	CA	496	U
57	CA	497	A
57	CA	498	U
57	CA	500	U
57	CA	502	U
57	CA	505	U
57	CA	507	A
57	CA	509	U
57	CA	510	A
57	CA	513	U
57	CA	514	A
57	CA	517	U
57	CA	518	G
57	CA	519	U
57	CA	520	A
57	CA	532	A
57	CA	535	U
57	CA	536	U
57	CA	537	A
57	CA	538	A
57	CA	539	A
57	CA	540	A
57	CA	544	U
57	CA	546	U
57	CA	547	U
57	CA	548	G
57	CA	555	A
57	CA	556	C
57	CA	558	A
57	CA	560	U
57	CA	564	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	CA	565	A
57	CA	566	U
57	CA	567	A
57	CA	570	A
57	CA	576	A
57	CA	581	G
57	CA	586	A
57	CA	587	A
57	CA	588	U
57	CA	590	A
57	CA	602	A
57	CA	603	A
57	CA	611	U
57	CA	613	U
57	CA	614	U
57	CA	615	U
57	CA	616	U
57	CA	617	U
57	CA	618	U
57	CA	619	U
57	CA	620	U
102	AA	2	U
102	AA	3	U
102	AA	4	U
102	AA	5	U
102	AA	10	A
102	AA	11	U
102	AA	12	U
102	AA	13	A
102	AA	16	A
102	AA	17	A
102	AA	18	G
102	AA	19	A
102	AA	20	A
102	AA	21	U
102	AA	27	A
102	AA	28	A
102	AA	29	U
102	AA	32	U
102	AA	33	G
102	AA	34	G
102	AA	38	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	40	U
102	AA	41	U
102	AA	42	A
102	AA	43	U
102	AA	44	A
102	AA	50	A
102	AA	53	A
102	AA	54	A
102	AA	57	A
102	AA	58	U
102	AA	59	U
102	AA	60	U
102	AA	64	U
102	AA	65	U
102	AA	66	C
102	AA	68	G
102	AA	69	U
102	AA	70	G
102	AA	71	U
102	AA	72	A
102	AA	73	G
102	AA	74	U
102	AA	75	A
102	AA	77	A
102	AA	78	U
102	AA	79	U
102	AA	80	U
102	AA	81	A
102	AA	82	U
102	AA	84	A
102	AA	85	U
102	AA	86	U
102	AA	88	G
102	AA	89	U
102	AA	98	U
102	AA	101	A
102	AA	104	A
102	AA	105	G
102	AA	106	G
102	AA	107	U
102	AA	111	U
102	AA	112	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	113	A
102	AA	114	U
102	AA	115	A
102	AA	116	U
102	AA	119	A
102	AA	120	A
102	AA	123	U
102	AA	124	U
102	AA	125	U
102	AA	126	A
102	AA	127	A
102	AA	130	U
102	AA	131	U
102	AA	133	U
102	AA	134	U
102	AA	135	G
102	AA	136	U
102	AA	137	U
102	AA	146	A
102	AA	148	A
102	AA	149	U
102	AA	152	A
102	AA	154	A
102	AA	159	U
102	AA	162	A
102	AA	164	U
102	AA	168	A
102	AA	170	A
102	AA	171	U
102	AA	172	U
102	AA	174	A
102	AA	176	A
102	AA	177	U
102	AA	178	A
102	AA	179	A
102	AA	183	U
102	AA	186	A
102	AA	187	A
102	AA	189	A
102	AA	282	A
102	AA	283	A
102	AA	284	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	285	A
102	AA	288	G
102	AA	289	U
102	AA	290	A
102	AA	296	A
102	AA	297	U
102	AA	299	U
102	AA	301	A
102	AA	319	A
102	AA	327	U
102	AA	328	U
102	AA	330	U
102	AA	331	C
102	AA	336	U
102	AA	342	U
102	AA	344	A
102	AA	370	U
102	AA	371	A
102	AA	375	A
102	AA	378	A
102	AA	380	G
102	AA	381	U
102	AA	383	A
102	AA	384	U
102	AA	385	A
102	AA	387	A
102	AA	388	U
102	AA	393	A
102	AA	394	U
102	AA	397	A
102	AA	411	A
102	AA	414	A
102	AA	418	G
102	AA	419	U
102	AA	420	A
102	AA	423	A
102	AA	424	G
102	AA	425	U
102	AA	426	A
102	AA	427	U
102	AA	428	A
102	AA	438	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	440	U
102	AA	441	A
102	AA	446	A
102	AA	447	U
102	AA	448	A
102	AA	455	U
102	AA	456	U
102	AA	458	U
102	AA	460	U
102	AA	461	U
102	AA	462	U
102	AA	463	U
102	AA	468	A
102	AA	470	G
102	AA	472	A
102	AA	473	A
102	AA	474	A
102	AA	475	U
102	AA	476	G
102	AA	477	A
102	AA	481	G
102	AA	483	A
102	AA	484	U
102	AA	485	A
102	AA	486	A
102	AA	488	U
102	AA	489	G
102	AA	490	G
102	AA	491	A
102	AA	492	U
102	AA	493	A
102	AA	494	U
102	AA	495	A
102	AA	496	A
102	AA	497	C
102	AA	498	U
102	AA	499	U
102	AA	503	A
102	AA	504	U
102	AA	509	U
102	AA	513	U
102	AA	514	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	515	U
102	AA	516	U
102	AA	518	A
102	AA	519	A
102	AA	520	U
102	AA	523	A
102	AA	524	A
102	AA	525	A
102	AA	526	G
102	AA	527	U
102	AA	529	U
102	AA	530	U
102	AA	531	U
102	AA	532	U
102	AA	533	A
102	AA	535	U
102	AA	536	A
102	AA	537	U
102	AA	538	U
102	AA	540	U
102	AA	545	U
102	AA	546	A
102	AA	548	A
102	AA	549	G
102	AA	551	A
102	AA	554	A
102	AA	555	U
102	AA	556	U
102	AA	557	A
102	AA	559	A
102	AA	560	G
102	AA	562	G
102	AA	563	U
102	AA	564	A
102	AA	565	U
102	AA	566	A
102	AA	567	G
102	AA	568	U
102	AA	570	U
102	AA	571	U
102	AA	572	U
102	AA	573	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	574	A
102	AA	575	A
102	AA	583	A
102	AA	800	A
102	AA	801	A
102	AA	802	G
102	AA	803	U
102	AA	814	A
102	AA	815	U
102	AA	816	C
102	AA	818	A
102	AA	819	A
102	AA	825	A
102	AA	826	A
102	AA	827	U
102	AA	828	A
102	AA	830	A
102	AA	836	A
102	AA	837	A
102	AA	838	A
102	AA	845	A
102	AA	883	U
102	AA	884	A
102	AA	885	U
102	AA	886	G
102	AA	887	A
102	AA	891	G
102	AA	892	U
102	AA	893	A
102	AA	948	A
102	AA	949	U
102	AA	950	U
102	AA	951	C
102	AA	952	U
102	AA	953	U
102	AA	954	U
102	AA	955	G
102	AA	1100	U
102	AA	1106	U
102	AA	1107	U
102	AA	1111	A
102	AA	1112	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	1113	U
102	AA	1157	A
102	AA	1158	G
102	AA	1159	A
102	AA	1160	A
102	AA	1163	A
102	AA	1164	A
102	AA	1165	G
102	AA	1166	A
102	AA	1168	U
102	AA	1169	A
102	AA	1171	A
102	AA	1172	A
102	AA	1173	U
102	AA	1174	U
102	AA	1175	U

