



Full wwPDB EM Validation Report ⓘ

Mar 20, 2025 – 01:27 pm GMT

PDB ID : 9HNY
EMDB ID : EMD-10180
Title : Mitoribosomal small subunit in complex with Mettl15 and Mettl17
Authors : Zgadzay, Y.; Aibara, S.; Gahura, O.; Amunts, A.
Deposited on : 2024-12-11
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

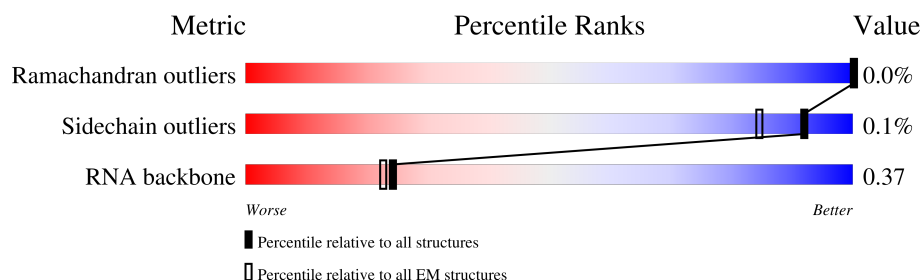
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.5

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	CA	620	<div> <div>20%</div> <div>49%</div> <div>32%</div> <div>19%</div> </div>
2	CC	74	<div> <div>32%</div> <div>91%</div> <div>9%</div> </div>
3	CE	435	<div> <div>8%</div> <div>85%</div> <div>15%</div> </div>
4	CF	160	<div> <div>99%</div> </div>
5	CH	282	<div> <div>76%</div> <div>24%</div> </div>
6	CI	443	<div> <div>13%</div> <div>94%</div> <div>6%</div> </div>
7	CJ	817	<div> <div>21%</div> <div>85%</div> <div>15%</div> </div>
8	CK	326	<div> <div>11%</div> <div>63%</div> <div>37%</div> </div>

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Mol	Chain	Length	Quality of chain
9	CN	158	
10	CO	429	
11	CP	188	
12	CQ	336	
13	CR	320	
14	CS	244	
15	Ca	602	
16	Cb	311	
17	Cd	440	
18	Cg	490	
19	Ci	181	
20	Cj	257	
21	Ck	874	
22	Cn	250	
23	Cp	187	
24	DB	1181	
25	DC	1165	
26	DD	812	
27	DE	747	
28	DF	666	
29	DG	631	
30	DH	581	
31	DI	407	
32	DJ	396	
33	DK	324	

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Mol	Chain	Length	Quality of chain
34	DL	307	
35	DO	282	
36	DP	274	
37	DR	270	
38	DT	247	
39	DU	228	
40	DV	183	
41	DW	179	
42	DX	169	
43	DY	163	
44	DZ	94	
45	F1	1041	
46	F2	1024	
47	F3	966	
48	F4	811	
49	F5	754	
50	F6	676	
51	F7	679	
52	F8	726	
53	F9	608	
54	FA	642	
55	FB	588	
55	FC	588	
56	FD	579	
57	FE	553	

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Mol	Chain	Length	Quality of chain
58	FF	474	
59	FG	463	
60	FH	457	
61	FI	445	
62	FJ	362	
63	FK	372	
64	FL	353	
65	FM	370	
65	FN	370	
66	FO	334	
67	FP	349	
68	FQ	307	
68	FR	307	
68	FS	307	
68	FT	307	
68	FU	307	
69	FV	264	
70	FW	263	
71	FX	239	
72	FY	189	
73	FZ	178	
74	Fa	171	
75	Fb	151	
76	Fc	148	
77	Fd	143	

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Mol	Chain	Length	Quality of chain
78	Fe	123	<div> <div>24%</div> <div>97%</div> </div>
79	Fi	629	<div> <div>65%</div> <div>66%</div> <div>34%</div> </div>
80	UA	27	<div> <div>70%</div> <div>100%</div> </div>
81	UB	6	<div> <div>33%</div> <div>100%</div> </div>
82	UC	10	<div> <div>100%</div> </div>
83	UF	11	<div> <div>27%</div> <div>100%</div> </div>
84	UG	16	<div> <div>12%</div> <div>100%</div> </div>
84	UJ	16	<div> <div>38%</div> <div>100%</div> </div>
85	UI	8	<div> <div>100%</div> </div>
86	UK	24	<div> <div>67%</div> <div>100%</div> </div>
87	UL	22	<div> <div>18%</div> <div>100%</div> </div>
88	UM	9	<div> <div>11%</div> <div>100%</div> </div>
88	UQ	9	<div> <div>22%</div> <div>100%</div> </div>
89	UN	7	<div> <div>14%</div> <div>100%</div> </div>
90	UO	30	<div> <div>37%</div> <div>100%</div> </div>
91	UP	45	<div> <div>64%</div> <div>100%</div> </div>
92	UY	85	<div> <div>98%</div> <div>98%</div> </div>
93	Ud	59	<div> <div>64%</div> <div>100%</div> </div>
94	Ug	167	<div> <div>42%</div> <div>100%</div> </div>
95	Uh	263	<div> <div>99%</div> <div>100%</div> </div>
96	Uk	31	<div> <div>55%</div> <div>100%</div> </div>
97	Ul	14	<div> <div>86%</div> <div>100%</div> </div>

2 Entry composition

There are 104 unique types of molecules in this entry. The entry contains 454141 atoms, of which 221033 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 RNA chain called 9S RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	CA	502	Total	C	H	N	O	P	0	0
			15241	4551	5079	1648	3461	502		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	614	U	A	conflict	GB X02547.1
CA	615	U	G	conflict	GB X02547.1
CA	616	U	C	conflict	GB X02547.1
CA	618	U	A	conflict	GB X02547.1
CA	619	U	A	conflict	GB X02547.1
CA	620	U	A	conflict	GB X02547.1

- Molecule 2 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CC	67	Total	C	H	N	O	0	0
			1195	410	610	87	88		

- Molecule 3 is a protein called Small ribosomal subunit protein uS5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	CE	370	Total	C	H	N	O	S	0	0
			5998	1916	2979	553	535	15		

- Molecule 4 is a protein called bS6m.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	CF	159	Total	C	H	N	O	S	0	0
			2626	835	1309	234	242	6		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	CH	214	Total	C	H	N	O	S	0	0
			3495	1105	1737	337	307	9		

- Molecule 6 is a protein called Ribosomal protein S9/S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	CI	418	Total	C	H	N	O	S	0	0
			6606	2087	3283	596	623	17		

- Molecule 7 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	CJ	691	Total	C	H	N	O	S	0	0
			11059	3556	5432	1001	1048	22		

- Molecule 8 is a protein called uS11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	CK	205	Total	C	H	N	O	S	0	0
			3335	1063	1652	306	304	10		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 9 is a protein called uS14m.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	CN	148	Total	C	H	N	O	S	0	0
			2483	799	1233	236	208	7		

- Molecule 10 is a protein called Mitochondrial ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	CO	356	Total	C	H	N	O	S	0	0
			5926	1883	2960	555	512	16		

- Molecule 11 is a protein called bS16m.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	CP	180	Total	C	H	N	O	S	0	0
			2999	956	1510	274	250	9		

- Molecule 12 is a protein called uS17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	CQ	236	Total	C	H	N	O	S	0	0
			3857	1230	1927	360	331	9		

- Molecule 13 is a protein called Mitochondrial ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	CR	134	Total	C	H	N	O	S	0	0
			2280	746	1127	210	195	2		

- Molecule 14 is a protein called uS19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	CS	85	Total	C	H	N	O	S	0	0
			1396	463	688	121	121	3		

- Molecule 15 is a protein called Chromosome passenger complex (CPC) protein INCENP N terminal.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Ca	494	Total	C	H	N	O	S	0	0
			8283	2705	4061	750	746	21		

- Molecule 16 is a protein called mS23.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Cb	152	Total	C	H	N	O	S	0	0
			2550	816	1283	230	215	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cb	6	VAL	GLU	conflict	UNP A0A3L6L708

- Molecule 17 is a protein called mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Cd	186	Total	C	H	N	O	S	0	0
			3199	1037	1574	298	282	8		

- Molecule 18 is a protein called Mitochondrial SSU ribosomal protein 29.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Cg	483	Total	C	H	N	O	S	0	0
			7704	2503	3793	686	702	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2

- Molecule 19 is a protein called mS33.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Ci	147	Total	C	H	N	O	S	0	0
			2414	770	1192	226	218	8		

- Molecule 20 is a protein called mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Cj	225	Total	C	H	N	O	S	0	0
			3522	1133	1737	309	339	4		

- Molecule 21 is a protein called mS35.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Ck	529	Total	C	H	N	O	S	0	0
			8539	2688	4281	764	788	18		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 22 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Cn	25	Total	C	H	N	O	0	0
			408	143	196	36	33		

- Molecule 23 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	Cp	171	Total	C	H	N	O	S	0	0
			2859	919	1408	262	265	5		

- Molecule 24 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	DB	588	Total	C	H	N	O	S	0	0
			9775	3118	4798	941	900	18		

- Molecule 25 is a protein called mS50.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	DC	1021	Total	C	H	N	O	S	0	0
			16155	5161	7983	1445	1536	30		

- Molecule 26 is a protein called mS51.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	DD	780	Total	C	H	N	O	S	0	0
			12633	4076	6198	1155	1164	40		

- Molecule 27 is a protein called Mitochondrial SSU ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	DE	581	Total	C	H	N	O	S	0	0
			8987	2930	4393	823	825	16		

- Molecule 28 is a protein called mS53.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	DF	487	Total	C	H	N	O	S	0	0
			7877	2487	3932	732	702	24		

- Molecule 29 is a protein called mS54.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	DG	560	Total	C	H	N	O	S	0	0
			8989	2853	4455	826	824	31		

- Molecule 30 is a protein called mS55.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	DH	501	Total	C	H	N	O	S	0	0
			8098	2567	4021	754	738	18		

- Molecule 31 is a protein called mS56.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	DI	390	Total	C	H	N	O	S	0	0
			6330	2018	3152	554	592	14		

- Molecule 32 is a protein called mS57.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	DJ	311	Total	C	H	N	O	S	0	0
			5012	1615	2481	450	452	14		

- Molecule 33 is a protein called mS58.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	DK	227	Total	C	H	N	O	S	0	0
			3589	1134	1797	321	332	5		

- Molecule 34 is a protein called mS59.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	DL	199	Total	C	H	N	O	S	0	0
			3211	1038	1590	286	287	10		

- Molecule 35 is a protein called mS62.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	DO	192	Total	C	H	N	O	S	0	0
			3067	972	1521	277	287	10		

- Molecule 36 is a protein called mS63.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	DP	212	Total	C	H	N	O	S	0	0
			3562	1155	1765	321	312	9		

- Molecule 37 is a protein called mS65.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	DR	251	Total	C	H	N	O	S	0	0
			4056	1305	2027	367	347	10		

- Molecule 38 is a protein called Rhodanese domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	DT	221	Total	C	H	N	O	S	0	0
			3704	1232	1792	334	336	10		

- Molecule 39 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	DU	218	Total	C	H	N	O	S	0	0
			3373	1093	1638	307	331	4		

- Molecule 40 is a protein called mS69.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	DV	144	Total	C	H	N	O	S	0	0
			2398	771	1185	222	216	4		

- Molecule 41 is a protein called mS70.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	DW	132	Total	C	H	N	O	S	0	0
			2236	725	1106	212	188	5		

- Molecule 42 is a protein called mS71.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	DX	88	Total	C	H	N	O	S	0	0
			1493	479	749	136	123	6		

- Molecule 43 is a protein called mS72.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	DY	154	Total	C	H	N	O	S	0	0
			2580	827	1287	245	216	5		

- Molecule 44 is a protein called mS73.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	DZ	28	Total	C	H	N	O	S	0	0
			451	157	213	38	42	1		

- Molecule 45 is a protein called Mitochondrial small ribosomal subunit Rsm22.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	F1	860	Total	C	H	N	O	S	0	0
			14086	4376	7088	1342	1240	40		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	695	ARG	CYS	conflict	UNP D0A703
F1	707	SER	GLY	conflict	UNP D0A703

- Molecule 46 is a protein called Pentacotriptide-repeat region of PRORP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	F2	888	Total	C	H	N	O	S	0	0
			14071	4470	6971	1247	1344	39		

- Molecule 47 is a protein called mt-SAF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	F3	886	Total	C	H	N	O	S	0	0
			13695	4291	6834	1217	1301	52		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	44	THR	ALA	conflict	UNP Q38E61
F3	190	VAL	ILE	conflict	UNP Q38E61
F3	303	ALA	SER	conflict	UNP Q38E61
F3	418	ASP	ASN	conflict	UNP Q38E61

- Molecule 48 is a protein called Methyltransfer_dom domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	F4	522	Total	C	H	N	O	S	0	0
			8425	2717	4169	743	775	21		

- Molecule 49 is a protein called Kinteoplast poly(A) polymerase complex 1 subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	F5	517	Total	C	H	N	O	S	0	0
			7167	2348	3398	709	697	15		

- Molecule 50 is a protein called DUF4460 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	F6	456	Total	C	H	N	O	S	0	0
			7255	2311	3609	635	686	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F6	88	VAL	ALA	conflict	UNP A0A3L6L7Z3
F6	192	VAL	LEU	conflict	UNP A0A3L6L7Z3
F6	246	VAL	LEU	conflict	UNP A0A3L6L7Z3
F6	291	ILE	THR	conflict	UNP A0A3L6L7Z3

- Molecule 51 is a protein called mt-SAF7 (KRIPP10).

Mol	Chain	Residues	Atoms						AltConf	Trace
51	F7	645	Total	C	H	N	O	S	0	0
			10208	3254	5096	896	928	34		

- Molecule 52 is a protein called Cupin type-1 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	F8	475	Total	C	H	N	O	S	0	0
			7316	2327	3651	668	655	15		

- Molecule 53 is a protein called Trichohyalin.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	F9	211	Total	C	H	N	O	S	0	0
			3379	1056	1671	322	325	5		

- Molecule 54 is a protein called mt-SAF10.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	FA	580	Total	C	H	N	O	S	0	0
			8975	2806	4550	787	810	22		

- Molecule 55 is a protein called tRNA pseudouridine synthase A-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	FB	383	Total	C	H	N	O	S	0	0
			6160	1967	3051	580	552	10		
55	FC	344	Total	C	H	N	O	S	0	0
			5623	1781	2801	538	495	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FB	385	THR	ALA	conflict	UNP A0A1G4II72
FC	375	THR	ALA	conflict	UNP A0A1G4II72

- Molecule 56 is a protein called PPR_long domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	FD	448	Total	C	H	N	O	S	0	0
			6998	2229	3482	626	639	22		

- Molecule 57 is a protein called mt-SAF13.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	FE	430	Total	C	H	N	O	S	0	0
			6905	2241	3425	600	621	18		

- Molecule 58 is a protein called S-adenosyl-methyltransferase mraW-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	FF	405	Total	C	H	N	O	S	0	0
			6416	2036	3179	580	597	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	106	GLY	CYS	conflict	UNP A0A3L6L433
FF	259	ALA	VAL	conflict	UNP A0A3L6L433

- Molecule 59 is a protein called mt-SAF15.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	FG	174	Total	C	H	N	O	S	0	0
			2828	878	1426	269	246	9		

- Molecule 60 is a protein called mt-SAF16 (P32).

Mol	Chain	Residues	Atoms						AltConf	Trace
60	FH	305	Total	C	H	N	O	S	0	0
			4734	1500	2338	424	453	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FH	169	ASP	HIS	conflict	UNP D0A6K1
FH	260	MET	ARG	conflict	UNP D0A6K1

- Molecule 61 is a protein called mt-SAF17.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	FI	350	Total	C	H	N	O	S	0	0
			5514	1731	2716	511	543	13		

- Molecule 62 is a protein called mt-SAF18 (RbfA).

Mol	Chain	Residues	Atoms						AltConf	Trace
62	FJ	353	Total	C	H	N	O	S	0	0
			5886	1844	2968	550	515	9		

- Molecule 63 is a protein called Mitochondrial glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	FK	209	Total	C	H	N	O	S	0	0
			3303	1089	1595	285	328	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FK	38	HIS	ARG	conflict	UNP Q57XS8

- Molecule 64 is a protein called Metallo-beta-lactamase domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	FL	314	Total	C	H	N	O	S	0	0
			4986	1586	2478	455	450	17		

- Molecule 65 is a protein called mt-SAF21.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	FM	323	Total	C	H	N	O	S	0	0
			4839	1498	2415	444	462	20		
65	FN	317	Total	C	H	N	O	S	0	0
			4742	1471	2363	434	454	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FM	326	HIS	ARG	conflict	UNP C9ZJW2
FN	326	HIS	ARG	conflict	UNP C9ZJW2

- Molecule 66 is a protein called mt-SAF22.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	FO	312	Total	C	H	N	O	S	0	0
			5145	1623	2560	495	454	13		

- Molecule 67 is a protein called ADP-ribosylglycohydrolase.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	FP	326	Total	C	H	N	O	S	0	0
			5001	1609	2474	444	464	10		

- Molecule 68 is a protein called Potassium voltage-gated channel, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	FQ	229	Total	C	H	N	O	S	0	0
			3661	1173	1817	330	334	7		
68	FR	216	Total	C	H	N	O	S	0	0
			3495	1120	1736	317	315	7		
68	FS	254	Total	C	H	N	O	S	0	0
			4088	1306	2027	374	373	8		
68	FT	215	Total	C	H	N	O	S	0	0
			3469	1112	1720	316	314	7		
68	FU	234	Total	C	H	N	O	S	0	0
			3766	1204	1871	344	339	8		

- Molecule 69 is a protein called mt-SAF25.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	FV	209	Total	C	H	N	O	S	0	0
			3185	1033	1561	281	299	11		

- Molecule 70 is a protein called Low molecular weight protein tyrosine phosphatase.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	FW	242	Total	C	H	N	O	S	0	0
			3985	1245	1991	379	364	6		

- Molecule 71 is a protein called PPR_long domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	FX	211	Total	C	H	N	O	S	0	0
			3272	1037	1616	305	300	14		

- Molecule 72 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	FY	154	Total	C	H	N	O	S	0	0
			2480	784	1243	221	226	6		

- Molecule 73 is a protein called mt-SAF29.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	FZ	128	Total	C	H	N	O	S	0	0
			1804	592	854	176	180	2		

- Molecule 74 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	Fa	161	Total	C	H	N	O	S	0	0
			2635	853	1324	234	220	4		

- Molecule 75 is a protein called Complex 1 protein (LYR family).

Mol	Chain	Residues	Atoms						AltConf	Trace
75	Fb	126	Total	C	H	N	O	S	0	0
			2140	691	1068	195	179	7		

- Molecule 76 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	Fc	84	Total	C	H	N	O	S	0	0
			1333	427	664	106	135	1		

- Molecule 77 is a protein called Probable Zinc-ribbon domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	Fd	91	Total	C	H	N	O	S	0	0
			1444	459	722	138	117	8		

- Molecule 78 is a protein called mt-SAF34.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	Fe	119	Total	C	H	N	O	S	0	0
			1997	631	985	196	179	6		

- Molecule 79 is a protein called mt-SAF38.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	Fi	417	Total	C	H	N	O	S	0	0
			6663	2132	3315	605	589	22		

- Molecule 80 is a protein called UNK-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	UA	27	Total	C	H	N	O	0	0
			164	81	29	27	27		

- Molecule 81 is a protein called UNK-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	UB	6	Total	C	H	N	O	0	0
			38	18	8	6	6		

- Molecule 82 is a protein called UNK-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	UC	10	Total	C	H	N	O	0	0
			65	30	15	10	10		

- Molecule 83 is a protein called UNK-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	UF	11	Total	C	H	N	O	0	0
			72	33	17	11	11		

- Molecule 84 is a protein called UNK-G,J.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	UG	16	Total	C	H	N	O	0	0
			100	48	20	16	16		
84	UJ	16	Total	C	H	N	O	0	0
			102	48	22	16	16		

- Molecule 85 is a protein called UNK-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	UI	8	Total	C	H	N	O	0	0
			52	24	12	8	8		

- Molecule 86 is a protein called UNK-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	UK	24	Total	C	H	N	O	0	0
			149	72	29	24	24		

- Molecule 87 is a protein called UNK-L.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	UL	22	Total	C	H	N	O	0	0
			135	66	25	22	22		

- Molecule 88 is a protein called UNK-M,Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	UM	9	Total	C	H	N	O	0	0
			59	27	14	9	9		
88	UQ	9	Total	C	H	N	O	0	0
			56	27	11	9	9		

- Molecule 89 is a protein called UNK-N.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	UN	7	Total	C	H	N	O	0	0
			45	21	10	7	7		

- Molecule 90 is a protein called UNK-O.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	UO	30	Total	C	H	N	O	0	0
			183	90	33	30	30		

- Molecule 91 is a protein called UNK-P.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	UP	45	Total	C	H	N	O	0	0
			278	135	53	45	45		

- Molecule 92 is a protein called UNK-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	UY	83	Total	C	H	N	O	0	0
			507	249	92	83	83		

- Molecule 93 is a protein called UNK-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	Ud	59	Total	C	H	N	O	0	0
			357	177	62	59	59		

- Molecule 94 is a protein called UNK-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	Ug	167	Total	C	H	N	O	0	0
			1023	501	188	167	167		

- Molecule 95 is a protein called UNK-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	Uh	263	Total	C	H	N	O	0	0
			1619	789	304	263	263		

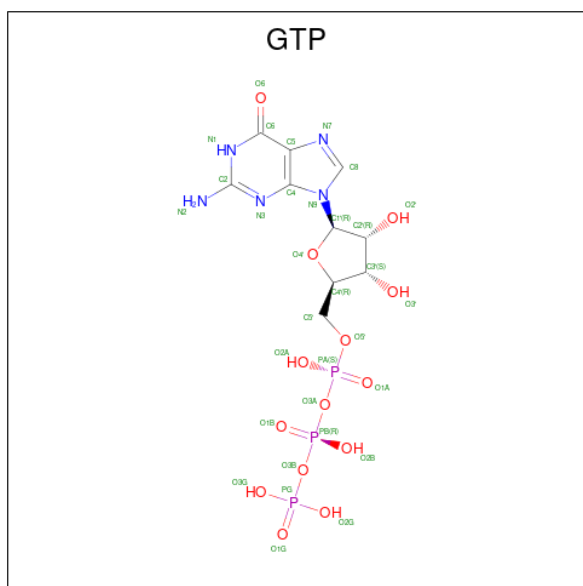
- Molecule 96 is a protein called UNK-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	Uk	31	Total	C	H	N	O	0	0
			188	93	33	31	31		

- Molecule 97 is a protein called UNK-l.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	U1	14	Total	C	H	N	O	0	0
			86	42	16	14	14		

- Molecule 98 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



Mol	Chain	Residues	Atoms						AltConf
98	Cg	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

- Molecule 99 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

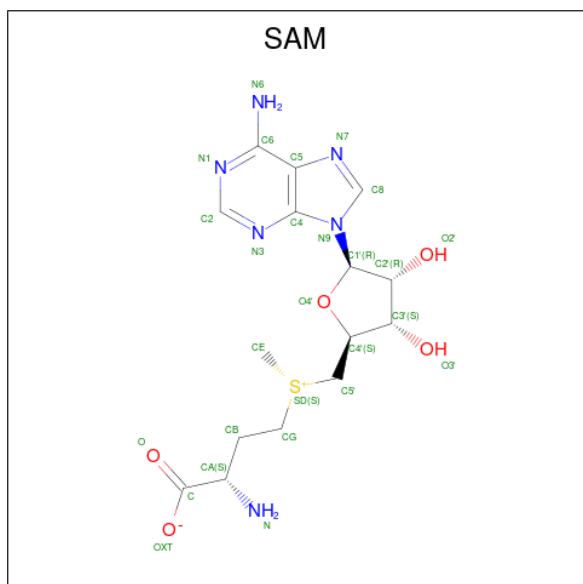
Mol	Chain	Residues	Atoms	AltConf
99	Cg	1	Total Mg 1 1	0

- Molecule 100 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



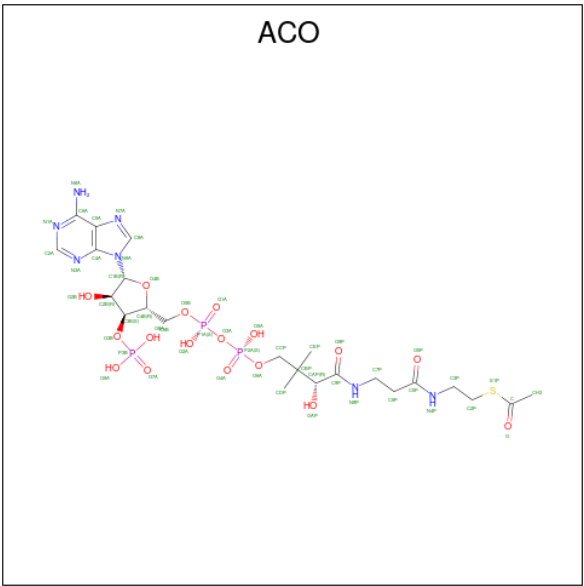
Mol	Chain	Residues	Atoms			AltConf
100	F1	1	Total	Fe	S	0
			8	4	4	

- Molecule 101 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
101	F1	1	Total 46	C 15	H 19	N 6	O 5	S 1	0
101	FF	1	Total 46	C 15	H 19	N 6	O 5	S 1	0

- Molecule 102 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).

