



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 02:27 pm GMT

PDB ID : 7AIH
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:

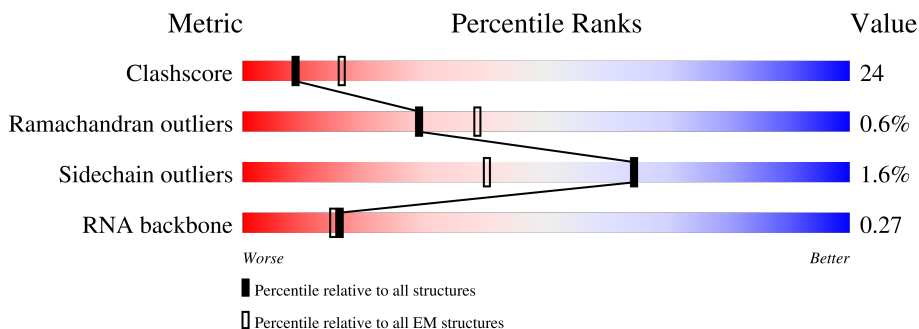
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	467	
2	B	436	
3	C	262	
4	D	204	
5	E	346	
6	F	171	
7	G	374	

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Mol	Chain	Length	Quality of chain
8	H	168	29% 52% 43%
9	I	305	24% 44% 39% 16%
10	J	144	22% 51% 44%
11	K	194	24% 57% 34% 8%
12	L	186	16% 62% 33%
13	M	279	17% 48% 43% 7%
14	N	252	17% 50% 24% 25%
15	O	476	36% 37% 26% 36%
16	P	185	23% 52% 37% 11%
17	Q	234	19% 56% 35% 7%
18	R	480	30% 60% 38%
19	S	409	6% 25% 12% 63%
20	T	83	11% 35% 31% 34%
21	U	118	30% 42% 30% 5% 22%
22	V	151	23% 50% 41% 7%
23	W	186	6% 18% 11% 71%
24	X	513	28% 58% 32% 9%
25	Y	292	35% 58% 29% 13%
26	Z	197	18% 44% 30% 24%
27	BA	167	28% 35% 44% 17%
28	UA	203	19% 81% 19%
29	BB	156	24% 40% 36% 22%
30	Aw	187	22% 98%
31	Bj	185	40% 89% 9%
32	An	331	24% 90% 5% 5%

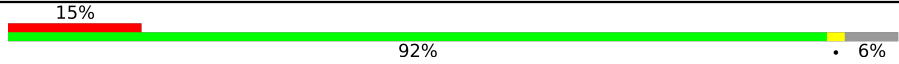
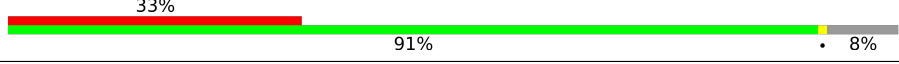



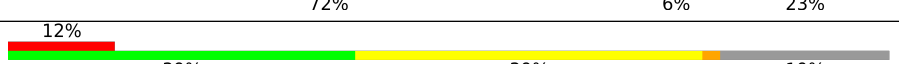
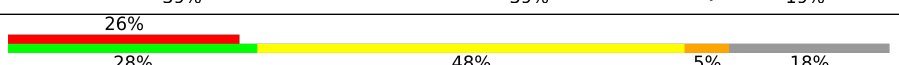
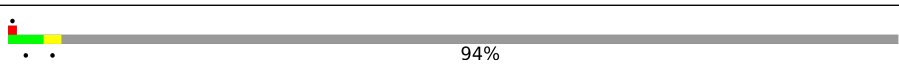
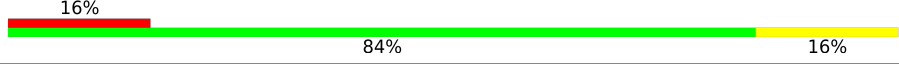
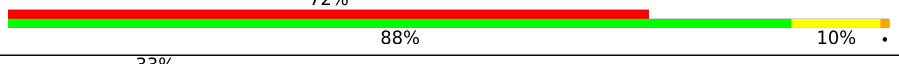
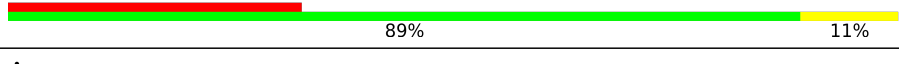


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Mol	Chain	Length	Quality of chain
33	Al	346	14% 75% 24%
34	BI	266	12% 47% 23% 30%
35	Az	152	14% 88% 9%
36	At	183	15% 90% 10%
37	BC	147	26% 61% 33% 5%
38	Ab	262	14% 99%
39	Ai	479	21% 99%
40	Ap	240	30% 89% 11%
41	Au	186	14% 85% 9% 5%
42	Aa	195	36% 87% 9%
43	Ao	284	13% 95%
44	BM	457	61% 40% 44% 15%
45	Ar	205	15% 95% 5%
46	Aj	503	15% 67% 32%
47	BH	229	23% 59% 34% 7%
48	Am	340	13% 96%
49	Aq	341	25% 72% 24%
50	BE	118	16% 42% 28% 29%
51	Ak	323	32% 92% 7%
52	BP	254	20% 46% 30% 23%
53	Ad	237	27% 86% 13%
54	BF	109	33% 57% 36% 7%
55	Av	192	24% 81% 19%
56	Af	155	27% 88% 10%
57	As	249	12% 39% 61%

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Mol	Chain	Length	Quality of chain
58	Ae	311	
59	Ac	291	
60	Ah	570	
61	BD	102	
62	Ay	174	
63	Ag	244	
64	Ax	216	
65	BL	380	
66	BO	190	
67	BG	1347	
68	UB	67	
69	UC	144	
70	UD	95	
71	1	9070	

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	Total	C	N	O	S	0	0
			2996	1929	496	556	15		

- Molecule 2 is a protein called uL4m.

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

- 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	Total	C	N	O	S	0	0
			1772	1144	303	321	4		

- Molecule 4 is a protein called uL10m.

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

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

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

- 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	Total	C	N	O	S	0	0
			1435	919	261	243	12		

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

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

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

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

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

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

- Molecule 10 is a protein called bL19m.

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

- Molecule 11 is a protein called bL20.

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

- Molecule 12 is a protein called bL21m.

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

- Molecule 13 is a protein called uL22m.

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

- 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
			Total	C	N	O		
28	UA	203	1015	609	203	203	0	0

- Molecule 29 is a protein called mL95.

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

- Molecule 30 is a protein called mL89.

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

- Molecule 31 is a protein called bL31m.

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

- Molecule 32 is a protein called mL76.

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

- Molecule 33 is a protein called mL74.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BI	186	1409	895	242	264	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
			Total	C	N	O	S		
42	Aa	178	1417	884	270	256	7	0	0

- Molecule 43 is a protein called mL79.

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

- Molecule 44 is a protein called mL70.

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

- Molecule 45 is a protein called mL84.

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

- Molecule 46 is a protein called mL72.

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

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

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

- Molecule 48 is a protein called mL75.

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

- Molecule 49 is a protein called mL82.

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

- Molecule 50 is a protein called mL98.

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

- Molecule 51 is a protein called mL73.

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

- Molecule 52 is a protein called mL52,mL52.

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

- Molecule 53 is a protein called mL49.

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

- Molecule 54 is a protein called mL99.

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

- Molecule 55 is a protein called mL88.

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

- 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
			Total	C	N	O	S		
63	Ag	231	1916	1211	356	340	9	0	0

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

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

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

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

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

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

- Molecule 67 is a protein called mL100.

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

- Molecule 68 is a protein called UB.

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

- Molecule 69 is a protein called UC.

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

- Molecule 70 is a protein called UD.

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

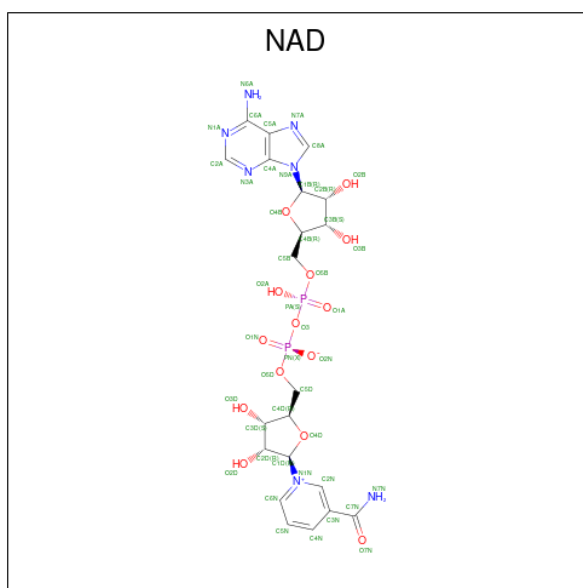
- Molecule 71 is a RNA chain called Ribosomal RNA.

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

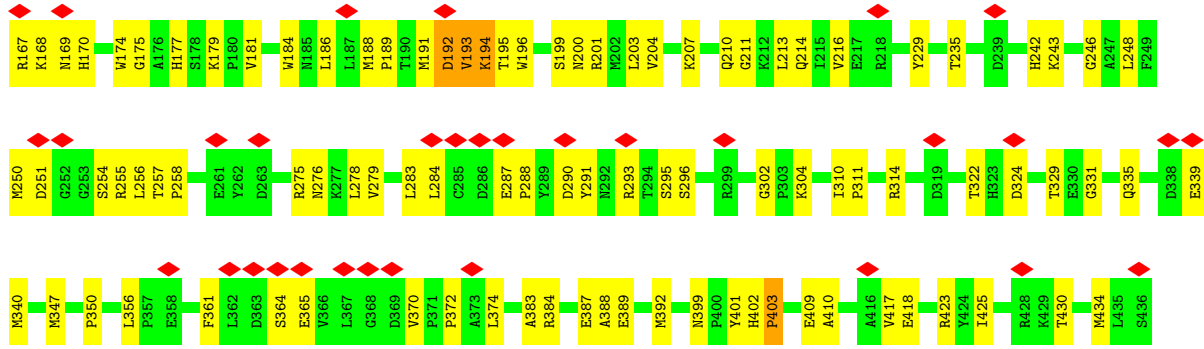
- Molecule 72 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

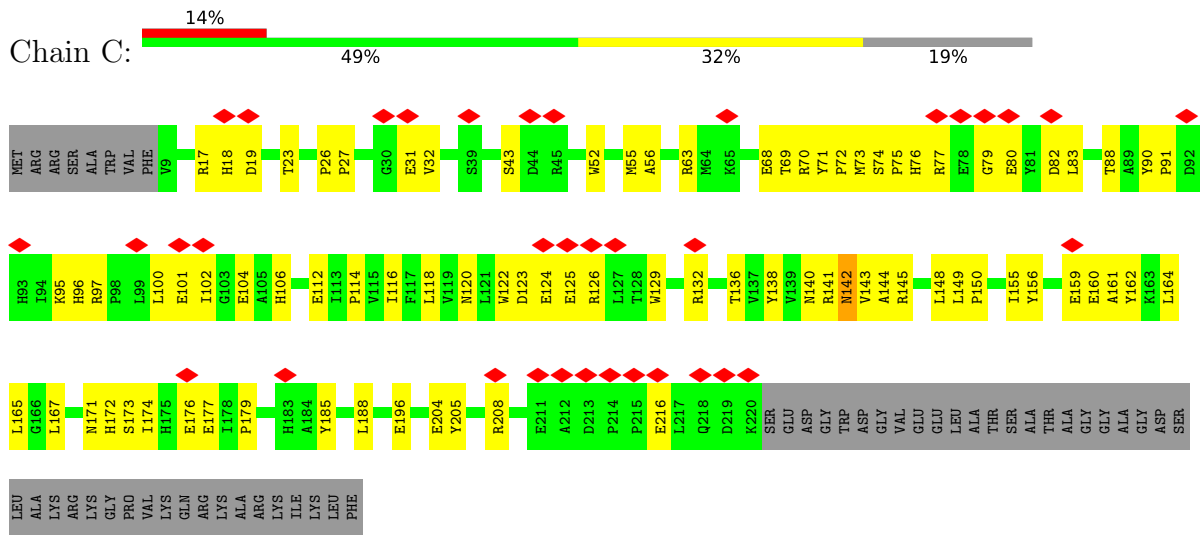
- Molecule 73 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



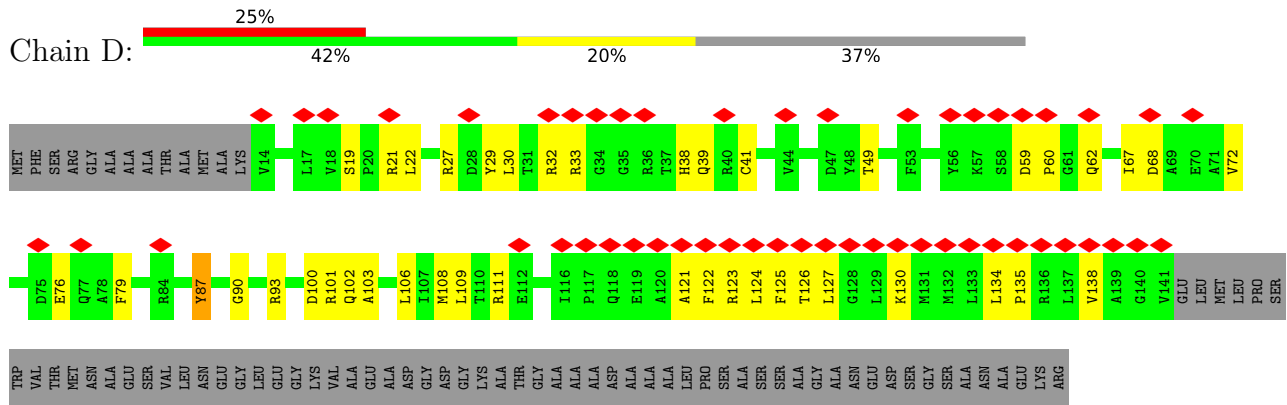
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
73	Ag	1	44	21	7	14	2	0



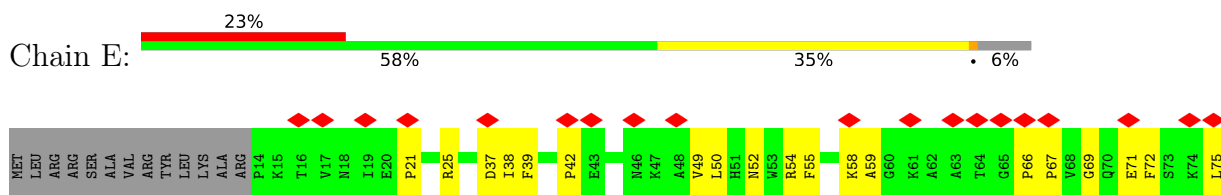
• Molecule 3: RIBOSOMAL_L9 domain-containing protein

