Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 11:00 am GMT

PDB ID	:	6YWY
EMDB ID	:	EMD-10985
Title	:	The structure of the mitoribosome from Neurospora crassa with bound tRNA at the P-site
Authors	:	Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on	:	2020-04-30
Resolution	:	3.05 Å(reported)

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

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

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

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

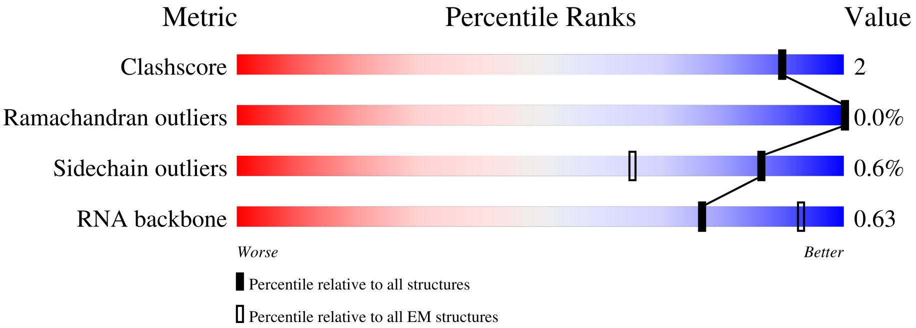
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance ⓘ

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

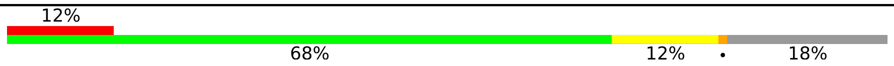
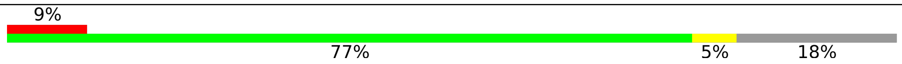
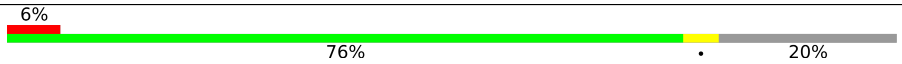
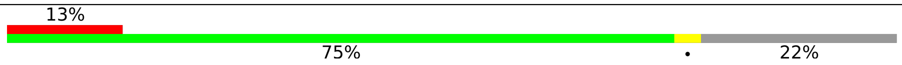
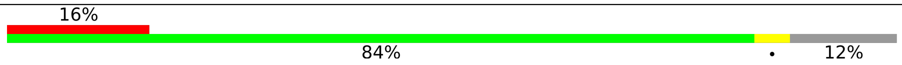
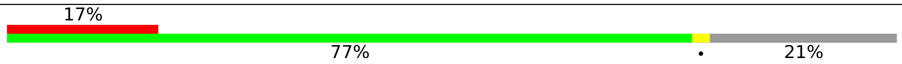
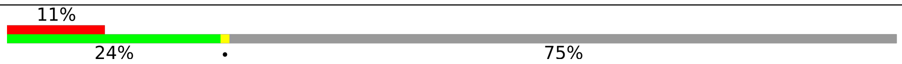
The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	3464	
2	B	383	
3	C	384	
4	D	325	
5	E	352	
6	F	255	
7	G	300	

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Mol	Chain	Length	Quality of chain
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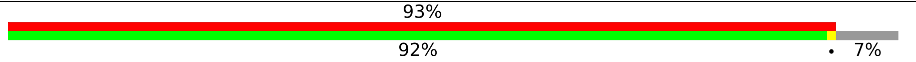
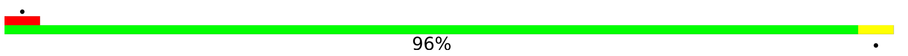
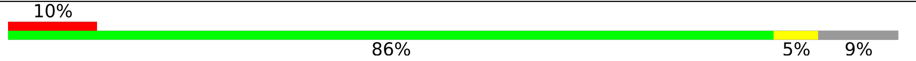
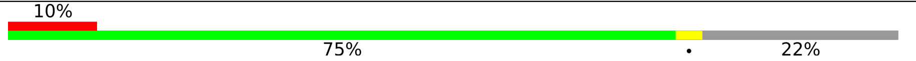
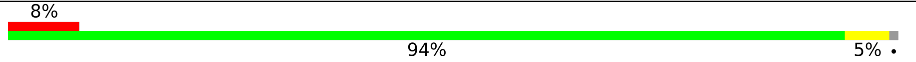
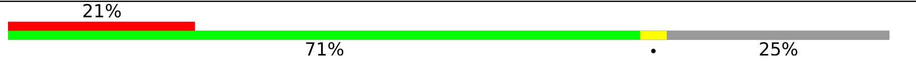
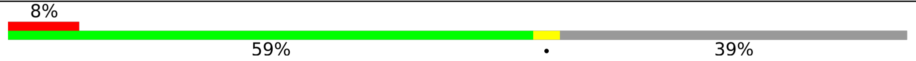
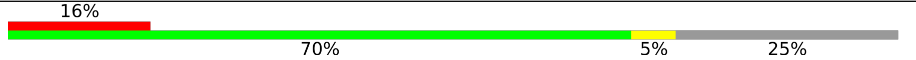
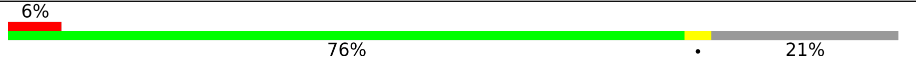
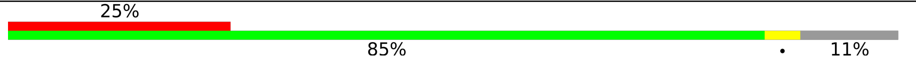
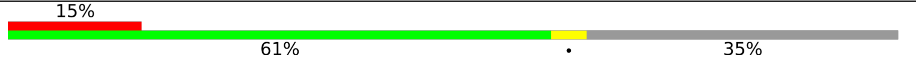
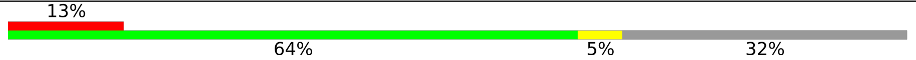
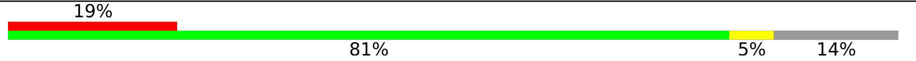
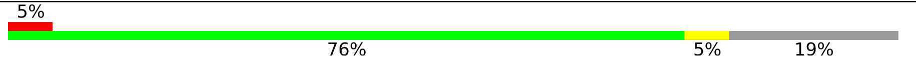
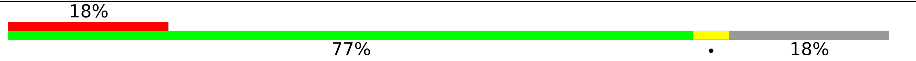
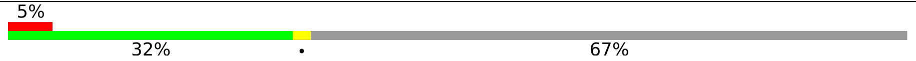
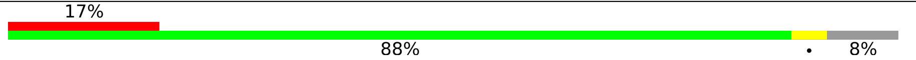
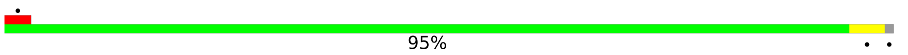
9	g	158	
10	H	183	
11	I	131	
12	J	312	
13	K	249	
14	L	193	
15	M	258	
16	N	217	
17	O	364	
18	P	228	
19	Q	396	
20	R	447	
21	S	274	
22	T	263	
23	U	161	
24	V	219	
25	W	129	
26	X	59	
27	Y	140	
28	0	124	
29	1	449	
30	2	370	
31	3	103	
32	4	138	

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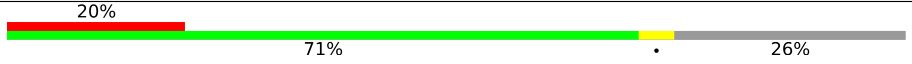
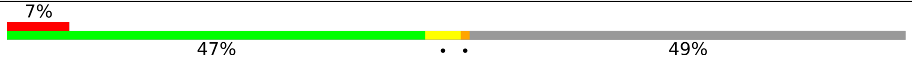
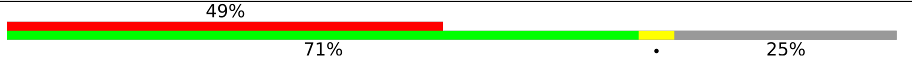
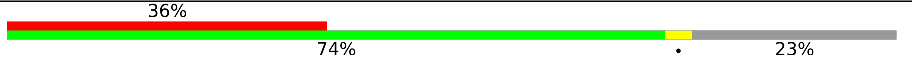
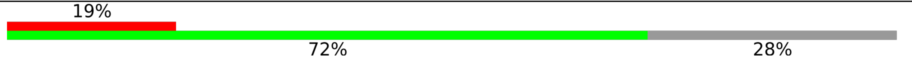
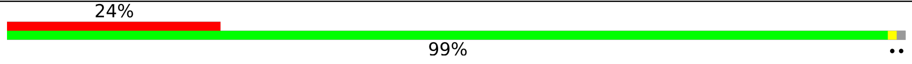
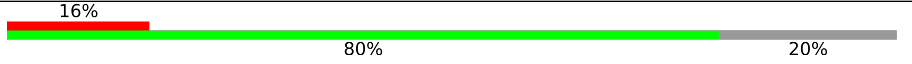
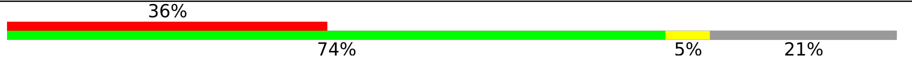
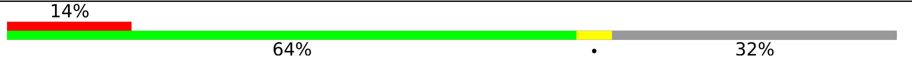
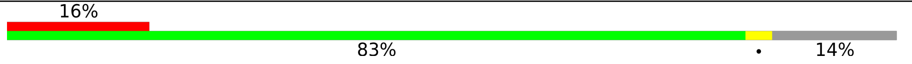
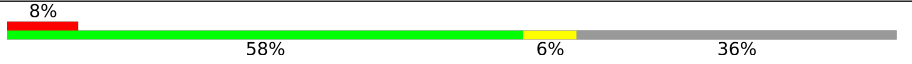
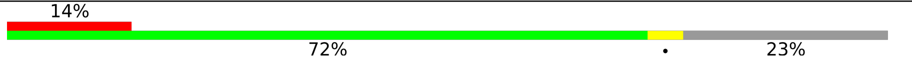
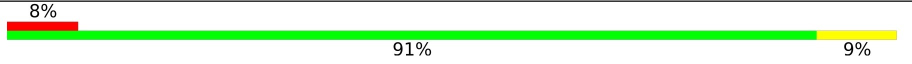
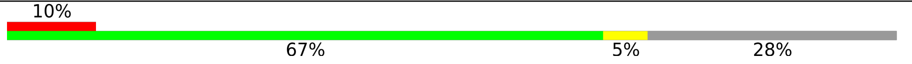
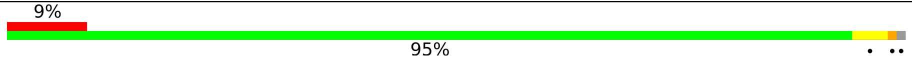
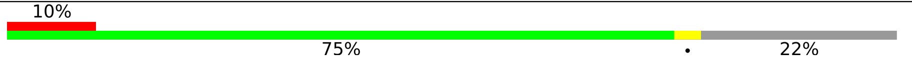
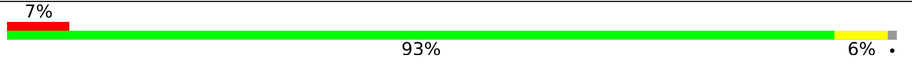
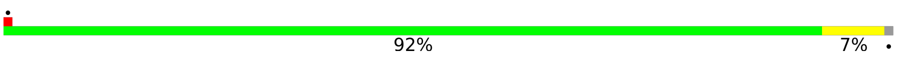
Mol	Chain	Length	Quality of chain
33	5	439	
34	6	368	
35	7	165	
36	8	443	
37	h	98	
38	i	218	
39	9	267	
40	a	225	
41	b	162	
42	c	110	
43	d	292	
44	AA	470	
45	BB	428	
46	CC	508	
47	DD	453	
48	EE	477	
49	FF	117	
50	GG	309	
51	HH	161	
52	II	315	
53	JJ	268	
54	KK	376	
55	LL	174	
56	MM	119	
57	NN	113	

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Mol	Chain	Length	Quality of chain
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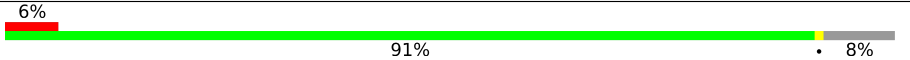
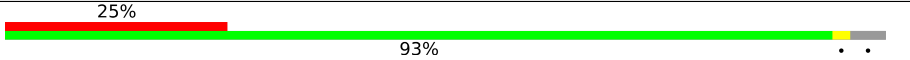
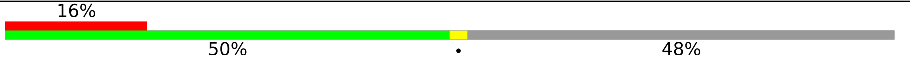
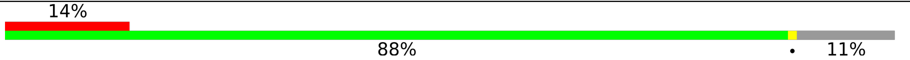
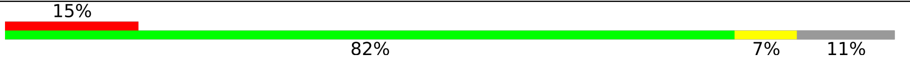
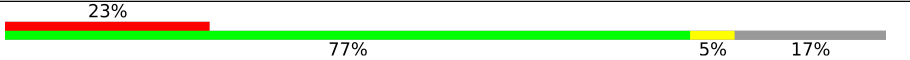
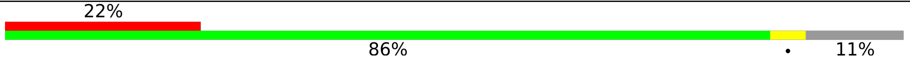
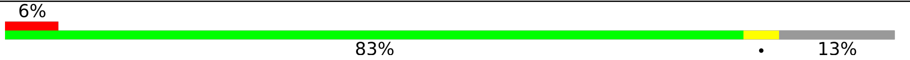
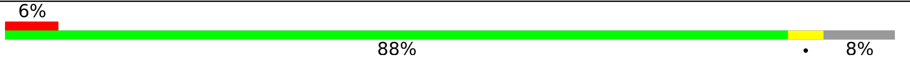
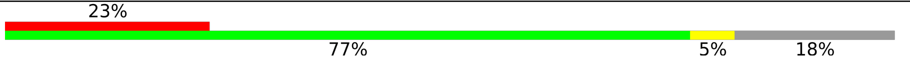
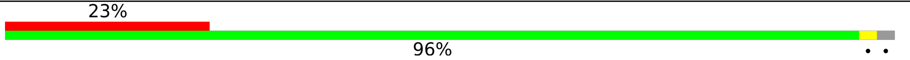
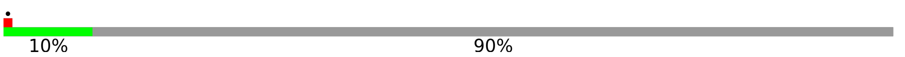
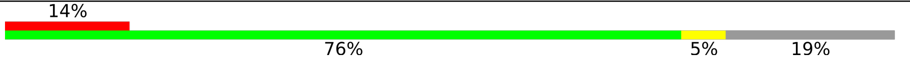
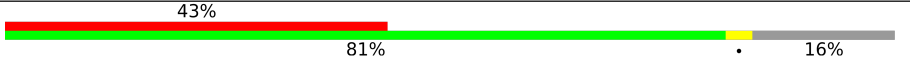
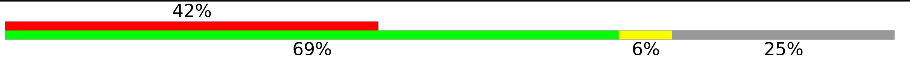
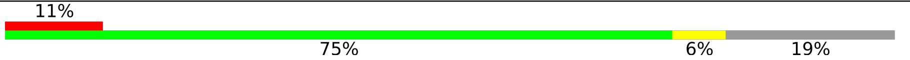
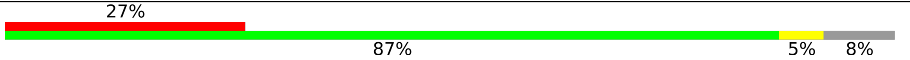
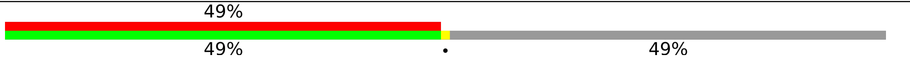
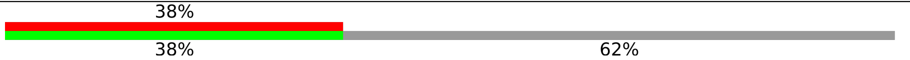
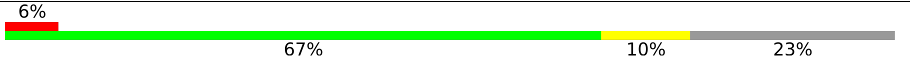
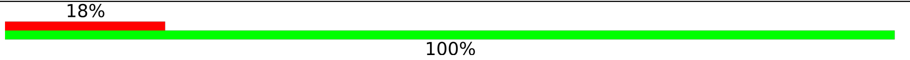
59	PP	107	
60	QQ	165	
61	RR	256	
62	SS	91	
63	TT	236	
64	UU	253	
65	VV	316	
66	WW	396	
67	XX	469	
68	YY	108	
69	ZZ	382	
70	11	90	
71	22	344	
72	33	236	
73	44	310	
73	55	310	
74	66	348	
75	77	414	
76	88	508	
77	00	95	
77	99	95	
78	aa	1864	
79	bb	73	
80	ee	11	

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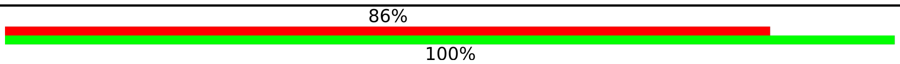
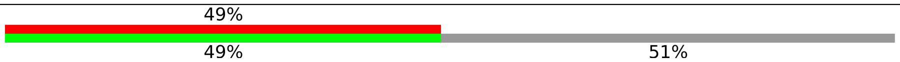
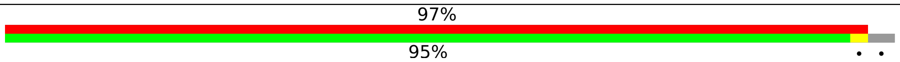
Mol	Chain	Length	Quality of chain
81	cc	7	
82	e	303	
83	j	201	

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 392401 atoms, of which 174325 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 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2843	Total 91056	C 27190	H 30416	N 10878	O 19729	P 2843	0	0

- Molecule 2 is a protein called 60S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	315	Total 4964	C 1527	H 2508	N 500	O 415	S 14	0	0

- Molecule 3 is a protein called Related to ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	307	Total 4757	C 1468	H 2421	N 447	O 413	S 8	0	0

- Molecule 4 is a protein called 60S ribosomal protein L4, variant.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	254	Total 4068	C 1280	H 2040	N 372	O 371	S 5	0	0

- Molecule 5 is a protein called Related to ribosomal protein L5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	309	Total 4910	C 1558	H 2461	N 436	O 443	S 12	0	0

- Molecule 6 is a protein called uL6m.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	201	Total 3253	C 1022	H 1645	N 290	O 288	S 8	0	0

- Molecule 7 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	74	1245	390	627	121	104	3	0	0

- Molecule 8 is a protein called Related to ribosomal protein YmL11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	f	245	3801	1202	1925	325	346	3	0	0

- Molecule 9 is a protein called uL11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	g	147	2257	700	1154	203	196	4	0	0

- Molecule 10 is a protein called uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	H	183	2885	899	1459	268	251	8	0	0

- Molecule 11 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	I	119	1898	564	985	182	159	8	0	0

- Molecule 12 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	J	243	3827	1198	1939	346	343	1	0	0

- Molecule 13 is a protein called Related to ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	K	168	2751	850	1401	263	231	6	0	0

- Molecule 14 is a protein called uL17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	L	192	3135	960	1590	294	285	6	0	0

- Molecule 15 is a protein called bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	M	194	3164	981	1628	292	253	10	0	0

- Molecule 16 is a protein called Related to ribosomal protein YmL49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	N	133	2176	673	1120	195	182	6	0	0

- Molecule 17 is a protein called Mitochondrial large ribosomal subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	O	272	4532	1392	2323	424	387	6	0	0

- Molecule 18 is a protein called uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	P	180	2975	953	1494	270	254	4	0	0

- Molecule 19 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	Q	353	5829	1786	2961	547	524	11	0	0

- Molecule 20 is a protein called Related to 60s ribosomal protein L2 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	R	249	4195	1283	2149	412	347	4	0	0

- Molecule 21 is a protein called bL28m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	S	179	2979	937	1507	281	252	2	0	0

- Molecule 22 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	T	180	2950	937	1453	279	278	3	0	0

- Molecule 23 is a protein called Related to ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	U	138	2263	698	1164	213	185	3	0	0

- Molecule 24 is a protein called Related to ribosomal protein YmL36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	V	94	1485	472	735	136	140	2	0	0

- Molecule 25 is a protein called Related to ribosomal protein YmL32 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	W	59	949	282	489	98	72	8	0	0

- Molecule 26 is a protein called bL33m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	X	48	836	263	433	71	65	4	0	0

- Molecule 27 is a protein called Related to ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	Y	46	777	224	412	84	56	1	0	0

- Molecule 28 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	0	46	797	240	409	86	58	4	0	0

- Molecule 29 is a protein called PEBP-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	1	367	6014	1899	3029	547	531	8	0	0

- Molecule 30 is a protein called mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	2	123	2101	660	1055	211	171	4	0	0

- Molecule 31 is a protein called mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	3	95	1536	489	773	135	137	2	0	0

- Molecule 32 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	4	137	2139	671	1087	192	183	6	0	0

- Molecule 33 is a protein called Ribonuclease III.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	5	350	5429	1740	2710	477	493	9	0	0

- Molecule 34 is a protein called mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	6	273	4474	1418	2248	399	401	8	0	0

- Molecule 35 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	7	84	Total 1383	C 431	H 709	N 130	O 113	0	0

- Molecule 36 is a protein called mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	8	331	Total 5374	C 1683	H 2714	N 480	O 489	S 8	0	0

- Molecule 37 is a protein called Probable ribosomal protein YmL44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	98	Total 1577	C 490	H 798	N 139	O 146	S 4	0	0

- Molecule 38 is a protein called mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	i	124	Total 1998	C 613	H 1022	N 181	O 177	S 5	0	0

- Molecule 39 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	9	206	Total 3341	C 1051	H 1698	N 295	O 290	S 7	0	0

- Molecule 40 is a protein called Related to ribosomal protein YmL20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	a	161	Total 2671	C 837	H 1340	N 253	O 235	S 6	0	0

- Molecule 41 is a protein called Mitoc_mL59 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	b	161	Total 2693	C 840	H 1379	N 249	O 221	S 4	0	0

- Molecule 42 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	c	98	Total	C	H	N	O	S	0	0
			1700	528	873	162	134	3		

- Molecule 43 is a protein called mL67.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	d	235	Total	C	H	N	O	S	0	0
			3797	1180	1909	363	339	6		

- Molecule 44 is a protein called bS1m.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	AA	372	Total	C	H	N	O	S	0	0
			5790	1827	2907	507	543	6		

- Molecule 45 is a protein called Mito ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	BB	290	Total	C	H	N	O	S	0	0
			4570	1426	2301	423	414	6		

- Molecule 46 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	CC	438	Total	C	H	N	O	S	0	0
			7538	2388	3897	636	612	5		

- Molecule 47 is a protein called S4 RNA-binding domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	DD	290	Total	C	H	N	O	S	0	0
			4715	1501	2373	430	400	11		

- Molecule 48 is a protein called Related to ribosomal protein S5 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
48	EE	367	Total	C	H	N	O	S	0	0
			5798	1799	2918	526	543	12		

- Molecule 49 is a protein called Ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	FF	117	1901	591	966	176	165	3	0	0

- Molecule 50 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	GG	223	3523	1098	1799	318	302	6	0	0

- Molecule 51 is a protein called uS8m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	HH	160	2521	783	1286	226	220	6	0	0

- Molecule 52 is a protein called uS9m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	II	247	3994	1253	2026	366	344	5	0	0

- Molecule 53 is a protein called 30S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	JJ	188	3105	998	1554	273	272	8	0	0

- Molecule 54 is a protein called Translational machinery component.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	KK	124	2020	625	1025	195	170	5	0	0

- Molecule 55 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	LL	128	1991	591	1032	198	165	5	0	0

- Molecule 56 is a protein called Probable ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	MM	118	1923	586	986	186	161	4	0	0

- Molecule 57 is a protein called Mitochondrial 37S ribosomal protein MRP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	NN	112	1875	573	961	184	150	7	0	0

- Molecule 58 is a protein called Related to ribosomal protein S15 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	OO	276	4428	1361	2230	431	401	5	0	0

- Molecule 59 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
59	PP	98	1612	510	826	141	135	0	0

- Molecule 60 is a protein called uS17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	QQ	158	2561	789	1314	234	219	5	0	0

- Molecule 61 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	RR	134	2169	679	1089	206	190	5	0	0

- Molecule 62 is a protein called Ribosomal protein S19/S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	SS	81	1325	422	677	118	107	1	0	0

- Molecule 63 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	TT	88	Total 1518	C 470	H 772	N 157	O 119	0	0

- Molecule 64 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	UU	224	Total 3687	C 1165	H 1843	N 342	O 330	S 7	0	0

- Molecule 65 is a protein called mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	VV	261	Total 4192	C 1300	H 2112	N 390	O 387	S 3	0	0

- Molecule 66 is a protein called mS27.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	WW	353	Total 5744	C 1804	H 2901	N 514	O 515	S 10	0	0

- Molecule 67 is a protein called Mitochondrial ribosomal protein DAP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	XX	408	Total 6446	C 2010	H 3271	N 562	O 587	S 16	0	0

- Molecule 68 is a protein called mS33.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	YY	99	Total 1609	C 491	H 823	N 152	O 142	S 1	0	0

- Molecule 69 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	ZZ	312	Total 5114	C 1631	H 2528	N 450	O 495	S 10	0	0

- Molecule 70 is a protein called 37S ribosomal protein mrp10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	11	88	Total 1358	C 417	H 686	N 128	O 121	S 6	0	0

- Molecule 71 is a protein called DUF1713 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	22	33	Total 660	C 187	H 359	N 70	O 43	S 1	0	0

- Molecule 72 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	33	191	Total 3134	C 978	H 1595	N 293	O 266	S 2	0	0

- Molecule 73 is a protein called Manganese and iron superoxide dismutase.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	44	260	Total 4045	C 1318	H 1983	N 355	O 378	S 11	0	0
73	55	232	Total 3652	C 1195	H 1794	N 316	O 337	S 10	0	0

- Molecule 74 is a protein called mS45.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	66	283	Total 4628	C 1455	H 2330	N 425	O 414	S 4	0	0

- Molecule 75 is a protein called mS46.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	77	179	Total 2796	C 893	H 1396	N 227	O 277	S 3	0	0

- Molecule 76 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	88	467	Total 7327	C 2340	H 3650	N 634	O 691	S 12	0	0

- Molecule 77 is a protein called IF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	00	48	Total 823	C 252	H 417	N 77	O 77	0	0
77	99	36	Total 639	C 191	H 333	N 59	O 56	0	0

- Molecule 78 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	aa	1435	Total 45981	C 13712	H 15373	N 5486	O 9975	P 1435	0	0

- Molecule 79 is a RNA chain called P-site-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	bb	73	Total 2346	C 697	H 789	N 284	O 503	P 73	0	0

- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	ee	11	Total 344	C 103	H 115	N 34	O 81	P 11	0	0

- Molecule 81 is a protein called Poly-Peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	cc	7	Total 69	C 21	H 34	N 7	O 7	0	0

- Molecule 82 is a protein called 60S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	e	148	Total 2396	C 751	H 1212	N 209	O 218	S 6	0	0

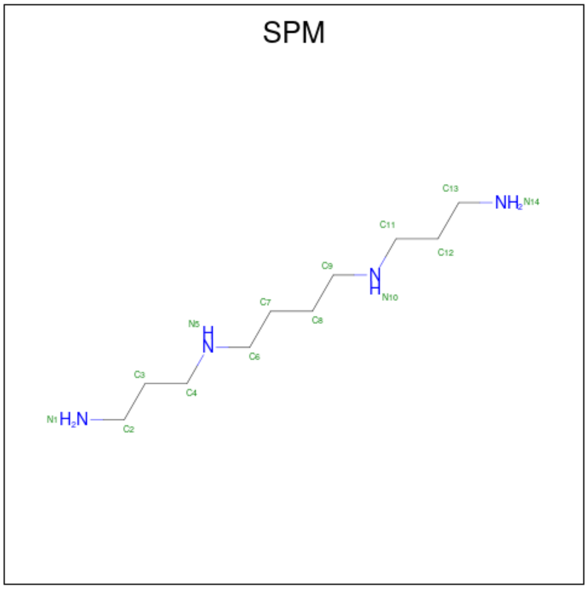
- Molecule 83 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	j	195	Total 3139	C 971	H 1586	N 290	O 284	S 8	0	0

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	A	144	Total 144	Mg 144	0
84	K	1	Total 1	Mg 1	0
84	L	1	Total 1	Mg 1	0
84	BB	1	Total 1	Mg 1	0
84	KK	1	Total 1	Mg 1	0
84	QQ	1	Total 1	Mg 1	0
84	XX	1	Total 1	Mg 1	0
84	YY	1	Total 1	Mg 1	0
84	00	1	Total 1	Mg 1	0
84	aa	97	Total 97	Mg 97	0
84	ee	1	Total 1	Mg 1	0

- Molecule 85 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
85	A	1	Total 40	C 10	H 26	N 4	0

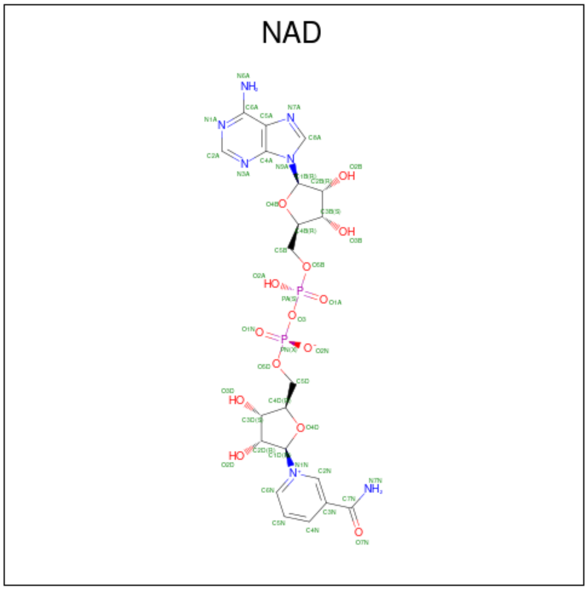
- Molecule 86 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
86	A	32	Total K 32 32	0
86	2	1	Total K 1 1	0
86	3	1	Total K 1 1	0
86	ZZ	1	Total K 1 1	0
86	88	1	Total K 1 1	0
86	aa	13	Total K 13 13	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

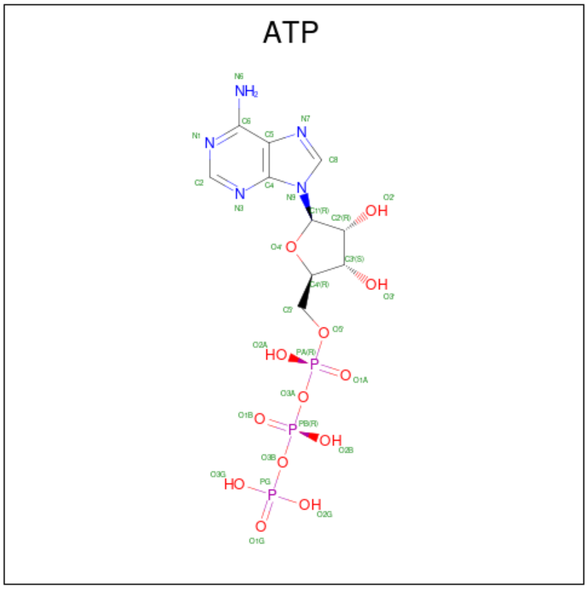
Mol	Chain	Residues	Atoms	AltConf
87	W	1	Total Zn 1 1	0
87	0	1	Total Zn 1 1	0

- Molecule 88 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
88	2	1	70	21	26	7	14	2	0

- Molecule 89 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



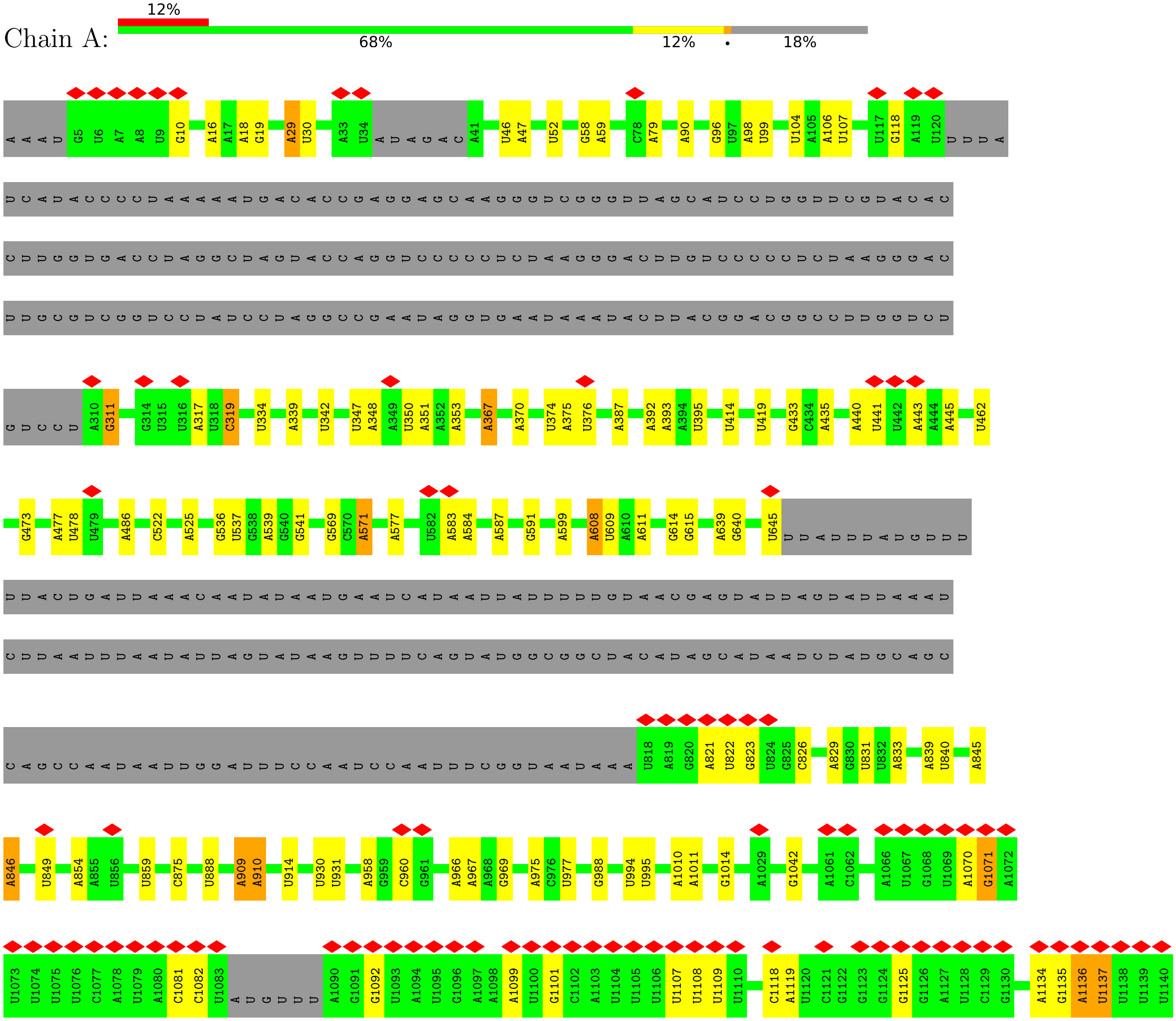
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
89	XX	1	43	10	12	5	13	3	0

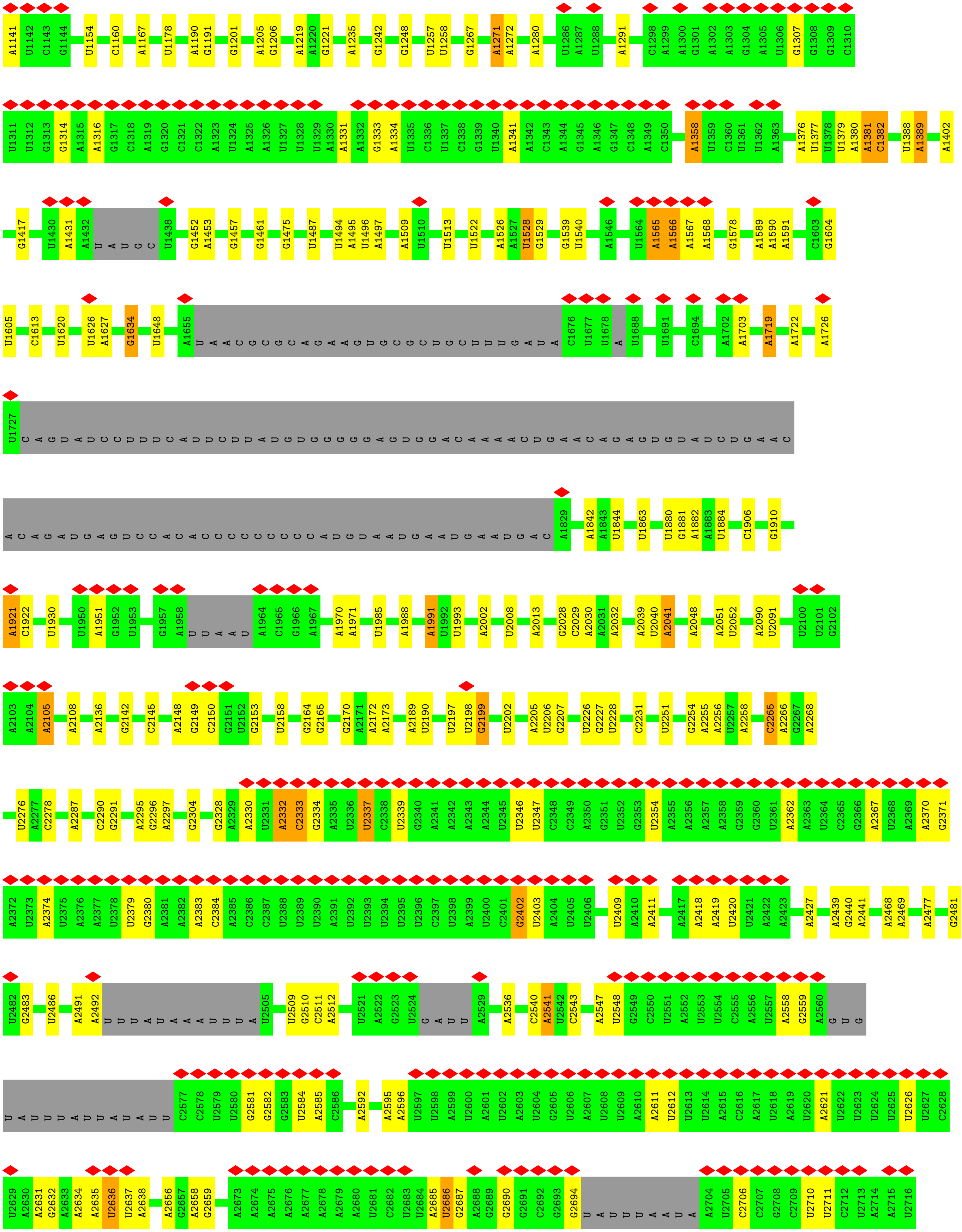
3 Residue-property plots ⓘ

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: 23S rRNA

Chain A:

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U1311 U1312 G1313 G1314 A1315 A1316 G1317 C1318 A1319 G1320 C1321 C1322 A1323 U1324 A1325 A1326 U1327 U1328 U1329 A1330 A1331 A1332 G1333 A1334 U1335 C1336 U1337 C1338 G1339 U1340 A1341 A1342 C1343 A1344 G1345 A1346 G1347 C1348 A1349 C1350 A1358 U1359 C1360 U1361 U1362 A1363 A1376 U1377 U1378 U1379 A1380 A1381 C1382 U1388 A1389 A1402
G1417 U1430 A1431 A1432 U A U G C U1438 G1452 A1453 G1457 G1461 G1475 U1487 U1494 A1495 U1496 A1497 A1509 U1510 U1513 U1522 A1526 A1527 U1528 G1529 G1539 U1540 A1546 U1564 A1565 A1566 A1567 A1568 G1578 A1589 A1590 A1591 C1603 G1604
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U A U U U A U U A U A U U C2577 C2578 U2579 U2580 G2581 G2582 G2583 U2584 A2585 C2586 A2592 A2595 A2596 U2597 U2598 A2599 U2600 A2601 U2602 A2603 U2604 G2605 U2606 A2607 U2608 U2609 A2610 A2611 U2612 U2613 U2614 A2615 C2616 A2617 U2618 A2619 U2620 A2621 U2622 U2623 U2624 U2625 U2626 U2627 C2628
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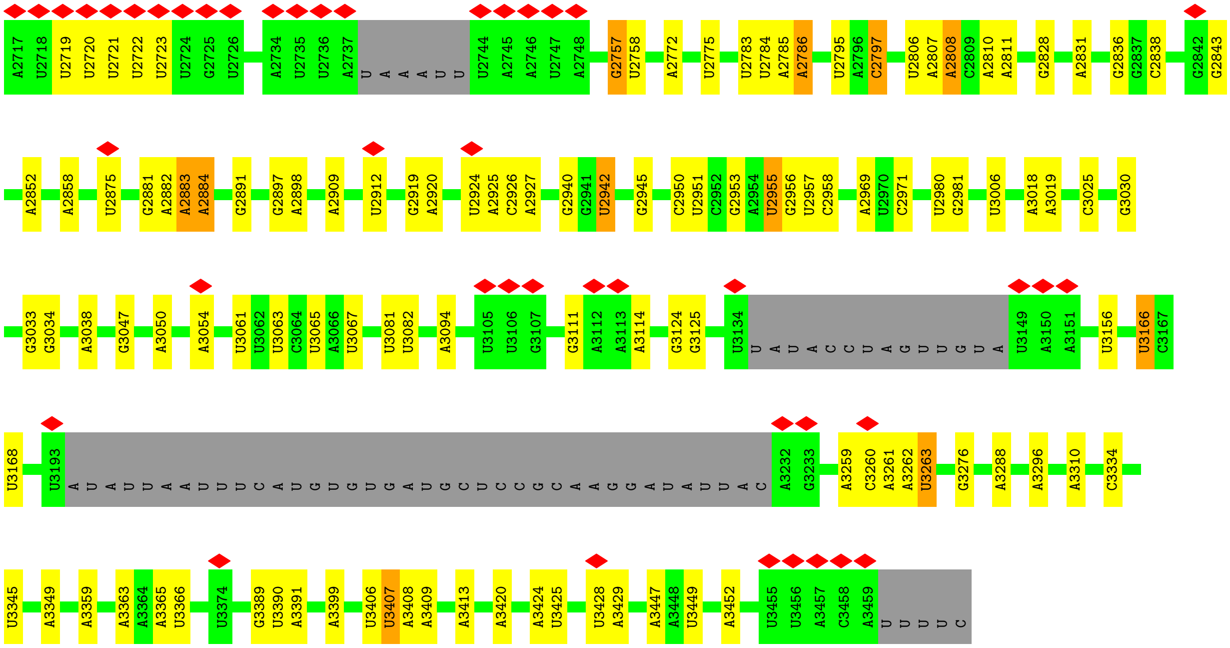
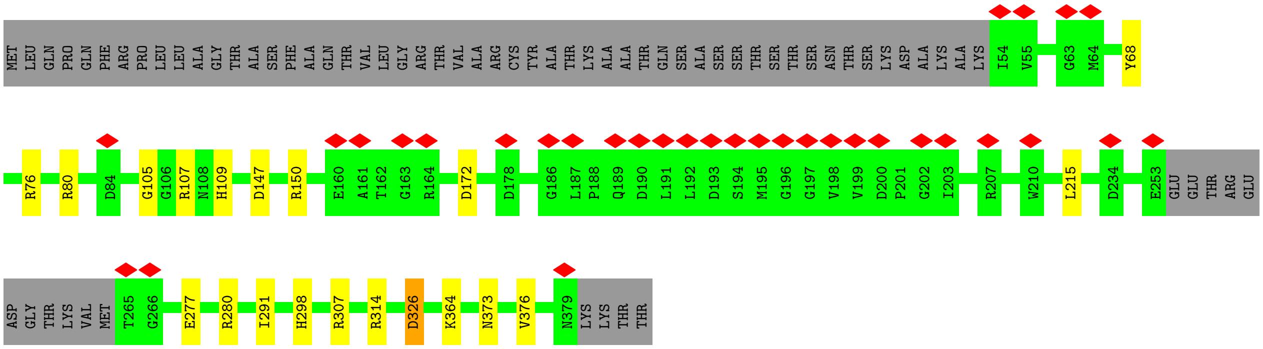


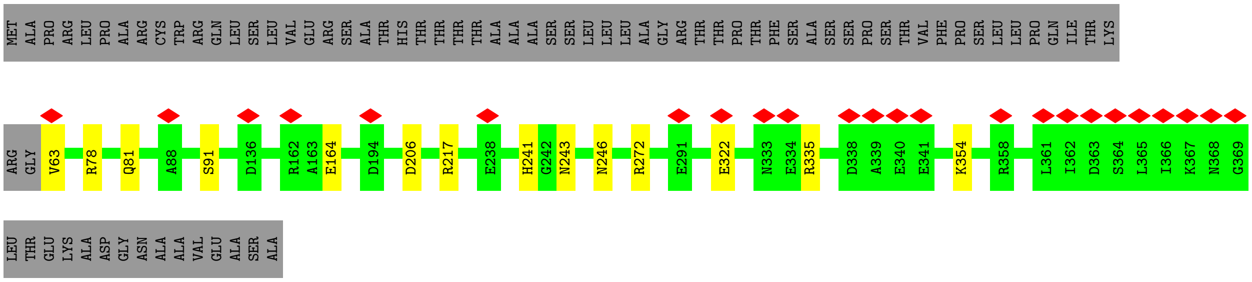
- Molecule 2: 60S ribosomal protein L2, mitochondrial

Chain B:



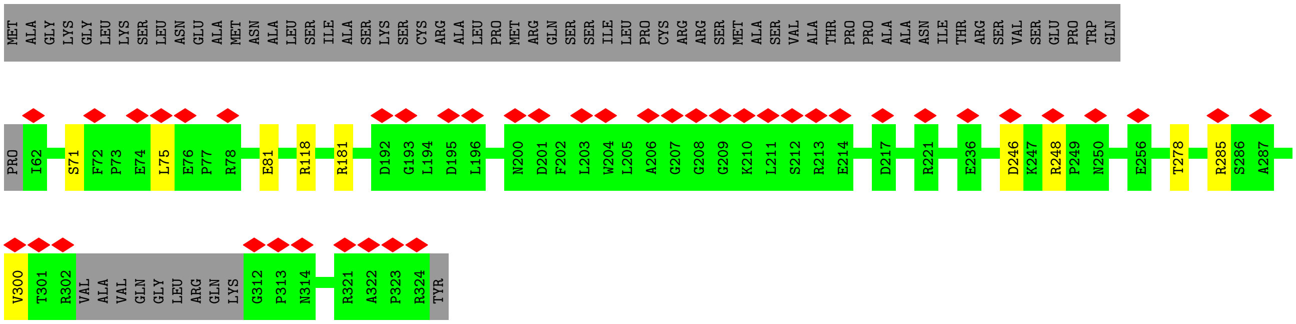
- Molecule 3: Related to ribosomal protein L3, mitochondrial

Chain C:



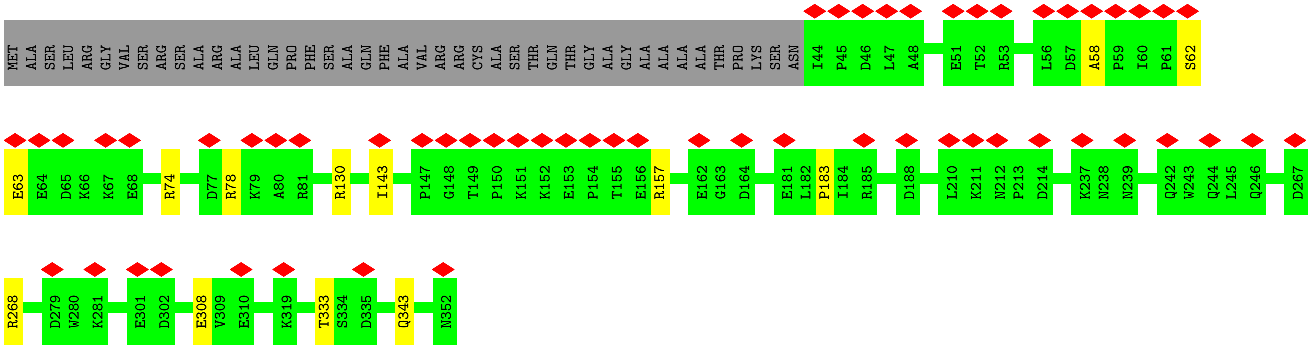
- Molecule 4: 60S ribosomal protein L4, variant

Chain D:



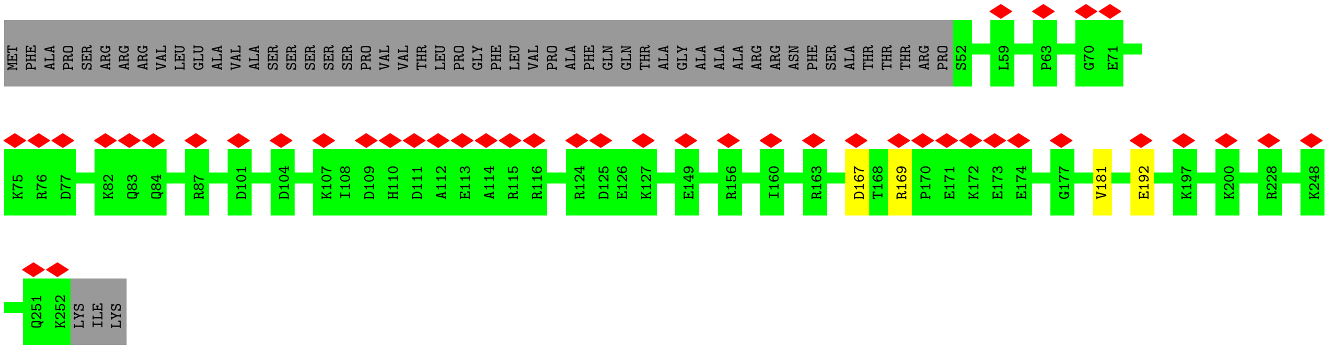
- Molecule 5: Related to ribosomal protein L5, mitochondrial

Chain E:



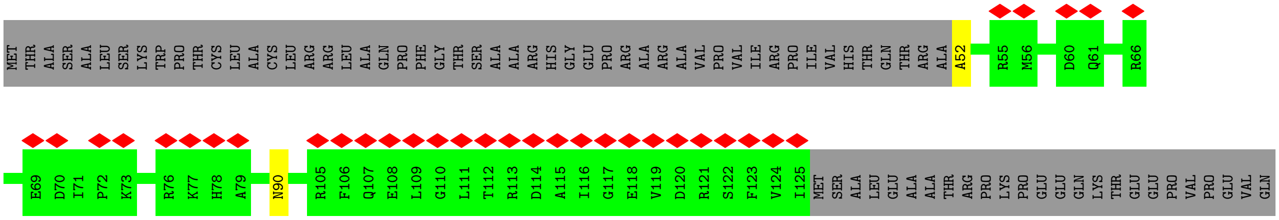
- Molecule 6: uL6m

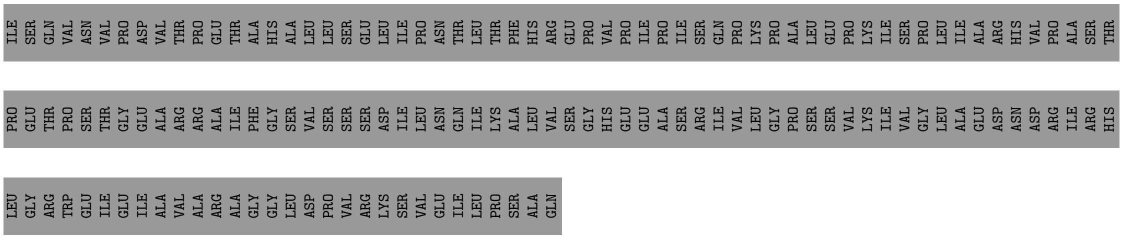
Chain F:



- Molecule 7: RIBOSOMAL_L9 domain-containing protein

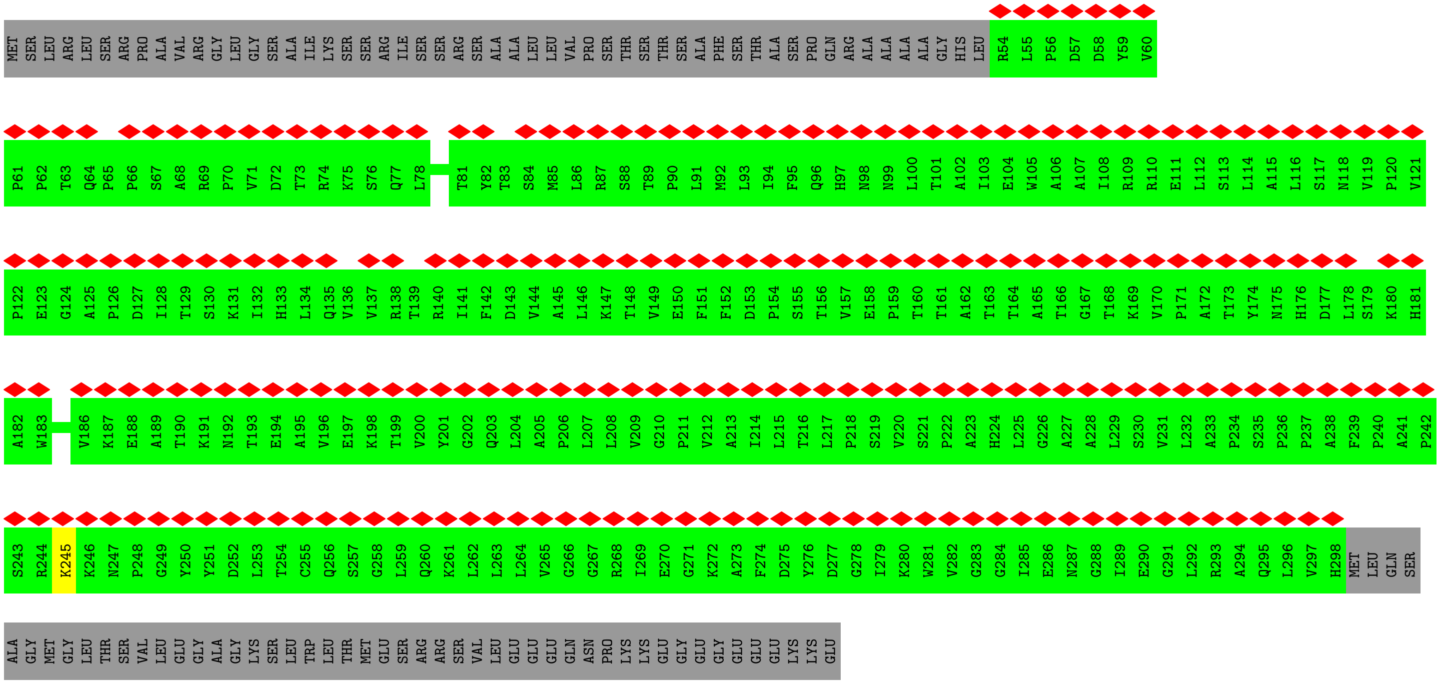
Chain G:





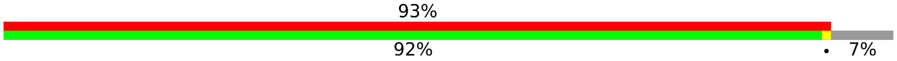
- Molecule 8: Related to ribosomal protein YmL11, mitochondrial

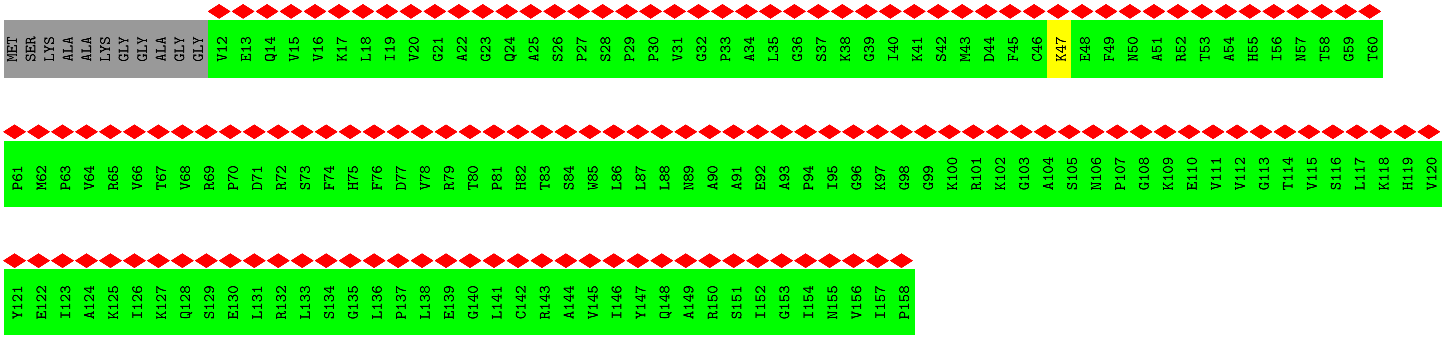
Chain f:



- Molecule 9: uL11m

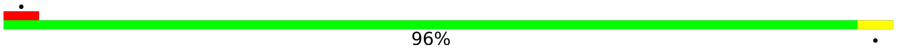
Chain g:

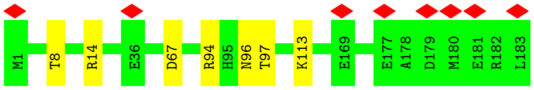




- Molecule 10: uL13m

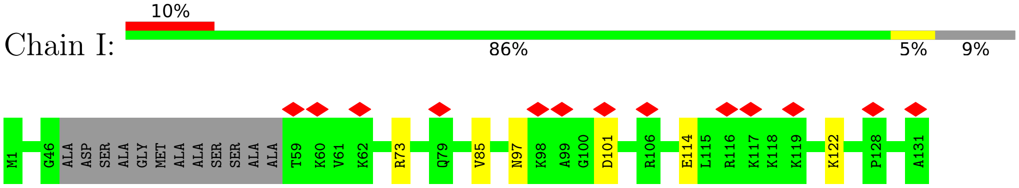
Chain H:





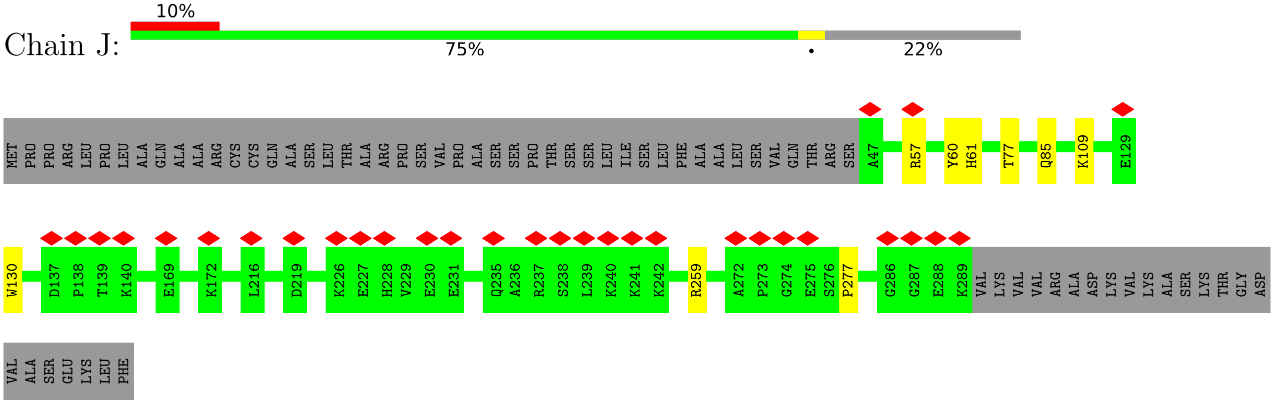
- Molecule 11: Ribosomal protein L14

Chain I:



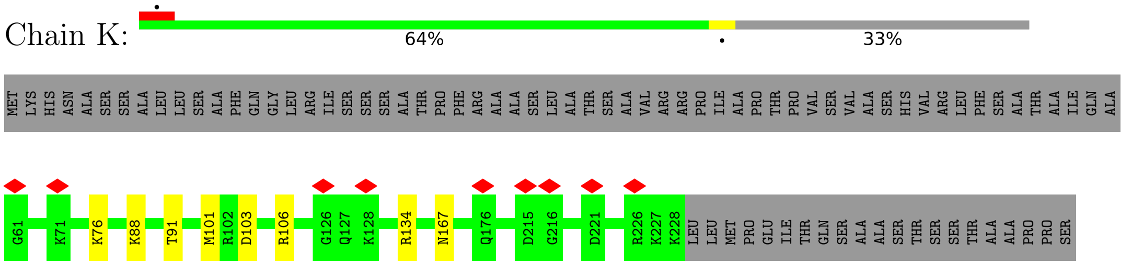
- Molecule 12: Ribosomal protein L15

Chain J:



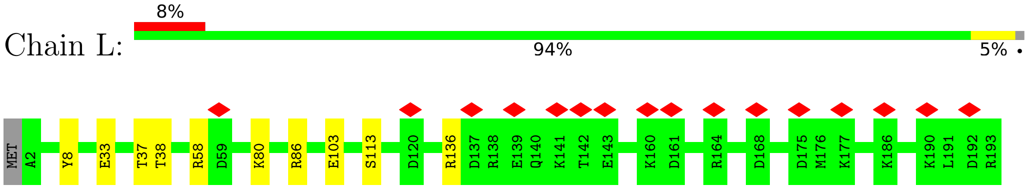
- Molecule 13: Related to ribosomal protein L16, mitochondrial

Chain K:



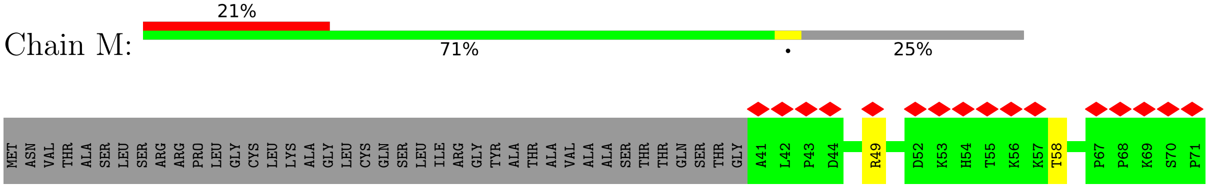
- Molecule 14: uL17m

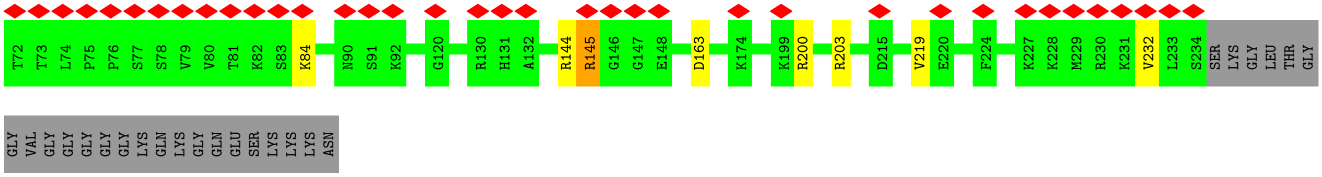
Chain L:



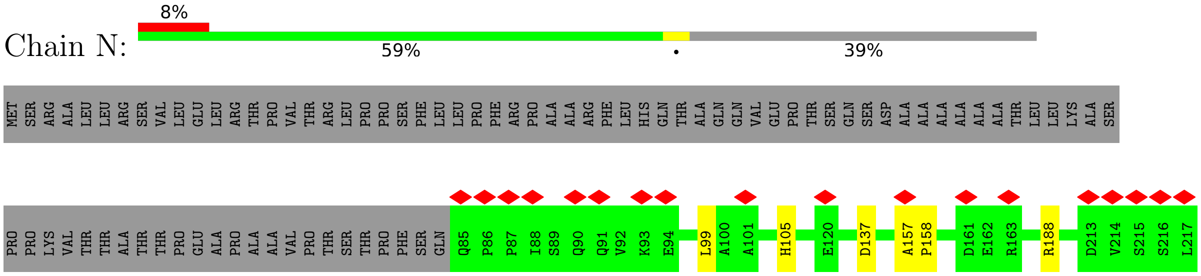
- Molecule 15: bL19m

Chain M:

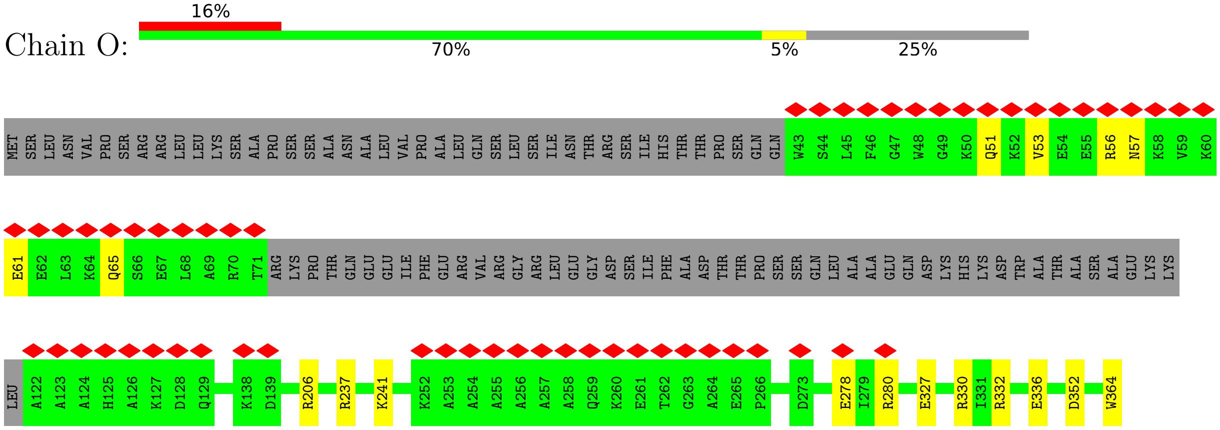




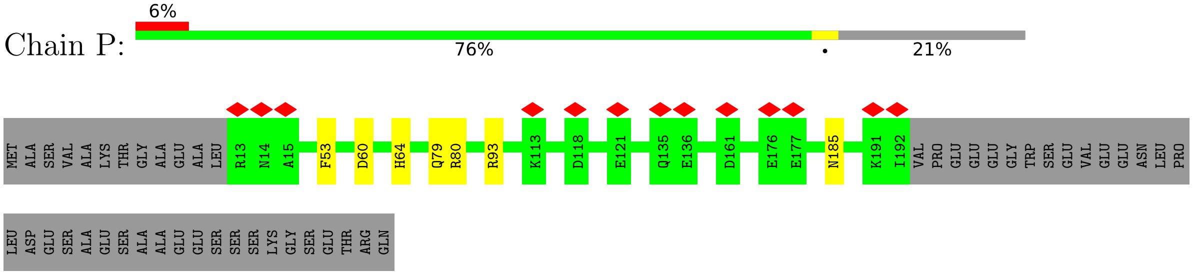
- Molecule 16: Related to ribosomal protein YmL49, mitochondrial



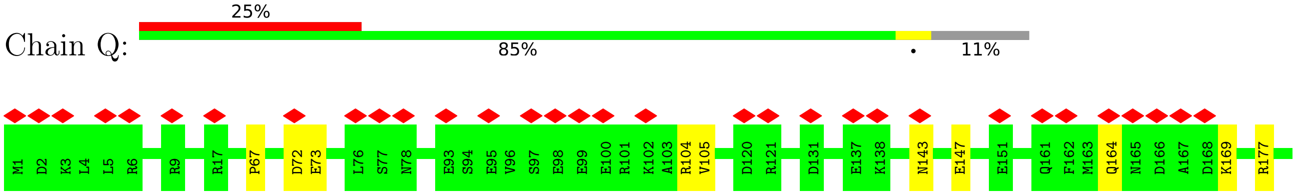
- Molecule 17: Mitochondrial large ribosomal subunit

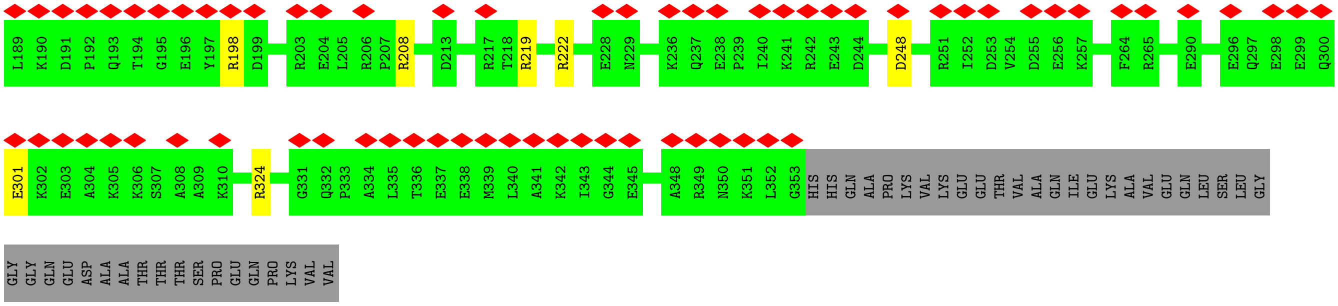


- Molecule 18: uL23m



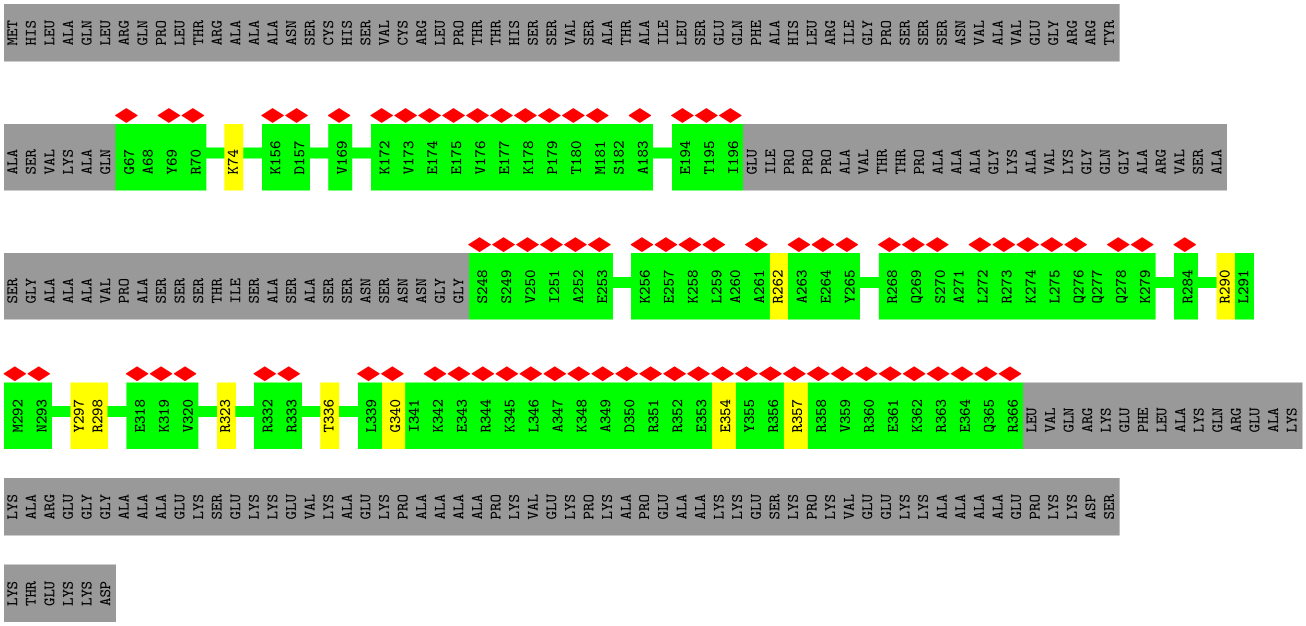
- Molecule 19: KOW domain-containing protein





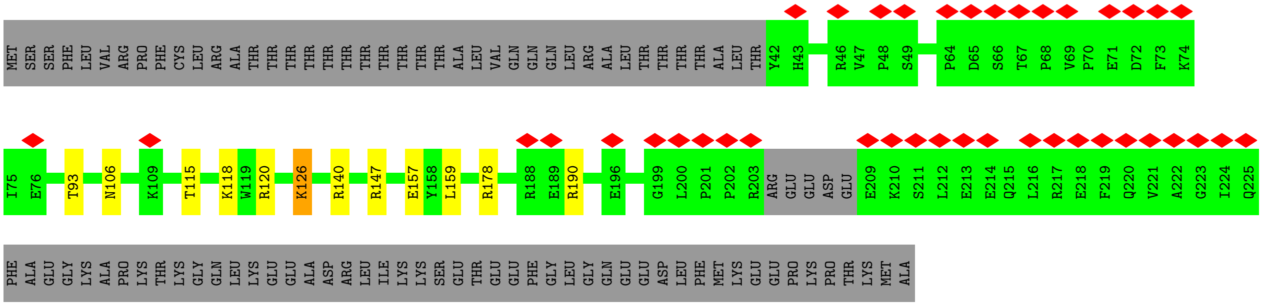
- Molecule 20: Related to 60s ribosomal protein L2 (Mitochondrial)

Chain R:



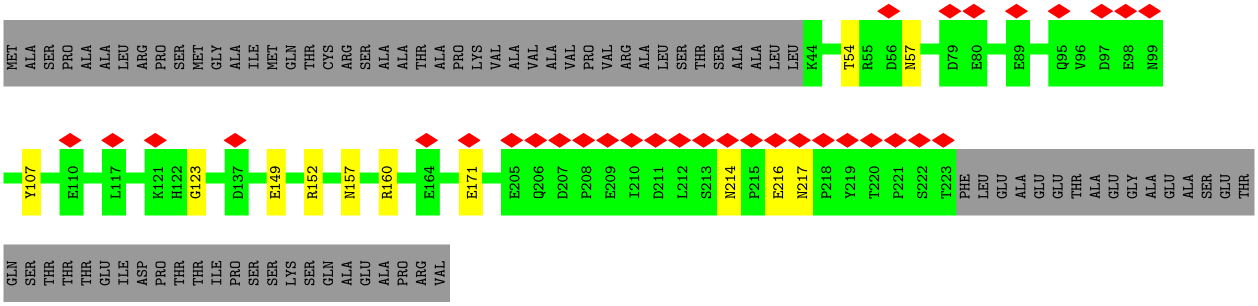
- Molecule 21: bL28m

Chain S:



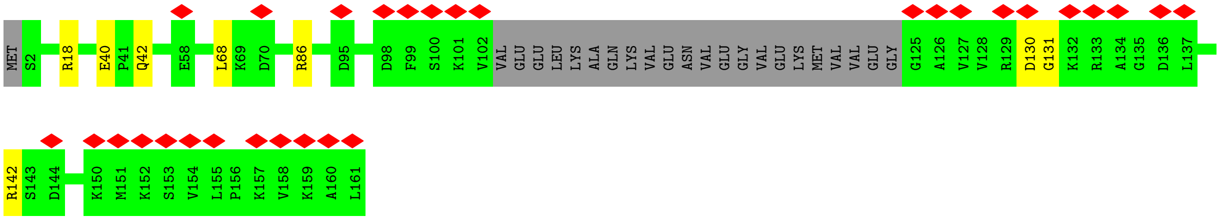
- Molecule 22: 54S ribosomal protein L4, mitochondrial

Chain T:



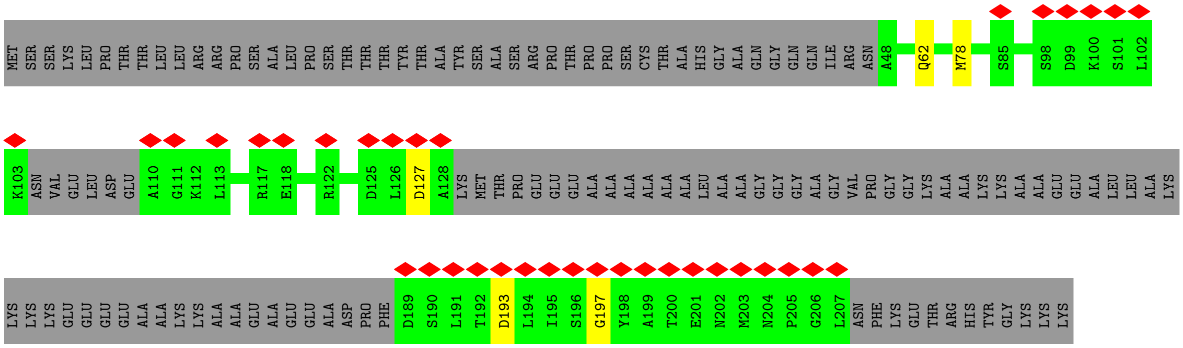
- Molecule 23: Related to ribosomal protein L30

Chain U:

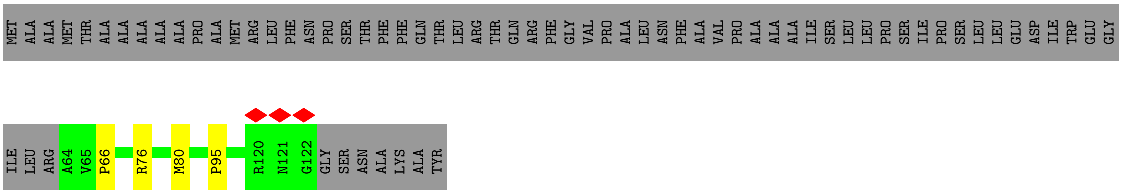
- Molecule 24: Related to ribosomal protein YmL36, mitochondrial

Chain V:

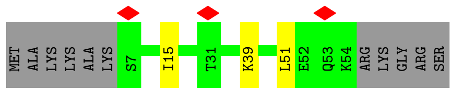
- Molecule 25: Related to ribosomal protein YmL32 (Mitochondrial)

Chain W:

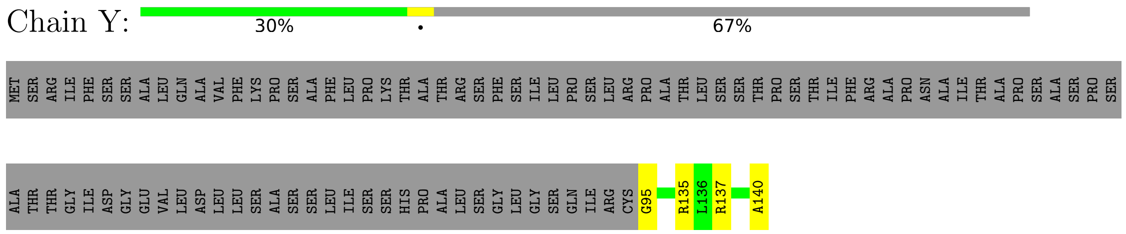



- Molecule 26: bL33m

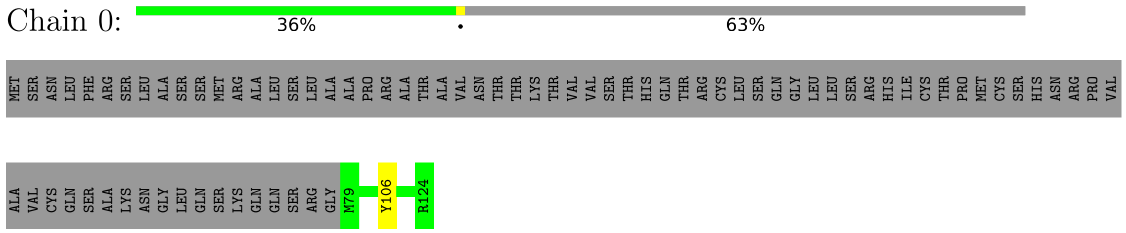
Chain X:

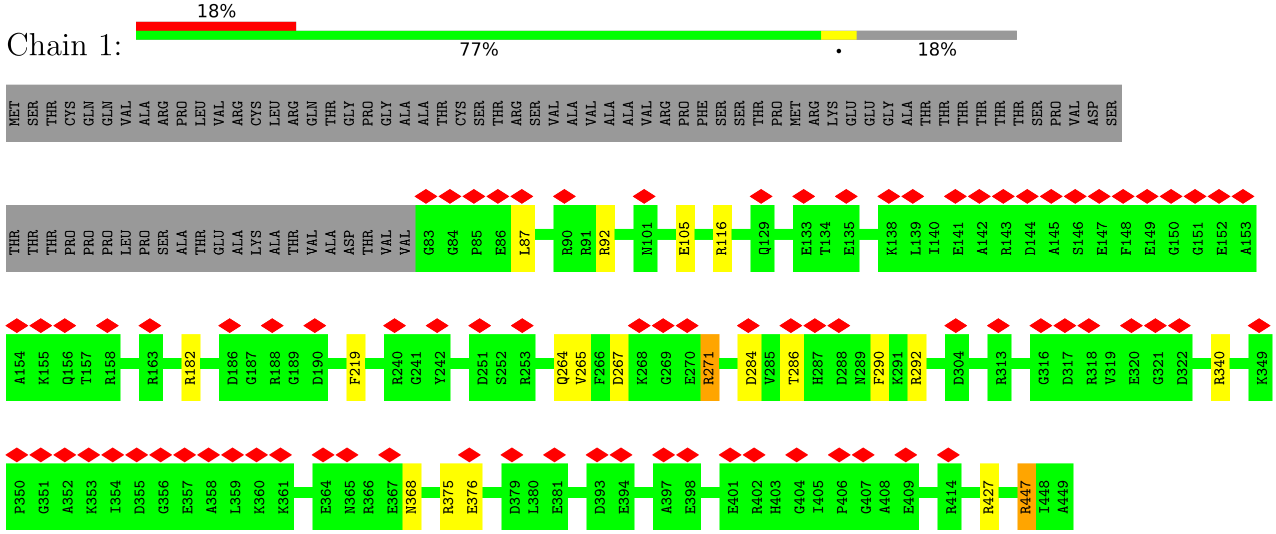
- Molecule 27: Related to ribosomal protein L34, mitochondrial