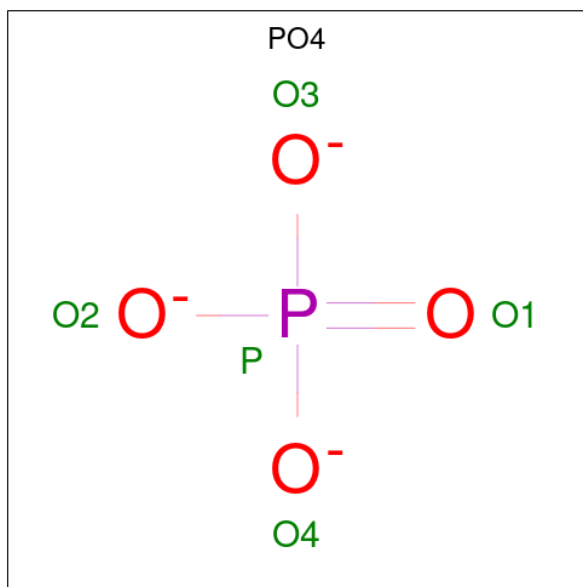


Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
102	F3	1	85	23	34	7	17	3	1	0

- Molecule 103 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
103	FG	1	Total	Zn	0
			1	1	
103	FL	1	Total	Zn	0
			1	1	
103	Fd	1	Total	Zn	0
			1	1	
103	Fe	1	Total	Zn	0
			1	1	

- Molecule 104 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

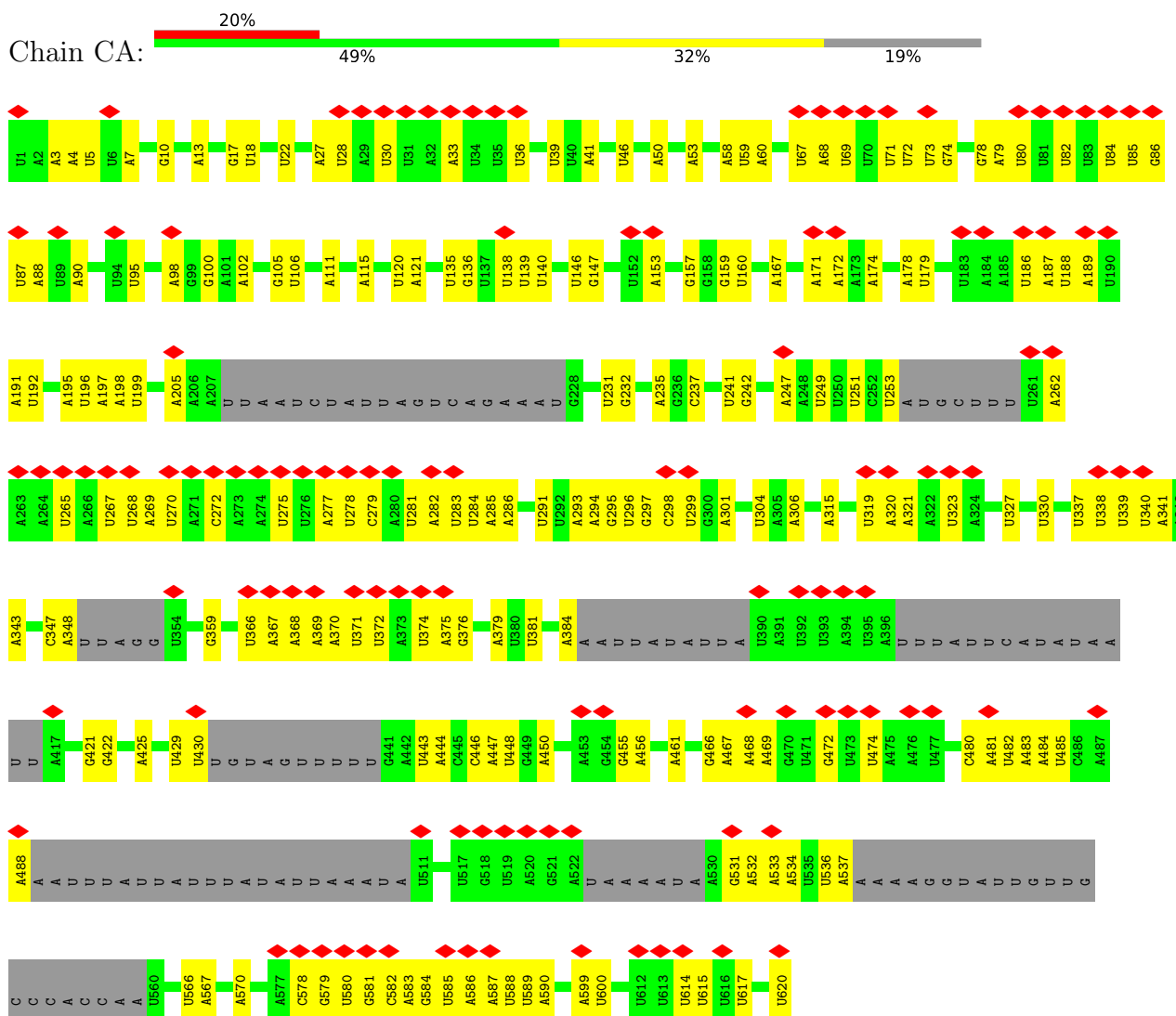


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
104	FW	1	5	4	1	0

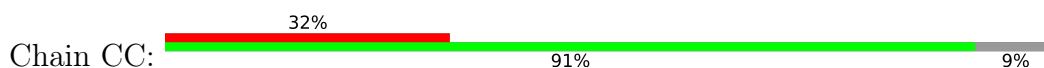
3 Residue-property plots [i](#)

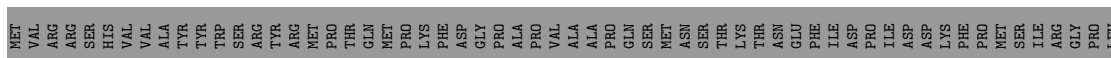
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

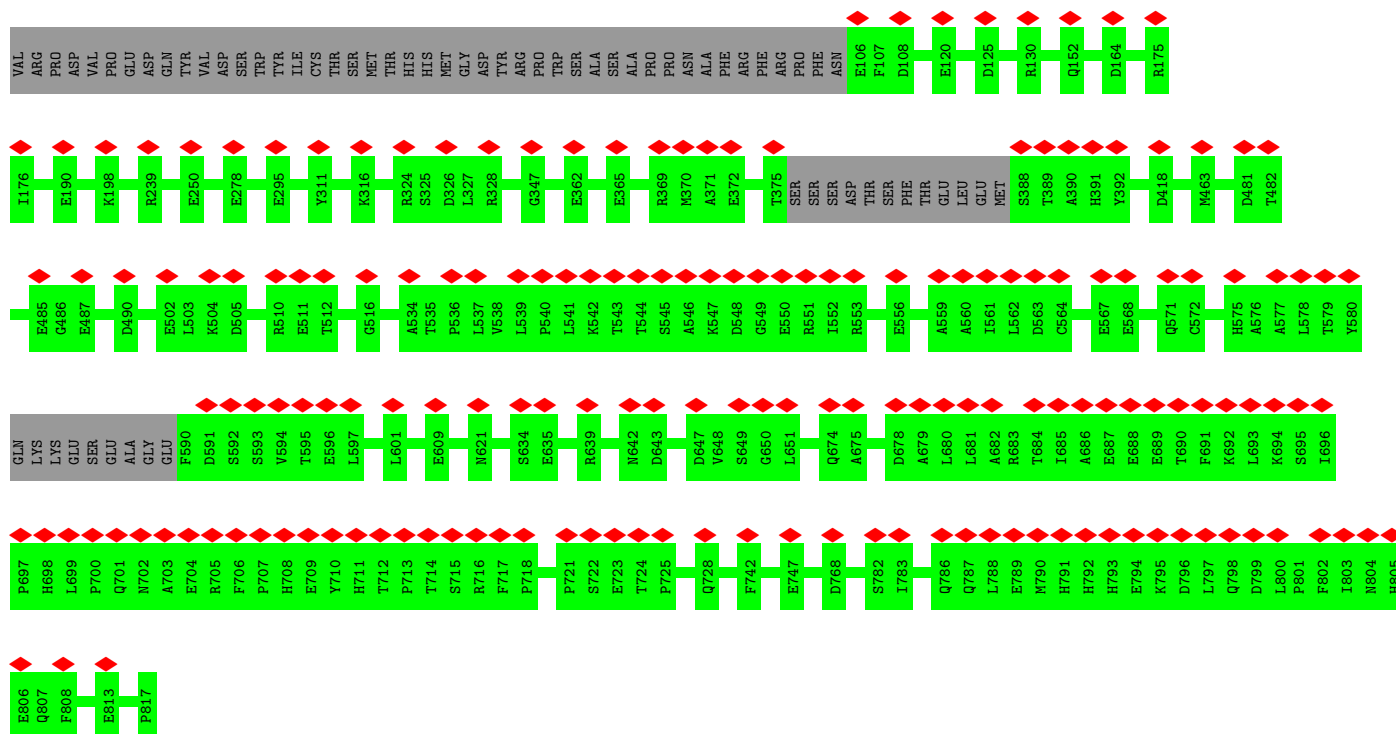
• Molecule 1: 9S RNA



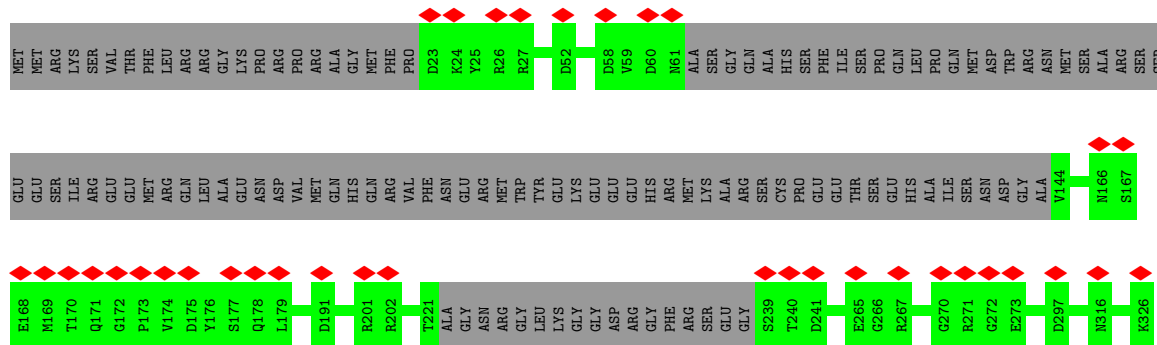
• Molecule 2: uS3m

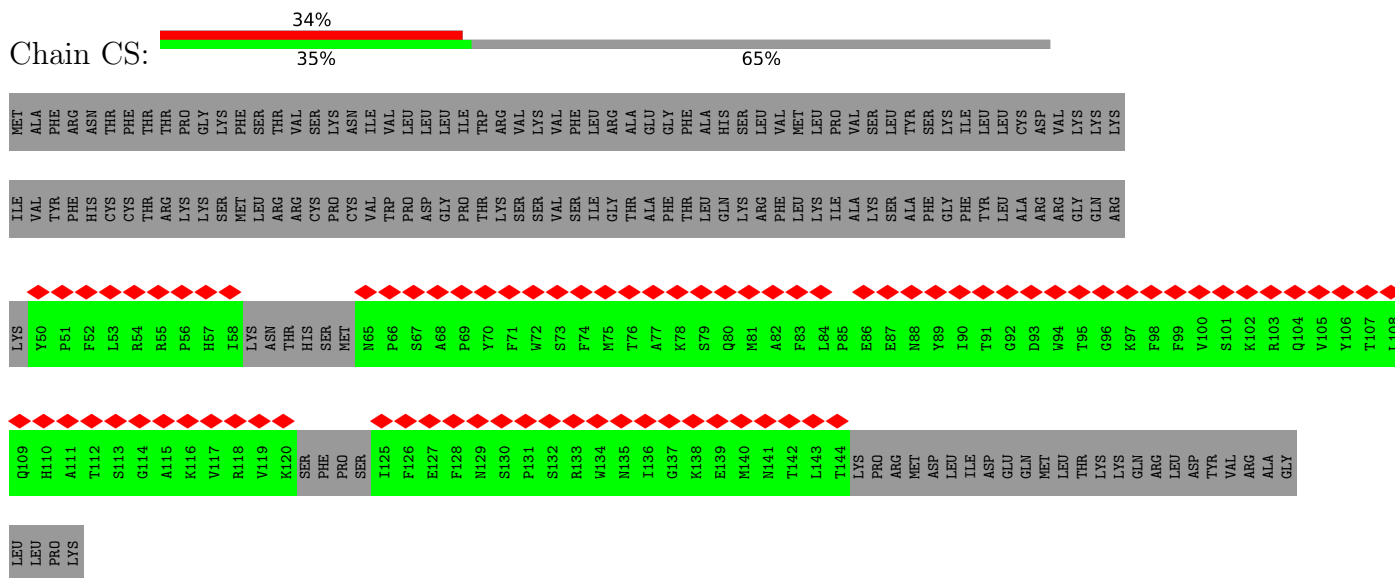




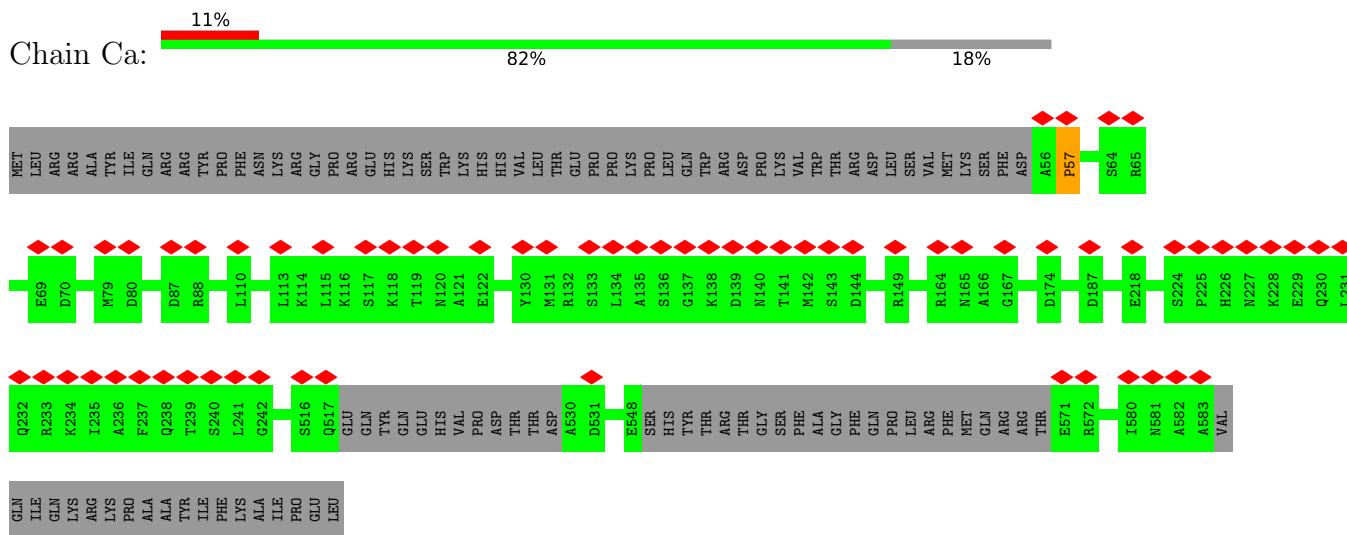


• Molecule 8: uS11m

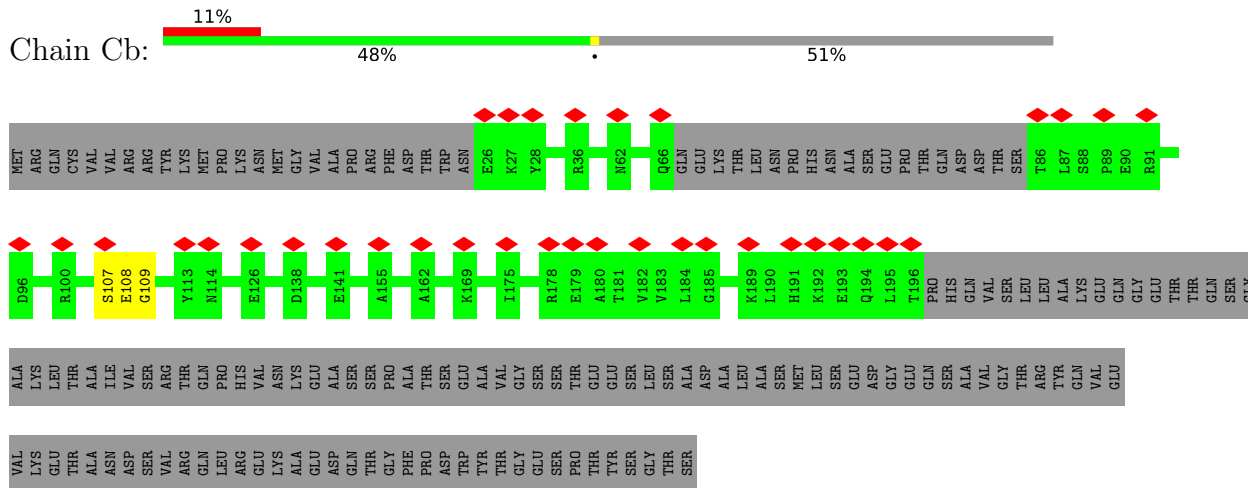




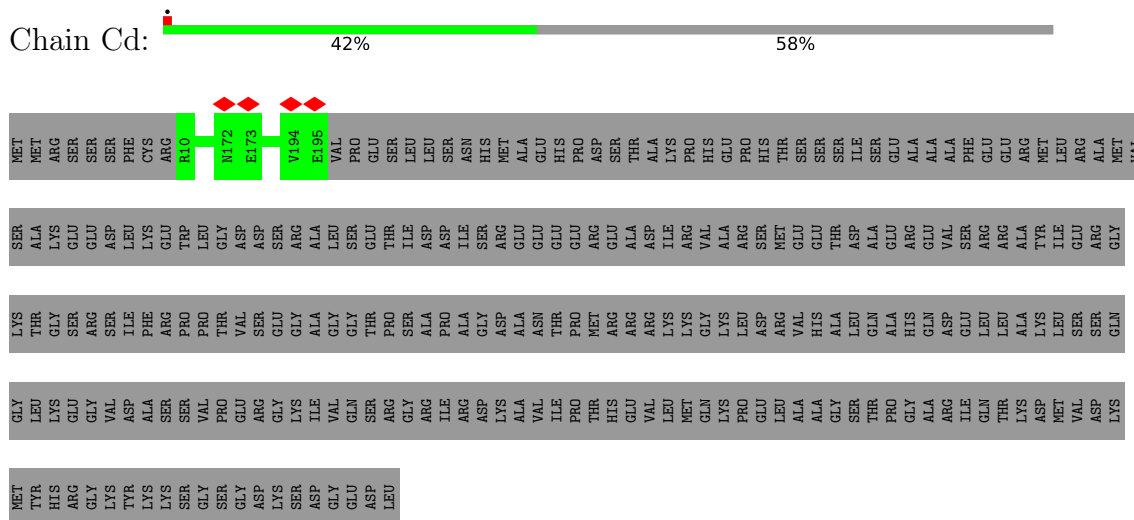
- Molecule 15: Chromosome passenger complex (CPC) protein INCENP N terminal



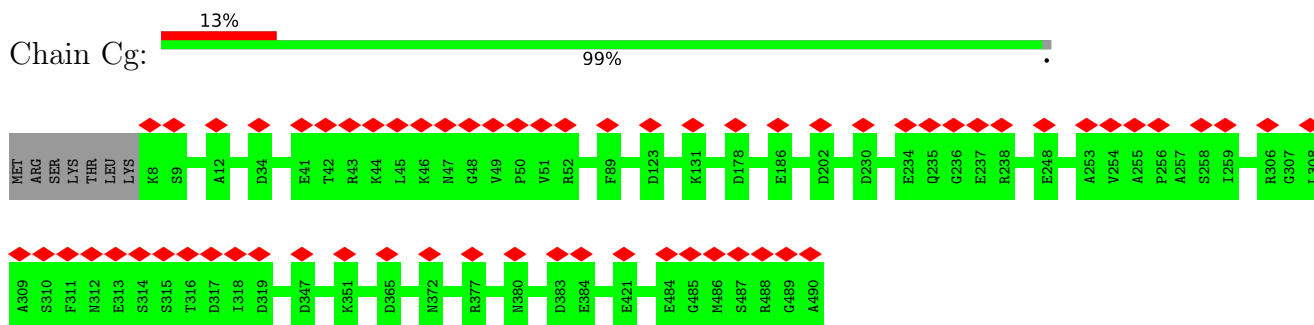
- Molecule 16: mS23



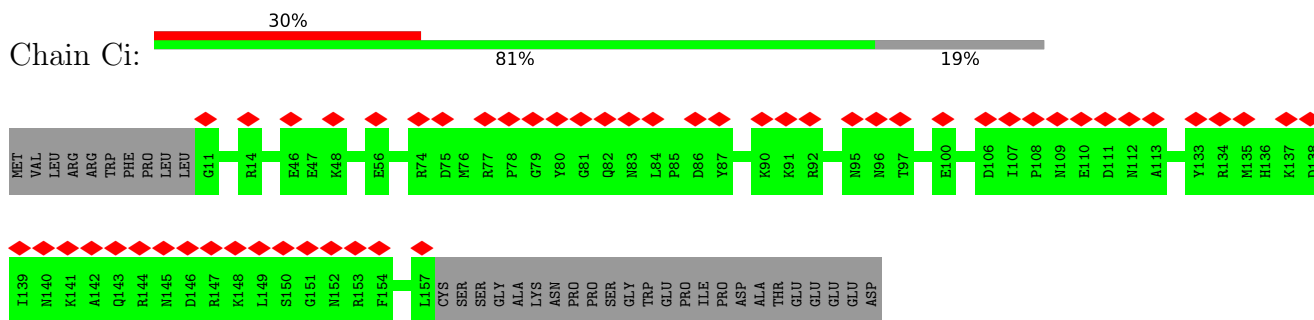
- Molecule 17: mS26



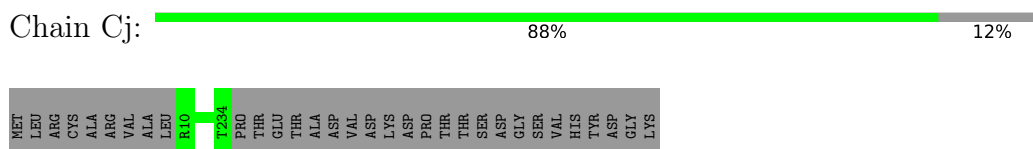
- Molecule 18: Mitochondrial SSU ribosomal protein 29



- Molecule 19: mS33

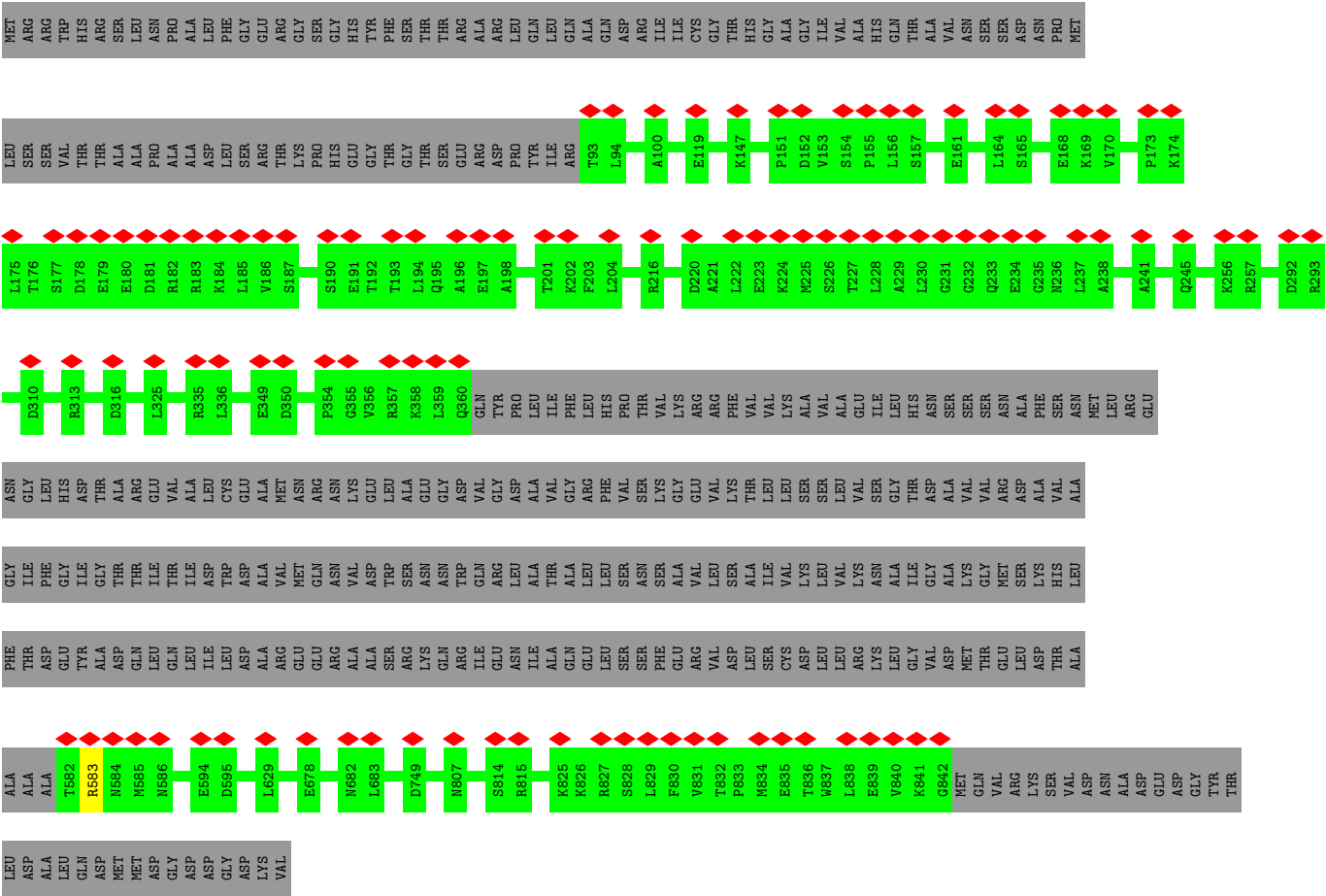


- Molecule 20: mS34

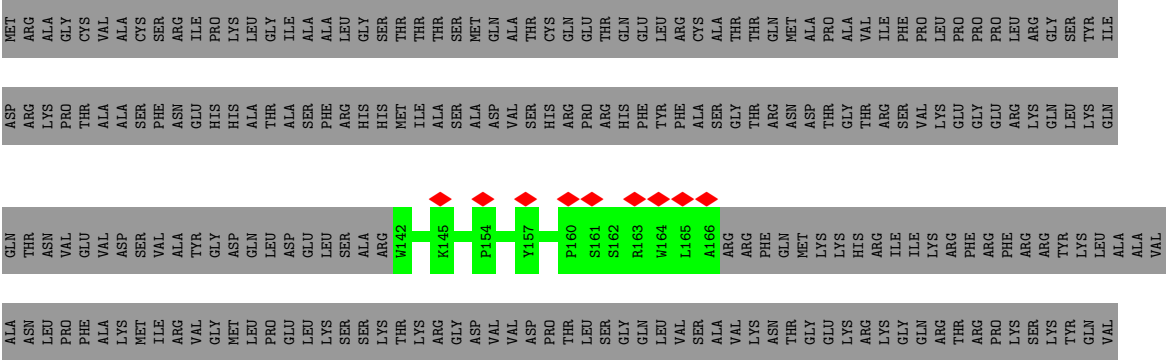


- Molecule 21: mS35

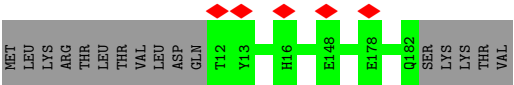
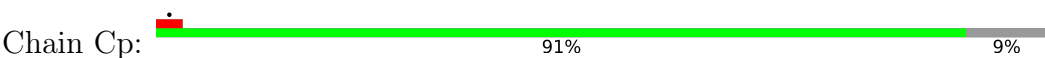




• Molecule 22: mS38

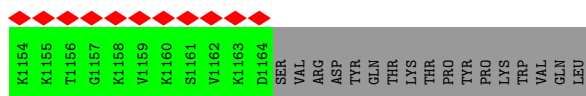


• Molecule 23: Protein FYV4, mitochondrial

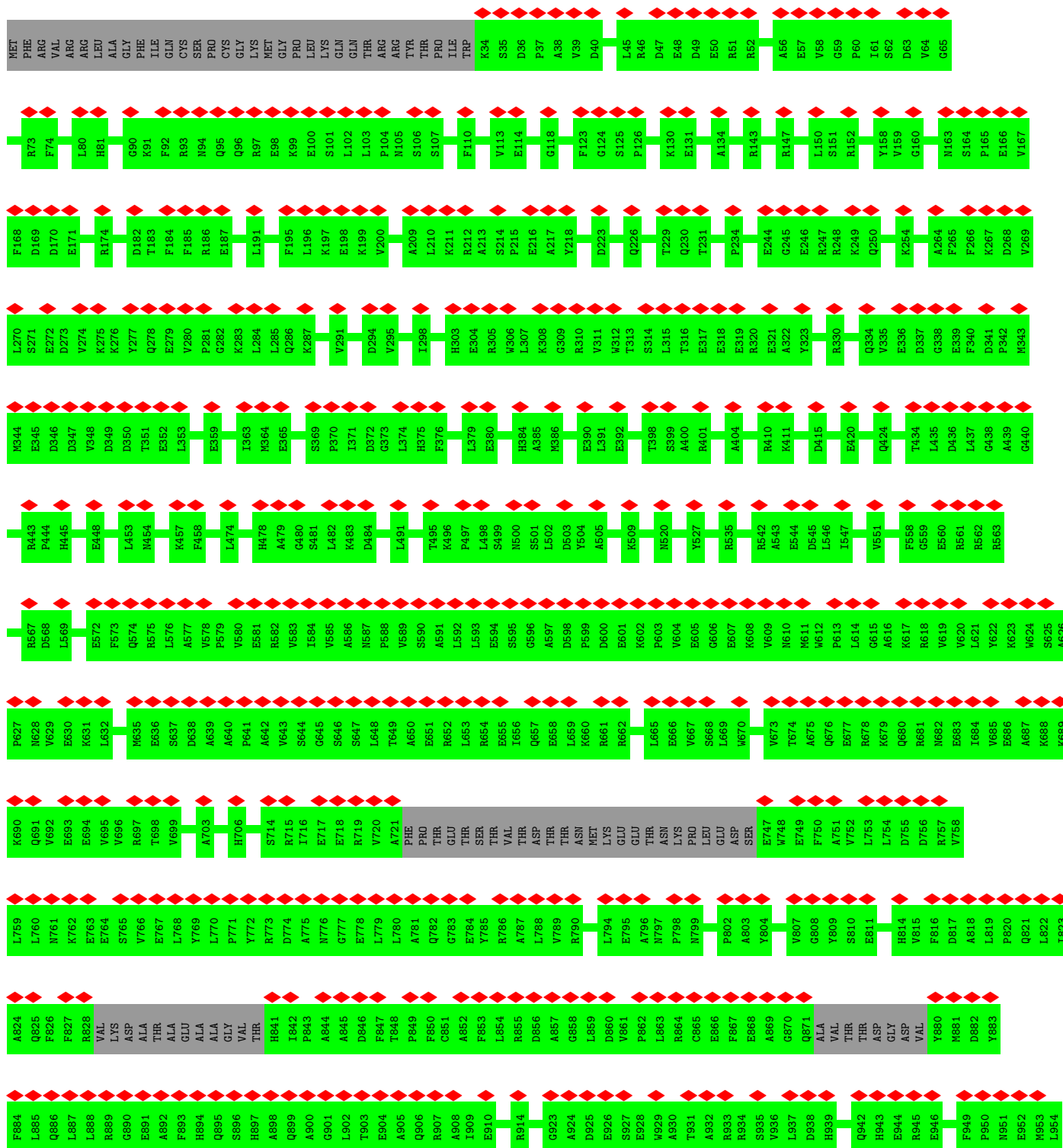


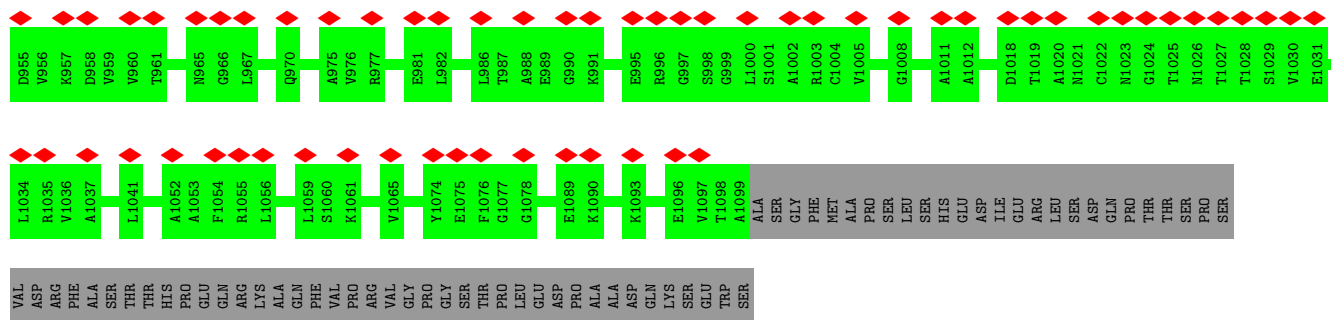
• Molecule 24: mS49

[illegible]