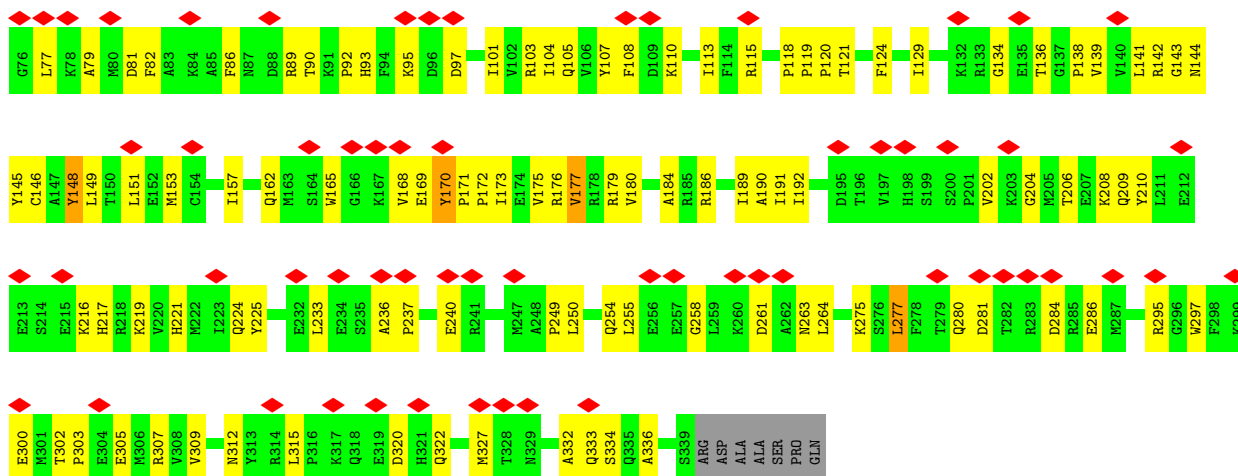


• Molecule 4: uL10m

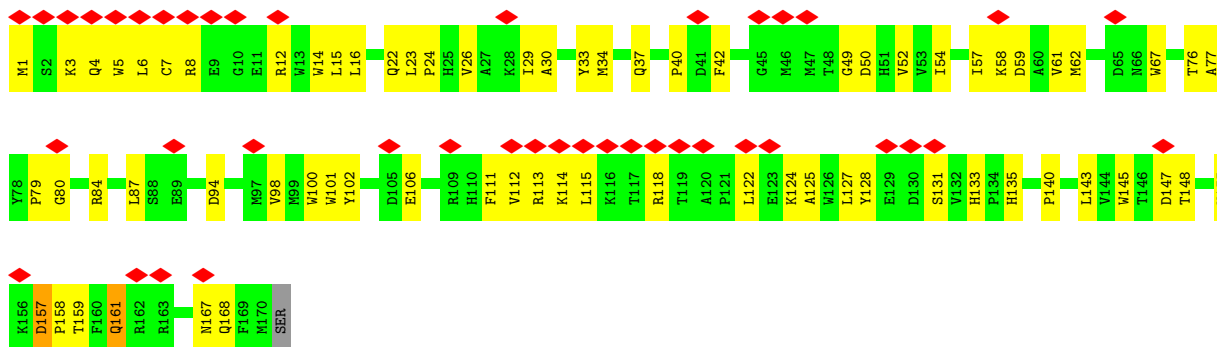


• Molecule 5: Putative ribosomal protein L11

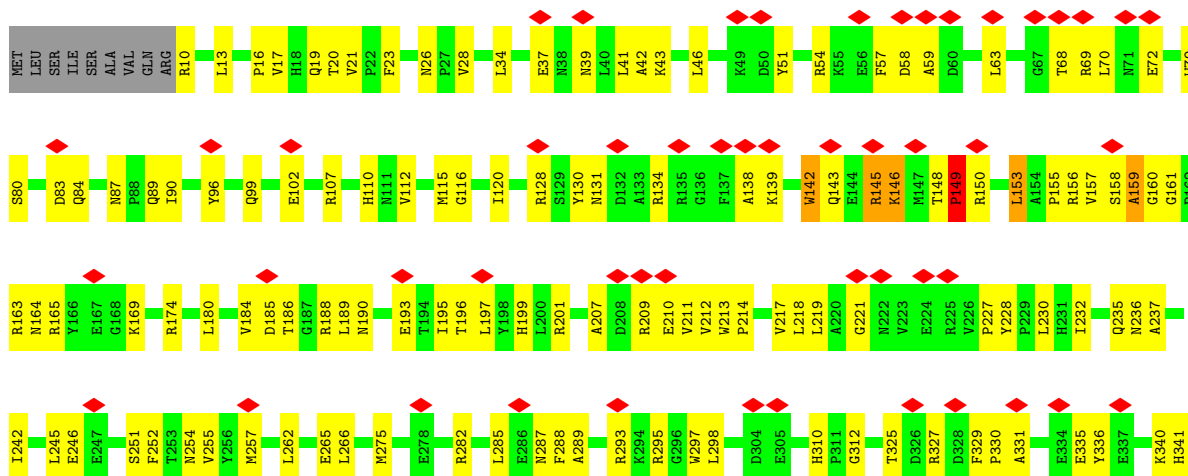


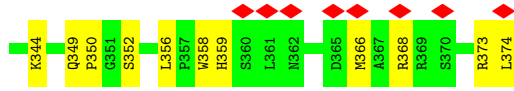


• Molecule 6: 50S ribosomal protein L13-like protein

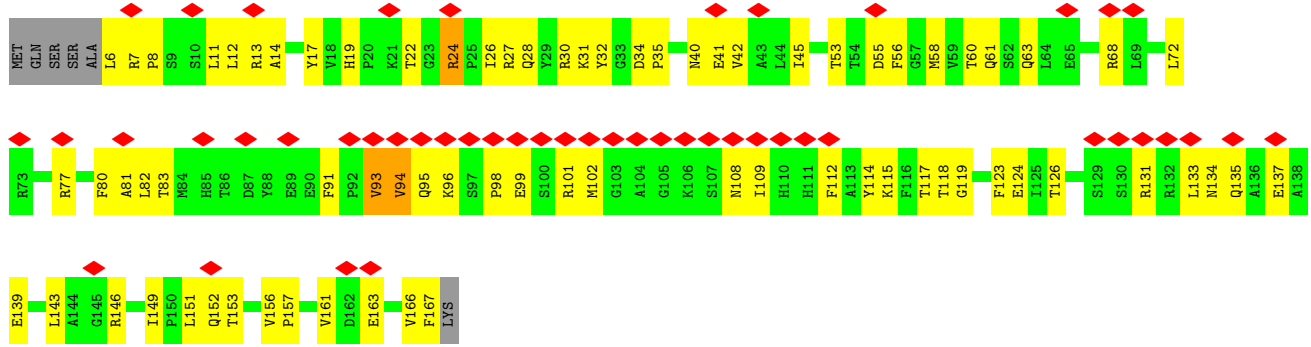


• Molecule 7: Ribosomal_L18e/L15P domain-containing protein

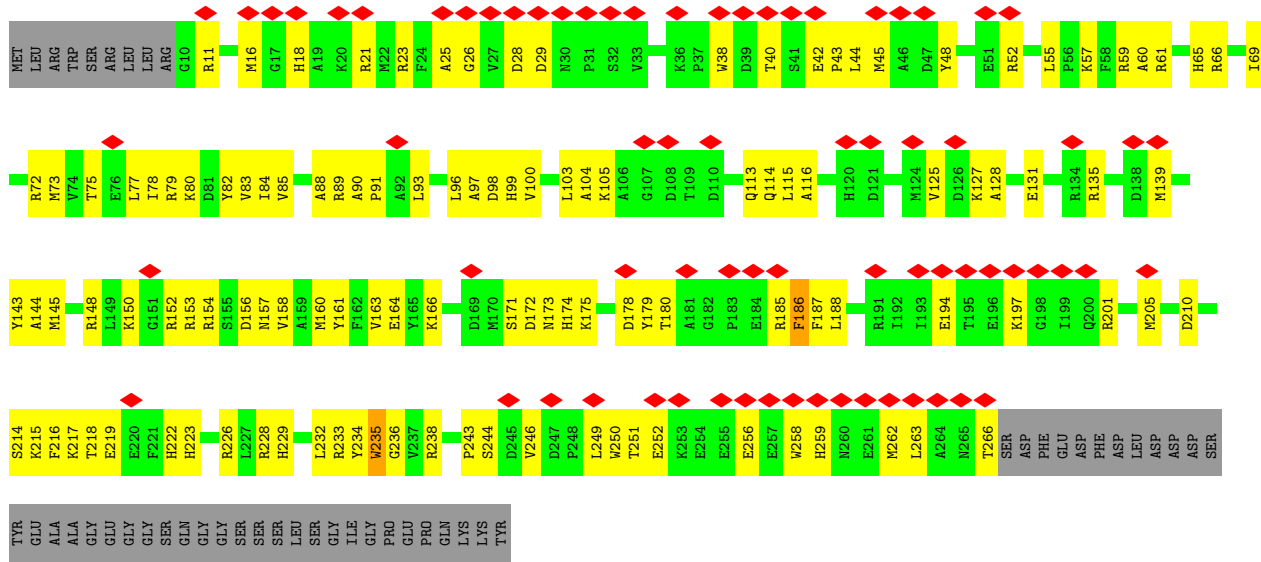




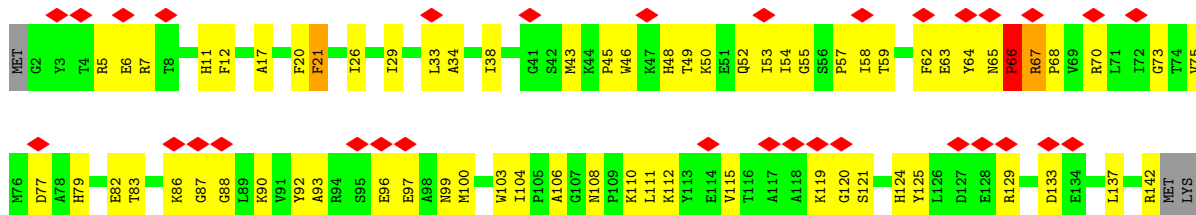
• Molecule 8: Ribosomal_L16 domain-containing protein

