wwPDB EM Validation Summary Report

Mar 20, 2026 – 10:26 AM UTC

PDB ID	:	7AIH / pdb_00007aih
EMDB ID	:	EMD-11796
Title	:	The Large subunit of the Kinetoplastid mitochondrial ribosome
Authors	:	Soufari, H.; Waltz, F.; Parrot, C.; Bochler, A.; Hashem, Y.
Deposited on	:	2020-09-27
Resolution	:	3.60 Å(reported)

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

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

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

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

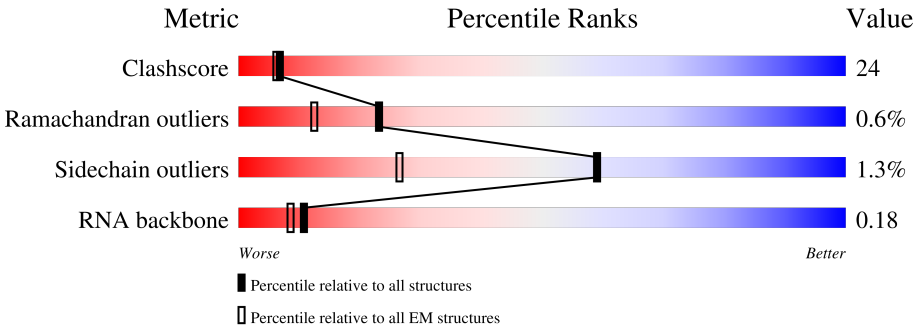
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

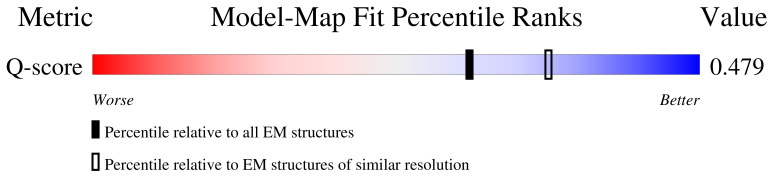
1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	A	467	10% 49% 28% • 21%
2	B	436	17% 55% 43% •
3	C	262	14% 43% 37% • 19%

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Mol	Chain	Length	Quality of chain
4	D	204	25% 35% 27% 37%
5	E	346	23% 51% 42% 6%
6	F	171	25% 50% 49%
7	G	374	16% 51% 44%
8	H	168	29% 49% 46%
9	I	305	24% 43% 41% 16%
10	J	144	22% 49% 47%
11	K	194	24% 45% 47% 8%
12	L	186	16% 55% 40%
13	M	279	17% 46% 46% 7%
14	N	252	17% 49% 26% 25%
15	O	476	36% 36% 26% 36%
16	P	185	23% 44% 45% 11%
17	Q	234	19% 51% 41% 7%
18	R	480	30% 58% 40%
19	S	409	6% 21% 16% 63%
20	T	83	11% 34% 33% 34%
21	U	118	30% 34% 36% 7% 22%
22	V	151	23% 46% 47% 7%
23	W	186	6% 18% 10% 71%
24	X	513	28% 54% 36% 9%
25	Y	292	35% 50% 37% 13%
26	Z	197	18% 41% 32% 24%
27	BA	167	28% 34% 46% 17%
28	UA	203	19% 79% 20%

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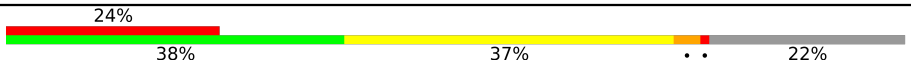
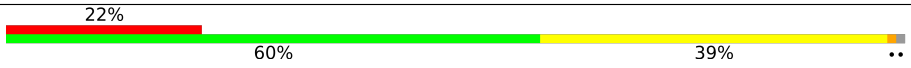
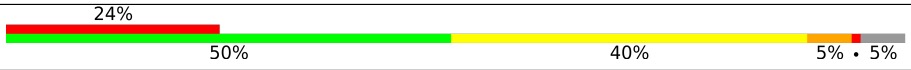
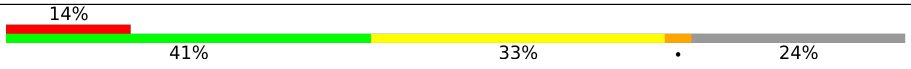
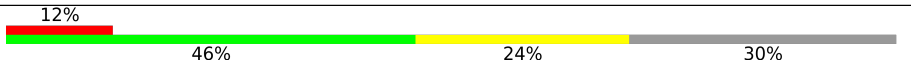
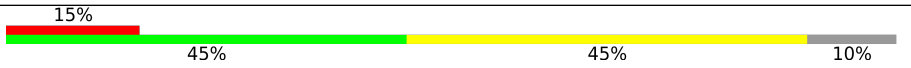
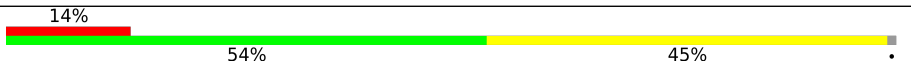
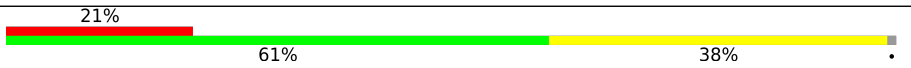
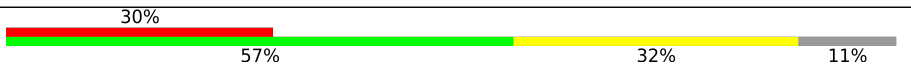
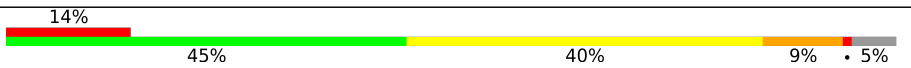
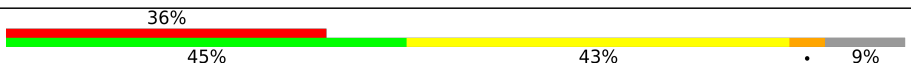
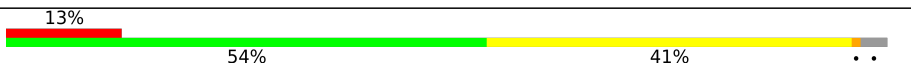
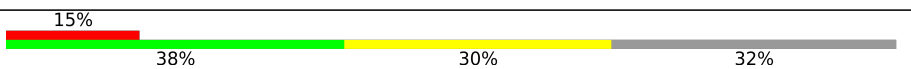
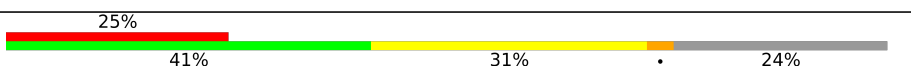
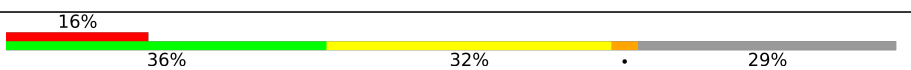
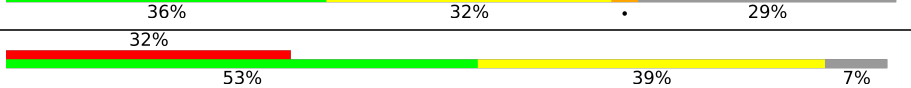
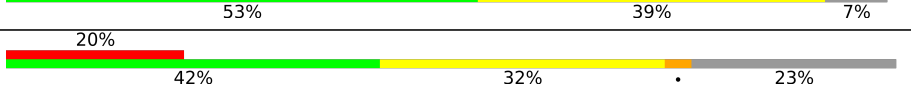
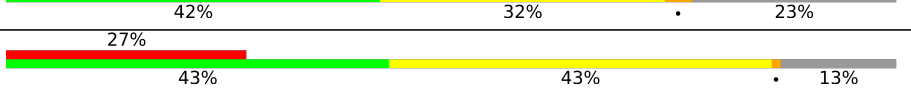
Mol	Chain	Length	Quality of chain
29	BB	156	
30	Aw	187	
31	Bj	185	
32	An	331	
33	Al	346	
34	BI	266	
35	Az	152	
36	At	183	
37	BC	147	
38	Ab	262	
39	Ai	479	
40	Ap	240	
41	Au	186	
42	Aa	195	
43	Ao	284	
44	BM	457	
45	Ar	205	
46	Aj	503	
47	BH	229	
48	Am	340	
49	Aq	341	
50	BE	118	
51	Ak	323	
52	BP	254	
53	Ad	237	

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Mol	Chain	Length	Quality of chain
54	BF	109	33% 54% 39% 7%
55	Av	192	24% 36% 44% 19%
56	Af	155	27% 49% 39% 10%
57	As	249	12% 19% 20% 61%
58	Ae	311	15% 64% 30% 6%
59	Ac	291	33% 51% 42% 8%
60	Ah	570	26% 42% 35% 21%
61	BD	102	17% 54% 41% 5%
62	Ay	174	18% 48% 32% 18%
63	Ag	244	20% 53% 41% 5%
64	Ax	216	11% 36% 34% 6% 23%
65	BL	380	12% 38% 39% 19%
66	BO	190	26% 26% 52% 18%
67	BG	1347	94%
68	UB	67	16% 84% 16%
69	UC	144	72% 88% 10%
70	UD	95	33% 87% 13%
71	1	9070	5% 5% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
72	ZN	BG	1401	-	-	X	-
72	ZN	T	101	-	-	X	-

2 Entry composition (i)

There are 73 unique types of molecules in this entry. The entry contains 143667 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 Ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	368	2996	1929	496	556	15	0	0

- Molecule 2 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	435	3513	2237	615	642	19	0	0

- Molecule 3 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	212	1772	1144	303	321	4	0	0

- Molecule 4 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1036	656	198	177	5	0	0

- Molecule 5 is a protein called Putative ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	326	2668	1704	480	470	14	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	170	1435	919	261	243	12	0	0

- Molecule 7 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	365	Total	C	N	O	S	0	0
			3012	1917	555	531	9		

- Molecule 8 is a protein called Ribosomal_L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	162	Total	C	N	O	S	0	0
			1305	836	239	226	4		

- Molecule 9 is a protein called Putative 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	257	Total	C	N	O	S	0	0
			2153	1362	406	372	13		

- Molecule 10 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1146	727	211	202	6		

- Molecule 11 is a protein called bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	179	Total	C	N	O	S	0	0
			1467	910	289	258	10		

- Molecule 12 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	178	Total	C	N	O	S	0	0
			1419	907	257	250	5		

- Molecule 13 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	259	Total	C	N	O	S	0	0
			2116	1345	385	371	15		

- Molecule 14 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	189	Total	C	N	O	S	0	0
			1599	1031	296	269	3		

- Molecule 15 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	307	Total	C	N	O	S	0	0
			2537	1600	455	475	7		

- Molecule 16 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	165	Total	C	N	O	S	0	0
			1367	856	266	238	7		

- Molecule 17 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	217	Total	C	N	O	S	0	0
			1785	1127	331	316	11		

- Molecule 18 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	472	Total	C	N	O	S	0	0
			3755	2377	662	704	12		

- Molecule 19 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	150	Total	C	N	O	S	0	0
			1244	782	247	207	8		

- Molecule 20 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	55	Total	C	N	O	S	0	0
			487	311	93	78	5		

- Molecule 21 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	92	Total	C	N	O	S	0	0
			744	472	142	125	5		

- Molecule 22 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	141	Total	C	N	O	S	0	0
			1202	755	242	197	8		

- Molecule 23 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	54	Total	C	N	O	S	0	0
			465	299	89	74	3		

- Molecule 24 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	468	Total	C	N	O	S	0	0
			3733	2365	657	694	17		

- Molecule 25 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	255	Total	C	N	O	S	0	0
			2067	1287	373	402	5		

- Molecule 26 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	150	Total	C	N	O	S	0	0
			1223	784	224	211	4		

- Molecule 27 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BA	138	Total	C	N	O	S	0	0
			1038	648	188	197	5		

- Molecule 28 is a protein called UA.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	UA	203	Total 1015	C 609	N 203	O 203	0	0

- Molecule 29 is a protein called mL95.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	BB	122	Total 1028	C 663	N 189	O 176	0	0

- Molecule 30 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Aw	185	Total 1509	C 949	N 289	O 268	S 3	0	0

- Molecule 31 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bj	168	Total 1358	C 865	N 255	O 231	S 7	0	0

- Molecule 32 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	An	314	Total 2605	C 1643	N 487	O 470	S 5	0	0

- Molecule 33 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Al	264	Total 2152	C 1371	N 374	O 399	S 8	0	0

- Molecule 34 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	186	Total 1409	C 895	N 242	O 264	S 8	0	0

- Molecule 35 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Az	138	Total	C	N	O	S	0	0
			1215	782	216	211	6		

- Molecule 36 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	At	165	Total	C	N	O	S	0	0
			1346	824	260	254	8		

- Molecule 37 is a protein called mL96.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	140	Total	C	N	O	S	0	0
			1114	693	205	207	9		

- Molecule 38 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ab	260	Total	C	N	O	S	0	0
			2185	1365	416	397	7		

- Molecule 39 is a protein called mL69.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ai	476	Total	C	N	O	S	0	0
			3789	2419	654	694	22		

- Molecule 40 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ap	214	Total	C	N	O	S	0	0
			1775	1111	327	328	9		

- Molecule 41 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Au	176	Total	C	N	O	S	0	0
			1490	945	292	245	8		

- Molecule 42 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Aa	178	Total	C	N	O	S	0	0
			1417	884	270	256	7		

- Molecule 43 is a protein called mL79.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ao	275	Total	C	N	O	S	0	0
			2276	1433	429	402	12		

- Molecule 44 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BM	389	Total	C	N	O	S	0	0
			3069	1954	548	551	16		

- Molecule 45 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ar	195	Total	C	N	O	S	0	0
			1644	1054	295	288	7		

- Molecule 46 is a protein called mL72.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Aj	341	Total	C	N	O	S	0	0
			2766	1756	508	491	11		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BH	214	Total	C	N	O	S	0	0
			1659	1050	290	310	9		

- Molecule 48 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Am	330	Total	C	N	O	S	0	0
			2708	1727	491	474	16		

- Molecule 49 is a protein called mL82.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Aq	258	Total	C	N	O	S	0	0
			2074	1296	406	360	12		

- Molecule 50 is a protein called mL98.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BE	84	Total	C	N	O	0	0
			700	447	125	128		

- Molecule 51 is a protein called mL73.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ak	300	Total	C	N	O	S	0	0
			2352	1489	421	429	13		

- Molecule 52 is a protein called mL52,mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BP	195	Total	C	N	O	S	0	0
			1593	1014	288	288	3		

- Molecule 53 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ad	207	Total	C	N	O	S	0	0
			1632	1049	289	286	8		

- Molecule 54 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BF	101	Total	C	N	O	S	0	0
			851	530	165	154	2		

- Molecule 55 is a protein called mL88.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Av	155	Total	C	N	O	S	0	0
			1300	828	230	234	8		

- Molecule 56 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Af	139	Total	C	N	O	S	0	0
			1132	709	215	207	1		

- Molecule 57 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	As	97	Total	C	N	O	S	0	0
			787	495	139	148	5		

- Molecule 58 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ae	291	Total	C	N	O	S	0	0
			2359	1526	418	404	11		

- Molecule 59 is a protein called MRP-L46 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ac	268	Total	C	N	O	S	0	0
			2174	1375	389	405	5		

- Molecule 60 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ah	452	Total	C	N	O	S	0	0
			3686	2338	651	679	18		

- Molecule 61 is a protein called mL97.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BD	97	Total	C	N	O	S	0	0
			807	499	160	140	8		

- Molecule 62 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Ay	142	Total	C	N	O	S	0	0
			1226	774	228	217	7		

- Molecule 63 is a protein called mL54/69.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Ag	231	Total	C	N	O	S	0	0
			1916	1211	356	340	9		

- Molecule 64 is a protein called LIM zinc-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ax	167	Total	C	N	O	S	0	0
			1388	876	268	233	11		

- Molecule 65 is a protein called Putative ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BL	309	Total	C	N	O	S	0	0
			2497	1594	464	427	12		

- Molecule 66 is a protein called Putative ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BO	155	Total	C	N	O	S	0	0
			1239	772	253	205	9		

- Molecule 67 is a protein called mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BG	85	Total	C	N	O	S	0	0
			643	400	122	115	6		

- Molecule 68 is a protein called UB.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	UB	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 69 is a protein called UC.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	UC	144	Total	C	N	O	0	0
			720	432	144	144		

- Molecule 70 is a protein called UD.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	UD	95	Total 475	C 285	N 95	O 95	0	0

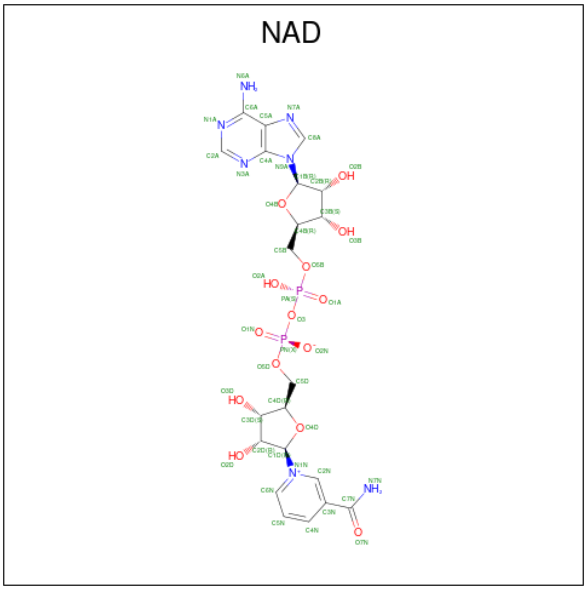
- Molecule 71 is a RNA chain called Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	1	1087	Total 22918	C 10319	N 3839	O 7673	P 1087	0	0

- Molecule 72 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
72	T	1	Total 1	Zn 1	0
72	W	1	Total 1	Zn 1	0
72	BD	1	Total 1	Zn 1	0
72	Ax	2	Total 2	Zn 2	0
72	BG	1	Total 1	Zn 1	0

- Molecule 73 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

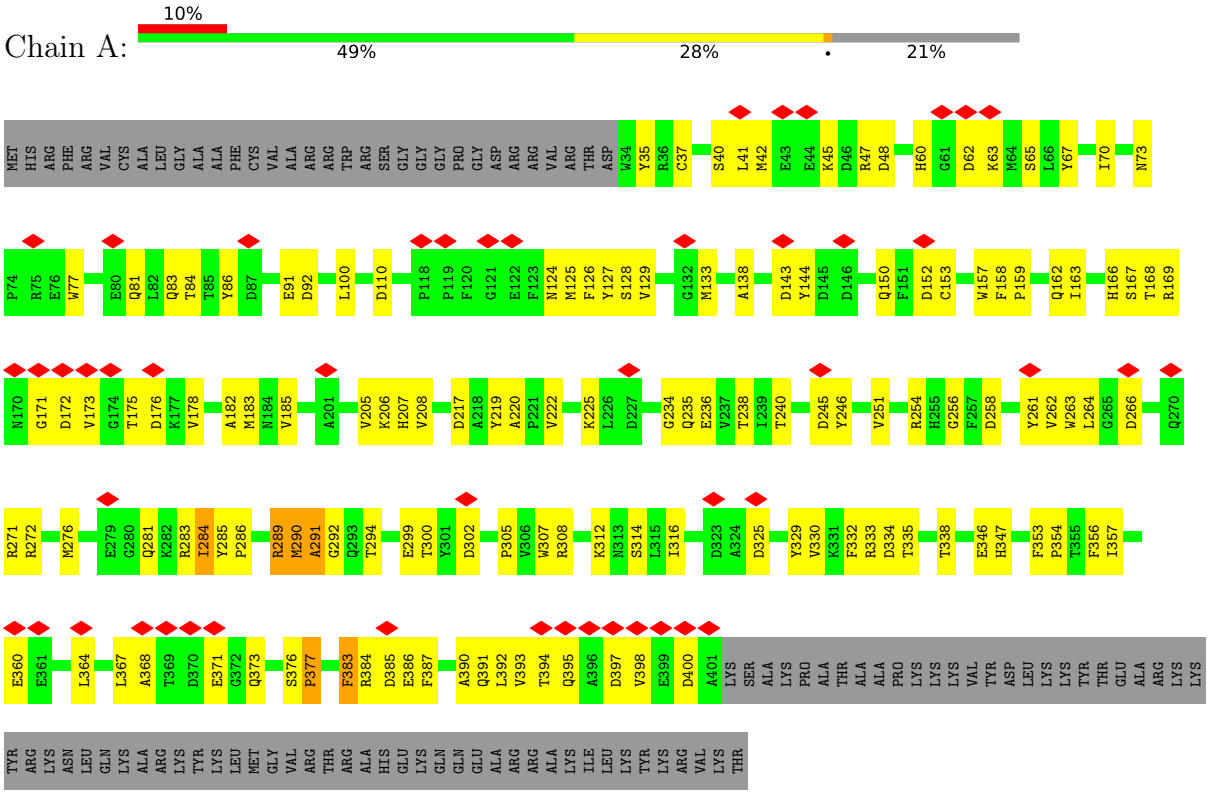


Mol	Chain	Residues	Atoms					AltConf
73	Ag	1	Total	C	N	O	P	0
			44	21	7	14	2	

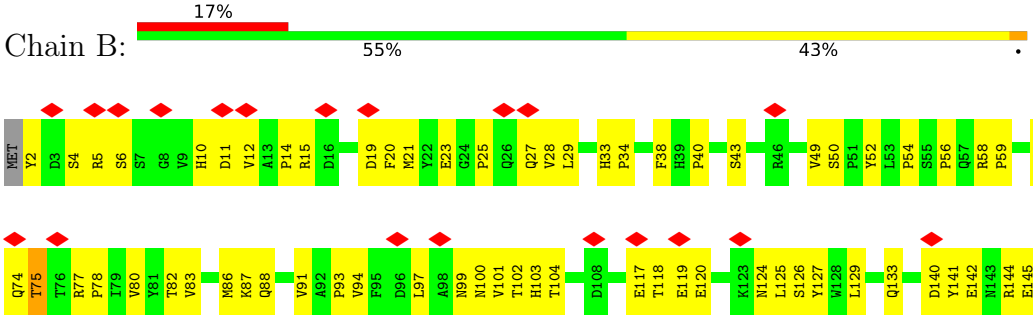
3 Residue-property plots (i)

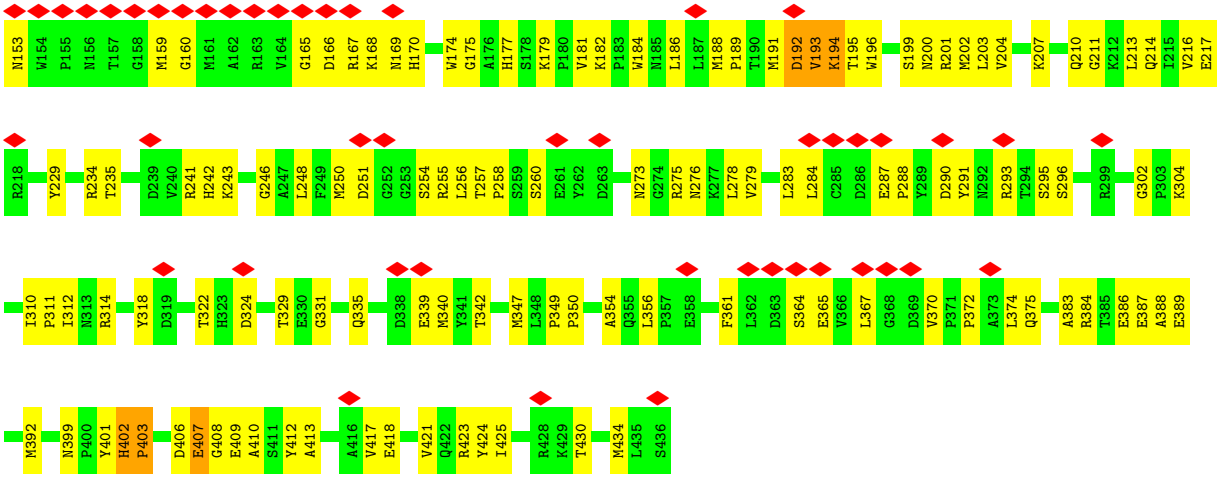
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ribosomal protein L3-like protein



• Molecule 2: uL4m

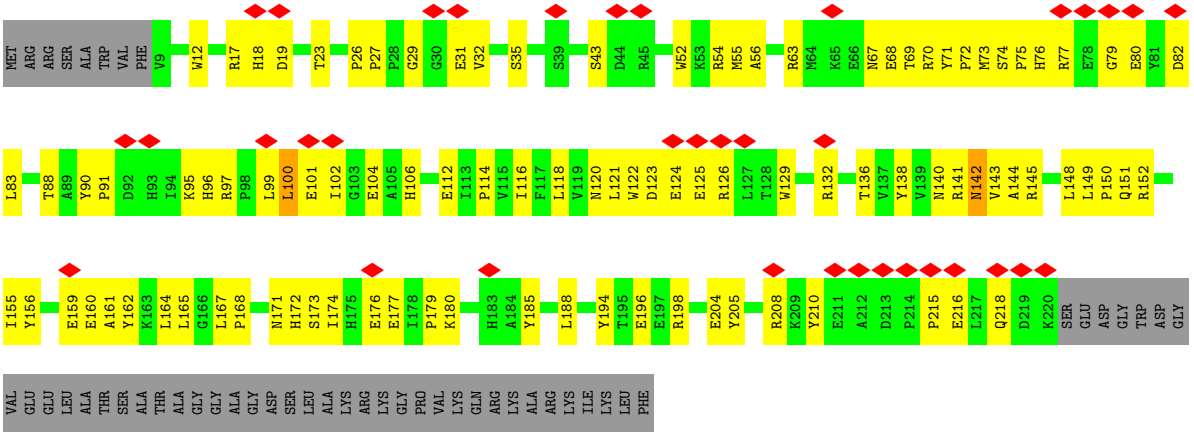




• Molecule 3: RIBOSOMAL_L9 domain-containing protein

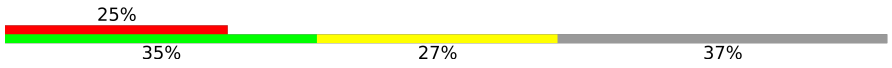
Chain C:

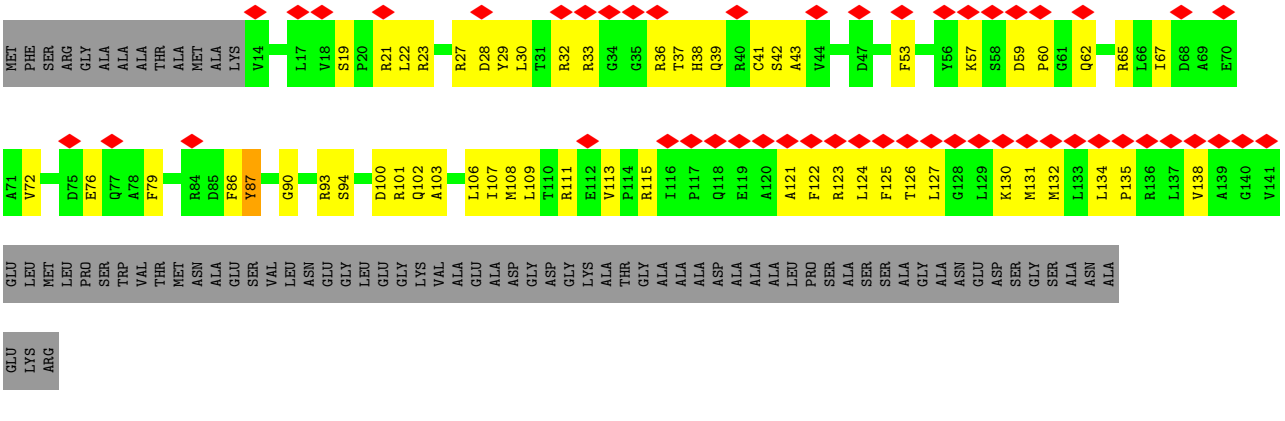




• Molecule 4: uL10m

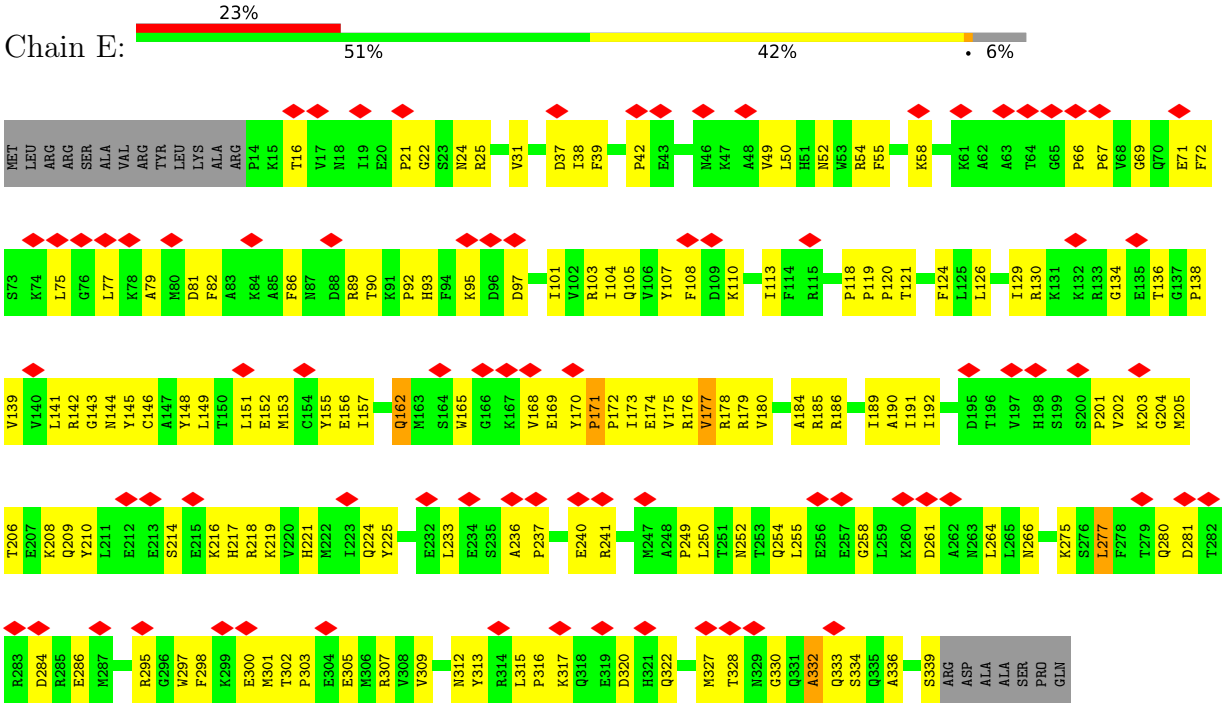
Chain D:





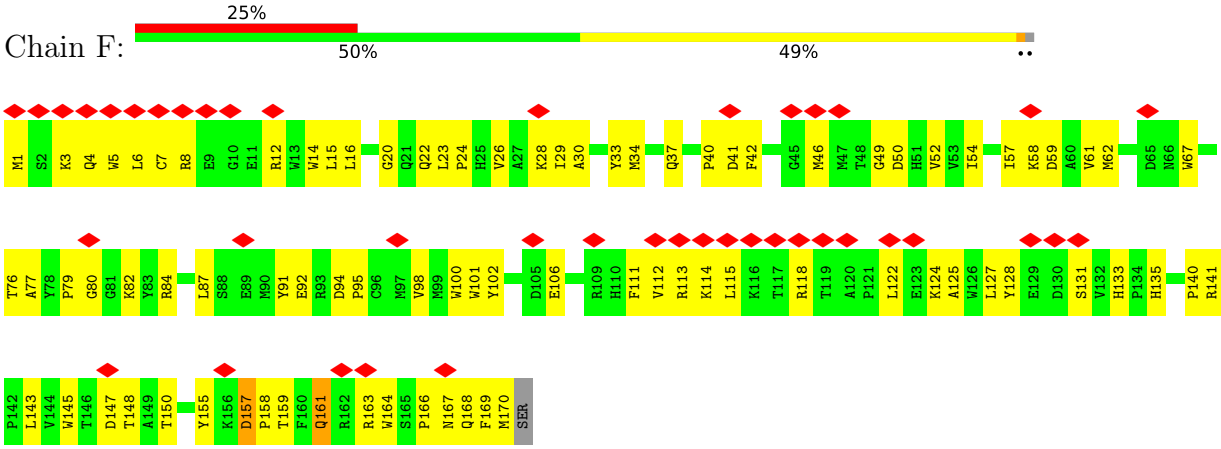
• Molecule 5: Putative ribosomal protein L11

Chain E:



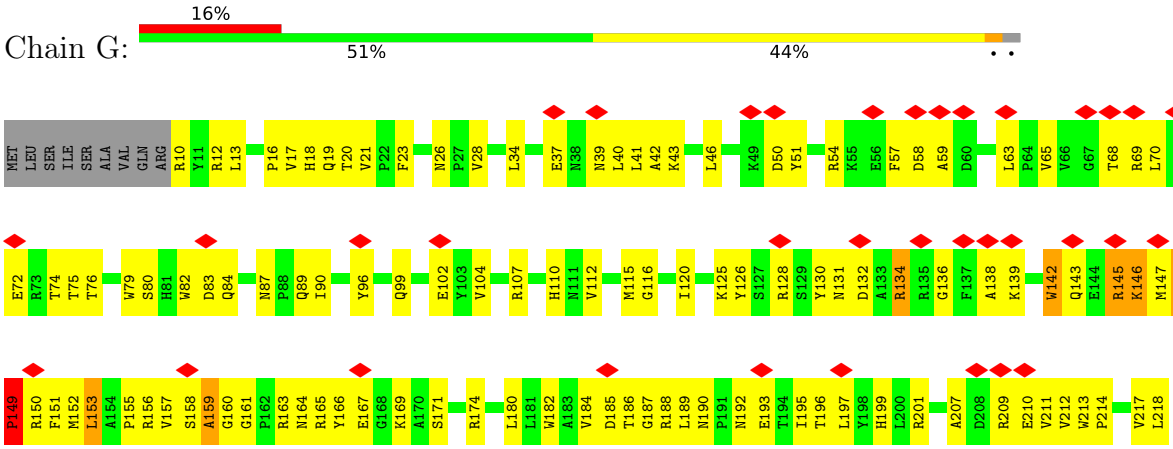
• Molecule 6: 50S ribosomal protein L13-like protein

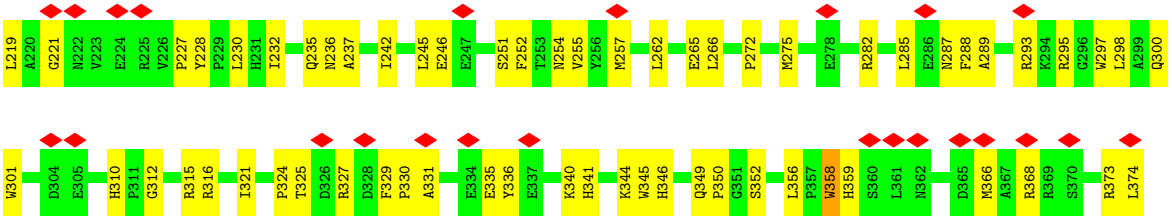
Chain F:



• Molecule 7: Ribosomal_L18e/L15P domain-containing protein

Chain G:

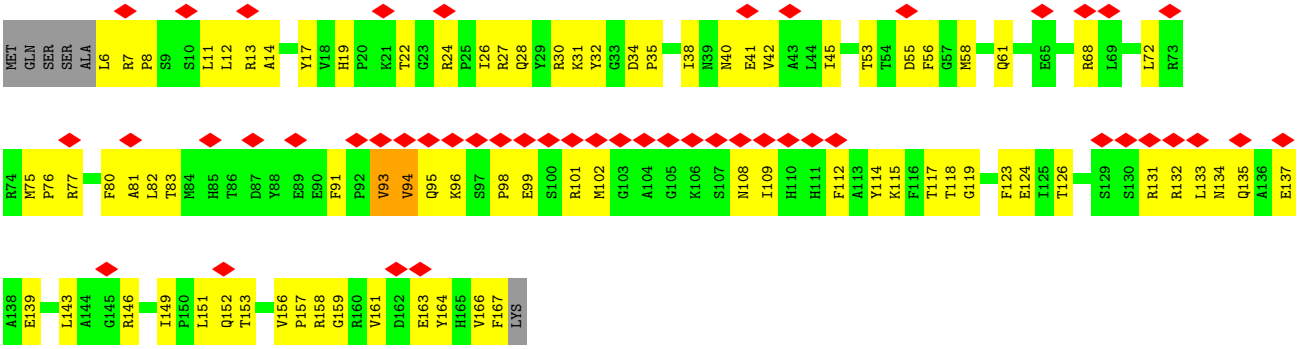




• Molecule 8: Ribosomal_L16 domain-containing protein

Chain H:

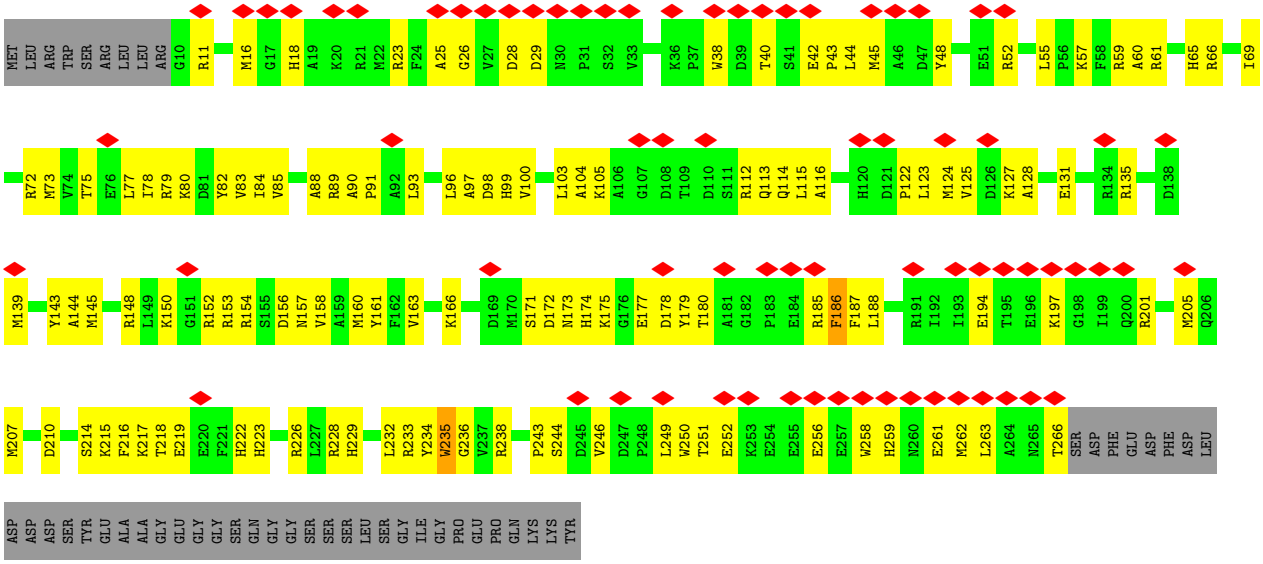




• Molecule 9: Putative 50S ribosomal protein L17

Chain I:

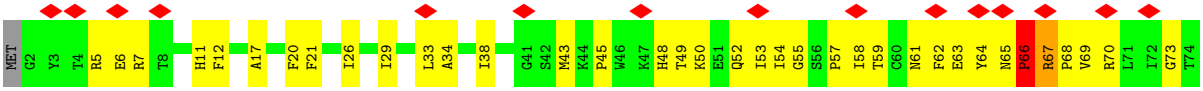


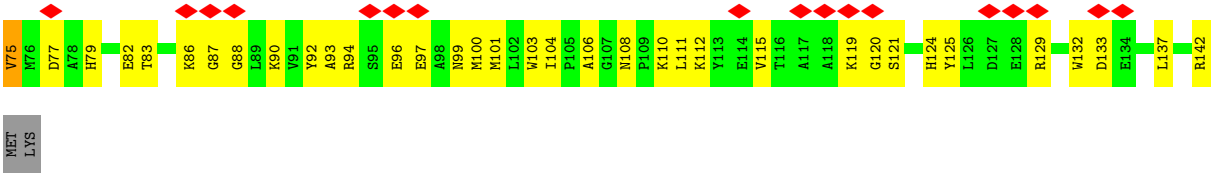


• Molecule 10: bL19m

Chain J:



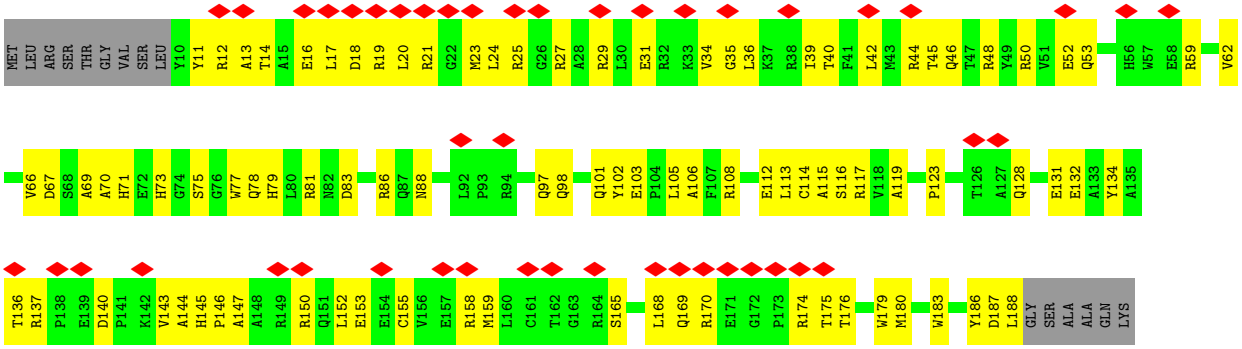




• Molecule 11: bL20

Chain K:

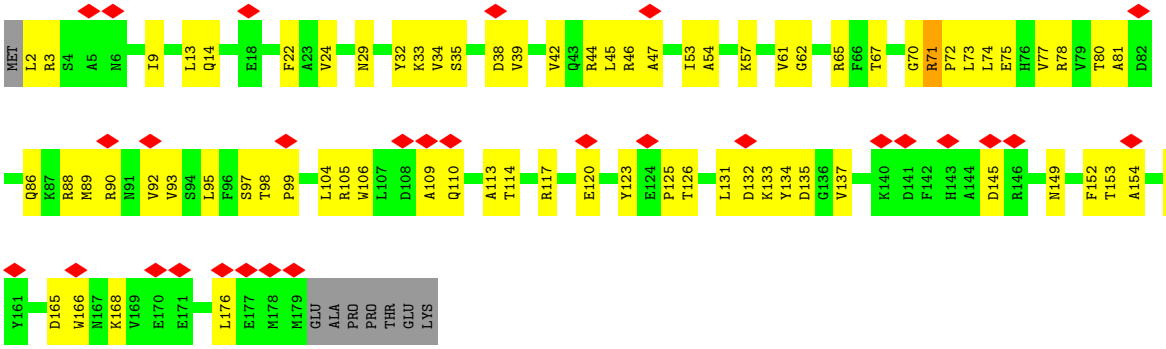




• Molecule 12: bL21m

Chain L:

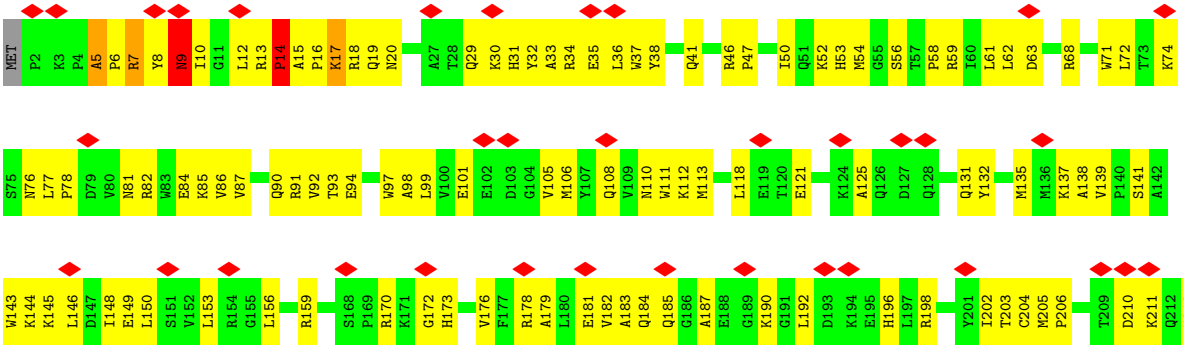


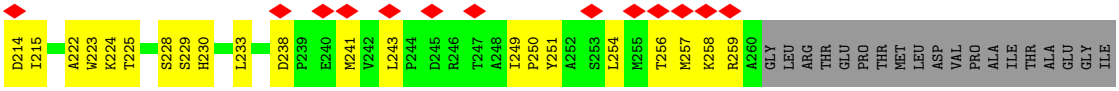


• Molecule 13: uL22m

Chain M:



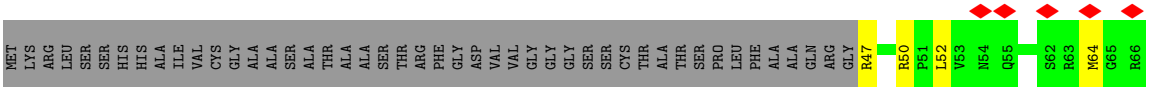


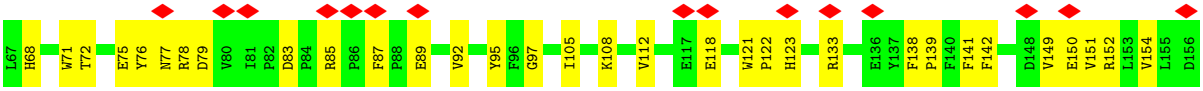


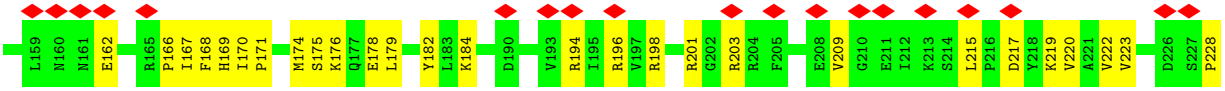
• Molecule 14: uL23m

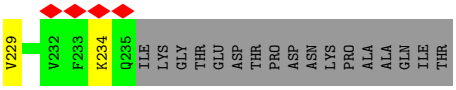
Chain N:





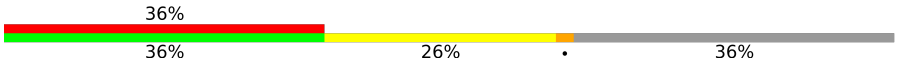


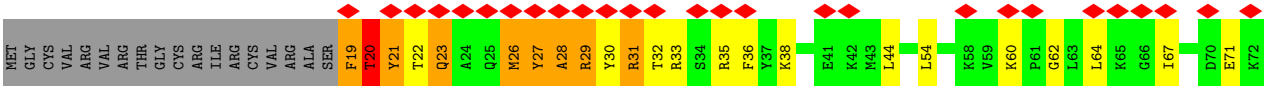


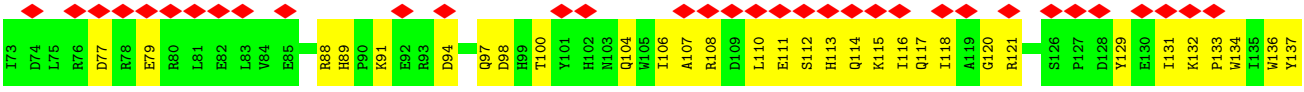


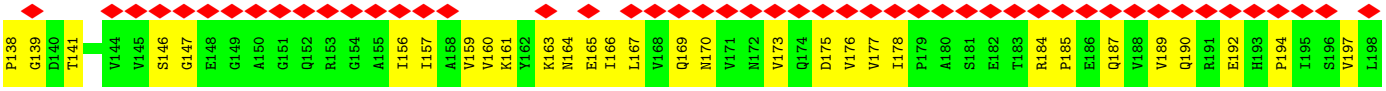
• Molecule 15: uL24m

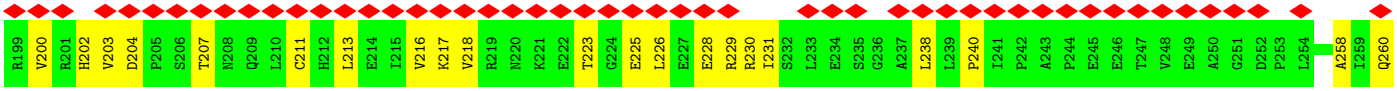
Chain O:













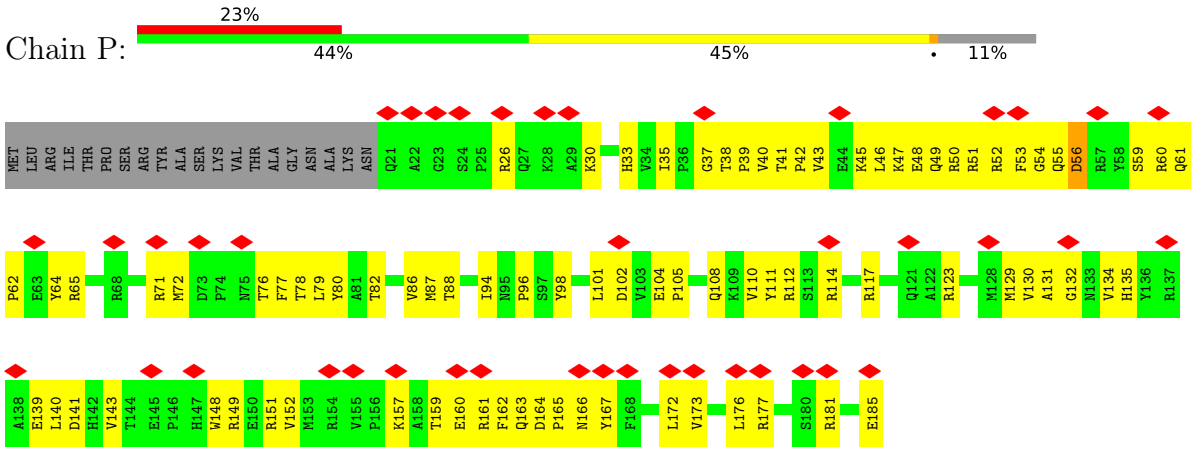






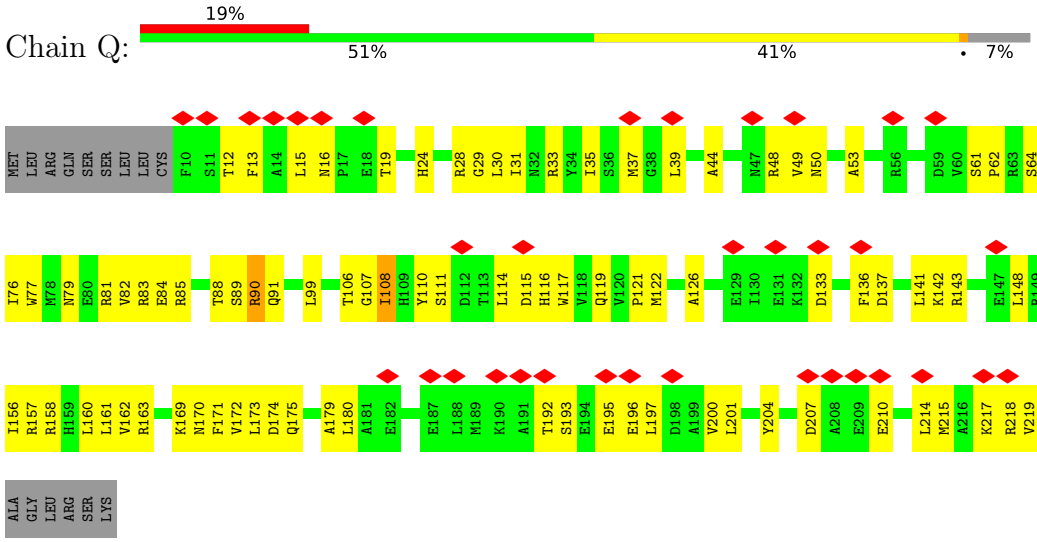
• Molecule 16: bL27m

Chain P:



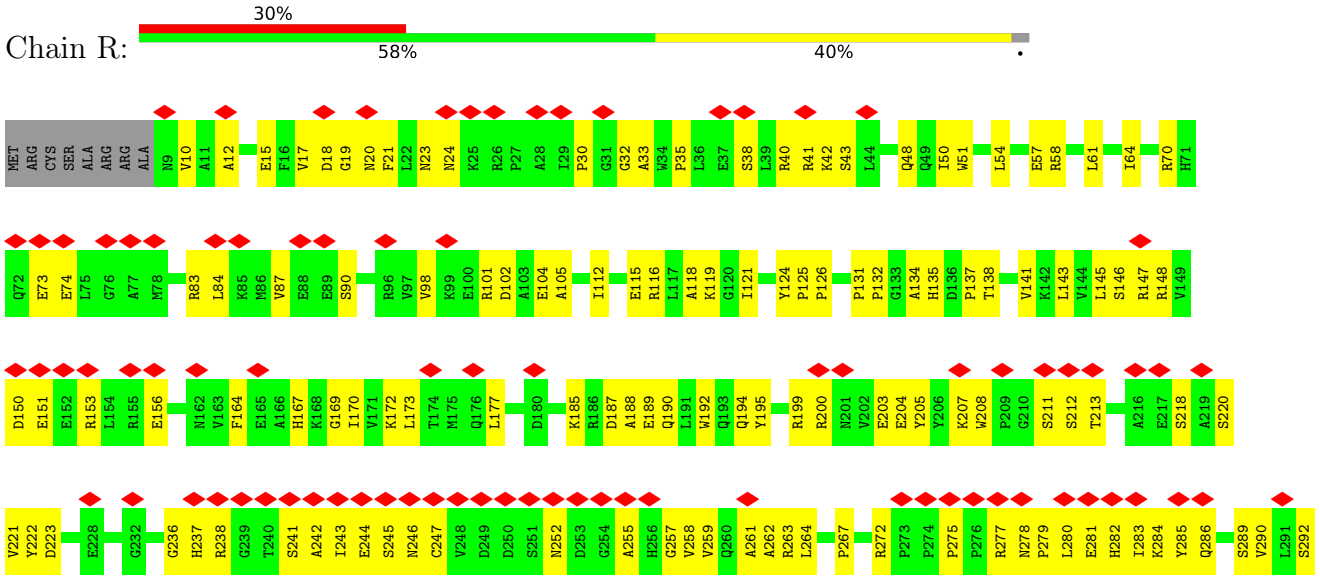
• Molecule 17: bL28m

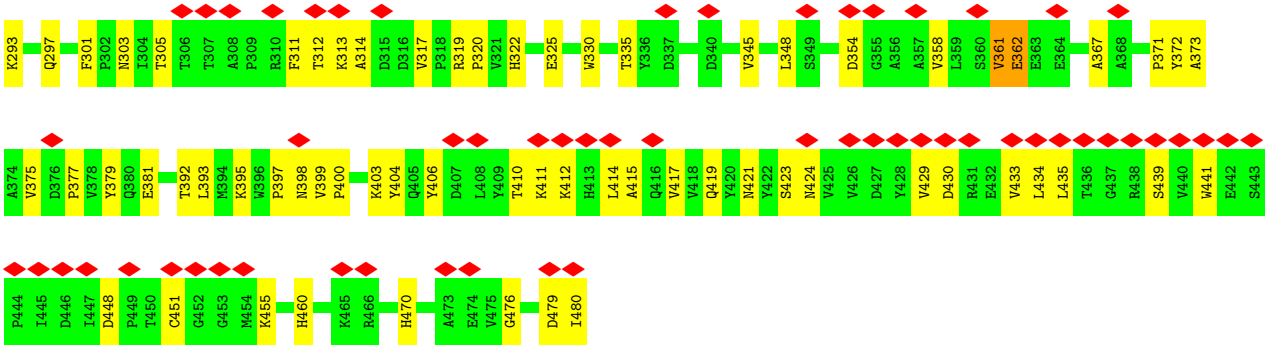
Chain Q:



• Molecule 18: uL29m

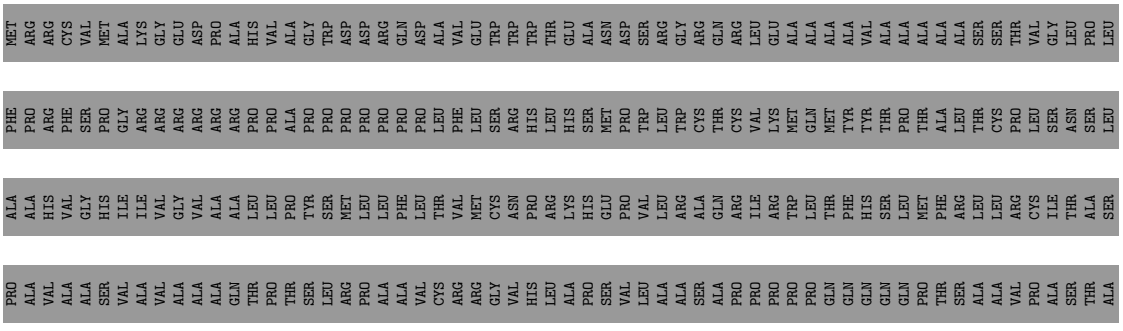
Chain R:

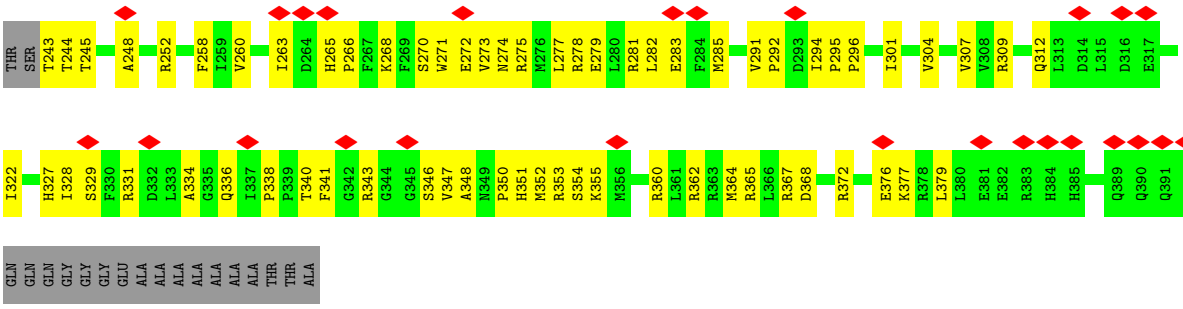




• Molecule 19: uL30m

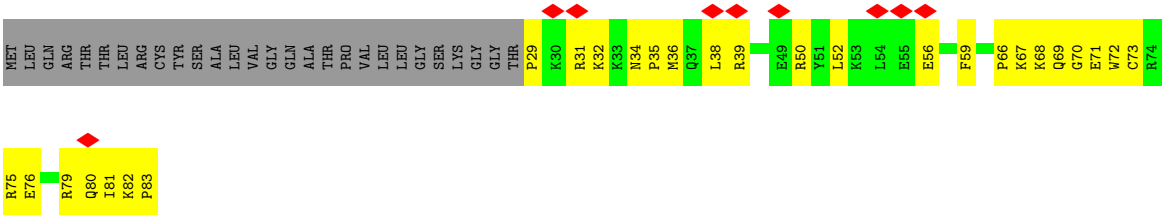






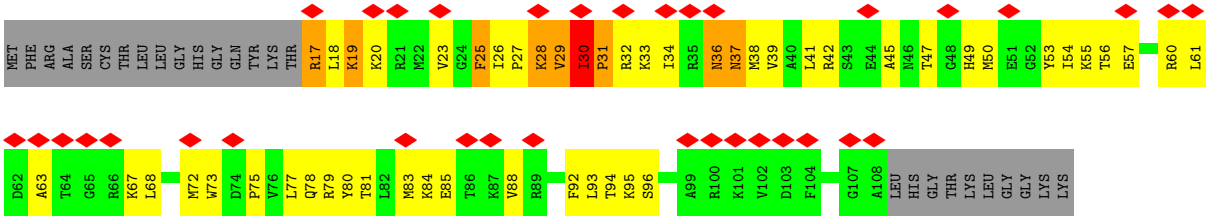
• Molecule 20: bL32m





• Molecule 21: bL33m





• Molecule 22: bL35m

Chain V:



• Molecule 23: bL36m

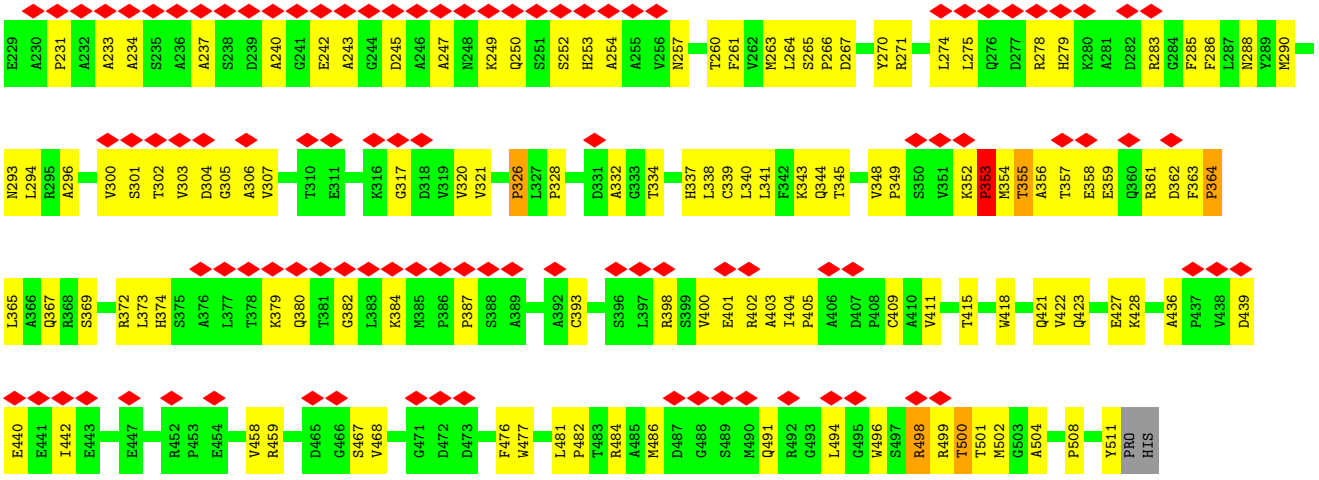
Chain W:



• Molecule 24: mL38

Chain X:

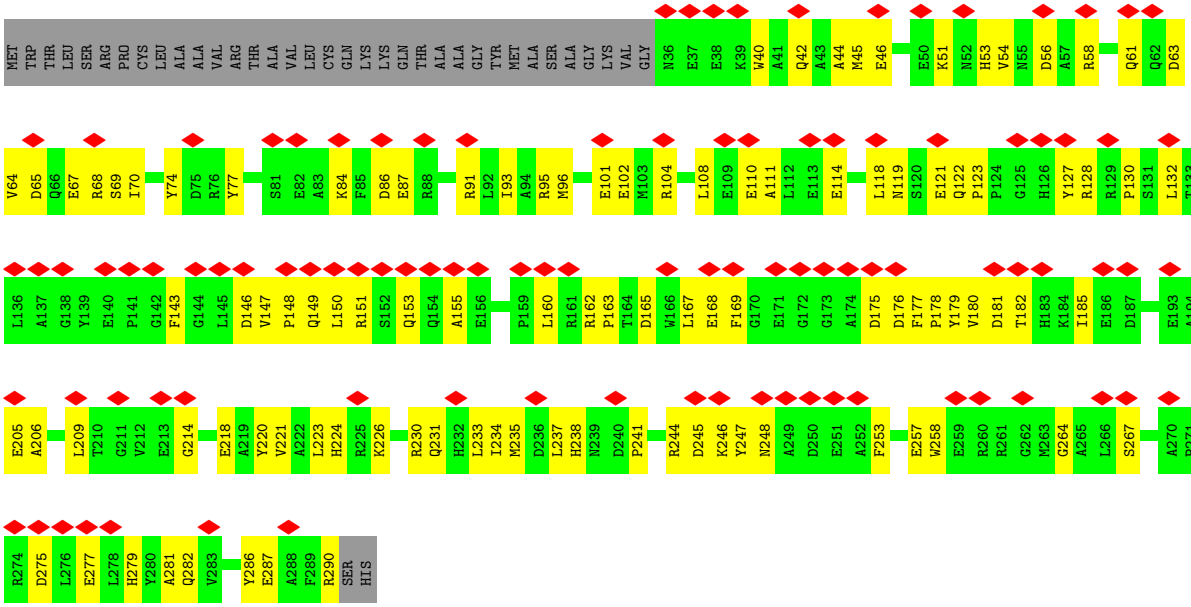




• Molecule 25: mL40

Chain Y:

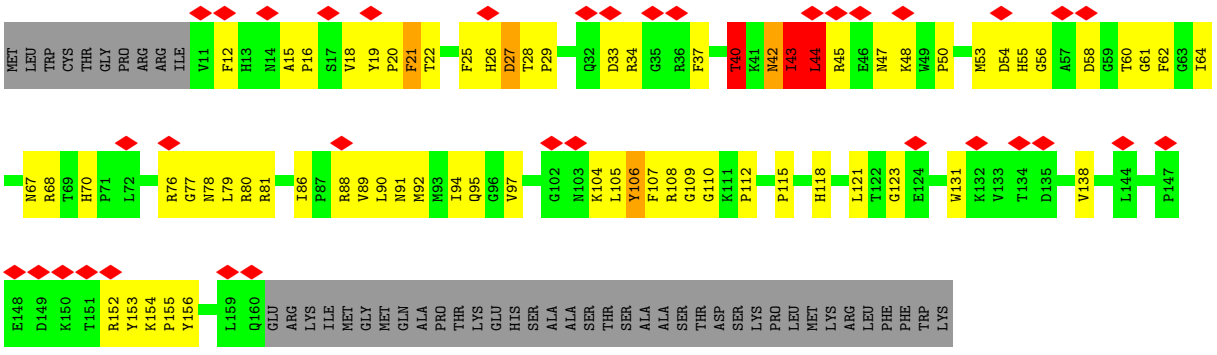




• Molecule 26: mL41

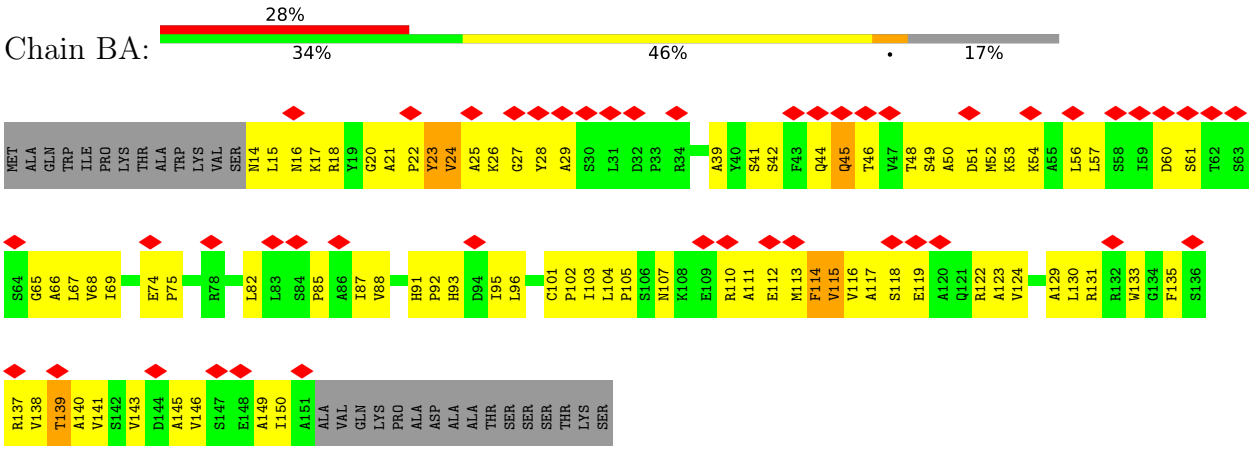
Chain Z:





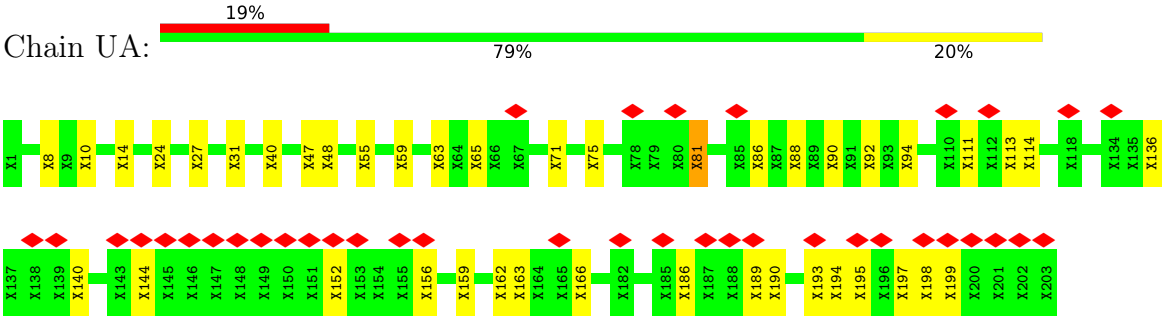
- Molecule 27: mL94

Chain BA:



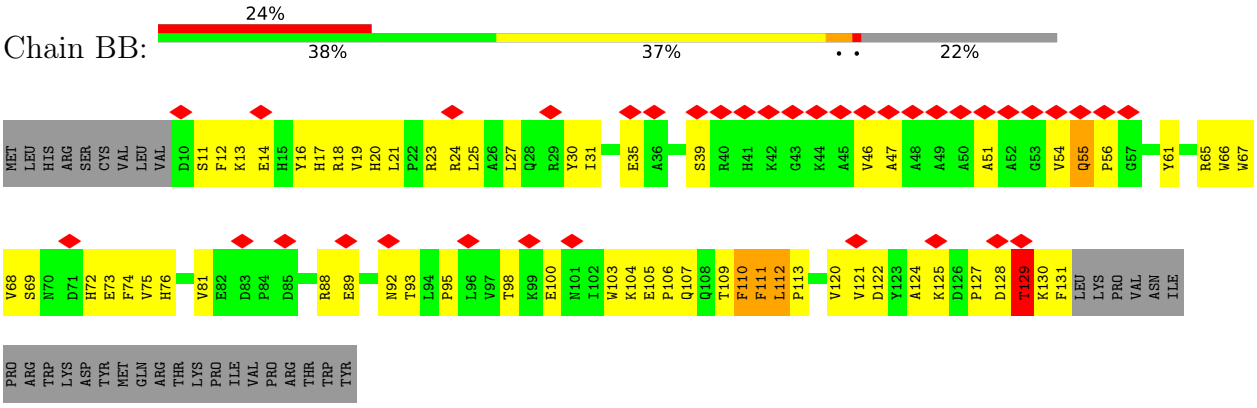
- Molecule 28: UA

Chain UA:



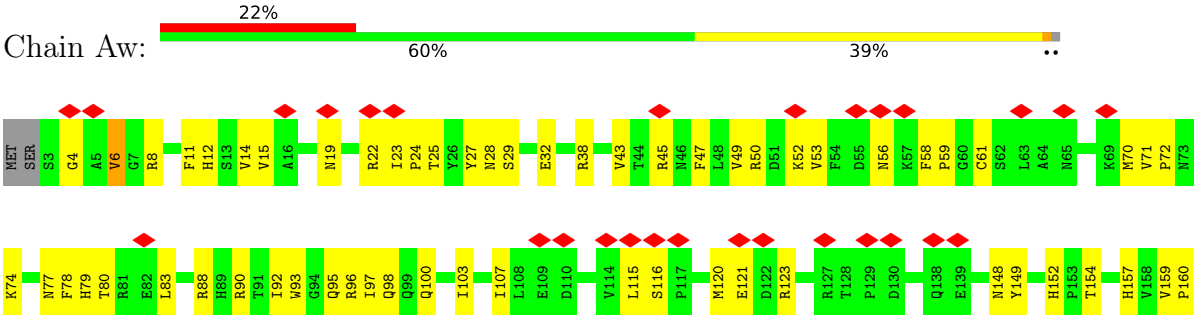
- Molecule 29: mL95

Chain BB:



- Molecule 30: mL89

Chain Aw:

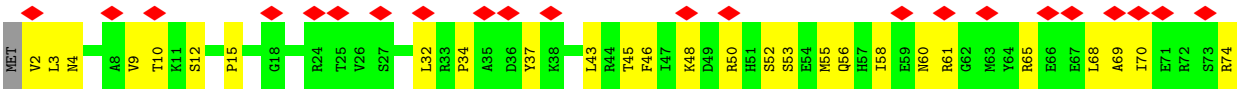


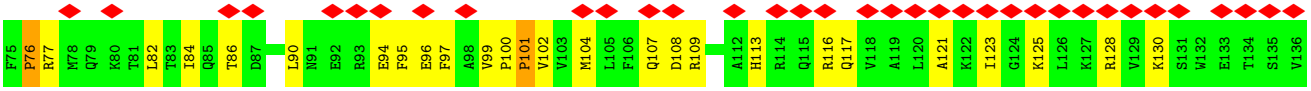


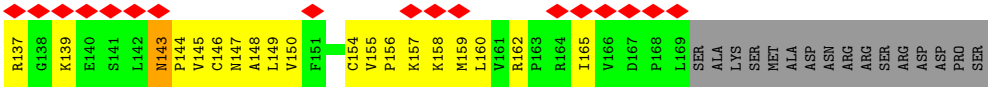
• Molecule 31: bL31m

Chain Bj:





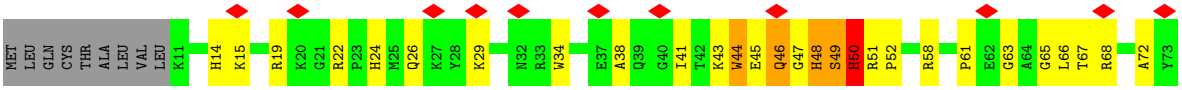


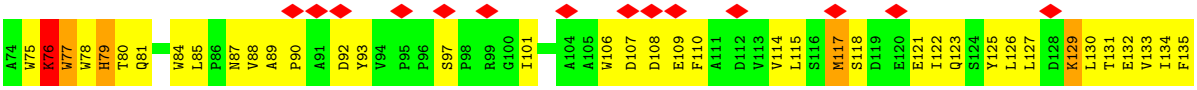


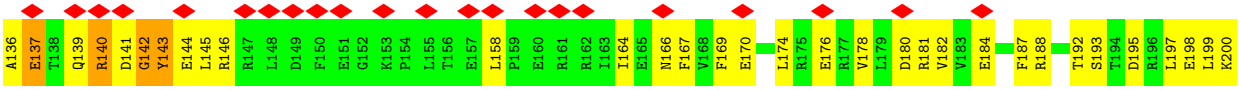
• Molecule 32: mL76

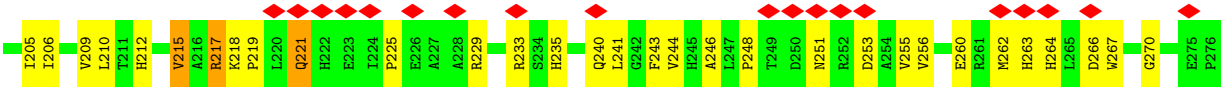
Chain An:

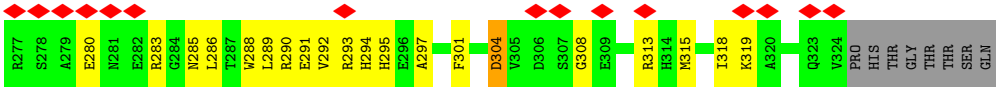








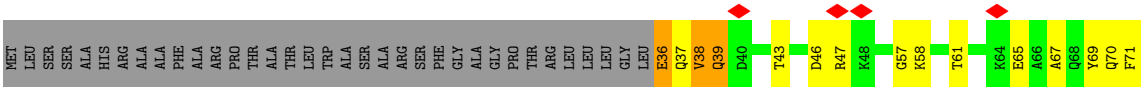


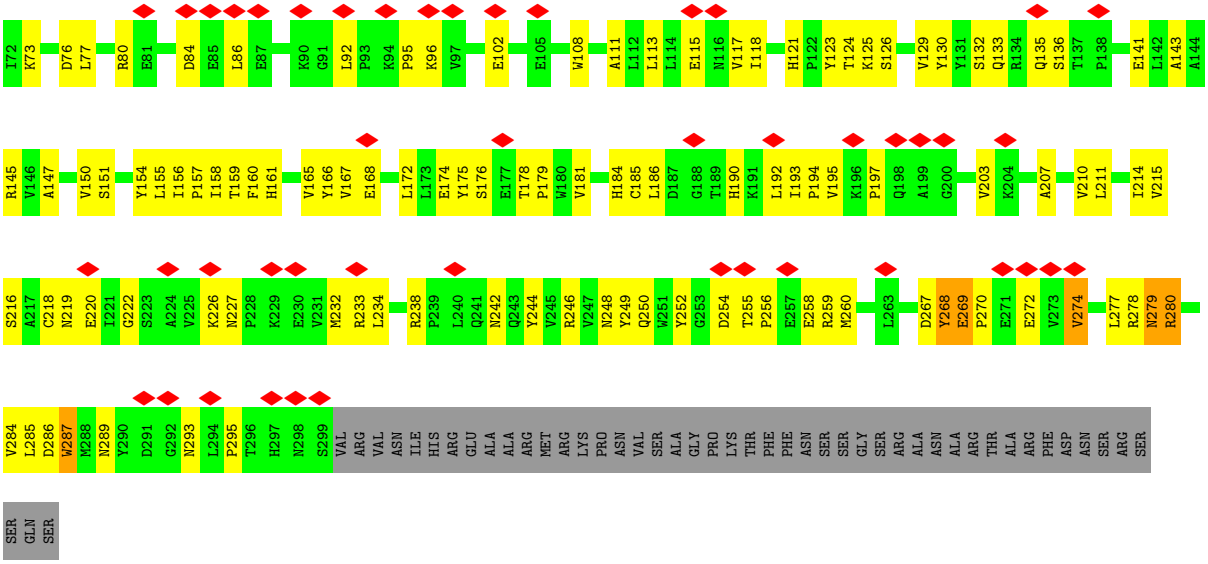


• Molecule 33: mL74

Chain Al:



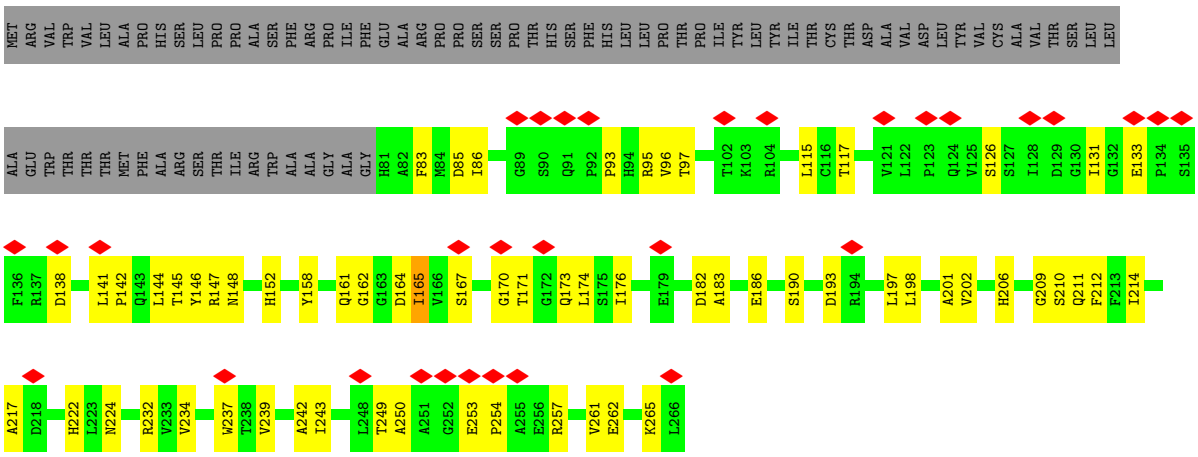




• Molecule 34: Peptidyl-prolyl cis-trans isomerase

Chain BI:

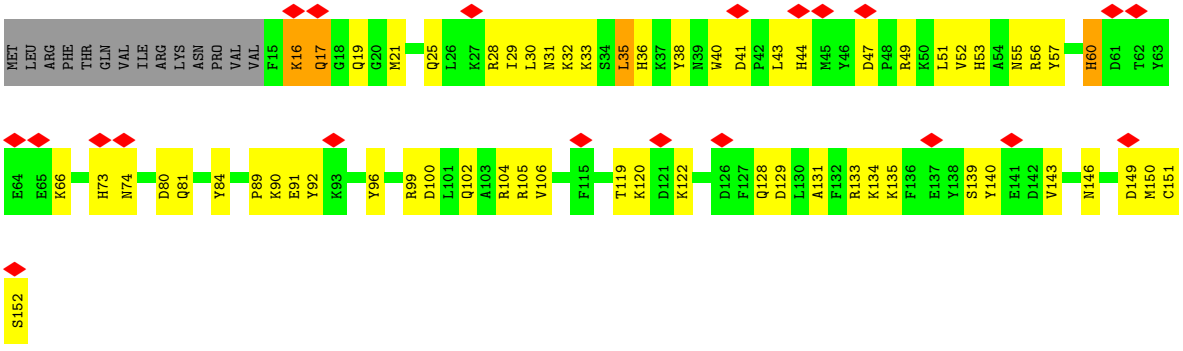




• Molecule 35: mL93

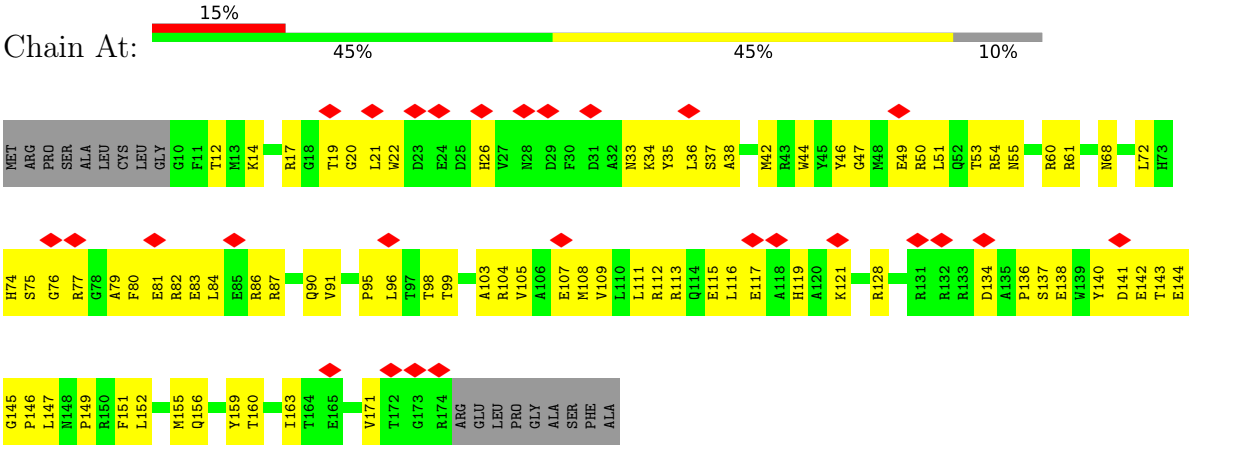
Chain Az:





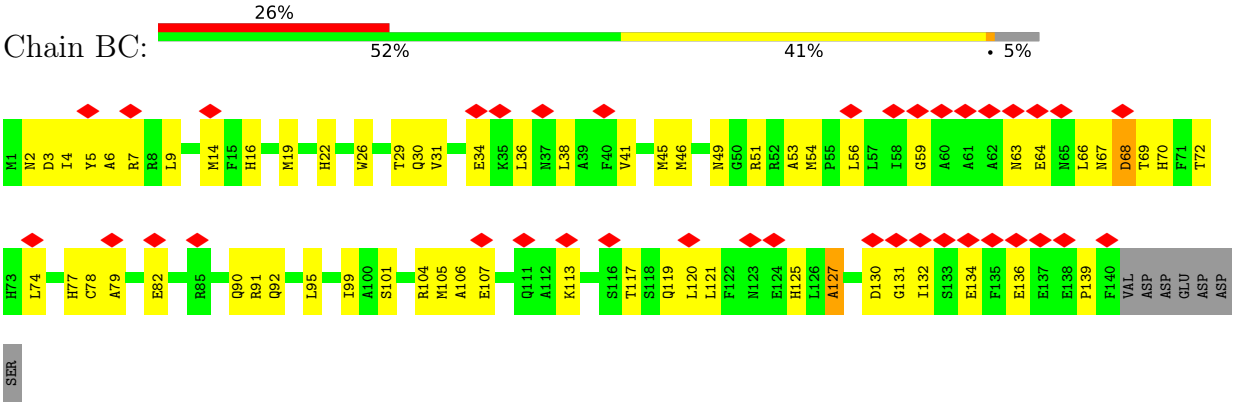
• Molecule 36: mL86

Chain At:



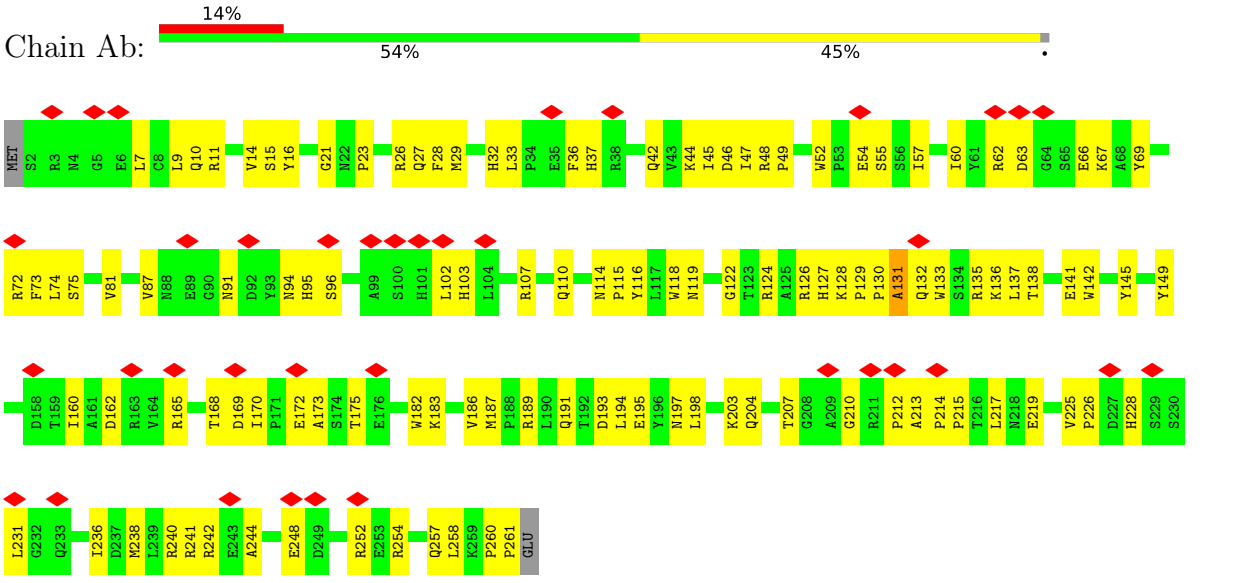
• Molecule 37: mL96

Chain BC:



• Molecule 38: L51_S25_CI-B8 domain-containing protein

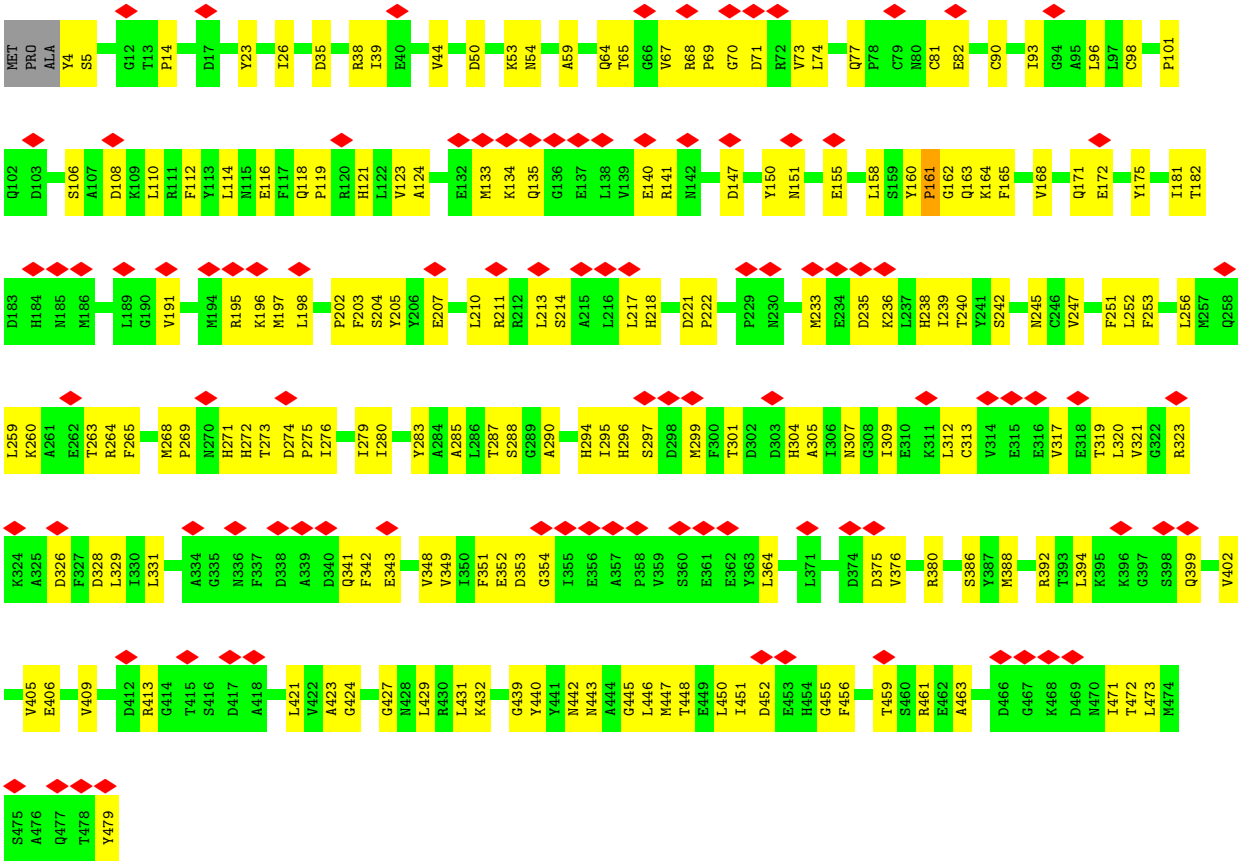
Chain Ab:



• Molecule 39: mL69

Chain Ai:

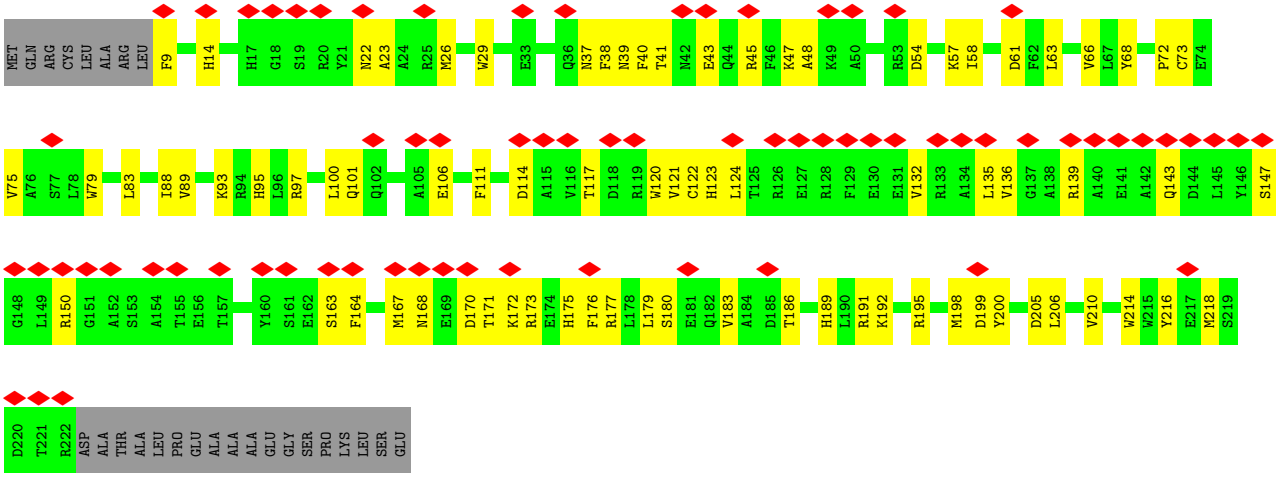




• Molecule 40: mL80

Chain Ap:

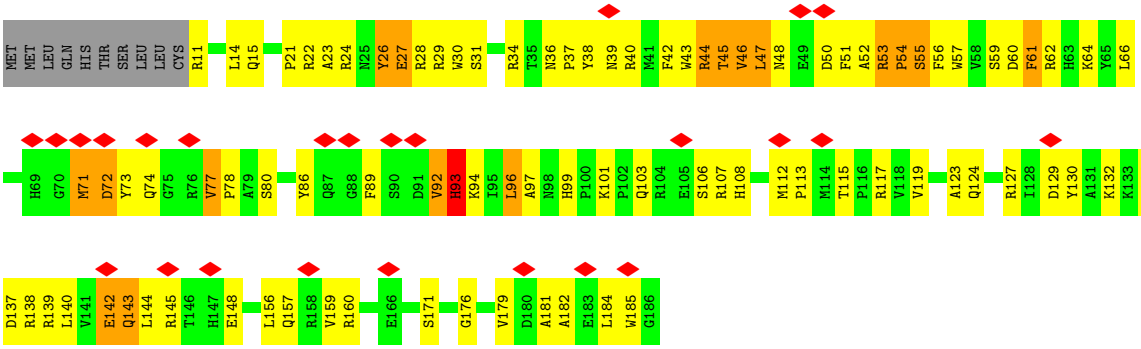




• Molecule 41: mL87

Chain Au:

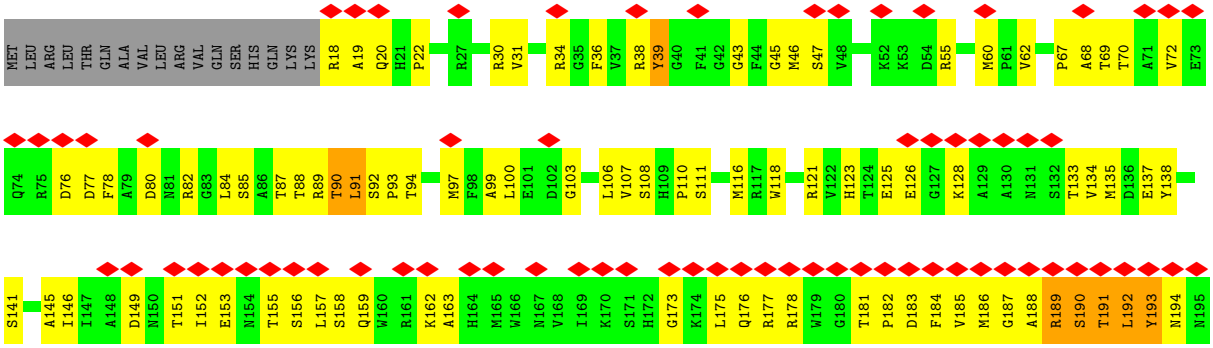




• Molecule 42: mL42

Chain Aa:

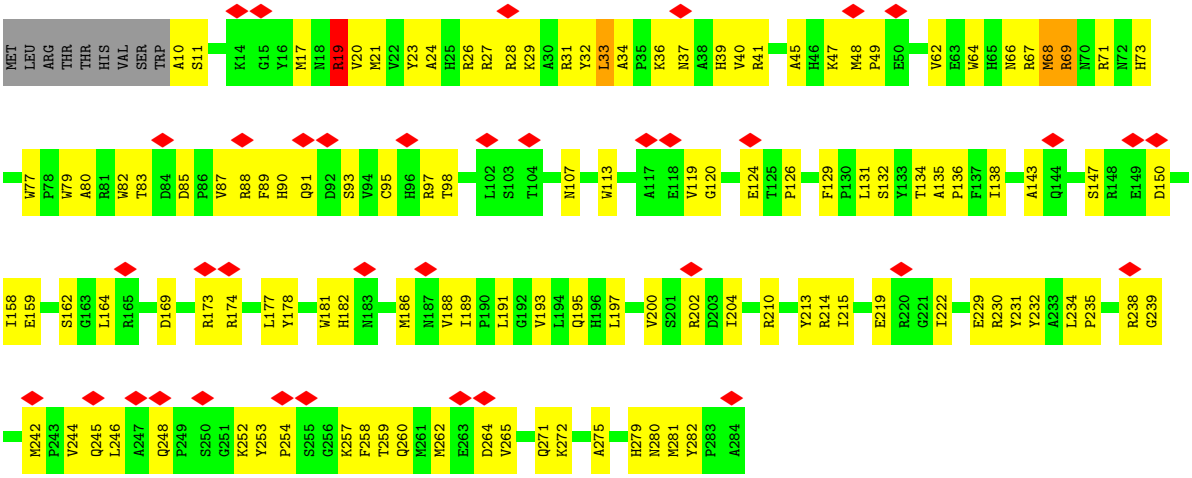




• Molecule 43: mL79

Chain Ao:



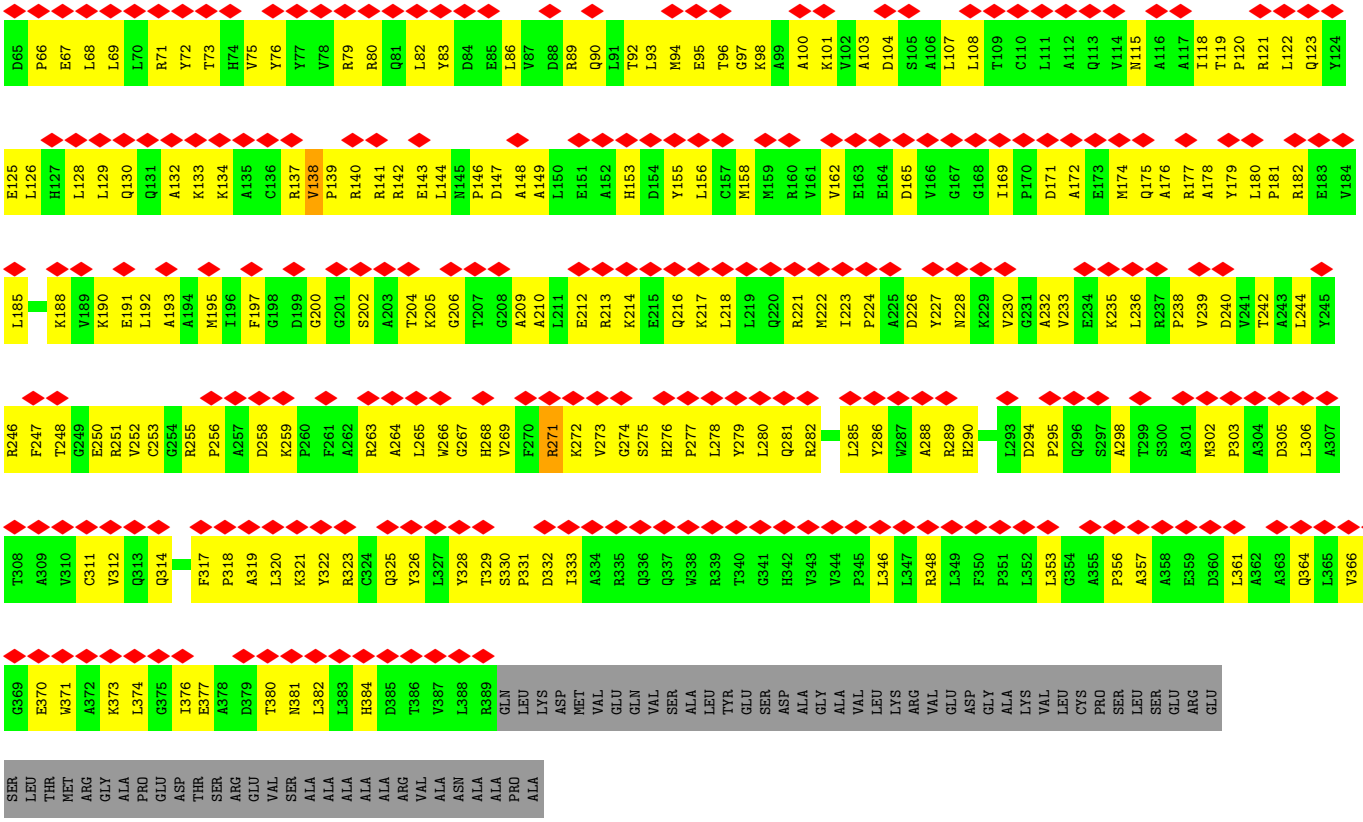


• Molecule 44: mL70

Chain BM:



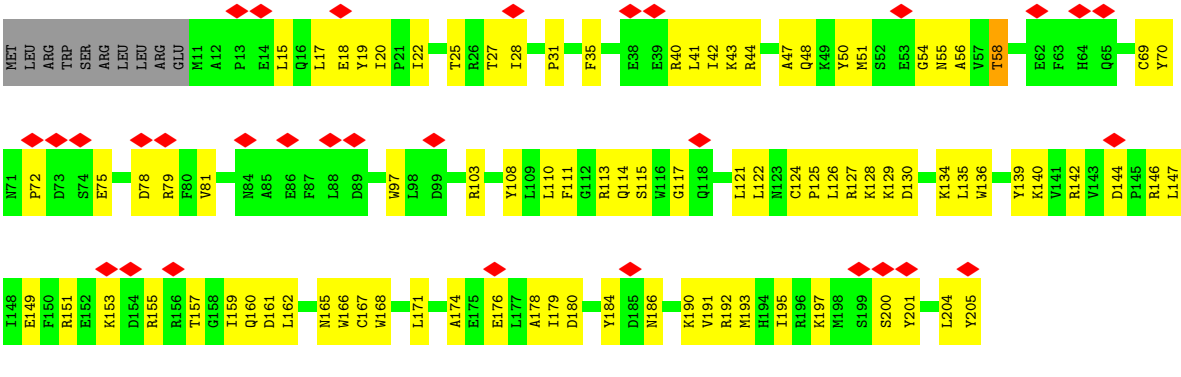




- Molecule 45: mL84

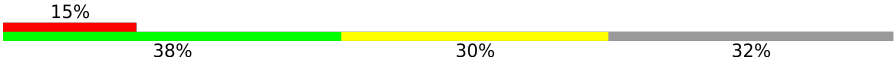
Chain Ar:

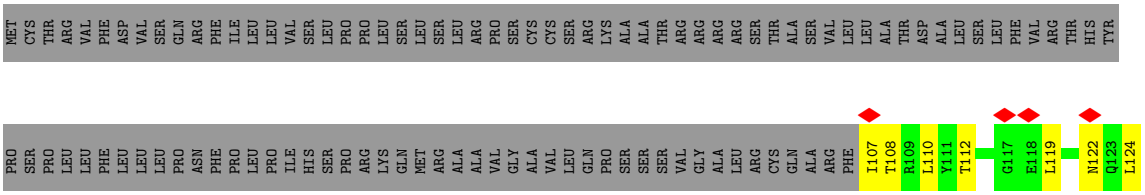


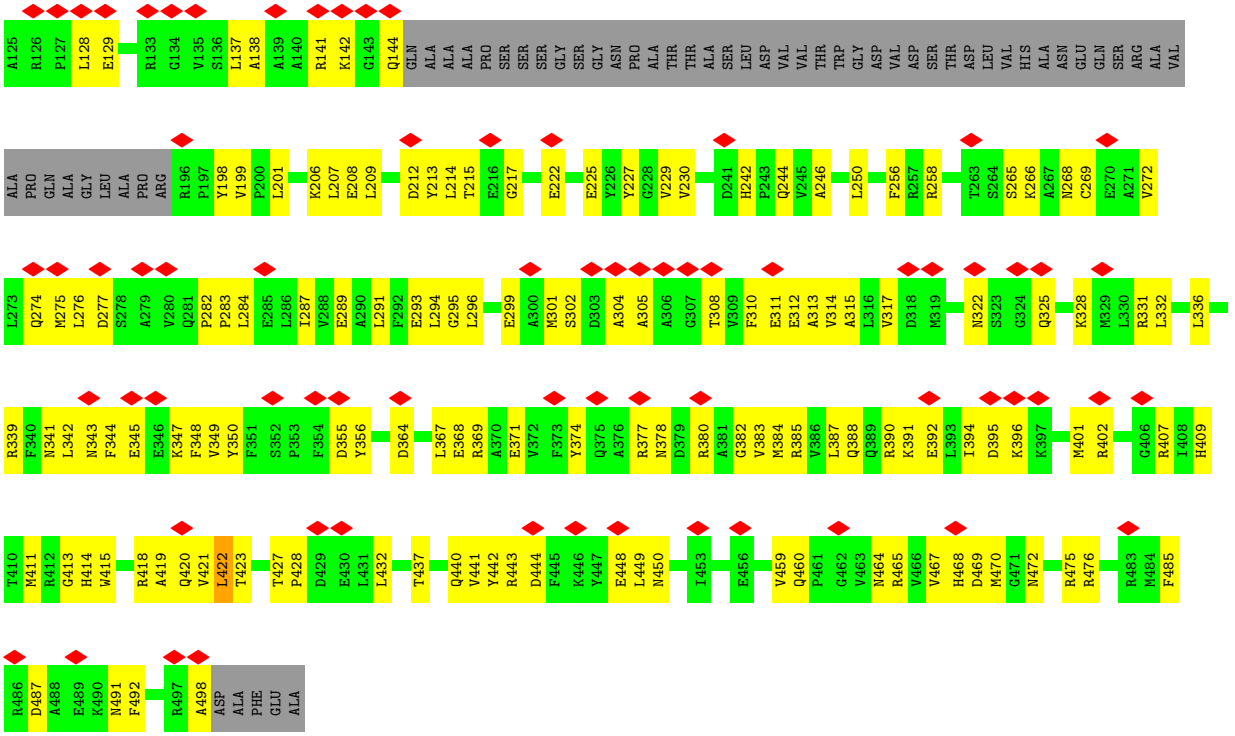


- Molecule 46: mL72

Chain Aj:



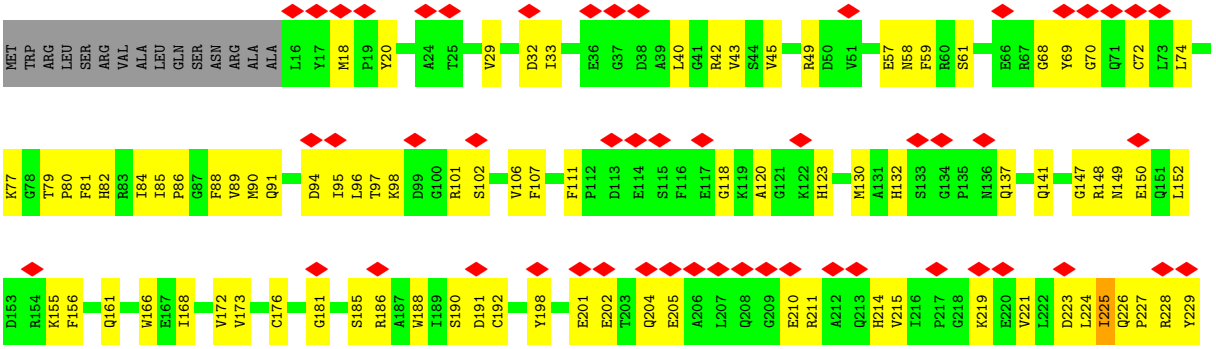




• Molecule 47: Peptidyl-prolyl cis-trans isomerase

Chain BH:

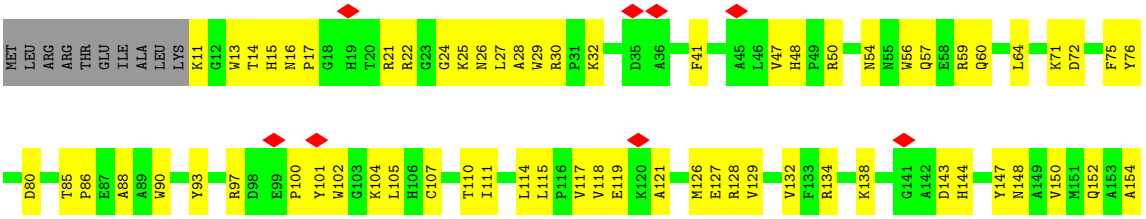


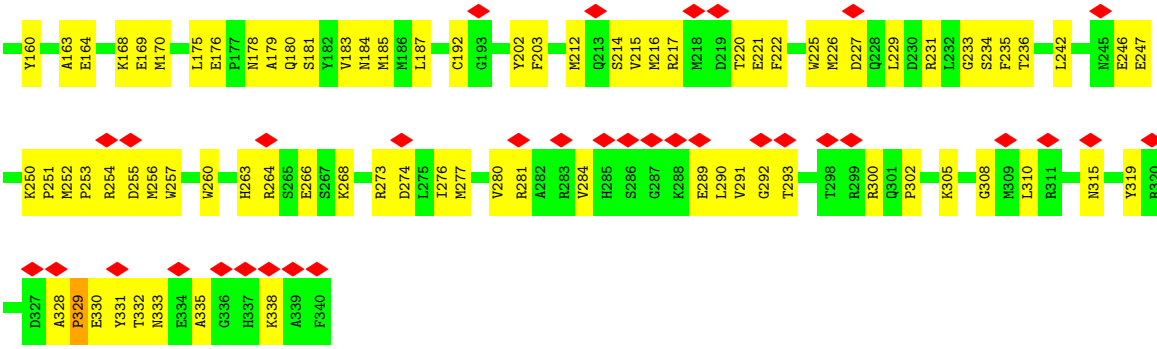


• Molecule 48: mL75

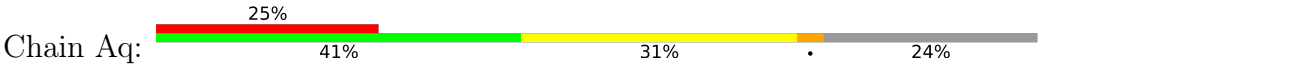
Chain Am:

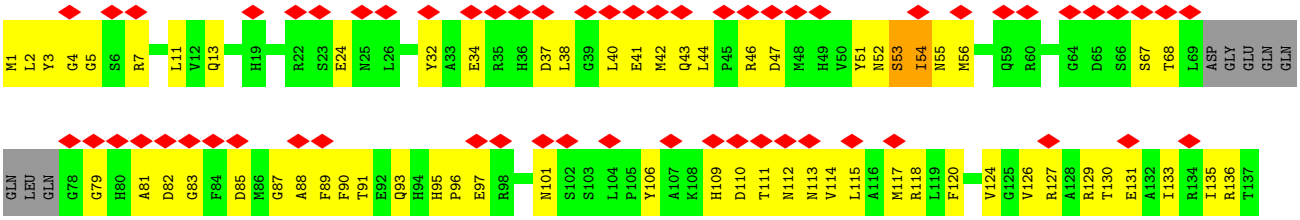






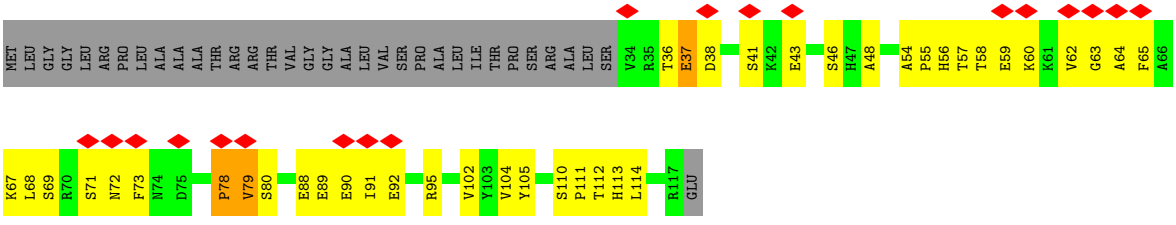
• Molecule 49: mL82





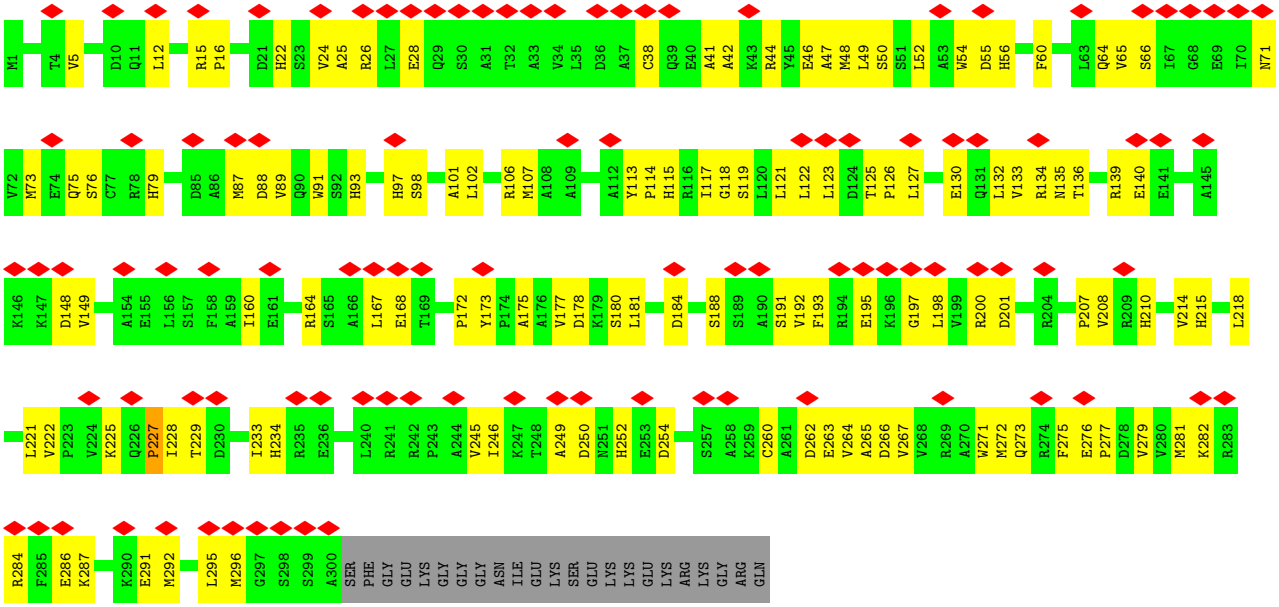
• Molecule 50: mL98





• Molecule 51: mL73

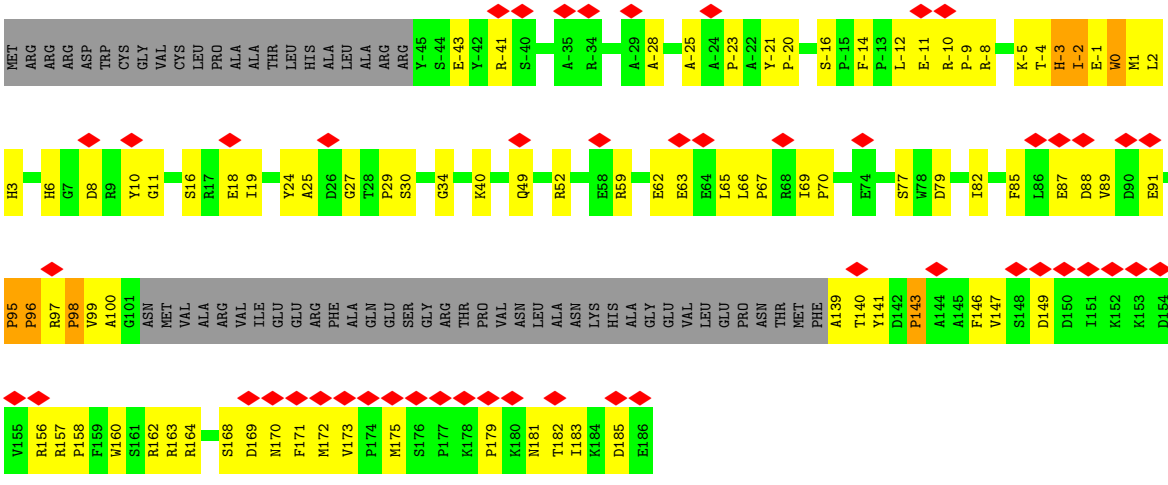




• Molecule 52: mL52,mL52

Chain BP:

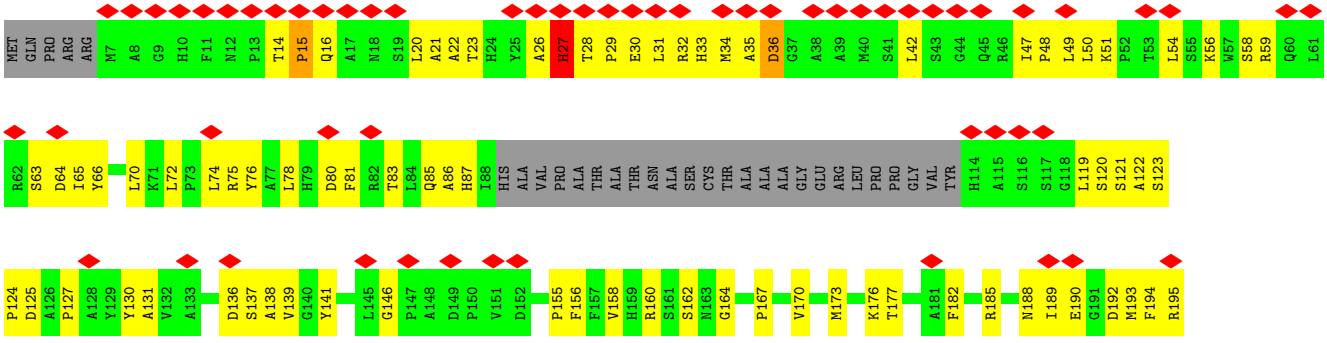


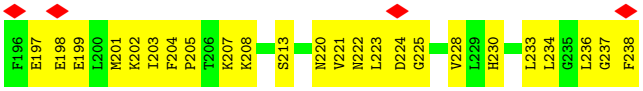


• Molecule 53: mL49

Chain Ad:



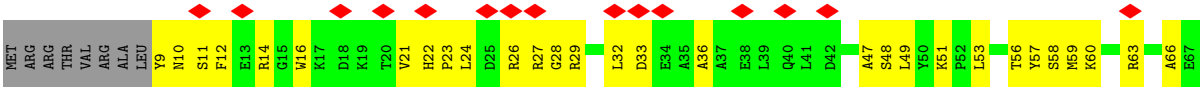


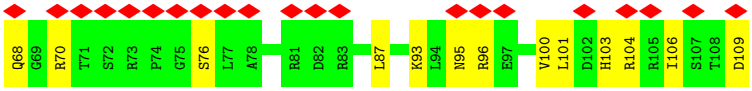


• Molecule 54: mL99

Chain BF:



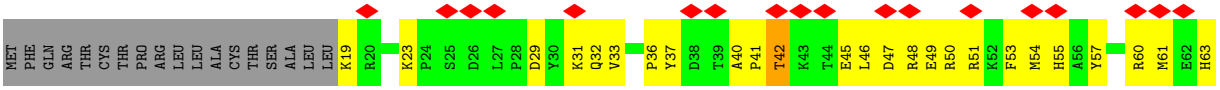


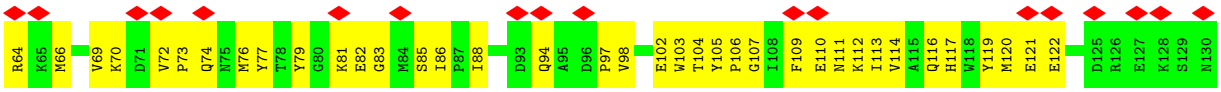


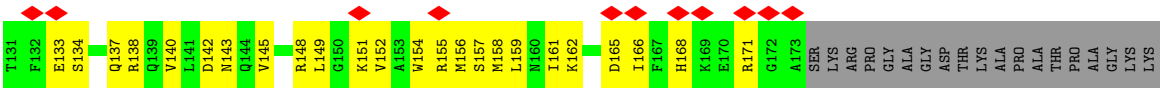
• Molecule 55: mL88

Chain Av:





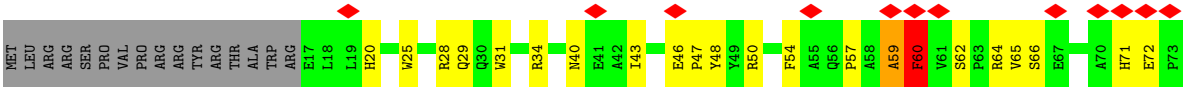


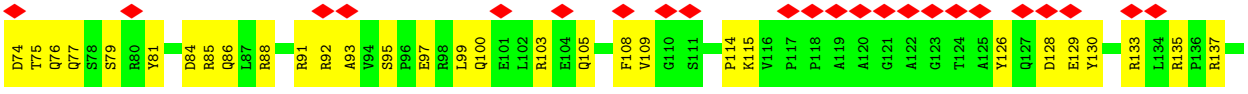


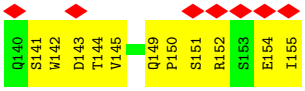
• Molecule 56: mL63

Chain Af:





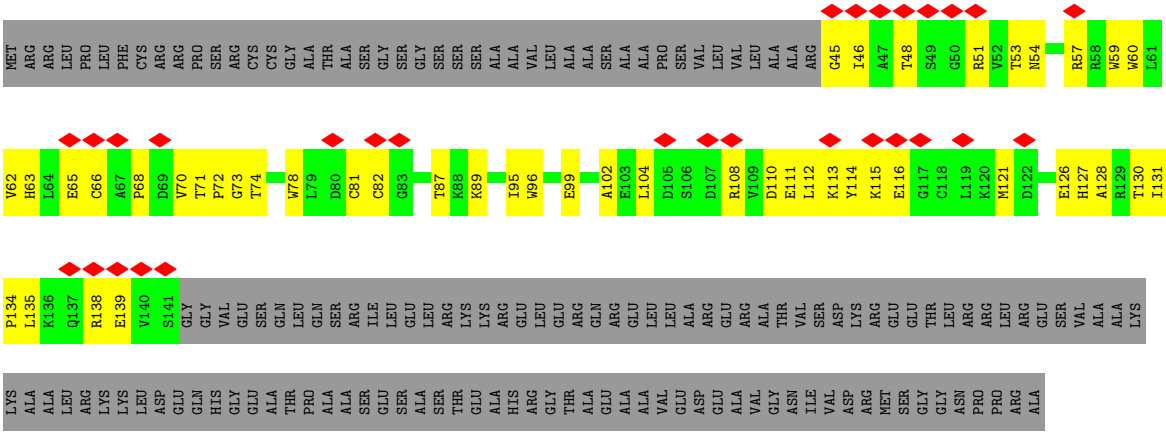




• Molecule 57: mL85

Chain As:

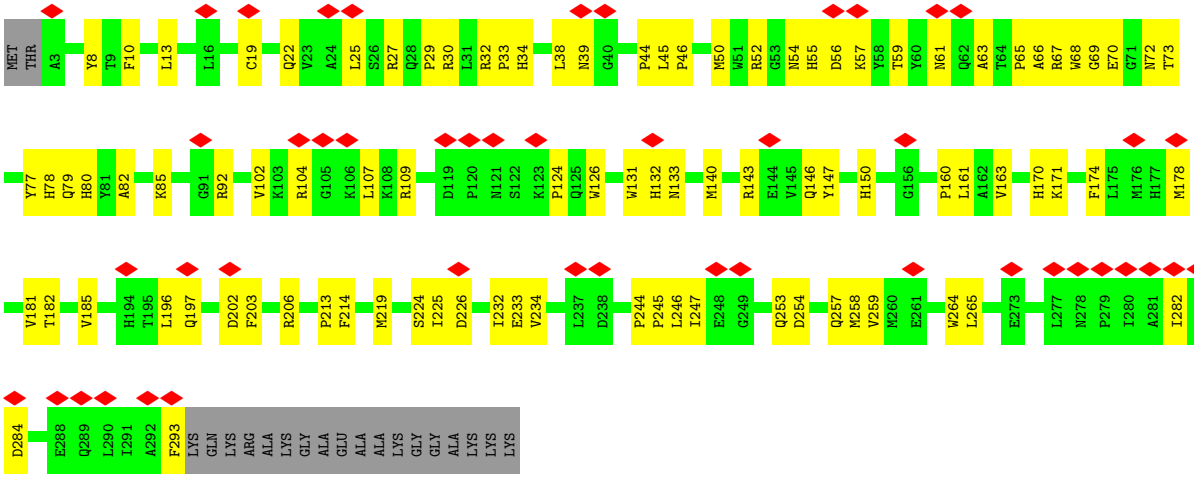




• Molecule 58: mL53

Chain Ae:

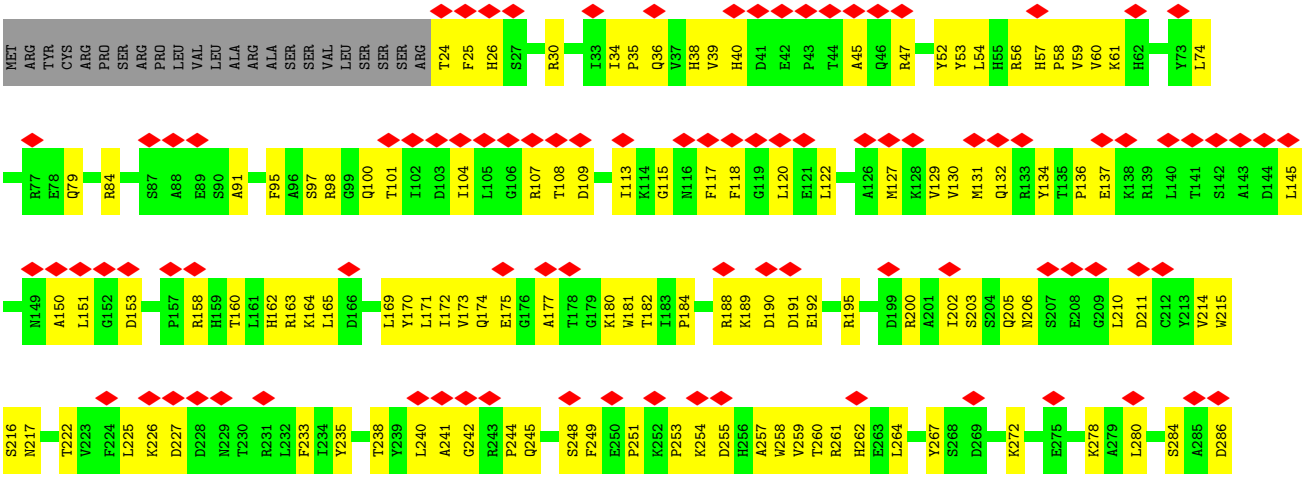


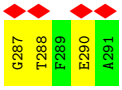


• Molecule 59: MRP-L46 domain-containing protein

Chain Ac:



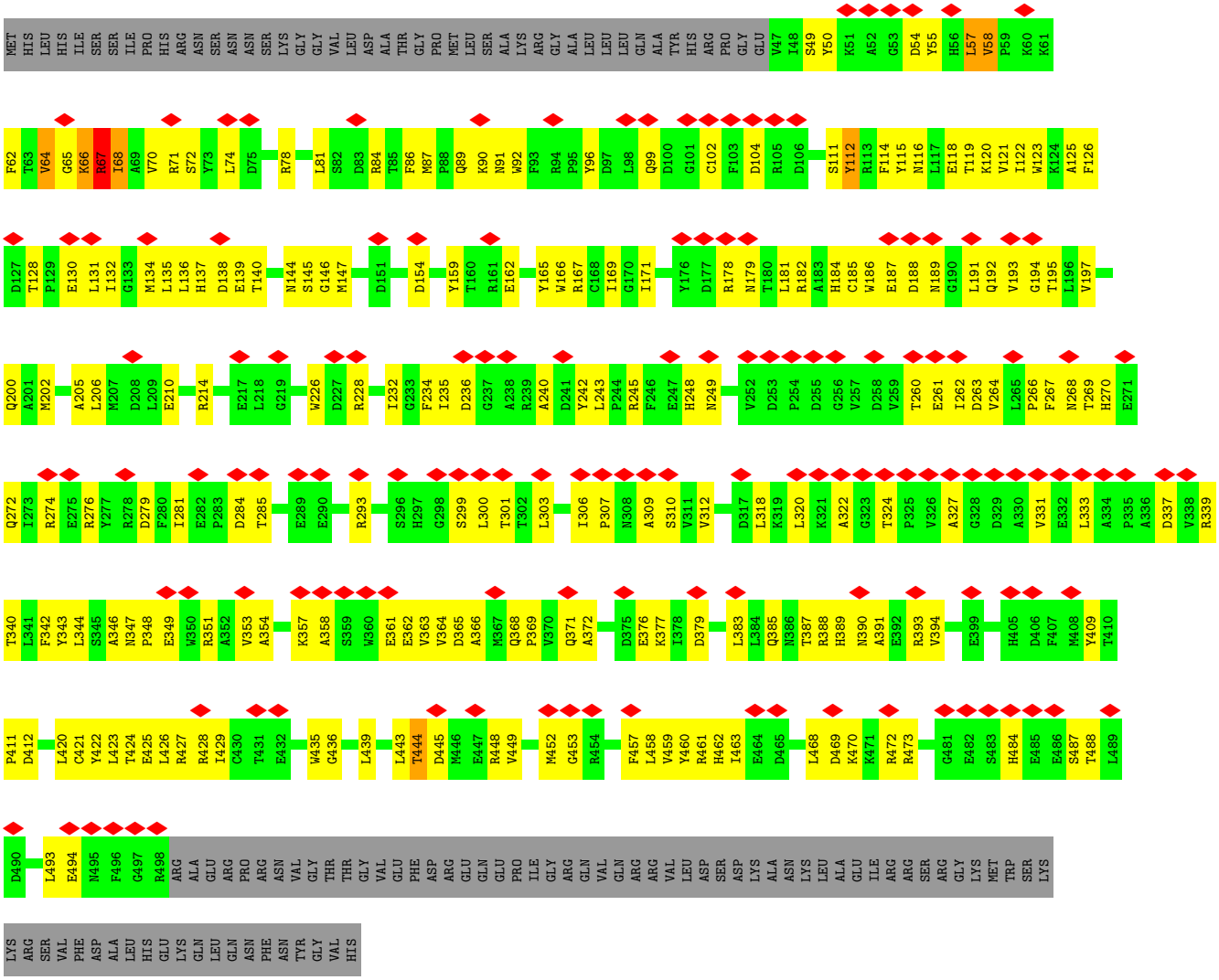




• Molecule 60: mL68

Chain Ah:

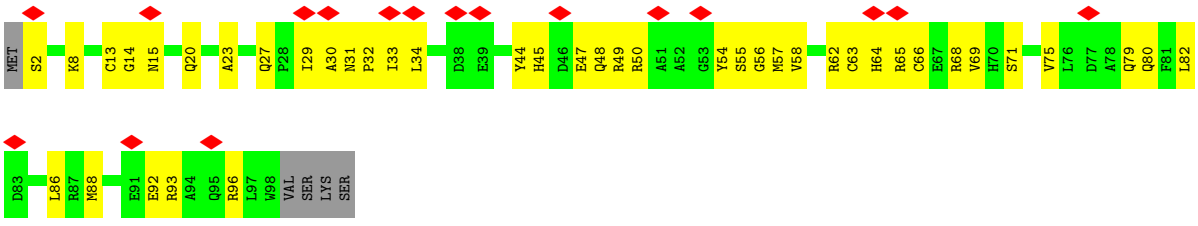




• Molecule 61: mL97

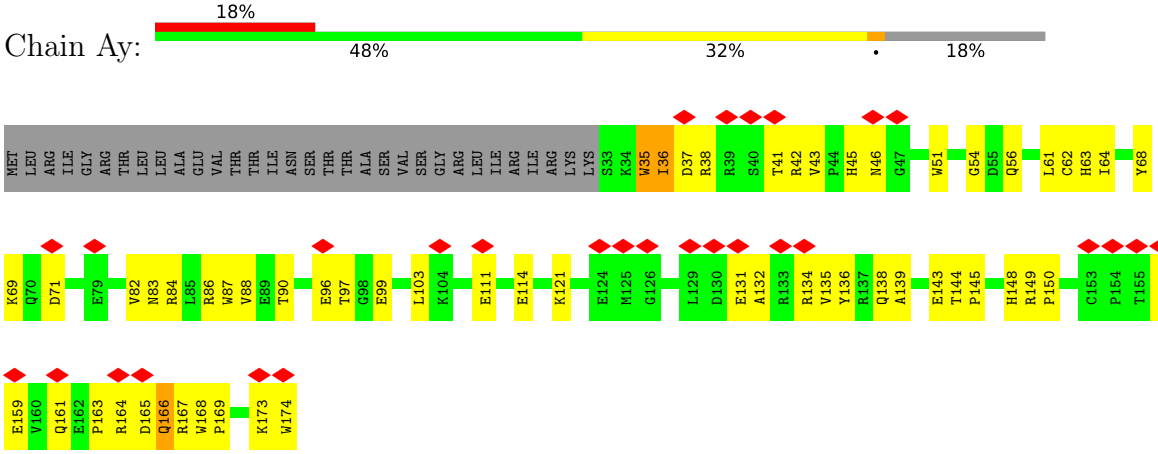
Chain BD:





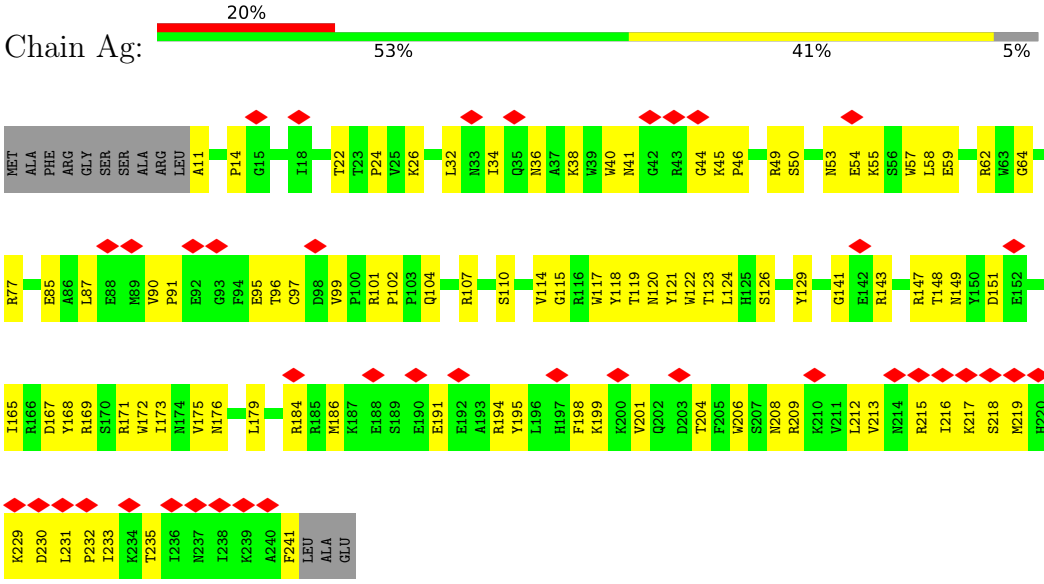
• Molecule 62: C2H2-type domain-containing protein

Chain Ay:



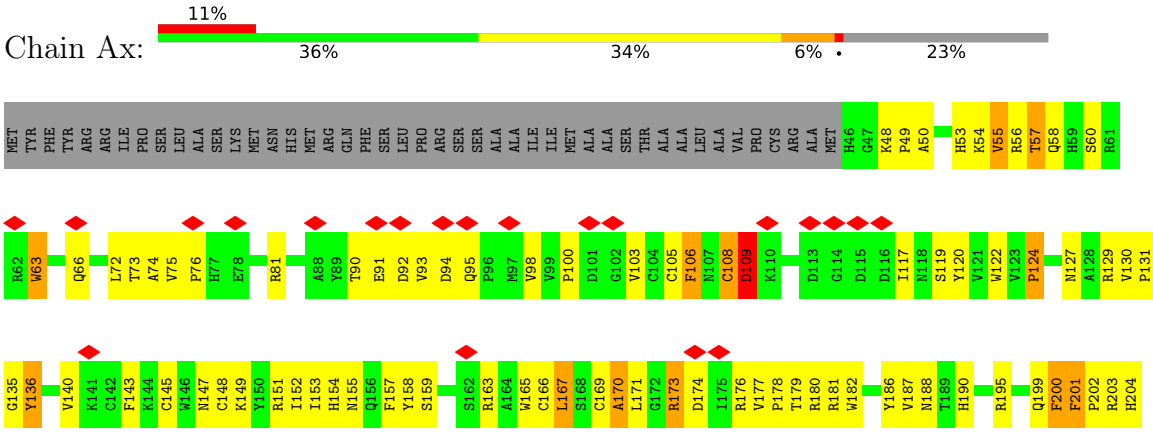
• Molecule 63: mL54/69

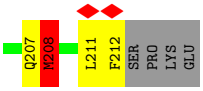
Chain Ag:



• Molecule 64: LIM zinc-binding domain-containing protein

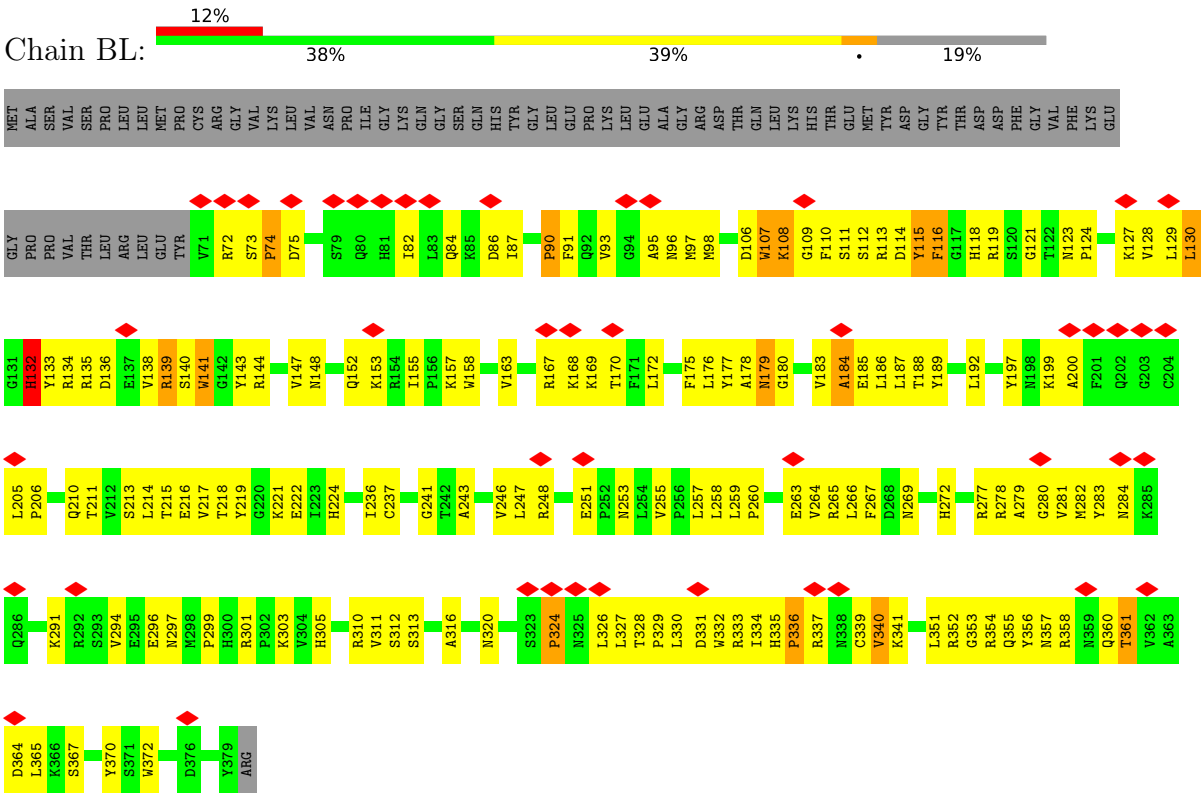
Chain Ax:





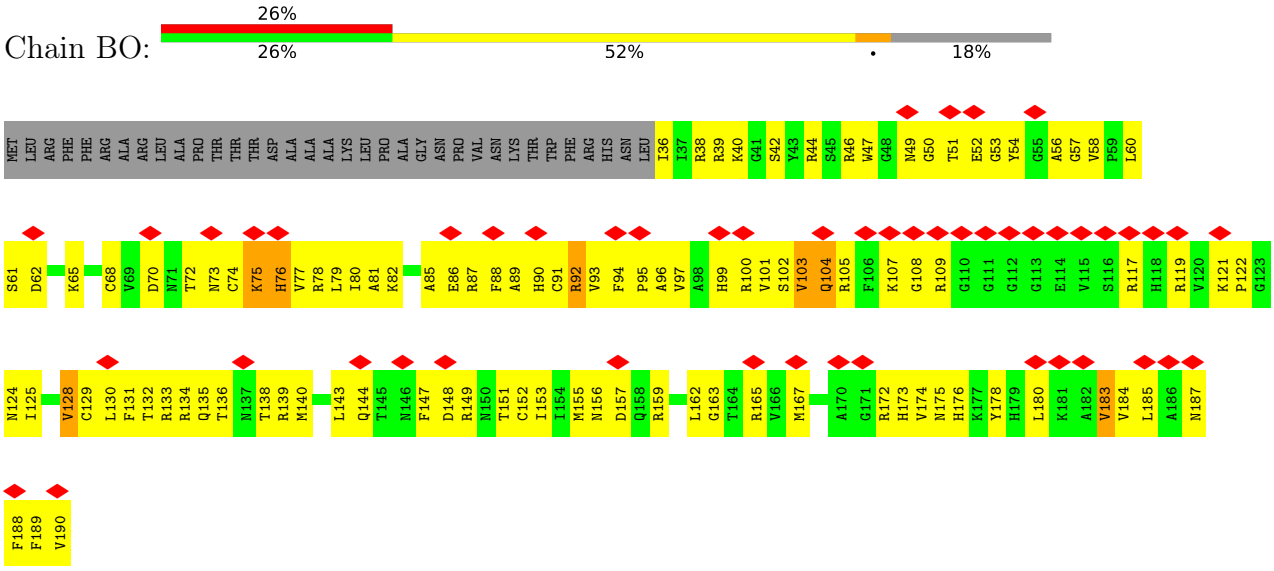
• Molecule 65: Putative ribosomal protein L2

Chain BL:



• Molecule 66: Putative ribosomal protein L14

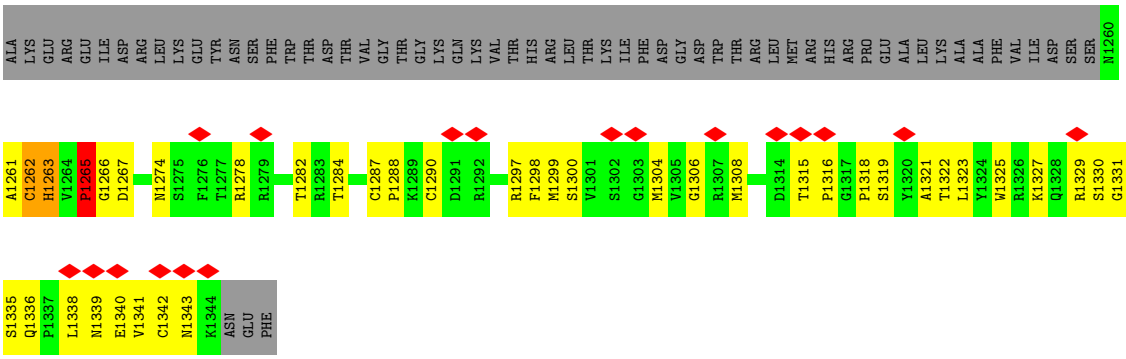
Chain BO:



• Molecule 67: mL100

Chain BG:

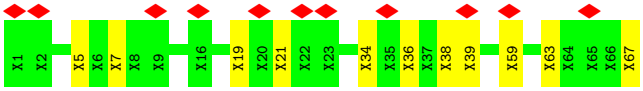




- Molecule 68: UB

Chain UB:

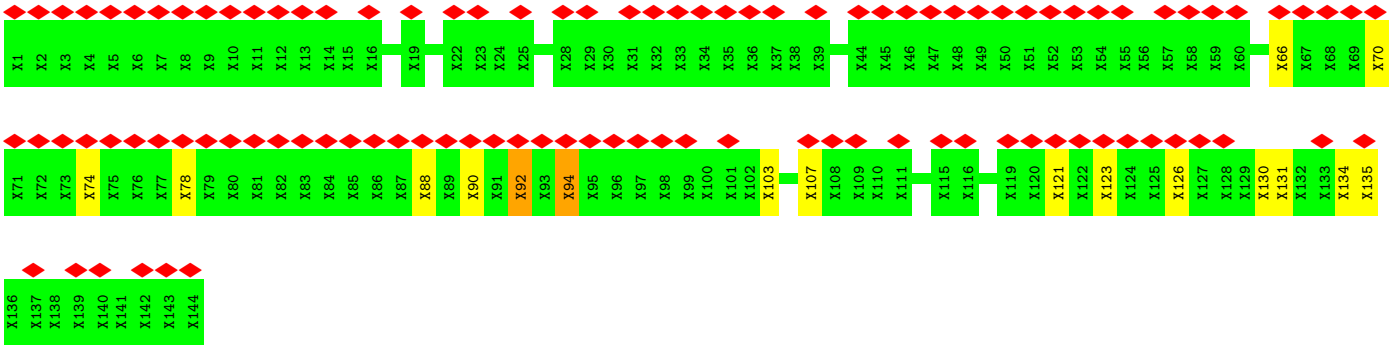




- Molecule 69: UC

Chain UC:

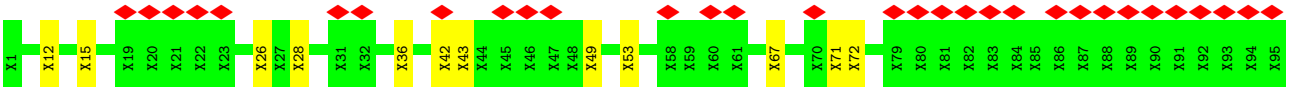




- Molecule 70: UD

Chain UD:

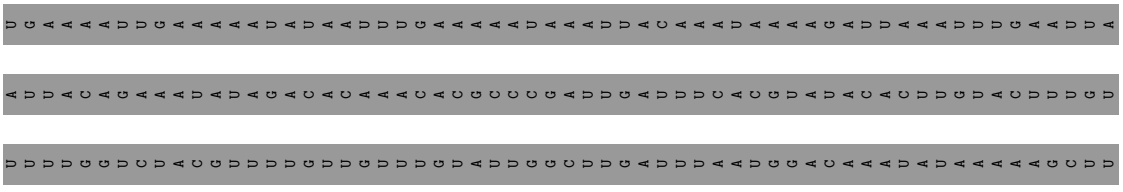


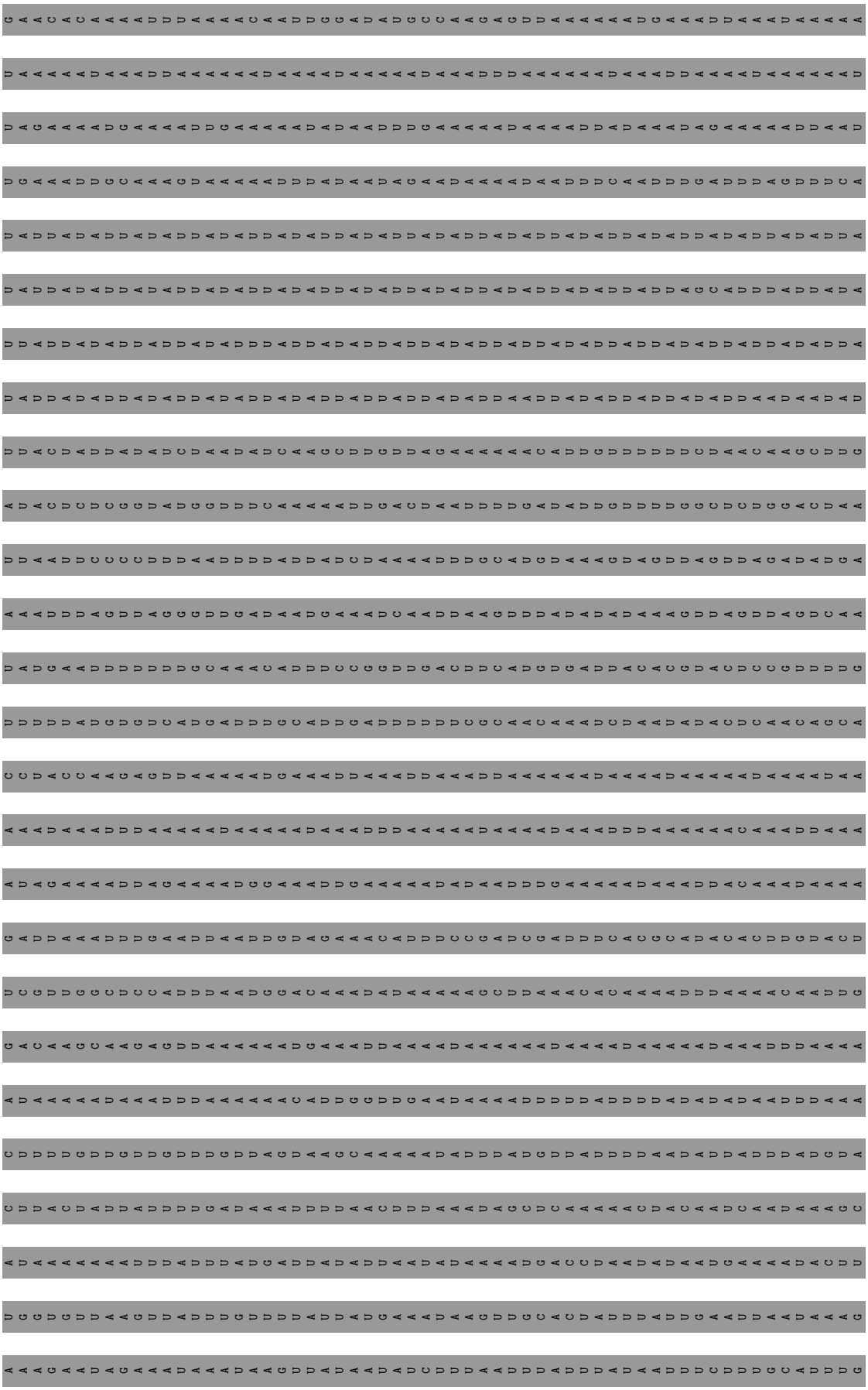


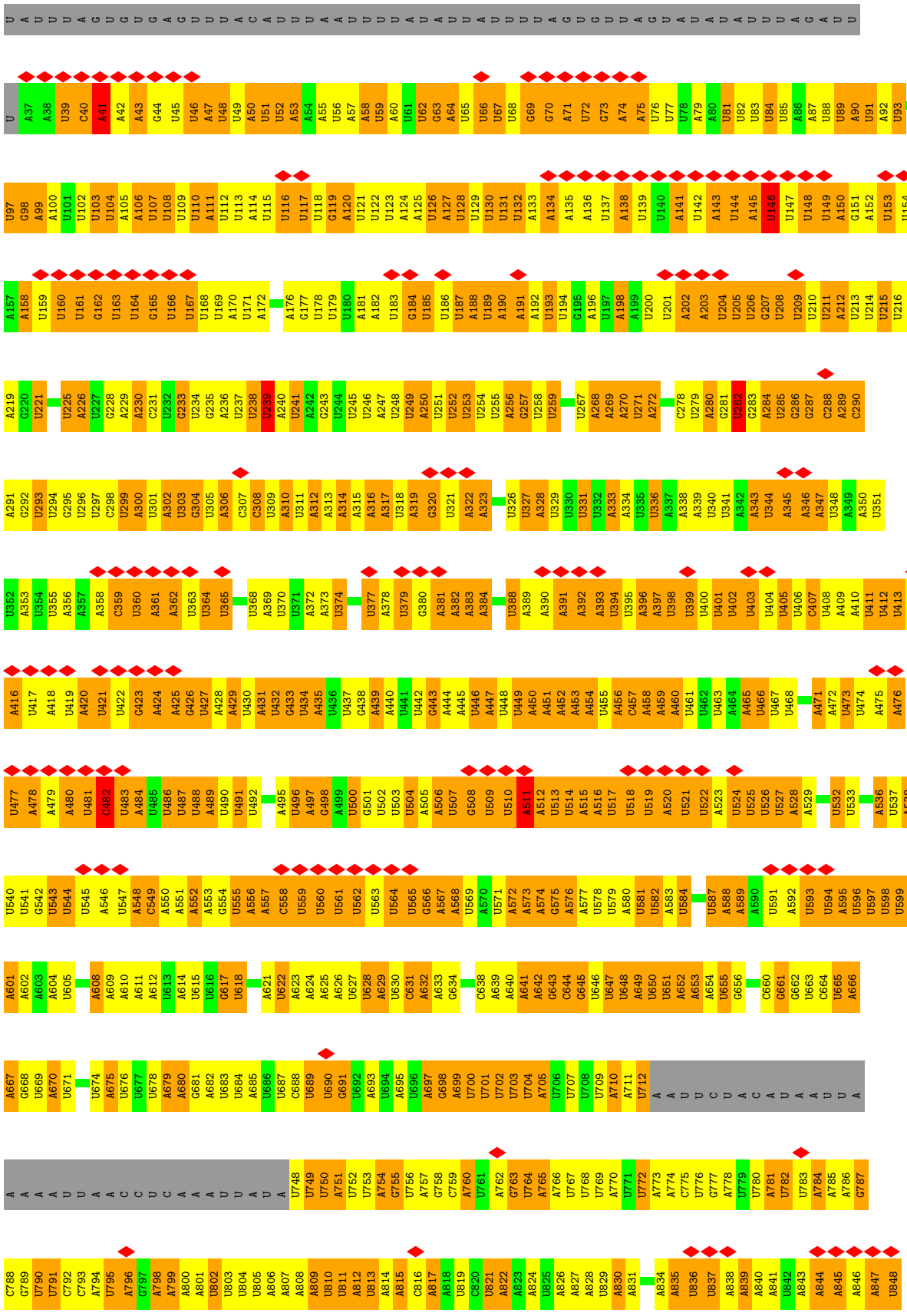
- Molecule 71: Ribosomal RNA

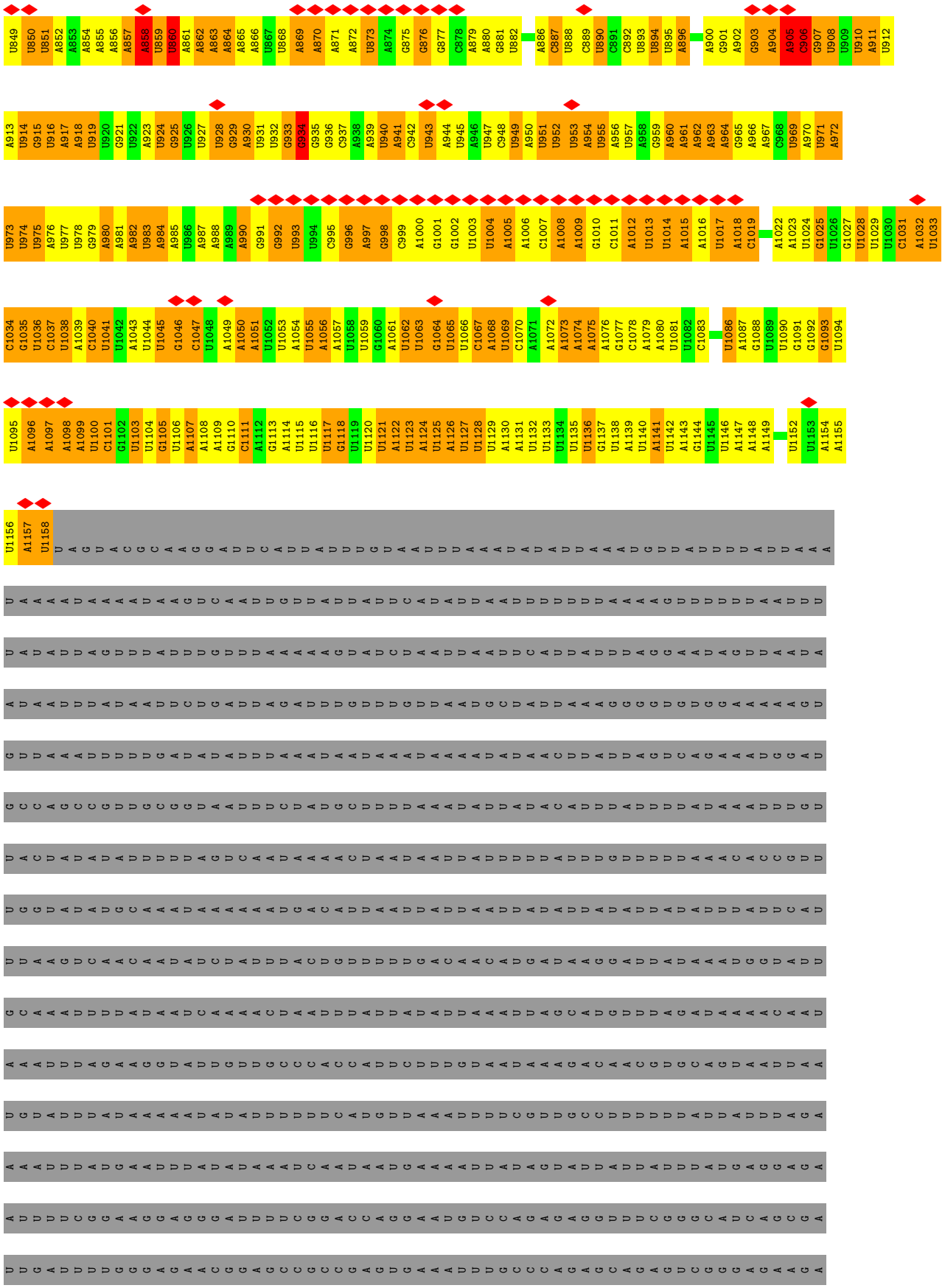
Chain 1:

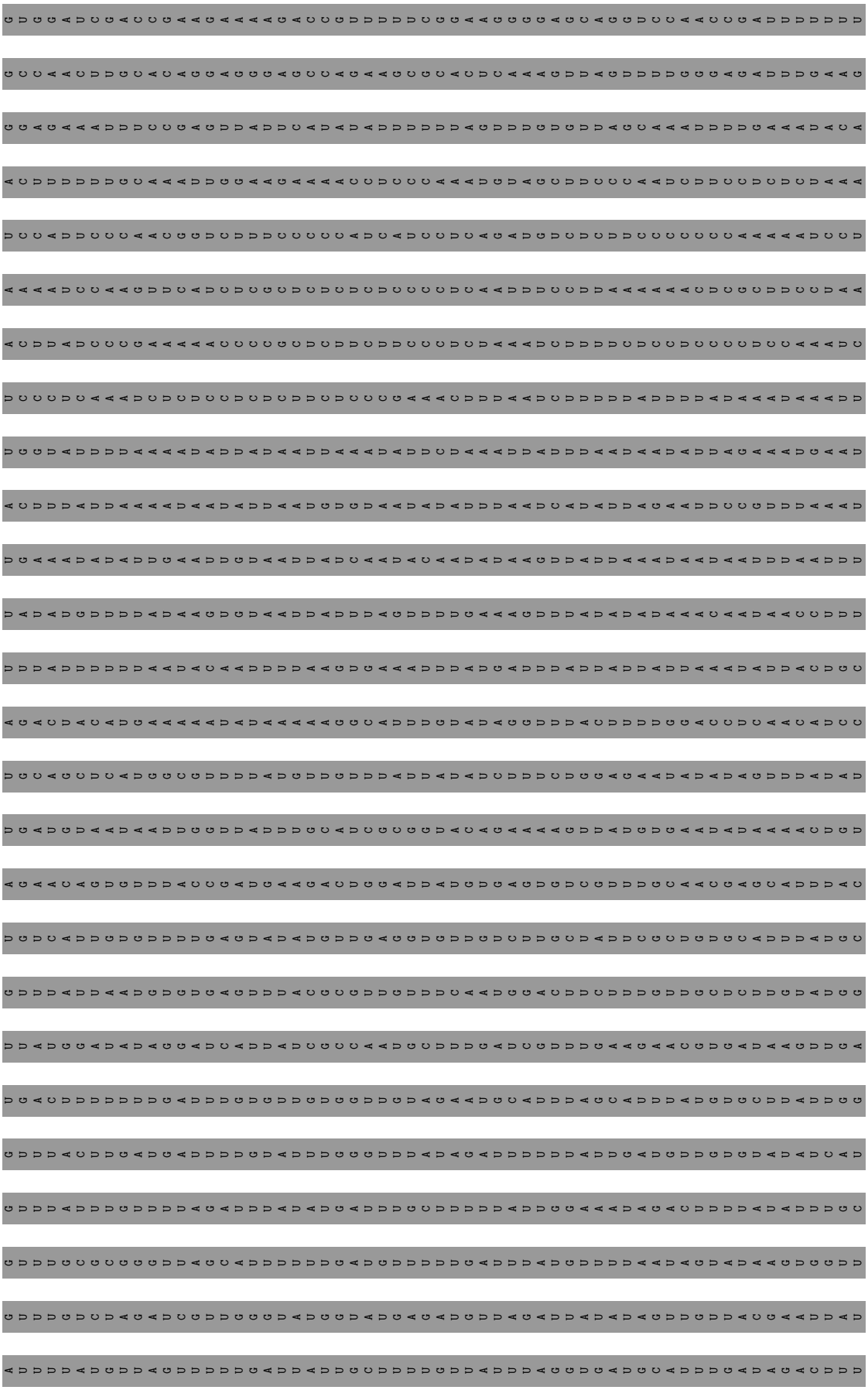


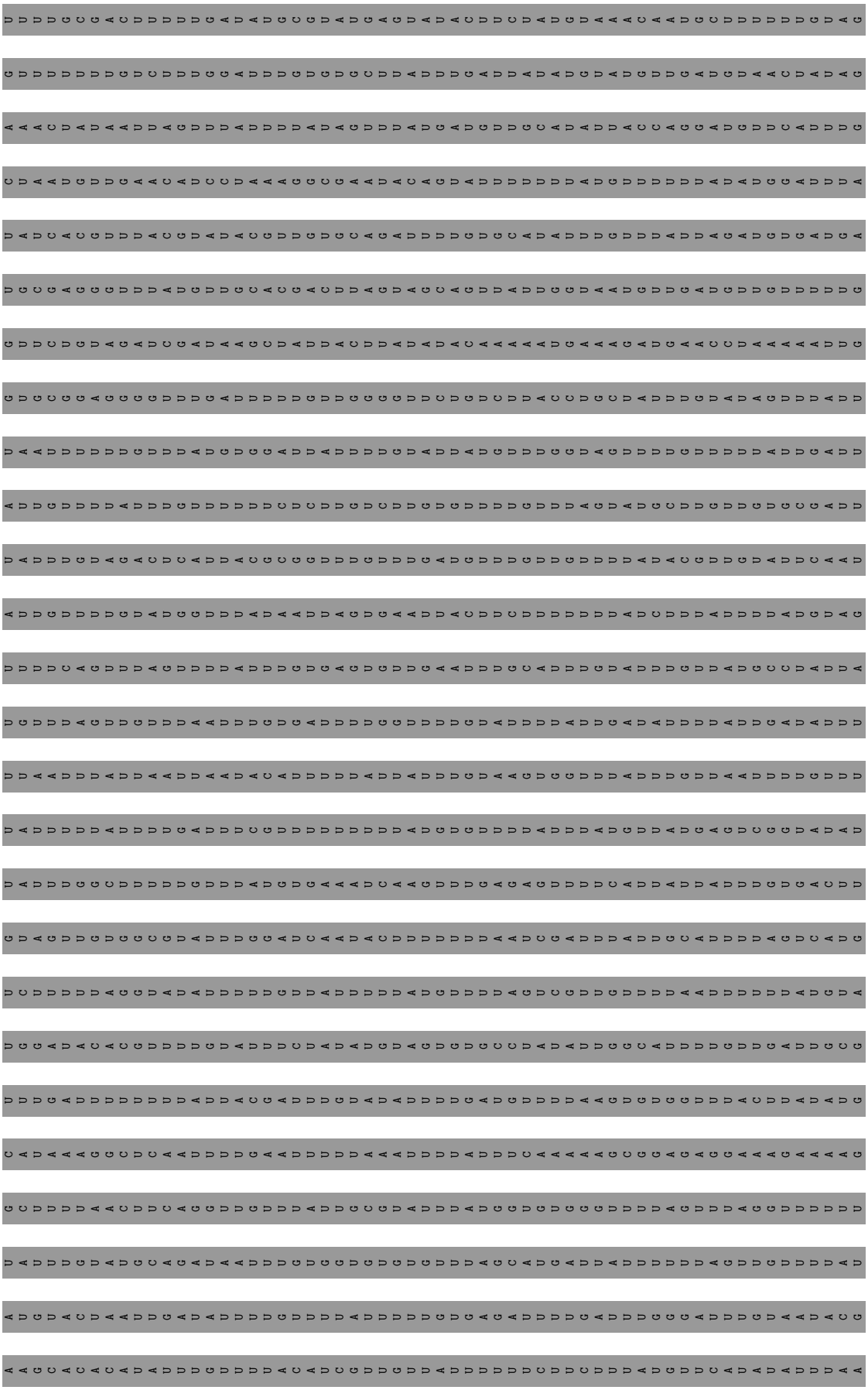

U G A A A A A U U G A A A A A A U A A A U U U G A A A A A U A A A U U U G A A A A A U A A A U U U G

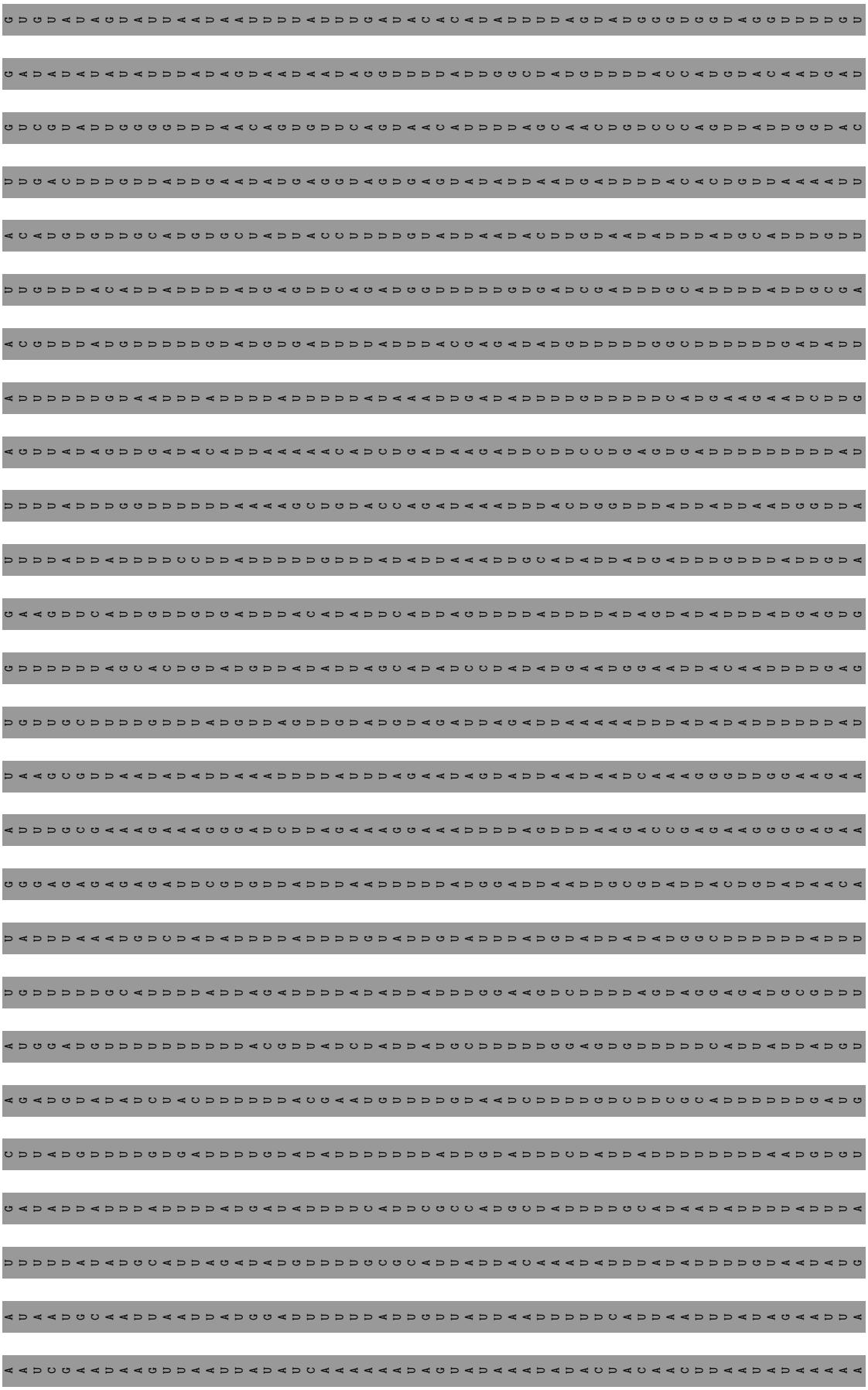


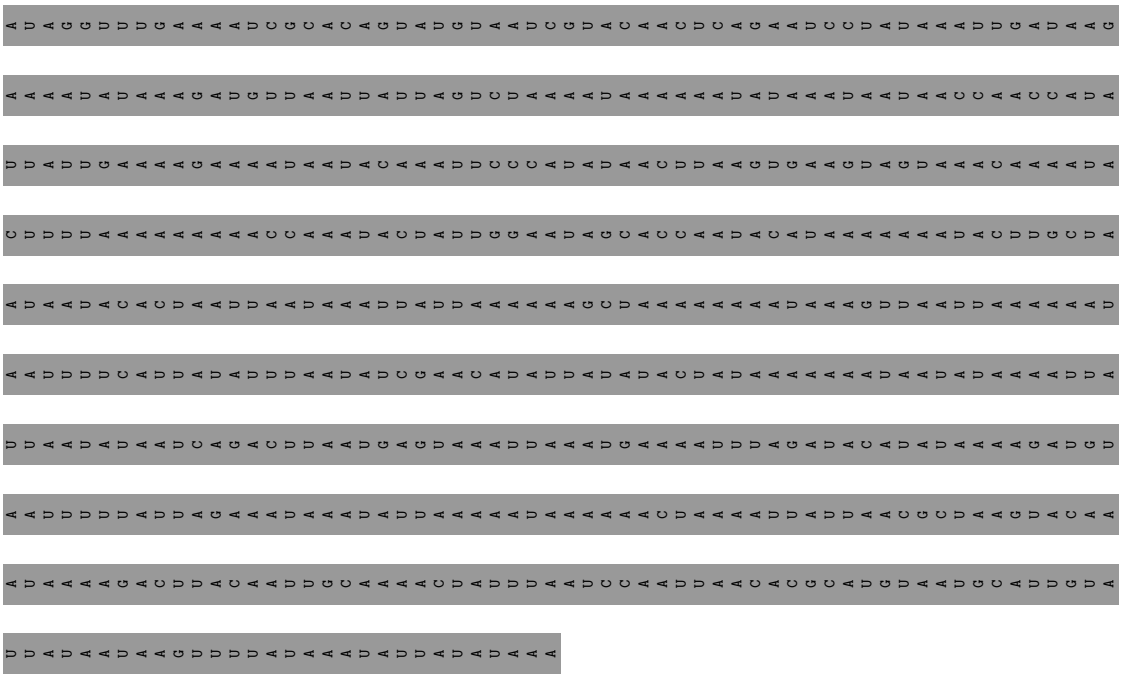



U849 U850 U851 A852 A853 A854 A855 A856 A857 A858 U859 U860 A861 A862 A863 A864 A865 A866 U867 U868 A869 A870 A871 A872 U873 A874 G875 G876 G877 C878 A879 A880 G881 U882 A886 C887 U888 C889 U890 C891 C892 U893 U894 U895 A896 A900 G901 A902 G903 A904 A905 C906 G907 U908 U909 U910 A911 U912
A913 U914 G915 U916 A917 A918 U919 U920 G921 U922 A923 U924 G925 U926 U927 U928 G929 A930 U931 U932 G933 G934 G935 G936 C937 A938 A939 U940 A941 C942 U943 A944 U945 A946 U947 C948 U949 A950 U951 U952 U953 A954 U955 A956 U957 A958 G959 A960 A961 A962 A963 A964 G965 A966 A967 C968 U969 A970 U971 A972
U973 U974 U975 A976 U977 U978 G979 A980 A981 A982 U983 A984 A985 U986 A987 A988 A989 A990 G991 G992 U993 U994 C995 G996 A997 G998 C999 A1000 G1001 G1002 U1003 U1004 A1005 A1006 C1007 A1008 A1009 G1010 C1011 A1012 U1013 U1014 A1015 A1016 U1017 A1018 C1019 A1022 A1023 U1024 G1025 U1026 G1027 U1028 U1029 U1030 C1031 A1032 U1033
C1034 G1035 U1036 C1037 U1038 A1039 C1040 U1041 U1042 A1043 U1044 U1045 G1046 C1047 U1048 A1049 A1050 A1051 U1052 U1053 A1054 U1055 A1056 A1057 U1058 U1059 G1060 A1061 U1062 U1063 G1064 U1065 U1066 C1067 A1068 U1069 C1070 A1071 A1072 A1073 A1074 A1075 A1076 G1077 C1078 A1079 A1080 U1081 U1082 C1083 U1086 A1087 G1088 U1089 U1090 G1091 G1092 G1093 U1094
U1095 A1096 A1097 A1098 A1099 U1100 C1101 G1102 U1103 U1104 G1105 U1106 A1107 A1108 A1109 G1110 C1111 A1112 G1113 A1114 U1115 U1116 U1117 G1118 U1119 U1120 U1121 A1122 U1123 A1124 U1125 A1126 U1127 U1128 U1129 A1130 A1131 U1132 U1133 U1134 U1135 U1136 G1137 U1138 A1139 U1140 A1141 U1142 A1143 G1144 U1145 U1146 A1147 A1148 A1149 U1152 U1153 A1154 A1155
U1156 A1157 U1158