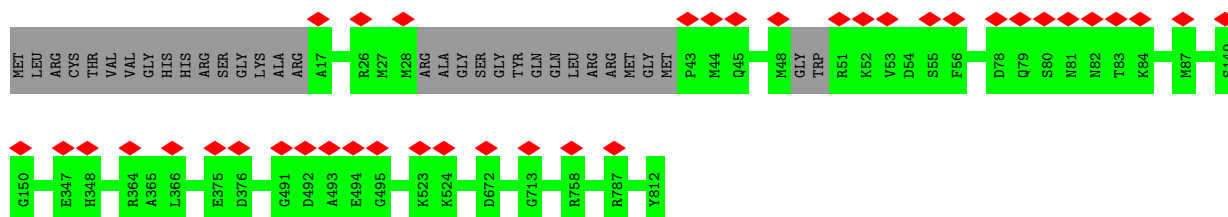


● Molecule 25: mS50

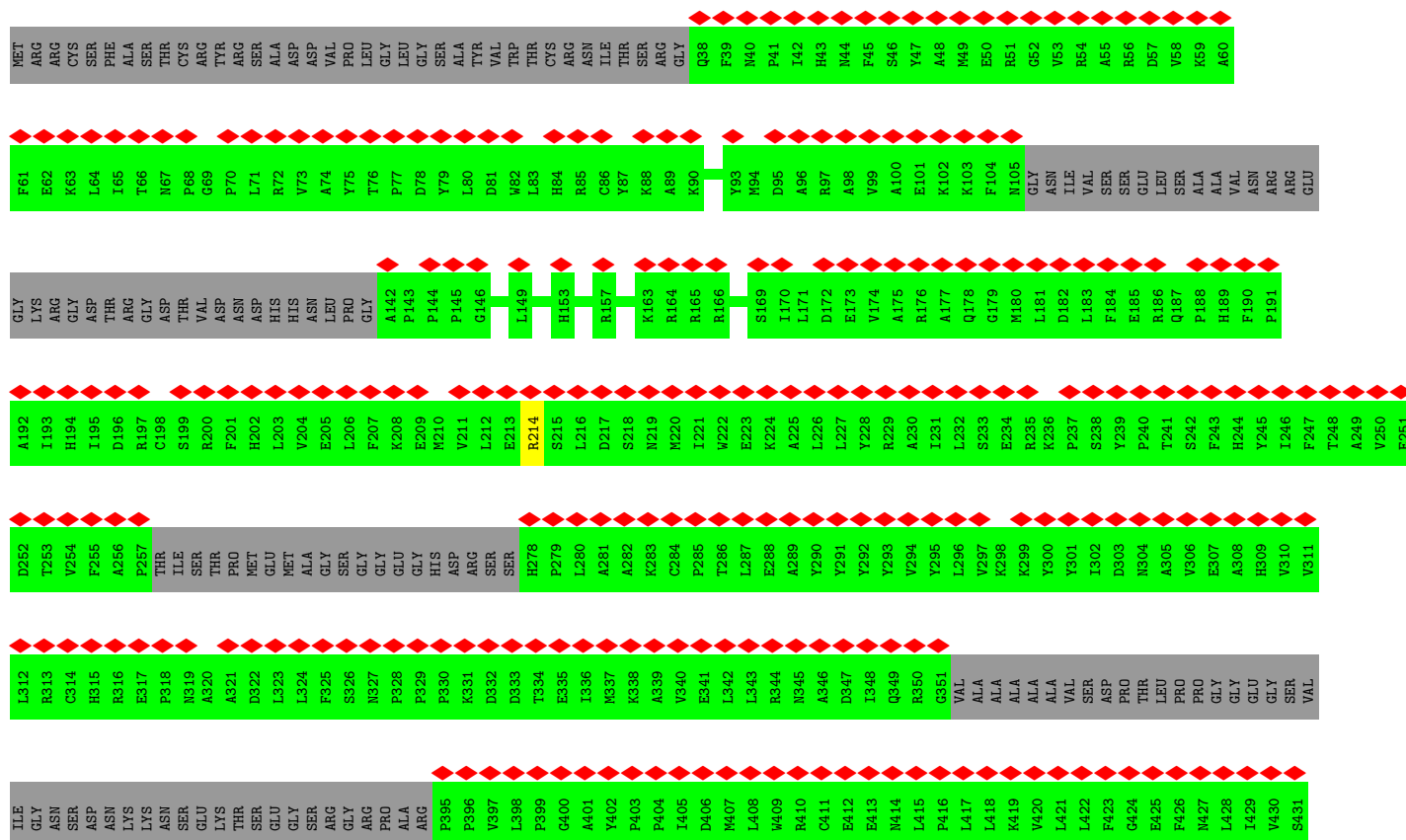
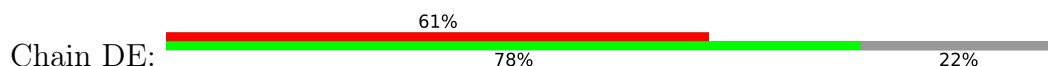




• Molecule 26: mS51

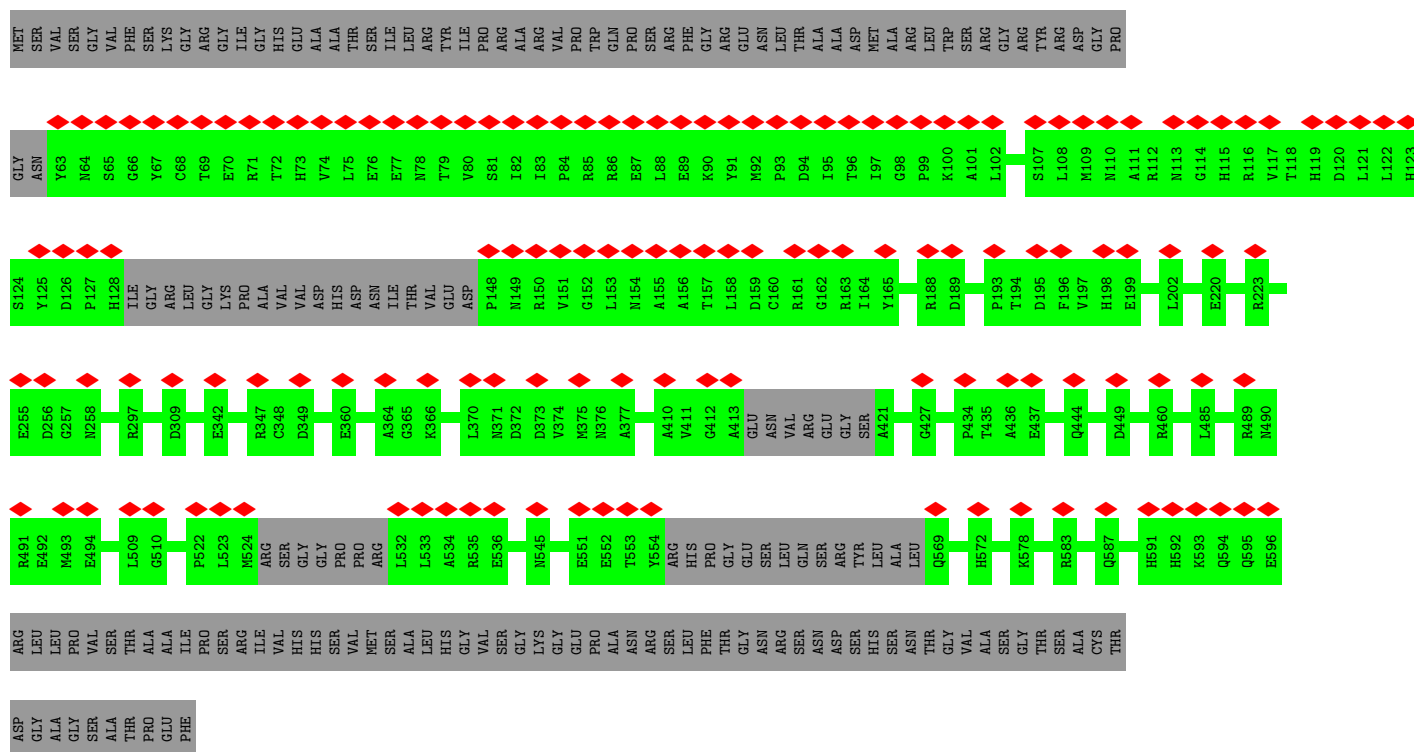
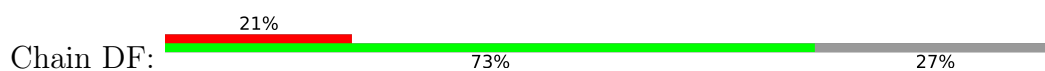


• Molecule 27: Mitochondrial SSU ribosomal protein

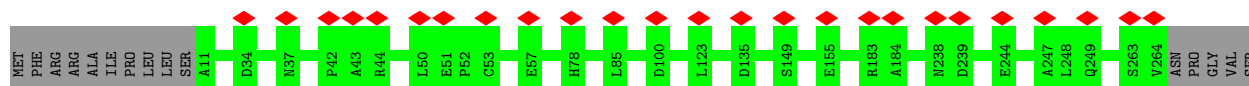
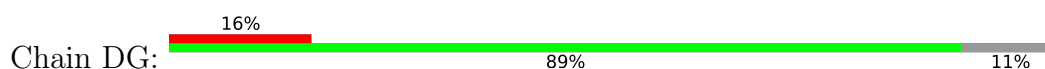


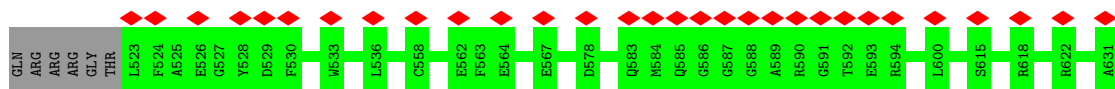
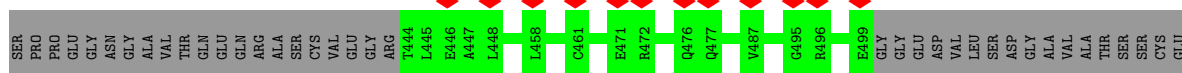
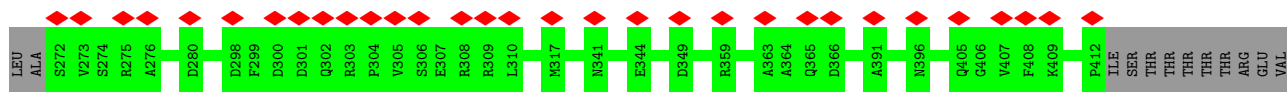


• Molecule 28: mS53

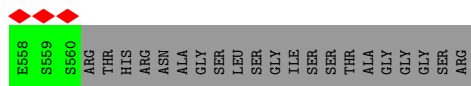
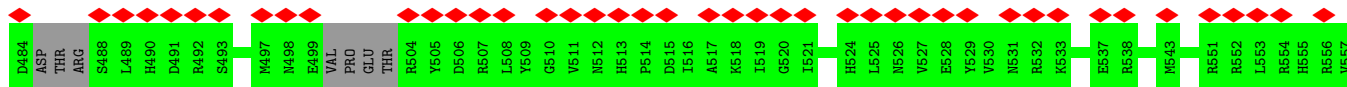
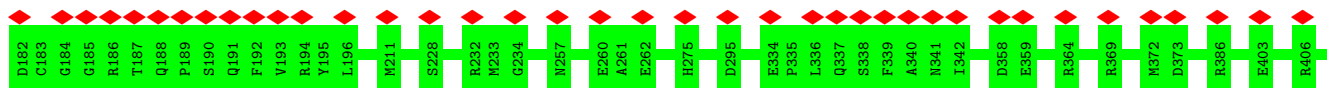
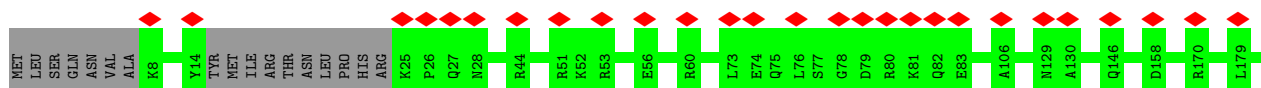


• Molecule 29: mS54

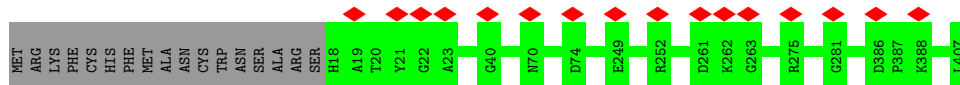




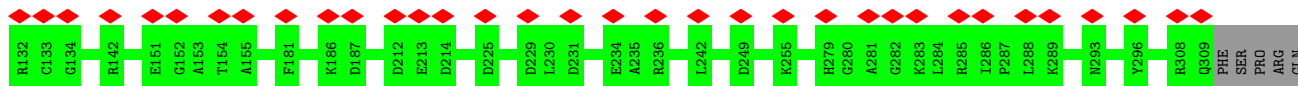
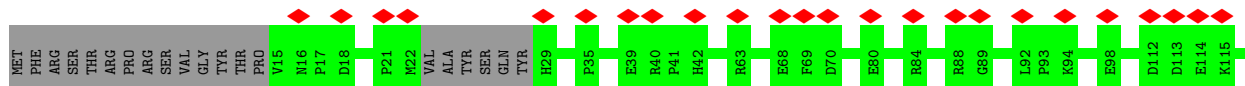
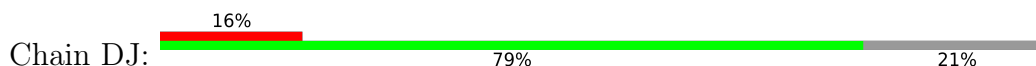
• Molecule 30: mS55

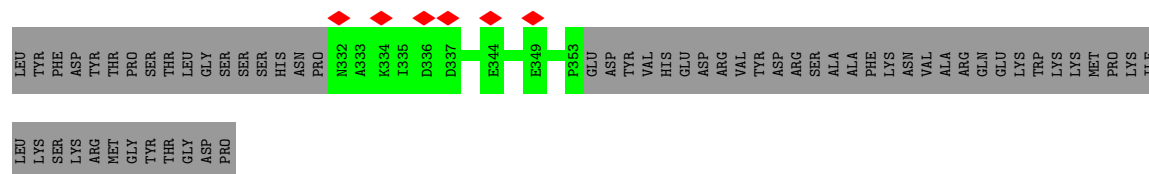


• Molecule 31: mS56

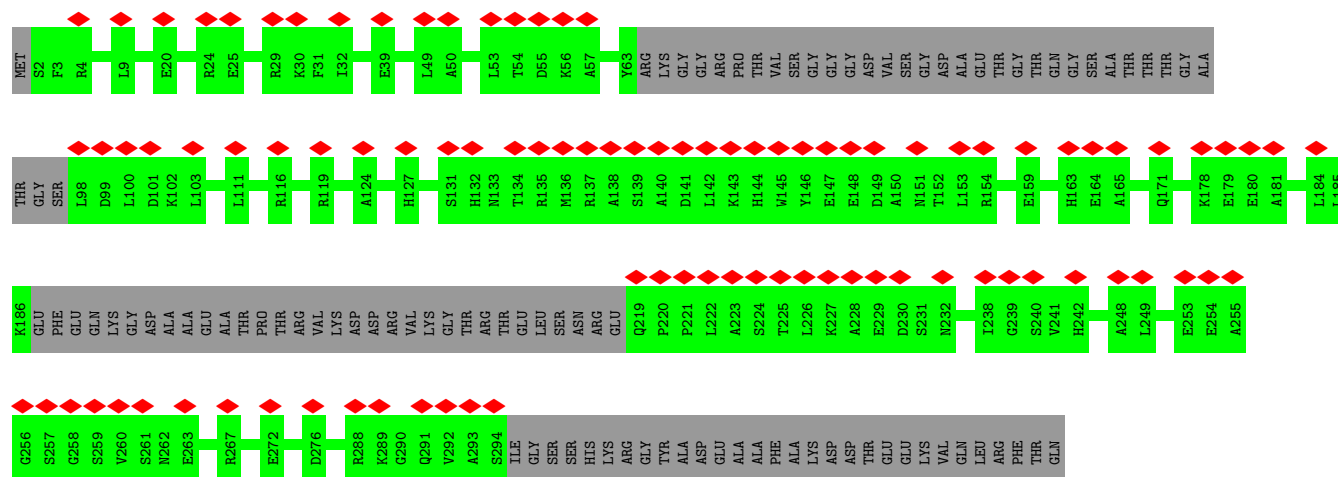
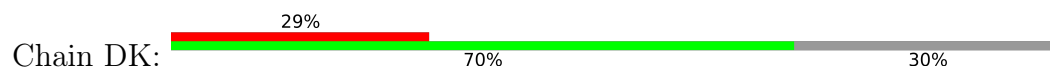


• Molecule 32: mS57

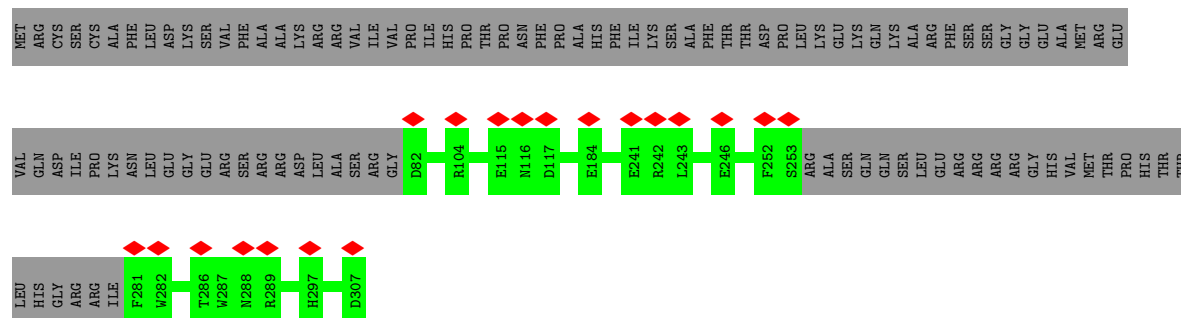




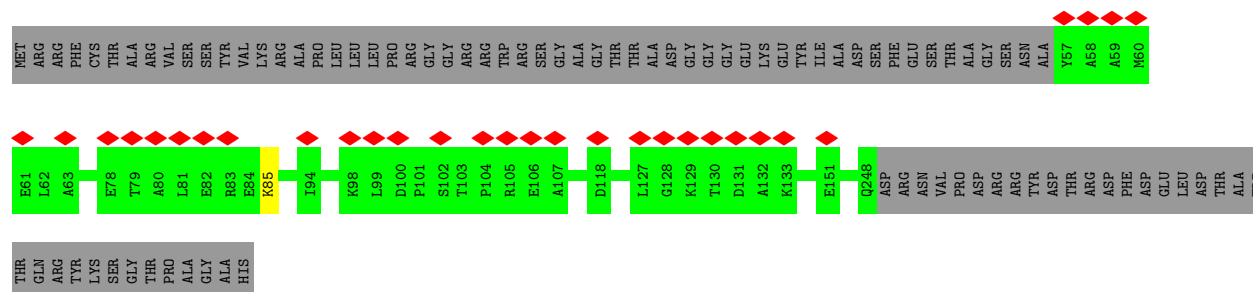
● Molecule 33: mS58




● Molecule 34: mS59

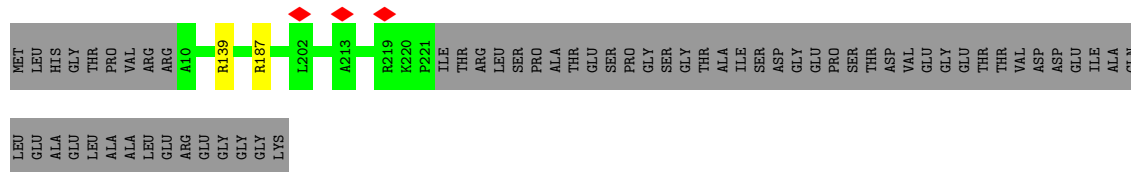


● Molecule 35: mS62



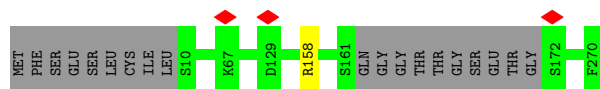
- Molecule 36: mS63

Chain DP:  77% 23%

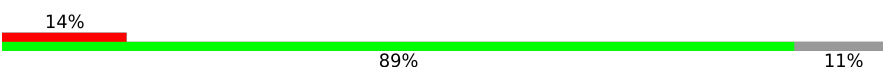


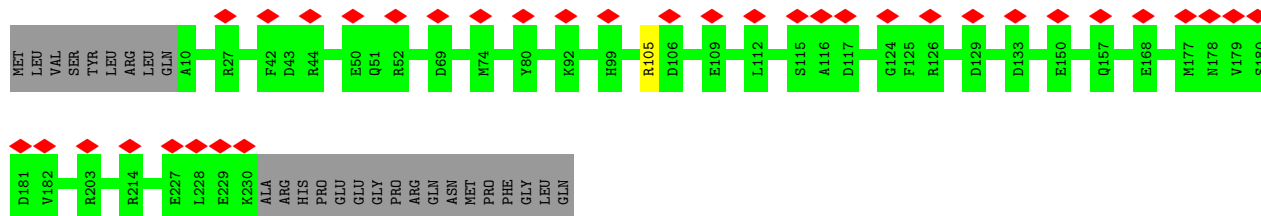
- Molecule 37: mS65

Chain DR:  93% 7%



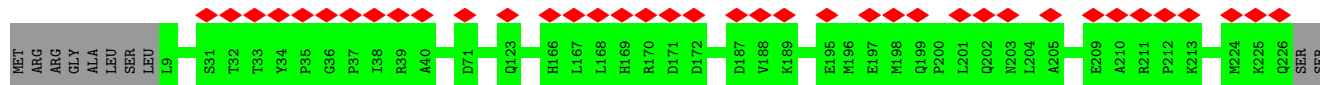
- Molecule 38: Rhodanese domain-containing protein

Chain DT:  14% 89% 11%




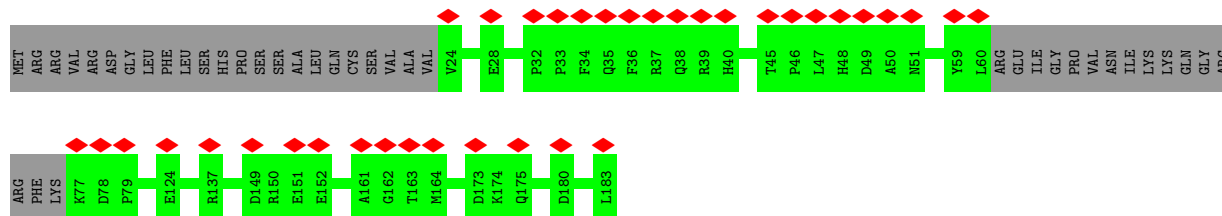
- Molecule 39: Ubiquitin-like domain-containing protein

Chain DU:  17% 96%




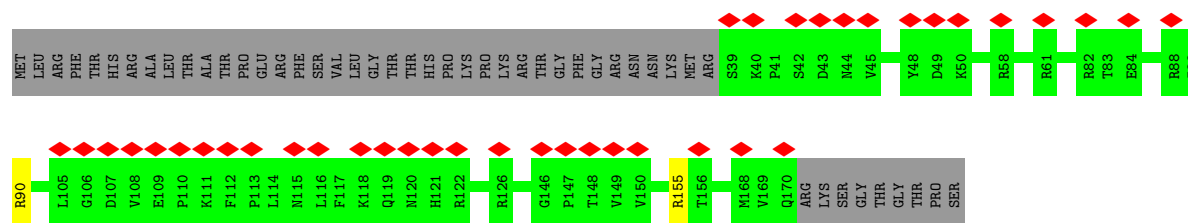
- Molecule 40: mS69

Chain DV:  20% 79% 21%

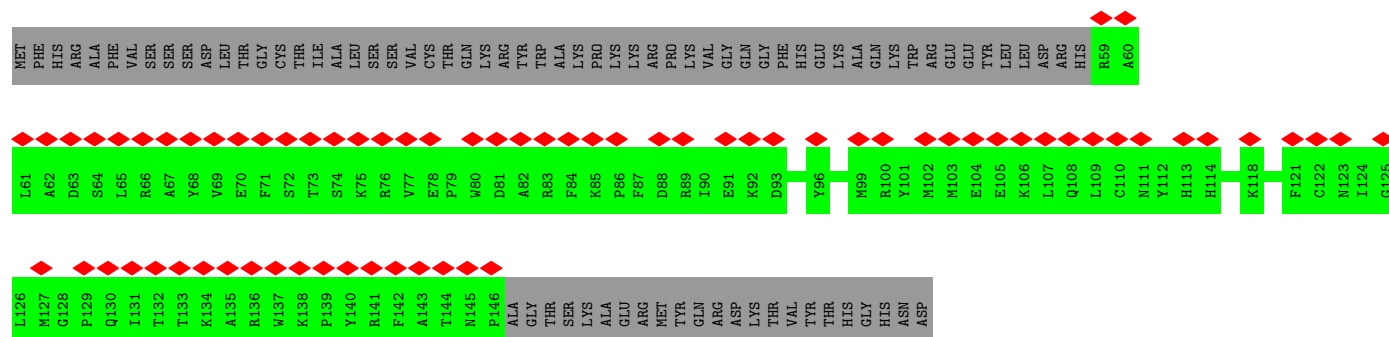
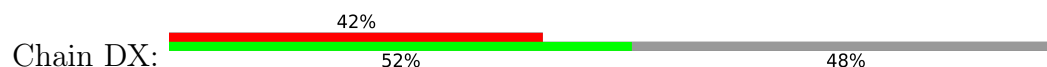


- Molecule 41: mS70

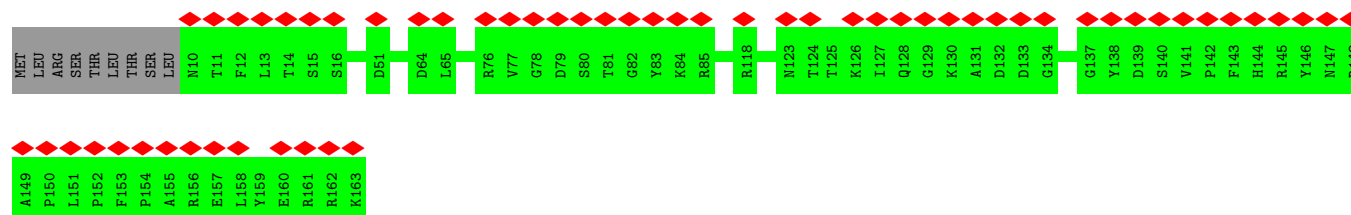
Chain DW:  22% 73% 26%



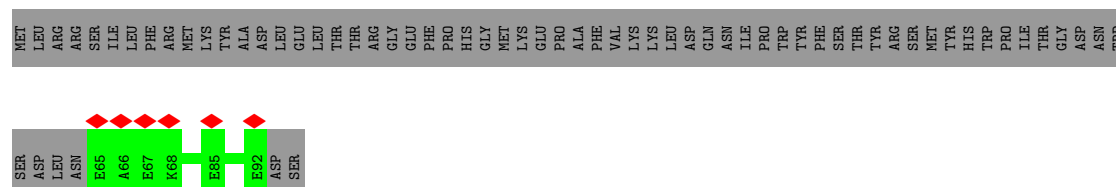
• Molecule 42: mS71



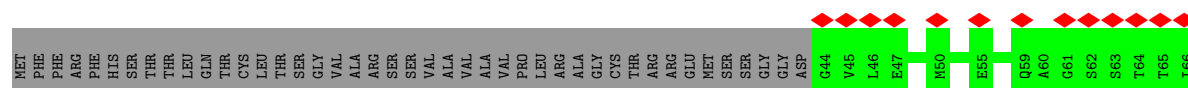
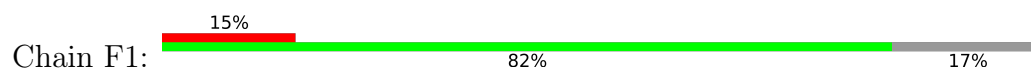
• Molecule 43: mS72