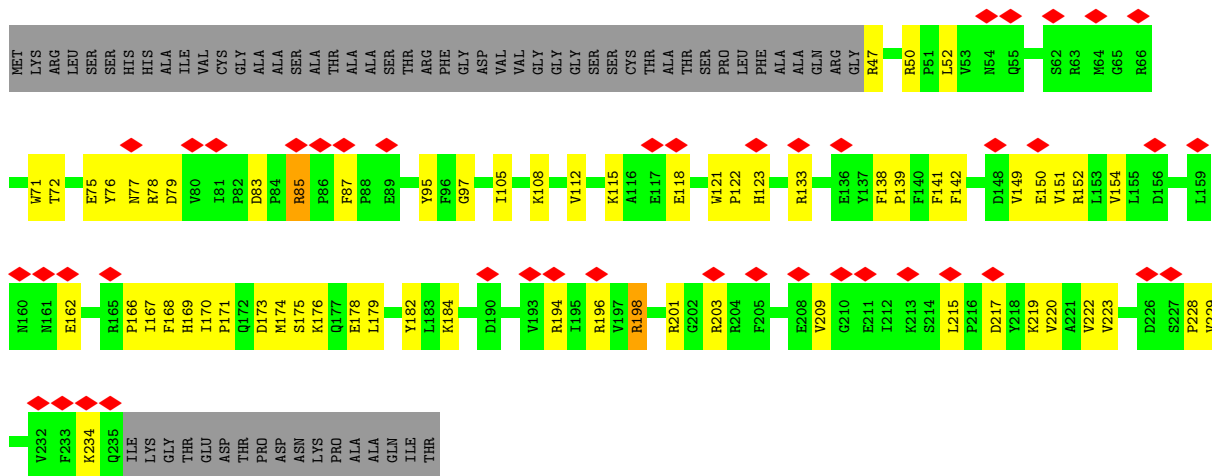


• Molecule 9: Putative 50S ribosomal protein L17

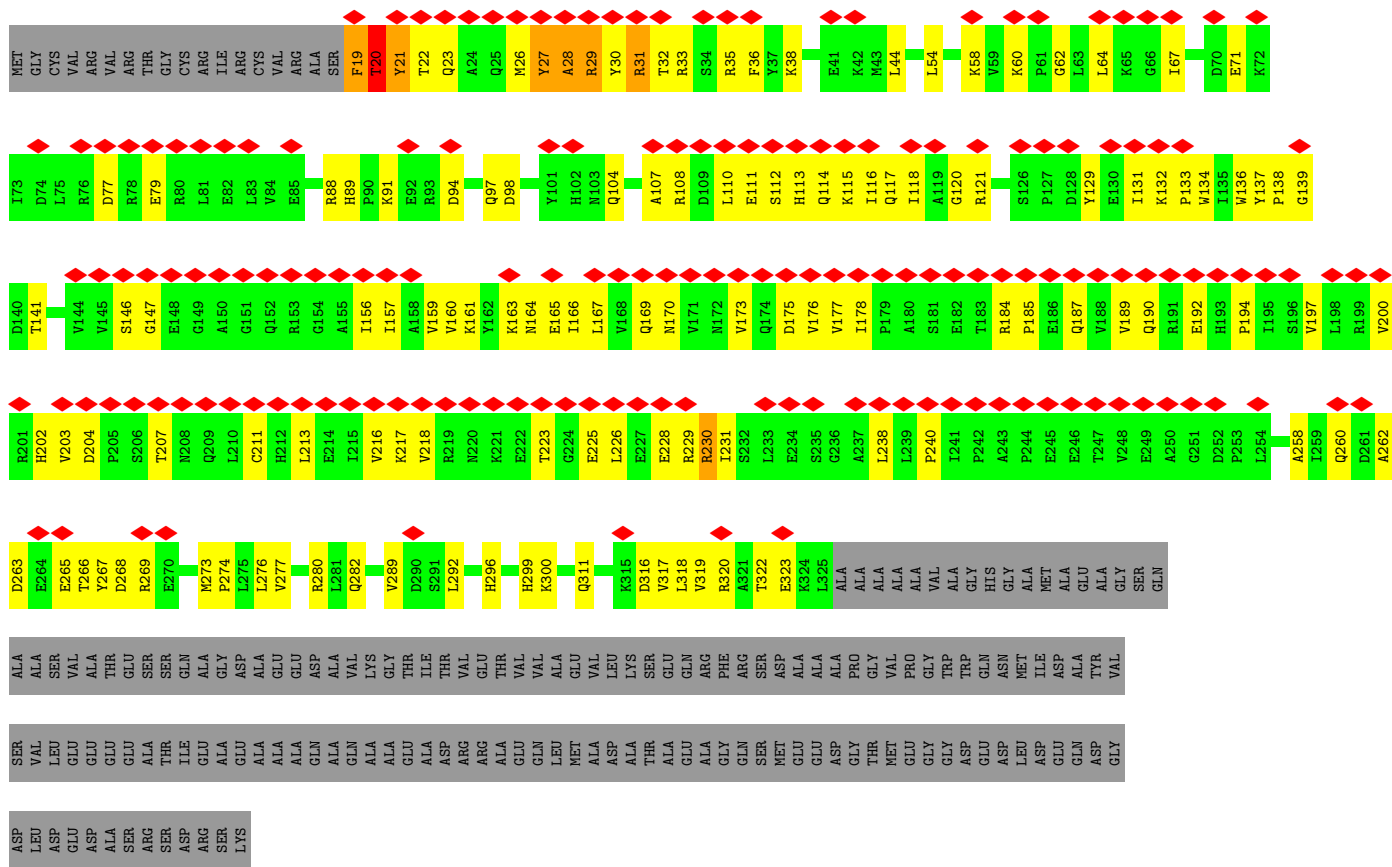


• Molecule 10: bL19m

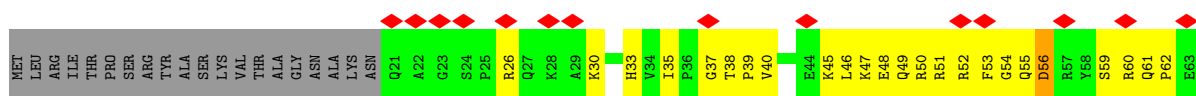


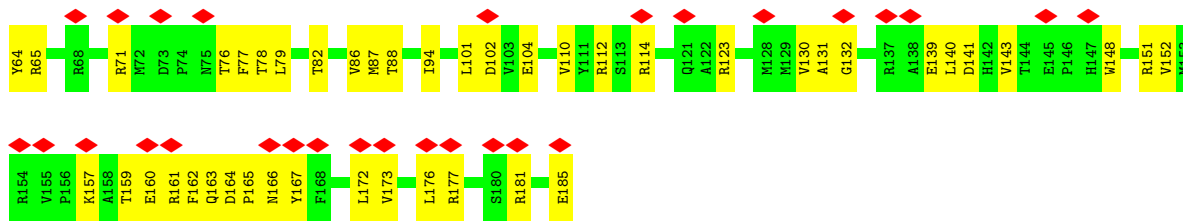


• Molecule 15: uL24m

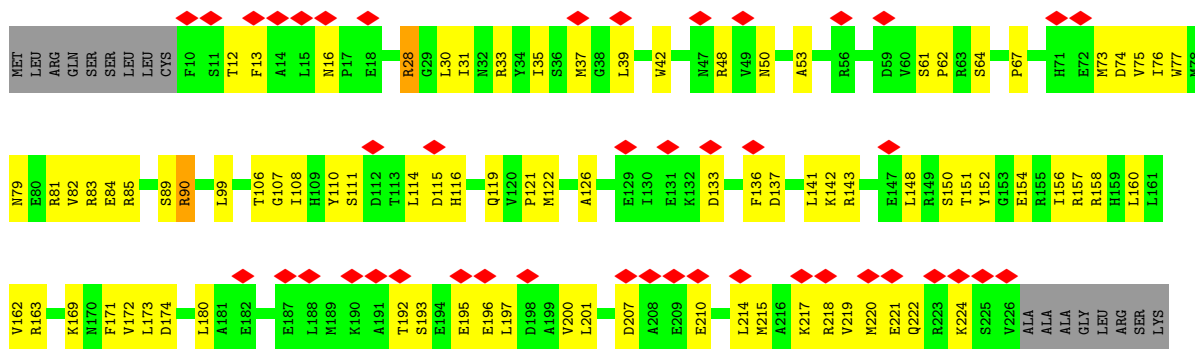


• Molecule 16: bL27m

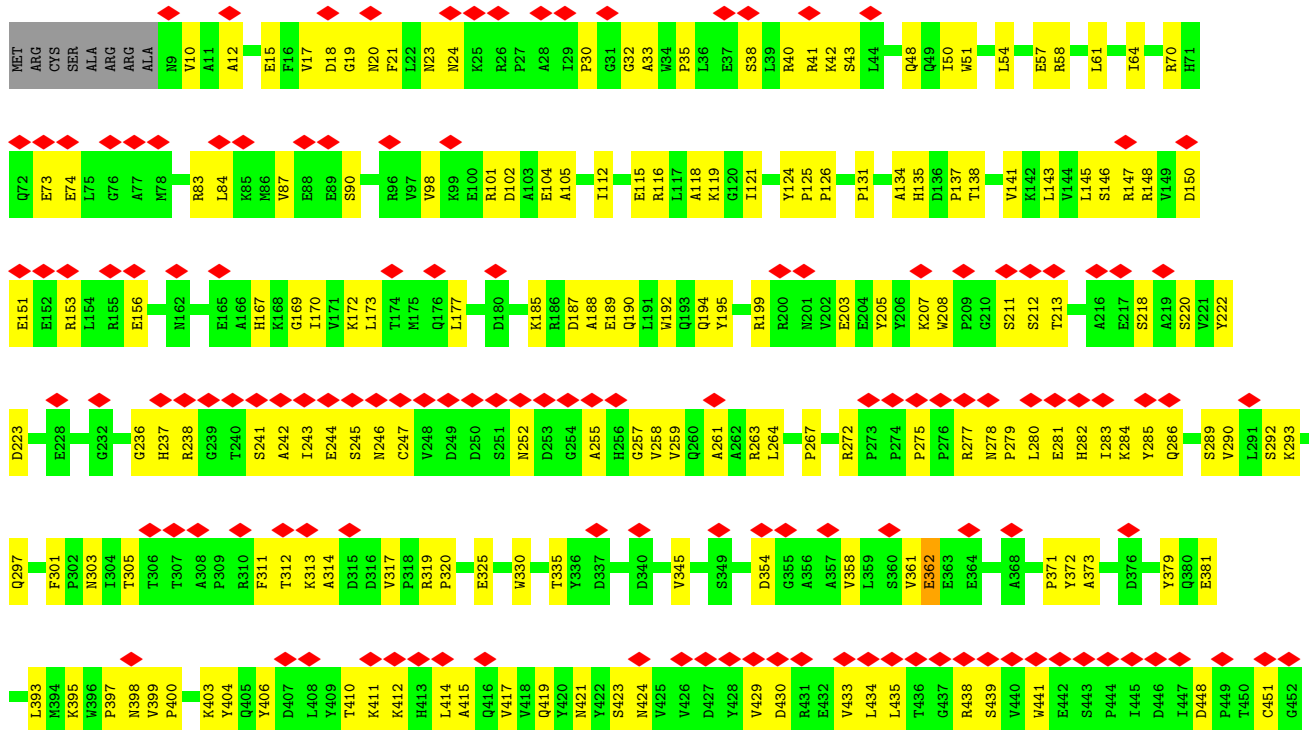


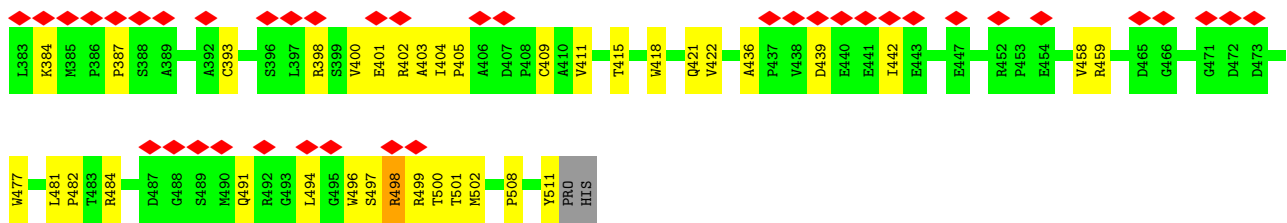


• Molecule 17: bL28m

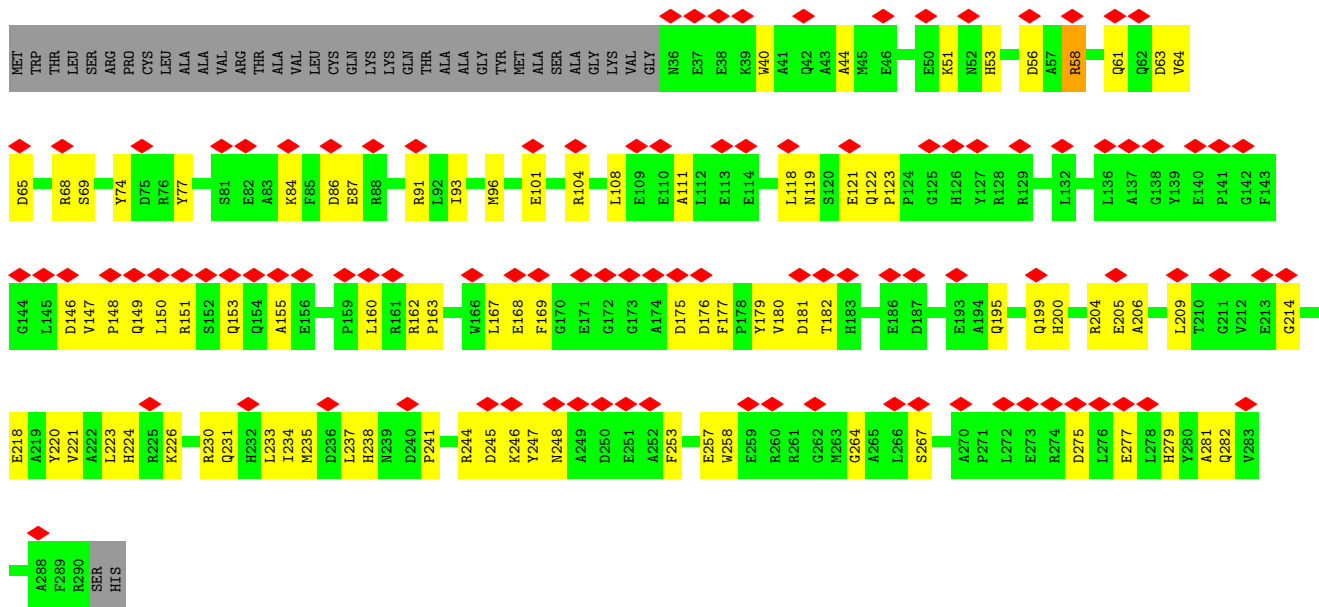


• Molecule 18: uL29m

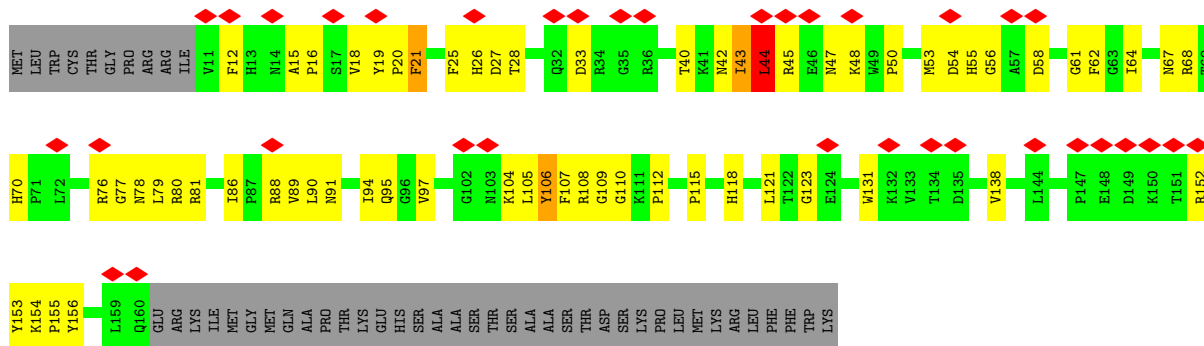




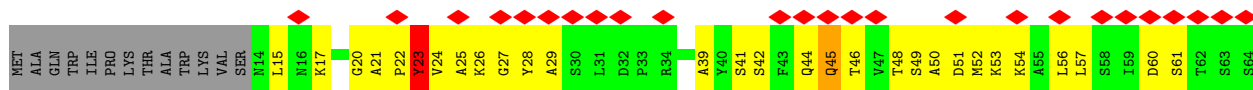
• Molecule 25: mL40

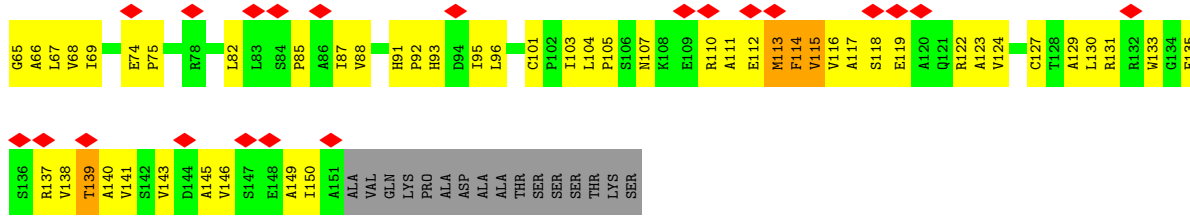


• Molecule 26: mL41

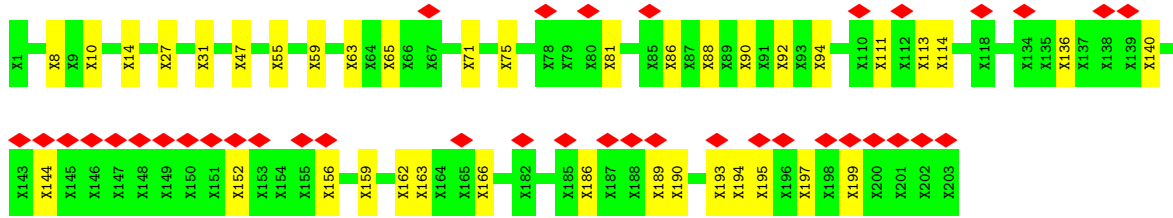
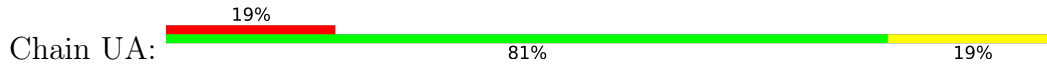


• Molecule 27: mL94

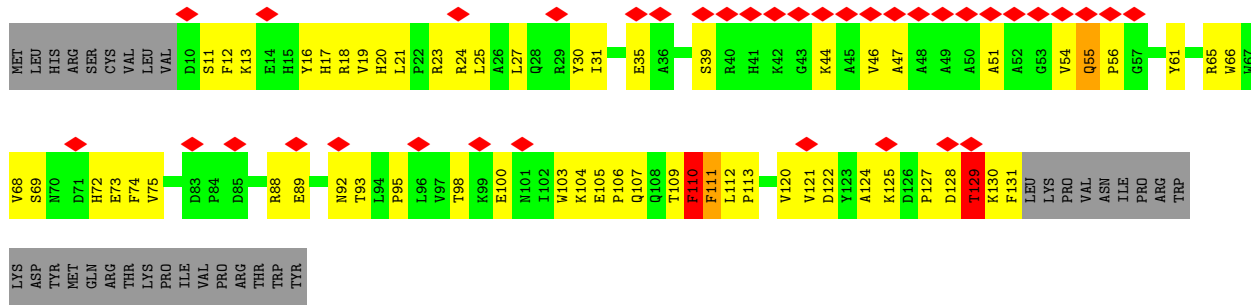




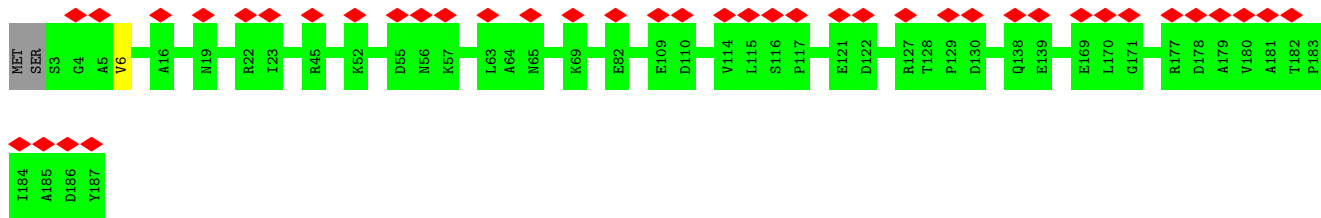
• Molecule 28: UA



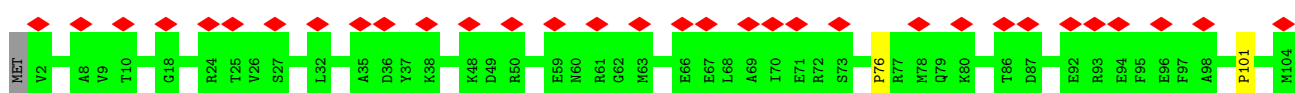
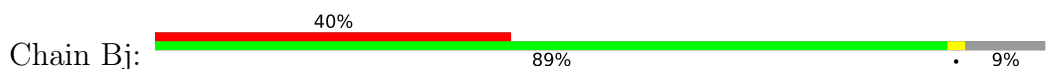
• Molecule 29: mL95

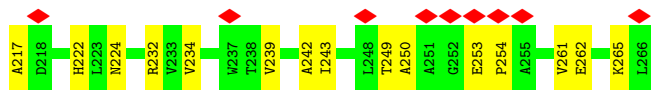


• Molecule 30: mL89

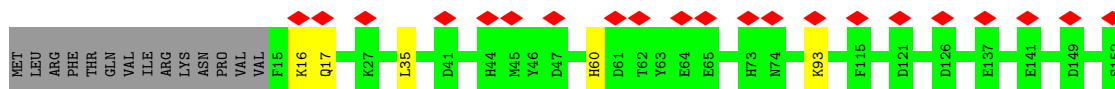
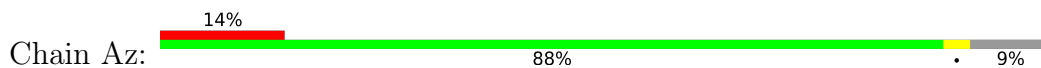


• Molecule 31: bL31m

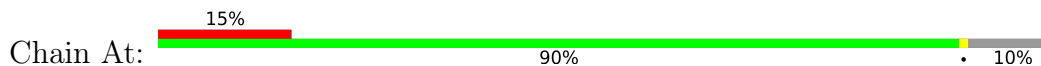




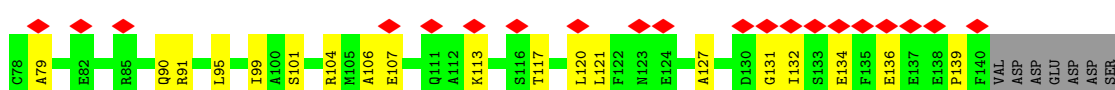
• Molecule 35: mL93



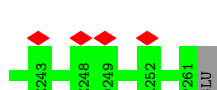
• Molecule 36: mL86



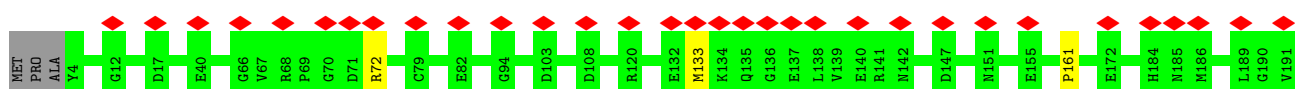
• Molecule 37: mL96

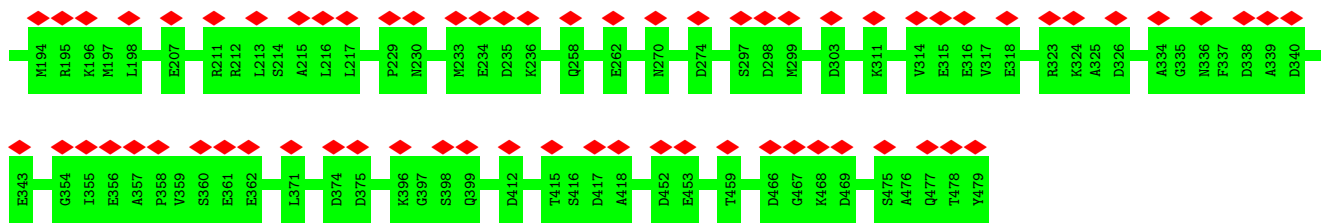


• Molecule 38: L51_S25_CI-B8 domain-containing protein

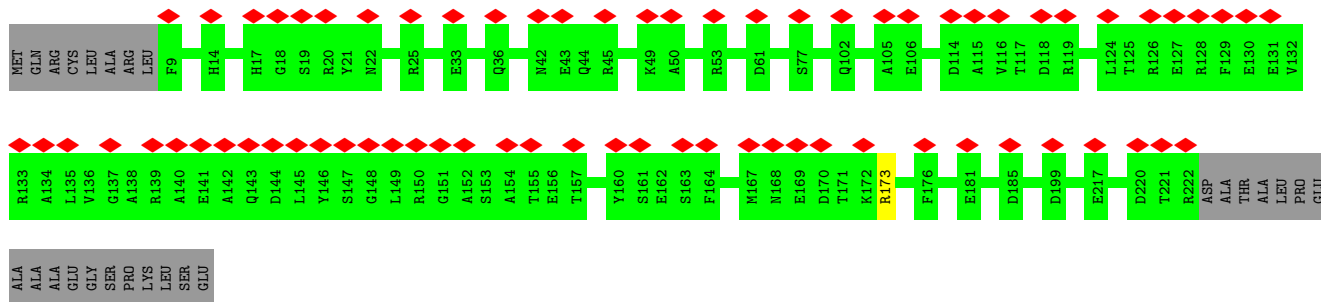
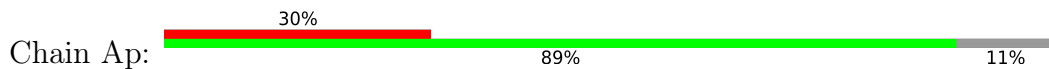


• Molecule 39: mL69

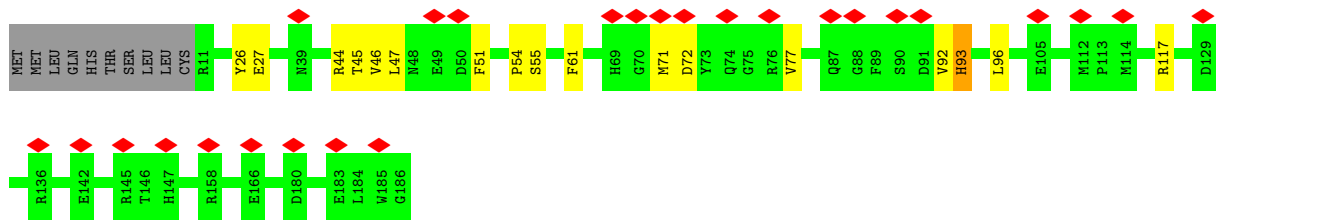
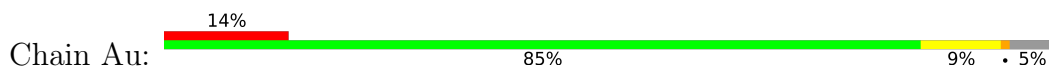