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	CA	14	A
57	CA	38	U
57	CA	80	U
57	CA	84	U
57	CA	198	A
57	CA	350	U
57	CA	512	G
57	CA	527	A
102	AA	40	U
102	AA	69	U
102	AA	171	U
102	AA	335	G
102	AA	379	U
102	AA	384	U
102	AA	387	A
102	AA	392	A
102	AA	418	G
102	AA	422	A
102	AA	425	U
102	AA	440	U
102	AA	485	A
102	AA	528	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
102	AA	534	U
102	AA	1162	G
102	AA	1164	A

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	-

All (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
150	DJ	401	UTP	C4-N3	3.67	1.39	1.33
150	DJ	401	UTP	O4'-C1'	3.67	1.46	1.41
154	Av	301	NAD	C2A-N1A	3.11	1.39	1.33
154	Av	301	NAD	C6A-C5A	-2.82	1.32	1.43
154	Av	301	NAD	C5A-C4A	-2.80	1.33	1.40
154	Av	301	NAD	C2B-C1B	-2.65	1.49	1.53
154	Av	301	NAD	C2D-C1D	-2.49	1.50	1.53
150	DJ	401	UTP	C2'-C1'	2.45	1.57	1.53
152	Cg	501	GTP	C4-N3	-2.33	1.31	1.37
150	DJ	401	UTP	PA-O5'	2.12	1.67	1.59
152	Cg	501	GTP	O4'-C4'	-2.06	1.40	1.45
150	DJ	401	UTP	PG-O3G	-2.04	1.47	1.54

All (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
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
154	Av	301	NAD	C2B-C3B-C4B	-3.31	96.21	102.64
154	Av	301	NAD	PN-O3-PA	-3.13	122.08	132.83
154	Av	301	NAD	C5A-C6A-N6A	-3.08	115.68	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
152	Cg	501	GTP	N2-C2-N3	-2.68	114.53	119.74
154	Av	301	NAD	C3N-C7N-N7N	-2.66	114.56	117.75
152	Cg	501	GTP	PB-O3B-PG	-2.66	123.70	132.83
152	Cg	501	GTP	PA-O3A-PB	-2.62	123.82	132.83
152	Cg	501	GTP	C8-N7-C5	2.62	107.99	102.99
152	Cg	501	GTP	O6-C6-C5	-2.55	119.40	124.37
150	DJ	401	UTP	O4'-C4'-C3'	-2.47	100.23	105.11
152	Cg	501	GTP	C5-C6-N1	2.46	118.30	113.95
154	Av	301	NAD	C2D-C3D-C4D	-2.39	98.00	102.64
152	Cg	501	GTP	O2G-PG-O1G	-2.36	101.43	110.68
152	Cg	501	GTP	N2-C2-N1	2.23	121.46	116.71
154	Av	301	NAD	O4B-C1B-C2B	-2.10	103.86	106.93
150	DJ	401	UTP	PB-O3B-PG	-2.09	125.66	132.83
150	DJ	401	UTP	C6-N1-C2	-2.02	118.00	121.20

There are no chirality outliers.

All (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
150	DJ	401	UTP	C2'-C1'-N1-C6
152	Cg	501	GTP	PB-O3B-PG-O2G
154	Av	301	NAD	O4D-C4D-C5D-O5D
150	DJ	401	UTP	C3'-C4'-C5'-O5'
153	CA	738	SPM	N10-C11-C12-C13
149	CA	735	SPD	N6-C7-C8-C9
153	CA	738	SPM	C2-C3-C4-N5
149	CA	735	SPD	C3-C4-C5-N6
154	Av	301	NAD	C3D-C4D-C5D-O5D
149	CA	736	SPD	C3-C4-C5-N6
153	CA	738	SPM	C7-C8-C9-N10
149	CA	735	SPD	C2-C3-C4-C5
153	CA	738	SPM	C6-C7-C8-C9
149	DL	401	SPD	C4-C5-N6-C7
149	CA	735	SPD	C4-C5-N6-C7
154	Av	301	NAD	C5D-O5D-PN-O3
149	CA	736	SPD	N1-C2-C3-C4
149	DL	401	SPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

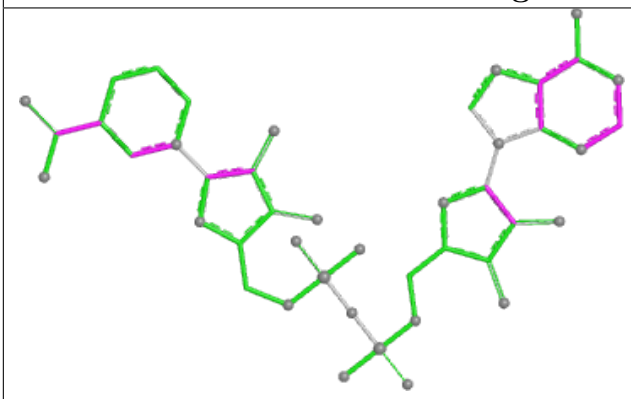
Mol	Chain	Res	Type	Atoms
152	Cg	501	GTP	PG-O3B-PB-O2B
149	CA	737	SPD	C3-C4-C5-N6
153	CA	738	SPM	C12-C11-N10-C9
149	CA	735	SPD	C7-C8-C9-N10
149	CA	736	SPD	C7-C8-C9-N10
149	CA	737	SPD	C7-C8-C9-N10
153	CA	738	SPM	C11-C12-C13-N14
154	Av	301	NAD	PA-O3-PN-O1N
153	CA	738	SPM	C7-C6-N5-C4
152	Cg	501	GTP	PB-O3B-PG-O1G
149	CA	736	SPD	C4-C5-N6-C7
149	CA	736	SPD	C8-C7-N6-C5
153	CA	738	SPM	N1-C2-C3-C4
150	DJ	401	UTP	C4'-C5'-O5'-PA
149	CA	737	SPD	C2-C3-C4-C5
154	Av	301	NAD	O4B-C4B-C5B-O5B
152	Cg	501	GTP	PG-O3B-PB-O1B
154	Av	301	NAD	PA-O3-PN-O2N
154	Av	301	NAD	C5D-O5D-PN-O1N
152	Cg	501	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

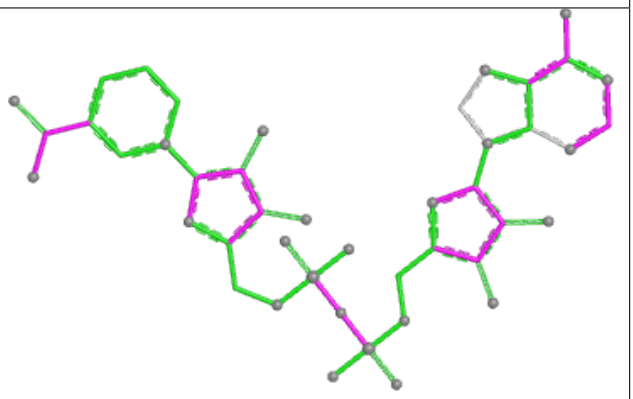
No monomer is involved in short contacts.

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.