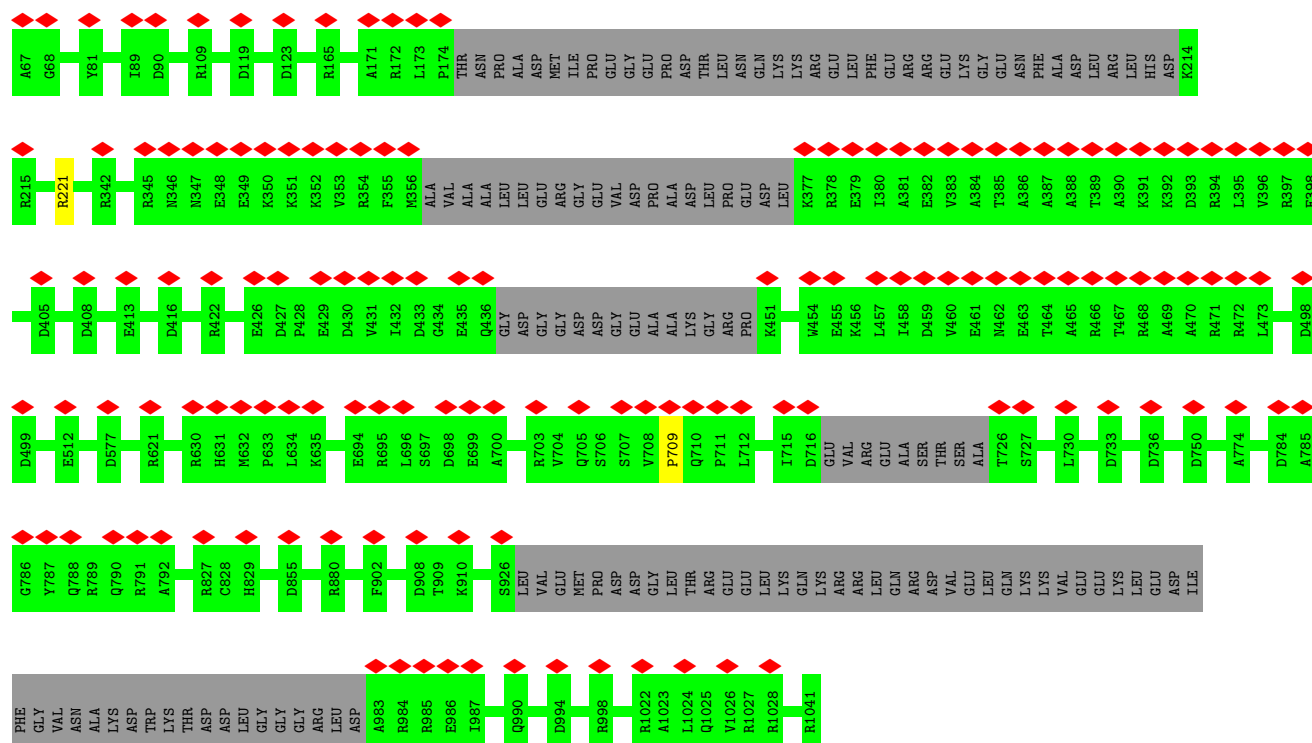


• Molecule 44: mS73



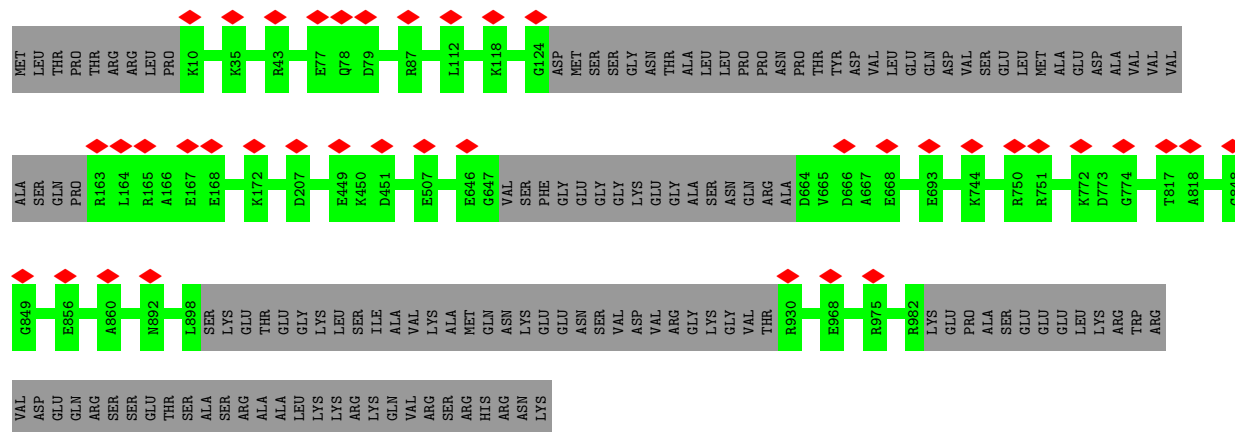
• Molecule 45: Mitochondrial small ribosomal subunit Rsm22





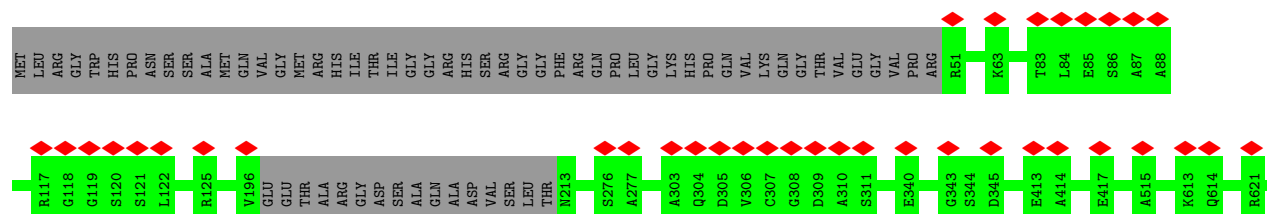
- Molecule 46: Pentacotriptide-repeat region of PRORP domain-containing protein

Chain F2: 87% 13%

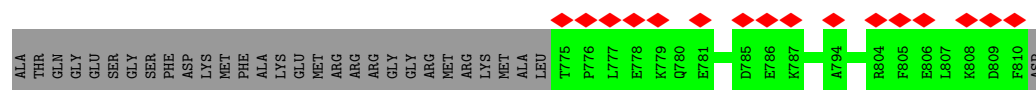


- Molecule 47: mt-SAF3

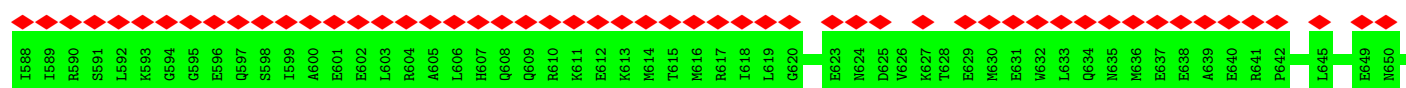
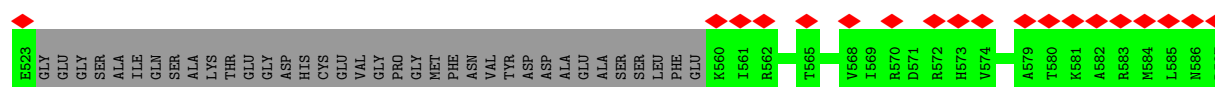
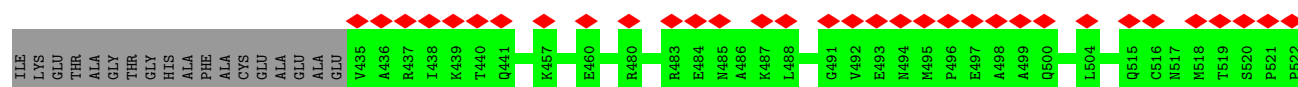
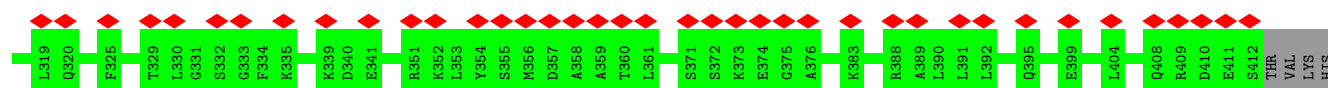
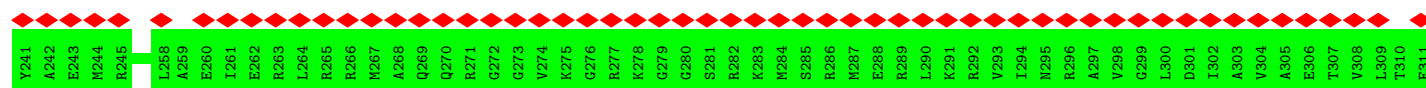
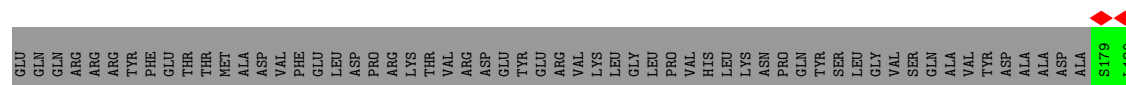
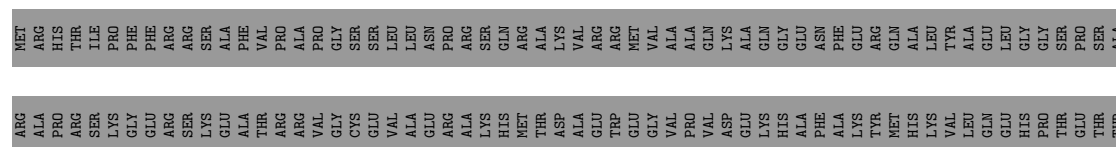
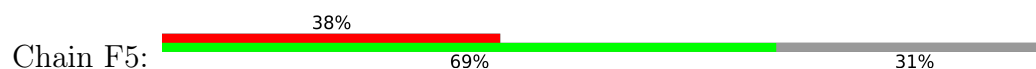
Chain F3: 11% 91% 8%

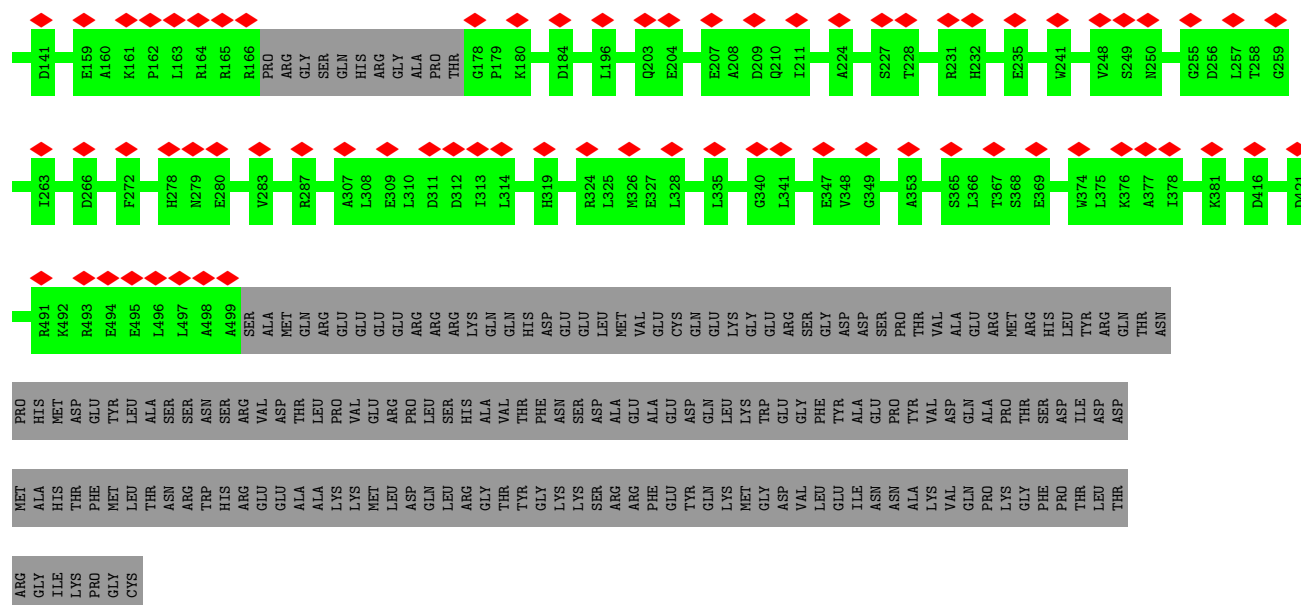




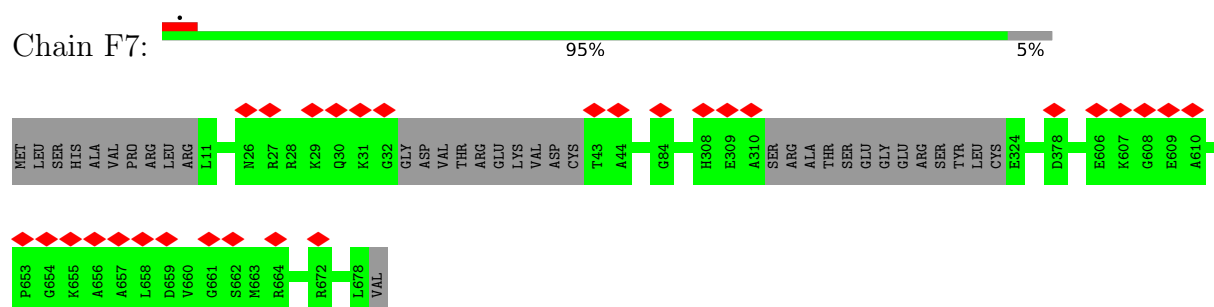


- Molecule 49: Kinteoplast poly(A) polymerase complex 1 subunit

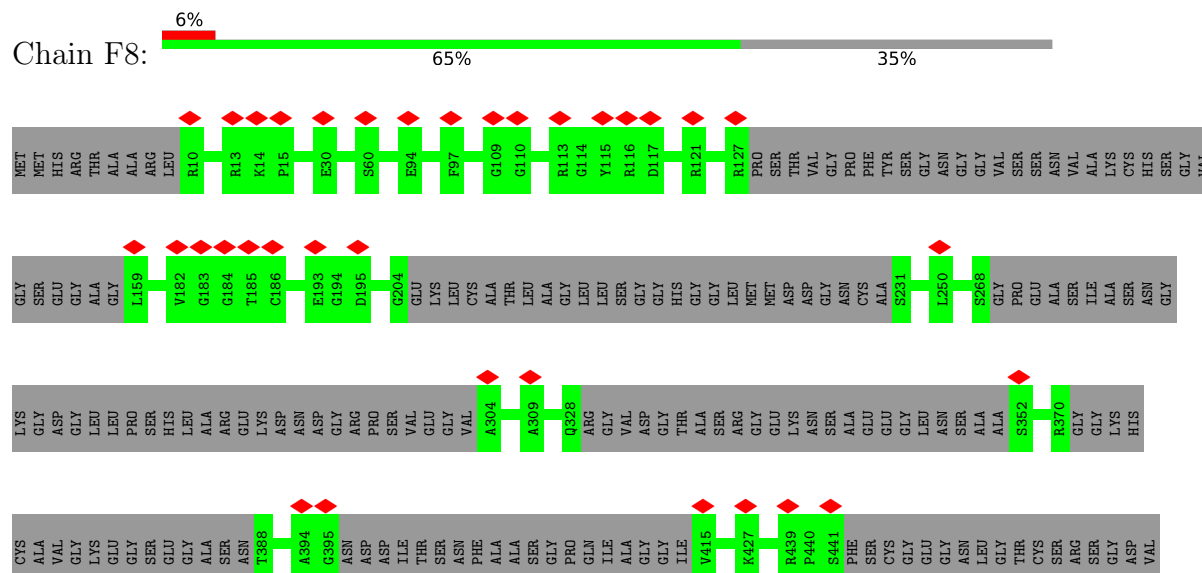


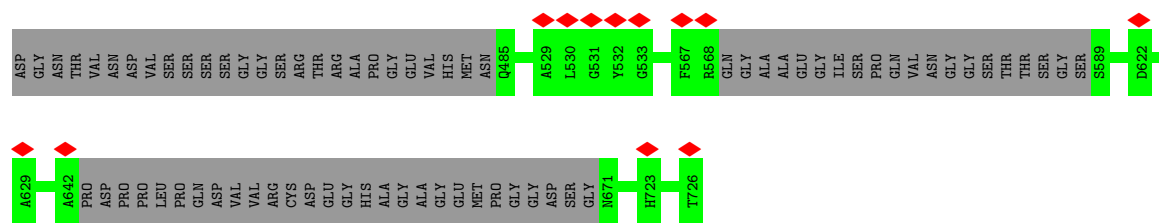


- Molecule 51: mt-SAF7 (KRIPP10)

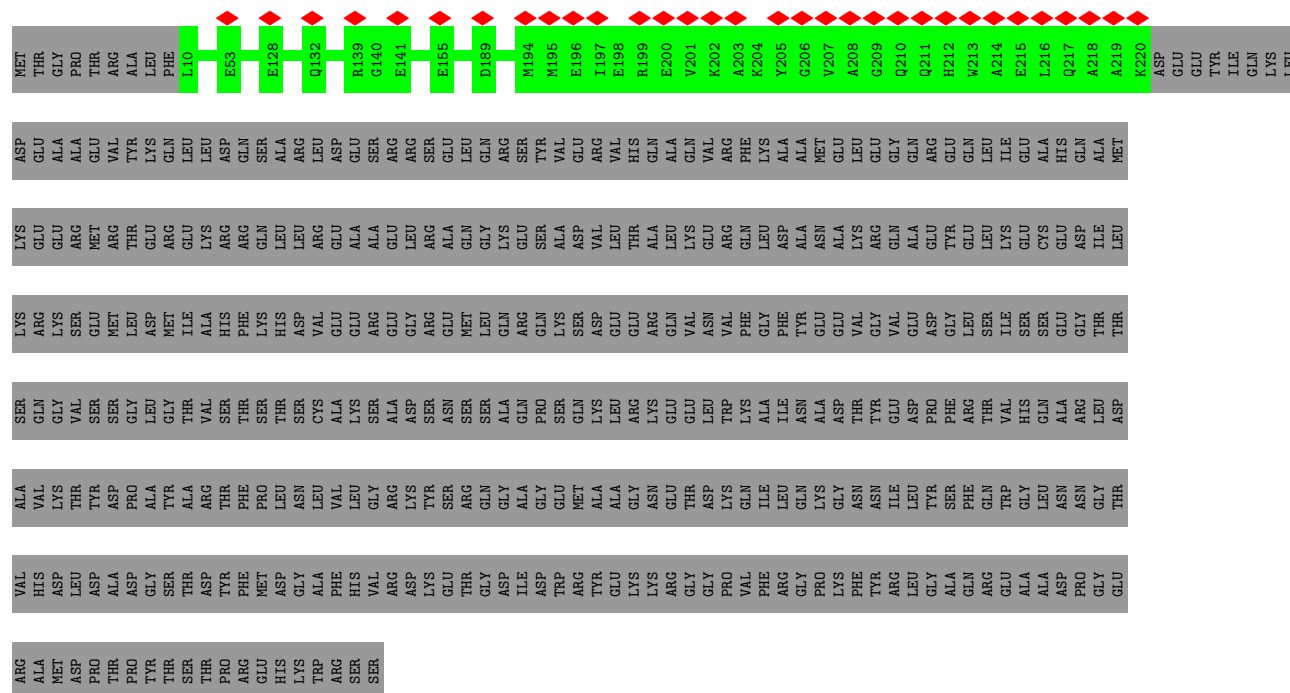


- Molecule 52: Cupin type-1 domain-containing protein

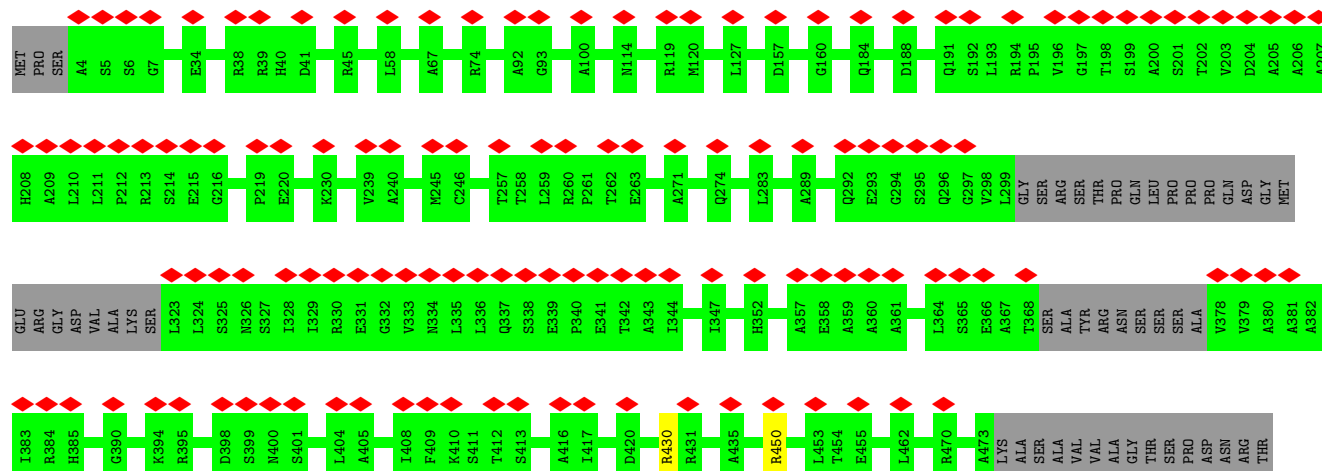
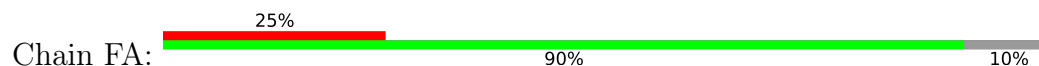


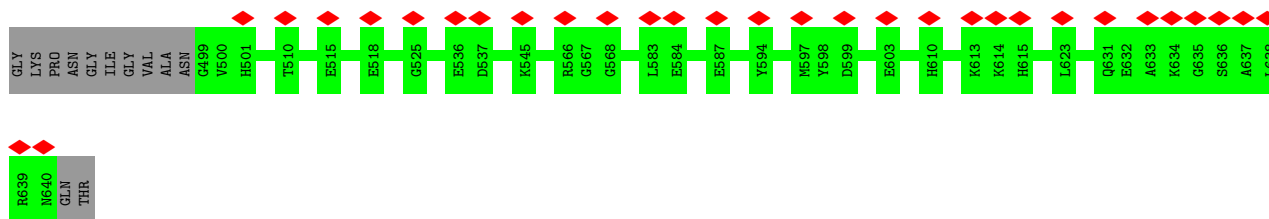


• Molecule 53: Trichohyalin

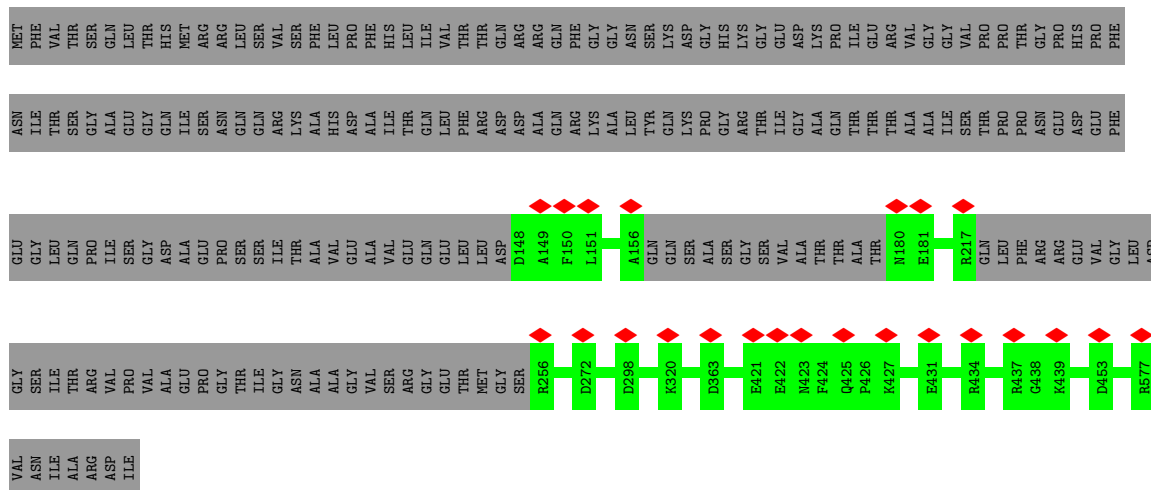


• Molecule 54: mt-SAF10

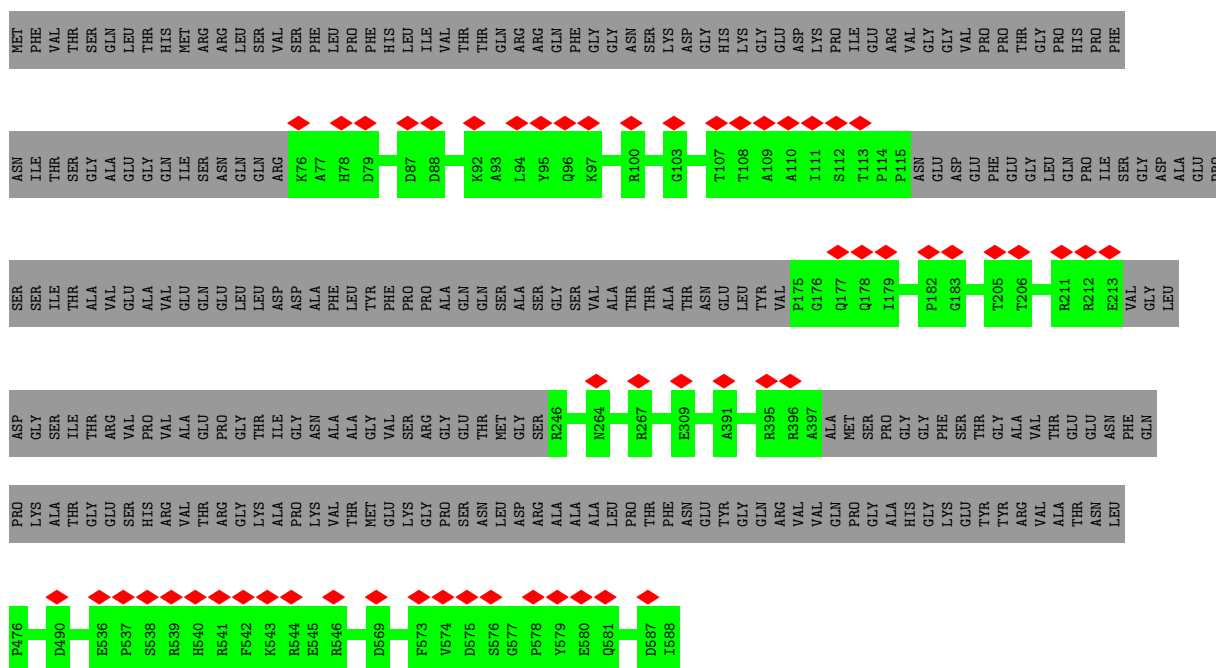




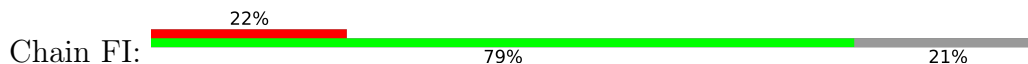
- Molecule 55: tRNA pseudouridine synthase A-like protein

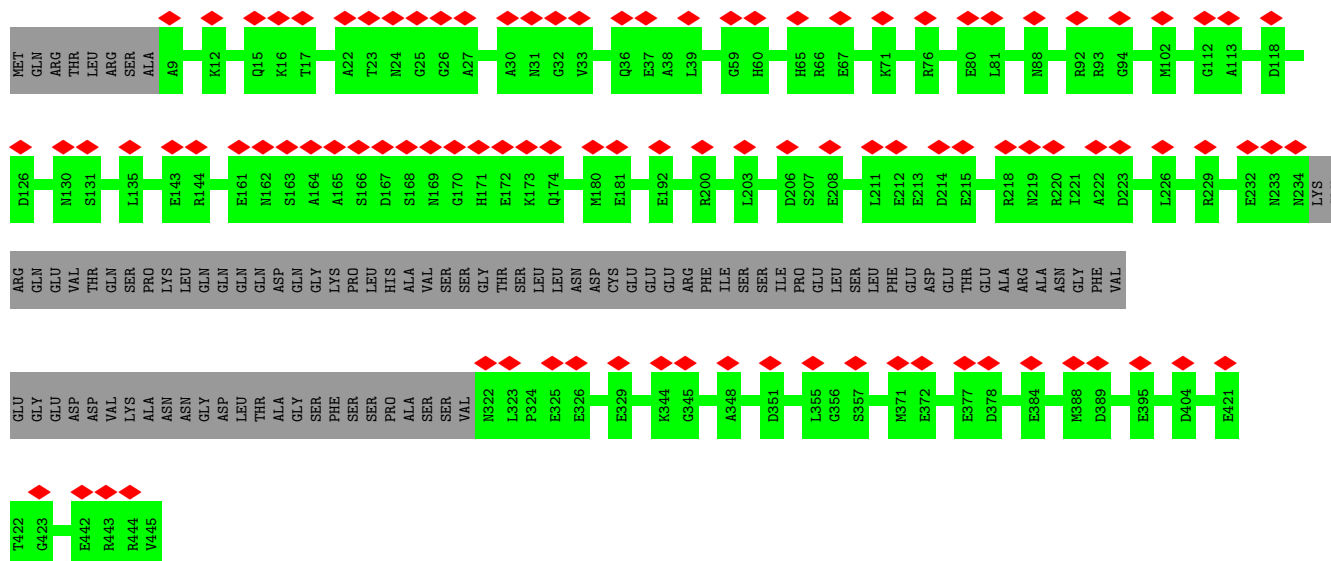


- Molecule 55: tRNA pseudouridine synthase A-like protein



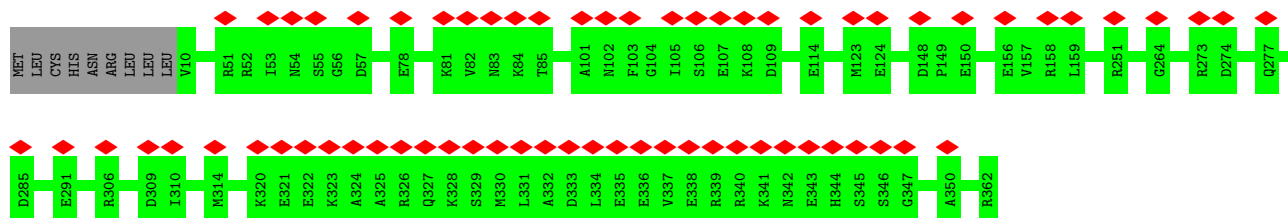
- Molecule 56: PPR long domain-containing protein





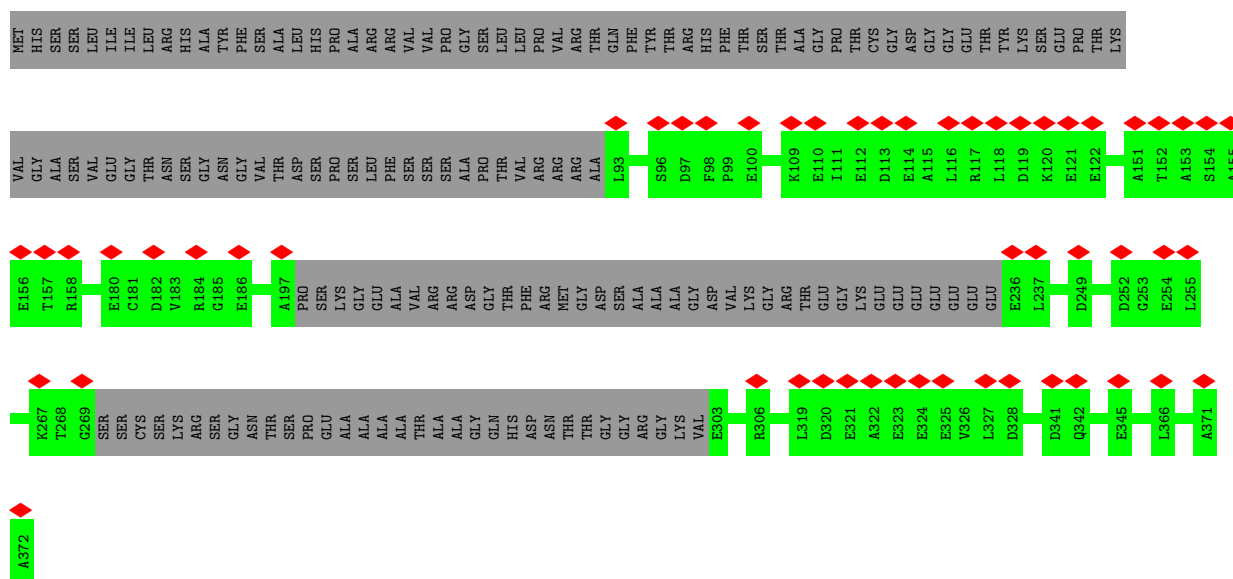
• Molecule 62: mt-SAF18 (RbfA)

Chain FJ: 19% 98% .