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	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	0.245	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	476.00003, 476.00003, 476.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	0/3098	0.68	6/4217 (0.1%)
2	B	0.47	0/3623	0.59	3/4931 (0.1%)
3	C	0.44	0/1831	0.57	0/2498
4	D	0.41	0/1062	0.66	1/1438 (0.1%)
5	E	0.50	0/2734	0.77	4/3687 (0.1%)
6	F	0.51	0/1485	0.70	1/2019 (0.0%)
7	G	0.52	0/3110	0.77	7/4223 (0.2%)
8	H	0.40	0/1338	0.60	0/1808
9	I	0.45	0/2220	0.62	0/2998
10	J	0.48	0/1175	0.76	1/1582 (0.1%)
11	K	0.42	0/1499	0.52	0/2026
12	L	0.44	0/1452	0.53	0/1970
13	M	0.49	0/2168	0.75	9/2928 (0.3%)
14	N	0.46	0/1650	0.54	0/2242
15	O	0.38	0/2591	0.60	2/3507 (0.1%)
16	P	0.45	0/1402	0.60	0/1892
17	Q	0.47	0/1827	0.58	0/2463
18	R	0.44	0/3852	0.64	4/5243 (0.1%)
19	S	0.44	0/1271	0.52	0/1712
20	T	0.43	0/501	0.52	0/665
21	U	0.60	0/756	1.00	4/1011 (0.4%)
22	V	0.50	0/1231	0.68	0/1645
23	W	0.64	0/483	1.00	1/657 (0.2%)
24	X	0.49	0/3846	0.72	3/5250 (0.1%)
25	Y	0.36	0/2116	0.53	0/2866
26	Z	0.51	0/1268	0.92	7/1725 (0.4%)
27	BA	0.36	0/1056	0.68	0/1435
29	BB	0.49	0/1061	0.80	3/1438 (0.2%)
30	Aw	0.44	0/1552	0.57	0/2107
31	Bj	0.37	0/1389	0.51	0/1878
32	An	0.54	0/2677	0.93	8/3633 (0.2%)
33	Al	0.46	0/2212	0.67	3/3013 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BI	0.35	0/1440	0.48	0/1953
35	Az	0.52	0/1259	0.61	0/1700
36	At	0.41	0/1373	0.53	0/1848
37	BC	0.39	0/1135	0.56	1/1532 (0.1%)
38	Ab	0.42	0/2249	0.51	1/3044 (0.0%)
39	Ai	0.42	0/3879	0.49	0/5258
40	Ap	0.33	0/1819	0.48	0/2458
41	Au	0.54	0/1542	0.93	6/2082 (0.3%)
42	Aa	0.62	1/1454 (0.1%)	0.93	9/1968 (0.5%)
43	Ao	0.47	0/2351	0.73	2/3196 (0.1%)
44	BM	0.26	0/3136	0.59	1/4259 (0.0%)
45	Ar	0.47	0/1689	0.56	1/2280 (0.0%)
46	Aj	0.40	0/2826	0.50	0/3807
47	BH	0.42	0/1700	0.54	0/2301
48	Am	0.42	0/2791	0.55	2/3775 (0.1%)
49	Aq	0.46	0/2128	0.76	2/2876 (0.1%)
50	BE	0.38	0/723	0.75	0/981
51	Ak	0.31	0/2403	0.50	0/3265
52	BP	0.46	0/1648	0.78	7/2238 (0.3%)
53	Ad	0.48	0/1682	0.70	0/2283
54	BF	0.38	0/871	0.61	0/1170
55	Av	0.34	0/1335	0.49	0/1797
56	Af	0.45	0/1165	0.92	3/1585 (0.2%)
57	As	0.37	0/804	0.48	0/1093
58	Ae	0.41	0/2441	0.51	0/3324
59	Ac	0.34	0/2236	0.49	0/3038
60	Ah	0.39	0/3780	0.62	2/5125 (0.0%)
61	BD	0.44	0/826	0.53	0/1109
62	Ay	0.51	0/1269	0.74	2/1724 (0.1%)
63	Ag	0.46	0/1968	0.58	0/2661
64	Ax	0.65	0/1439	1.11	15/1952 (0.8%)
65	BL	0.52	0/2572	0.86	8/3482 (0.2%)
66	BO	0.48	0/1266	0.86	0/1702
67	BG	0.48	0/657	0.98	4/888 (0.5%)
71	1	0.46	1/25626 (0.0%)	0.59	20/39842 (0.1%)
All	All	0.45	2/147018 (0.0%)	0.65	153/204303 (0.1%)

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
3	C	0	1
9	I	0	1
12	L	0	1
18	R	0	1
26	Z	0	1
27	BA	0	2
28	UA	0	2
29	BB	0	2
31	Bj	0	1
32	An	0	2
41	Au	0	3
43	Ao	0	1
48	Am	0	1
49	Aq	0	2
50	BE	0	3
51	Ak	0	1
53	Ad	0	1
56	Af	0	1
65	BL	0	3
66	BO	0	5
69	UC	0	2
70	UD	0	1
All	All	0	38

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Aa	193	TYR	N-CA	15.63	1.66	1.46
71	1	482	C	C1'-N1	5.46	1.56	1.48

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Af	60	PHE	N-CA-C	-18.27	81.82	110.14
42	Aa	91	LEU	N-CA-C	-15.60	88.17	109.54
7	G	214	PRO	N-CA-C	-12.90	91.32	110.80
56	Af	59	ALA	N-CA-C	-11.87	86.89	108.02
6	F	158	PRO	N-CA-C	-11.03	93.84	111.38

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	142	ASN	Peptide
9	I	235	TRP	Peptide
12	L	71	ARG	Peptide
18	R	125	PRO	Peptide
26	Z	21	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	2807	144	0
2	B	3513	0	3413	192	0
3	C	1772	0	1734	101	0
4	D	1036	0	1038	49	0
5	E	2668	0	2697	126	0
6	F	1435	0	1396	84	0
7	G	3012	0	2917	182	0
8	H	1305	0	1315	96	0
9	I	2153	0	2089	146	0
10	J	1146	0	1145	91	0
11	K	1467	0	1469	101	0
12	L	1419	0	1443	82	0
13	M	2116	0	2150	139	0
14	N	1599	0	1591	80	0
15	O	2537	0	2530	142	0
16	P	1367	0	1374	102	0
17	Q	1785	0	1784	106	0
18	R	3755	0	3722	183	0
19	S	1244	0	1272	63	0
20	T	487	0	496	27	0
21	U	744	0	798	80	0
22	V	1202	0	1224	90	0
23	W	465	0	446	17	0
24	X	3733	0	3604	192	0
25	Y	2067	0	1955	111	0
26	Z	1223	0	1192	82	0
27	BA	1038	0	1052	80	0
28	UA	1015	0	213	30	0
29	BB	1028	0	1003	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Aw	1509	0	1470	83	0
31	Bj	1358	0	1422	85	0
32	An	2605	0	2536	180	0
33	Al	2152	0	2112	132	0
34	BI	1409	0	1400	49	0
35	Az	1215	0	1144	67	0
36	At	1346	0	1299	92	0
37	BC	1114	0	1096	63	0
38	Ab	2185	0	2095	143	0
39	Ai	3789	0	3752	157	0
40	Ap	1775	0	1699	66	0
41	Au	1490	0	1450	127	0
42	Aa	1417	0	1377	115	0
43	Ao	2276	0	2176	124	0
44	BM	3069	0	3105	213	0
45	Ar	1644	0	1608	102	0
46	Aj	2766	0	2765	149	0
47	BH	1659	0	1607	73	0
48	Am	2708	0	2634	139	0
49	Aq	2074	0	2050	148	0
50	BE	700	0	665	43	0
51	Ak	2352	0	2369	109	0
52	BP	1593	0	1529	106	0
53	Ad	1632	0	1607	120	0
54	BF	851	0	831	49	0
55	Av	1300	0	1284	92	0
56	Af	1132	0	1108	66	0
57	As	787	0	777	47	0
58	Ae	2359	0	2328	97	0
59	Ac	2174	0	2096	120	0
60	Ah	3686	0	3572	205	0
61	BD	807	0	772	35	0
62	Ay	1226	0	1157	67	0
63	Ag	1916	0	1888	106	0
64	Ax	1388	0	1308	111	0
65	BL	2497	0	2489	182	0
66	BO	1239	0	1246	154	0
67	BG	643	0	617	37	0
68	UB	335	0	73	8	0
69	UC	720	0	151	10	0
70	UD	475	0	105	11	0
71	1	22918	0	11465	1258	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	Ax	2	0	0	0	0
72	BD	1	0	0	0	0
72	BG	1	0	0	2	0
72	T	1	0	0	2	0
72	W	1	0	0	0	0
73	Ag	44	0	26	10	0
All	All	143667	0	128129	6601	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 6601 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Aq:68:THR:HG21	53:Ad:30:GLU:OE1	1.38	1.22
11:K:46:GLN:OE1	42:Aa:191:THR:O	1.61	1.18
43:Ao:238:ARG:HG2	52:BP:98:PRO:HG3	1.27	1.13
48:Am:319:TYR:HB3	71:1:482:C:H5	1.01	1.13
48:Am:319:TYR:CD2	71:1:482:C:N4	2.16	1.12

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	366/467 (78%)	315 (86%)	48 (13%)	3 (1%)	16 49
2	B	433/436 (99%)	380 (88%)	52 (12%)	1 (0%)	43 72
3	C	210/262 (80%)	179 (85%)	31 (15%)	0	100 100
4	D	126/204 (62%)	108 (86%)	18 (14%)	0	100 100
5	E	324/346 (94%)	294 (91%)	30 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	168/171 (98%)	152 (90%)	15 (9%)	1 (1%)	21 54
7	G	363/374 (97%)	313 (86%)	48 (13%)	2 (1%)	21 54
8	H	160/168 (95%)	144 (90%)	14 (9%)	2 (1%)	9 39
9	I	255/305 (84%)	224 (88%)	31 (12%)	0	100 100
10	J	139/144 (96%)	102 (73%)	36 (26%)	1 (1%)	18 51
11	K	177/194 (91%)	158 (89%)	19 (11%)	0	100 100
12	L	176/186 (95%)	157 (89%)	18 (10%)	1 (1%)	21 54
13	M	257/279 (92%)	217 (84%)	39 (15%)	1 (0%)	30 61
14	N	187/252 (74%)	163 (87%)	24 (13%)	0	100 100
15	O	305/476 (64%)	271 (89%)	29 (10%)	5 (2%)	7 36
16	P	163/185 (88%)	145 (89%)	17 (10%)	1 (1%)	21 54
17	Q	215/234 (92%)	192 (89%)	22 (10%)	1 (0%)	24 57
18	R	470/480 (98%)	409 (87%)	60 (13%)	1 (0%)	43 72
19	S	148/409 (36%)	132 (89%)	16 (11%)	0	100 100
20	T	53/83 (64%)	50 (94%)	3 (6%)	0	100 100
21	U	90/118 (76%)	75 (83%)	13 (14%)	2 (2%)	5 30
22	V	139/151 (92%)	119 (86%)	20 (14%)	0	100 100
23	W	52/186 (28%)	46 (88%)	6 (12%)	0	100 100
24	X	466/513 (91%)	418 (90%)	45 (10%)	3 (1%)	21 54
25	Y	253/292 (87%)	234 (92%)	19 (8%)	0	100 100
26	Z	148/197 (75%)	117 (79%)	28 (19%)	3 (2%)	6 32
27	BA	136/167 (81%)	103 (76%)	29 (21%)	4 (3%)	3 26
29	BB	120/156 (77%)	95 (79%)	23 (19%)	2 (2%)	7 35
30	Aw	183/187 (98%)	161 (88%)	22 (12%)	0	100 100
31	Bj	166/185 (90%)	143 (86%)	22 (13%)	1 (1%)	21 54
32	An	312/331 (94%)	256 (82%)	49 (16%)	7 (2%)	5 30
33	Al	262/346 (76%)	219 (84%)	43 (16%)	0	100 100
34	BI	184/266 (69%)	155 (84%)	29 (16%)	0	100 100
35	Az	136/152 (90%)	109 (80%)	25 (18%)	2 (2%)	8 37
36	At	163/183 (89%)	145 (89%)	18 (11%)	0	100 100
37	BC	138/147 (94%)	127 (92%)	11 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	Ab	258/262 (98%)	226 (88%)	32 (12%)	0	100	100
39	Ai	474/479 (99%)	413 (87%)	60 (13%)	1 (0%)	43	72
40	Ap	212/240 (88%)	188 (89%)	24 (11%)	0	100	100
41	Au	174/186 (94%)	132 (76%)	36 (21%)	6 (3%)	3	23
42	Aa	176/195 (90%)	142 (81%)	32 (18%)	2 (1%)	11	43
43	Ao	273/284 (96%)	233 (85%)	38 (14%)	2 (1%)	18	51
44	BM	387/457 (85%)	326 (84%)	61 (16%)	0	100	100
45	Ar	193/205 (94%)	167 (86%)	26 (14%)	0	100	100
46	Aj	337/503 (67%)	292 (87%)	45 (13%)	0	100	100
47	BH	212/229 (93%)	185 (87%)	27 (13%)	0	100	100
48	Am	328/340 (96%)	275 (84%)	53 (16%)	0	100	100
49	Aq	250/341 (73%)	199 (80%)	45 (18%)	6 (2%)	4	29
50	BE	82/118 (70%)	56 (68%)	25 (30%)	1 (1%)	10	41
51	Ak	298/323 (92%)	254 (85%)	44 (15%)	0	100	100
52	BP	191/254 (75%)	162 (85%)	28 (15%)	1 (0%)	24	57
53	Ad	203/237 (86%)	163 (80%)	38 (19%)	2 (1%)	12	45
54	BF	99/109 (91%)	79 (80%)	20 (20%)	0	100	100
55	Av	153/192 (80%)	128 (84%)	25 (16%)	0	100	100
56	Af	137/155 (88%)	119 (87%)	18 (13%)	0	100	100
57	As	95/249 (38%)	87 (92%)	8 (8%)	0	100	100
58	Ae	289/311 (93%)	253 (88%)	36 (12%)	0	100	100
59	Ac	266/291 (91%)	234 (88%)	32 (12%)	0	100	100
60	Ah	450/570 (79%)	386 (86%)	62 (14%)	2 (0%)	30	61
61	BD	95/102 (93%)	85 (90%)	10 (10%)	0	100	100
62	Ay	140/174 (80%)	117 (84%)	18 (13%)	5 (4%)	2	22
63	Ag	229/244 (94%)	204 (89%)	25 (11%)	0	100	100
64	Ax	165/216 (76%)	134 (81%)	31 (19%)	0	100	100
65	BL	307/380 (81%)	235 (76%)	66 (22%)	6 (2%)	6	32
66	BO	153/190 (80%)	105 (69%)	45 (29%)	3 (2%)	6	32
67	BG	83/1347 (6%)	57 (69%)	23 (28%)	3 (4%)	2	22
All	All	14352/18415 (78%)	12263 (85%)	2005 (14%)	84 (1%)	23	54

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ILE
6	F	167	ASN
8	H	94	VAL
10	J	66	PRO
21	U	30	ILE

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	A	314/394 (80%)	313 (100%)	1 (0%)	86	83
2	B	380/381 (100%)	375 (99%)	5 (1%)	61	72
3	C	190/227 (84%)	189 (100%)	1 (0%)	81	80
4	D	106/154 (69%)	105 (99%)	1 (1%)	70	76
5	E	285/301 (95%)	273 (96%)	12 (4%)	26	53
6	F	151/152 (99%)	149 (99%)	2 (1%)	61	72
7	G	315/323 (98%)	303 (96%)	12 (4%)	29	55
8	H	138/143 (96%)	138 (100%)	0	100	100
9	I	223/262 (85%)	222 (100%)	1 (0%)	84	81
10	J	119/122 (98%)	115 (97%)	4 (3%)	32	57
11	K	151/162 (93%)	151 (100%)	0	100	100
12	L	151/158 (96%)	151 (100%)	0	100	100
13	M	226/242 (93%)	222 (98%)	4 (2%)	51	68
14	N	175/220 (80%)	175 (100%)	0	100	100
15	O	278/397 (70%)	273 (98%)	5 (2%)	51	68
16	P	147/163 (90%)	145 (99%)	2 (1%)	59	71
17	Q	191/204 (94%)	189 (99%)	2 (1%)	68	75
18	R	406/412 (98%)	402 (99%)	4 (1%)	68	75
19	S	135/336 (40%)	135 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	52/74 (70%)	52 (100%)	0	100	100
21	U	80/100 (80%)	74 (92%)	6 (8%)	12	39
22	V	125/135 (93%)	123 (98%)	2 (2%)	55	69
23	W	50/164 (30%)	46 (92%)	4 (8%)	11	37
24	X	402/438 (92%)	393 (98%)	9 (2%)	45	65
25	Y	209/236 (89%)	208 (100%)	1 (0%)	81	80
26	Z	132/172 (77%)	129 (98%)	3 (2%)	44	64
27	BA	112/135 (83%)	111 (99%)	1 (1%)	70	76
29	BB	106/140 (76%)	105 (99%)	1 (1%)	70	76
30	Aw	157/159 (99%)	155 (99%)	2 (1%)	61	72
31	Bj	150/165 (91%)	149 (99%)	1 (1%)	76	78
32	An	274/289 (95%)	263 (96%)	11 (4%)	28	54
33	Al	236/299 (79%)	228 (97%)	8 (3%)	32	57
34	BI	153/221 (69%)	152 (99%)	1 (1%)	76	78
35	Az	129/143 (90%)	127 (98%)	2 (2%)	55	69
36	At	140/153 (92%)	140 (100%)	0	100	100
37	BC	117/124 (94%)	116 (99%)	1 (1%)	70	76
38	Ab	233/235 (99%)	232 (100%)	1 (0%)	84	81
39	Ai	408/410 (100%)	407 (100%)	1 (0%)	87	85
40	Ap	189/208 (91%)	188 (100%)	1 (0%)	81	80
41	Au	154/164 (94%)	148 (96%)	6 (4%)	28	54
42	Aa	150/166 (90%)	147 (98%)	3 (2%)	48	66
43	Ao	236/245 (96%)	235 (100%)	1 (0%)	84	81
44	BM	319/370 (86%)	318 (100%)	1 (0%)	86	83
45	Ar	169/179 (94%)	168 (99%)	1 (1%)	78	79
46	Aj	286/420 (68%)	284 (99%)	2 (1%)	76	78
47	BH	177/189 (94%)	176 (99%)	1 (1%)	78	79
48	Am	278/287 (97%)	276 (99%)	2 (1%)	76	78
49	Aq	221/276 (80%)	218 (99%)	3 (1%)	59	71
50	BE	76/100 (76%)	76 (100%)	0	100	100
51	Ak	254/272 (93%)	254 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	BP	167/215 (78%)	166 (99%)	1 (1%)	78 79
53	Ad	172/193 (89%)	170 (99%)	2 (1%)	63 73
54	BF	88/95 (93%)	87 (99%)	1 (1%)	65 74
55	Av	141/169 (83%)	140 (99%)	1 (1%)	76 78
56	Af	120/135 (89%)	120 (100%)	0	100 100
57	As	88/204 (43%)	88 (100%)	0	100 100
58	Ae	249/261 (95%)	247 (99%)	2 (1%)	73 77
59	Ac	232/253 (92%)	232 (100%)	0	100 100
60	Ah	385/485 (79%)	378 (98%)	7 (2%)	51 68
61	BD	85/90 (94%)	85 (100%)	0	100 100
62	Ay	130/158 (82%)	129 (99%)	1 (1%)	73 77
63	Ag	202/211 (96%)	200 (99%)	2 (1%)	68 75
64	Ax	150/190 (79%)	141 (94%)	9 (6%)	17 45
65	BL	268/329 (82%)	262 (98%)	6 (2%)	45 65
66	BO	130/158 (82%)	128 (98%)	2 (2%)	57 70
67	BG	67/1047 (6%)	64 (96%)	3 (4%)	24 51
All	All	12529/15614 (80%)	12360 (99%)	169 (1%)	59 72

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	Au	72	ASP
60	Ah	112	TYR
42	Aa	46	MET
49	Aq	339	ARG
64	Ax	57	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 343 such sidechains are listed below:

Mol	Chain	Res	Type
45	Ar	96	GLN
55	Av	137	GLN
46	Aj	210	GLN
48	Am	184	ASN
59	Ac	57	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
71	1	1085/9070 (11%)	639 (58%)	127 (11%)

5 of 639 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
71	1	39	U
71	1	40	C
71	1	41	A
71	1	42	A
71	1	43	A

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
71	1	506	A
71	1	944	A
71	1	617	G
71	1	932	U
71	1	1074	A

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
73	NAD	Ag	301	-	46,48,48	0.50	0	64,73,73	0.79	3 (4%)

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
73	NAD	Ag	301	-	-	11/30/62/62	0/5/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	Ag	301	NAD	C4D-O4D-C1D	-3.26	106.94	109.92
73	Ag	301	NAD	C6N-N1N-C2N	-2.24	119.97	121.88
73	Ag	301	NAD	O4B-C4B-C3B	-2.10	100.98	105.15

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
73	Ag	301	NAD	C5B-O5B-PA-O3
73	Ag	301	NAD	C2D-C1D-N1N-C2N
73	Ag	301	NAD	C4B-C5B-O5B-PA
73	Ag	301	NAD	PN-O3-PA-O5B
73	Ag	301	NAD	PA-O3-PN-O5D

There are no ring outliers.

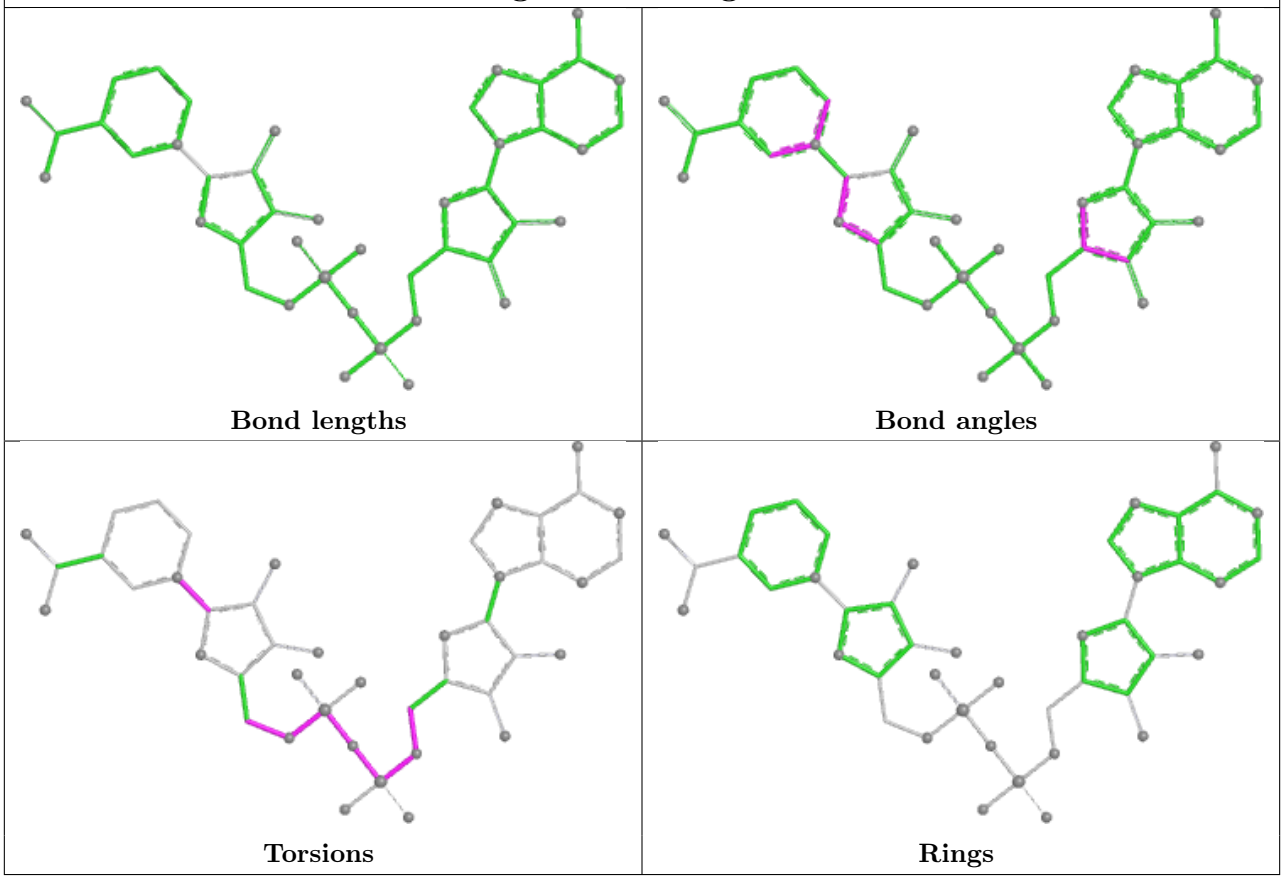
1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	Ag	301	NAD	10	0

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 Ag 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

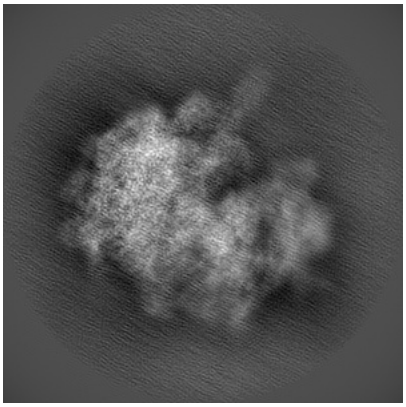
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11796. These allow visual inspection of the internal detail of the map and identification of artifacts.