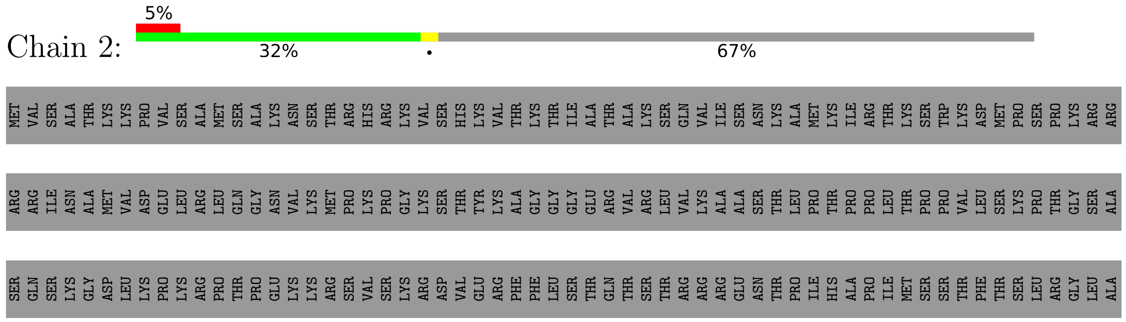
- Molecule 28: Ribosomal protein

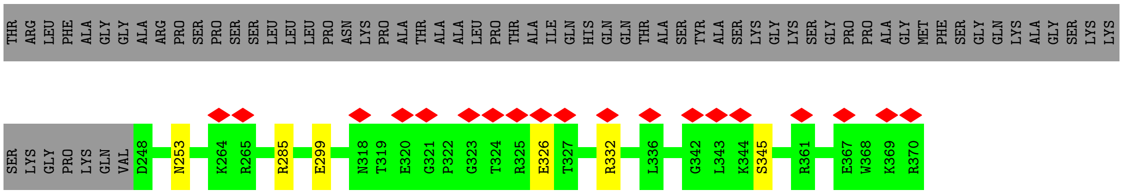


- Molecule 29: PEBP-like protein



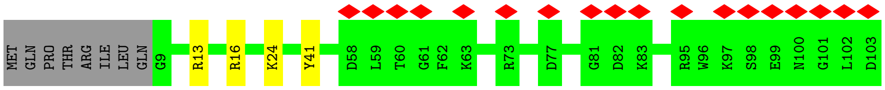
- Molecule 30: mL40





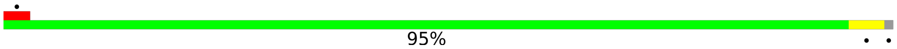
- Molecule 31: mL41

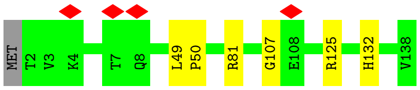
Chain 3:



- Molecule 32: L51_S25_CI-B8 domain-containing protein

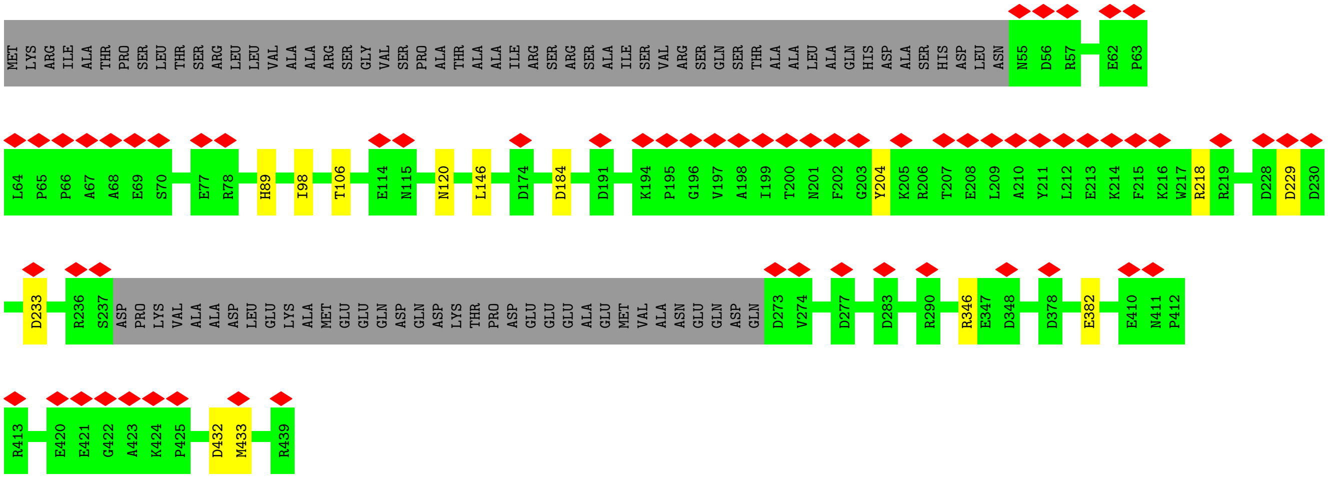
Chain 4:





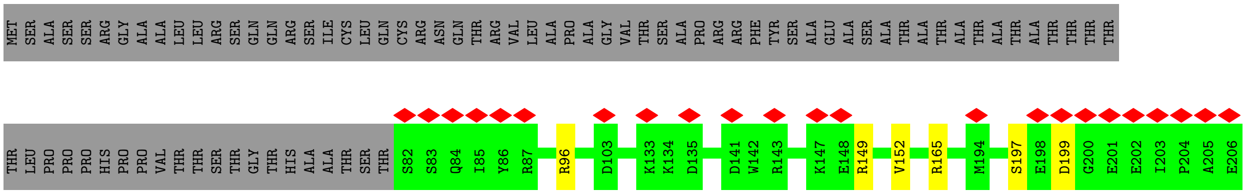
- Molecule 33: Ribonuclease III

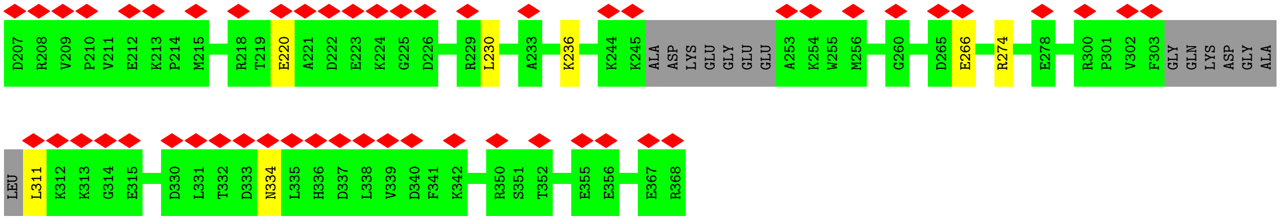
Chain 5:



- Molecule 34: mL46

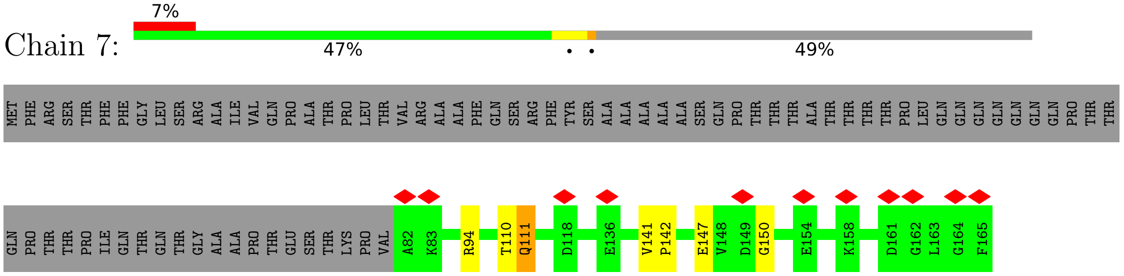
Chain 6:





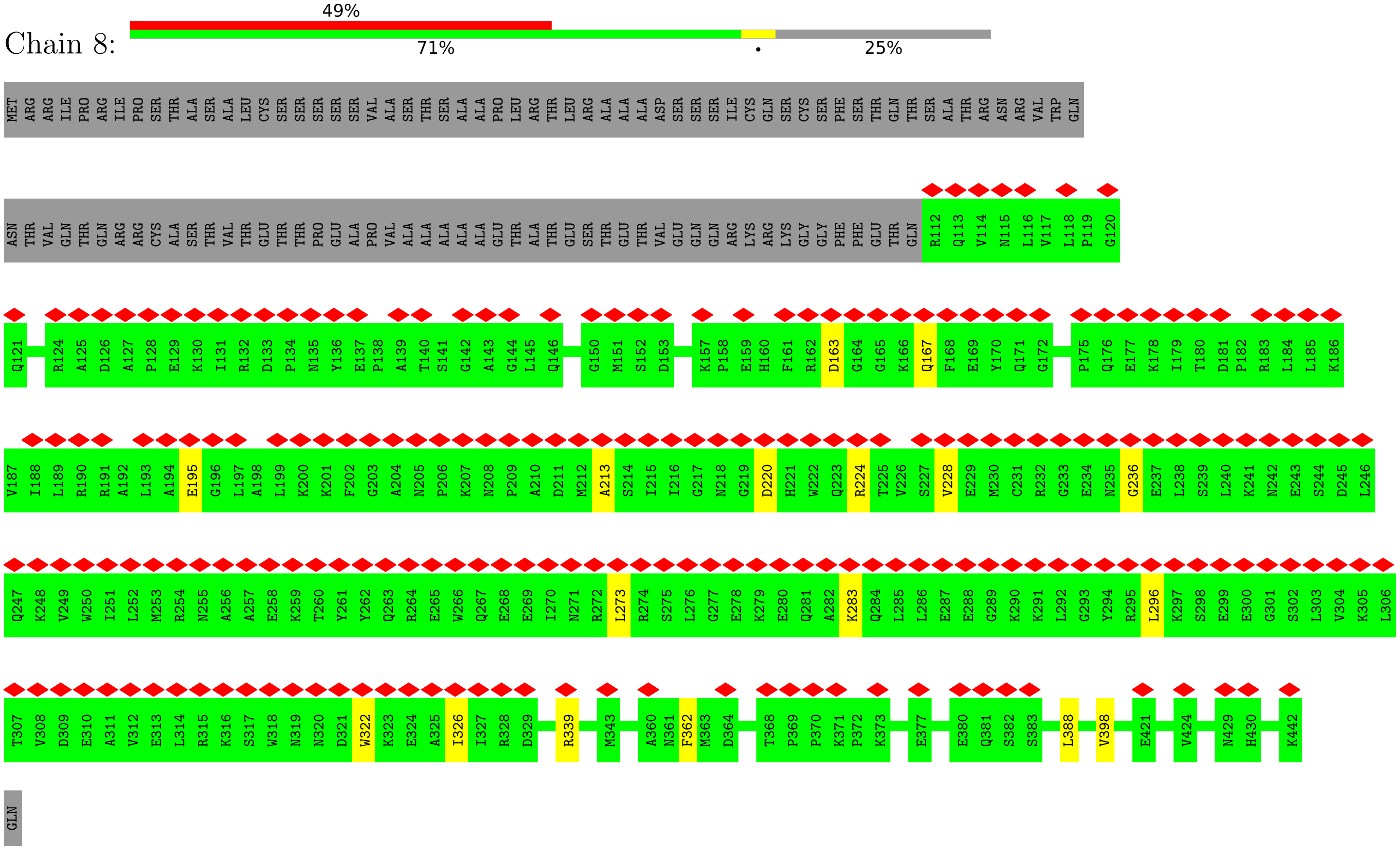
- Molecule 35: mL49

Chain 7:



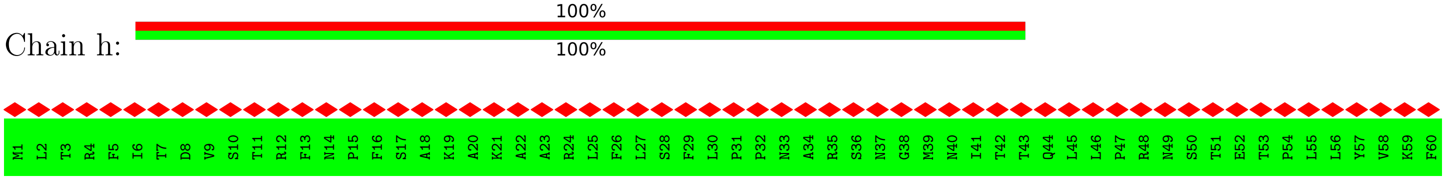
- Molecule 36: mL50

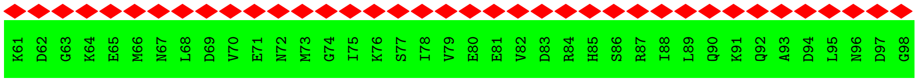
Chain 8:



- Molecule 37: Probable ribosomal protein YmL44, mitochondrial

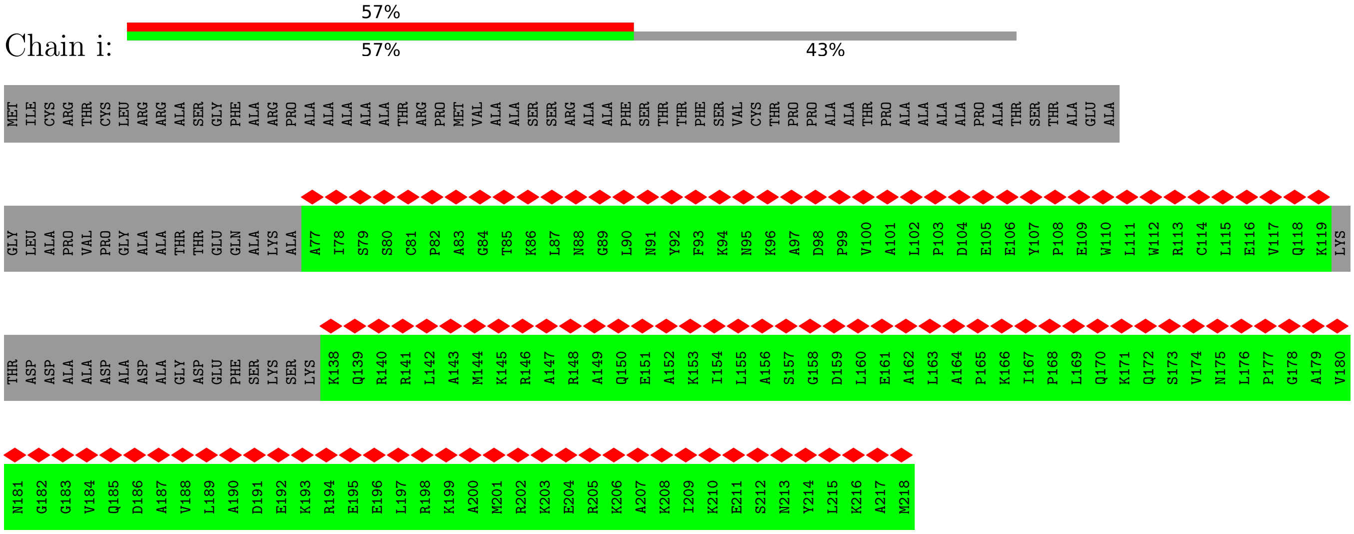
Chain h:





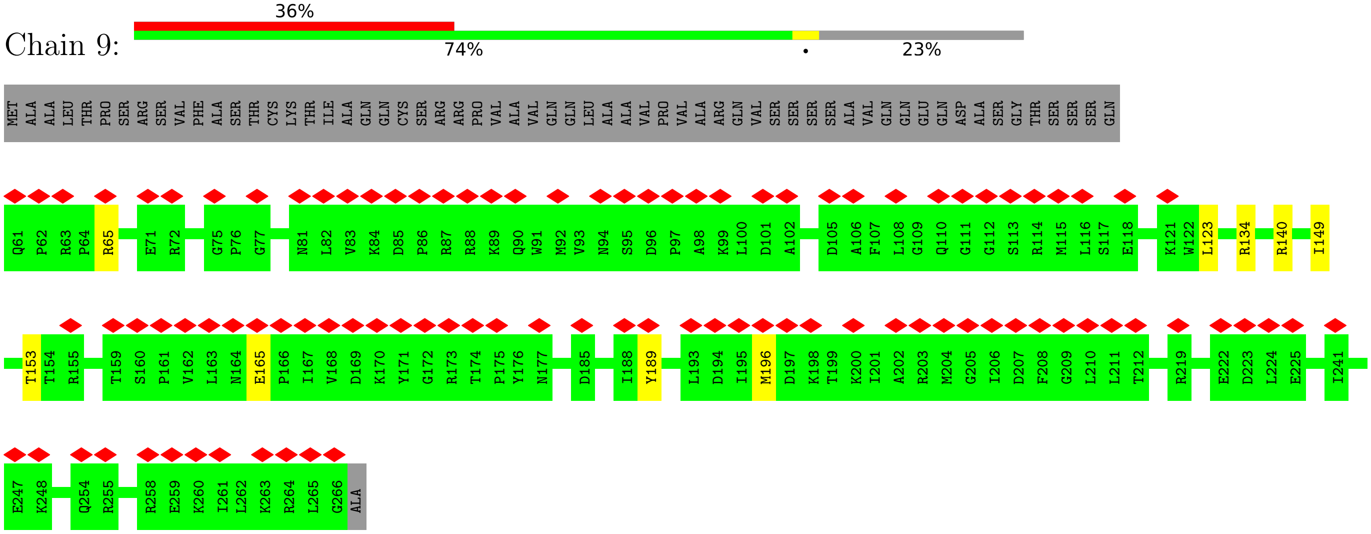
- Molecule 38: mL54

Chain i:



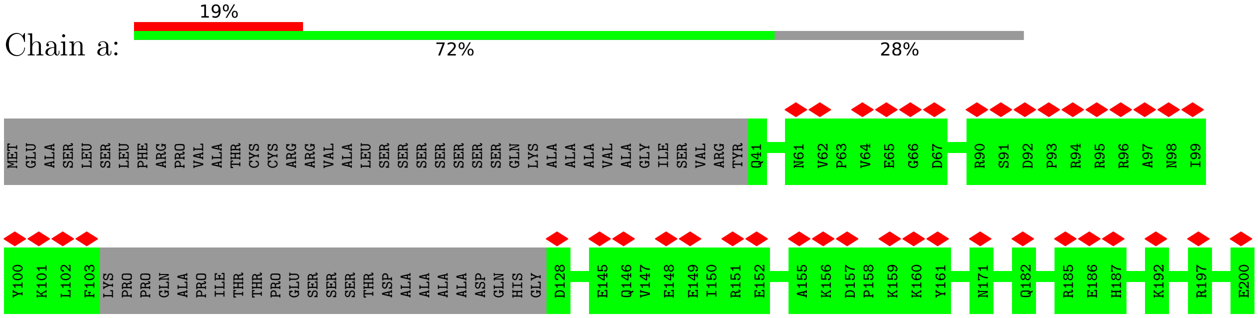
- Molecule 39: RNase III domain-containing protein

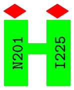
Chain 9:



- Molecule 40: Related to ribosomal protein YmL20, mitochondrial

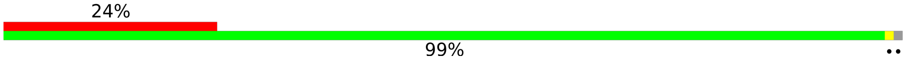
Chain a:

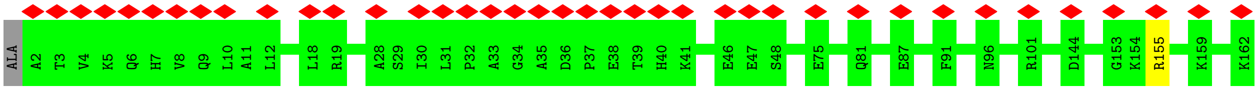




- Molecule 41: Mitoc_mL59 domain-containing protein

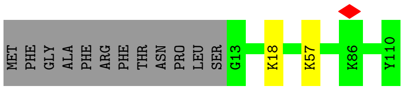
Chain b:





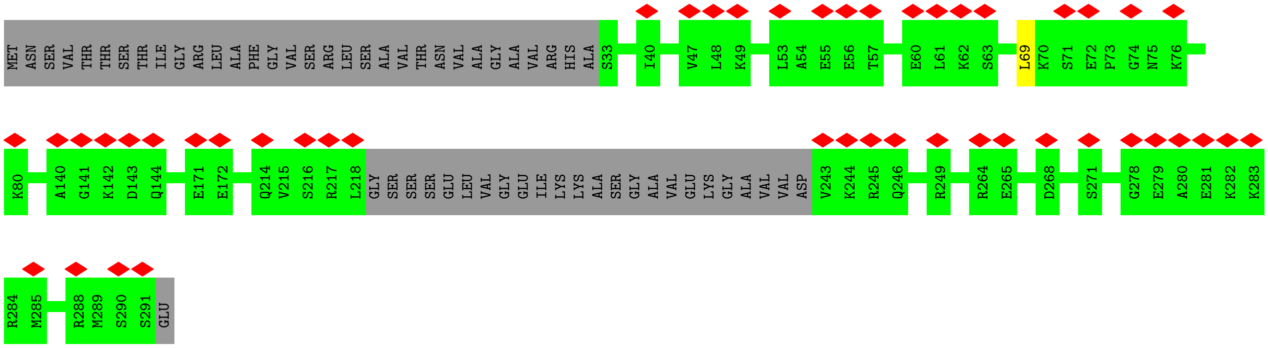
- Molecule 42: 54S ribosomal protein L31, mitochondrial

Chain c:



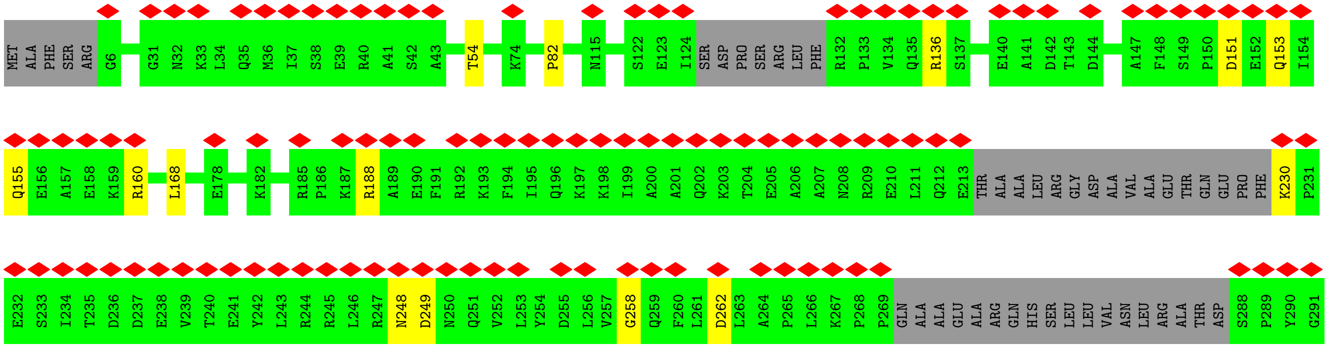
- Molecule 43: mL67

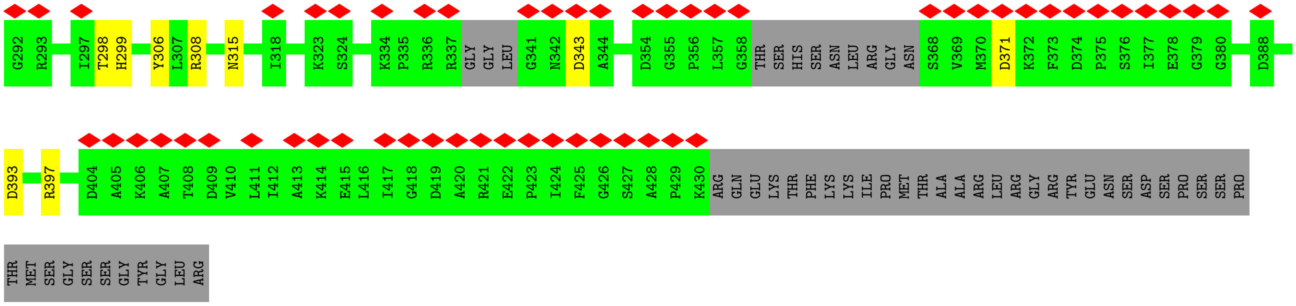
Chain d:



- Molecule 44: bS1m

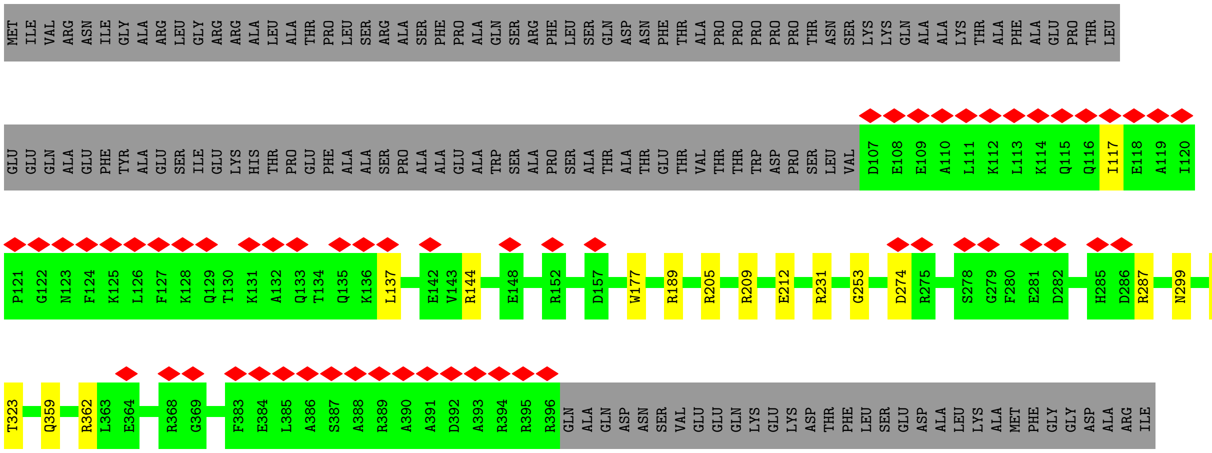
Chain AA:





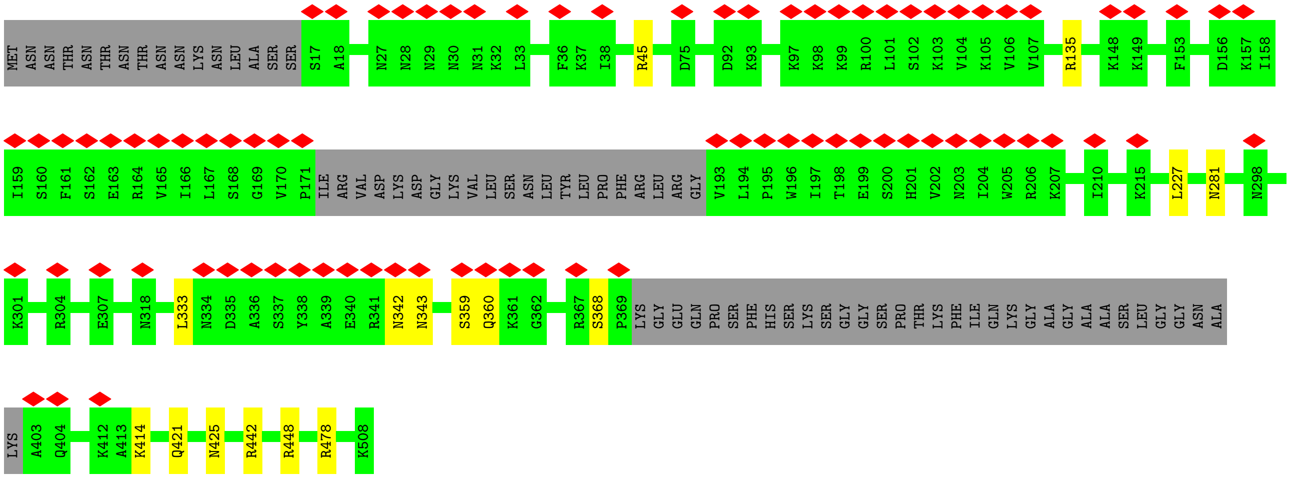
- Molecule 45: Mito ribosomal protein S2

Chain BB:



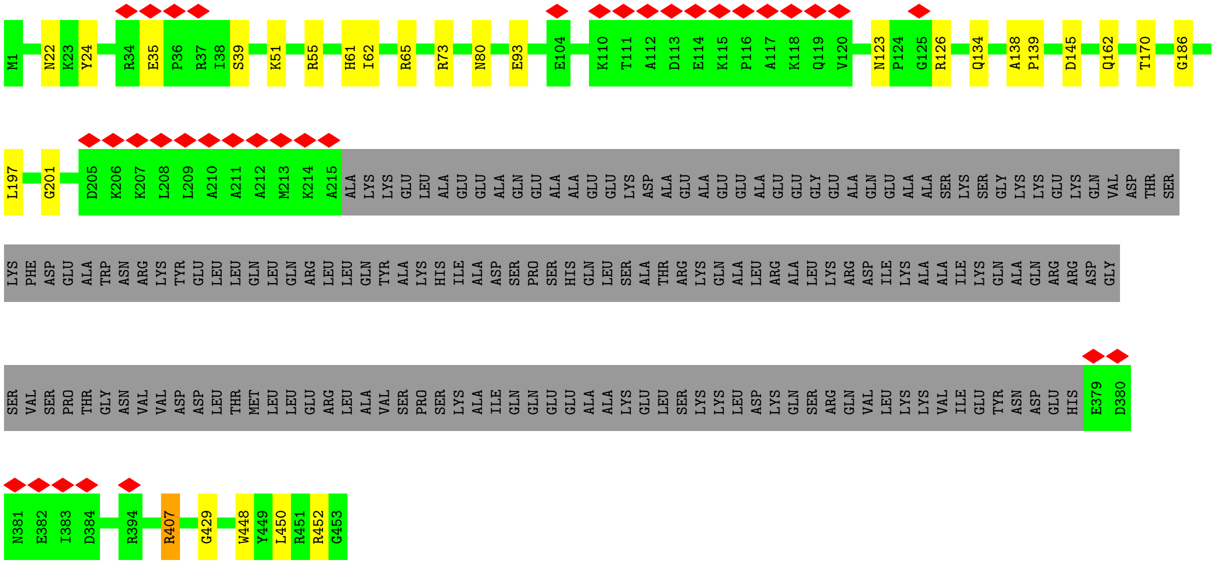
- Molecule 46: Ribosomal protein S5

Chain CC:



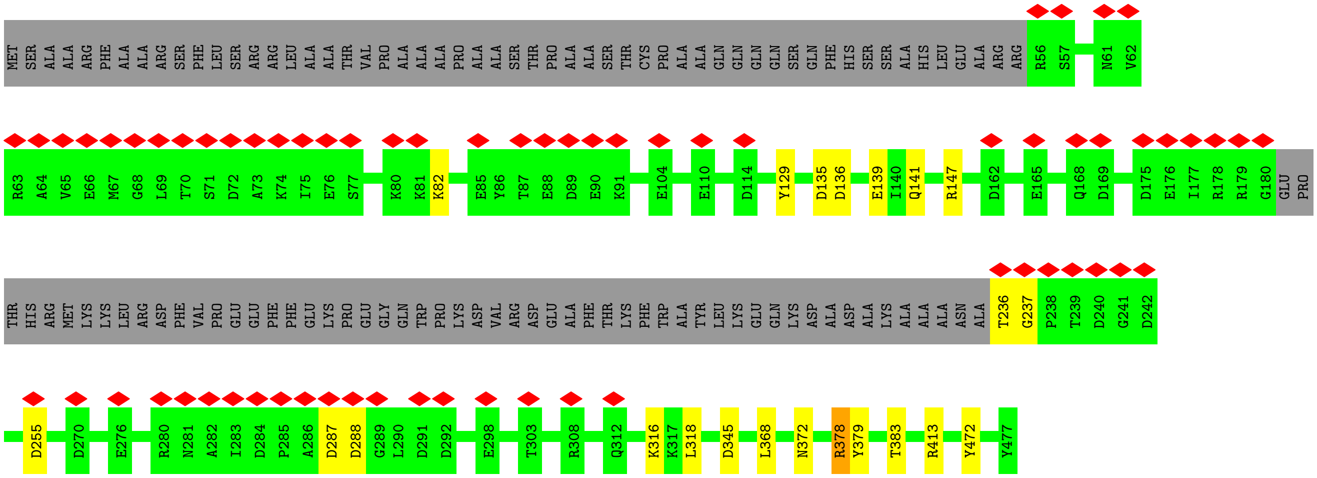
- Molecule 47: S4 RNA-binding domain-containing protein

Chain DD:



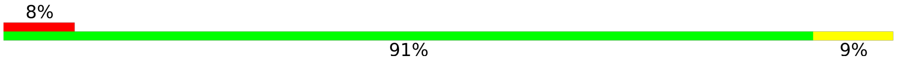
- Molecule 48: Related to ribosomal protein S5 (Mitochondrial)

Chain EE:



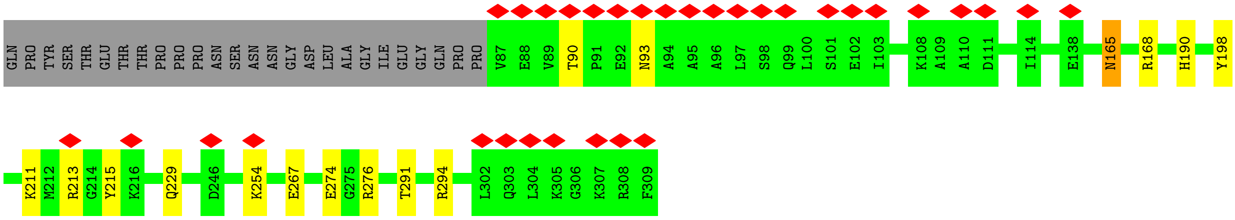
- Molecule 49: Ribosomal protein S6

Chain FF:

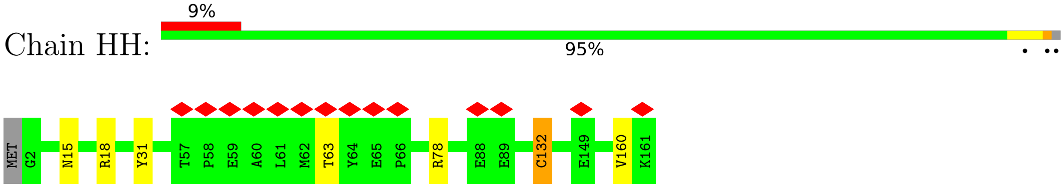


- Molecule 50: Ribosomal_S7 domain-containing protein

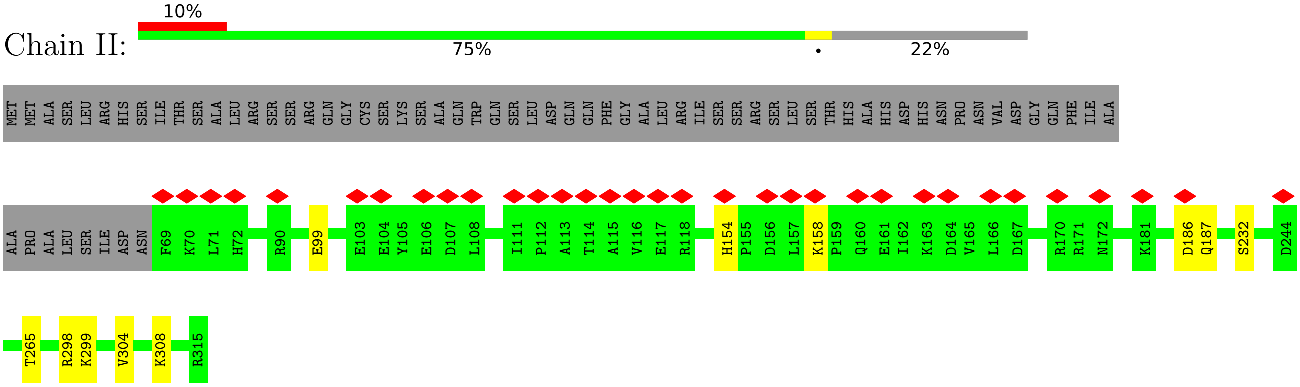
Chain GG:



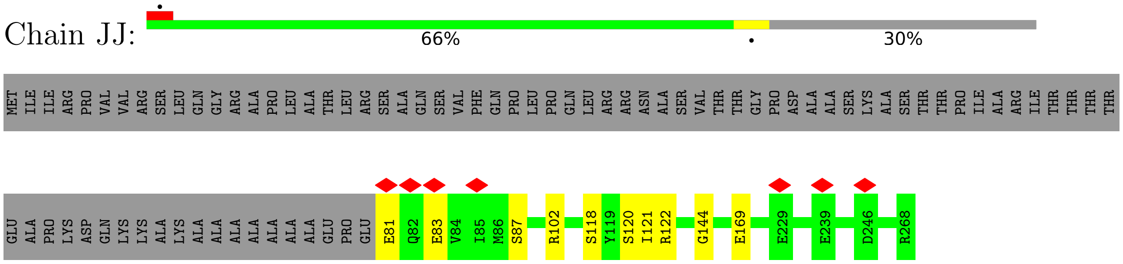
- Molecule 51: uS8m



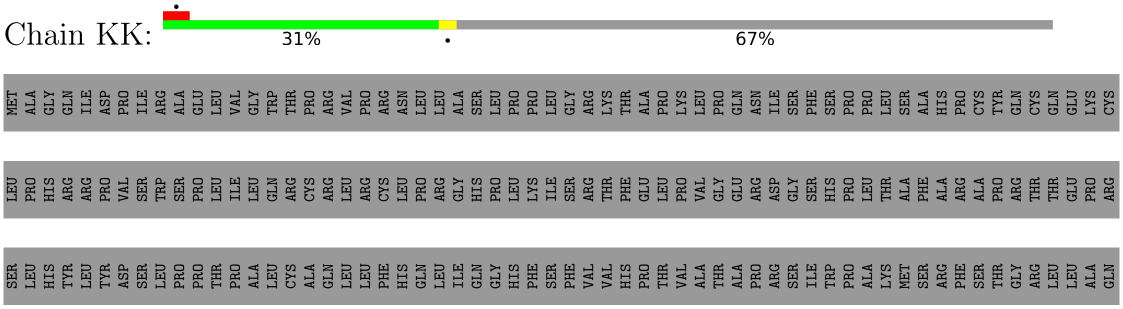
- Molecule 52: uS9m

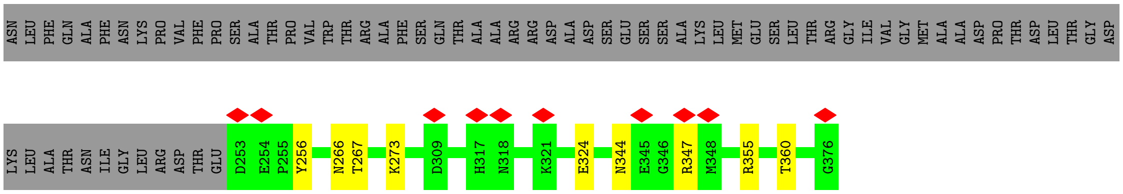


- Molecule 53: 30S ribosomal protein S10, mitochondrial



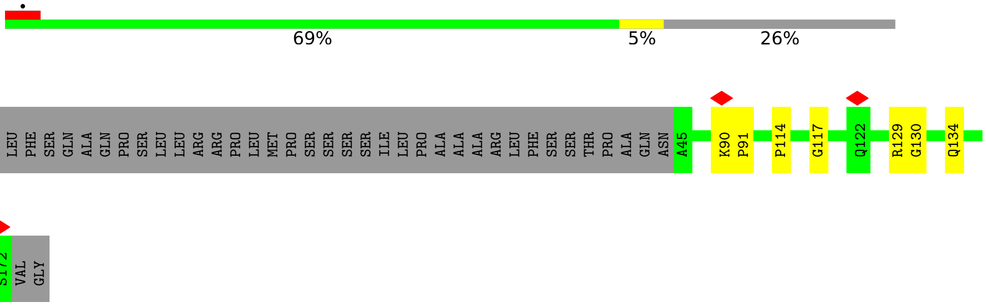
- Molecule 54: Translational machinery component





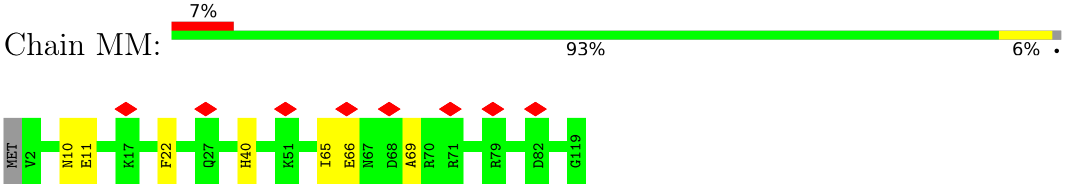
- Molecule 55: Ribosomal protein S12

Chain LL:



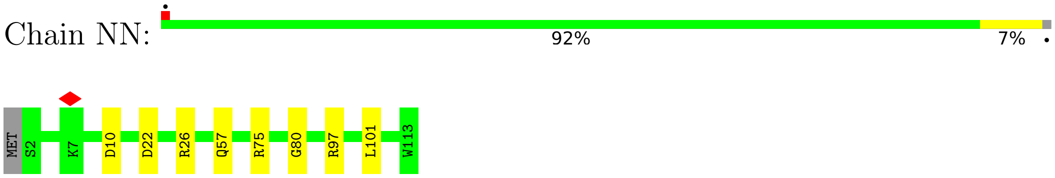
- Molecule 56: Probable ribosomal protein S13

Chain MM:



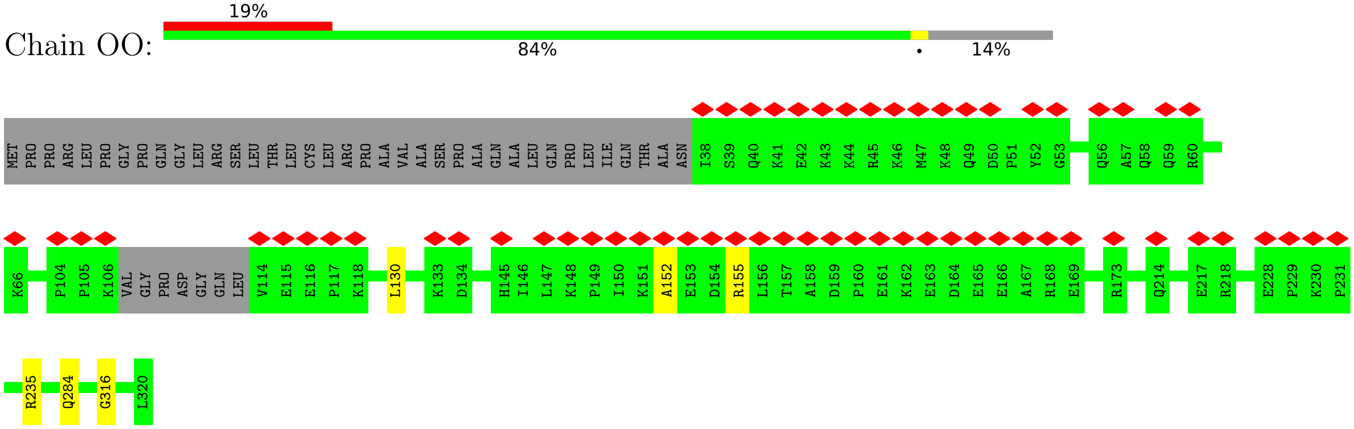
- Molecule 57: Mitochondrial 37S ribosomal protein MRP2

Chain NN:



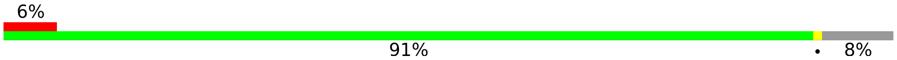
- Molecule 58: Related to ribosomal protein S15 (Mitochondrial)

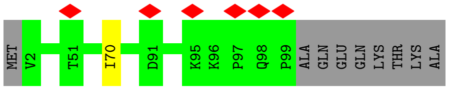
Chain OO:



- Molecule 59: bS16m

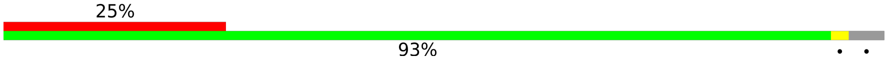
Chain PP:

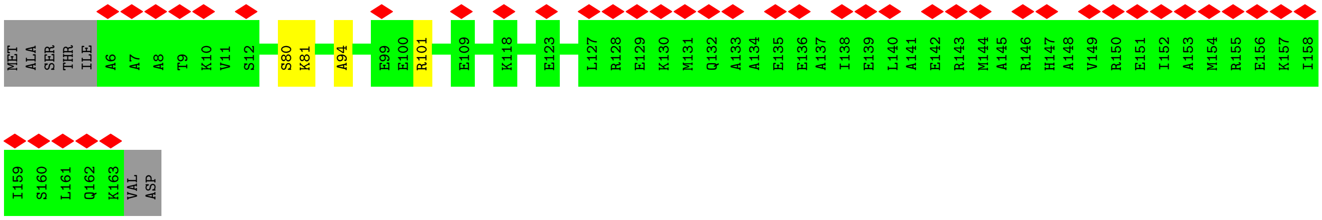




- Molecule 60: uS17m

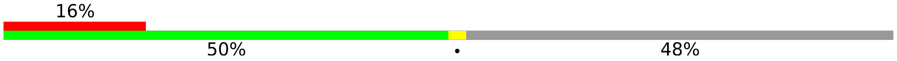
Chain QQ:

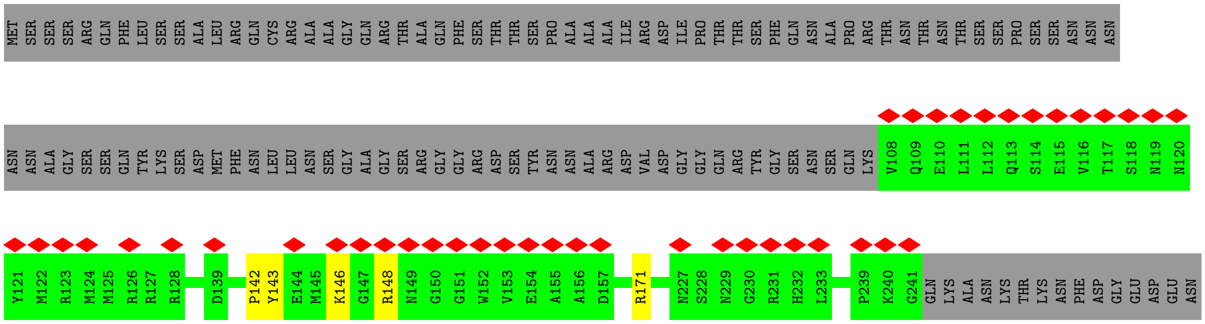




- Molecule 61: Ribosomal protein S18

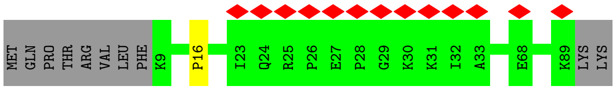
Chain RR:





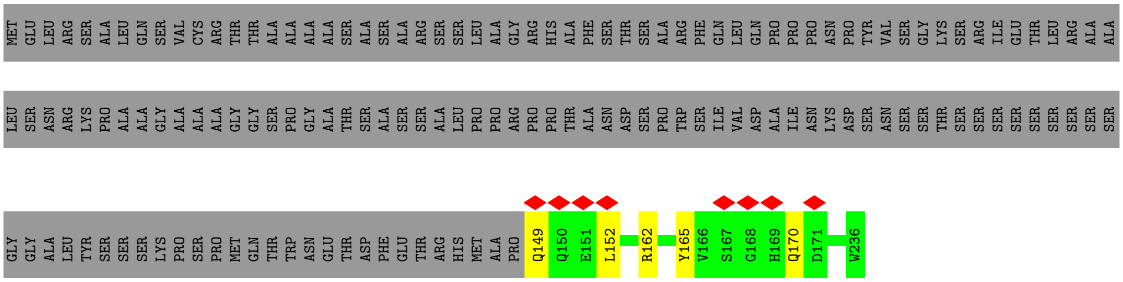
- Molecule 62: Ribosomal protein S19/S15

Chain SS:



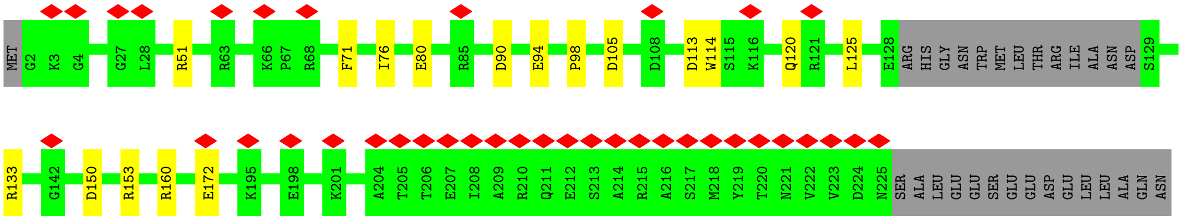
- Molecule 63: bS21m

Chain TT:



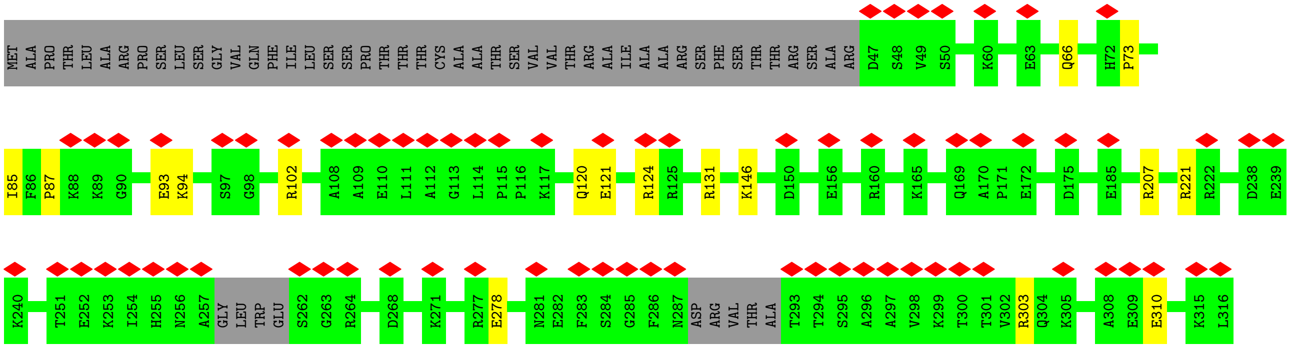
- Molecule 64: 37S ribosomal protein S25, mitochondrial

Chain UU:



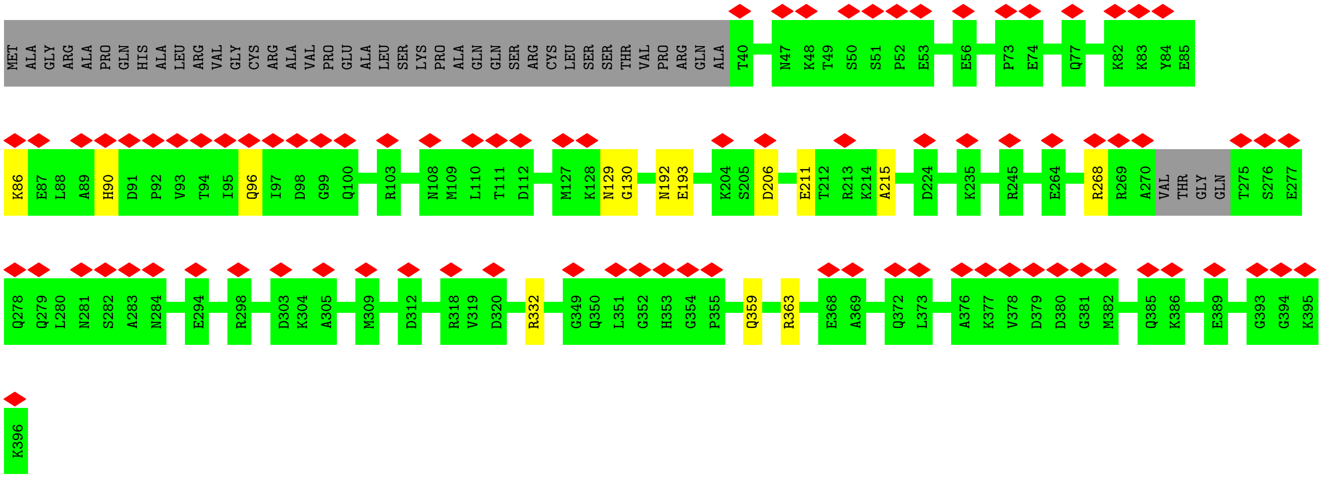
- Molecule 65: mS26

Chain VV:



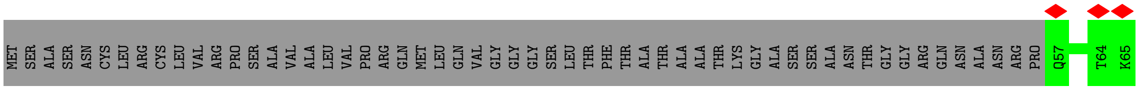
- Molecule 66: mS27

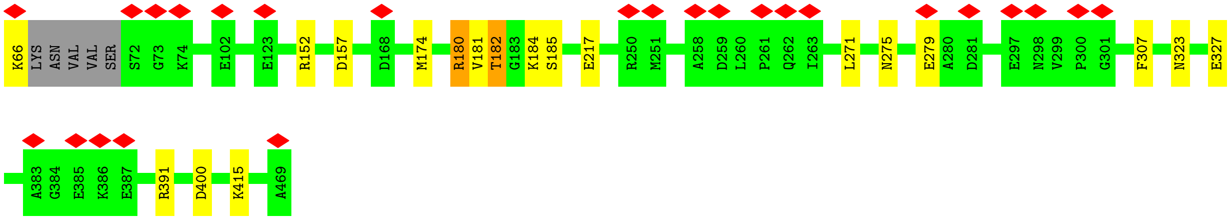
Chain WW:



- Molecule 67: Mitochondrial ribosomal protein DAP3

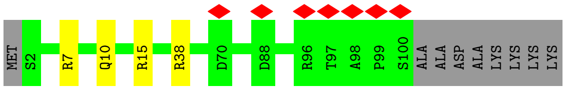
Chain XX:





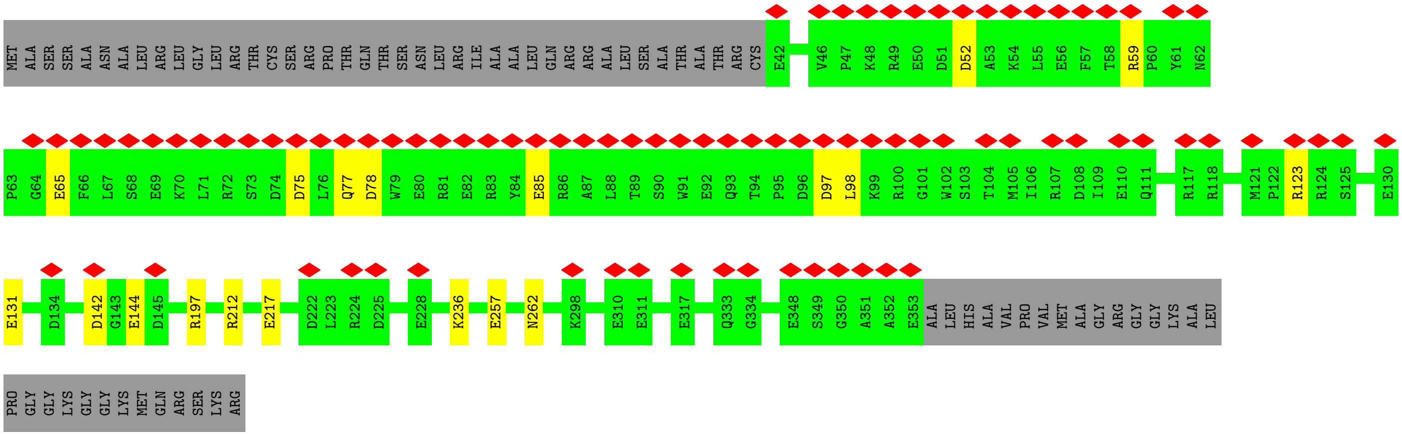
- Molecule 68: mS33

Chain YY:



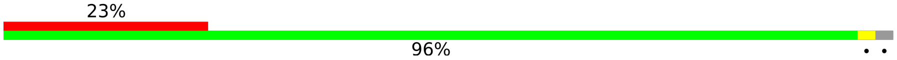
- Molecule 69: 37S ribosomal protein S24, mitochondrial

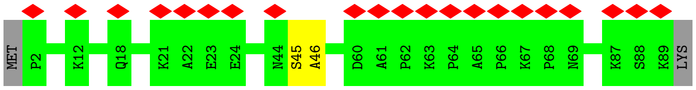
Chain ZZ:



- Molecule 70: 37S ribosomal protein mrp10, mitochondrial

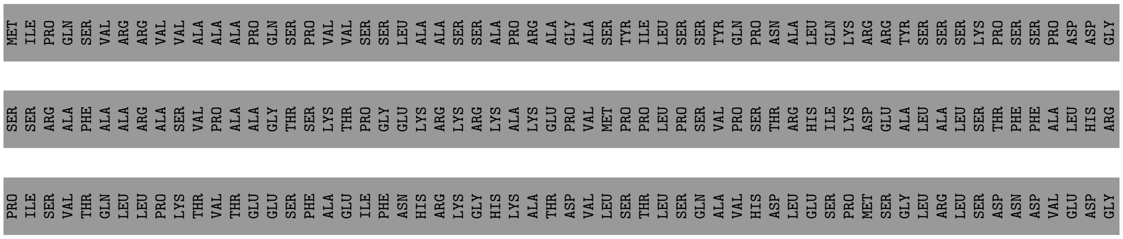
Chain 11:

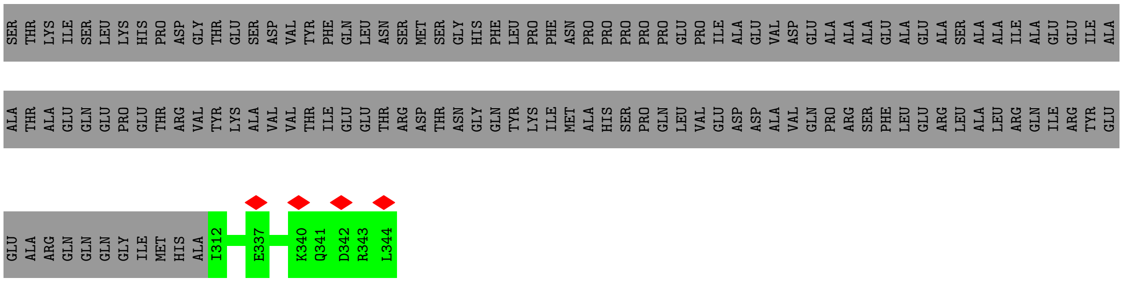




- Molecule 71: DUF1713 domain-containing protein

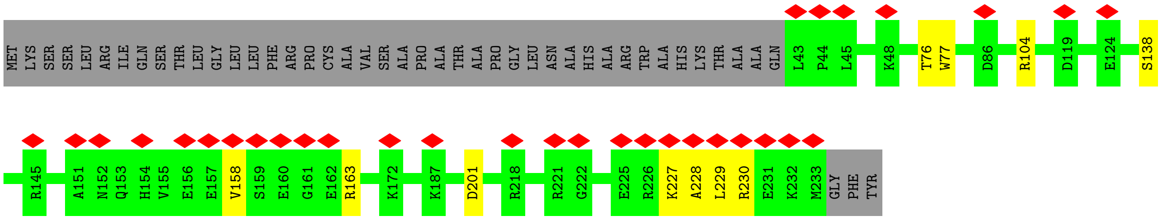
Chain 22:





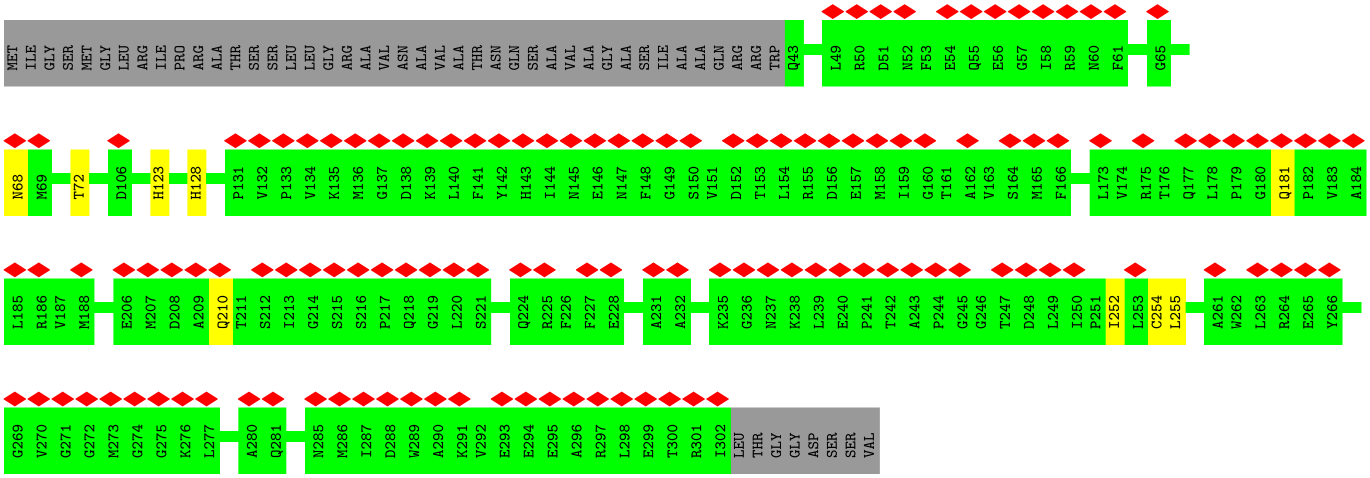
- Molecule 72: Protein FYV4, mitochondrial

Chain 33:



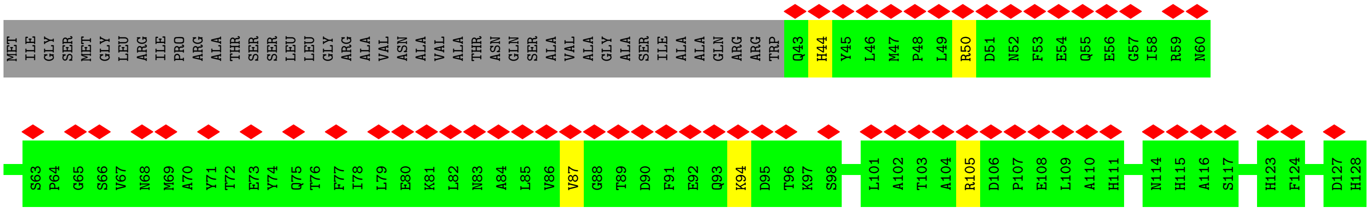
- Molecule 73: Manganese and iron superoxide dismutase

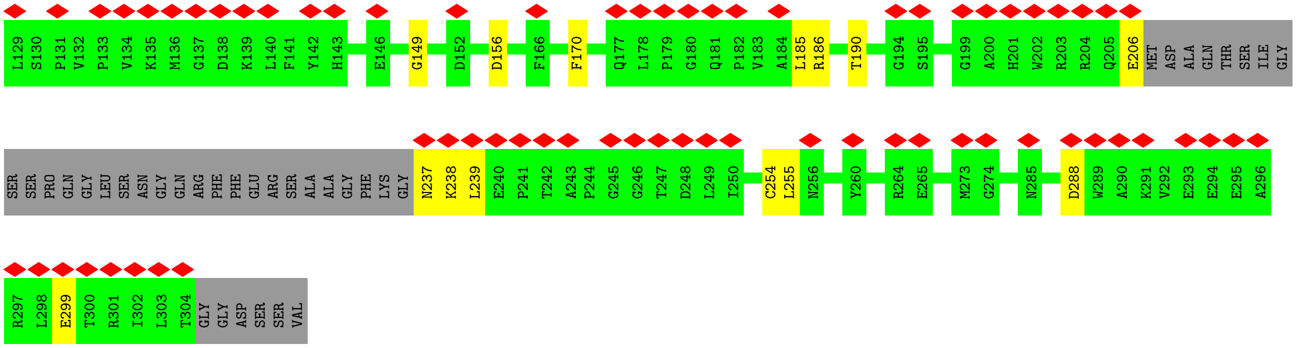
Chain 44:



- Molecule 73: Manganese and iron superoxide dismutase

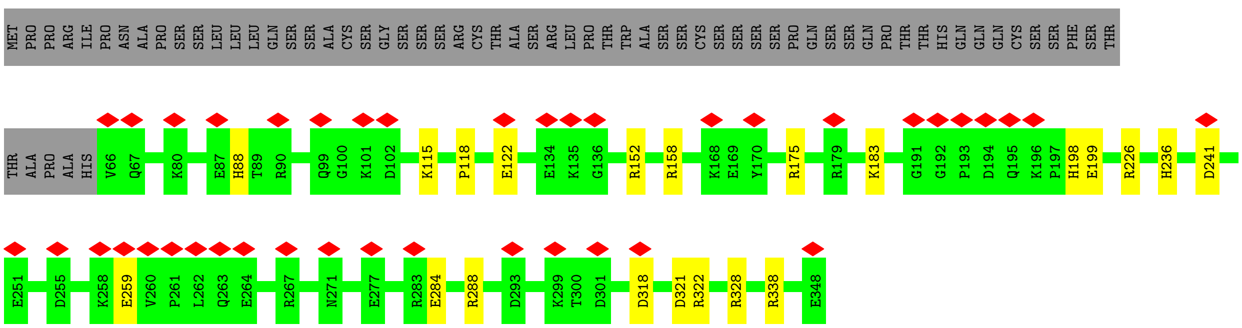
Chain 55:





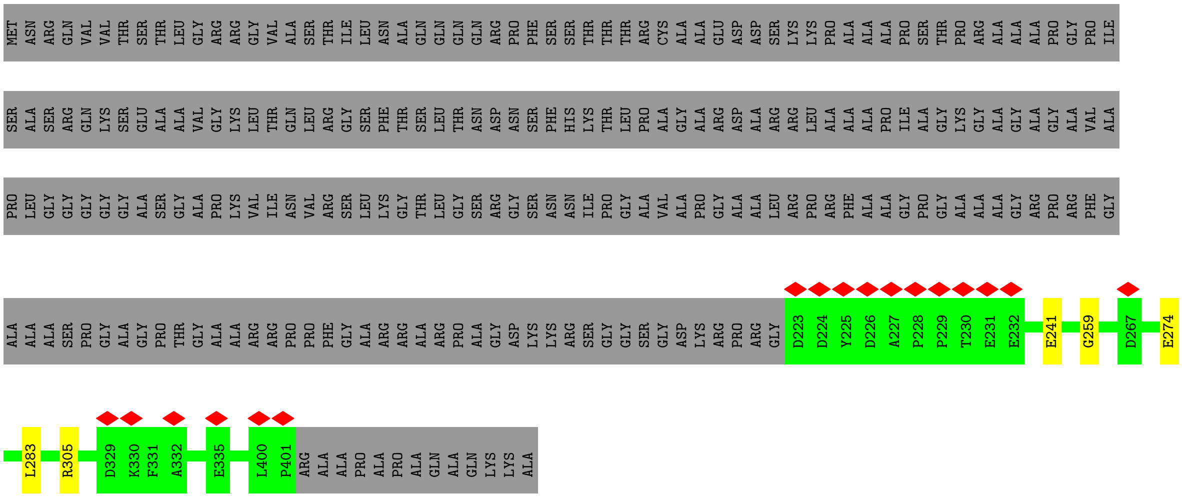
- Molecule 74: mS45

Chain 66:



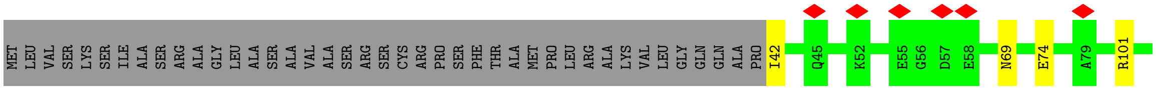
- Molecule 75: mS46

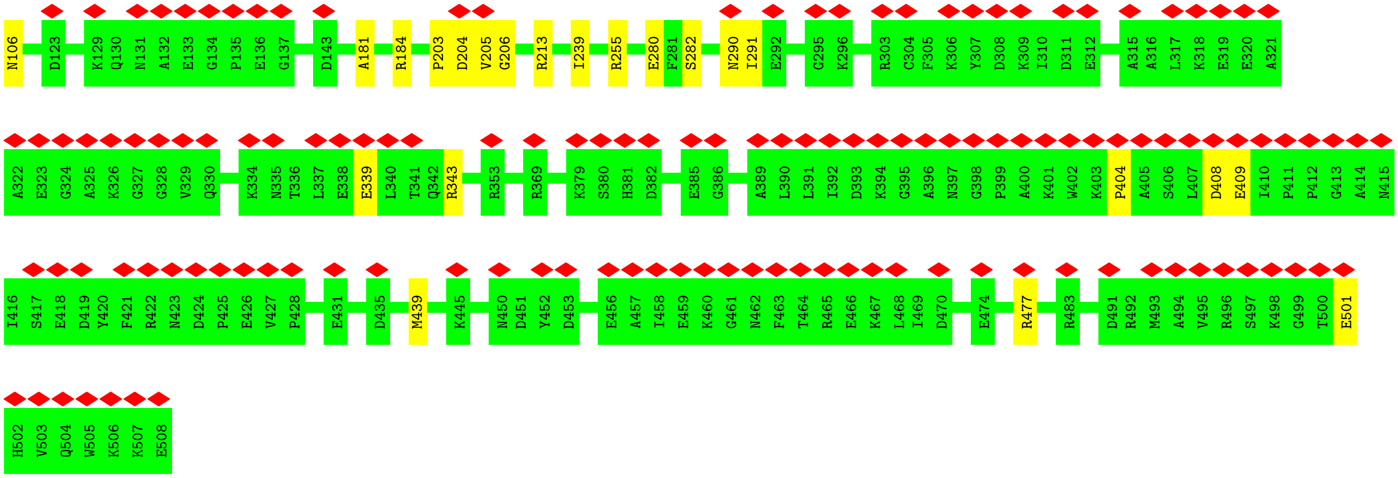
Chain 77:



- Molecule 76: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial

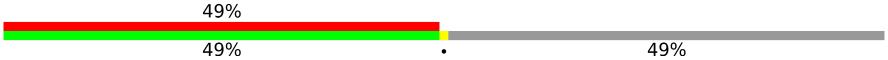
Chain 88:

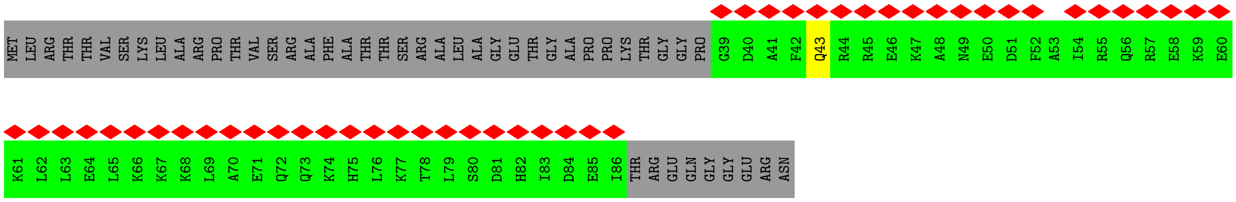




- Molecule 77: IF1

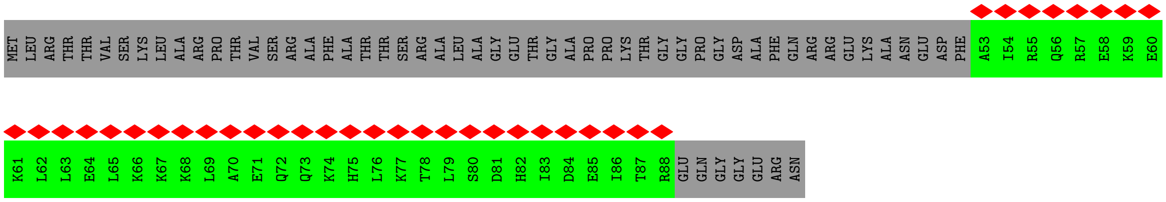
Chain 00:





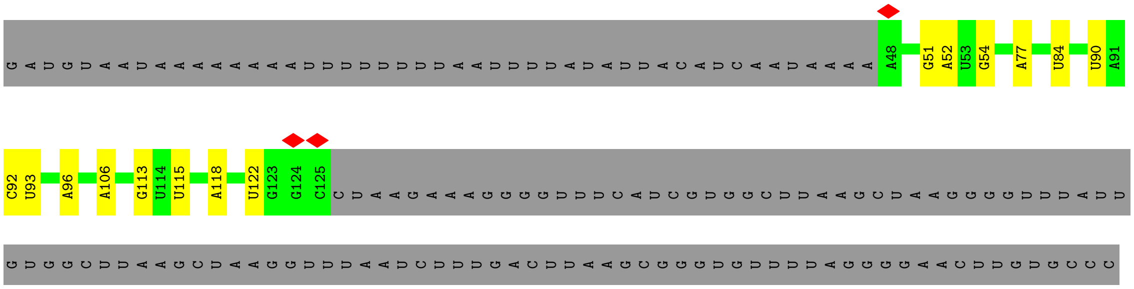
- Molecule 77: IF1

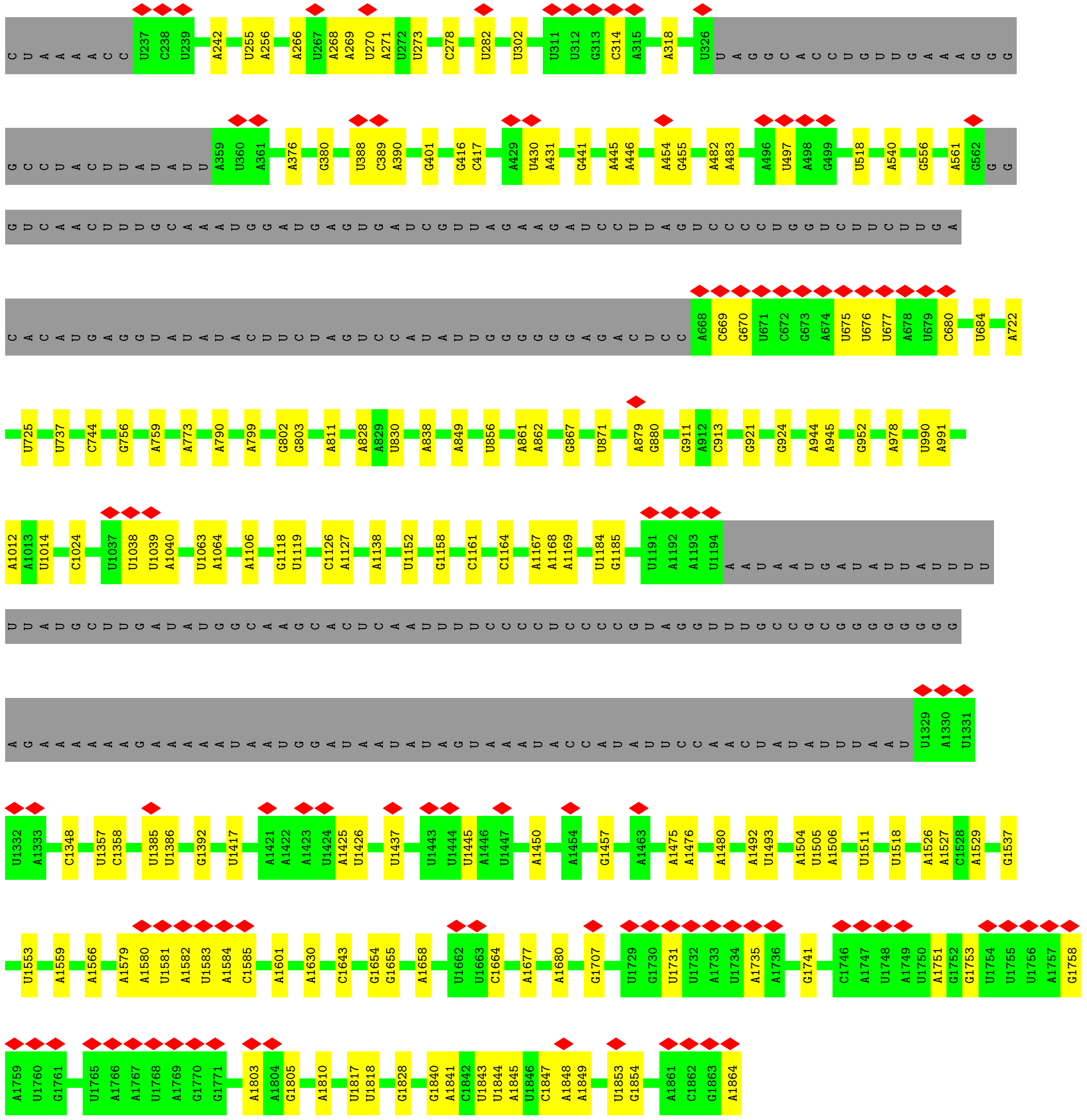
Chain 99:



- Molecule 78: 16S rRNA

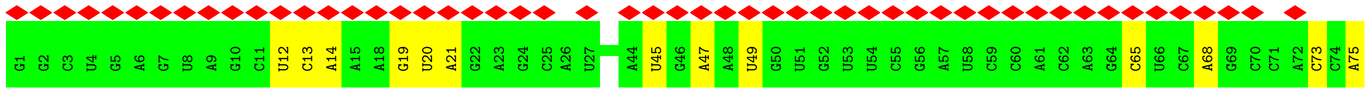
Chain aa:





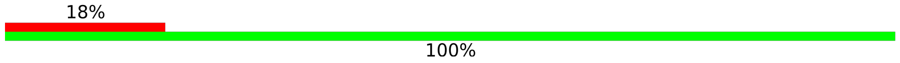
- Molecule 79: P-site-tRNA

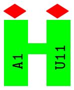
Chain bb:



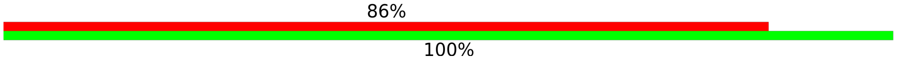
- Molecule 80: mRNA

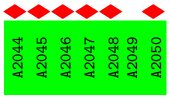
Chain ee:



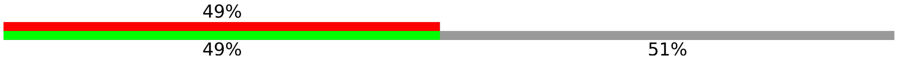

A1 U11

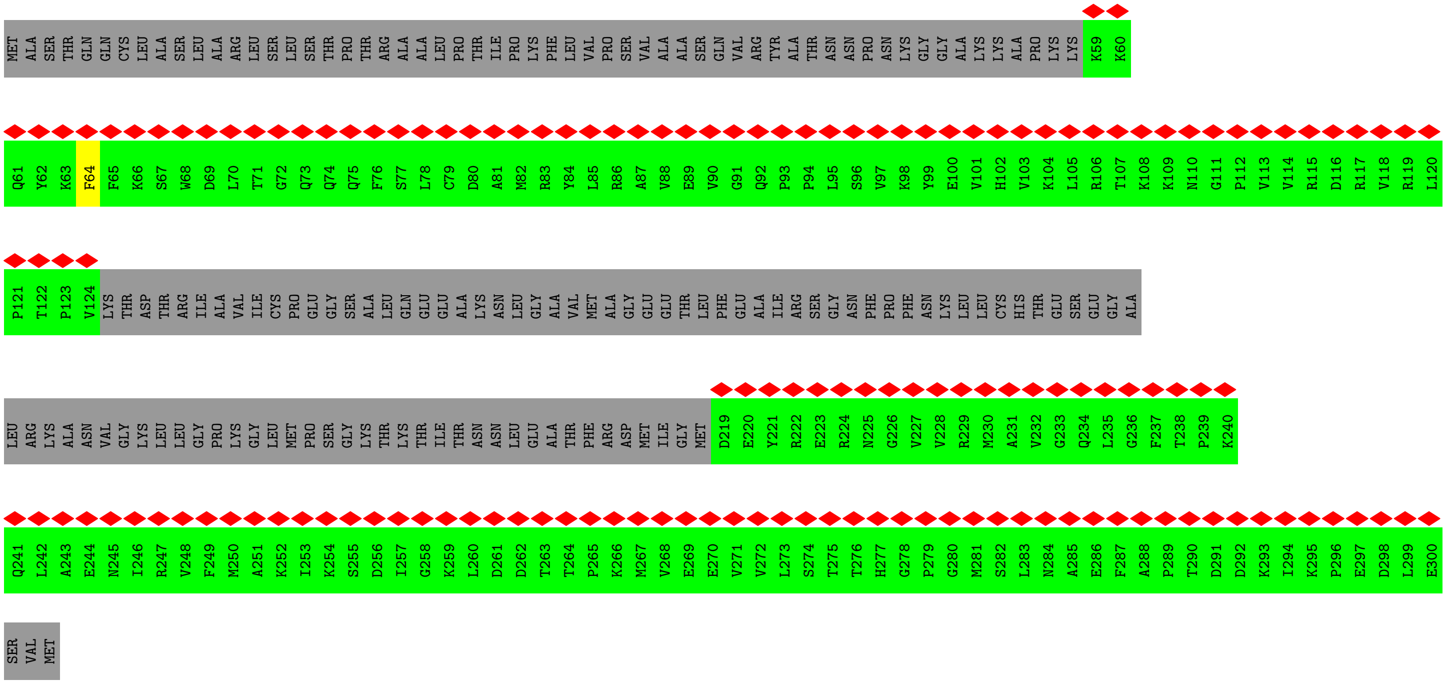
- Molecule 81: Poly-Peptide

Chain cc:



A2044 A2045 A2046 A2047 A2048 A2049 A2050

- Molecule 82: 60S ribosomal protein L1, mitochondrial

Chain e:



MET ALA SER THR GLN GLN CYS LEU ALA SER LEU ALA ARG LEU SER LEU SER THR PRO THR ARG ALA ALA LEU PRO THR ILE PRO LYS PHE LEU VAL PRO SER VAL ALA ALA SER GLN VAL ARG TYR ALA THR ASN PRO ASN LYS GLY GLY ALA LYS LYS ALA PRO LYS LYS K59 K60

Q61 Y62 K63 F64 F65 K66 S67 W68 D69 L70 T71 G72 Q73 Q74 Q75 F76 S77 L78 C79 D80 A81 M82 R83 Y84 L85 R86 A87 V88 E89 V90 G91 Q92 P93 P94 L95 S96 V97 K98 Y99 E100 V101 H102 V103 K104 L105 R106 T107 K108 K109 N110 G111 P112 V113 V114 R115 D116 R117 V118 R119 L120

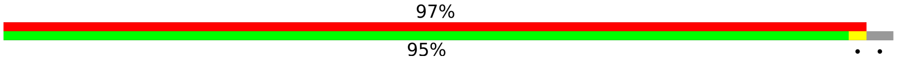
P121 T122 P123 V124 LYS THR ASP THR ARG ILE ALA VAL ILE CYS PRO GLU GLY SER ALA LEU GLN GLU GLU ALA LYS ASN LEU GLY ALA VAL MET ALA GLY GLU GLU THR LEU PHE GLU ALA ILE ARG SER GLY ASN PHE PRO PHE ASN LYS LEU LEU CYS HIS THR GLU SER GLU GLY ALA

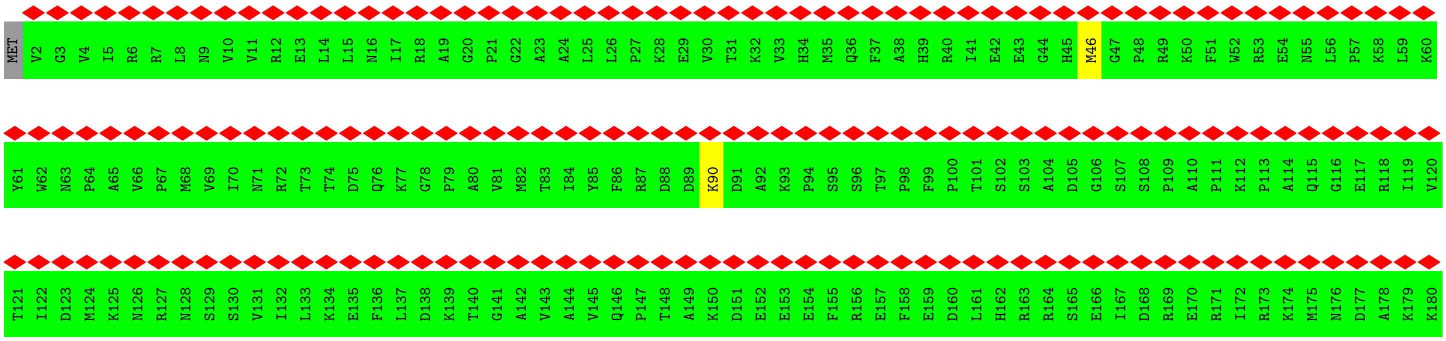
LEU ARG LYS ALA ASN VAL GLY LYS LEU LEU GLY PRO LYS GLY LEU MET PRO SER GLY LYS THR LYS THR ILE THR ASN LEU GLU ALA THR PHE ARG ASP MET ILE GLY MET D219 E220 Y221 R222 E223 R224 N225 G226 V227 V228 R229 M230 A231 V232 G233 Q234 L235 G236 F237 T238 P239 K240