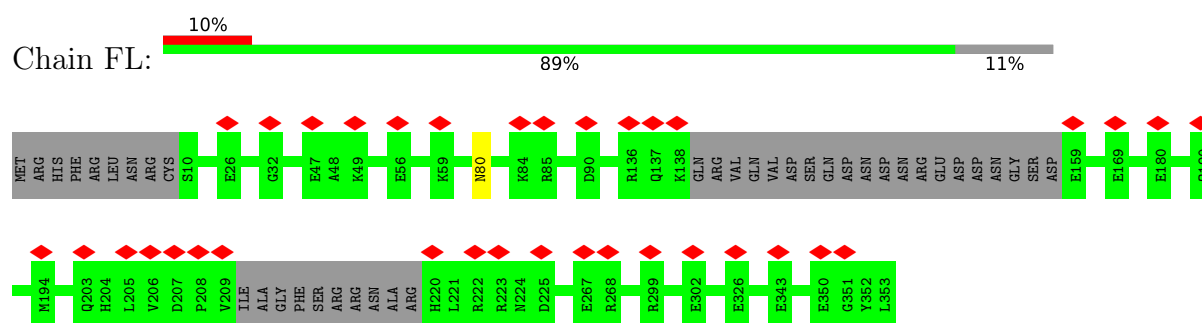


• Molecule 63: Mitochondrial glycoprotein

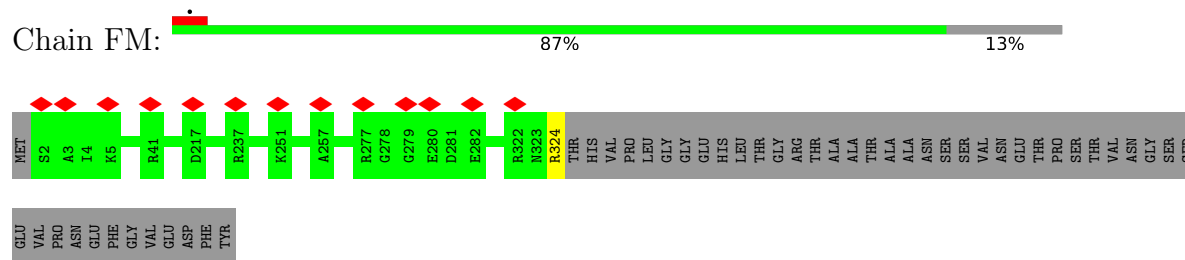
Chain FK: 15% 56% 44%



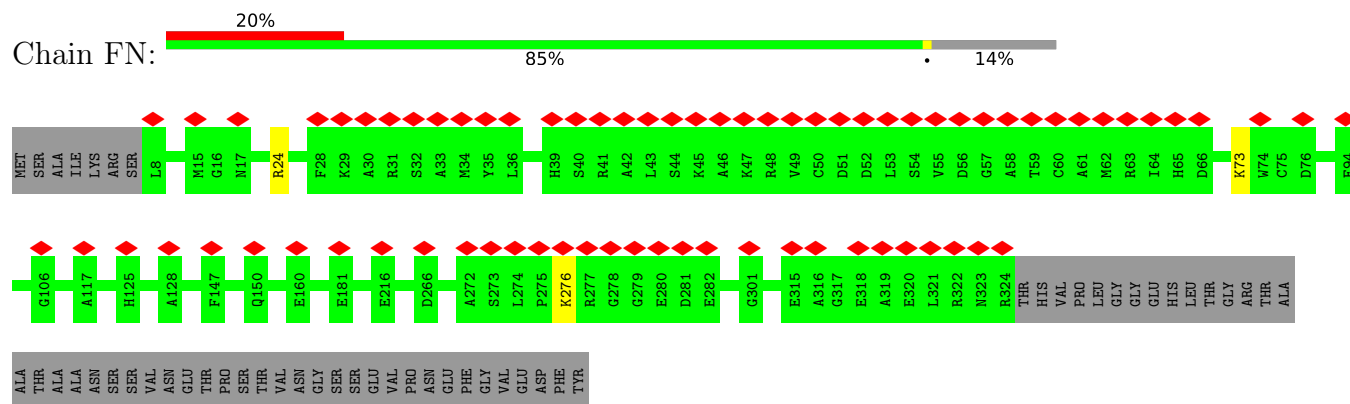
• Molecule 64: Metallo-beta-lactamase domain-containing protein



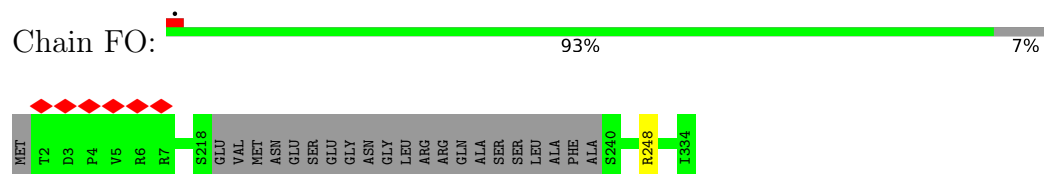
- Molecule 65: mt-SAF21



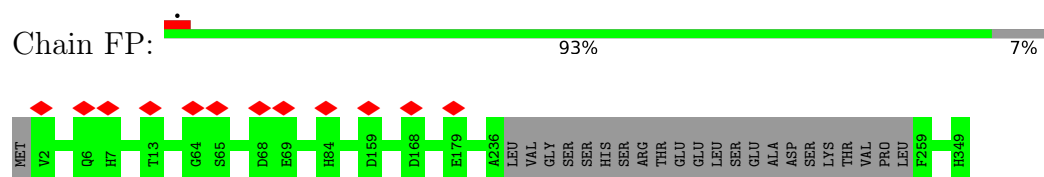
- Molecule 65: mt-SAF21



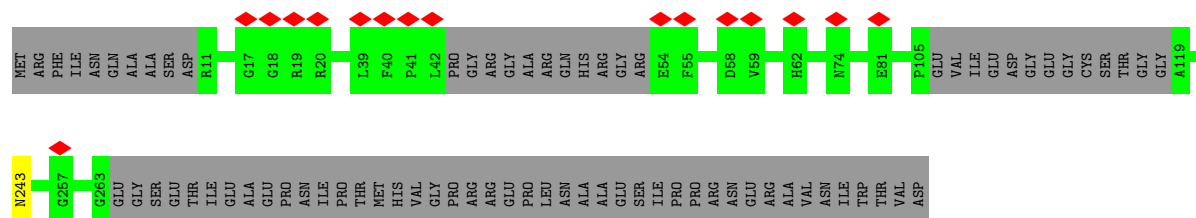
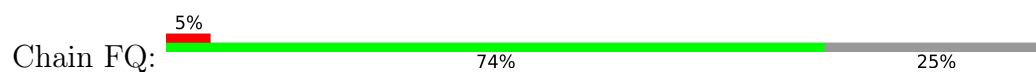
- Molecule 66: mt-SAF22



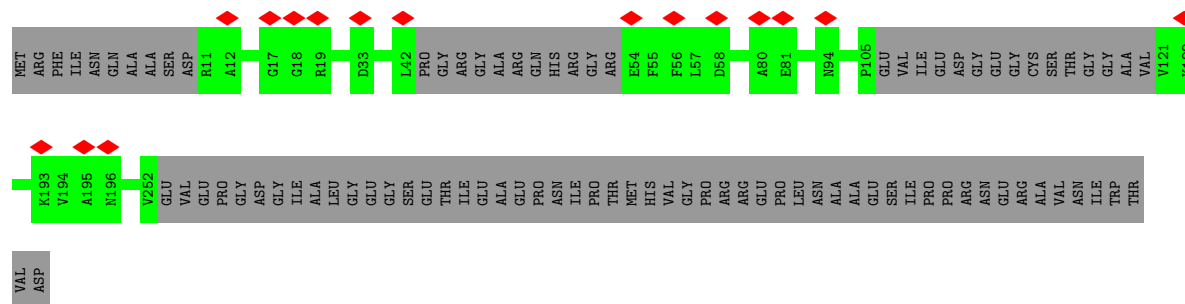
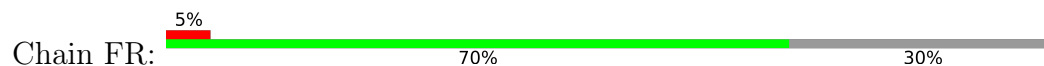
- Molecule 67: ADP-ribosylglycohydrolase



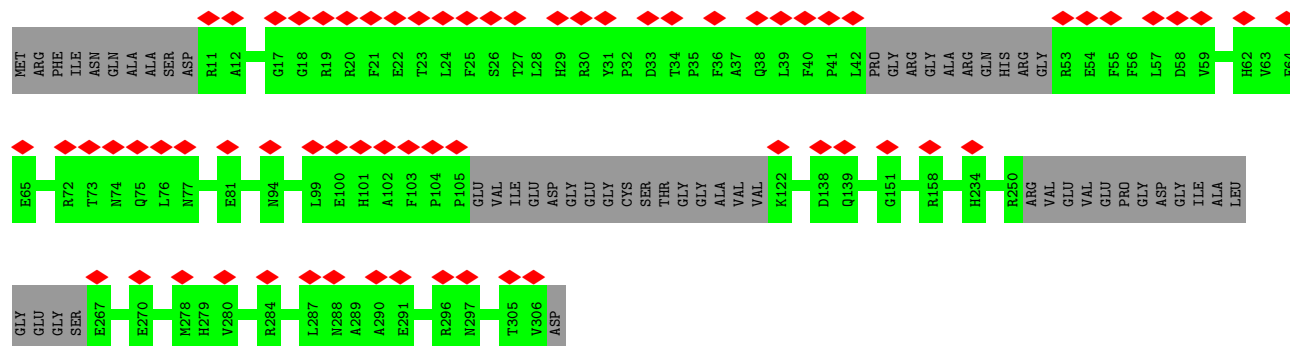
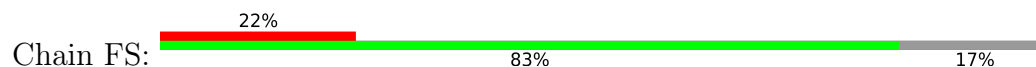
- Molecule 68: Potassium voltage-gated channel, putative



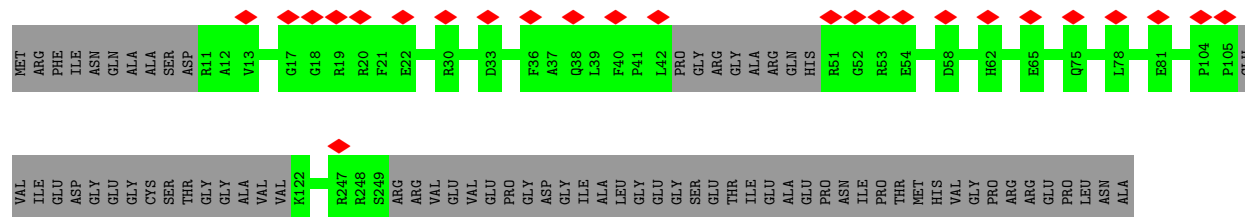
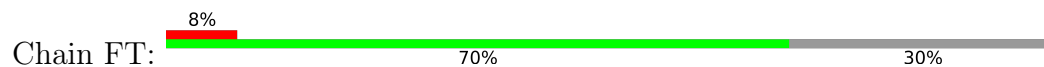
- Molecule 68: Potassium voltage-gated channel, putative



- Molecule 68: Potassium voltage-gated channel, putative




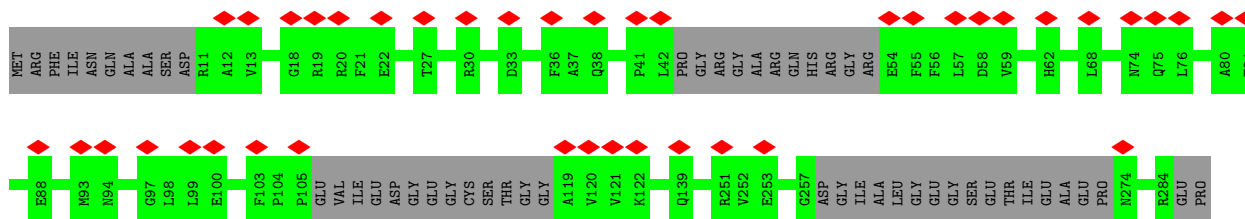
- Molecule 68: Potassium voltage-gated channel, putative



ALA
GLU
SER
ILE
PRO
PRO
ARG
GLU
ASN
ARG
ASP
ALA
VAL
ASN
ILE
TRP
VAL
ASP


- Molecule 68: Potassium voltage-gated channel, putative

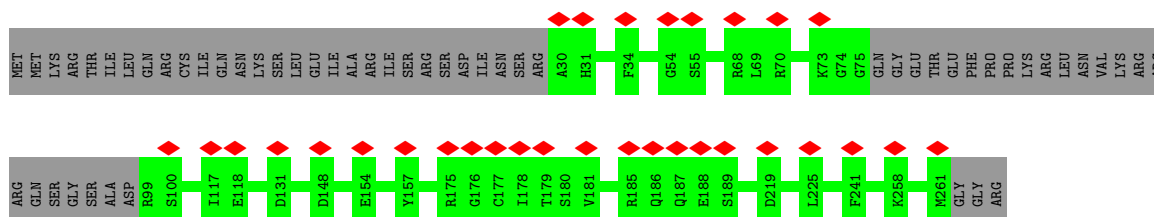
Chain FU: 



LEU
ASN
ALA
GLU
SER
ILE
PRO
PRO
ASN
GLU
ARG
ALA
VAL
ASN
ILE
TRP
THR
VAL
ASP

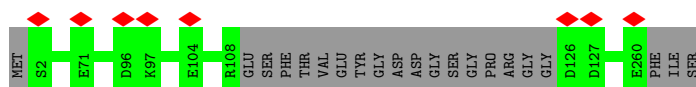
- Molecule 69: mt-SAF25

Chain FV: 




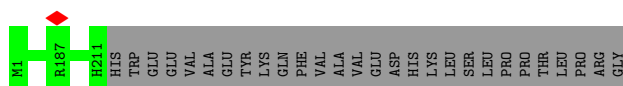
- Molecule 70: Low molecular weight protein tyrosine phosphatase

Chain FW: 




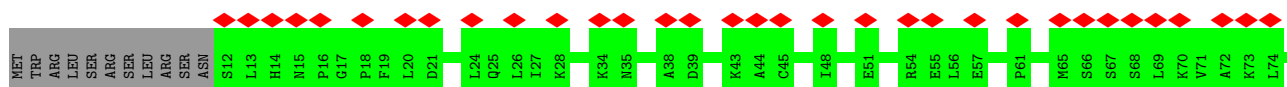
- Molecule 71: PPR_long domain-containing protein

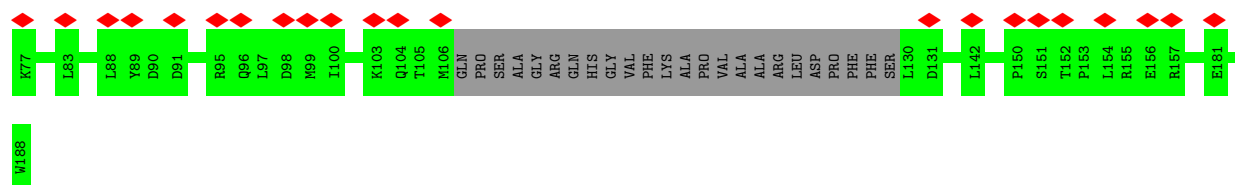
Chain FX: 



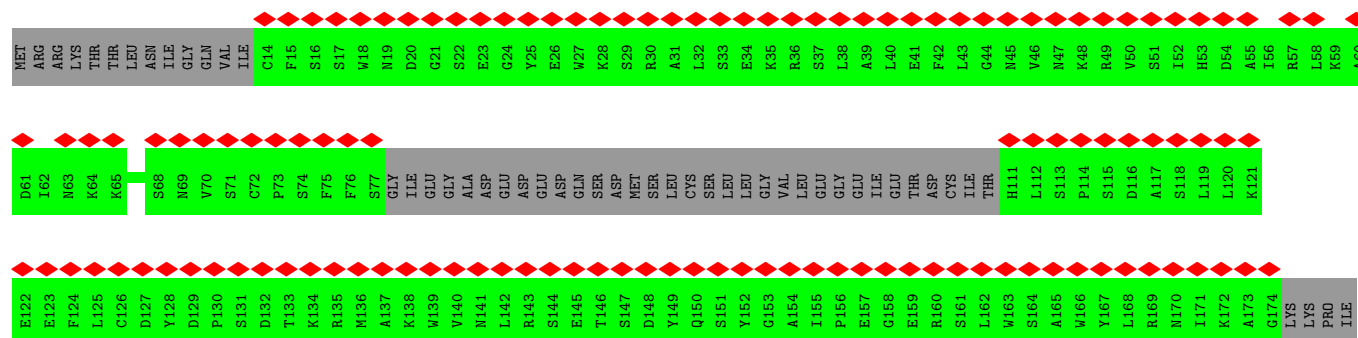
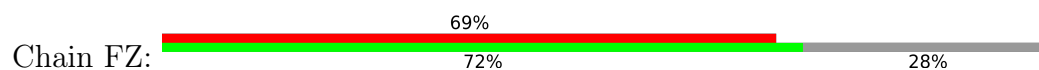
- Molecule 72: mt-SAF28

Chain FY: 

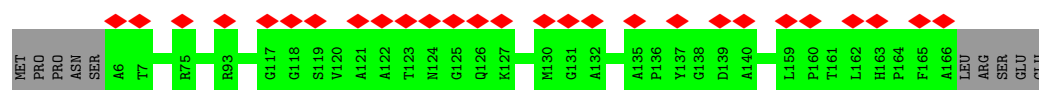




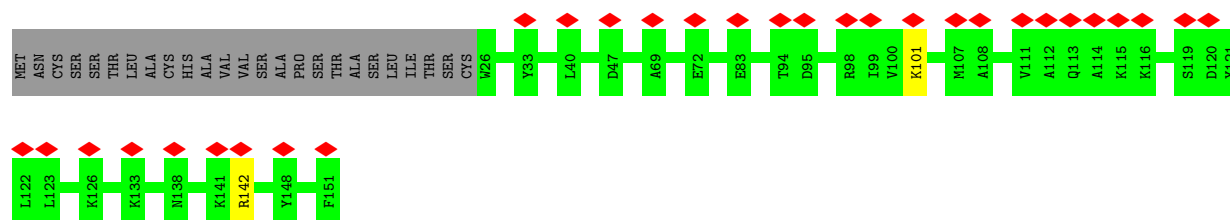
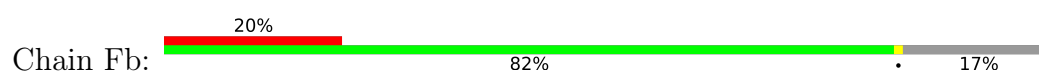
- Molecule 73: mt-SAF29



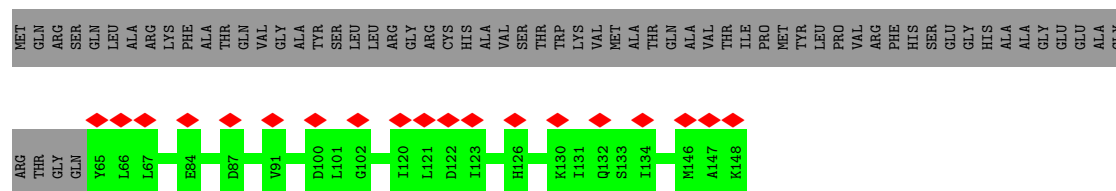
- Molecule 74: mt-SAF30



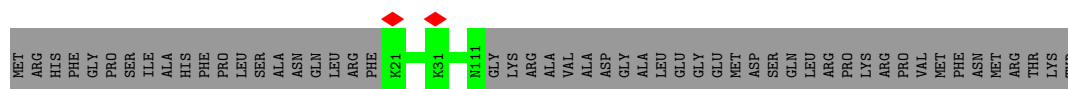
- Molecule 75: Complex 1 protein (LYR family)



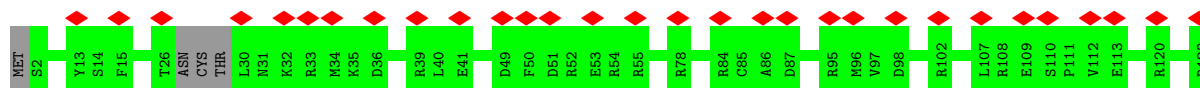
- Molecule 76: Acyl carrier protein



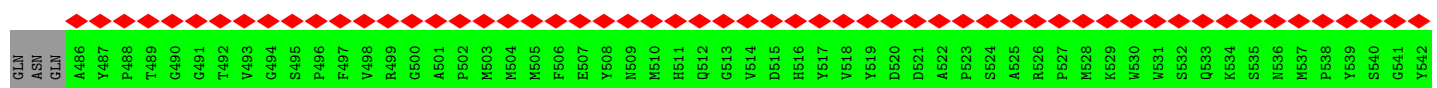
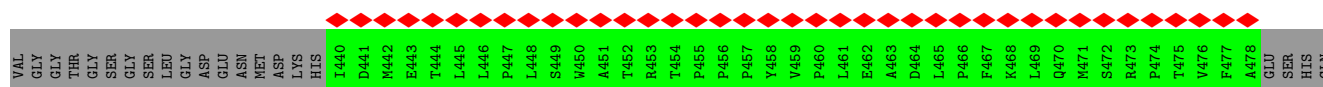
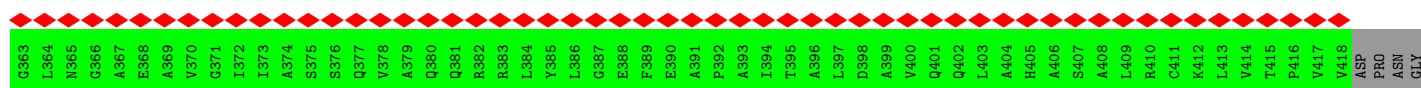
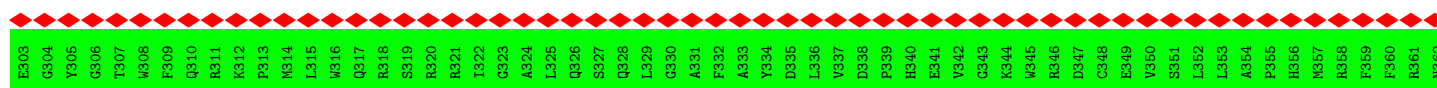
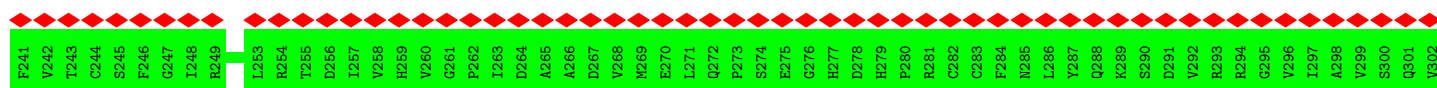
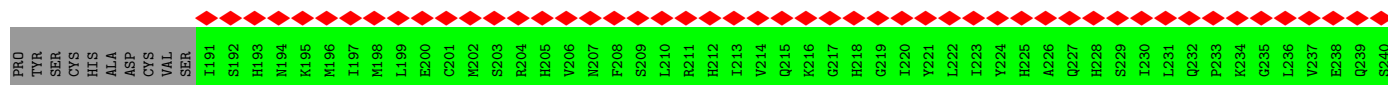
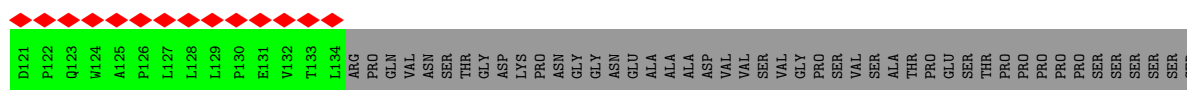
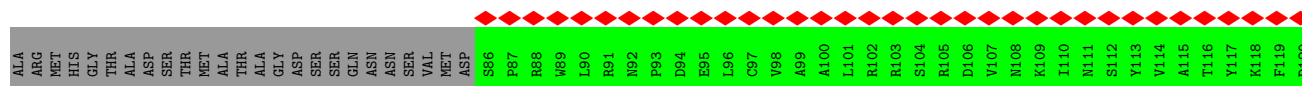
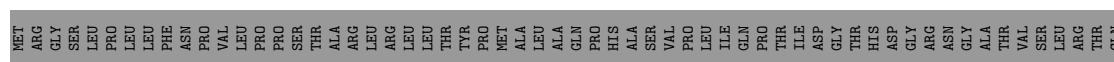
- Molecule 77: Probable Zinc-ribbon domain-containing protein

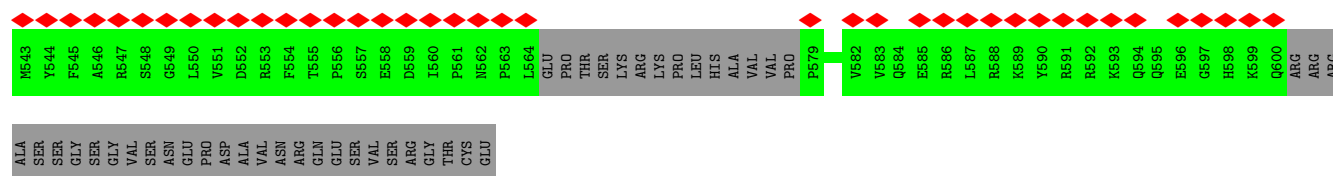


• Molecule 78: mt-SAF34

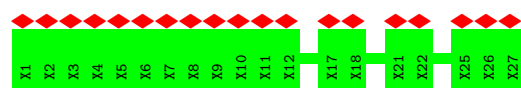
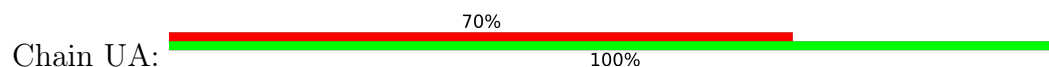


• Molecule 79: mt-SAF38





- Molecule 80: UNK-A



- Molecule 81: UNK-B

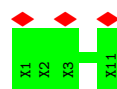


- Molecule 82: UNK-C



There are no outlier residues recorded for this chain.