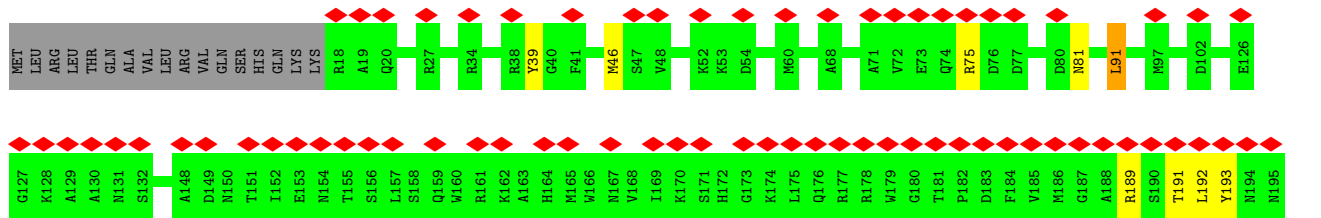
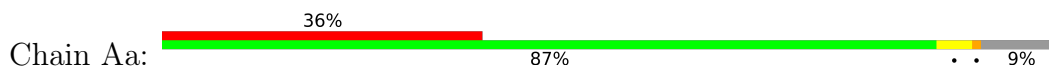
• Molecule 40: mL80



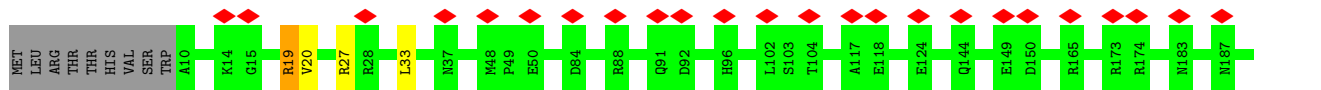
• Molecule 41: mL87

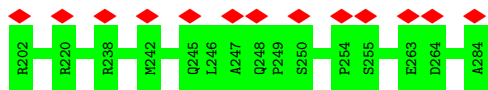


• Molecule 42: mL42

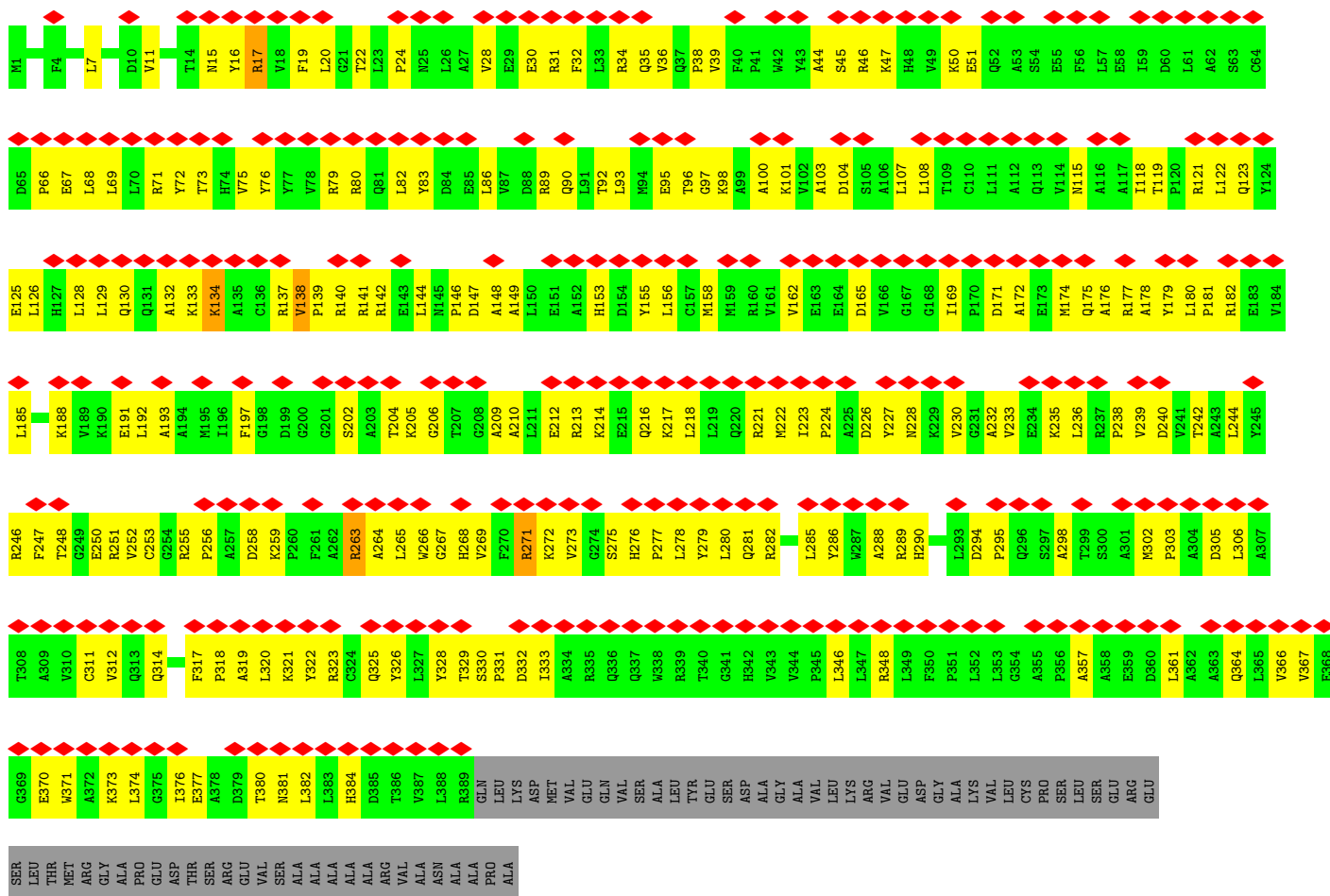
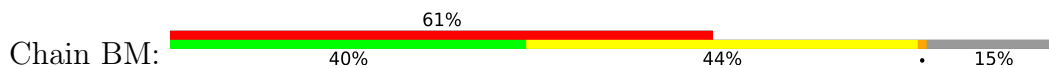


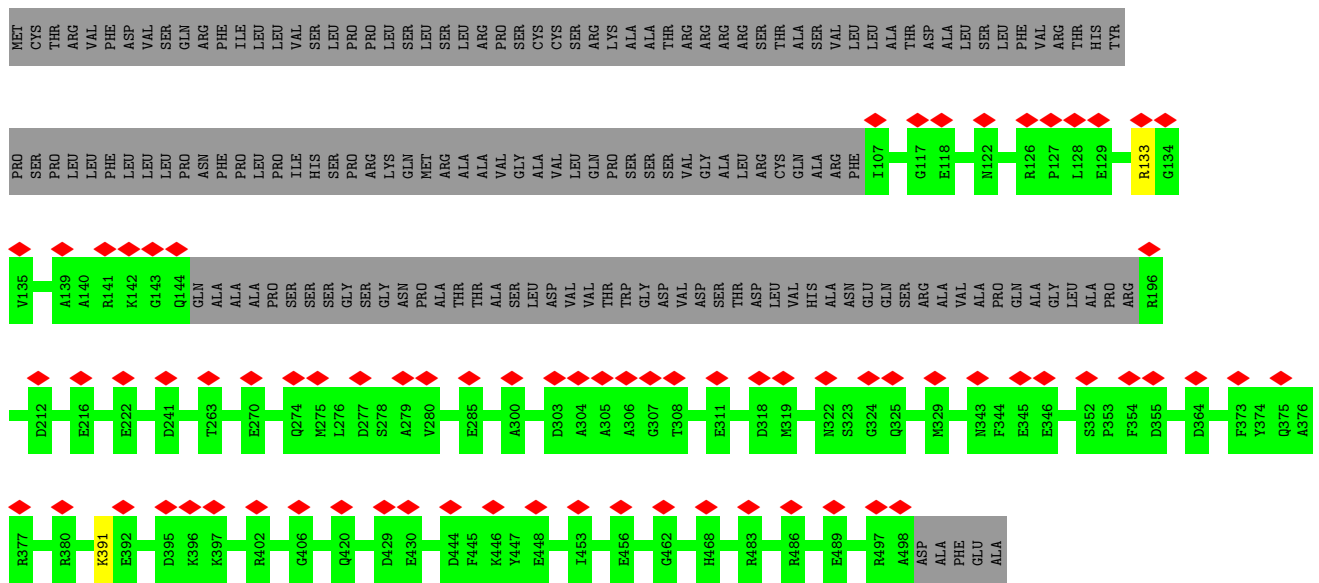
• Molecule 43: mL79



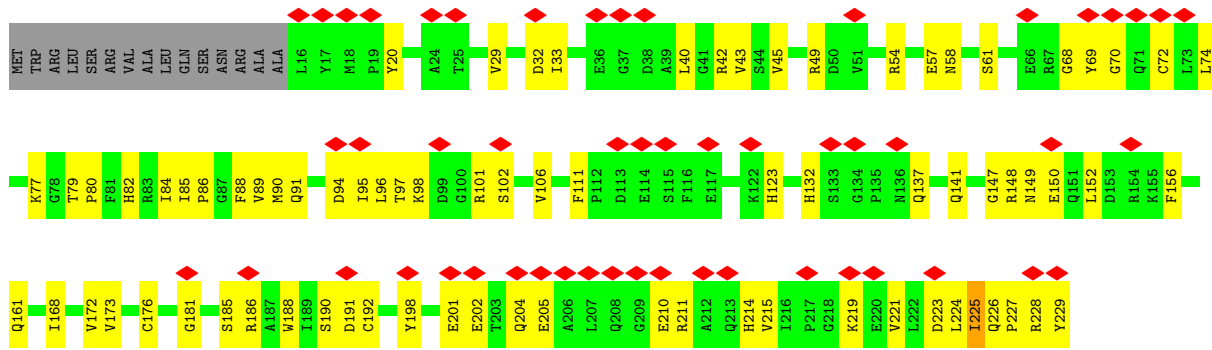


• Molecule 44: mL70

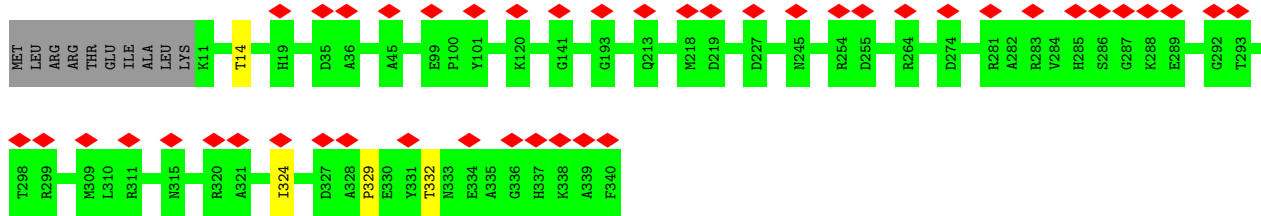




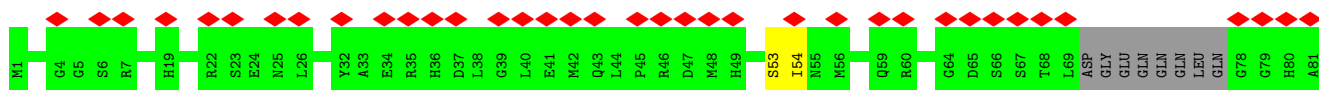
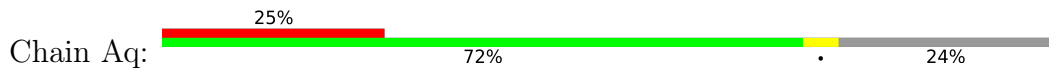
• Molecule 47: Peptidyl-prolyl cis-trans isomerase

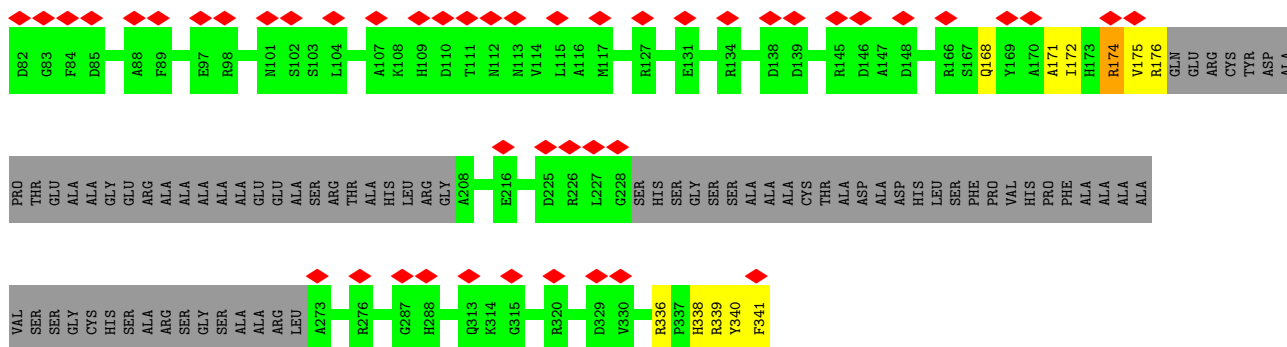


• Molecule 48: mL75

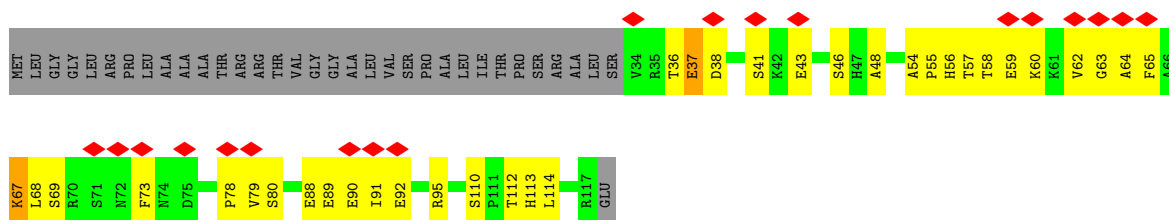


• Molecule 49: mL82

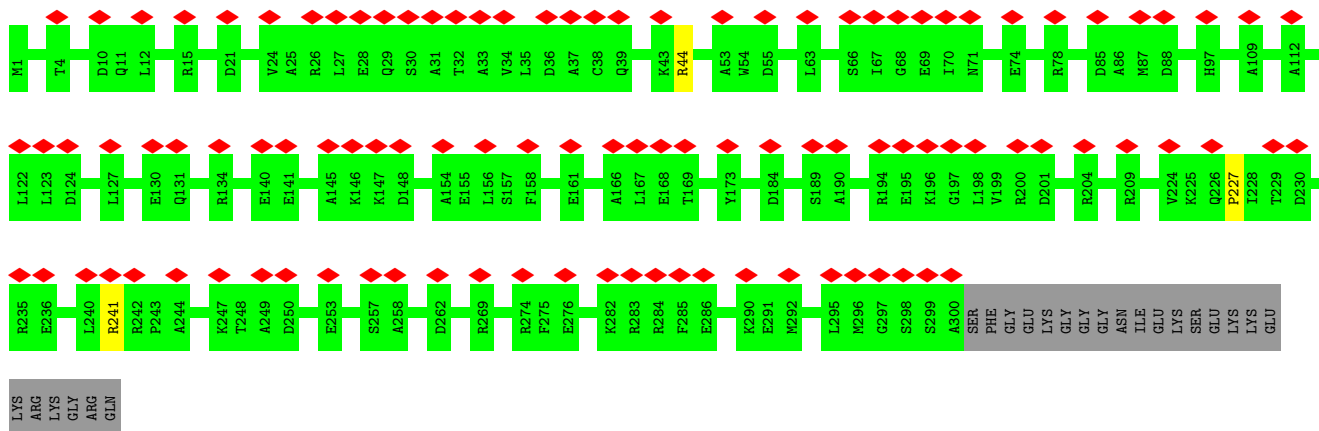




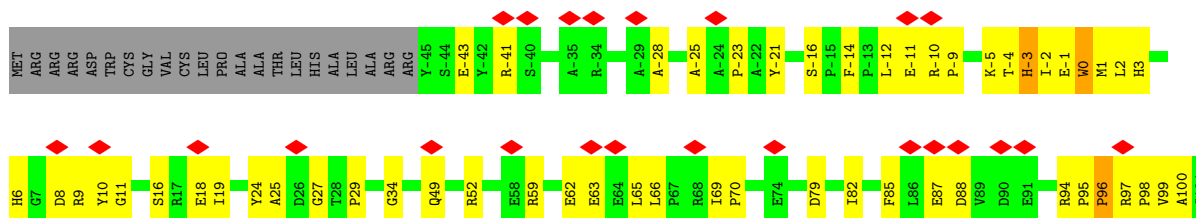
• Molecule 50: mL98

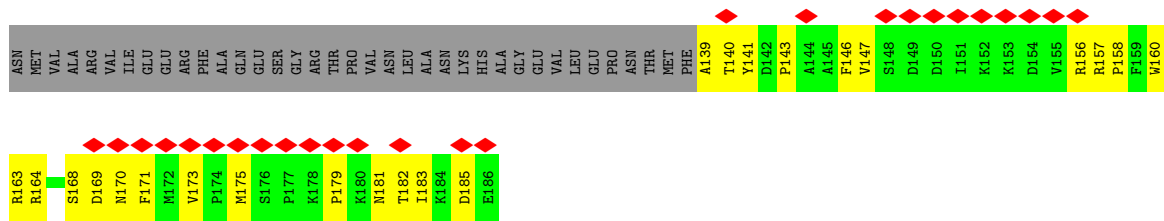


• Molecule 51: mL73

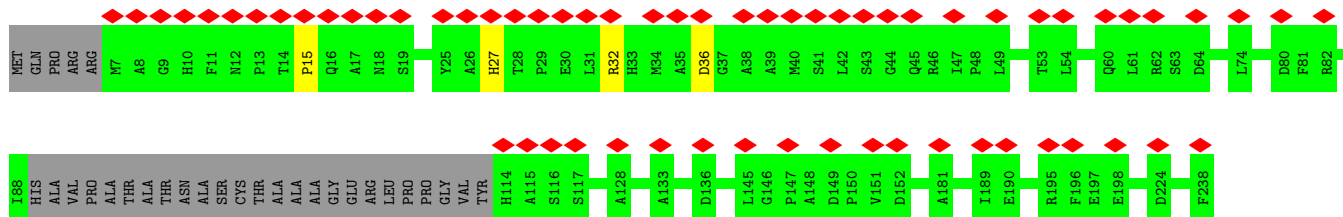
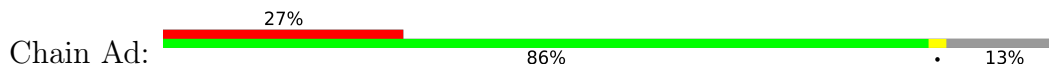