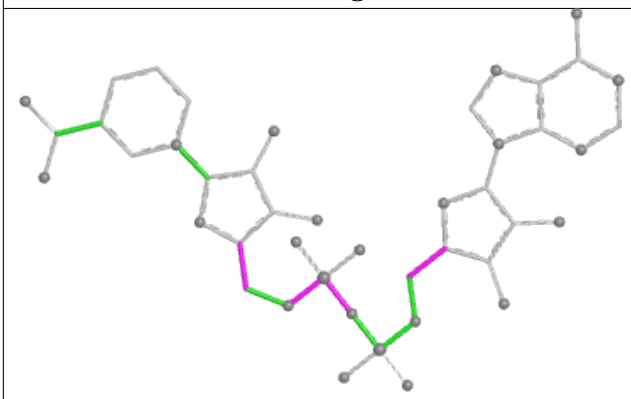
Ligand NAD Av 301



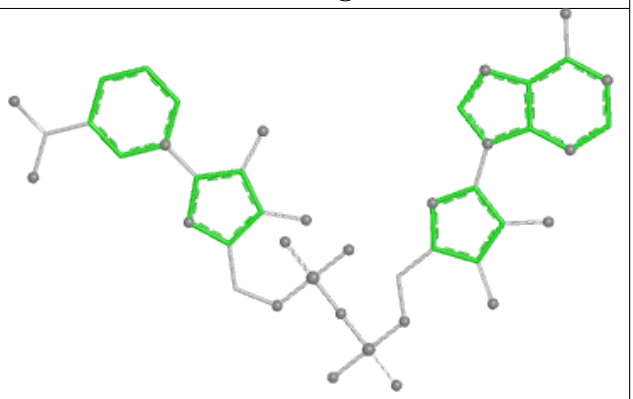
Bond lengths



Bond angles

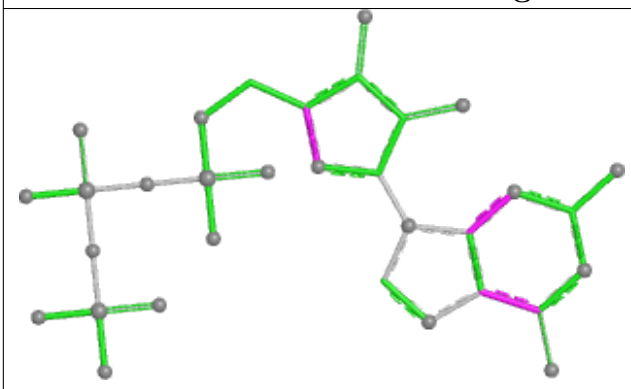


Torsions

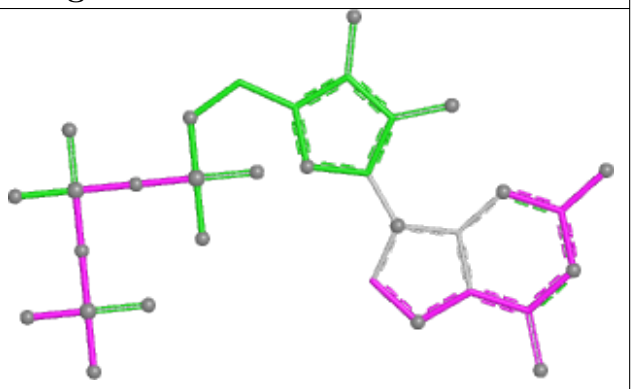


Rings

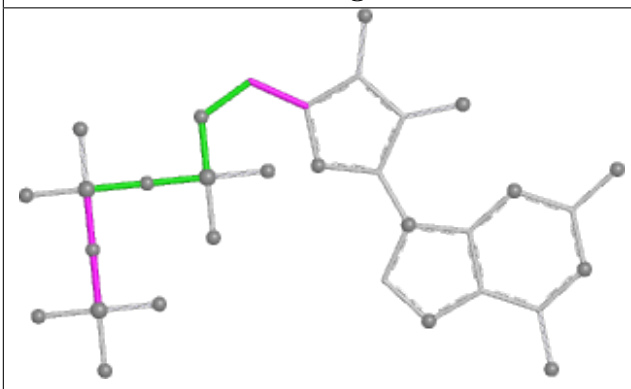
Ligand GTP Cg 501



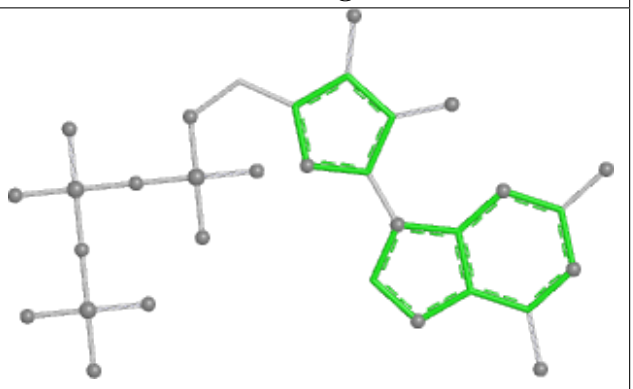
Bond lengths



Bond angles

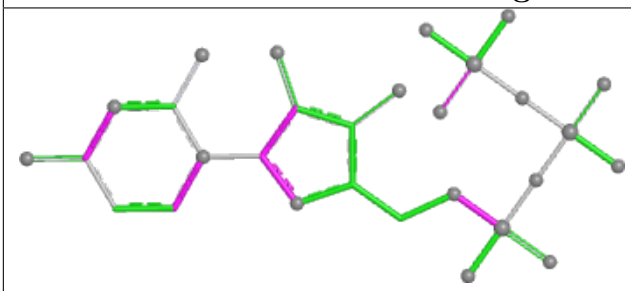


Torsions

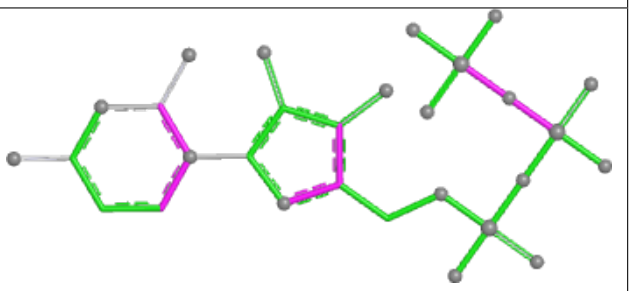


Rings

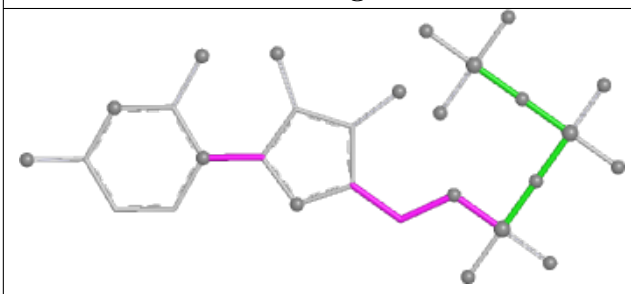
Ligand UTP DJ 401



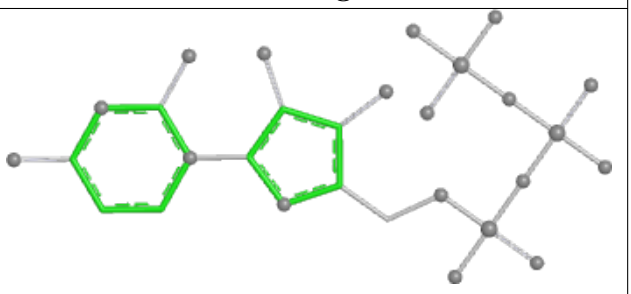
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All 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
1	AV	56:ALA	C	57:ASN	N	5.01

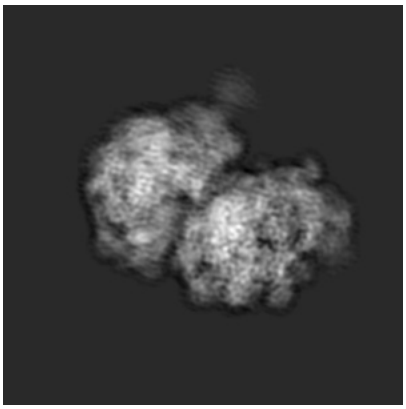
6 Map visualisation

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.