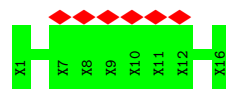
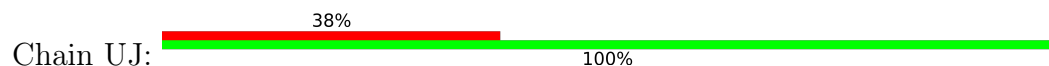
- Molecule 83: UNK-F




- Molecule 84: UNK-G,J



- Molecule 84: UNK-G,J



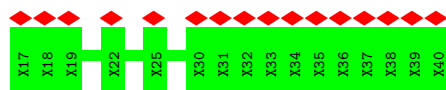
- Molecule 85: UNK-I

Chain UI:  100%

There are no outlier residues recorded for this chain.

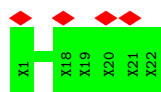
- Molecule 86: UNK-K

Chain UK:  67%
100%



- Molecule 87: UNK-L

Chain UL:  18%
100%



- Molecule 88: UNK-M,Q

Chain UM:  11%
100%



- Molecule 88: UNK-M,Q

Chain UQ:  22%
100%



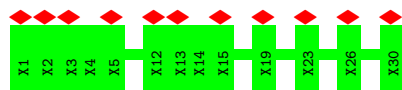
- Molecule 89: UNK-N

Chain UN:  14%
100%

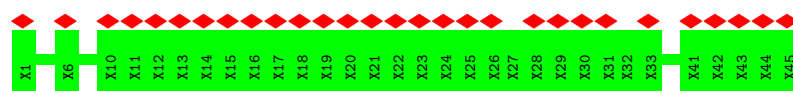


- Molecule 90: UNK-O

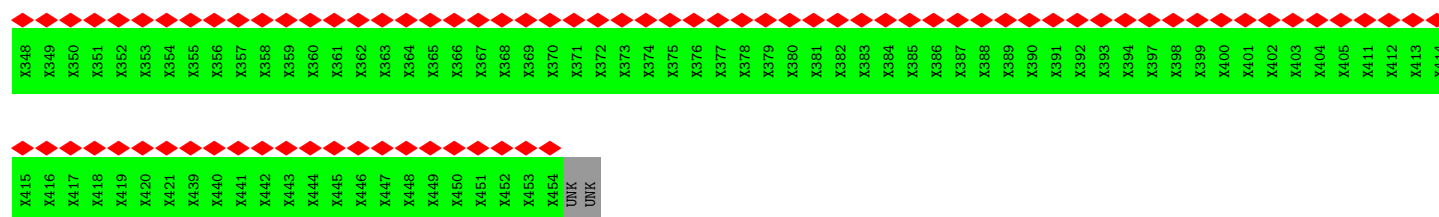
Chain UO:  37%
100%



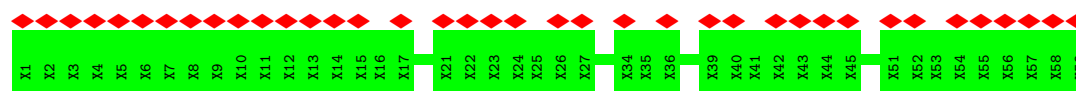
- Molecule 91: UNK-P



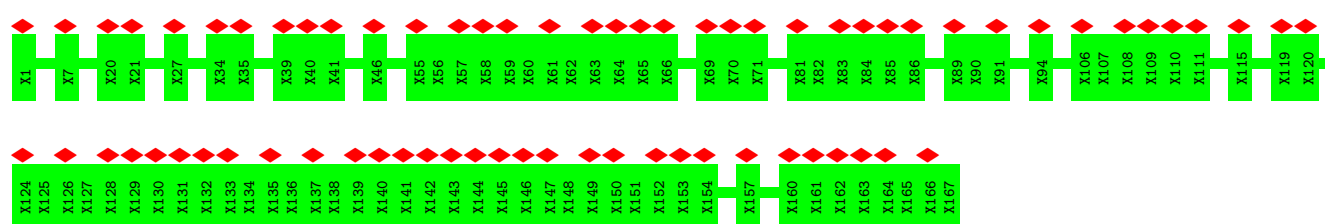
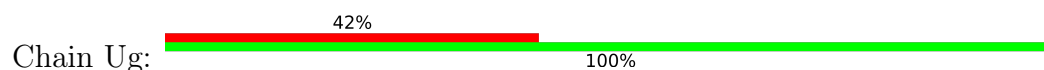
• Molecule 92: UNK-Y



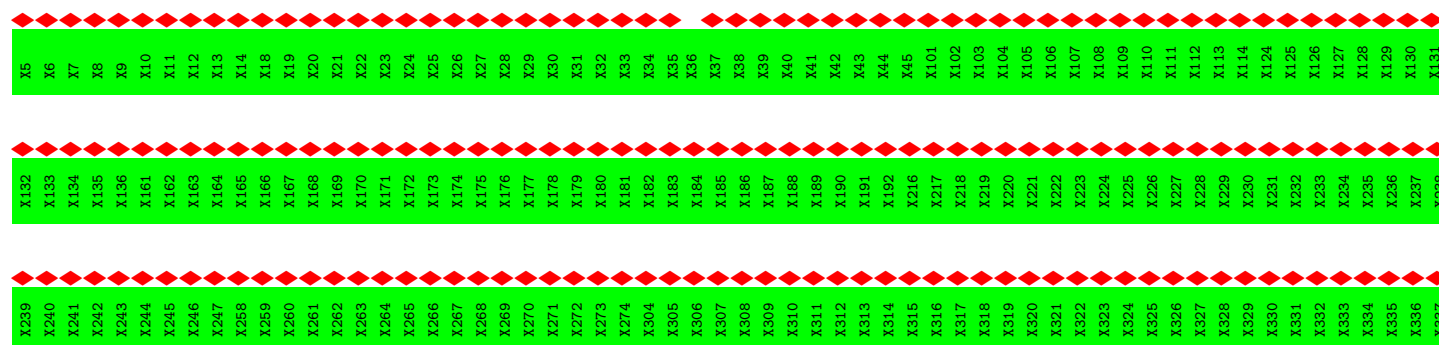
• Molecule 93: UNK-d

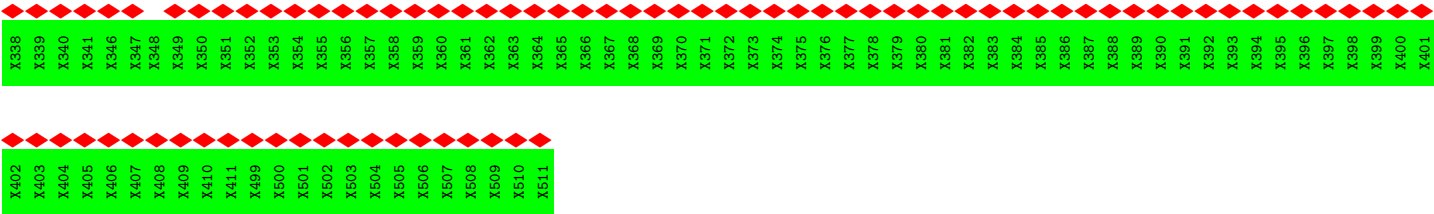


• Molecule 94: UNK-g

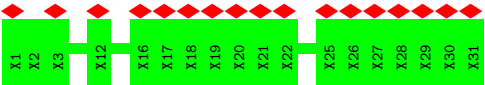


• Molecule 95: UNK-h

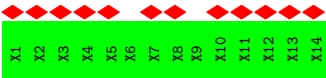
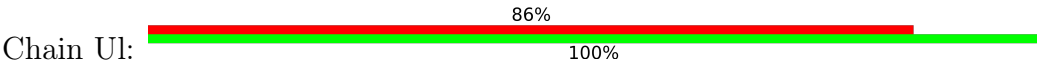




● Molecule 96: UNK-k



● Molecule 97: UNK-l



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.613	Depositor
Minimum map value	-0.285	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, SAM, ZN, ACO, PO4, GTP

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	CA	0.23	0/11345	0.70	0/17617
2	CC	0.27	0/603	0.46	0/814
3	CE	0.27	0/3095	0.54	0/4184
4	CF	0.27	0/1344	0.54	0/1813
5	CH	0.26	0/1797	0.57	0/2421
6	CI	0.26	0/3388	0.51	0/4576
7	CJ	0.25	0/5781	0.50	0/7862
8	CK	0.26	0/1722	0.53	0/2321
9	CN	0.24	0/1287	0.49	0/1740
10	CO	0.27	0/3044	0.52	0/4104
11	CP	0.27	0/1533	0.53	0/2074
12	CQ	0.27	0/1985	0.51	0/2687
13	CR	0.26	0/1189	0.53	0/1609
14	CS	0.25	0/731	0.46	0/987
15	Ca	0.27	0/4351	0.52	1/5880 (0.0%)
16	Cb	0.28	0/1298	0.55	0/1744
17	Cd	0.27	0/1671	0.48	0/2246
18	Cg	0.26	0/4032	0.48	0/5475
19	Ci	0.25	0/1256	0.52	0/1695
20	Cj	0.28	0/1834	0.51	0/2499
21	Ck	0.24	0/4340	0.50	0/5871
22	Cn	0.28	0/223	0.48	0/305
23	Cp	0.27	0/1496	0.51	0/2030
24	DB	0.25	0/5108	0.55	0/6905
25	DC	0.25	0/8359	0.49	0/11333
26	DD	0.27	0/6621	0.51	0/8972
27	DE	0.25	0/4710	0.51	0/6396
28	DF	0.24	0/4031	0.52	0/5459
29	DG	0.25	0/4633	0.52	0/6280
30	DH	0.24	0/4169	0.51	0/5641
31	DI	0.26	0/3244	0.52	0/4395
32	DJ	0.25	0/2599	0.48	0/3519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	DK	0.25	0/1828	0.49	0/2474
34	DL	0.27	0/1664	0.53	0/2247
35	DO	0.26	0/1576	0.51	0/2124
36	DP	0.26	0/1851	0.51	0/2507
37	DR	0.28	0/2093	0.53	0/2853
38	DT	0.26	0/1982	0.49	0/2685
39	DU	0.27	0/1777	0.52	0/2412
40	DV	0.25	0/1246	0.51	0/1691
41	DW	0.25	0/1172	0.50	0/1599
42	DX	0.24	0/765	0.51	0/1030
43	DY	0.26	0/1334	0.54	0/1810
44	DZ	0.24	0/247	0.40	0/333
45	F1	0.25	0/7134	0.55	0/9607
46	F2	0.26	0/7256	0.50	0/9804
47	F3	0.25	0/6980	0.50	0/9447
48	F4	0.25	0/4358	0.50	0/5894
49	F5	0.25	0/3829	0.48	0/5192
50	F6	0.26	0/3728	0.50	0/5060
51	F7	0.26	0/5227	0.50	0/7077
52	F8	0.27	0/3747	0.53	0/5074
53	F9	0.26	0/1737	0.53	0/2333
54	FA	0.24	0/4509	0.49	0/6141
55	FB	0.26	0/3190	0.54	0/4328
55	FC	0.25	0/2889	0.55	0/3913
56	FD	0.25	0/3604	0.50	0/4905
57	FE	0.27	0/3583	0.51	0/4872
58	FF	0.26	0/3307	0.53	0/4461
59	FG	0.24	0/1429	0.52	0/1926
60	FH	0.27	0/2445	0.53	0/3315
61	FI	0.25	0/2847	0.53	0/3842
62	FJ	0.26	0/2987	0.54	0/4030
63	FK	0.27	0/1757	0.50	0/2390
64	FL	0.26	0/2567	0.53	0/3479
65	FM	0.25	0/2462	0.52	0/3326
65	FN	0.25	0/2417	0.51	0/3267
66	FO	0.27	0/2647	0.57	0/3579
67	FP	0.27	0/2593	0.49	0/3544
68	FQ	0.26	0/1886	0.54	0/2562
68	FR	0.26	0/1800	0.53	0/2444
68	FS	0.26	0/2110	0.53	0/2869
68	FT	0.25	0/1790	0.54	0/2429
68	FU	0.26	0/1939	0.54	0/2633
69	FV	0.27	0/1668	0.49	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	FW	0.25	0/2036	0.55	0/2751
71	FX	0.25	0/1693	0.49	0/2287
72	FY	0.25	0/1267	0.50	0/1715
73	FZ	0.29	0/966	0.51	0/1305
74	Fa	0.26	0/1351	0.53	0/1837
75	Fb	0.25	0/1104	0.50	0/1487
76	Fc	0.27	0/679	0.46	0/923
77	Fd	0.26	0/743	0.49	0/1007
78	Fe	0.26	0/1035	0.58	0/1389
79	Fi	0.25	0/3438	0.52	0/4660
All	All	0.26	0/235088	0.53	1/320588 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
58	FF	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Ca	57	PRO	N-CA-CB	5.75	110.20	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	FF	222	ASP	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CC	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
3	CE	364/435 (84%)	341 (94%)	23 (6%)	0	100	100
4	CF	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
5	CH	208/282 (74%)	197 (95%)	11 (5%)	0	100	100
6	CI	414/443 (94%)	404 (98%)	10 (2%)	0	100	100
7	CJ	685/817 (84%)	664 (97%)	21 (3%)	0	100	100
8	CK	199/326 (61%)	190 (96%)	9 (4%)	0	100	100
9	CN	146/158 (92%)	141 (97%)	5 (3%)	0	100	100
10	CO	352/429 (82%)	339 (96%)	13 (4%)	0	100	100
11	CP	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
12	CQ	232/336 (69%)	226 (97%)	6 (3%)	0	100	100
13	CR	128/320 (40%)	127 (99%)	1 (1%)	0	100	100
14	CS	79/244 (32%)	73 (92%)	6 (8%)	0	100	100
15	Ca	488/602 (81%)	465 (95%)	22 (4%)	1 (0%)	44	71
16	Cb	148/311 (48%)	136 (92%)	9 (6%)	3 (2%)	6	28
17	Cd	184/440 (42%)	176 (96%)	8 (4%)	0	100	100
18	Cg	481/490 (98%)	461 (96%)	20 (4%)	0	100	100
19	Ci	145/181 (80%)	138 (95%)	7 (5%)	0	100	100
20	Cj	223/257 (87%)	216 (97%)	7 (3%)	0	100	100
21	Ck	525/874 (60%)	511 (97%)	14 (3%)	0	100	100
22	Cn	23/250 (9%)	20 (87%)	3 (13%)	0	100	100
23	Cp	169/187 (90%)	162 (96%)	7 (4%)	0	100	100
24	DB	578/1181 (49%)	553 (96%)	25 (4%)	0	100	100
25	DC	1013/1165 (87%)	990 (98%)	23 (2%)	0	100	100
26	DD	774/812 (95%)	741 (96%)	33 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	DE	571/747 (76%)	522 (91%)	48 (8%)	1 (0%)	44	71
28	DF	477/666 (72%)	465 (98%)	12 (2%)	0	100	100
29	DG	552/631 (88%)	531 (96%)	21 (4%)	0	100	100
30	DH	489/581 (84%)	471 (96%)	18 (4%)	0	100	100
31	DI	388/407 (95%)	379 (98%)	9 (2%)	0	100	100
32	DJ	305/396 (77%)	296 (97%)	9 (3%)	0	100	100
33	DK	221/324 (68%)	217 (98%)	4 (2%)	0	100	100
34	DL	195/307 (64%)	193 (99%)	2 (1%)	0	100	100
35	DO	190/282 (67%)	179 (94%)	11 (6%)	0	100	100
36	DP	210/274 (77%)	194 (92%)	16 (8%)	0	100	100
37	DR	247/270 (92%)	233 (94%)	14 (6%)	0	100	100
38	DT	219/247 (89%)	197 (90%)	22 (10%)	0	100	100
39	DU	216/228 (95%)	203 (94%)	13 (6%)	0	100	100
40	DV	140/183 (76%)	130 (93%)	10 (7%)	0	100	100
41	DW	130/179 (73%)	124 (95%)	6 (5%)	0	100	100
42	DX	86/169 (51%)	79 (92%)	7 (8%)	0	100	100
43	DY	152/163 (93%)	146 (96%)	6 (4%)	0	100	100
44	DZ	26/94 (28%)	24 (92%)	2 (8%)	0	100	100
45	F1	848/1041 (82%)	811 (96%)	36 (4%)	1 (0%)	48	76
46	F2	880/1024 (86%)	845 (96%)	35 (4%)	0	100	100
47	F3	880/966 (91%)	843 (96%)	36 (4%)	1 (0%)	48	76
48	F4	500/811 (62%)	480 (96%)	20 (4%)	0	100	100
49	F5	511/754 (68%)	483 (94%)	28 (6%)	0	100	100
50	F6	450/676 (67%)	432 (96%)	18 (4%)	0	100	100
51	F7	639/679 (94%)	612 (96%)	27 (4%)	0	100	100
52	F8	455/726 (63%)	439 (96%)	16 (4%)	0	100	100
53	F9	209/608 (34%)	206 (99%)	3 (1%)	0	100	100
54	FA	572/642 (89%)	553 (97%)	19 (3%)	0	100	100
55	FB	377/588 (64%)	362 (96%)	15 (4%)	0	100	100
55	FC	336/588 (57%)	320 (95%)	16 (5%)	0	100	100
56	FD	444/579 (77%)	424 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	FE	428/553 (77%)	418 (98%)	10 (2%)	0	100	100
58	FF	401/474 (85%)	378 (94%)	22 (6%)	1 (0%)	44	71
59	FG	172/463 (37%)	158 (92%)	14 (8%)	0	100	100
60	FH	299/457 (65%)	274 (92%)	25 (8%)	0	100	100
61	FI	346/445 (78%)	338 (98%)	8 (2%)	0	100	100
62	FJ	351/362 (97%)	340 (97%)	11 (3%)	0	100	100
63	FK	203/372 (55%)	194 (96%)	9 (4%)	0	100	100
64	FL	308/353 (87%)	289 (94%)	19 (6%)	0	100	100
65	FM	321/370 (87%)	309 (96%)	12 (4%)	0	100	100
65	FN	315/370 (85%)	309 (98%)	6 (2%)	0	100	100
66	FO	308/334 (92%)	294 (96%)	14 (4%)	0	100	100
67	FP	322/349 (92%)	309 (96%)	13 (4%)	0	100	100
68	FQ	223/307 (73%)	216 (97%)	7 (3%)	0	100	100
68	FR	210/307 (68%)	203 (97%)	7 (3%)	0	100	100
68	FS	246/307 (80%)	238 (97%)	8 (3%)	0	100	100
68	FT	209/307 (68%)	203 (97%)	6 (3%)	0	100	100
68	FU	226/307 (74%)	209 (92%)	17 (8%)	0	100	100
69	FV	205/264 (78%)	194 (95%)	11 (5%)	0	100	100
70	FW	238/263 (90%)	226 (95%)	12 (5%)	0	100	100
71	FX	209/239 (87%)	199 (95%)	10 (5%)	0	100	100
72	FY	150/189 (79%)	143 (95%)	7 (5%)	0	100	100
73	FZ	124/178 (70%)	119 (96%)	5 (4%)	0	100	100
74	Fa	159/171 (93%)	152 (96%)	7 (4%)	0	100	100
75	Fb	124/151 (82%)	123 (99%)	1 (1%)	0	100	100
76	Fc	82/148 (55%)	79 (96%)	3 (4%)	0	100	100
77	Fd	89/143 (62%)	84 (94%)	5 (6%)	0	100	100
78	Fe	115/123 (94%)	112 (97%)	3 (3%)	0	100	100
79	Fi	407/629 (65%)	384 (94%)	23 (6%)	0	100	100
All	All	26661/35727 (75%)	25542 (96%)	1111 (4%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Ca	57	PRO
16	Cb	107	SER
45	F1	709	PRO
47	F3	722	SER
16	Cb	109	GLY
27	DE	214	ARG
16	Cb	108	GLU
58	FF	223	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CC	66/73 (90%)	66 (100%)	0	100	100
3	CE	317/372 (85%)	316 (100%)	1 (0%)	91	94
4	CF	143/144 (99%)	143 (100%)	0	100	100
5	CH	187/246 (76%)	187 (100%)	0	100	100
6	CI	353/372 (95%)	353 (100%)	0	100	100
7	CJ	609/723 (84%)	609 (100%)	0	100	100
8	CK	182/284 (64%)	182 (100%)	0	100	100
9	CN	134/143 (94%)	134 (100%)	0	100	100
10	CO	313/377 (83%)	313 (100%)	0	100	100
11	CP	160/168 (95%)	160 (100%)	0	100	100
12	CQ	208/297 (70%)	208 (100%)	0	100	100
13	CR	120/279 (43%)	119 (99%)	1 (1%)	79	87
14	CS	76/220 (34%)	76 (100%)	0	100	100
15	Ca	441/543 (81%)	441 (100%)	0	100	100
16	Cb	131/267 (49%)	131 (100%)	0	100	100
17	Cd	169/381 (44%)	169 (100%)	0	100	100
18	Cg	424/432 (98%)	424 (100%)	0	100	100
19	Ci	130/160 (81%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Cj	192/219 (88%)	192 (100%)	0	100	100
21	Ck	464/747 (62%)	463 (100%)	1 (0%)	92	95
22	Cn	20/210 (10%)	20 (100%)	0	100	100
23	Cp	159/175 (91%)	159 (100%)	0	100	100
24	DB	532/1027 (52%)	531 (100%)	1 (0%)	92	95
25	DC	862/986 (87%)	862 (100%)	0	100	100
26	DD	687/712 (96%)	687 (100%)	0	100	100
27	DE	464/644 (72%)	464 (100%)	0	100	100
28	DF	418/559 (75%)	418 (100%)	0	100	100
29	DG	486/543 (90%)	486 (100%)	0	100	100
30	DH	436/505 (86%)	436 (100%)	0	100	100
31	DI	349/364 (96%)	349 (100%)	0	100	100
32	DJ	270/347 (78%)	270 (100%)	0	100	100
33	DK	189/262 (72%)	189 (100%)	0	100	100
34	DL	170/263 (65%)	170 (100%)	0	100	100
35	DO	159/229 (69%)	158 (99%)	1 (1%)	84	90
36	DP	190/239 (80%)	188 (99%)	2 (1%)	70	82
37	DR	222/237 (94%)	221 (100%)	1 (0%)	86	91
38	DT	205/228 (90%)	204 (100%)	1 (0%)	86	91
39	DU	179/201 (89%)	179 (100%)	0	100	100
40	DV	132/166 (80%)	132 (100%)	0	100	100
41	DW	123/163 (76%)	121 (98%)	2 (2%)	58	76
42	DX	79/149 (53%)	79 (100%)	0	100	100
43	DY	137/146 (94%)	137 (100%)	0	100	100
44	DZ	23/84 (27%)	23 (100%)	0	100	100
45	F1	746/895 (83%)	745 (100%)	1 (0%)	92	96
46	F2	750/866 (87%)	750 (100%)	0	100	100
47	F3	746/809 (92%)	743 (100%)	3 (0%)	89	93
48	F4	469/704 (67%)	469 (100%)	0	100	100
49	F5	324/642 (50%)	324 (100%)	0	100	100
50	F6	401/590 (68%)	401 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	F7	546/576 (95%)	546 (100%)	0	100	100
52	F8	381/557 (68%)	381 (100%)	0	100	100
53	F9	171/506 (34%)	171 (100%)	0	100	100
54	FA	478/527 (91%)	476 (100%)	2 (0%)	89	93
55	FB	327/493 (66%)	327 (100%)	0	100	100
55	FC	298/493 (60%)	298 (100%)	0	100	100
56	FD	379/494 (77%)	377 (100%)	2 (0%)	86	91
57	FE	382/486 (79%)	382 (100%)	0	100	100
58	FF	345/400 (86%)	345 (100%)	0	100	100
59	FG	153/414 (37%)	152 (99%)	1 (1%)	81	88
60	FH	259/390 (66%)	259 (100%)	0	100	100
61	FI	299/380 (79%)	299 (100%)	0	100	100
62	FJ	314/323 (97%)	314 (100%)	0	100	100
63	FK	182/308 (59%)	182 (100%)	0	100	100
64	FL	275/310 (89%)	274 (100%)	1 (0%)	89	93
65	FM	254/292 (87%)	253 (100%)	1 (0%)	89	93
65	FN	249/292 (85%)	246 (99%)	3 (1%)	67	80
66	FO	273/290 (94%)	272 (100%)	1 (0%)	89	93
67	FP	265/286 (93%)	265 (100%)	0	100	100
68	FQ	202/264 (76%)	201 (100%)	1 (0%)	86	91
68	FR	194/264 (74%)	194 (100%)	0	100	100
68	FS	227/264 (86%)	227 (100%)	0	100	100
68	FT	192/264 (73%)	192 (100%)	0	100	100
68	FU	209/264 (79%)	209 (100%)	0	100	100
69	FV	182/231 (79%)	182 (100%)	0	100	100
70	FW	218/234 (93%)	218 (100%)	0	100	100
71	FX	169/195 (87%)	169 (100%)	0	100	100
72	FY	136/165 (82%)	136 (100%)	0	100	100
73	FZ	86/156 (55%)	86 (100%)	0	100	100
74	Fa	140/150 (93%)	140 (100%)	0	100	100
75	Fb	114/135 (84%)	112 (98%)	2 (2%)	54	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	Fc	78/127 (61%)	78 (100%)	0	100	100
77	Fd	76/119 (64%)	76 (100%)	0	100	100
78	Fe	111/115 (96%)	111 (100%)	0	100	100
79	Fi	361/537 (67%)	361 (100%)	0	100	100
All	All	23271/30693 (76%)	23242 (100%)	29 (0%)	92	96

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CE	143	ASN
13	CR	55	ARG
21	Ck	583	ARG
24	DB	705	LYS
35	DO	85	LYS
36	DP	139	ARG
36	DP	187	ARG
37	DR	158	ARG
38	DT	105	ARG
41	DW	90	ARG
41	DW	155	ARG
45	F1	221	ARG
47	F3	750	ARG
47	F3	777	ARG
47	F3	892	ARG
54	FA	430	ARG
54	FA	450	ARG
56	FD	4	ARG
56	FD	14	ARG
59	FG	181	ARG
64	FL	80	ASN
65	FM	324	ARG
65	FN	24	ARG
65	FN	73	LYS
65	FN	276	LYS
66	FO	248	ARG
68	FQ	243	ASN
75	Fb	101	LYS
75	Fb	142	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
6	CI	44	HIS
6	CI	329	HIS
7	CJ	642	ASN
7	CJ	781	HIS
11	CP	84	GLN
11	CP	131	ASN
12	CQ	87	GLN
15	Ca	475	GLN
18	Cg	458	HIS
20	Cj	142	ASN
21	Ck	589	GLN
21	Ck	801	HIS
23	Cp	16	HIS
24	DB	684	GLN
24	DB	711	GLN
25	DC	894	HIS
26	DD	387	GLN
27	DE	315	HIS
27	DE	695	ASN
29	DG	26	ASN
30	DH	114	HIS
30	DH	142	HIS
30	DH	221	HIS
31	DI	209	HIS
34	DL	144	HIS
35	DO	159	HIS
36	DP	143	ASN
37	DR	43	HIS
38	DT	167	ASN
41	DW	99	HIS
46	F2	579	HIS
48	F4	334	GLN
49	F5	485	ASN
50	F6	471	ASN
51	F7	542	ASN
54	FA	145	GLN
54	FA	274	GLN
54	FA	385	HIS
55	FB	367	GLN
56	FD	100	HIS
56	FD	194	GLN
57	FE	125	GLN
63	FK	164	HIS

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Mol	Chain	Res	Type
64	FL	74	ASN
66	FO	318	GLN
68	FQ	139	GLN
69	FV	187	GLN
69	FV	196	ASN
73	FZ	53	HIS
75	Fb	102	HIS
79	Fi	111	ASN
79	Fi	402	GLN
79	Fi	405	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	492/620 (79%)	198 (40%)	6 (1%)

All (198) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	CA	3	A
1	CA	4	A
1	CA	5	U
1	CA	7	A
1	CA	10	G
1	CA	13	A
1	CA	17	G
1	CA	18	U
1	CA	22	U
1	CA	28	U
1	CA	30	U
1	CA	33	A
1	CA	36	U
1	CA	39	U
1	CA	41	A
1	CA	46	U
1	CA	50	A
1	CA	53	A
1	CA	58	A
1	CA	59	U
1	CA	60	A
1	CA	67	U

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Mol	Chain	Res	Type
1	CA	68	A
1	CA	69	U
1	CA	71	U
1	CA	72	U
1	CA	73	U
1	CA	74	G
1	CA	78	G
1	CA	79	A
1	CA	80	U
1	CA	82	U
1	CA	84	U
1	CA	85	U
1	CA	86	G
1	CA	87	U
1	CA	88	A
1	CA	90	A
1	CA	95	U
1	CA	98	A
1	CA	100	G
1	CA	102	A
1	CA	105	G
1	CA	106	U
1	CA	111	A
1	CA	115	A
1	CA	120	U
1	CA	121	A
1	CA	135	U
1	CA	136	G
1	CA	138	U
1	CA	139	U
1	CA	140	U
1	CA	146	U
1	CA	147	G
1	CA	153	A
1	CA	157	G
1	CA	159	G
1	CA	160	U
1	CA	167	A
1	CA	171	A
1	CA	172	A
1	CA	174	A
1	CA	178	A