• Molecule 52: mL52,mL52

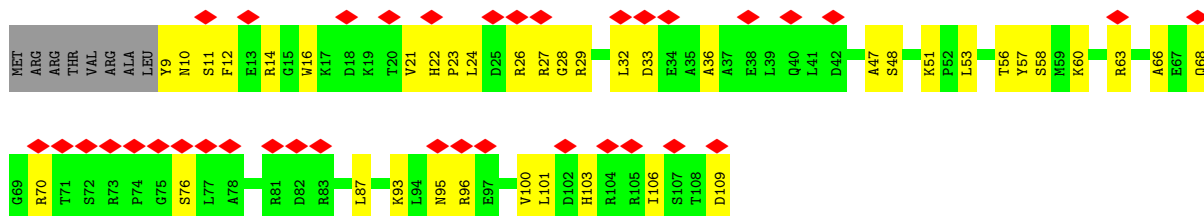




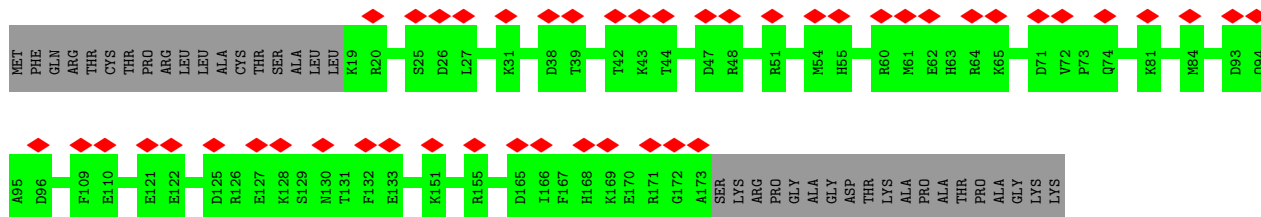
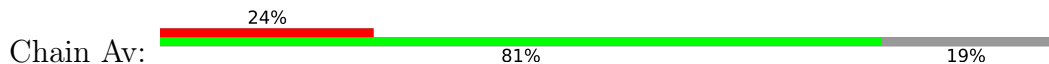
• Molecule 53: mL49



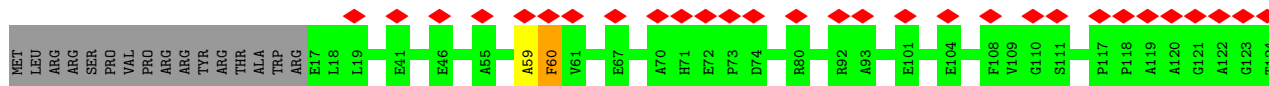
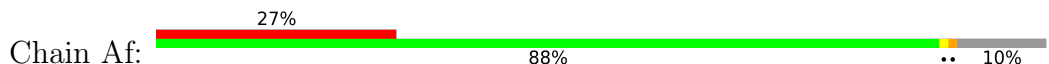
• Molecule 54: mL99

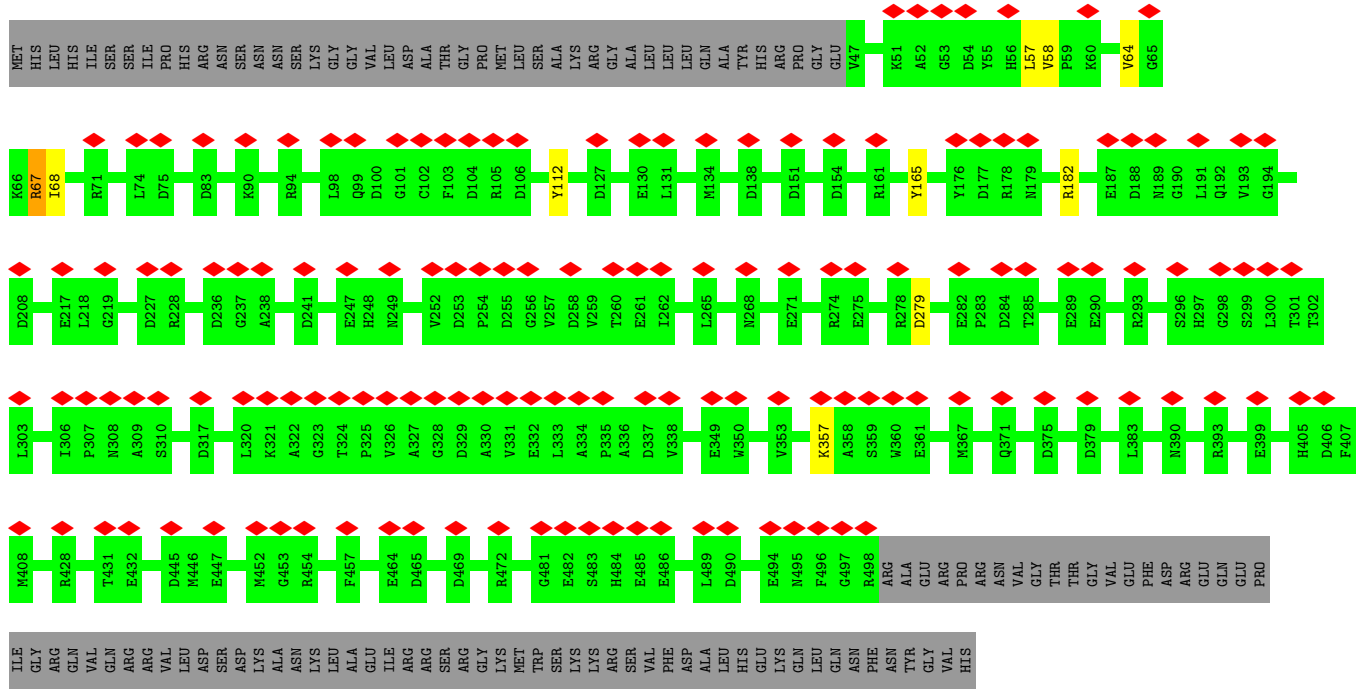


• Molecule 55: mL88

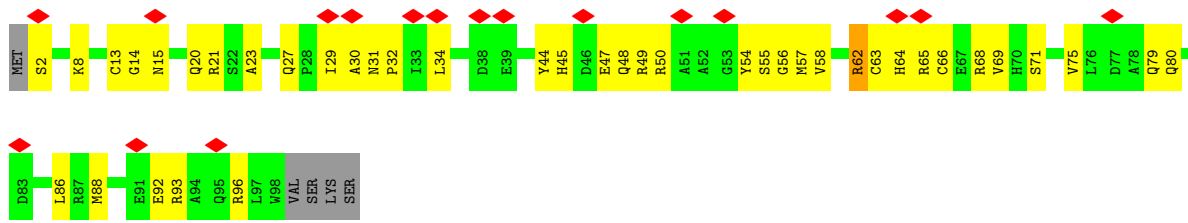


• Molecule 56: mL63

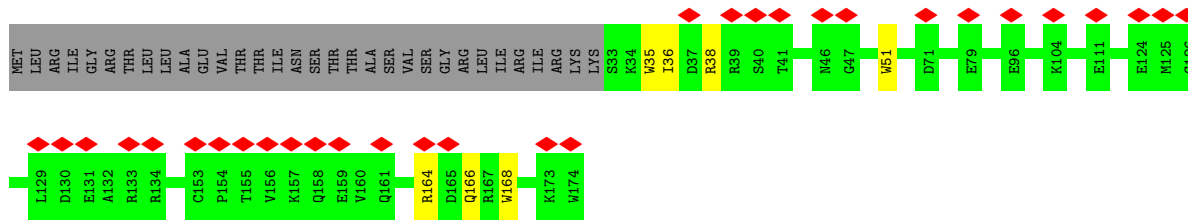
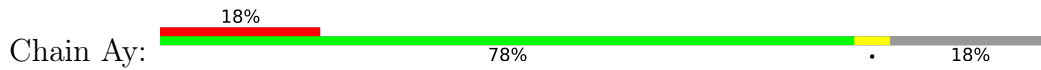




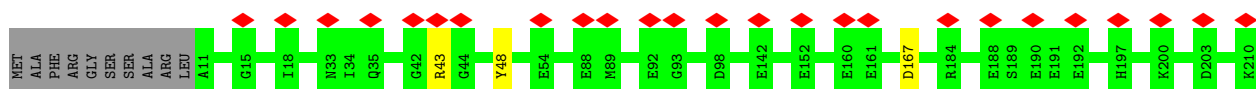
• Molecule 61: mL97

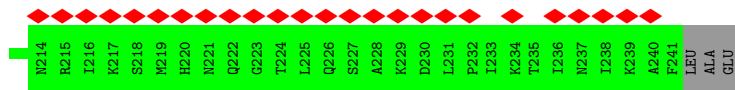


• Molecule 62: C2H2-type domain-containing protein

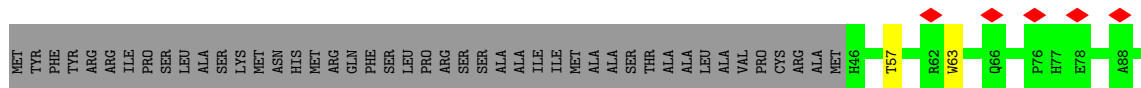
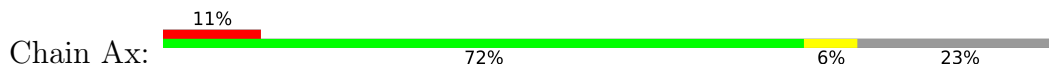


• Molecule 63: mL54/69

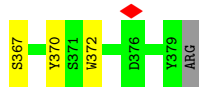
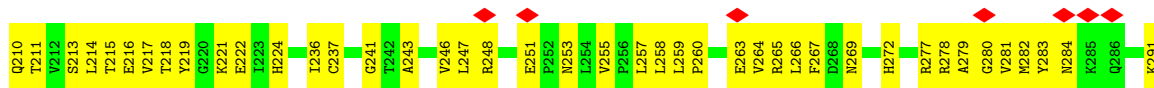
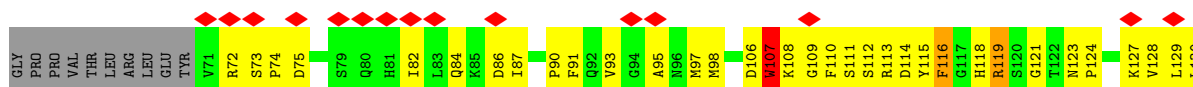




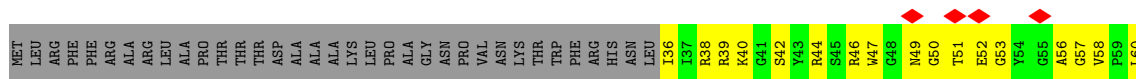
• Molecule 64: LIM zinc-binding domain-containing protein



• Molecule 65: Putative ribosomal protein L2



• Molecule 66: Putative ribosomal protein L14

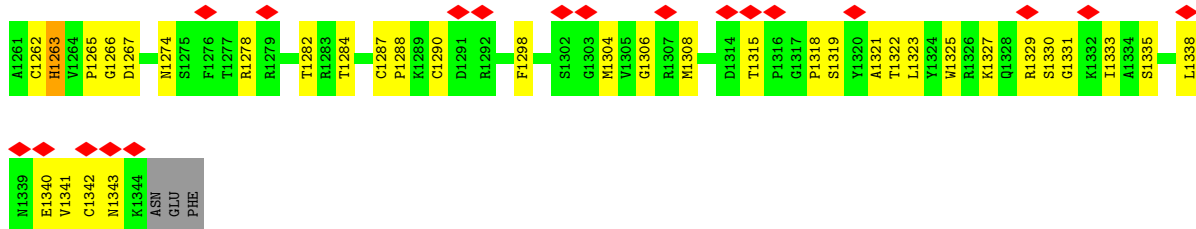


ASP PRO ALA THR THR VAL VAL VAL VAL VAL VAL ILE ILE ILE
GLU LEU MET ARG ARG LYS LYS LYS LYS LYS LYS LYS LYS

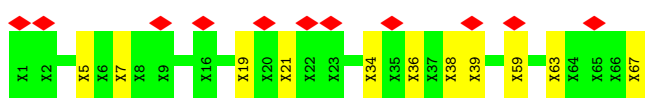
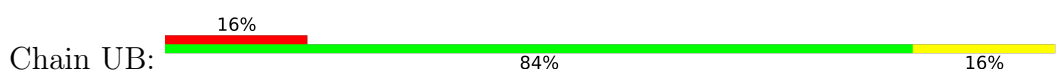
ARG GLU MET ASN ARG ALA LYS LEU LEU LEU LEU LEU LEU
LEU LEU VAL VAL PHE LEU LEU LEU LEU LEU LEU LEU LEU

ASP GLU LEU LEU ASN ASN LYS LEU LEU LEU LEU LEU LEU
GLU VAL VAL GLY LEU LEU LEU LEU LEU LEU LEU LEU LEU

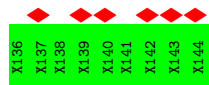
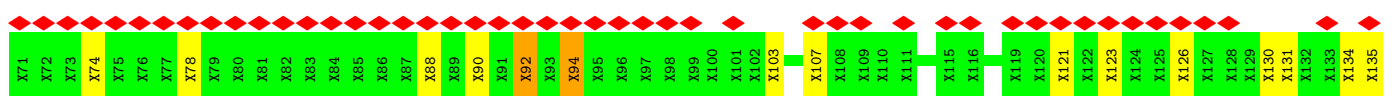
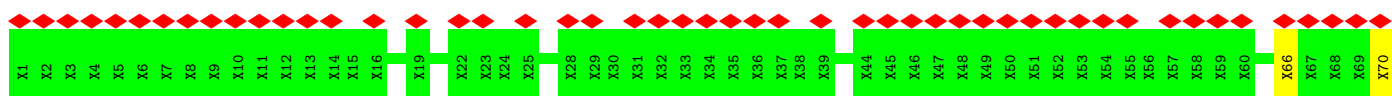
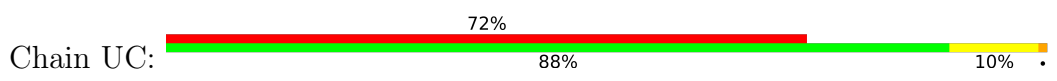
ALA LYS GLU ARG ARG ILE ASP ARG ARG ARG ARG ARG ARG
LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU



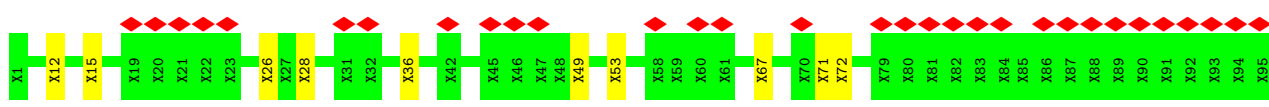
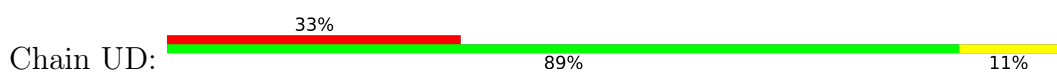
• Molecule 68: UB