Q241 L242 A243 E244 N245 I246 R247 V248 F249 M250 A251 K252 I253 K254 S255 D256 I257 G258 K259 L260 D261 D262 T263 T264 P265 K266 M267 V268 E269 E270 V271 V272 L273 S274 T275 I276 H277 G278 P279 G280 M281 S282 L283 N284 A285 E286 F287 A288 P289 T290 D291 D292 K293 I294 K295 P296 E297 D298 L299 E300

SER VAL MET

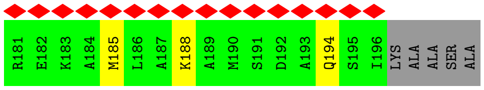
- Molecule 83: L51_S25_CI-B8 domain-containing protein

Chain j:



MET V2 G3 V4 I5 R6 R7 L8 N9 V10 V11 R12 E13 L14 L15 N16 I17 R18 A19 G20 P21 G22 A23 A24 L25 L26 P27 K28 E29 V30 T31 K32 V33 H34 M35 Q36 F37 A38 H39 R40 I41 E42 E43 G44 H45 M46 G47 P48 R49 K50 F51 W52 R53 E54 N55 L56 P57 K58 L59 K60

Y61 W62 N63 P64 A65 V66 P67 M68 V69 I70 N71 R72 T73 T74 D75 Q76 K77 G78 P79 A80 V81 M82 T83 I84 Y85 F86 R87 D88 D89 K90 D91 A92 K93 P94 S95 S96 T97 P98 F99 P100 T101 S102 S103 A104 D105 G106 S107 S108 P109 A110 P111 K112 P113 A114 Q115 G116 E117 R118 I119 V120

T121 I122 D123 M124 K125 N126 R127 N128 S129 S130 V131 I132 L133 K134 E135 F136 L137 D138 K139 T140 G141 A142 V143 A144 V145 Q146 P147 T148 A149 K150 D151 E152 E153 E154 F155 R156 E157 F158 E159 D160 L161 H162 R163 R164 S165 E166 I167 D168 R169 E170 R171 I172 R173 K174 M175 N176 D177 A178 K179 K180


R181
E182
K183
A184
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K188
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M190
S191
D192
A193
Q194
S195
I196
LYS
ALA
ALA
SER
ALA

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.193	Depositor
Minimum map value	-22.800	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.186	Depositor
Recommended contour level	4.77	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/67912	0.68	0/105757
2	B	0.26	0/2514	0.44	0/3388
3	C	0.27	0/2380	0.44	0/3209
4	D	0.25	0/2072	0.40	0/2794
5	E	0.25	0/2518	0.40	0/3427
6	F	0.25	0/1644	0.41	0/2218
7	G	0.24	0/630	0.44	0/842
8	f	0.24	0/1923	0.39	0/2631
9	g	0.24	0/1126	0.41	0/1525
10	H	0.27	0/1460	0.42	0/1975
11	I	0.26	0/918	0.45	0/1225
12	J	0.26	0/1931	0.42	0/2597
13	K	0.27	0/1376	0.42	0/1842
14	L	0.25	0/1569	0.39	0/2106
15	M	0.25	0/1572	0.41	0/2117
16	N	0.27	0/1077	0.44	0/1452
17	O	0.25	0/2248	0.40	0/3015
18	P	0.26	0/1523	0.40	0/2058
19	Q	0.24	0/2916	0.39	0/3927
20	R	0.25	0/2083	0.40	0/2789
21	S	0.25	0/1510	0.40	0/2042
22	T	0.23	0/1538	0.38	0/2086
23	U	0.25	0/1117	0.42	0/1496
24	V	0.24	0/766	0.40	0/1034
25	W	0.25	0/467	0.41	0/616
26	X	0.27	0/411	0.43	0/551
27	Y	0.26	0/368	0.44	0/485
28	0	0.27	0/395	0.46	0/523
29	1	0.25	0/3053	0.39	0/4108
30	2	0.24	0/1074	0.37	0/1449
31	3	0.27	0/783	0.42	0/1056
32	4	0.27	0/1077	0.41	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	5	0.25	0/2790	0.39	0/3794
34	6	0.25	0/2274	0.40	0/3062
35	7	0.25	0/686	0.42	0/919
36	8	0.24	0/2714	0.38	0/3657
37	h	0.25	0/791	0.37	0/1065
38	i	0.23	0/989	0.37	0/1324
39	9	0.24	0/1678	0.38	0/2267
40	a	0.24	0/1364	0.39	0/1842
41	b	0.24	0/1348	0.37	0/1816
42	c	0.27	0/846	0.40	0/1134
43	d	0.24	0/1930	0.40	0/2597
44	AA	0.25	0/2948	0.40	0/3995
45	BB	0.25	0/2314	0.40	0/3142
46	CC	0.27	0/3712	0.40	0/4978
47	DD	0.28	0/2408	0.39	0/3255
48	EE	0.26	0/2928	0.41	0/3947
49	FF	0.25	0/952	0.42	0/1285
50	GG	0.25	0/1765	0.39	0/2392
51	HH	0.27	0/1259	0.42	0/1707
52	II	0.26	0/2012	0.40	0/2720
53	JJ	0.28	0/1590	0.39	0/2140
54	KK	0.26	0/1015	0.43	0/1357
55	LL	0.27	0/973	0.44	0/1305
56	MM	0.25	0/950	0.41	0/1274
57	NN	0.27	0/929	0.40	0/1243
58	OO	0.24	0/2242	0.38	0/3016
59	PP	0.28	0/806	0.43	0/1096
60	QQ	0.25	0/1268	0.39	0/1701
61	RR	0.25	0/1105	0.38	0/1491
62	SS	0.26	0/667	0.42	0/902
63	TT	0.25	0/761	0.37	0/1015
64	UU	0.25	0/1890	0.37	0/2554
65	VV	0.24	0/2120	0.37	0/2851
66	WW	0.24	0/2897	0.36	0/3911
67	XX	0.26	0/3234	0.40	0/4374
68	YY	0.25	0/797	0.39	0/1070
69	ZZ	0.25	0/2645	0.38	0/3566
70	11	0.24	0/686	0.36	0/929
71	22	0.24	0/301	0.39	0/388
72	33	0.26	0/1573	0.43	0/2119
73	44	0.24	0/2121	0.38	0/2879
73	55	0.24	0/1912	0.38	0/2600
74	66	0.26	0/2348	0.38	0/3163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	77	0.27	0/1431	0.39	0/1934
76	88	0.25	0/3760	0.39	0/5085
77	00	0.22	0/409	0.33	0/540
77	99	0.22	0/307	0.33	0/405
78	aa	0.25	0/34270	0.68	0/53383
79	bb	0.15	0/1741	0.65	0/2708
80	ee	0.17	0/254	0.70	0/392
81	cc	0.25	0/34	0.35	0/46
82	e	0.24	0/1206	0.40	0/1624
83	j	0.24	0/1583	0.41	0/2130
All	All	0.25	0/231484	0.55	0/333882