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Mol	Chain	Res	Type
1	CA	179	U
1	CA	186	U
1	CA	187	A
1	CA	188	U
1	CA	189	A
1	CA	191	A
1	CA	192	U
1	CA	195	A
1	CA	196	U
1	CA	197	A
1	CA	198	A
1	CA	199	U
1	CA	205	A
1	CA	231	U
1	CA	232	G
1	CA	235	A
1	CA	237	C
1	CA	241	U
1	CA	242	G
1	CA	247	A
1	CA	249	U
1	CA	251	U
1	CA	253	U
1	CA	262	A
1	CA	265	U
1	CA	267	U
1	CA	268	U
1	CA	269	A
1	CA	270	U
1	CA	272	C
1	CA	275	U
1	CA	277	A
1	CA	278	U
1	CA	279	C
1	CA	281	U
1	CA	282	A
1	CA	283	U
1	CA	284	U
1	CA	285	A
1	CA	286	A
1	CA	291	U
1	CA	293	A

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Mol	Chain	Res	Type
1	CA	294	A
1	CA	296	U
1	CA	297	G
1	CA	298	C
1	CA	299	U
1	CA	301	A
1	CA	304	U
1	CA	306	A
1	CA	315	A
1	CA	319	U
1	CA	320	A
1	CA	321	A
1	CA	323	U
1	CA	327	U
1	CA	330	U
1	CA	337	U
1	CA	338	U
1	CA	339	U
1	CA	340	U
1	CA	341	A
1	CA	343	A
1	CA	347	C
1	CA	348	A
1	CA	359	G
1	CA	366	U
1	CA	367	A
1	CA	368	A
1	CA	369	A
1	CA	370	A
1	CA	371	U
1	CA	372	U
1	CA	374	U
1	CA	375	A
1	CA	376	G
1	CA	379	A
1	CA	381	U
1	CA	384	A
1	CA	421	G
1	CA	422	G
1	CA	425	A
1	CA	429	U
1	CA	430	U

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Mol	Chain	Res	Type
1	CA	443	U
1	CA	444	A
1	CA	446	C
1	CA	447	A
1	CA	448	U
1	CA	450	A
1	CA	455	G
1	CA	456	A
1	CA	461	A
1	CA	466	G
1	CA	467	A
1	CA	468	A
1	CA	469	A
1	CA	472	G
1	CA	474	U
1	CA	480	C
1	CA	481	A
1	CA	482	U
1	CA	483	A
1	CA	484	A
1	CA	485	U
1	CA	488	A
1	CA	531	G
1	CA	532	A
1	CA	533	A
1	CA	534	A
1	CA	536	U
1	CA	537	A
1	CA	566	U
1	CA	567	A
1	CA	570	A
1	CA	578	C
1	CA	579	G
1	CA	580	U
1	CA	581	G
1	CA	582	C
1	CA	583	A
1	CA	584	G
1	CA	585	U
1	CA	586	A
1	CA	587	A
1	CA	588	U

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Mol	Chain	Res	Type
1	CA	589	U
1	CA	590	A
1	CA	599	A
1	CA	600	U
1	CA	614	U
1	CA	615	U
1	CA	617	U
1	CA	620	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	4	A
1	CA	27	A
1	CA	78	G
1	CA	285	A
1	CA	295	G
1	CA	483	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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
101	SAM	FF	501	-	24,29,29	1.20	3 (12%)	23,42,42	1.64	4 (17%)
100	SF4	F1	1101	45	0,12,12	-	-	-	-	-
102	ACO	F3	1001	-	45,53,53	4.06	14 (31%)	56,79,79	2.18	6 (10%)
101	SAM	F1	1102	-	24,29,29	1.20	3 (12%)	23,42,42	1.60	4 (17%)
104	PO4	FW	301	-	4,4,4	0.99	0	6,6,6	0.41	0
98	GTP	Cg	501	99	26,34,34	1.13	2 (7%)	32,54,54	1.71	7 (21%)

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
100	SF4	F1	1101	45	-	-	0/6/5/5
101	SAM	FF	501	-	-	5/12/33/33	0/3/3/3
102	ACO	F3	1001	-	-	21/47/67/67	0/3/3/3
101	SAM	F1	1102	-	-	3/12/33/33	0/3/3/3
98	GTP	Cg	501	99	-	0/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
102	F3	1001	ACO	O4B-C1B	17.32	1.65	1.41
102	F3	1001	ACO	C2B-C1B	-14.37	1.32	1.53
102	F3	1001	ACO	C9P-N8P	7.16	1.49	1.33
102	F3	1001	ACO	O4B-C4B	-6.70	1.30	1.45
102	F3	1001	ACO	C5P-N4P	5.21	1.45	1.33
102	F3	1001	ACO	P3B-O3B	5.07	1.68	1.59
98	Cg	501	GTP	C5-C6	-4.04	1.39	1.47
101	F1	1102	SAM	C2-N3	3.90	1.38	1.32
101	FF	501	SAM	C2-N3	3.87	1.38	1.32
102	F3	1001	ACO	O5P-C5P	-3.17	1.16	1.23
102	F3	1001	ACO	C6A-N6A	2.78	1.44	1.34
102	F3	1001	ACO	C5A-C4A	-2.65	1.33	1.40
102	F3	1001	ACO	O3B-C3B	-2.54	1.34	1.44
102	F3	1001	ACO	C6P-C5P	2.50	1.56	1.51
102	F3	1001	ACO	C3P-N4P	2.50	1.51	1.46
102	F3	1001	ACO	C3B-C4B	2.43	1.59	1.52
101	F1	1102	SAM	C2-N1	2.43	1.38	1.33
101	FF	501	SAM	C2-N1	2.31	1.38	1.33
101	FF	501	SAM	OXT-C	-2.23	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
101	F1	1102	SAM	OXT-C	-2.18	1.23	1.30
98	Cg	501	GTP	C2-N3	2.12	1.38	1.33
102	F3	1001	ACO	O2B-C2B	2.01	1.47	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
102	F3	1001	ACO	C5A-C6A-N6A	11.16	137.31	120.35
102	F3	1001	ACO	N6A-C6A-N1A	-7.60	102.80	118.57
101	FF	501	SAM	N3-C2-N1	-5.83	119.57	128.68
101	F1	1102	SAM	N3-C2-N1	-5.47	120.14	128.68
102	F3	1001	ACO	N3A-C2A-N1A	-5.27	120.44	128.68
98	Cg	501	GTP	PA-O3A-PB	-4.46	117.53	132.83
98	Cg	501	GTP	PB-O3B-PG	-3.90	119.43	132.83
98	Cg	501	GTP	C5-C6-N1	3.35	119.87	113.95
98	Cg	501	GTP	C3'-C2'-C1'	3.13	105.69	100.98
98	Cg	501	GTP	C2-N1-C6	-3.12	119.36	125.10
98	Cg	501	GTP	C8-N7-C5	3.01	108.73	102.99
101	F1	1102	SAM	OXT-C-O	-2.70	117.97	124.09
102	F3	1001	ACO	P2A-O3A-P1A	-2.68	123.62	132.83
102	F3	1001	ACO	C6P-C5P-N4P	2.61	120.81	116.42
101	FF	501	SAM	OXT-C-O	-2.57	118.25	124.09
101	F1	1102	SAM	C3'-C2'-C1'	2.41	104.61	100.98
101	FF	501	SAM	C3'-C2'-C1'	2.40	104.60	100.98
101	F1	1102	SAM	OXT-C-CA	2.32	121.28	113.38
98	Cg	501	GTP	O6-C6-C5	-2.21	120.06	124.37
101	FF	501	SAM	OXT-C-CA	2.16	120.76	113.38
102	F3	1001	ACO	O5P-C5P-N4P	-2.00	119.23	123.01

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
101	F1	1102	SAM	CB-CG-SD-CE
101	F1	1102	SAM	CB-CG-SD-C5'
101	F1	1102	SAM	C4'-C5'-SD-CG
101	FF	501	SAM	N-CA-CB-CG
101	FF	501	SAM	C-CA-CB-CG
102	F3	1001	ACO	C3B-O3B-P3B-O7A
102	F3	1001	ACO	C3B-C4B-C5B-O5B
102	F3	1001	ACO	OAP-CAP-CBP-CCP
102	F3	1001	ACO	C9P-CAP-CBP-CCP

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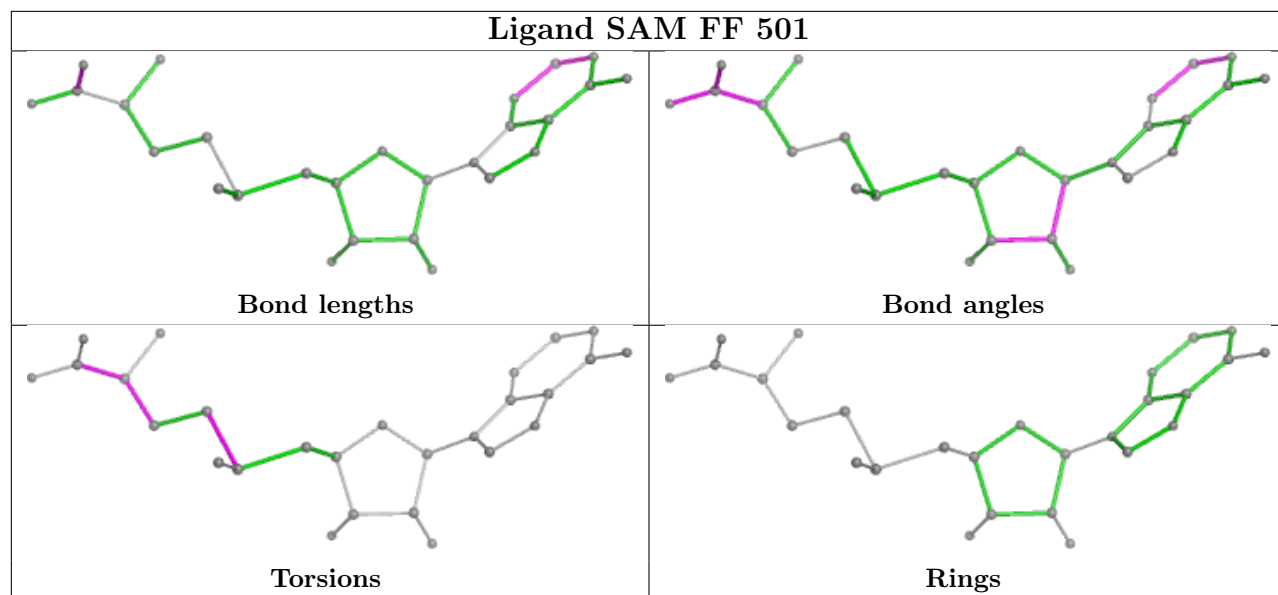
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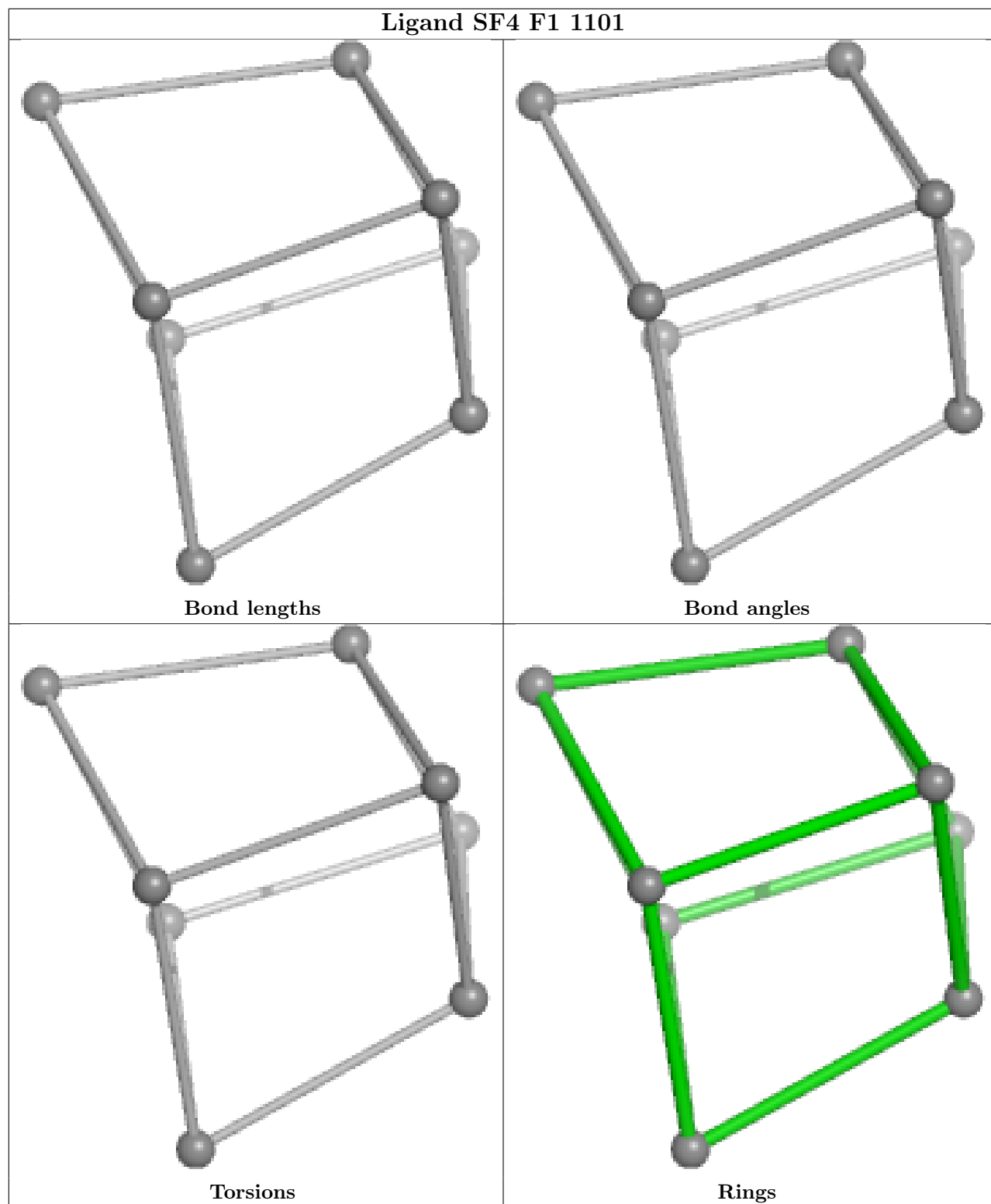
Mol	Chain	Res	Type	Atoms
102	F3	1001	ACO	OAP-CAP-CBP-CDP
102	F3	1001	ACO	C9P-CAP-CBP-CDP
102	F3	1001	ACO	C9P-CAP-CBP-CEP
102	F3	1001	ACO	C5P-C6P-C7P-N8P
102	F3	1001	ACO	C2B-C3B-O3B-P3B
102	F3	1001	ACO	C4B-C3B-O3B-P3B
102	F3	1001	ACO	O4B-C4B-C5B-O5B
102	F3	1001	ACO	OAP-CAP-CBP-CEP
102	F3	1001	ACO	N8P-C9P-CAP-CBP
101	FF	501	SAM	O-C-CA-N
102	F3	1001	ACO	C4B-C5B-O5B-P1A
101	FF	501	SAM	CB-CG-SD-CE
102	F3	1001	ACO	O5P-C5P-C6P-C7P
102	F3	1001	ACO	C3P-C2P-S1P-C
101	FF	501	SAM	OXT-C-CA-N
102	F3	1001	ACO	S1P-C2P-C3P-N4P
102	F3	1001	ACO	P1A-O3A-P2A-O4A
102	F3	1001	ACO	P1A-O3A-P2A-O5A
102	F3	1001	ACO	N4P-C5P-C6P-C7P
102	F3	1001	ACO	O9P-C9P-CAP-CBP

There are no ring outliers.

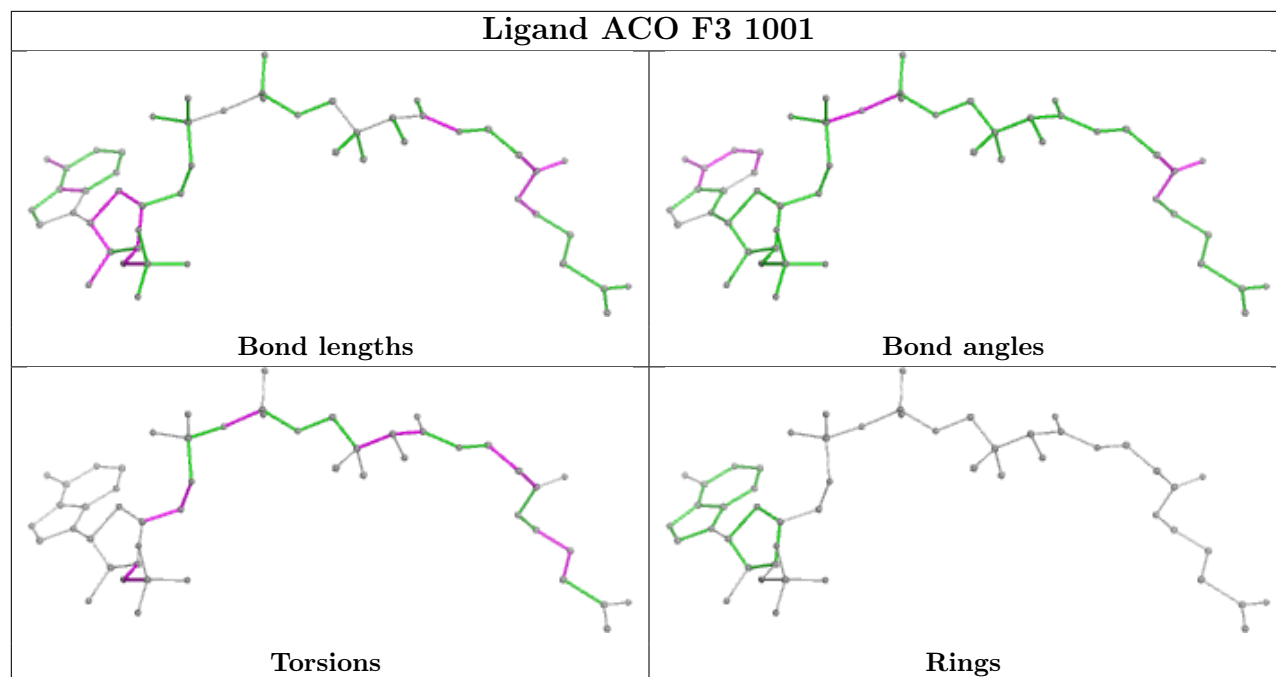
No monomer is involved in short contacts.

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.

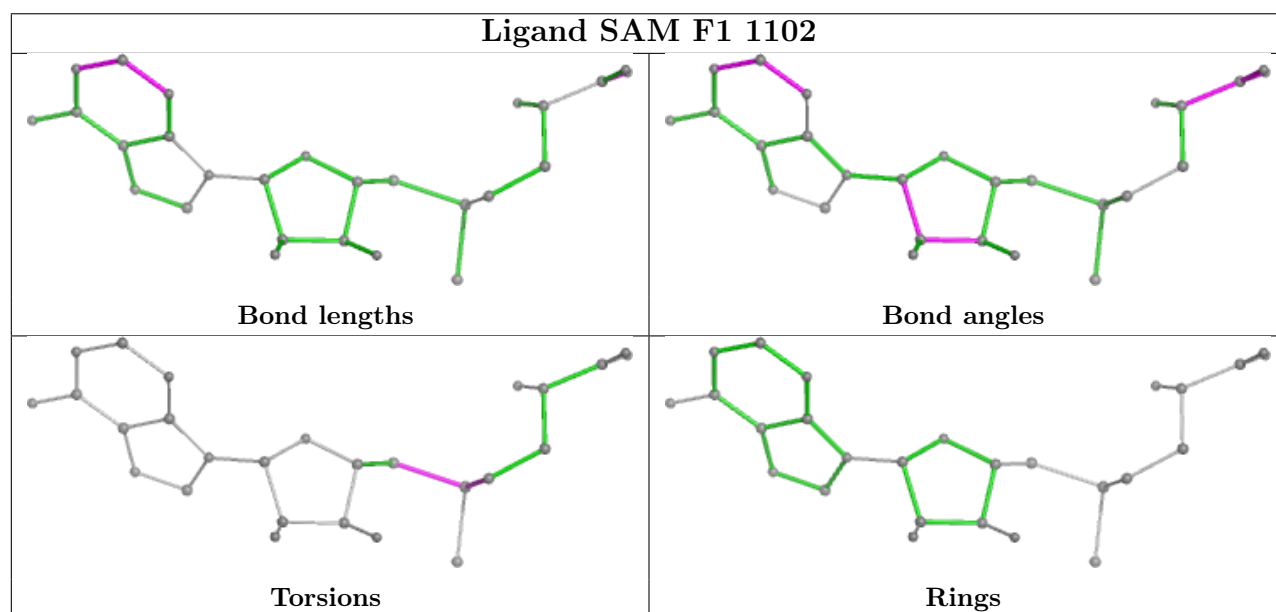


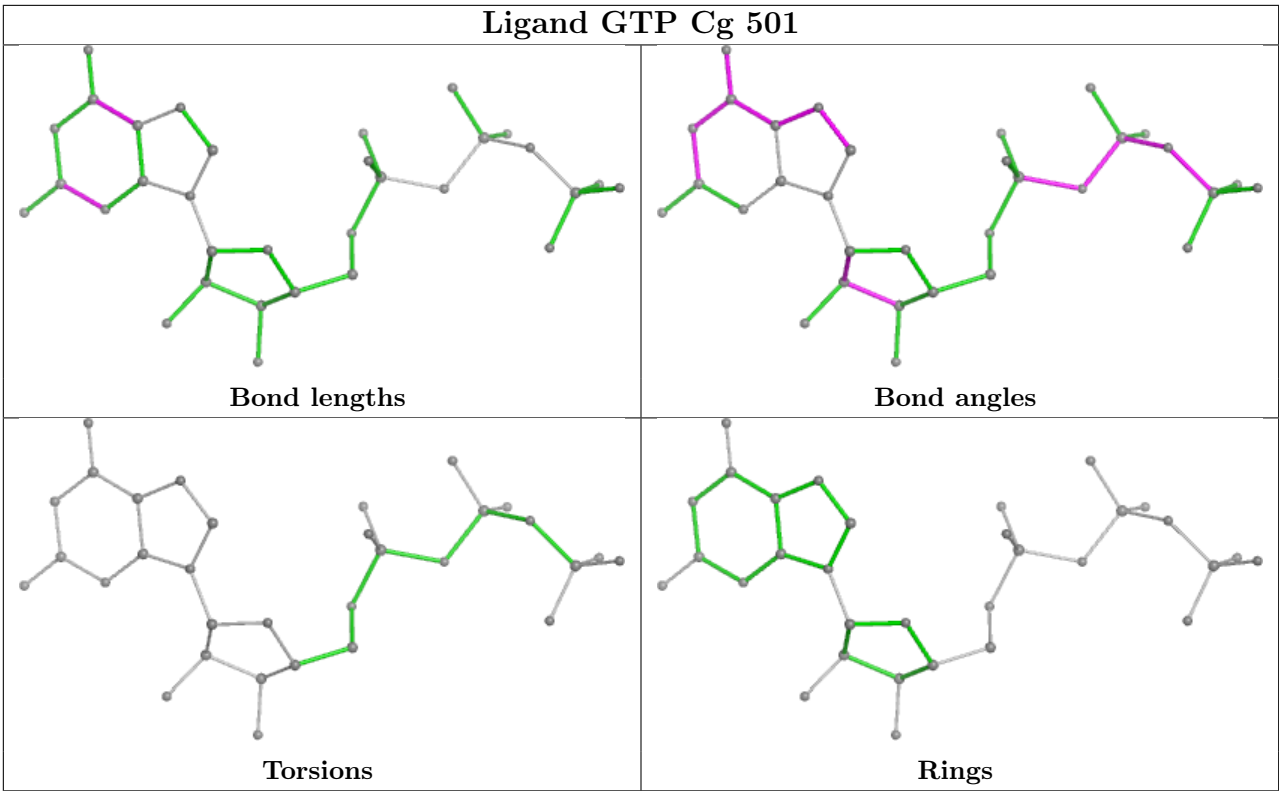


Ligand ACO F3 1001



Ligand SAM F1 1102





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
94	Ug	10
95	Uh	9
92	UY	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UY	421:UNK	C	439:UNK	N	57.87
1	UY	405:UNK	C	411:UNK	N	41.49
1	Uh	411:UNK	C	499:UNK	N	40.91
1	Ug	129:UNK	C	130:UNK	N	34.53
1	Uh	274:UNK	C	304:UNK	N	29.82
1	Ug	102:UNK	C	103:UNK	N	29.18
1	Ug	83:UNK	C	84:UNK	N	25.05

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Uh	45:UNK	C	101:UNK	N	21.70
1	Uh	136:UNK	C	161:UNK	N	20.48
1	Uh	192:UNK	C	216:UNK	N	17.84
1	Uh	247:UNK	C	258:UNK	N	15.50
1	Ug	52:UNK	C	53:UNK	N	14.17
1	UY	394:UNK	C	397:UNK	N	12.35
1	Ug	39:UNK	C	40:UNK	N	12.18
1	Ug	70:UNK	C	71:UNK	N	12.15
1	Ug	26:UNK	C	27:UNK	N	8.05
1	Uh	14:UNK	C	18:UNK	N	7.74
1	Uh	114:UNK	C	124:UNK	N	7.25
1	Ug	46:UNK	C	47:UNK	N	6.24
1	Uh	341:UNK	C	346:UNK	N	5.59
1	Ug	145:UNK	C	146:UNK	N	5.06
1	Ug	33:UNK	C	34:UNK	N	4.81

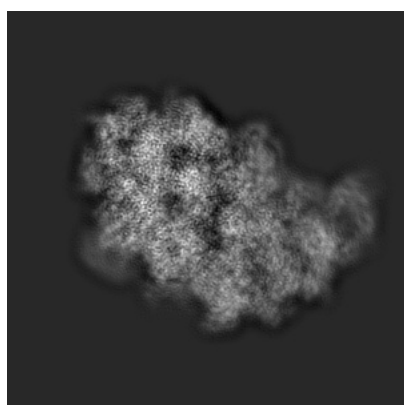
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10180. These allow visual inspection of the internal detail of the map and identification of artifacts.