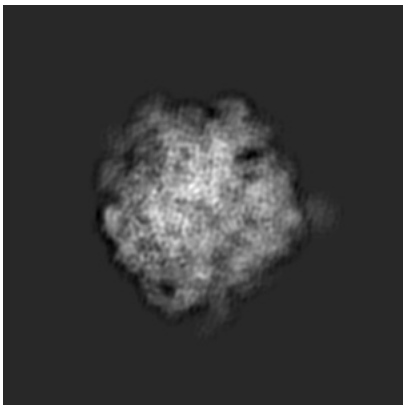
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

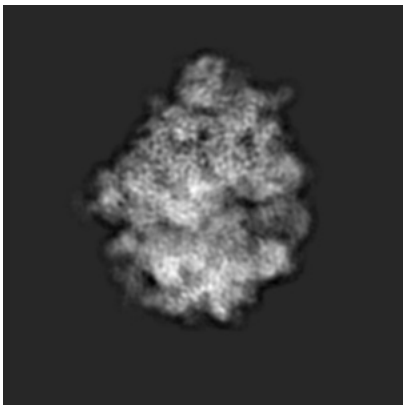
6.1.1 Primary map



X

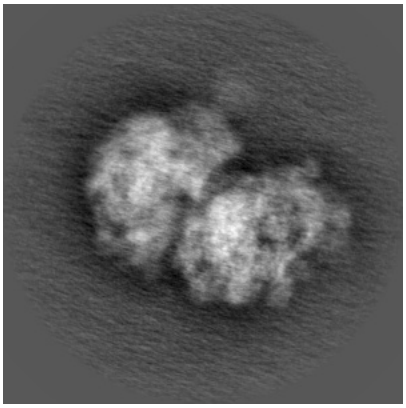


Y

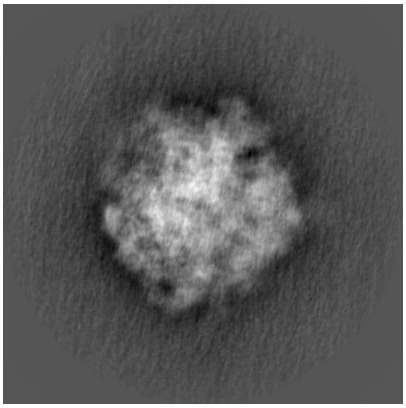


Z

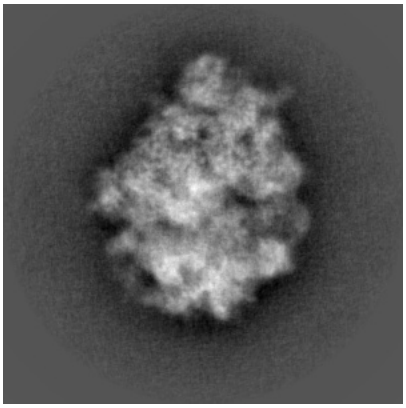
6.1.2 Raw map



X



Y

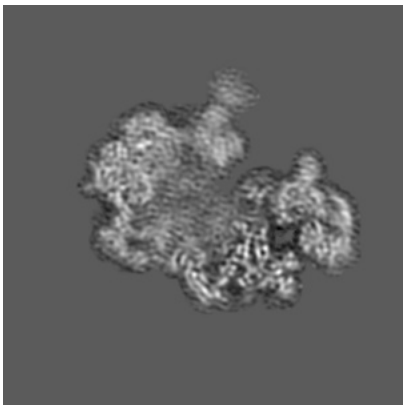


Z

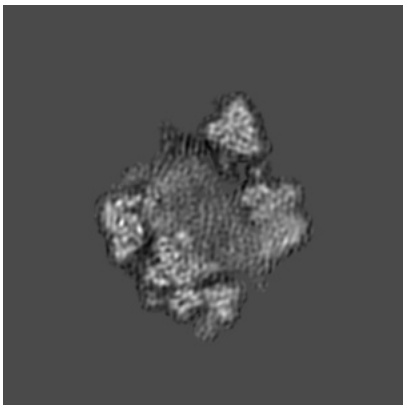
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