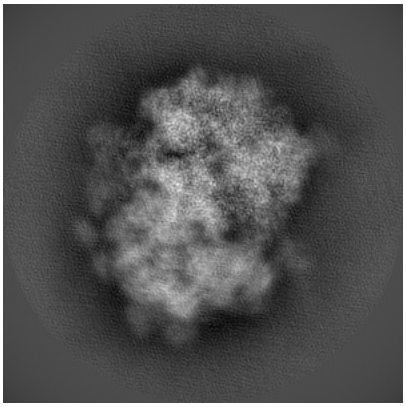
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

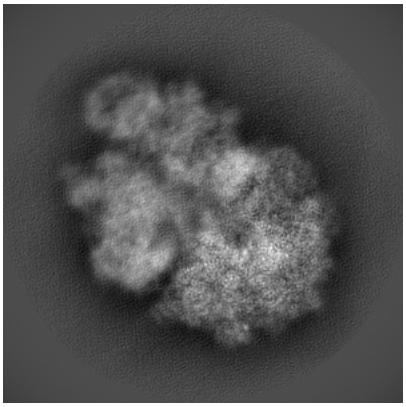
6.1.1 Primary map



X



Y

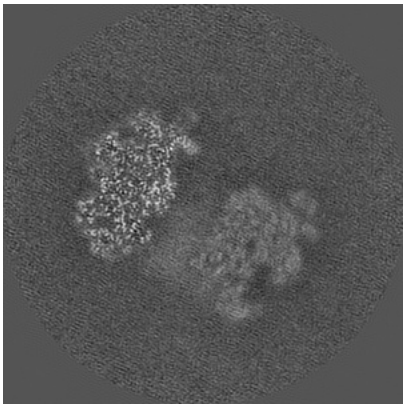


Z

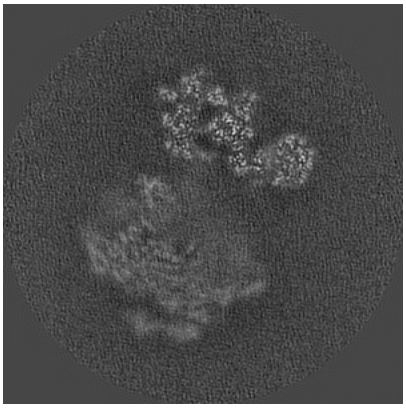
The images above show the map projected in three orthogonal directions.

6.2 Central slices

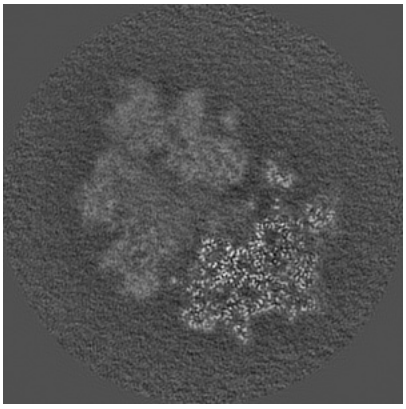
6.2.1 Primary map



X Index: 200



Y Index: 200

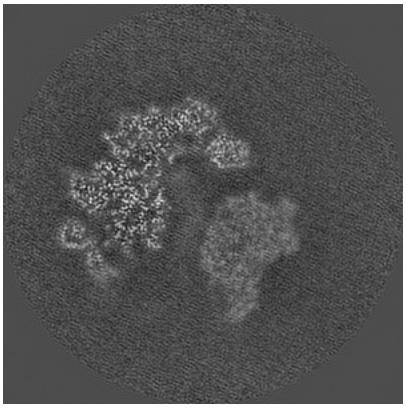


Z Index: 200

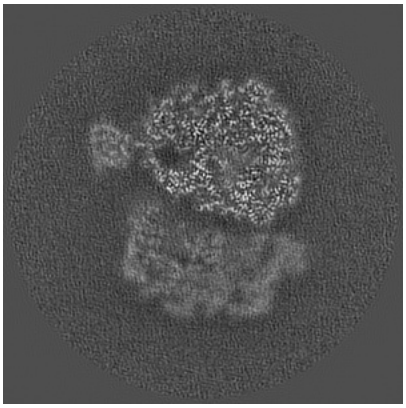
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

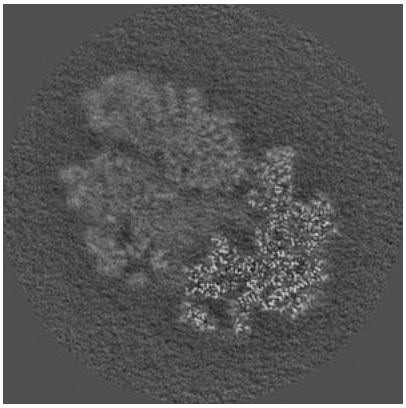
6.3.1 Primary map



X Index: 224



Y Index: 150

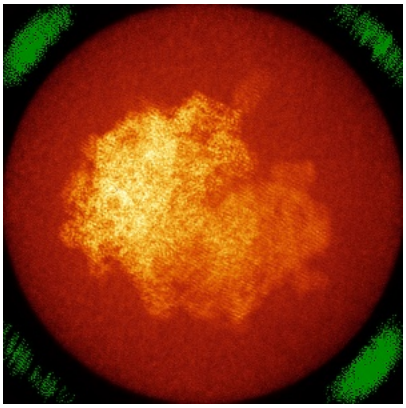


Z Index: 185

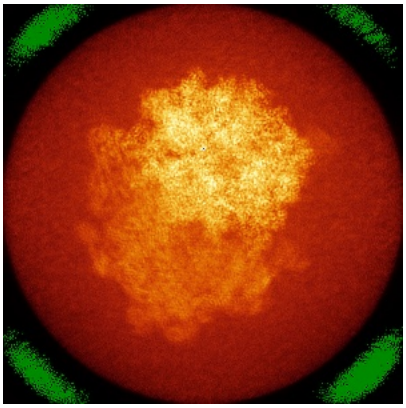
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

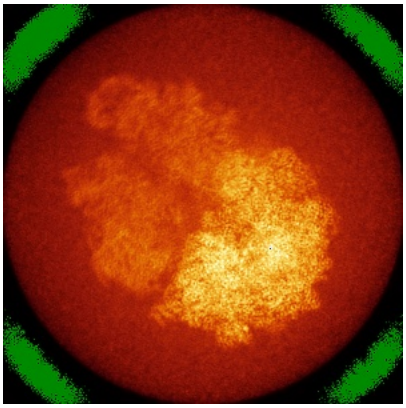
6.4.1 Primary map



X



Y

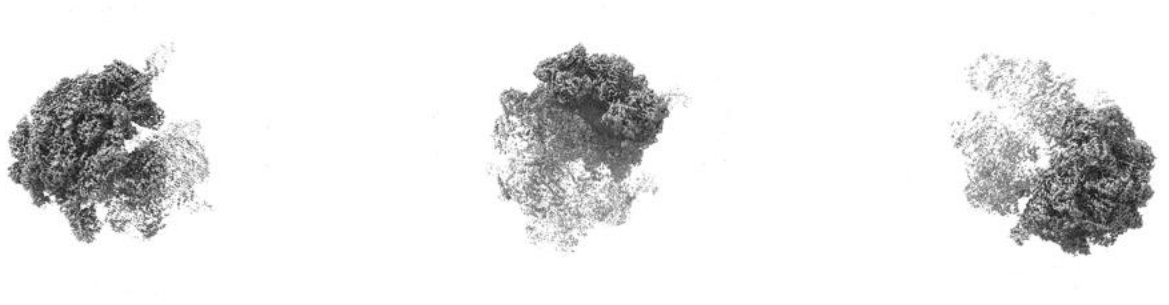


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

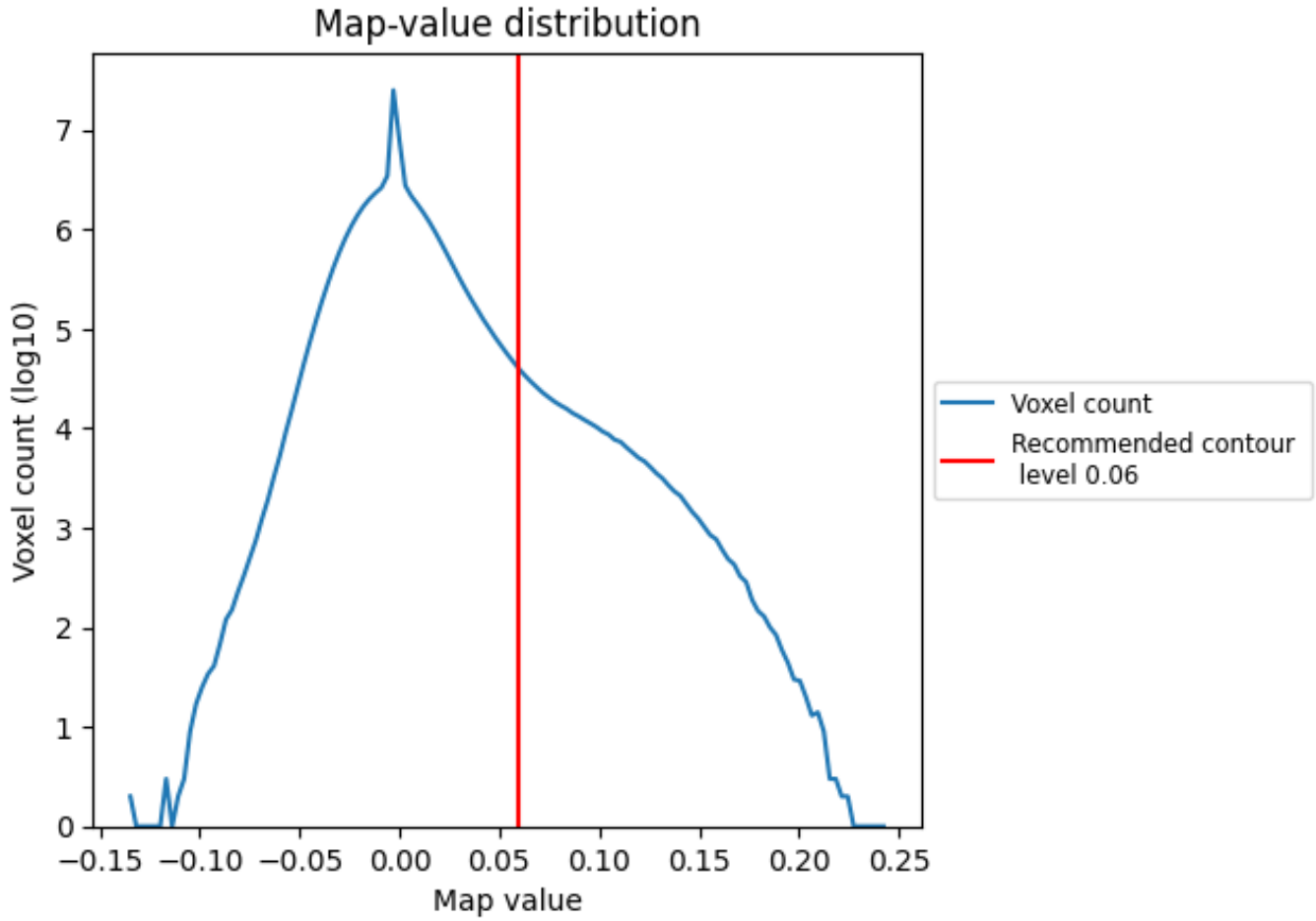
6.6 Mask visualisation (i)

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

7 Map analysis

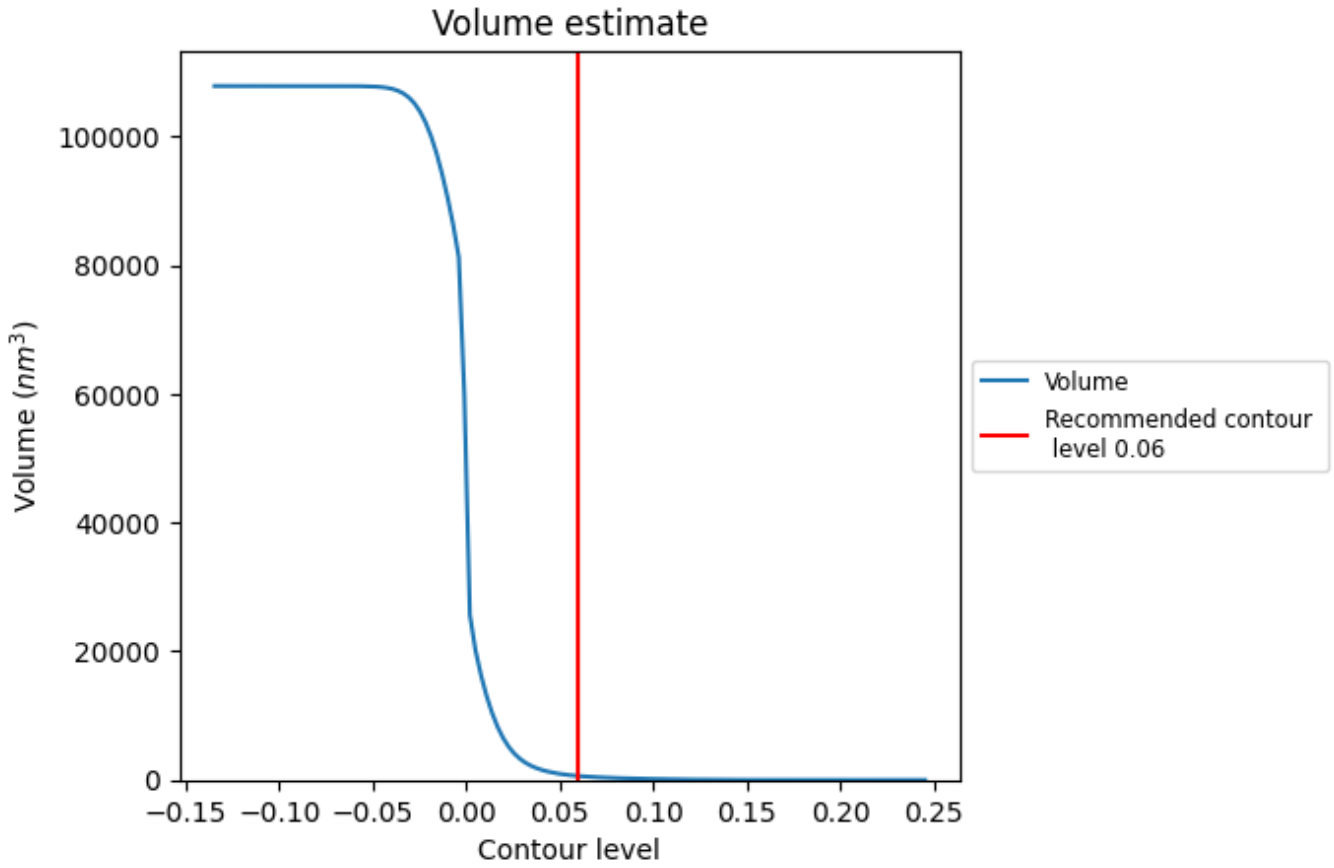
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

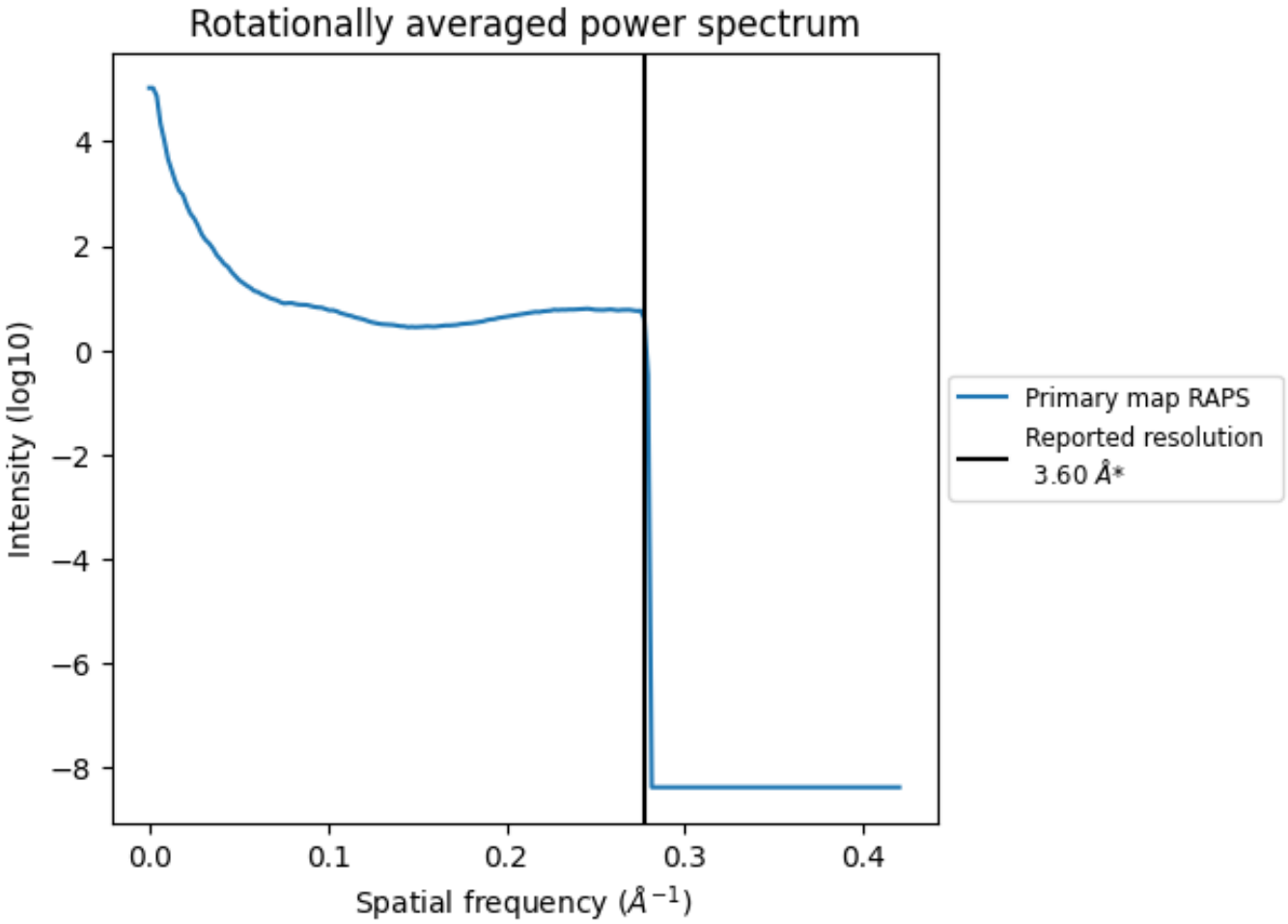
7.2 Volume estimate (i)



The volume at the recommended contour level is 617 nm^3; this corresponds to an approximate mass of 557 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 0.278 Å^{-1}

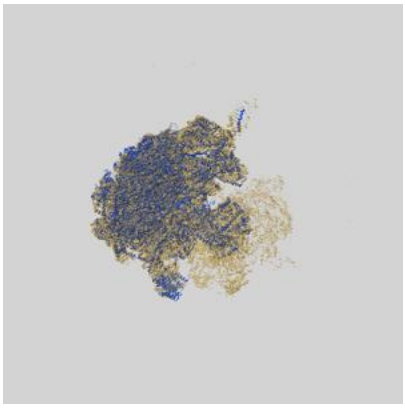
8 Fourier-Shell correlation

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

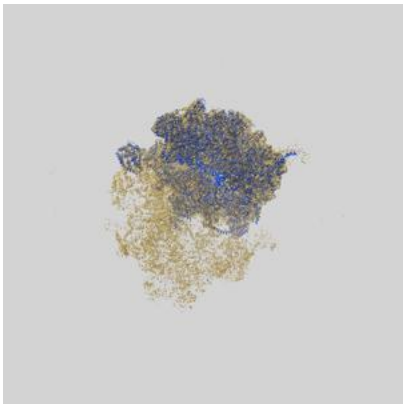
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11796 and PDB model 7AIH. Per-residue inclusion information can be found in section 3 on page 18.

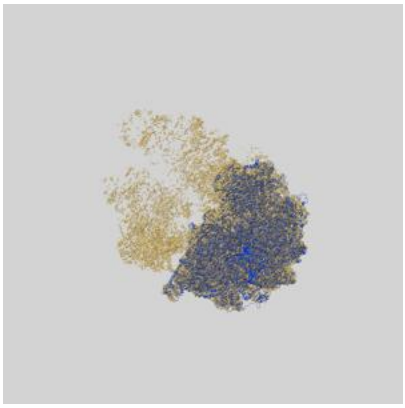
9.1 Map-model overlay



X



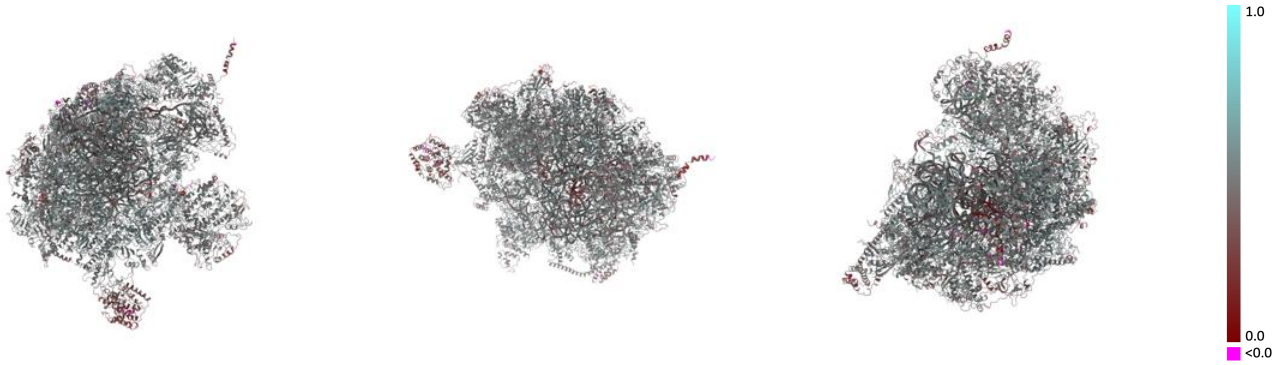
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

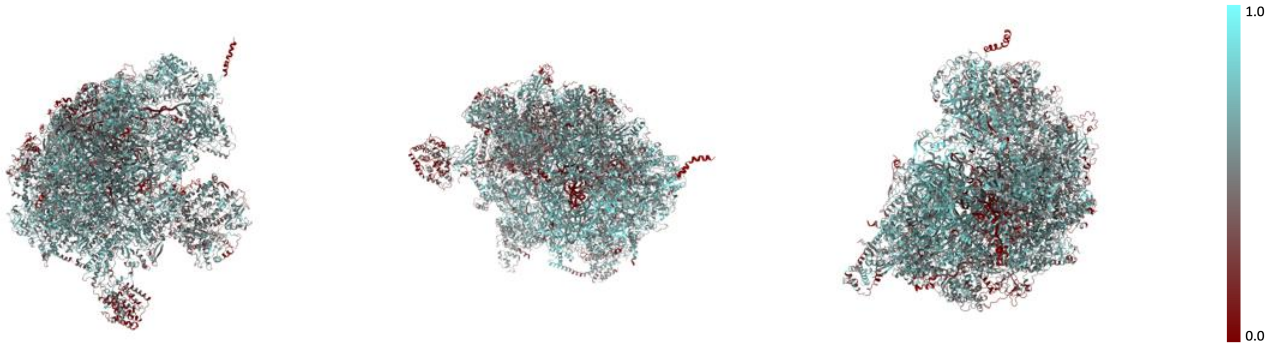
9.2 Q-score mapped to coordinate model (i)



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.

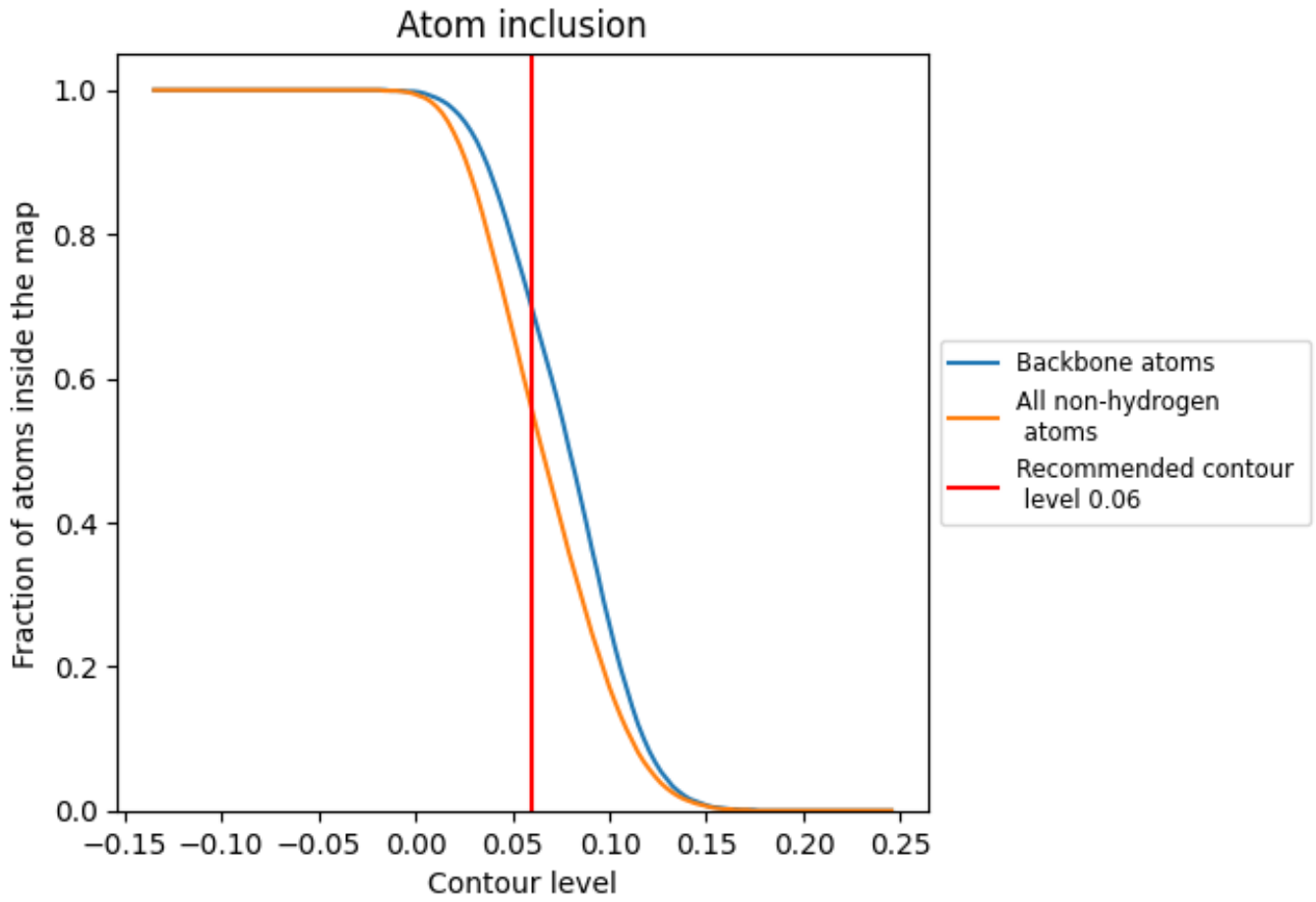
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5560	0.4790
1	0.6140	0.4520
A	0.6480	0.5200
Aa	0.4530	0.4490
Ab	0.6170	0.5000
Ac	0.4800	0.4600
Ad	0.5160	0.4950
Ae	0.6230	0.5110
Af	0.5220	0.4740
Ag	0.5740	0.5060
Ah	0.5280	0.4630
Ai	0.5570	0.5060
Aj	0.5570	0.4990
Ak	0.4720	0.4440
Al	0.5900	0.4970
Am	0.6380	0.4910
An	0.5490	0.4840
Ao	0.6240	0.5100
Ap	0.4920	0.4530
Aq	0.5040	0.5020
Ar	0.6090	0.5180
As	0.5420	0.4690
At	0.5910	0.4980
Au	0.6160	0.5040
Av	0.5240	0.4600
Aw	0.6010	0.4990
Ax	0.6050	0.4990
Ay	0.5880	0.4910
Az	0.6370	0.5210
B	0.5880	0.5130
BA	0.4920	0.4510
BB	0.5560	0.4620
BC	0.4970	0.4860
BD	0.6090	0.5130
BE	0.5690	0.4430



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Chain	Atom inclusion	Q-score
BF	0.4960	0.4800
BG	0.5610	0.4930
BH	0.5450	0.4970
BI	0.5760	0.4760
BL	0.5950	0.5110
BM	0.2680	0.3150
BO	0.5190	0.4600
BP	0.5470	0.4990
Bj	0.4450	0.4790
C	0.6010	0.5080
D	0.4770	0.4210
E	0.5620	0.4670
F	0.5610	0.5100
G	0.5960	0.5200
H	0.4930	0.4920
I	0.5470	0.4970
J	0.5650	0.4970
K	0.5550	0.4920
L	0.5850	0.5030
M	0.5720	0.5010
N	0.5680	0.4990
O	0.3660	0.4270
P	0.5370	0.5070
Q	0.5680	0.4970
R	0.5170	0.4670
S	0.5550	0.5110
T	0.6370	0.5140
U	0.4740	0.4910
UA	0.6620	0.4690
UB	0.6780	0.5100
UC	0.2810	0.3630
UD	0.5450	0.3890
V	0.5570	0.5230
W	0.5620	0.5070
X	0.5120	0.4770
Y	0.4660	0.4700
Z	0.5640	0.5010