• Molecule 69: UC



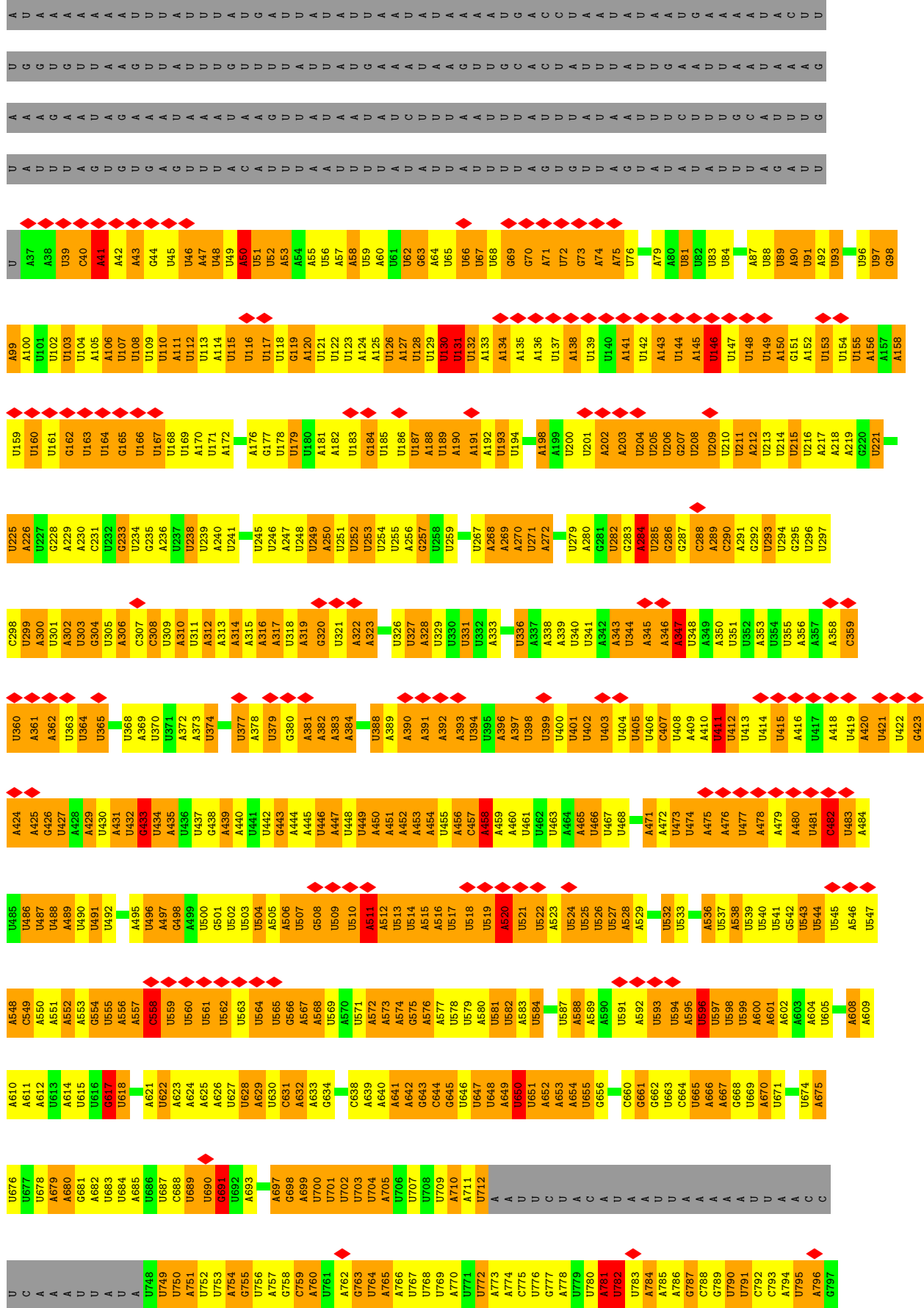
• Molecule 70: UD



• Molecule 71: Ribosomal RNA



U G A A A A A U U G A A A A A A U U U U G G A A A A A A U U U U U U U U A A A G A A U U U U A
A U U A A C A G A A A A A U A G A A C A C A A A A A C C C C G A U U G A U U U C A C A U D U G U A C U U G U
U U U U G G U C U A A A C G U U U U U G U U G U U G U A A U U U G G C C U U A A U U G G A A A A A A A G C U U
G A A C A C A A A A A U U U A A A A A C A A A U U G G A A U A A G G C C A A A G A A A A A A A A A A A
U A A A A A U A U
U A G A A A A U G A A A A A U U U A U
U G A A A U U G C A A A A G U A A A A A A A U U U A
U A U U A A A A U U A
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U A U U A A A A U U A
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4 Experimental information

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 ($e^-/\text{\AA}^2$)	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: ZN, NAD

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	0.58	0/3098	0.56	1/4217 (0.0%)
2	B	0.52	0/3623	0.54	1/4931 (0.0%)
3	C	0.52	0/1831	0.53	0/2498
4	D	0.45	0/1062	0.56	0/1438
5	E	0.46	0/2734	0.57	0/3687
6	F	0.53	0/1485	0.59	1/2019 (0.0%)
7	G	0.51	0/3110	0.61	2/4223 (0.0%)
8	H	0.46	0/1338	0.57	0/1808
9	I	0.50	0/2220	0.53	0/2998
10	J	0.48	0/1175	0.61	1/1582 (0.1%)
11	K	0.46	0/1499	0.50	0/2026
12	L	0.52	0/1452	0.55	0/1970
13	M	0.50	0/2168	0.60	2/2928 (0.1%)
14	N	0.55	0/1650	0.51	0/2242
15	O	0.42	0/2591	0.53	0/3507
16	P	0.51	0/1402	0.52	0/1892
17	Q	0.51	0/1827	0.54	0/2463
18	R	0.46	0/3852	0.54	1/5243 (0.0%)
19	S	0.48	0/1271	0.50	0/1712
20	T	0.51	0/501	0.49	0/665
21	U	0.49	0/756	0.74	1/1011 (0.1%)
22	V	0.53	0/1231	0.57	0/1645
23	W	0.51	0/483	0.69	0/657
24	X	0.49	0/3846	0.58	3/5250 (0.1%)
25	Y	0.41	0/2116	0.48	0/2866
26	Z	0.53	0/1268	0.69	0/1725
27	BA	0.42	0/1056	0.59	0/1435
29	BB	0.53	0/1061	0.62	0/1438
30	Aw	0.50	0/1552	0.52	0/2107
31	Bj	0.45	0/1389	0.50	0/1878
32	An	0.47	0/2677	0.65	0/3633
33	Al	0.49	0/2212	0.56	0/3013

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BI	0.42	0/1440	0.53	0/1953
35	Az	0.61	0/1259	0.55	0/1700
36	At	0.45	0/1373	0.51	1/1848 (0.1%)
37	BC	0.38	0/1135	0.51	0/1532
38	Ab	0.48	0/2249	0.49	0/3044
39	Ai	0.48	0/3879	0.51	0/5258
40	Ap	0.40	0/1819	0.47	0/2458
41	Au	0.53	0/1542	0.65	0/2082
42	Aa	0.52	1/1454 (0.1%)	0.71	4/1968 (0.2%)
43	Ao	0.52	0/2351	0.56	0/3196
44	BM	0.31	0/3136	0.53	1/4259 (0.0%)
45	Ar	0.55	0/1689	0.55	0/2280
46	Aj	0.47	0/2826	0.50	0/3807
47	BH	0.50	0/1700	0.53	0/2301
48	Am	0.48	0/2791	0.52	1/3775 (0.0%)
49	Aq	0.45	0/2128	0.61	1/2876 (0.0%)
50	BE	0.47	0/723	0.63	0/981
51	Ak	0.38	0/2403	0.50	0/3265
52	BP	0.48	0/1648	0.60	1/2238 (0.0%)
53	Ad	0.52	0/1682	0.60	0/2283
54	BF	0.47	0/871	0.52	0/1170
55	Av	0.40	0/1335	0.48	0/1797
56	Af	0.47	0/1165	0.71	3/1585 (0.2%)
57	As	0.42	0/804	0.53	0/1093
58	Ae	0.48	0/2441	0.51	0/3324
59	Ac	0.41	0/2236	0.49	0/3038
60	Ah	0.44	0/3780	0.54	0/5125
61	BD	0.50	0/826	0.48	0/1109
62	Ay	0.51	0/1269	0.58	0/1724
63	Ag	0.52	0/1968	0.52	0/2661
64	Ax	0.56	0/1439	0.82	3/1952 (0.2%)
65	BL	0.53	0/2572	0.67	3/3482 (0.1%)
66	BO	0.49	0/1266	0.68	0/1702
67	BG	0.46	0/657	0.70	0/888
71	1	0.91	9/25626 (0.0%)	1.08	102/39842 (0.3%)
All	All	0.58	10/147018 (0.0%)	0.70	133/204303 (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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Aa	193	TYR	N-CA	10.00	1.66	1.46
71	1	654	A	N9-C4	-7.40	1.33	1.37
71	1	886	A	N9-C4	-6.49	1.33	1.37
71	1	799	A	N9-C4	-5.76	1.34	1.37
71	1	814	A	N9-C4	-5.70	1.34	1.37

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	1	146	U	N1-C1'-C2'	-11.88	98.56	114.00
56	Af	60	PHE	N-CA-C	-10.81	81.82	111.00
52	BP	-3	HIS	CB-CA-C	10.28	130.95	110.40
71	1	359	C	C2-N1-C1'	9.27	129.00	118.80
56	Af	59	ALA	N-CA-C	-8.93	86.89	111.00

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	124	0
2	B	3513	0	3413	129	0
3	C	1772	0	1734	71	0
4	D	1036	0	1038	28	0
5	E	2668	0	2697	94	0
6	F	1435	0	1396	63	0
7	G	3012	0	2917	125	0
8	H	1305	0	1315	82	0
9	I	2153	0	2089	133	0
10	J	1146	0	1145	81	0
11	K	1467	0	1469	59	0
12	L	1419	0	1443	50	0
13	M	2116	0	2150	122	0
14	N	1599	0	1591	75	0
15	O	2537	0	2530	131	0
16	P	1367	0	1374	70	0
17	Q	1785	0	1784	79	0
18	R	3755	0	3722	152	0
19	S	1244	0	1272	40	0
20	T	487	0	496	26	0
21	U	744	0	798	71	0
22	V	1202	0	1224	78	0
23	W	465	0	446	13	0
24	X	3733	0	3604	142	0
25	Y	2067	0	1955	67	0
26	Z	1223	0	1192	73	0
27	BA	1038	0	1052	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	UA	1015	0	213	22	0
29	BB	1028	0	1003	66	0
30	Aw	1509	0	1470	0	0
31	Bj	1358	0	1422	0	0
32	An	2605	0	2536	0	0
33	Al	2152	0	2112	0	0
34	BI	1409	0	1400	46	0
35	Az	1215	0	1144	0	0
36	At	1346	0	1299	0	0
37	BC	1114	0	1096	43	0
38	Ab	2185	0	2095	0	0
39	Ai	3789	0	3752	0	0
40	Ap	1775	0	1699	0	0
41	Au	1490	0	1450	0	0
42	Aa	1417	0	1377	0	0
43	Ao	2276	0	2176	0	0
44	BM	3069	0	3105	196	0
45	Ar	1644	0	1608	0	0
46	Aj	2766	0	2765	0	0
47	BH	1659	0	1607	64	0
48	Am	2708	0	2634	0	0
49	Aq	2074	0	2050	0	0
50	BE	700	0	665	35	0
51	Ak	2352	0	2369	0	0
52	BP	1593	0	1529	80	0
53	Ad	1632	0	1607	0	0
54	BF	851	0	831	41	0
55	Av	1300	0	1284	0	0
56	Af	1132	0	1108	0	0
57	As	787	0	777	0	0
58	Ae	2359	0	2328	0	0
59	Ac	2174	0	2096	0	0
60	Ah	3686	0	3572	0	0
61	BD	807	0	772	32	0
62	Ay	1226	0	1157	0	0
63	Ag	1916	0	1888	0	0
64	Ax	1388	0	1308	0	0
65	BL	2497	0	2489	163	0
66	BO	1239	0	1246	148	0
67	BG	643	0	617	24	0
68	UB	335	0	73	8	0
69	UC	720	0	151	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	UD	475	0	105	8	0
71	1	22918	0	11465	1051	0
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	0	0
All	All	143667	0	128129	3654	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 3654 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)
21:U:25:PHE:HD1	71:1:933:G:N2	1.46	1.10
21:U:25:PHE:HB3	71:1:972:A:H61	1.09	1.09
21:U:39:VAL:HG21	21:U:85:GLU:HB2	1.36	1.03
10:J:67:ARG:HG2	10:J:68:PRO:HD2	1.38	1.02
10:J:67:ARG:CG	10:J:68:PRO:HD2	1.90	1.01

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%)	19	59
2	B	433/436 (99%)	380 (88%)	52 (12%)	1 (0%)	47	79
3	C	210/262 (80%)	179 (85%)	31 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	126/204 (62%)	108 (86%)	18 (14%)	0	100	100
5	E	324/346 (94%)	294 (91%)	30 (9%)	0	100	100
6	F	168/171 (98%)	152 (90%)	15 (9%)	1 (1%)	25	64
7	G	363/374 (97%)	313 (86%)	48 (13%)	2 (1%)	25	64
8	H	160/168 (95%)	144 (90%)	14 (9%)	2 (1%)	12	50
9	I	255/305 (84%)	224 (88%)	31 (12%)	0	100	100
10	J	139/144 (96%)	102 (73%)	36 (26%)	1 (1%)	22	61
11	K	177/194 (91%)	158 (89%)	19 (11%)	0	100	100
12	L	176/186 (95%)	157 (89%)	18 (10%)	1 (1%)	25	64
13	M	257/279 (92%)	217 (84%)	39 (15%)	1 (0%)	34	71
14	N	187/252 (74%)	163 (87%)	24 (13%)	0	100	100
15	O	305/476 (64%)	271 (89%)	29 (10%)	5 (2%)	9	46
16	P	163/185 (88%)	145 (89%)	17 (10%)	1 (1%)	25	64
17	Q	215/234 (92%)	192 (89%)	22 (10%)	1 (0%)	29	68
18	R	470/480 (98%)	409 (87%)	60 (13%)	1 (0%)	47	79
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%)	6	39
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%)	25	64
25	Y	253/292 (87%)	234 (92%)	19 (8%)	0	100	100
26	Z	148/197 (75%)	117 (79%)	28 (19%)	3 (2%)	7	41
27	BA	136/167 (81%)	103 (76%)	29 (21%)	4 (3%)	4	33
29	BB	120/156 (77%)	95 (79%)	23 (19%)	2 (2%)	9	45
30	Aw	183/187 (98%)	161 (88%)	22 (12%)	0	100	100
31	Bj	166/185 (90%)	143 (86%)	22 (13%)	1 (1%)	25	64
32	An	312/331 (94%)	256 (82%)	49 (16%)	7 (2%)	6	39
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%)	10	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	At	163/183 (89%)	145 (89%)	18 (11%)	0	100	100
37	BC	138/147 (94%)	127 (92%)	11 (8%)	0	100	100
38	Ab	258/262 (98%)	226 (88%)	32 (12%)	0	100	100
39	Ai	474/479 (99%)	413 (87%)	60 (13%)	1 (0%)	47	79
40	Ap	212/240 (88%)	188 (89%)	24 (11%)	0	100	100
41	Au	174/186 (94%)	132 (76%)	36 (21%)	6 (3%)	3	31
42	Aa	176/195 (90%)	142 (81%)	32 (18%)	2 (1%)	14	53
43	Ao	273/284 (96%)	233 (85%)	38 (14%)	2 (1%)	22	61
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%)	6	37
50	BE	82/118 (70%)	56 (68%)	25 (30%)	1 (1%)	13	51
51	Ak	298/323 (92%)	254 (85%)	44 (15%)	0	100	100
52	BP	191/254 (75%)	162 (85%)	28 (15%)	1 (0%)	29	68
53	Ad	203/237 (86%)	163 (80%)	38 (19%)	2 (1%)	15	55
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%)	34	71
61	BD	95/102 (93%)	85 (90%)	10 (10%)	0	100	100
62	Ay	140/174 (80%)	117 (84%)	18 (13%)	5 (4%)	3	29
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%)	7	41
66	BO	153/190 (80%)	105 (69%)	45 (29%)	3 (2%)	7	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	BG	83/1347 (6%)	57 (69%)	23 (28%)	3 (4%)	3	29
All	All	14352/18415 (78%)	12263 (85%)	2005 (14%)	84 (1%)	29	64