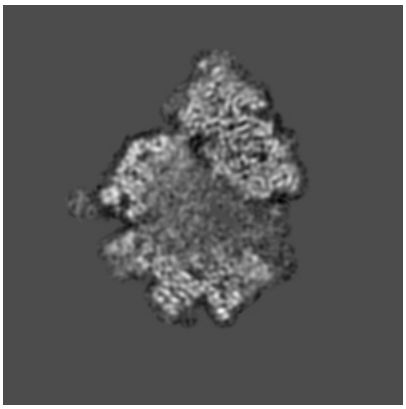
6.2.1 Primary map



X Index: 200

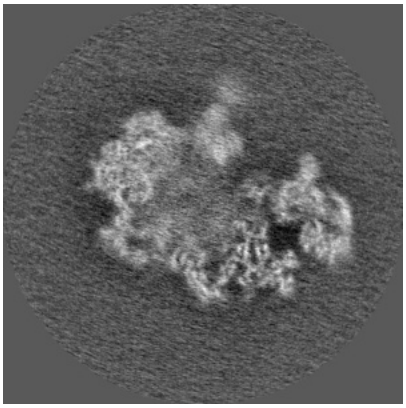


Y Index: 200

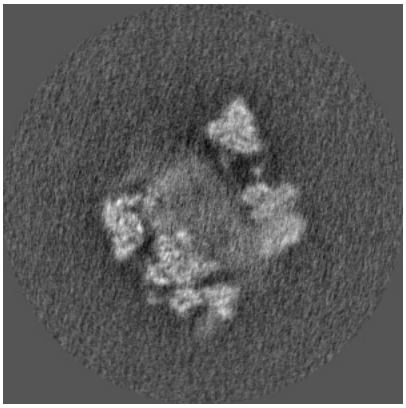


Z Index: 200

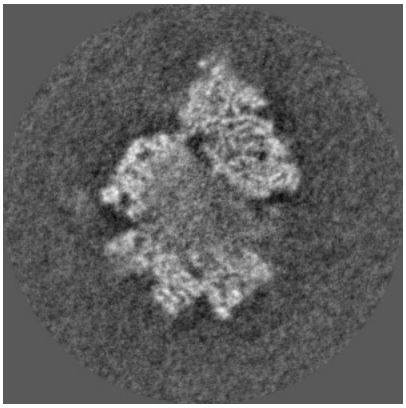
6.2.2 Raw map



X Index: 200



Y Index: 200

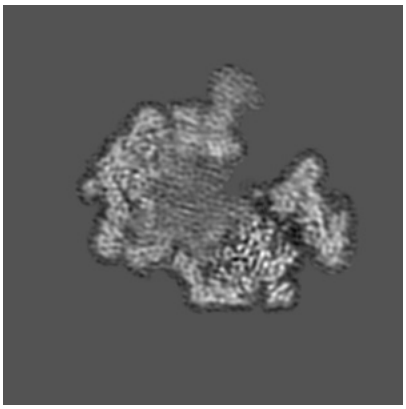


Z Index: 200

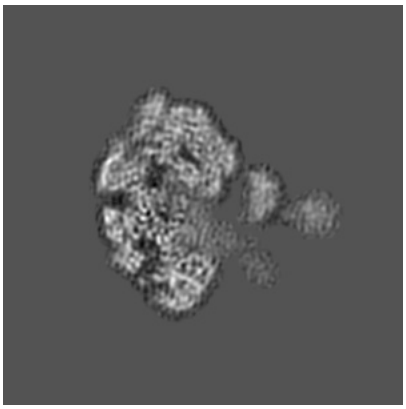
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

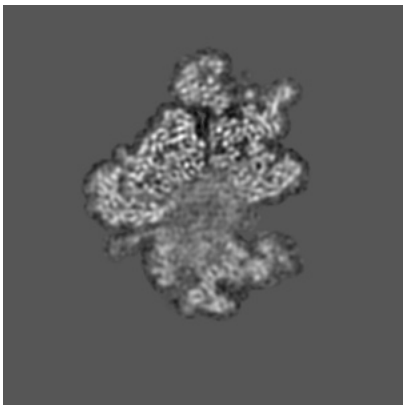
6.3.1 Primary map



X Index: 192

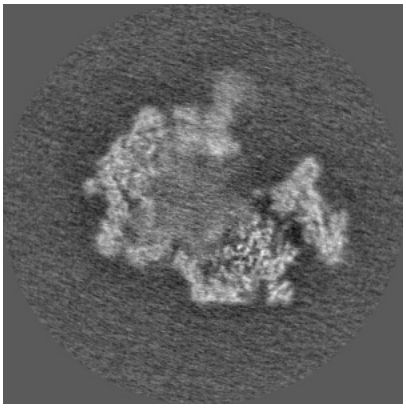


Y Index: 231

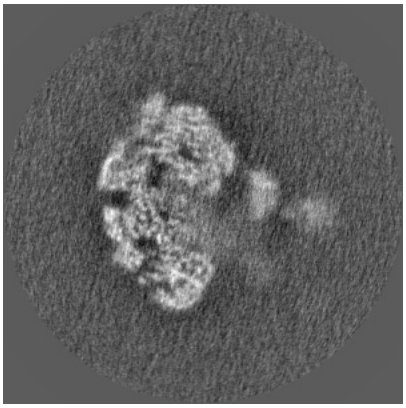


Z Index: 174

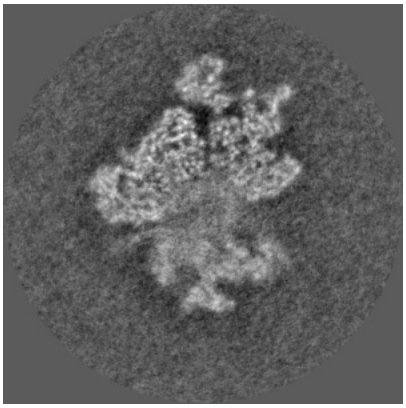
6.3.2 Raw map



X Index: 192



Y Index: 230

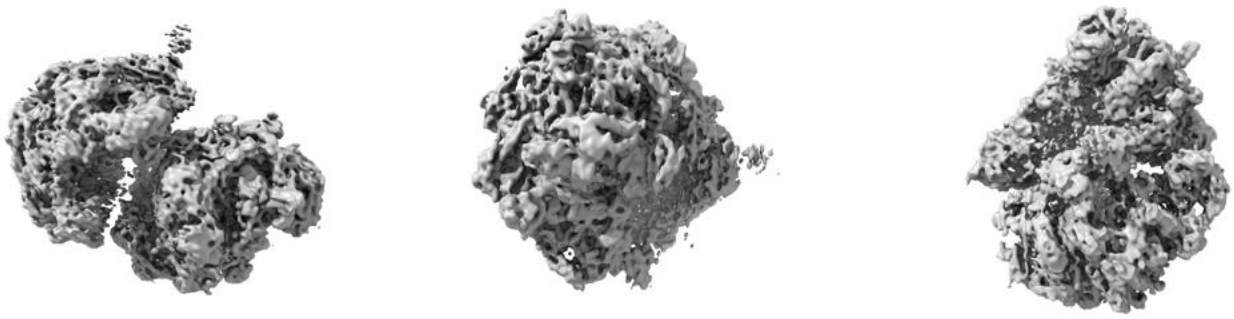


Z Index: 173

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.

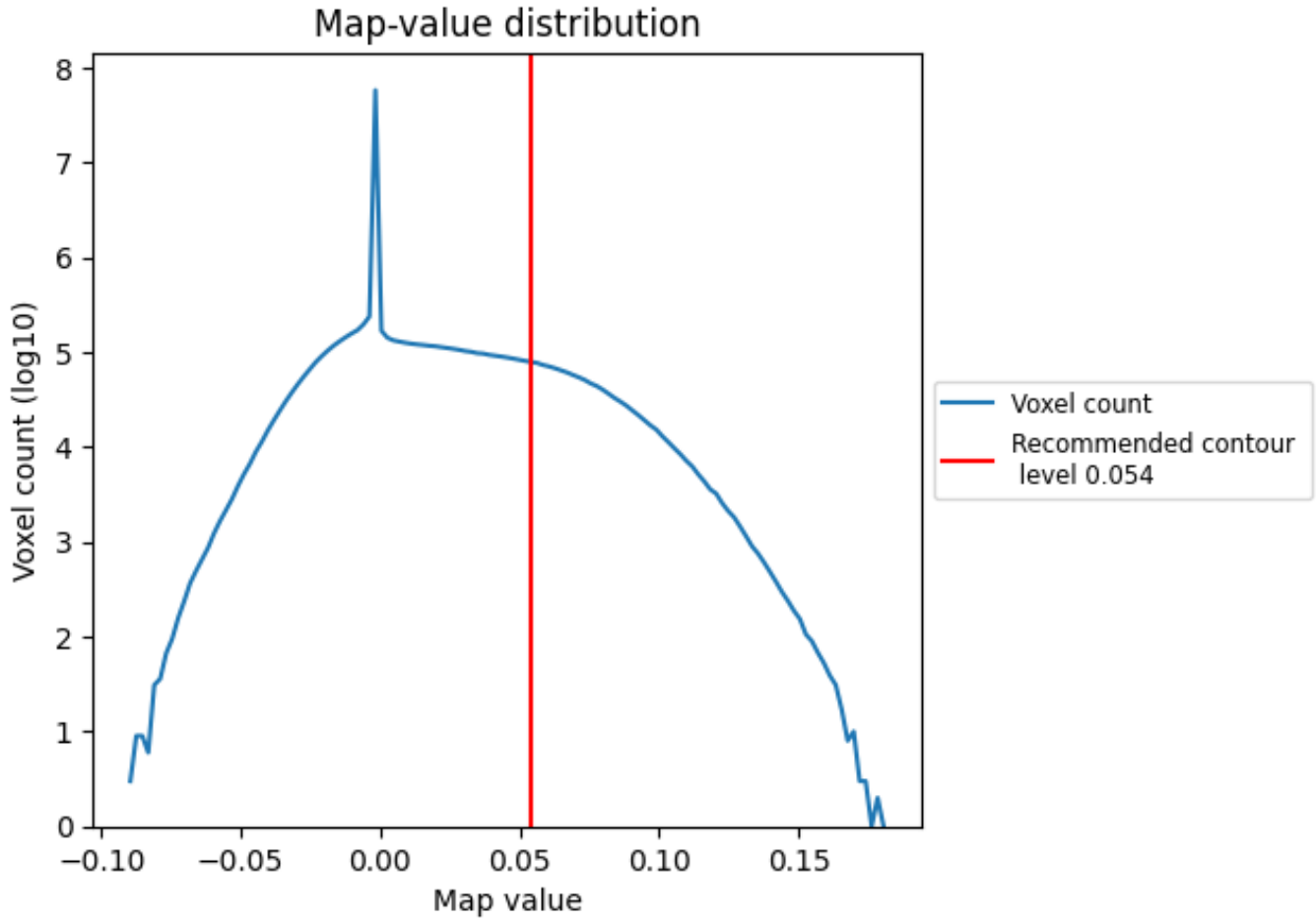
6.5 Mask visualisation (i)