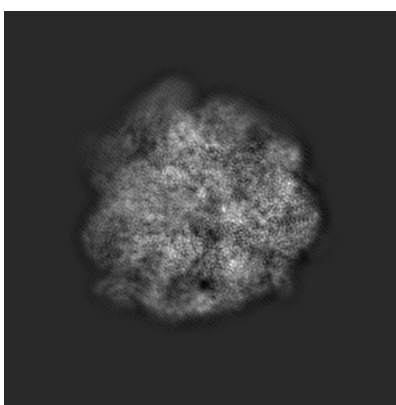
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

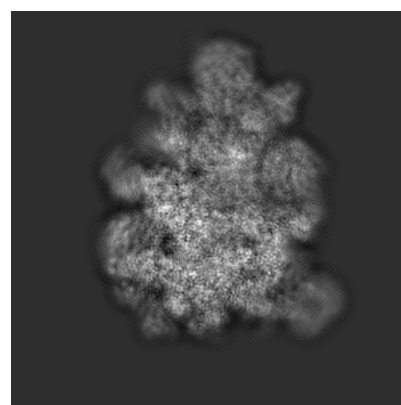
6.1.1 Primary map



X



Y

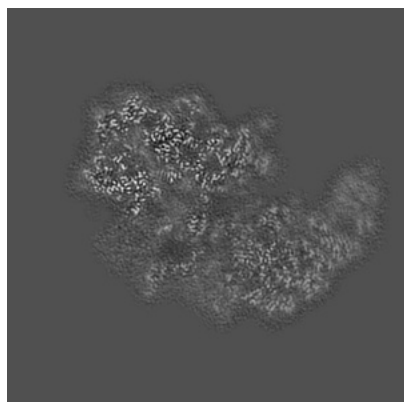


Z

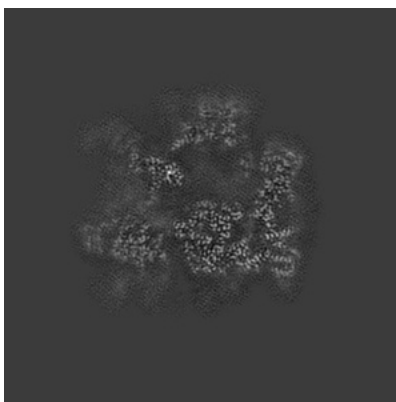
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

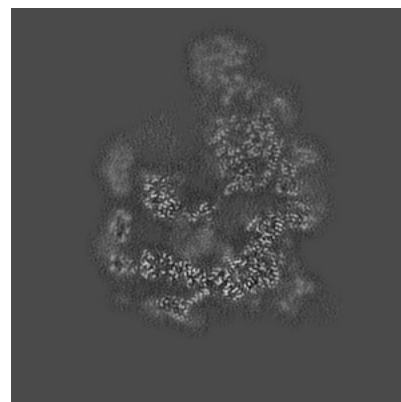
6.2.1 Primary map



X Index: 160



Y Index: 160

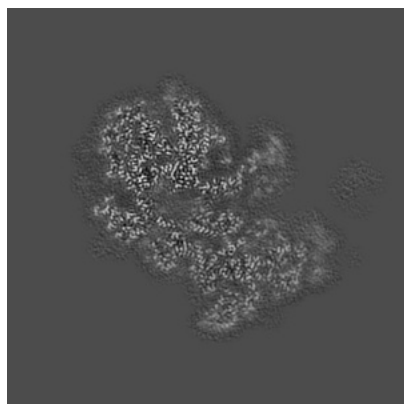


Z Index: 160

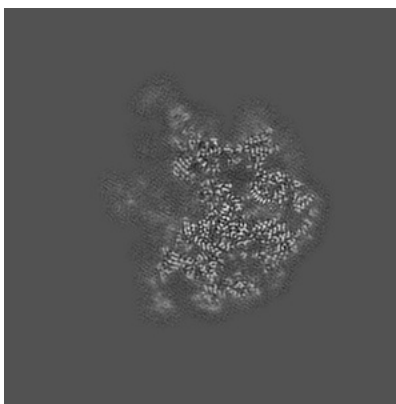
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

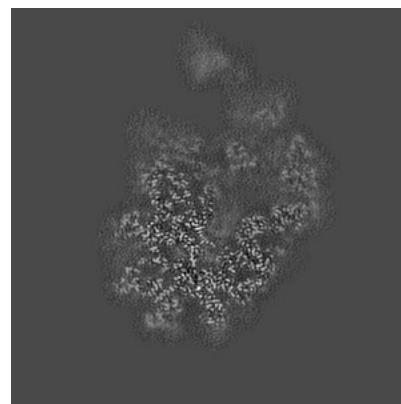
6.3.1 Primary map



X Index: 137



Y Index: 109

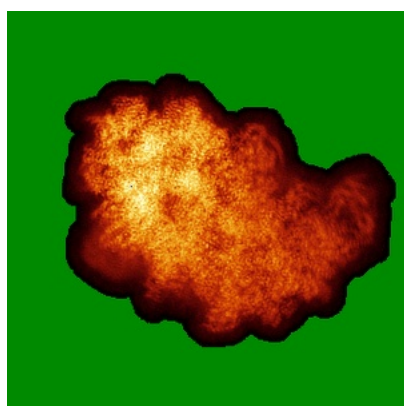


Z Index: 181

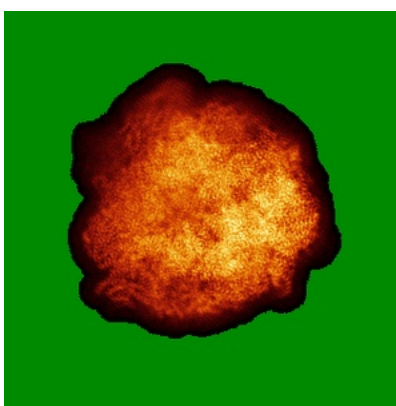
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

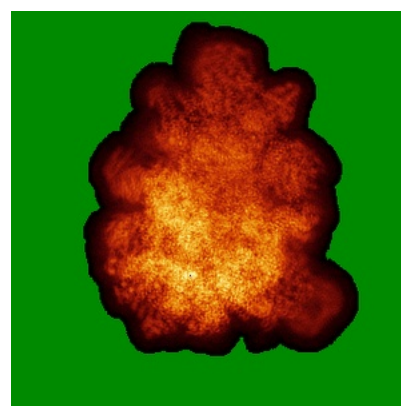
6.4.1 Primary map



X



Y

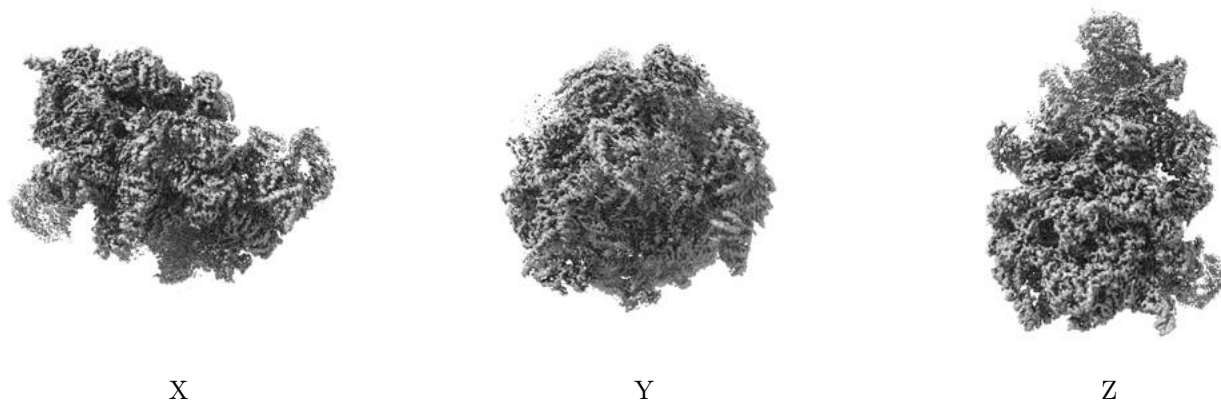


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

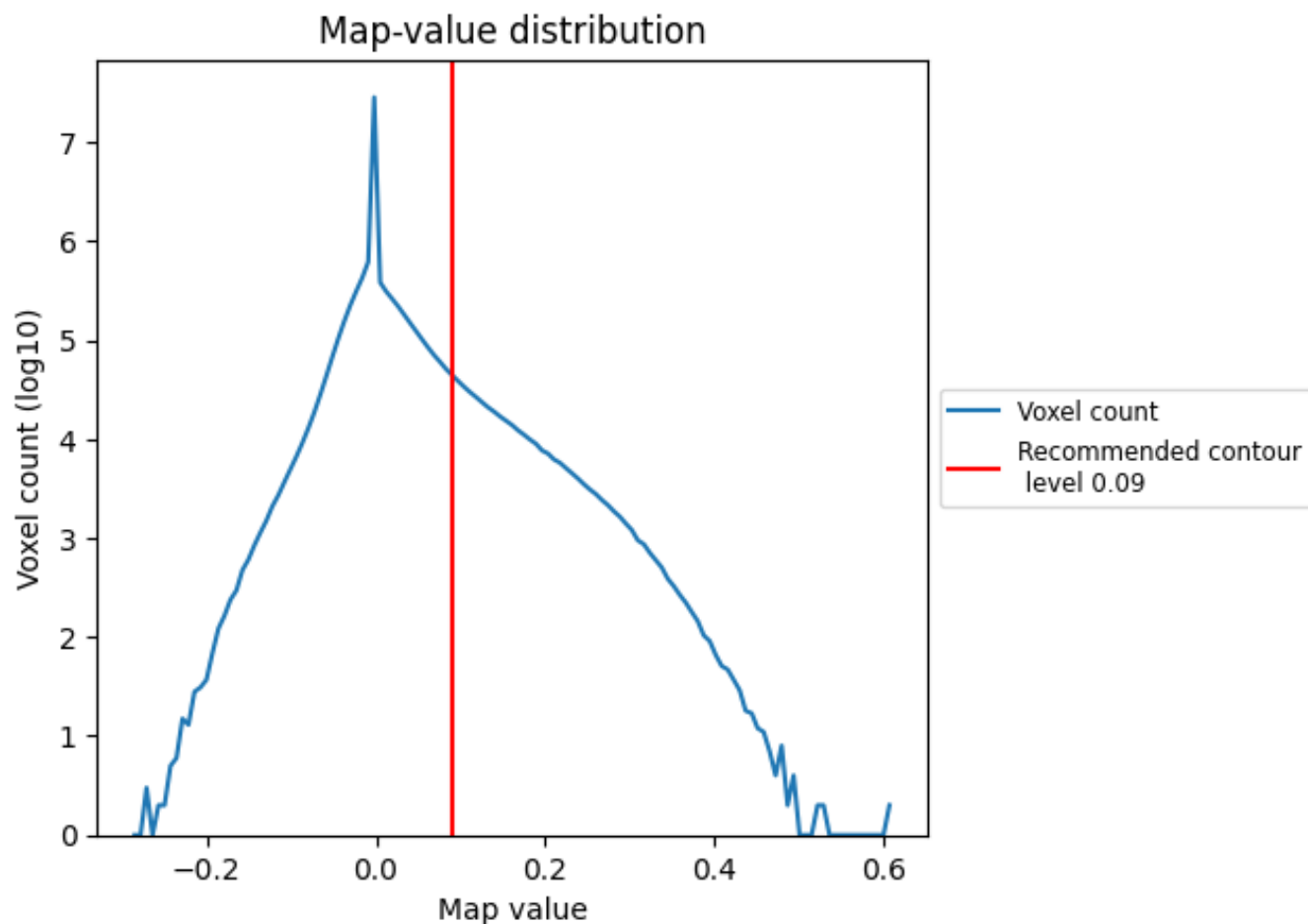
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

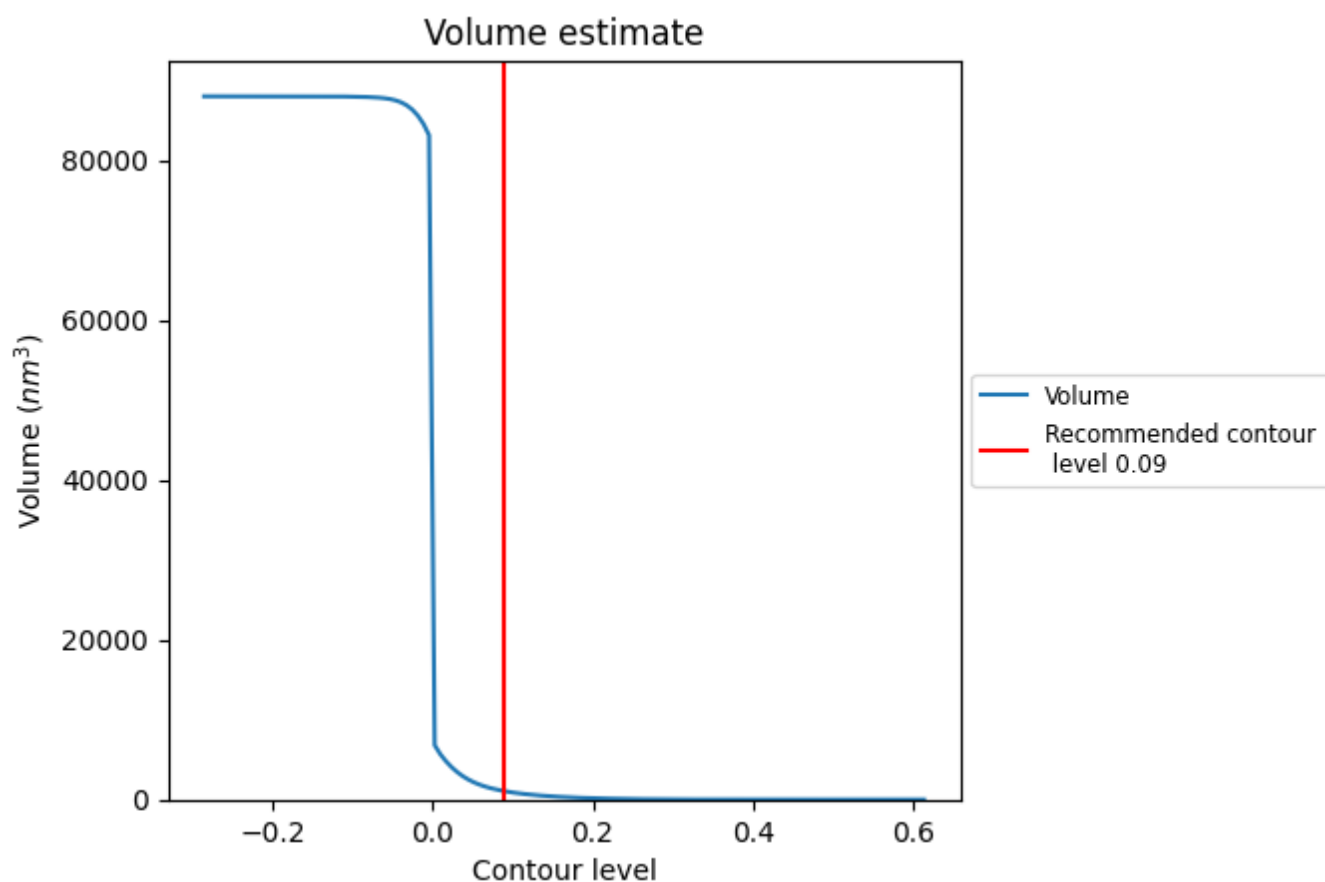
This section contains the results of statistical analysis of the map.

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.

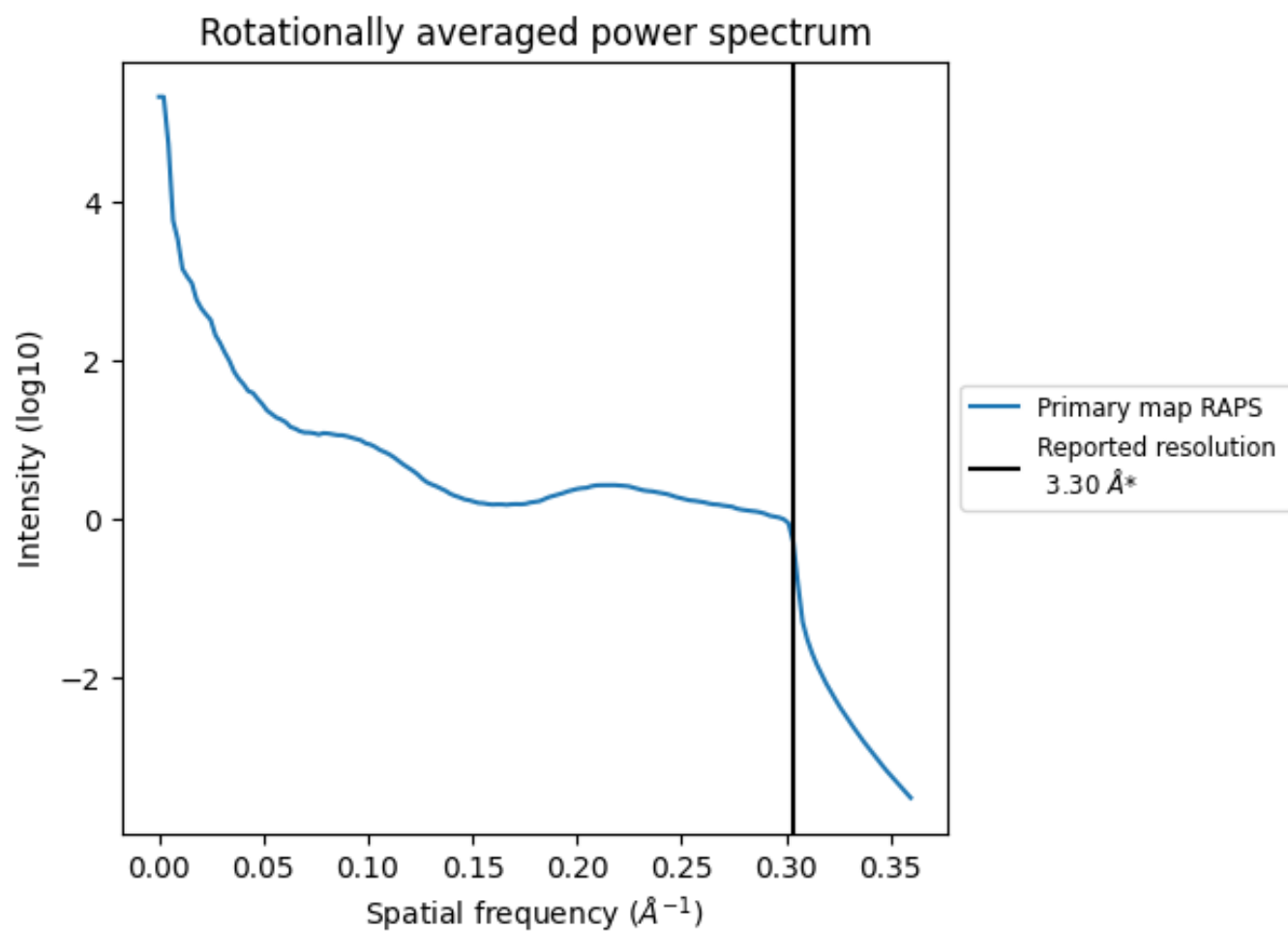
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1051 nm³; this corresponds to an approximate mass of 949 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

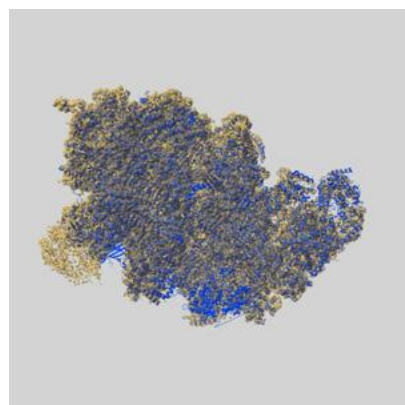
8 Fourier-Shell correlation ⓘ

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

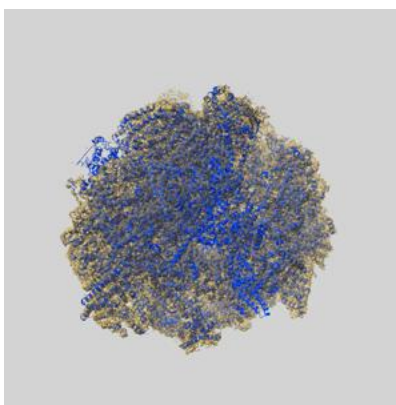
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10180 and PDB model 9HNY. Per-residue inclusion information can be found in section [3](#) on page [27](#).

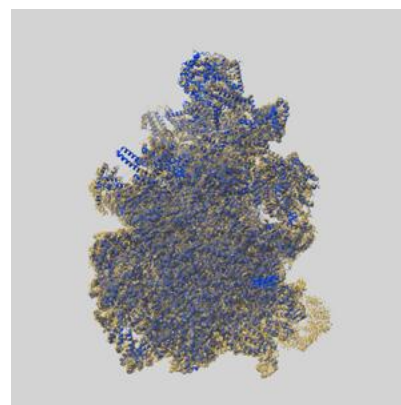
9.1 Map-model overlay [i](#)



X



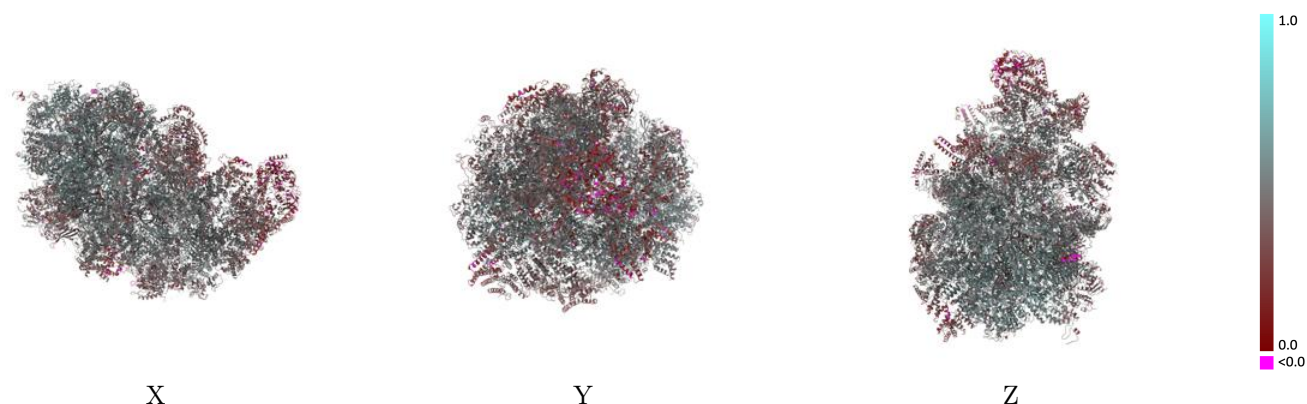
Y



Z

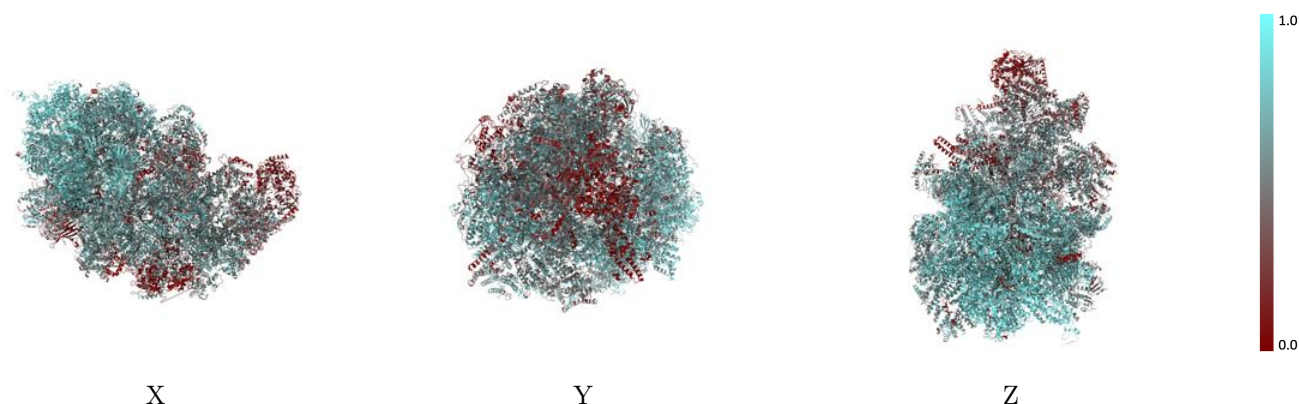
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



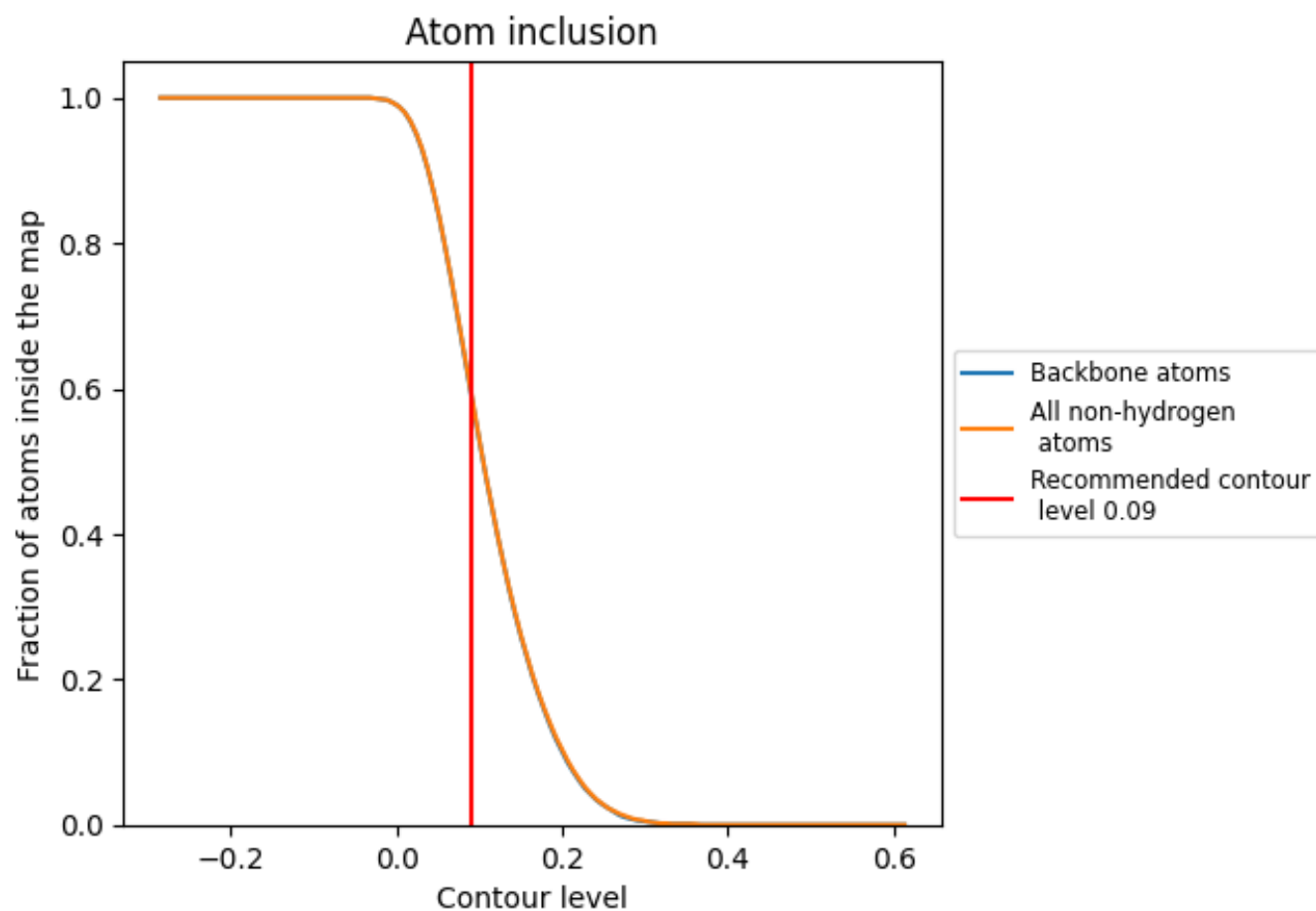
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5940	 0.4590
CA	 0.6720	 0.4820
CC	 0.4410	 0.4800
CE	 0.7040	 0.5180
CF	 0.7400	 0.5050
CH	 0.7910	 0.5470
CI	 0.6450	 0.4850
CJ	 0.5700	 0.4790
CK	 0.6240	 0.4620
CN	 0.2720	 0.4680
CO	 0.7710	 0.5260
CP	 0.8140	 0.5480
CQ	 0.6780	 0.5230
CR	 0.6580	 0.4700
CS	 0.0120	 0.3370
Ca	 0.6930	 0.4860
Cb	 0.5820	 0.4160
Cd	 0.8130	 0.5330
Cg	 0.6490	 0.4730
Ci	 0.5250	 0.4880
Cj	 0.8440	 0.5440
Ck	 0.5960	 0.4500
Cn	 0.4530	 0.4740
Cp	 0.7760	 0.5220
DB	 0.4250	 0.4100
DC	 0.3700	 0.3290
DD	 0.7960	 0.5310
DE	 0.2210	 0.2520
DF	 0.5230	 0.4640
DG	 0.5930	 0.4080
DH	 0.5240	 0.4680
DI	 0.7570	 0.4970
DJ	 0.5810	 0.4510
DK	 0.4480	 0.4070
DL	 0.6880	 0.5240





























































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Chain	Atom inclusion	Q-score
DO	 0.6440	 0.4180
DP	 0.8280	 0.4920
DR	 0.8260	 0.5280
DT	 0.6040	 0.5060
DU	 0.6880	 0.4980
DV	 0.5720	 0.4810
DW	 0.5440	 0.4570
DX	 0.2190	 0.3910
DY	 0.5000	 0.4540
DZ	 0.5870	 0.4890
F1	 0.5990	 0.4900
F2	 0.7520	 0.4980
F3	 0.6940	 0.4550
F4	 0.4200	 0.3880
F5	 0.3830	 0.3400
F6	 0.5730	 0.3700
F7	 0.7580	 0.4980
F8	 0.7120	 0.4940
F9	 0.6670	 0.4860
FA	 0.5270	 0.4170
FB	 0.7210	 0.5220
FC	 0.6430	 0.4520
FD	 0.4780	 0.4050
FE	 0.7200	 0.5220
FF	 0.5950	 0.4950
FG	 0.6330	 0.4970
FH	 0.5780	 0.4650
FI	 0.5160	 0.4700
FJ	 0.6120	 0.4960
FK	 0.5730	 0.4660
FL	 0.6190	 0.5260
FM	 0.7130	 0.4870
FN	 0.5510	 0.3910
FO	 0.8250	 0.5430
FP	 0.7990	 0.5030
FQ	 0.7190	 0.4880
FR	 0.6840	 0.4850
FS	 0.5830	 0.4480
FT	 0.6670	 0.4560
FU	 0.6140	 0.4460
FV	 0.6050	 0.4660
FW	 0.7640	 0.5180

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Chain	Atom inclusion	Q-score
FX	 0.8150	 0.4960
FY	 0.5230	 0.4310
FZ	 0.1370	 0.3760
Fa	 0.6630	 0.5190
Fb	 0.5750	 0.3460
Fc	 0.5470	 0.3300
Fd	 0.7780	 0.5080
Fe	 0.5190	 0.4630
Fi	 0.0260	 0.3430
UA	 0.3260	 0.2760
UB	 0.6670	 0.4610
UC	 0.8400	 0.5010
UF	 0.6360	 0.4620
UG	 0.7620	 0.4630
UI	 0.8750	 0.5310
UJ	 0.5500	 0.4920
UK	 0.3080	 0.4190
UL	 0.7360	 0.4790
UM	 0.7110	 0.4770
UN	 0.7710	 0.4670
UO	 0.5530	 0.3720
UP	 0.3420	 0.3700
UQ	 0.6220	 0.4100
UY	 0.0190	 0.3990
Ud	 0.3590	 0.4010
Ug	 0.5290	 0.3820
Uh	 0.0520	 0.4180
Uk	 0.3810	 0.4290
Ul	 0.2140	 0.3520