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%)	92	97
2	B	380/381 (100%)	375 (99%)	5 (1%)	69	86
3	C	190/227 (84%)	190 (100%)	0	100	100
4	D	106/154 (69%)	104 (98%)	2 (2%)	57	80
5	E	285/301 (95%)	270 (95%)	15 (5%)	22	58
6	F	151/152 (99%)	149 (99%)	2 (1%)	69	86
7	G	315/323 (98%)	305 (97%)	10 (3%)	39	70
8	H	138/143 (96%)	137 (99%)	1 (1%)	84	93
9	I	223/262 (85%)	221 (99%)	2 (1%)	78	90
10	J	119/122 (98%)	115 (97%)	4 (3%)	37	69
11	K	151/162 (93%)	149 (99%)	2 (1%)	69	86
12	L	151/158 (96%)	151 (100%)	0	100	100
13	M	226/242 (93%)	222 (98%)	4 (2%)	59	81
14	N	175/220 (80%)	172 (98%)	3 (2%)	60	82
15	O	278/397 (70%)	272 (98%)	6 (2%)	52	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	147/163 (90%)	147 (100%)	0	100	100
17	Q	191/204 (94%)	189 (99%)	2 (1%)	76	88
18	R	406/412 (98%)	403 (99%)	3 (1%)	84	93
19	S	135/336 (40%)	135 (100%)	0	100	100
20	T	52/74 (70%)	52 (100%)	0	100	100
21	U	80/100 (80%)	75 (94%)	5 (6%)	18	53
22	V	125/135 (93%)	120 (96%)	5 (4%)	31	65
23	W	50/164 (30%)	46 (92%)	4 (8%)	12	43
24	X	402/438 (92%)	395 (98%)	7 (2%)	60	82
25	Y	209/236 (89%)	207 (99%)	2 (1%)	76	88
26	Z	132/172 (77%)	128 (97%)	4 (3%)	41	71
27	BA	112/135 (83%)	108 (96%)	4 (4%)	35	67
29	BB	106/140 (76%)	103 (97%)	3 (3%)	43	72
30	Aw	157/159 (99%)	156 (99%)	1 (1%)	86	94
31	Bj	150/165 (91%)	149 (99%)	1 (1%)	84	93
32	An	274/289 (95%)	265 (97%)	9 (3%)	38	69
33	Al	236/299 (79%)	230 (98%)	6 (2%)	47	75
34	BI	153/221 (69%)	152 (99%)	1 (1%)	84	93
35	Az	129/143 (90%)	126 (98%)	3 (2%)	50	76
36	At	140/153 (92%)	140 (100%)	0	100	100
37	BC	117/124 (94%)	116 (99%)	1 (1%)	78	90
38	Ab	233/235 (99%)	233 (100%)	0	100	100
39	Ai	408/410 (100%)	406 (100%)	2 (0%)	88	95
40	Ap	189/208 (91%)	188 (100%)	1 (0%)	88	95
41	Au	154/164 (94%)	145 (94%)	9 (6%)	20	55
42	Aa	150/166 (90%)	145 (97%)	5 (3%)	38	69
43	Ao	236/245 (96%)	234 (99%)	2 (1%)	81	91
44	BM	319/370 (86%)	315 (99%)	4 (1%)	69	86
45	Ar	169/179 (94%)	168 (99%)	1 (1%)	86	94
46	Aj	286/420 (68%)	284 (99%)	2 (1%)	84	93
47	BH	177/189 (94%)	175 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Am	278/287 (97%)	276 (99%)	2 (1%)	84	93
49	Aq	221/276 (80%)	216 (98%)	5 (2%)	50	76
50	BE	76/100 (76%)	75 (99%)	1 (1%)	69	86
51	Ak	254/272 (93%)	252 (99%)	2 (1%)	81	91
52	BP	167/215 (78%)	165 (99%)	2 (1%)	71	87
53	Ad	172/193 (89%)	171 (99%)	1 (1%)	86	94
54	BF	88/95 (93%)	87 (99%)	1 (1%)	73	88
55	Av	141/169 (83%)	141 (100%)	0	100	100
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%)	244 (98%)	5 (2%)	55	79
59	Ac	232/253 (92%)	230 (99%)	2 (1%)	78	90
60	Ah	385/485 (79%)	376 (98%)	9 (2%)	50	76
61	BD	85/90 (94%)	83 (98%)	2 (2%)	49	75
62	Ay	130/158 (82%)	128 (98%)	2 (2%)	65	84
63	Ag	202/211 (96%)	199 (98%)	3 (2%)	65	84
64	Ax	150/190 (79%)	141 (94%)	9 (6%)	19	54
65	BL	268/329 (82%)	261 (97%)	7 (3%)	46	74
66	BO	130/158 (82%)	125 (96%)	5 (4%)	33	66
67	BG	67/1047 (6%)	65 (97%)	2 (3%)	41	71
All	All	12529/15614 (80%)	12323 (98%)	206 (2%)	64	83

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	Az	60	HIS
46	Aj	391	LYS
66	BO	105	ARG
39	Ai	133	MET
42	Aa	39	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 307 such sidechains are listed below:

Mol	Chain	Res	Type
48	Am	106	HIS
64	Ax	85	HIS
48	Am	278	GLN
56	Af	20	HIS
66	BO	124	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
71	1	1085/9070 (11%)	638 (58%)	127 (11%)

5 of 638 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 [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 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	-	42,48,48	0.61	0	50,73,73	1.12	5 (10%)

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	-	-	11/26/62/62	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
73	Ag	301	NAD	O4D-C1D-C2D	-4.10	100.93	106.93
73	Ag	301	NAD	C3D-C2D-C1D	3.28	105.91	100.98
73	Ag	301	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
73	Ag	301	NAD	C5A-C6A-N6A	2.15	123.62	120.35
73	Ag	301	NAD	O4B-C4B-C3B	-2.09	100.98	105.11

There are no chirality outliers.

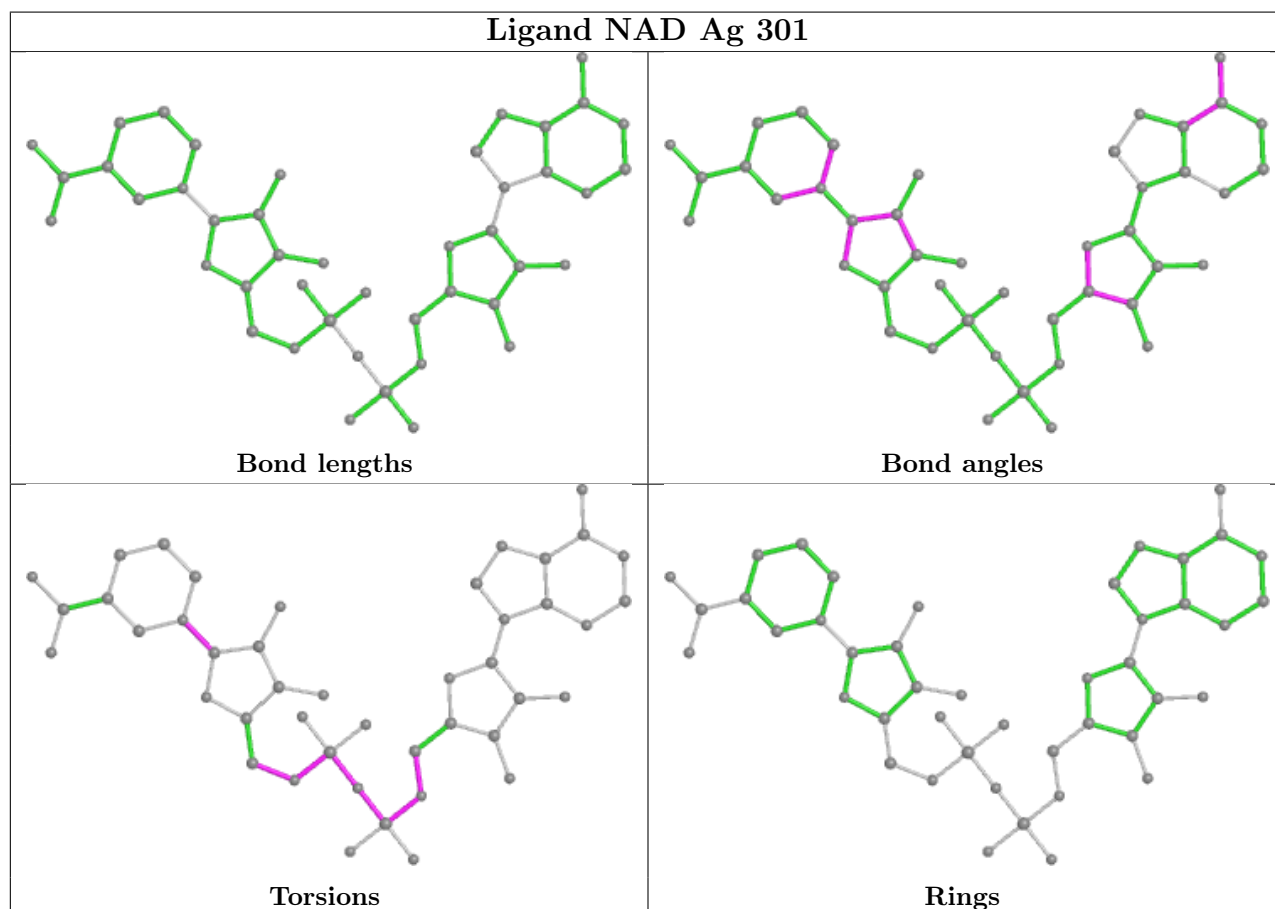
5 of 11 torsion outliers are listed below:

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.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

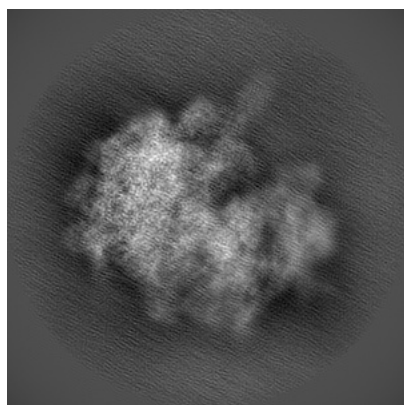
6 Map visualisation [i](#)

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.

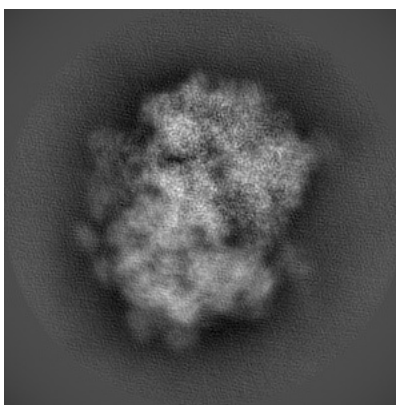
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

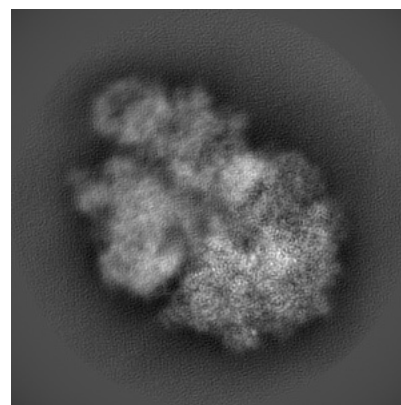
6.1.1 Primary map



X



Y

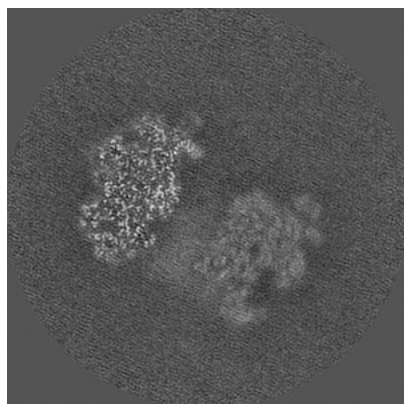


Z

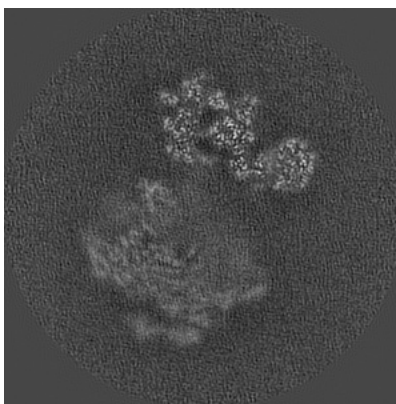
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

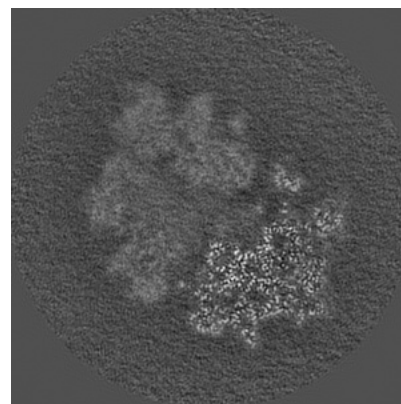
6.2.1 Primary map



X Index: 200



Y Index: 200

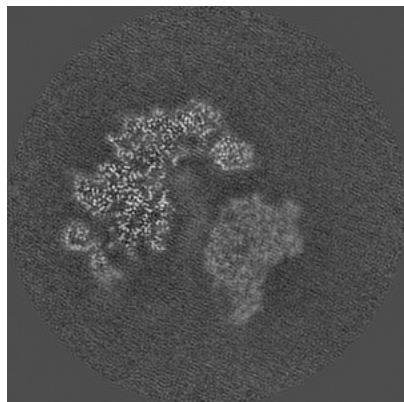


Z Index: 200

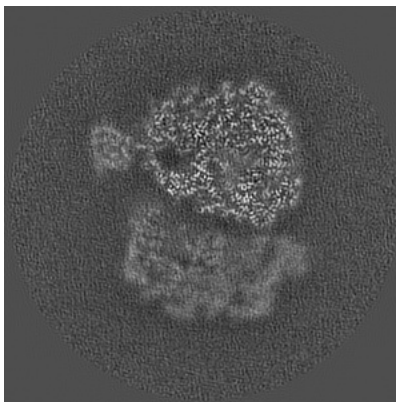
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

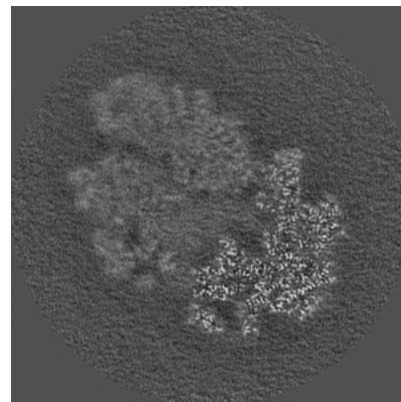
6.3.1 Primary map



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 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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

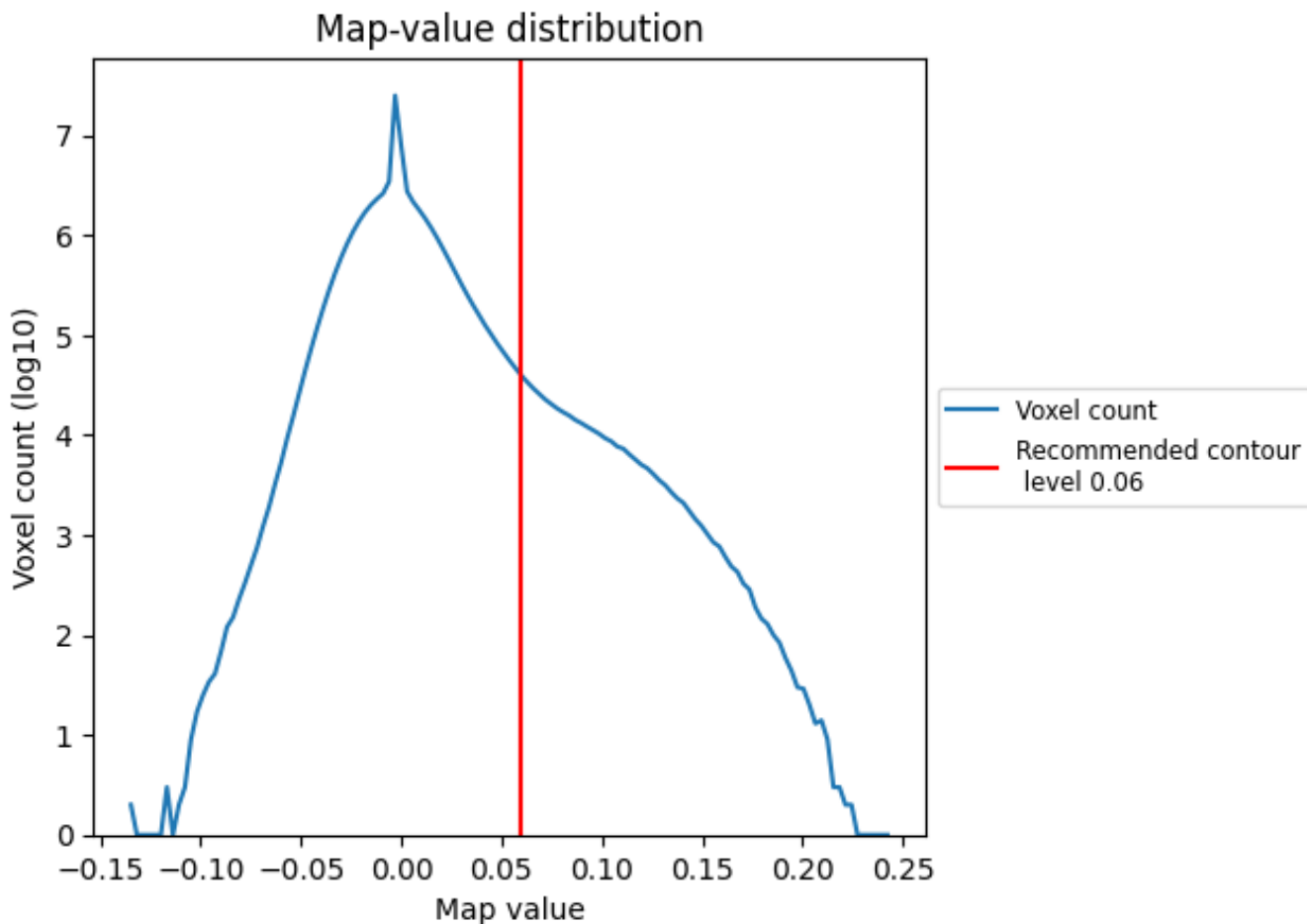
6.5 Mask visualisation

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

7 Map analysis [i](#)

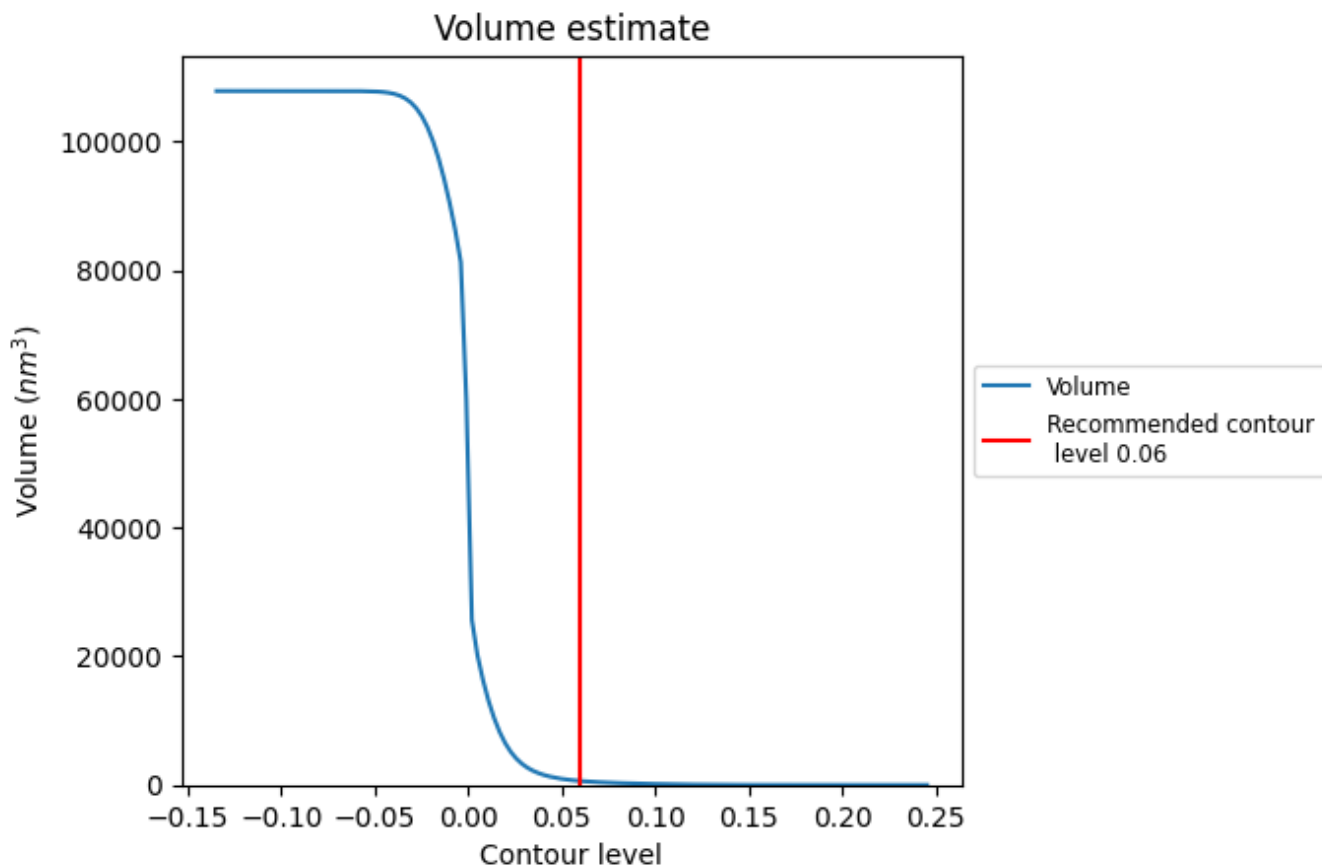
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