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

7 Map analysis

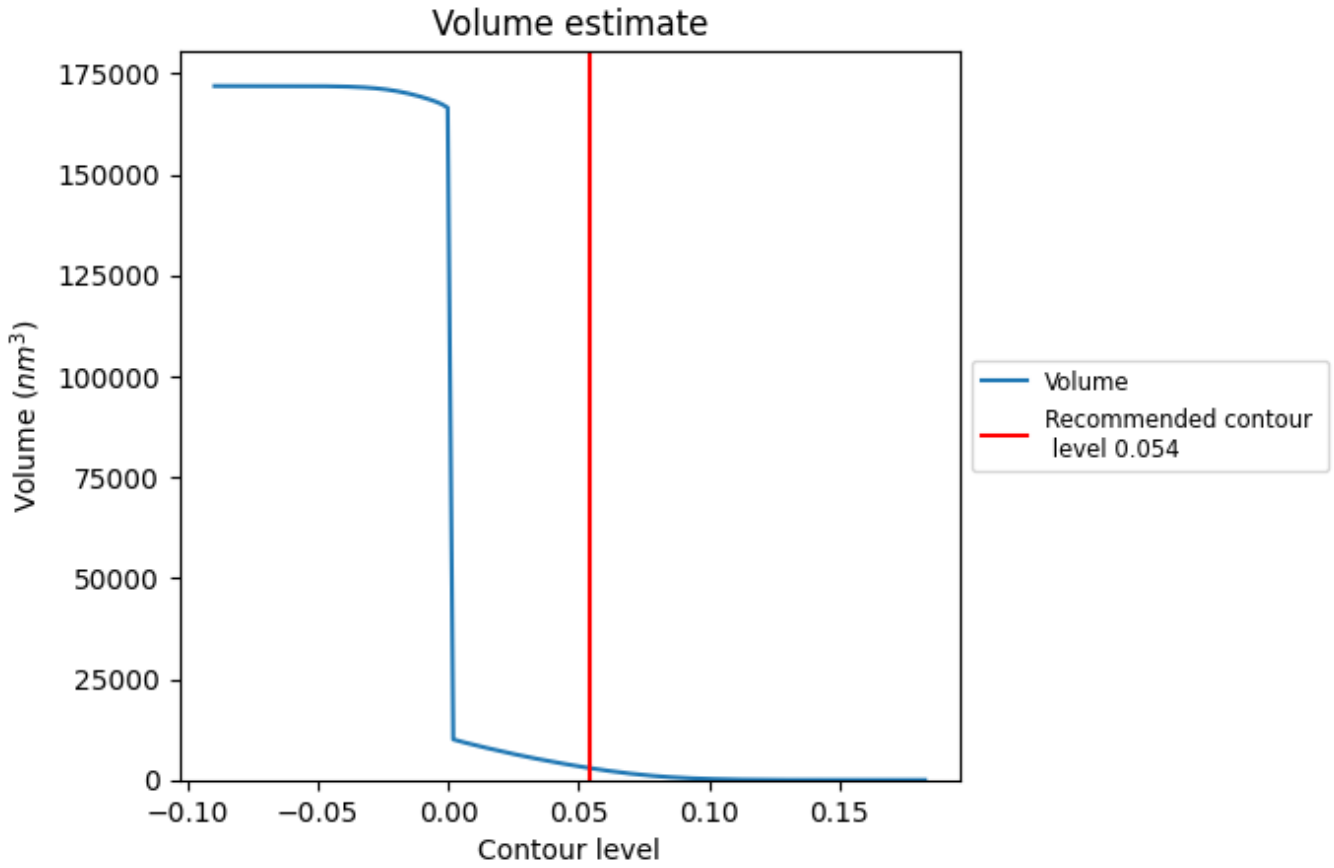
This section contains the results of statistical analysis of the map.

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.

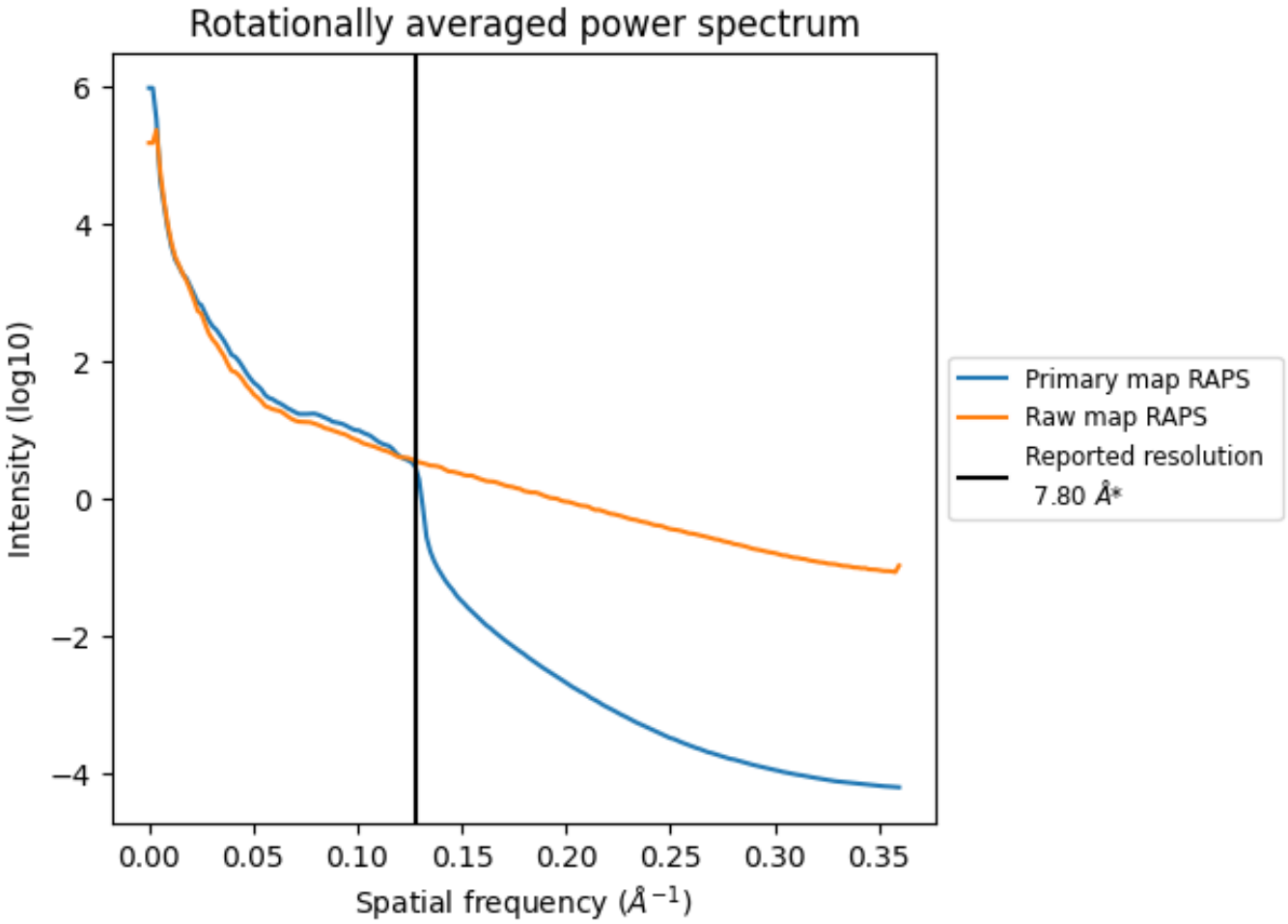
7.2 Volume estimate



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)

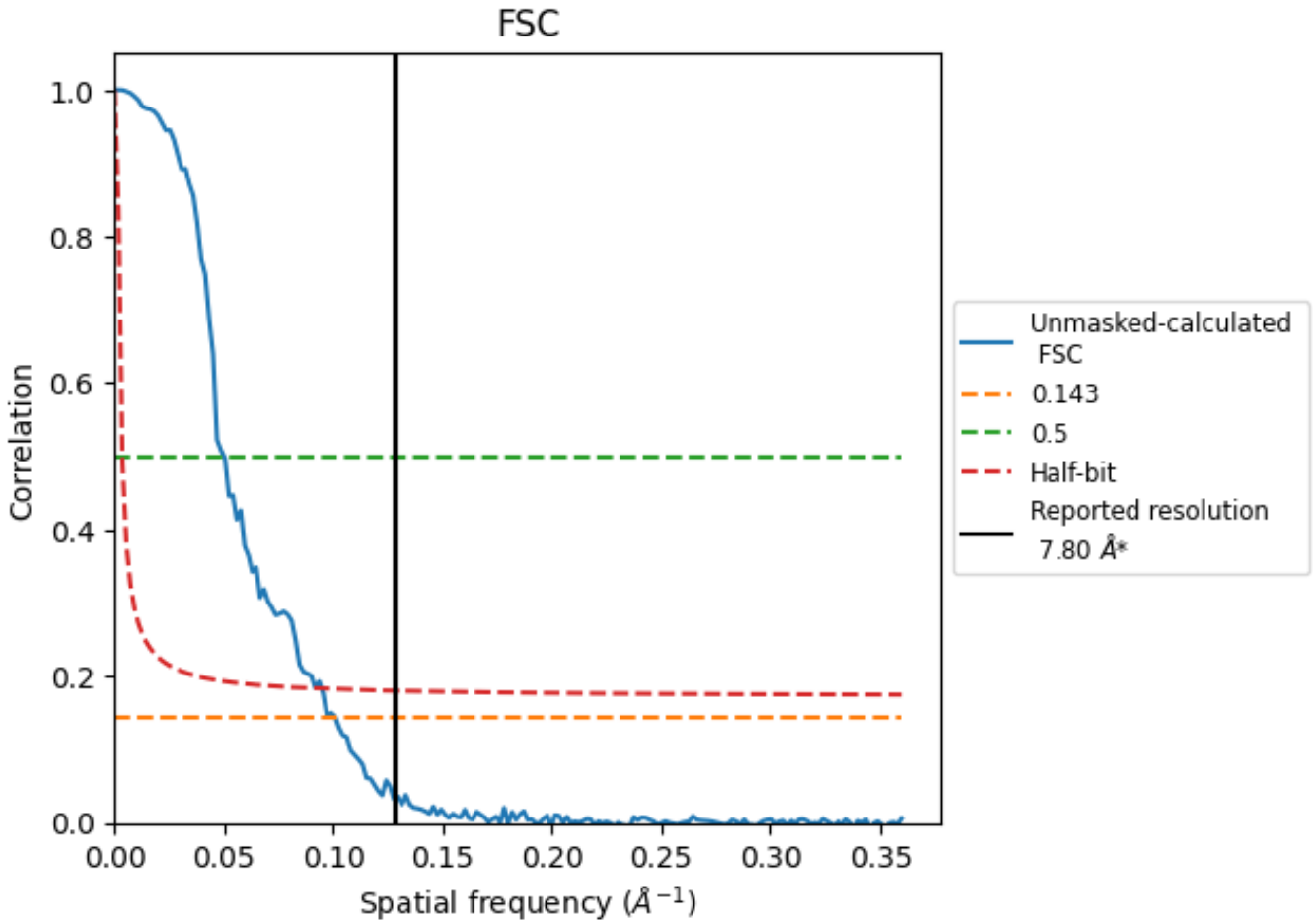


*Reported resolution corresponds to spatial frequency of 0.128 Å^{-1}

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)

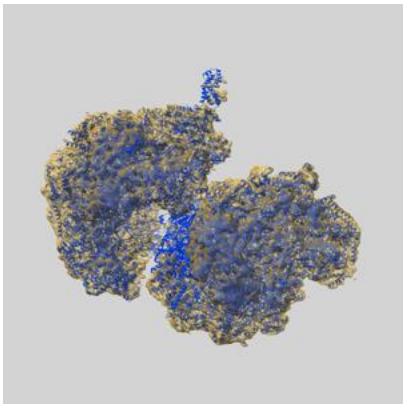
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.90	20.04	10.57

*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 %

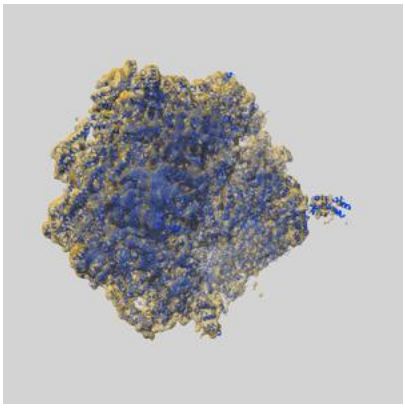
9 Map-model fit

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.