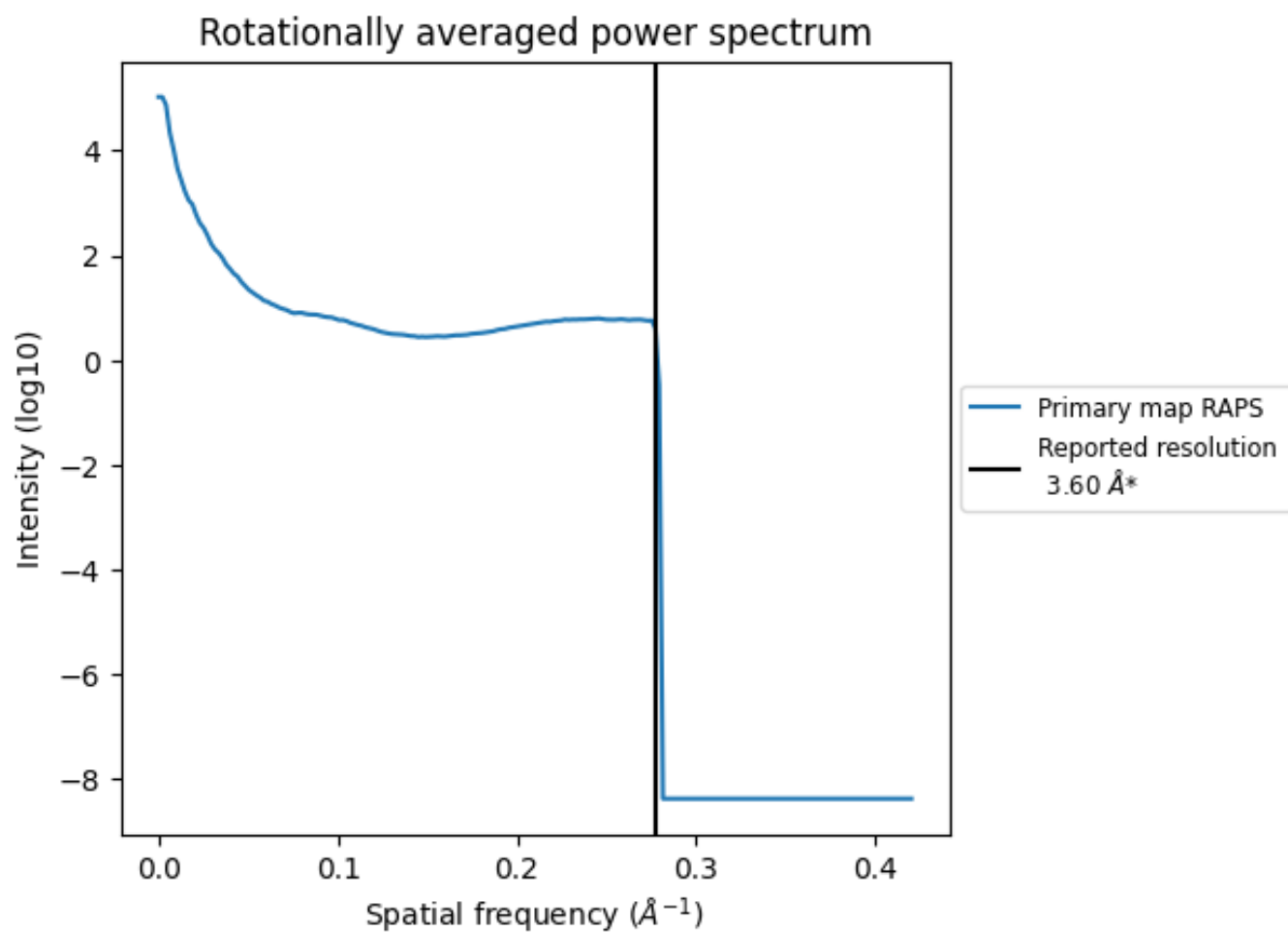
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; 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

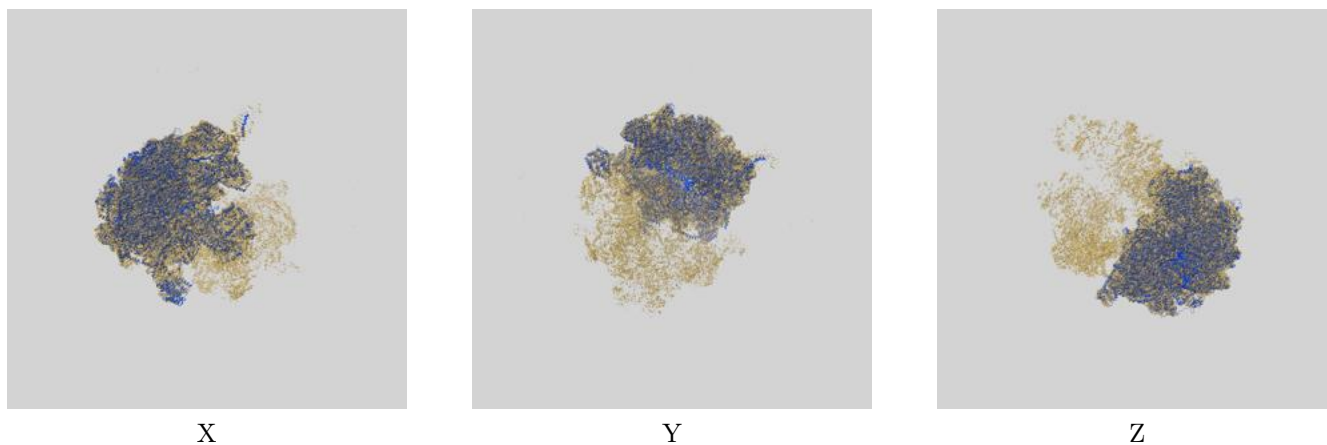
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

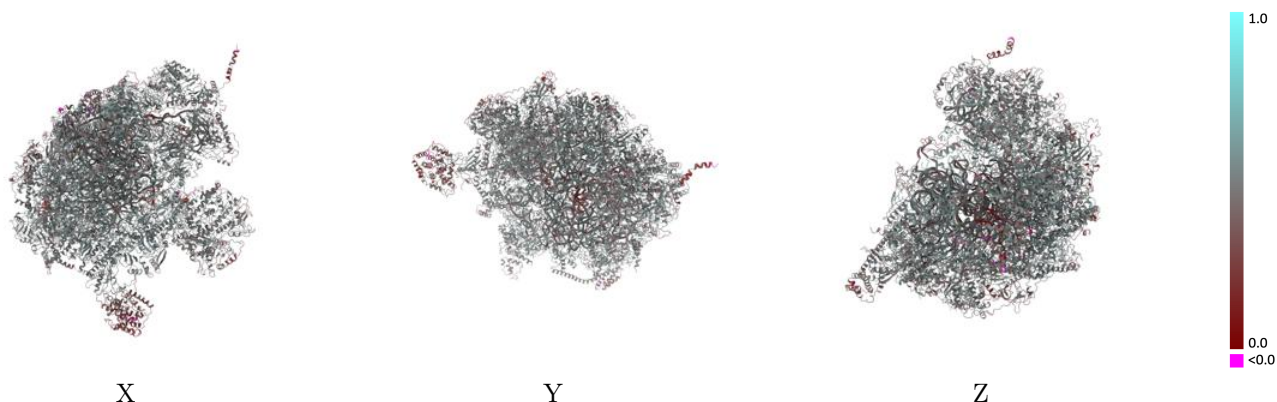
This section contains information regarding the fit between EMDB map EMD-11796 and PDB model 7AIH. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



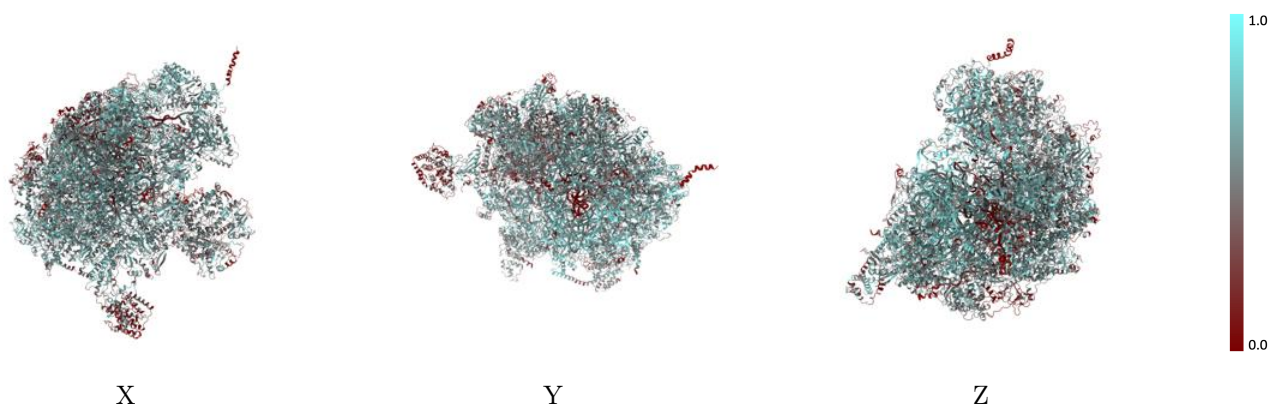
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



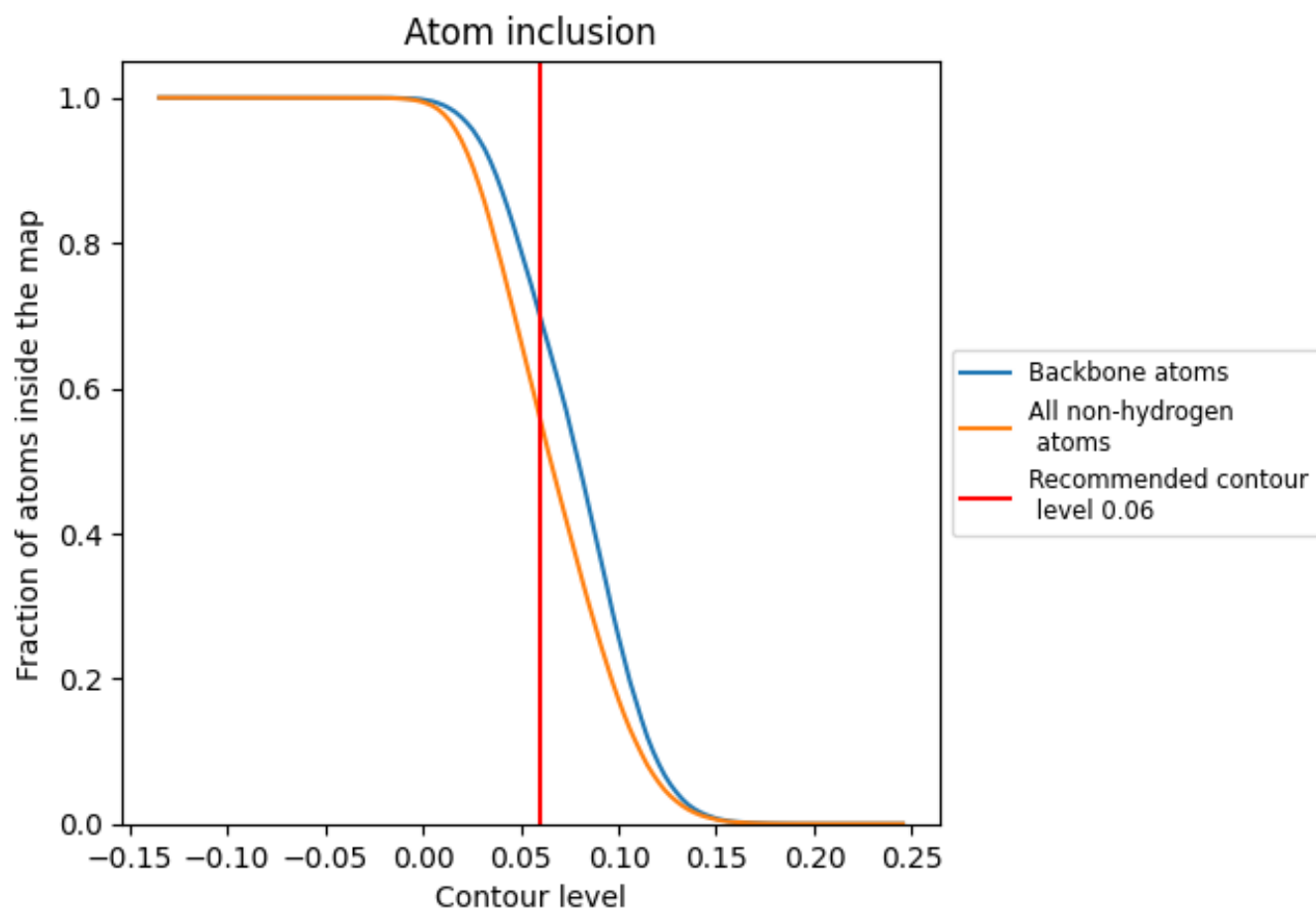
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































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	 0.5559	 0.4790
1	 0.6135	 0.4520
A	 0.6485	 0.5200
Aa	 0.4527	 0.4490
Ab	 0.6170	 0.5000
Ac	 0.4805	 0.4600
Ad	 0.5163	 0.4950
Ae	 0.6225	 0.5110
Af	 0.5225	 0.4740
Ag	 0.5739	 0.5060
Ah	 0.5277	 0.4630
Ai	 0.5569	 0.5060
Aj	 0.5566	 0.4990
Ak	 0.4718	 0.4440
Al	 0.5895	 0.4970
Am	 0.6382	 0.4910
An	 0.5486	 0.4840
Ao	 0.6244	 0.5100
Ap	 0.4922	 0.4530
Aq	 0.5037	 0.5020
Ar	 0.6093	 0.5180
As	 0.5424	 0.4690
At	 0.5907	 0.4980
Au	 0.6162	 0.5040
Av	 0.5245	 0.4600
Aw	 0.6012	 0.4990
Ax	 0.6048	 0.4990
Ay	 0.5883	 0.4910
Az	 0.6374	 0.5210
B	 0.5877	 0.5130
BA	 0.4916	 0.4510
BB	 0.5561	 0.4620
BC	 0.4968	 0.4860
BD	 0.6093	 0.5130
BE	 0.5691	 0.4430



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Chain	Atom inclusion	Q-score
BF	0.4963	0.4800
BG	0.5609	0.4930
BH	0.5450	0.4970
BI	0.5760	0.4760
BL	0.5948	0.5110
BM	0.2679	0.3150
BO	0.5193	0.4600
BP	0.5468	0.4990
Bj	0.4445	0.4790
C	0.6005	0.5080
D	0.4773	0.4210
E	0.5621	0.4670
F	0.5609	0.5100
G	0.5959	0.5200
H	0.4929	0.4920
I	0.5467	0.4970
J	0.5653	0.4970
K	0.5551	0.4920
L	0.5848	0.5030
M	0.5721	0.5010
N	0.5678	0.4990
O	0.3662	0.4270
P	0.5374	0.5070
Q	0.5676	0.4970
R	0.5171	0.4670
S	0.5555	0.5110
T	0.6375	0.5140
U	0.4743	0.4910
UA	0.6621	0.4690
UB	0.6776	0.5100
UC	0.2806	0.3630
UD	0.5453	0.3890
V	0.5567	0.5230
W	0.5617	0.5070
X	0.5125	0.4770
Y	0.4661	0.4700
Z	0.5639	0.5010