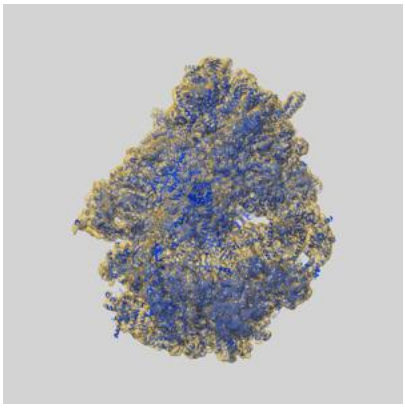
9.1 Map-model overlay



X



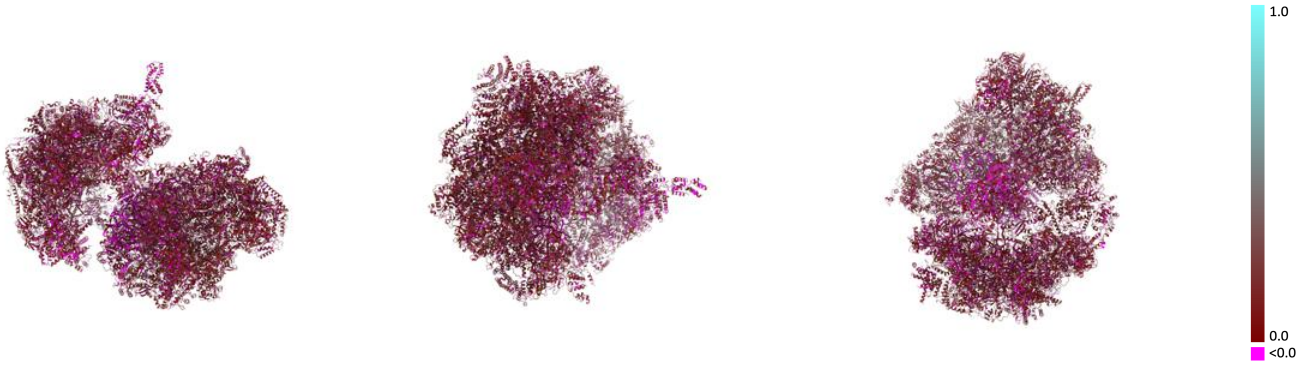
Y



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.

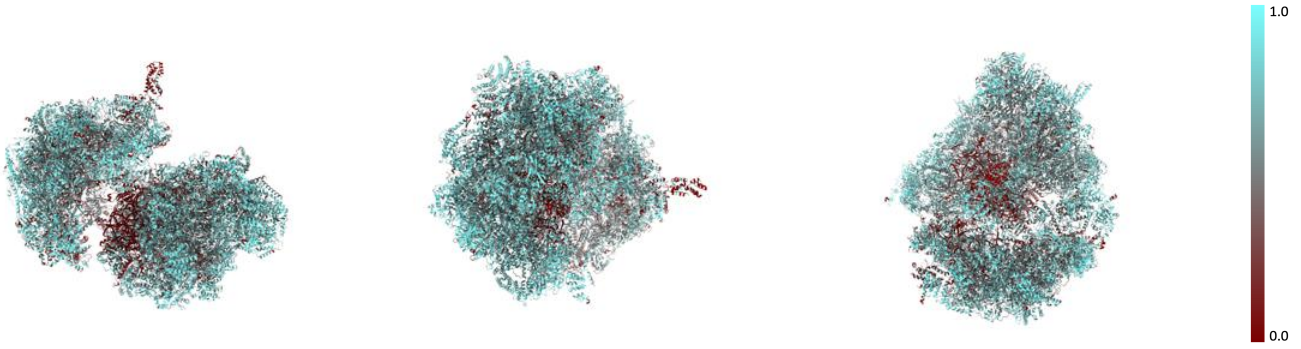
9.2 Q-score mapped to coordinate model



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.

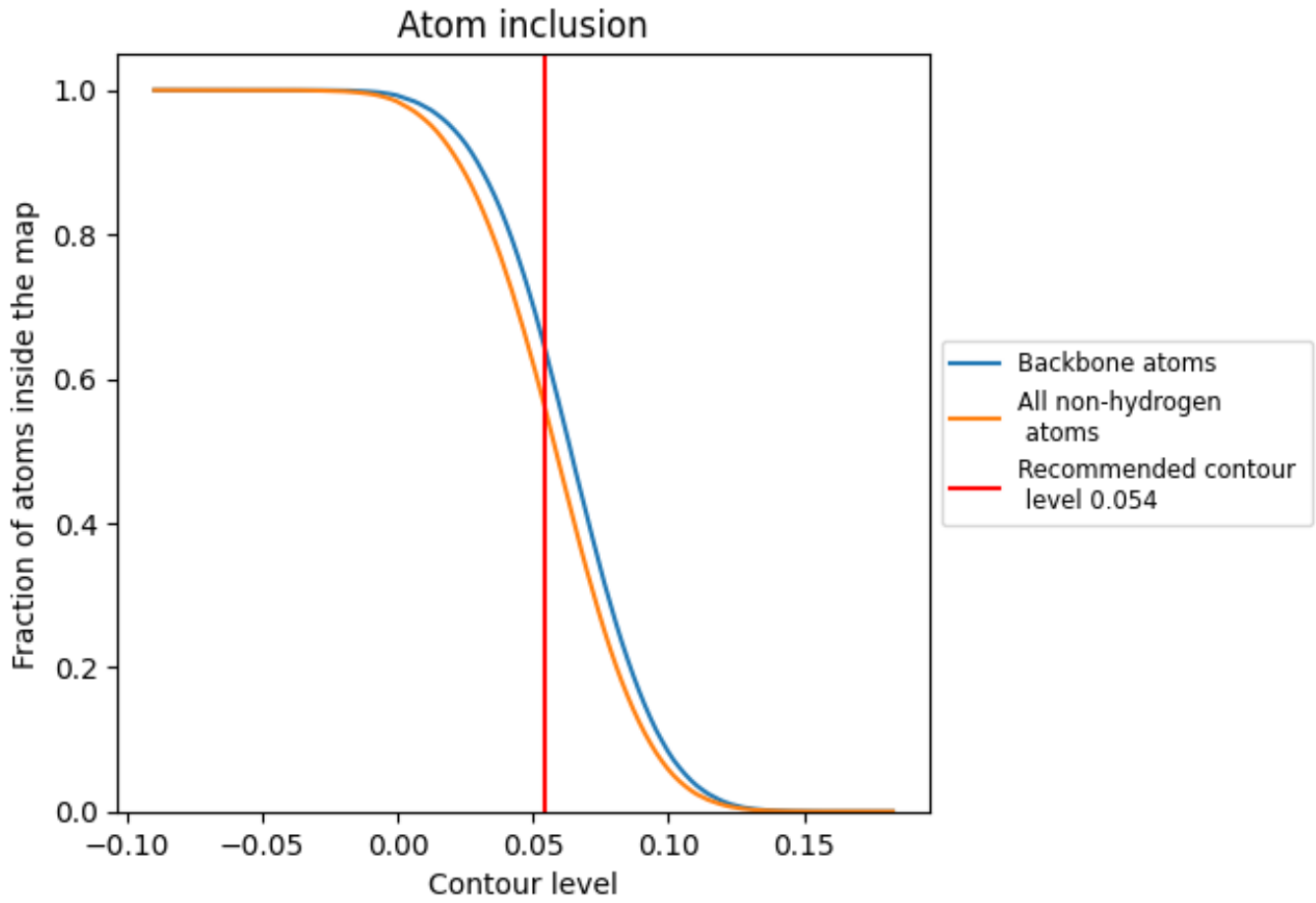
9.3 Atom inclusion mapped to coordinate model



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

Continued on next page...

Continued from previous page...

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...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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