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60640	30416	30431	128	0
2	B	2456	2508	2508	11	0
3	C	2336	2421	2420	13	0
4	D	2028	2040	2040	6	0
5	E	2449	2461	2461	10	0
6	F	1608	1645	1645	2	0
7	G	618	627	627	2	0
8	f	1876	1925	1925	0	0
9	g	1103	1154	1154	0	0
10	H	1426	1459	1459	5	0
11	I	913	985	985	4	0
12	J	1888	1939	1939	6	0
13	K	1350	1401	1401	6	0
14	L	1545	1590	1590	5	0
15	M	1536	1628	1628	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	1056	1120	1120	5	0
17	O	2209	2323	2323	11	0
18	P	1481	1494	1494	4	0
19	Q	2868	2961	2961	14	0
20	R	2046	2149	2149	7	0
21	S	1472	1507	1507	8	0
22	T	1497	1453	1453	9	0
23	U	1099	1164	1164	5	0
24	V	750	735	735	5	0
25	W	460	489	488	4	0
26	X	403	433	433	2	0
27	Y	365	412	412	3	0
28	0	388	409	409	0	0
29	1	2985	3029	3029	13	0
30	2	1046	1055	1055	4	0
31	3	763	773	773	3	0
32	4	1052	1087	1087	4	0
33	5	2719	2710	2710	10	0
34	6	2226	2248	2248	6	0
35	7	674	709	709	4	0
36	8	2660	2714	2714	8	0
37	h	779	798	798	0	0
38	i	976	1022	1022	0	0
39	9	1643	1698	1698	6	0
40	a	1331	1340	1340	0	0
41	b	1314	1379	1379	0	0
42	c	827	873	873	0	0
43	d	1888	1909	1909	0	0
44	AA	2883	2907	2907	19	0
45	BB	2269	2301	2301	13	0
46	CC	3641	3897	3897	11	0
47	DD	2342	2373	2373	17	0
48	EE	2880	2918	2918	15	0
49	FF	935	966	966	6	0
50	GG	1724	1799	1799	7	0
51	HH	1235	1286	1286	3	0
52	II	1968	2026	2026	7	0
53	JJ	1551	1554	1554	7	0
54	KK	995	1025	1025	5	0
55	LL	959	1032	1032	5	0
56	MM	937	986	986	5	0
57	NN	914	961	961	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	OO	2198	2230	2230	4	0
59	PP	786	826	826	1	0
60	QQ	1247	1314	1314	2	0
61	RR	1080	1089	1089	3	0
62	SS	648	677	677	1	0
63	TT	746	772	772	3	0
64	UU	1844	1843	1842	11	0
65	VV	2080	2112	2112	14	0
66	WW	2843	2901	2900	7	0
67	XX	3175	3271	3271	10	0
68	YY	786	823	823	2	0
69	ZZ	2586	2528	2528	13	0
70	11	672	686	686	1	0
71	22	301	359	359	0	0
72	33	1539	1595	1595	4	0
73	44	2062	1983	1982	7	0
73	55	1858	1794	1793	11	0
74	66	2298	2330	2330	17	0
75	77	1400	1396	1396	3	0
76	88	3677	3650	3650	14	0
77	00	406	417	417	1	0
77	99	306	333	333	0	0
78	aa	30608	15373	15377	0	0
79	bb	1557	789	790	0	0
80	ee	229	115	115	0	0
81	cc	35	34	34	0	0
82	e	1184	1212	1212	0	0
83	j	1553	1586	1586	0	0
84	00	1	0	0	0	0
84	A	144	0	0	0	0
84	BB	1	0	0	0	0
84	K	1	0	0	0	0
84	KK	1	0	0	0	0
84	L	1	0	0	0	0
84	QQ	1	0	0	0	0
84	XX	1	0	0	0	0
84	YY	1	0	0	0	0
84	aa	97	0	0	0	0
84	ee	1	0	0	0	0
85	A	14	26	26	0	0
86	2	1	0	0	0	0
86	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	88	1	0	0	0	0
86	A	32	0	0	0	0
86	ZZ	1	0	0	0	0
86	aa	13	0	0	0	0
87	0	1	0	0	0	0
87	W	1	0	0	0	0
88	2	44	26	26	3	0
89	XX	31	12	12	2	0
All	All	218076	174325	174339	473	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:NN:75:ARG:NH1	57:NN:80:GLY:O	2.08	0.86
67:XX:152:ARG:NH1	67:XX:415:LYS:O	2.09	0.85
1:A:2337:U:O2'	1:A:2339:U:OP1	1.96	0.83
69:ZZ:212:ARG:NH1	69:ZZ:257:GLU:OE1	2.12	0.82
57:NN:22:ASP:OD2	57:NN:26:ARG:NH1	2.12	0.82
1:A:3094:A:OP1	10:H:94:ARG:NH1	2.14	0.81
14:L:136:ARG:NH1	25:W:95:PRO:O	2.13	0.81
47:DD:407:ARG:NH1	74:66:198:HIS:O	2.14	0.81
1:A:2757:G:OP2	30:2:285:ARG:NH1	2.15	0.80
5:E:268:ARG:NH2	5:E:308:GLU:OE1	2.14	0.80
1:A:445:A:OP2	19:Q:324:ARG:NH2	2.16	0.79
1:A:3452:A:OP2	33:5:218:ARG:NH1	2.17	0.78
33:5:146:LEU:O	39:9:140:ARG:NH2	2.18	0.77
46:CC:478:ARG:NH1	57:NN:101:LEU:O	2.17	0.77
1:A:29:A:O3'	3:C:78:ARG:NH1	2.17	0.77
5:E:343:GLN:OE1	30:2:345:SER:OG	2.03	0.76
1:A:2797:C:OP1	26:X:39:LYS:NZ	2.18	0.76
14:L:58:ARG:O	14:L:86:ARG:NH1	2.19	0.76
67:XX:180:ARG:O	67:XX:182:THR:N	2.19	0.76
74:66:284:GLU:OE2	74:66:288:ARG:NH2	2.20	0.76
21:S:93:THR:OG1	21:S:140:ARG:NH1	2.19	0.75
29:1:219:PHE:O	29:1:340:ARG:NH1	2.19	0.75
58:OO:130:LEU:O	65:VV:221:ARG:NH1	2.18	0.75
64:UU:150:ASP:OD1	64:UU:153:ARG:NH2	2.20	0.74
15:M:232:VAL:O	66:WW:96:GLN:NE2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:DD:126:ARG:NH2	48:EE:472:TYR:O	2.21	0.74
1:A:2481:G:O2'	1:A:2483:G:OP2	2.05	0.73
33:5:229:ASP:OD1	33:5:233:ASP:N	2.21	0.73
19:Q:164:GLN:NE2	19:Q:169:LYS:O	2.21	0.73
47:DD:80:ASN:O	47:DD:126:ARG:NH1	2.20	0.73
44:AA:168:LEU:O	65:VV:303:ARG:NH1	2.21	0.73
50:GG:165:ASN:OD1	50:GG:168:ARG:NH2	2.22	0.72
1:A:2536:A:OP1	20:R:262:ARG:NH1	2.23	0.71
5:E:268:ARG:NH1	24:V:62:GLN:OE1	2.23	0.71
48:EE:147:ARG:NH2	75:77:241:GLU:O	2.24	0.70
1:A:2925:A:OP2	1:A:2926:C:N4	2.24	0.70
1:A:3334:C:OP1	3:C:217:ARG:NH1	2.25	0.70
29:1:375:ARG:NH1	29:1:376:GLU:OE2	2.25	0.70
1:A:1291:A:N6	1:A:1358:A:OP2	2.25	0.70
1:A:2008:U:OP2	1:A:2013:A:N6	2.22	0.70
46:CC:333:LEU:O	48:EE:82:LYS:NZ	2.24	0.69
1:A:2276:U:OP1	3:C:63:VAL:N	2.25	0.69
49:FF:76:GLU:OE1	49:FF:79:ARG:NH1	2.25	0.69
46:CC:343:ASN:ND2	53:JJ:87:SER:O	2.26	0.69
29:1:292:ARG:NH2	29:1:368:ASN:OD1	2.25	0.69
1:A:3363:A:O2'	1:A:3365:A:OP2	2.11	0.69
49:FF:112:ARG:NH1	65:VV:278:GLU:OE1	2.24	0.69
1:A:2153:G:OP2	1:A:2153:G:N2	2.25	0.68
45:BB:209:ARG:NH2	76:88:280:GLU:OE2	2.25	0.68
1:A:831:U:OP1	1:A:854:A:O2'	2.12	0.68
54:KK:324:GLU:OE1	54:KK:355:ARG:NH1	2.27	0.67
51:HH:15:ASN:OD1	51:HH:18:ARG:NH2	2.28	0.67
45:BB:359:GLN:OE1	45:BB:362:ARG:NH2	2.27	0.67
1:A:2951:U:O2'	1:A:2955:U:OP1	2.12	0.67
29:1:105:GLU:O	29:1:116:ARG:NH1	2.27	0.67
17:O:364:TRP:O	32:4:125:ARG:NH1	2.28	0.67
1:A:2512:A:OP2	29:1:182:ARG:NH2	2.27	0.67
47:DD:186:GLY:O	74:66:158:ARG:NH1	2.27	0.66
48:EE:318:LEU:O	48:EE:413:ARG:NH2	2.29	0.66
48:EE:129:TYR:OH	53:JJ:122:ARG:NH1	2.29	0.66
29:1:267:ASP:OD1	29:1:271:ARG:NH2	2.29	0.65
55:LL:129:ARG:NH2	55:LL:130:GLY:O	2.29	0.65
76:88:42:ILE:O	76:88:101:ARG:NH2	2.29	0.65
51:HH:63:THR:OG1	76:88:74:GLU:OE2	2.14	0.65
1:A:3033:G:N2	1:A:3033:G:OP2	2.30	0.64
1:A:1271:A:OP1	1:A:1382:C:O2'	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:A:OP1	2:B:314:ARG:NH1	2.30	0.64
1:A:3166:U:O2'	15:M:163:ASP:OD2	2.15	0.64
35:7:111:GLN:NE2	35:7:147:GLU:OE2	2.30	0.64
69:ZZ:212:ARG:O	69:ZZ:262:ASN:ND2	2.30	0.64
53:JJ:102:ARG:NH2	53:JJ:144:GLY:O	2.31	0.64
1:A:2492:A:O2'	1:A:2634:A:N6	2.31	0.63
44:AA:160:ARG:NH2	44:AA:262:ASP:OD1	2.31	0.63
67:XX:271:LEU:O	67:XX:275:ASN:ND2	2.31	0.63
1:A:2380:G:N1	1:A:2383:A:OP2	2.31	0.63
47:DD:407:ARG:NH2	74:66:118:PRO:O	2.32	0.63
2:B:280:ARG:NH2	2:B:364:LYS:O	2.32	0.63
1:A:2332:A:H4'	1:A:2332:A:OP1	1.98	0.63
32:4:81:ARG:NH1	32:4:107:GLY:O	2.32	0.62
73:44:181:GLN:N	73:44:181:GLN:OE1	2.33	0.62
73:44:68:ASN:ND2	73:44:72:THR:OG1	2.31	0.62
76:88:339:GLU:O	76:88:343:ARG:NH2	2.32	0.62
1:A:3366:U:O4	3:C:272:ARG:NH2	2.31	0.62
13:K:91:THR:O	13:K:134:ARG:NH1	2.32	0.62
6:F:169:ARG:NE	6:F:192:GLU:OE2	2.33	0.61
1:A:2584:U:O4	1:A:2585:A:N6	2.33	0.61
11:I:114:GLU:N	11:I:114:GLU:OE2	2.33	0.61
55:LL:134:GLN:N	55:LL:134:GLN:OE1	2.33	0.61
67:XX:184:LYS:NZ	89:XX:501:ATP:O1G	2.33	0.61
34:6:149:ARG:NH2	34:6:152:VAL:O	2.32	0.61
66:WW:129:ASN:OD1	66:WW:130:GLY:N	2.34	0.61
1:A:846:A:OP2	20:R:298:ARG:NH2	2.33	0.61
29:1:264:GLN:NE2	29:1:265:VAL:O	2.33	0.61
63:TT:149:GLN:N	63:TT:152:LEU:O	2.33	0.61
45:BB:231:ARG:NH2	52:II:99:GLU:OE2	2.34	0.61
17:O:241:LYS:NZ	19:Q:72:ASP:OD1	2.34	0.60
59:PP:70:ILE:O	65:VV:131:ARG:NH1	2.33	0.60
46:CC:368:SER:O	53:JJ:81:GLU:N	2.35	0.60
67:XX:323:ASN:OD1	67:XX:327:GLU:N	2.34	0.60
19:Q:147:GLU:OE1	19:Q:177:ARG:NH1	2.34	0.60
76:88:69:ASN:ND2	76:88:106:ASN:OD1	2.34	0.60
1:A:3111:G:N2	1:A:3114:A:OP2	2.34	0.59
64:UU:113:ASP:O	64:UU:120:GLN:NE2	2.34	0.59
65:VV:87:PRO:O	65:VV:146:LYS:NZ	2.34	0.59
1:A:1314:G:N2	1:A:1341:A:O2'	2.36	0.59
65:VV:121:GLU:OE1	65:VV:124:ARG:NH1	2.36	0.59
1:A:1634:G:OP1	21:S:120:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:II:298:ARG:NH1	52:II:299:LYS:O	2.36	0.59
1:A:537:U:O2’	31:3:13:ARG:NH1	2.36	0.59
34:6:266:GLU:OE1	34:6:274:ARG:NH2	2.35	0.59
45:BB:137:LEU:O	73:44:123:HIS:ND1	2.35	0.59
4:D:81:GLU:OE2	4:D:285:ARG:NE	2.36	0.59
34:6:197:SER:OG	34:6:199:ASP:OD1	2.18	0.59
45:BB:117:ILE:O	52:II:154:HIS:NE2	2.36	0.59
1:A:614:G:OP1	1:A:1528:U:O2’	2.21	0.58
1:A:473:G:N7	21:S:147:ARG:NH2	2.52	0.58
1:A:2332:A:C8	1:A:2332:A:H5”	2.38	0.58
23:U:142:ARG:NH1	36:8:388:LEU:O	2.37	0.58
47:DD:73:ARG:NH1	47:DD:450:LEU:O	2.37	0.57
33:5:204:TYR:OH	39:9:196:MET:O	2.22	0.57
47:DD:65:ARG:O	74:66:338:ARG:NH1	2.37	0.57
1:A:3389:G:O2’	1:A:3409:A:N6	2.37	0.57
17:O:278:GLU:OE2	17:O:280:ARG:NH2	2.37	0.57
49:FF:4:GLU:OE2	61:RR:171:ARG:NE	2.37	0.57
1:A:833:A:OP1	12:J:109:LYS:NZ	2.38	0.57
36:8:195:GLU:OE1	36:8:339:ARG:NE	2.37	0.57
1:A:2785:A:O2’	1:A:2786:A:OP2	2.22	0.57
19:Q:248:ASP:OD1	22:T:123:GLY:N	2.37	0.56
1:A:2540:C:OP2	20:R:323:ARG:NH2	2.36	0.56
1:A:2251:U:O2’	25:W:66:PRO:O	2.23	0.56
50:GG:291:THR:O	50:GG:294:ARG:NH2	2.33	0.56
57:NN:57:GLN:NE2	62:SS:16:PRO:O	2.38	0.56
76:88:184:ARG:NE	76:88:239:ILE:O	2.33	0.56
22:T:214:ASN:ND2	22:T:217:ASN:O	2.39	0.56
1:A:1565:A:O2’	1:A:1566:A:OP2	2.21	0.56
1:A:2687:G:OP2	29:1:292:ARG:NH1	2.38	0.56
10:H:8:THR:N	17:O:352:ASP:OD1	2.37	0.56
65:VV:93:GLU:OE2	65:VV:102:ARG:NH1	2.38	0.56
17:O:332:ARG:NH1	17:O:336:GLU:OE1	2.39	0.56
58:OO:152:ALA:O	58:OO:155:ARG:NH2	2.39	0.56
1:A:2635:A:O2’	1:A:2636:U:O3’	2.24	0.56
56:MM:10:ASN:OD1	56:MM:11:GLU:N	2.39	0.55
45:BB:144:ARG:NH2	64:UU:105:ASP:OD1	2.40	0.55
76:88:213:ARG:NH1	76:88:439:MET:O	2.38	0.55
1:A:822:U:N3	1:A:823:G:O6	2.39	0.55
69:ZZ:52:ASP:OD1	69:ZZ:52:ASP:N	2.38	0.55
14:L:103:GLU:O	14:L:113:SER:OG	2.23	0.55
17:O:206:ARG:NH1	25:W:80:MET:SD	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:AA:155:GLN:N	44:AA:155:GLN:OE1	2.39	0.55
49:FF:37:ASP:OD1	49:FF:38:ILE:N	2.40	0.55
76:88:204:ASP:O	76:88:206:GLY:N	2.40	0.55
53:JJ:169:GLU:OE1	57:NN:97:ARG:NH2	2.38	0.55
18:P:60:ASP:OD1	18:P:64:HIS:ND1	2.39	0.55
12:J:109:LYS:O	29:1:447:ARG:NH1	2.40	0.55
44:AA:306:TYR:OH	64:UU:94:GLU:OE2	2.24	0.55
64:UU:125:LEU:O	64:UU:160:ARG:NH2	2.39	0.55
76:88:290:ASN:OD1	76:88:291:ILE:N	2.40	0.55
27:Y:137:ARG:NE	27:Y:140:ALA:O	2.40	0.54
66:WW:359:GLN:OE1	66:WW:363:ARG:NH1	2.40	0.54
10:H:14:ARG:NH1	10:H:67:ASP:O	2.40	0.54
36:8:163:ASP:OD2	36:8:167:GLN:NE2	2.41	0.54
44:AA:308:ARG:NH2	73:55:156:ASP:OD2	2.41	0.54
73:44:254:CYS:SG	73:44:255:LEU:N	2.81	0.54
1:A:1178:U:O2	1:A:1178:U:C2’	2.56	0.54
76:88:181:ALA:O	76:88:184:ARG:NH1	2.41	0.54
1:A:1014:G:O2’	12:J:85:GLN:OE1	2.26	0.54
44:AA:298:THR:OG1	44:AA:299:HIS:N	2.41	0.54
60:QQ:94:ALA:O	60:QQ:101:ARG:NH2	2.40	0.54
1:A:2362:A:N1	1:A:2374:A:O2’	2.40	0.53
30:2:299:GLU:OE2	88:2:4301:NAD:O2D	2.26	0.53
63:TT:165:TYR:O	63:TT:170:GLN:NE2	2.41	0.53
22:T:171:GLU:OE1	22:T:171:GLU:N	2.40	0.53
49:FF:54:GLN:N	49:FF:54:GLN:OE1	2.41	0.53
74:66:321:ASP:O	74:66:328:ARG:NH1	2.39	0.53
55:LL:117:GLY:O	55:LL:145:ARG:NH2	2.41	0.53
69:ZZ:123:ARG:NH2	69:ZZ:142:ASP:OD1	2.41	0.53
19:Q:104:ARG:NH1	19:Q:143:ASN:O	2.42	0.53
69:ZZ:197:ARG:NH1	69:ZZ:217:GLU:OE2	2.41	0.53
1:A:2541:A:OP2	20:R:323:ARG:NH1	2.42	0.53
47:DD:39:SER:O	48:EE:316:LYS:NZ	2.41	0.53
1:A:645:U:O2’	1:A:821:A:N6	2.42	0.53
1:A:1461:G:OP1	12:J:77:THR:OG1	2.24	0.53
67:XX:279:GLU:N	67:XX:279:GLU:OE1	2.42	0.53
1:A:2090:A:N7	7:G:52:ALA:N	2.57	0.53
1:A:2919:G:O2’	1:A:2920:A:OP2	2.23	0.53
44:AA:315:ASN:N	64:UU:172:GLU:OE2	2.39	0.53
4:D:71:SER:O	4:D:75:LEU:N	2.38	0.53
11:I:101:ASP:OD2	11:I:122:LYS:NZ	2.40	0.52
46:CC:414:LYS:NZ	48:EE:139:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:VV:85:ILE:O	65:VV:94:LYS:NZ	2.41	0.52
46:CC:281:ASN:ND2	69:ZZ:131:GLU:OE1	2.43	0.52
1:A:311:G:O6	19:Q:219:ARG:NH1	2.40	0.52
18:P:185:ASN:ND2	19:Q:67:PRO:O	2.38	0.52
47:DD:429:GLY:O	74:66:115:LYS:NZ	2.43	0.52
1:A:2379:U:N3	1:A:2383:A:N7	2.58	0.52
17:O:327:GLU:OE2	17:O:330:ARG:NH1	2.42	0.52
5:E:130:ARG:NH1	88:2:4301:NAD:O1A	2.40	0.52
58:OO:235:ARG:O	65:VV:207:ARG:NH1	2.42	0.52
1:A:3263:U:O2'	22:T:54:THR:O	2.28	0.51
73:44:128:HIS:NE2	73:44:252:ILE:O	2.43	0.51
73:55:185:LEU:O	73:55:186:ARG:NH1	2.43	0.51
65:VV:120:GLN:N	65:VV:120:GLN:OE1	2.42	0.51
1:A:2346:U:OP1	1:A:2354:U:N3	2.43	0.51
2:B:326:ASP:OD1	2:B:326:ASP:N	2.43	0.51
17:O:51:GLN:O	17:O:56:ARG:NH1	2.39	0.51
44:AA:343:ASP:N	44:AA:343:ASP:OD1	2.43	0.51
57:NN:10:ASP:OD1	57:NN:10:ASP:N	2.44	0.51
24:V:127:ASP:OD1	24:V:127:ASP:N	2.44	0.51
39:9:149:ILE:O	39:9:153:THR:OG1	2.28	0.51
29:1:87:LEU:O	29:1:92:ARG:NH2	2.44	0.51
1:A:339:A:N6	31:3:24:LYS:O	2.43	0.50
1:A:2772:A:N6	1:A:2783:U:O4	2.44	0.50
1:A:3345:U:OP2	3:C:354:LYS:NZ	2.45	0.50
61:RR:142:PRO:O	61:RR:146:LYS:N	2.40	0.50
66:WW:206:ASP:O	66:WW:268:ARG:NH1	2.44	0.50
19:Q:208:ARG:N	19:Q:222:ARG:O	2.43	0.50
48:EE:236:THR:OG1	48:EE:237:GLY:N	2.44	0.50
69:ZZ:77:GLN:N	69:ZZ:77:GLN:OE1	2.45	0.50
1:A:2510:G:OP2	5:E:78:ARG:NH1	2.41	0.50
44:AA:188:ARG:NE	65:VV:310:GLU:O	2.45	0.50
1:A:875:C:OP1	4:D:118:ARG:NH2	2.41	0.50
1:A:608:A:OP2	16:N:188:ARG:NH1	2.42	0.50
1:A:2883:A:O2'	1:A:2884:A:P	2.69	0.50
33:5:432:ASP:OD1	33:5:433:MET:N	2.44	0.50
60:QQ:80:SER:OG	60:QQ:81:LYS:N	2.45	0.50
50:GG:254:LYS:NZ	50:GG:267:GLU:OE1	2.41	0.50
1:A:1071:G:O6	1:A:1099:A:N6	2.45	0.50
2:B:373:ASN:ND2	2:B:376:VAL:O	2.39	0.49
34:6:96:ARG:NH1	34:6:230:LEU:O	2.41	0.49
36:8:213:ALA:O	36:8:339:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:237:ARG:NH1	19:Q:73:GLU:OE1	2.43	0.49
5:E:143:ILE:HD12	5:E:143:ILE:O	2.13	0.49
74:66:88:HIS:NE2	74:66:183:LYS:O	2.43	0.49
48:EE:379:TYR:N	48:EE:383:THR:O	2.44	0.49
75:77:283:LEU:O	75:77:305:ARG:NH2	2.45	0.49
70:11:45:SER:OG	70:11:46:ALA:N	2.45	0.49
46:CC:442:ARG:NH2	46:CC:448:ARG:O	2.36	0.49
53:JJ:118:SER:OG	53:JJ:120:SER:O	2.31	0.49
44:AA:136:ARG:NH2	73:55:149:GLY:O	2.46	0.48
48:EE:287:ASP:OD1	48:EE:288:ASP:N	2.46	0.48
73:44:68:ASN:O	73:44:72:THR:OG1	2.26	0.48
1:A:2924:U:O4	1:A:2925:A:N6	2.47	0.48
75:77:259:GLY:N	75:77:274:GLU:OE2	2.42	0.48
1:A:1906:C:O2	3:C:241:HIS:NE2	2.43	0.48
73:44:210:GLN:OE1	73:55:105:ARG:NH1	2.46	0.48
1:A:1201:G:O6	13:K:76:LYS:NZ	2.47	0.48
44:AA:54:THR:HG23	64:UU:98:PRO:HB3	1.95	0.48
3:C:206:ASP:OD2	3:C:335:ARG:NH2	2.41	0.48
47:DD:197:LEU:O	47:DD:201:GLY:N	2.43	0.48
74:66:226:ARG:NH2	74:66:241:ASP:OD2	2.46	0.48
1:A:59:A:OP1	25:W:76:ARG:NE	2.42	0.48
1:A:1930:U:O2'	2:B:76:ARG:NH1	2.47	0.48
24:V:193:ASP:OD1	24:V:193:ASP:N	2.46	0.48
45:BB:205:ARG:NH2	76:88:282:SER:O	2.46	0.48
2:B:105:GLY:O	2:B:107:ARG:NH1	2.45	0.48
16:N:157:ALA:HB3	16:N:158:PRO:CD	2.43	0.48
26:X:15:ILE:N	26:X:51:LEU:O	2.46	0.48
33:5:346:ARG:O	39:9:65:ARG:NH2	2.46	0.48
64:UU:114:TRP:O	64:UU:133:ARG:NH2	2.43	0.48
1:A:1071:G:N3	1:A:1101:G:N2	2.61	0.48
22:T:149:GLU:OE1	22:T:152:ARG:NH2	2.47	0.48
48:EE:135:ASP:OD1	48:EE:136:ASP:N	2.46	0.48
48:EE:255:ASP:OD1	48:EE:255:ASP:N	2.47	0.48
5:E:157:ARG:NH2	5:E:183:PRO:O	2.42	0.48
33:5:89:HIS:NE2	33:5:98:ILE:O	2.46	0.48
48:EE:345:ASP:OD1	48:EE:378:ARG:NH1	2.47	0.48
72:33:227:LYS:HD3	72:33:228:ALA:N	2.29	0.48
74:66:318:ASP:OD1	74:66:318:ASP:N	2.47	0.48
1:A:577:A:N6	1:A:591:G:O2'	2.47	0.47
1:A:1221:G:HO2'	1:A:1402:A:HO2'	1.62	0.47
36:8:236:GLY:O	36:8:326:ILE:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:88:408:ASP:OD1	76:88:409:GLU:N	2.47	0.47
1:A:3047:G:N2	1:A:3050:A:OP2	2.36	0.47
30:2:326:GLU:OE2	30:2:332:ARG:NH1	2.47	0.47
33:5:106:THR:O	33:5:120:ASN:ND2	2.47	0.47
12:J:259:ARG:NH2	12:J:277:PRO:O	2.47	0.47
21:S:157:GLU:OE2	21:S:190:ARG:NH1	2.43	0.47
39:9:165:GLU:O	39:9:189:TYR:OH	2.31	0.47
1:A:1135:G:O2'	1:A:1136:A:OP2	2.29	0.47
45:BB:189:ARG:NH2	64:UU:76:ILE:O	2.47	0.47
47:DD:448:TRP:O	47:DD:452:ARG:N	2.46	0.47
77:00:43:GLN:N	77:00:43:GLN:OE1	2.48	0.47
19:Q:301:GLU:OE2	19:Q:301:GLU:N	2.48	0.47
68:YY:7:ARG:NH2	68:YY:10:GLN:OE1	2.47	0.47
73:55:44:HIS:NE2	73:55:94:LYS:O	2.47	0.47
1:A:96:G:OP2	18:P:93:ARG:NH1	2.42	0.47
1:A:2333:C:H2'	1:A:2334:G:O4'	2.14	0.47
1:A:541:G:N7	27:Y:135:ARG:NH1	2.51	0.46
14:L:33:GLU:OE1	14:L:80:LYS:NZ	2.44	0.46
69:ZZ:78:ASP:N	69:ZZ:78:ASP:OD1	2.49	0.46
69:ZZ:97:ASP:OD1	69:ZZ:98:LEU:N	2.48	0.46
1:A:1921:A:H2'	1:A:1921:A:N3	2.31	0.46
4:D:300:VAL:HG23	4:D:300:VAL:O	2.15	0.46
44:AA:151:ASP:O	44:AA:153:GLN:NE2	2.48	0.46
76:88:501:GLU:OE2	76:88:501:GLU:N	2.47	0.46
47:DD:55:ARG:NH2	47:DD:62:ILE:O	2.42	0.46
1:A:1178:U:O2	1:A:1178:U:H2'	2.16	0.46
20:R:336:THR:O	20:R:340:GLY:N	2.48	0.46
72:33:104:ARG:NH1	72:33:201:ASP:OD2	2.48	0.46
11:I:97:ASN:OD1	11:I:101:ASP:N	2.47	0.45
15:M:49:ARG:NH2	15:M:58:THR:OG1	2.46	0.45
54:KK:344:ASN:O	54:KK:347:ARG:NH2	2.46	0.45
1:A:1991:A:N3	1:A:1991:A:H2'	2.30	0.45
18:P:79:GLN:O	18:P:80:ARG:NH2	2.49	0.45
46:CC:135:ARG:NH2	69:ZZ:144:GLU:OE1	2.49	0.45
69:ZZ:59:ARG:NH1	69:ZZ:65:GLU:OE1	2.45	0.45
16:N:157:ALA:HB3	16:N:158:PRO:HD3	1.98	0.45
1:A:2402:G:H2'	1:A:2403:U:C6	2.52	0.45
16:N:137:ASP:OD2	23:U:86:ARG:NH2	2.50	0.45
46:CC:421:GLN:O	46:CC:425:ASN:ND2	2.50	0.45
1:A:3390:U:OP2	15:M:200:ARG:NH1	2.50	0.45
2:B:68:TYR:OH	2:B:80:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:101:MET:O	13:K:167:ASN:N	2.47	0.45
50:GG:274:GLU:OE1	50:GG:276:ARG:NE	2.47	0.45
66:WW:193:GLU:OE1	66:WW:332:ARG:NH2	2.48	0.45
24:V:193:ASP:O	24:V:197:GLY:N	2.47	0.45
56:MM:65:ILE:O	56:MM:65:ILE:HG22	2.17	0.45
58:OO:284:GLN:NE2	58:OO:316:GLY:O	2.50	0.45
3:C:91:SER:OG	10:H:113:LYS:O	2.35	0.45
21:S:106:ASN:N	21:S:115:THR:O	2.45	0.45
1:A:826:C:O2'	1:A:859:U:OP1	2.35	0.45
22:T:107:TYR:OH	22:T:149:GLU:OE2	2.31	0.45
22:T:157:ASN:OD1	22:T:160:ARG:NH1	2.37	0.45
47:DD:22:ASN:OD1	47:DD:24:TYR:N	2.48	0.45
17:O:53:VAL:O	17:O:57:ASN:ND2	2.50	0.44
35:7:141:VAL:N	35:7:142:PRO:CD	2.81	0.44
1:A:2492:A:H2'	1:A:2492:A:N3	2.32	0.44
1:A:3406:U:H3'	1:A:3407:U:H5"	2.00	0.44
23:U:130:ASP:OD1	23:U:131:GLY:N	2.50	0.44
5:E:58:ALA:O	29:1:116:ARG:NH2	2.51	0.44
1:A:1388:U:H4'	1:A:1389:A:O4'	2.18	0.44
22:T:216:GLU:OE2	22:T:216:GLU:N	2.47	0.44
73:55:206:GLU:N	73:55:238:LYS:O	2.51	0.44
1:A:930:U:HO2'	1:A:3063:U:HO2'	1.62	0.44
1:A:2170:G:N2	1:A:2199:G:OP1	2.51	0.44
1:A:2686:U:N3	29:1:290:PHE:O	2.49	0.44
13:K:103:ASP:OD1	13:K:103:ASP:N	2.51	0.44
36:8:228:VAL:O	36:8:228:VAL:HG12	2.18	0.44
13:K:103:ASP:OD2	13:K:106:ARG:NH1	2.51	0.44
14:L:37:THR:OG1	14:L:38:THR:N	2.51	0.44
16:N:99:LEU:O	16:N:105:HIS:NE2	2.49	0.44
50:GG:213:ARG:NH1	50:GG:215:TYR:OH	2.51	0.44
53:JJ:83:GLU:OE1	53:JJ:83:GLU:N	2.51	0.44
1:A:1178:U:O2	1:A:1178:U:H3'	2.17	0.44
1:A:1272:A:O2'	1:A:1381:A:N6	2.50	0.44
1:A:2028:G:O2'	2:B:277:GLU:OE2	2.32	0.44
2:B:172:ASP:N	2:B:291:ILE:O	2.47	0.44
56:MM:66:GLU:O	56:MM:69:ALA:N	2.40	0.44
1:A:615:G:O2'	1:A:2254:G:OP1	2.30	0.44
17:O:61:GLU:O	17:O:65:GLN:NE2	2.51	0.44
36:8:220:ASP:OD2	36:8:224:ARG:NE	2.46	0.44
44:AA:371:ASP:OD1	44:AA:371:ASP:N	2.51	0.44
45:BB:253:GLY:N	45:BB:309:GLU:OE1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:219:VAL:HG12	15:M:219:VAL:O	2.18	0.43
1:A:1475:G:N2	1:A:1513:U:O4	2.51	0.43
1:A:2227:G:N2	1:A:2231:C:O2'	2.52	0.43
46:CC:359:SER:O	46:CC:360:GLN:HB3	2.18	0.43
47:DD:93:GLU:OE1	47:DD:93:GLU:N	2.45	0.43
65:VV:73:PRO:O	74:66:322:ARG:NH1	2.46	0.43
1:A:1539:G:O2'	1:A:1540:U:OP2	2.34	0.43
3:C:322:GLU:OE2	3:C:322:GLU:N	2.51	0.43
50:GG:211:LYS:N	50:GG:229:GLN:O	2.49	0.43
65:VV:73:PRO:O	74:66:322:ARG:NH2	2.49	0.43
69:ZZ:85:GLU:HA	69:ZZ:85:GLU:OE1	2.18	0.43
73:55:50:ARG:NH2	73:55:288:ASP:OD2	2.51	0.43
4:D:181:ARG:NH1	4:D:278:THR:O	2.49	0.43
45:BB:299:ASN:OD1	45:BB:299:ASN:N	2.51	0.43
1:A:367:A:N3	1:A:367:A:H2'	2.33	0.43
1:A:909:A:O2'	1:A:910:A:P	2.77	0.43
52:II:154:HIS:O	52:II:158:LYS:N	2.50	0.43
67:XX:391:ARG:NH1	67:XX:400:ASP:OD1	2.45	0.43
4:D:246:ASP:OD1	4:D:248:ARG:NH2	2.52	0.43
1:A:3168:U:H4'	11:I:85:VAL:HG21	2.01	0.43
44:AA:258:GLY:O	44:AA:262:ASP:N	2.51	0.43
47:DD:138:ALA:N	47:DD:139:PRO:CD	2.81	0.43
54:KK:266:ASN:OD1	54:KK:267:THR:N	2.49	0.43
1:A:1082:C:O2	1:A:1092:G:N1	2.51	0.43
1:A:1221:G:O2'	1:A:1402:A:O2'	2.33	0.43
1:A:2940:G:N2	1:A:2942:U:O4	2.38	0.43
32:4:49:LEU:N	32:4:50:PRO:CD	2.81	0.43
49:FF:66:ARG:NH1	49:FF:115:GLU:OE1	2.50	0.43
1:A:640:G:OP1	35:7:94:ARG:NH1	2.52	0.42
1:A:2040:U:OP1	21:S:118:LYS:NZ	2.51	0.42
1:A:2807:A:O2'	1:A:2808:A:OP1	2.29	0.42
7:G:90:ASN:OD1	21:S:126:LYS:NZ	2.52	0.42
44:AA:248:ASN:OD1	44:AA:249:ASP:N	2.52	0.42
73:55:254:CYS:SG	73:55:255:LEU:N	2.91	0.42
29:1:284:ASP:OD1	29:1:286:THR:OG1	2.33	0.42
33:5:184:ASP:N	33:5:184:ASP:OD1	2.52	0.42
52:II:232:SER:O	52:II:265:THR:OG1	2.31	0.42
64:UU:51:ARG:NH1	64:UU:71:PHE:O	2.48	0.42
1:A:374:U:OP2	1:A:375:A:O2'	2.34	0.42
15:M:84:LYS:O	15:M:84:LYS:CG	2.67	0.42
24:V:62:GLN:NE2	24:V:78:MET:SD	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:AA:393:ASP:OD1	44:AA:397:ARG:N	2.52	0.42
45:BB:212:GLU:OE2	76:88:477:ARG:NH2	2.51	0.42
68:YY:15:ARG:NH1	69:ZZ:236:LYS:O	2.45	0.42
47:DD:407:ARG:O	74:66:152:ARG:NH1	2.44	0.42
1:A:2197:U:O2’	1:A:2199:G:OP2	2.27	0.42
1:A:342:U:OP1	31:3:16:ARG:NH1	2.52	0.42
6:F:181:VAL:O	6:F:181:VAL:HG13	2.20	0.42
54:KK:256:TYR:O	54:KK:324:GLU:N	2.50	0.42
56:MM:40:HIS:NE2	67:XX:217:GLU:OE1	2.52	0.42
66:WW:86:LYS:O	66:WW:90:HIS:ND1	2.51	0.42
1:A:2481:G:N3	1:A:2481:G:H2’	2.33	0.42
20:R:354:GLU:OE2	20:R:357:ARG:NH2	2.52	0.42
61:RR:143:TYR:O	61:RR:148:ARG:NH1	2.53	0.42
10:H:96:ASN:O	10:H:97:THR:OG1	2.33	0.42
15:M:144:ARG:O	15:M:145:ARG:HG2	2.19	0.42
21:S:159:LEU:O	21:S:178:ARG:NH1	2.53	0.42
54:KK:360:THR:O	63:TT:162:ARG:NH1	2.49	0.42
1:A:2040:U:O2’	1:A:2041:A:OP2	2.30	0.41
1:A:2925:A:O2’	1:A:2926:C:O4’	2.36	0.41
12:J:60:TYR:O	12:J:61:HIS:ND1	2.53	0.41
55:LL:114:PRO:O	55:LL:145:ARG:NE	2.44	0.41
73:55:170:PHE:O	73:55:190:THR:OG1	2.37	0.41
1:A:30:U:O2	3:C:81:GLN:NE2	2.53	0.41
1:A:536:G:N2	1:A:539:A:OP2	2.38	0.41
3:C:78:ARG:O	3:C:81:GLN:NE2	2.51	0.41
34:6:96:ARG:NH2	34:6:236:LYS:O	2.51	0.41
45:BB:322:ASP:OD1	45:BB:323:THR:N	2.48	0.41
46:CC:342:ASN:OD1	46:CC:343:ASN:N	2.53	0.41
67:XX:180:ARG:C	67:XX:182:THR:H	2.21	0.41
1:A:2265:C:O2	1:A:2950:C:H5”	2.20	0.41
23:U:40:GLU:OE2	23:U:42:GLN:NE2	2.47	0.41
44:AA:54:THR:HG22	44:AA:82:PRO:O	2.20	0.41
48:EE:139:GLU:OE2	48:EE:141:GLN:NE2	2.53	0.41
1:A:2468:A:H4’	1:A:2469:A:O5’	2.20	0.41
35:7:110:THR:OG1	35:7:150:GLY:O	2.27	0.41
36:8:398:VAL:O	36:8:398:VAL:HG23	2.20	0.41
20:R:290:ARG:O	20:R:297:TYR:HA	2.19	0.41
1:A:1719:A:OP1	2:B:307:ARG:NH1	2.50	0.41
1:A:1863:U:OP1	22:T:57:ASN:ND2	2.53	0.41
3:C:164:GLU:OE2	3:C:164:GLU:N	2.53	0.41
50:GG:90:THR:N	50:GG:93:ASN:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:33:76:THR:OG1	72:33:77:TRP:N	2.54	0.41
1:A:975:A:OP1	27:Y:95:GLY:N	2.52	0.41
19:Q:105:VAL:O	19:Q:105:VAL:HG12	2.21	0.41
88:2:4301:NAD:O5D	88:2:4301:NAD:H2N	2.20	0.41
66:WW:211:GLU:O	66:WW:215:ALA:N	2.48	0.41
67:XX:185:SER:OG	89:XX:501:ATP:O2B	2.39	0.41
74:66:122:GLU:OE1	74:66:175:ARG:NH2	2.54	0.41
3:C:243:ASN:ND2	3:C:246:ASN:O	2.52	0.41
19:Q:72:ASP:OD1	19:Q:73:GLU:N	2.44	0.41
34:6:220:GLU:OE1	34:6:220:GLU:N	2.51	0.41
44:AA:151:ASP:N	44:AA:151:ASP:OD1	2.53	0.41
52:II:186:ASP:OD1	52:II:187:GLN:N	2.49	0.41
1:A:16:A:O3'	39:9:134:ARG:NH1	2.54	0.41
1:A:319:C:O2	19:Q:219:ARG:NH2	2.54	0.41
1:A:571:A:N6	1:A:2255:A:H4'	2.36	0.41
1:A:1154:U:OP2	13:K:88:LYS:NZ	2.44	0.41
5:E:62:SER:OG	5:E:63:GLU:N	2.53	0.41
56:MM:22:PHE:HB3	56:MM:65:ILE:HG22	2.03	0.41
73:55:87:VAL:O	73:55:87:VAL:HG13	2.21	0.41
74:66:152:ARG:NE	74:66:199:GLU:OE1	2.46	0.41
1:A:1167:A:OP2	23:U:18:ARG:NH1	2.54	0.41
51:HH:132:CYS:N	51:HH:160:VAL:O	2.53	0.41
47:DD:61:HIS:NE2	47:DD:145:ASP:OD2	2.50	0.40
1:A:1136:A:O2'	1:A:1137:U:OP2	2.30	0.40
2:B:147:ASP:OD2	2:B:150:ARG:NE	2.53	0.40
32:4:132:HIS:NE2	33:5:382:GLU:OE2	2.54	0.40
45:BB:274:ASP:OD1	45:BB:362:ARG:NH1	2.54	0.40
55:LL:90:LYS:HB2	55:LL:91:PRO:HD3	2.03	0.40
52:II:304:VAL:N	52:II:308:LYS:O	2.53	0.40
1:A:2105:A:H2'	1:A:2105:A:N3	2.36	0.40
1:A:2510:G:OP1	5:E:74:ARG:NH2	2.48	0.40
65:VV:66:GLN:NE2	74:66:236:HIS:O	2.54	0.40
73:55:237:ASN:OD1	73:55:239:LEU:N	2.54	0.40
74:66:259:GLU:OE1	74:66:259:GLU:N	2.54	0.40
1:A:2828:G:N2	1:A:2831:A:OP2	2.51	0.40
44:AA:298:THR:OG1	64:UU:90:ASP:O	2.38	0.40
48:EE:368:LEU:O	48:EE:372:ASN:ND2	2.54	0.40
72:33:158:VAL:O	72:33:163:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

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	B	311/383 (81%)	304 (98%)	7 (2%)	0	100	100
3	C	305/384 (79%)	300 (98%)	5 (2%)	0	100	100
4	D	250/325 (77%)	248 (99%)	2 (1%)	0	100	100
5	E	307/352 (87%)	303 (99%)	4 (1%)	0	100	100
6	F	199/255 (78%)	197 (99%)	2 (1%)	0	100	100
7	G	72/300 (24%)	72 (100%)	0	0	100	100
8	f	243/347 (70%)	240 (99%)	3 (1%)	0	100	100
9	g	145/158 (92%)	142 (98%)	3 (2%)	0	100	100
10	H	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
11	I	115/131 (88%)	113 (98%)	2 (2%)	0	100	100
12	J	241/312 (77%)	236 (98%)	5 (2%)	0	100	100
13	K	166/249 (67%)	166 (100%)	0	0	100	100
14	L	190/193 (98%)	189 (100%)	1 (0%)	0	100	100
15	M	192/258 (74%)	188 (98%)	4 (2%)	0	100	100
16	N	131/217 (60%)	125 (95%)	6 (5%)	0	100	100
17	O	268/364 (74%)	267 (100%)	1 (0%)	0	100	100
18	P	178/228 (78%)	178 (100%)	0	0	100	100
19	Q	351/396 (89%)	350 (100%)	1 (0%)	0	100	100
20	R	245/447 (55%)	240 (98%)	5 (2%)	0	100	100
21	S	175/274 (64%)	172 (98%)	3 (2%)	0	100	100
22	T	178/263 (68%)	177 (99%)	1 (1%)	0	100	100
23	U	134/161 (83%)	134 (100%)	0	0	100	100
24	V	88/219 (40%)	88 (100%)	0	0	100	100
25	W	57/129 (44%)	56 (98%)	1 (2%)	0	100	100
26	X	46/59 (78%)	44 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Y	44/140 (31%)	44 (100%)	0	0	100	100
28	0	44/124 (36%)	43 (98%)	1 (2%)	0	100	100
29	1	365/449 (81%)	362 (99%)	3 (1%)	0	100	100
30	2	121/370 (33%)	121 (100%)	0	0	100	100
31	3	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
32	4	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
33	5	346/439 (79%)	342 (99%)	4 (1%)	0	100	100
34	6	267/368 (73%)	264 (99%)	3 (1%)	0	100	100
35	7	82/165 (50%)	81 (99%)	1 (1%)	0	100	100
36	8	329/443 (74%)	323 (98%)	6 (2%)	0	100	100
37	h	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
38	i	120/218 (55%)	115 (96%)	5 (4%)	0	100	100
39	9	204/267 (76%)	198 (97%)	6 (3%)	0	100	100
40	a	157/225 (70%)	156 (99%)	1 (1%)	0	100	100
41	b	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
42	c	96/110 (87%)	94 (98%)	2 (2%)	0	100	100
43	d	231/292 (79%)	228 (99%)	3 (1%)	0	100	100
44	AA	360/470 (77%)	355 (99%)	5 (1%)	0	100	100
45	BB	288/428 (67%)	283 (98%)	5 (2%)	0	100	100
46	CC	432/508 (85%)	426 (99%)	6 (1%)	0	100	100
47	DD	286/453 (63%)	280 (98%)	6 (2%)	0	100	100
48	EE	363/477 (76%)	356 (98%)	7 (2%)	0	100	100
49	FF	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
50	GG	221/309 (72%)	220 (100%)	1 (0%)	0	100	100
51	HH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
52	II	245/315 (78%)	239 (98%)	6 (2%)	0	100	100
53	JJ	186/268 (69%)	182 (98%)	4 (2%)	0	100	100
54	KK	122/376 (32%)	119 (98%)	3 (2%)	0	100	100
55	LL	126/174 (72%)	120 (95%)	6 (5%)	0	100	100
56	MM	116/119 (98%)	112 (97%)	4 (3%)	0	100	100
57	NN	110/113 (97%)	110 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	OO	272/320 (85%)	270 (99%)	2 (1%)	0	100	100
59	PP	96/107 (90%)	95 (99%)	1 (1%)	0	100	100
60	QQ	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
61	RR	132/256 (52%)	130 (98%)	2 (2%)	0	100	100
62	SS	79/91 (87%)	77 (98%)	2 (2%)	0	100	100
63	TT	86/236 (36%)	85 (99%)	1 (1%)	0	100	100
64	UU	222/253 (88%)	219 (99%)	3 (1%)	0	100	100
65	VV	255/316 (81%)	255 (100%)	0	0	100	100
66	WW	349/396 (88%)	344 (99%)	5 (1%)	0	100	100
67	XX	404/469 (86%)	393 (97%)	8 (2%)	3 (1%)	22	52
68	YY	97/108 (90%)	96 (99%)	1 (1%)	0	100	100
69	ZZ	310/382 (81%)	308 (99%)	2 (1%)	0	100	100
70	11	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
71	22	31/344 (9%)	31 (100%)	0	0	100	100
72	33	189/236 (80%)	181 (96%)	8 (4%)	0	100	100
73	44	258/310 (83%)	253 (98%)	5 (2%)	0	100	100
73	55	228/310 (74%)	224 (98%)	4 (2%)	0	100	100
74	66	281/348 (81%)	279 (99%)	2 (1%)	0	100	100
75	77	177/414 (43%)	176 (99%)	1 (1%)	0	100	100
76	88	465/508 (92%)	449 (97%)	14 (3%)	2 (0%)	34	64
77	00	46/95 (48%)	46 (100%)	0	0	100	100
77	99	34/95 (36%)	34 (100%)	0	0	100	100
81	cc	5/7 (71%)	5 (100%)	0	0	100	100
82	e	144/303 (48%)	139 (96%)	5 (4%)	0	100	100
83	j	193/201 (96%)	187 (97%)	6 (3%)	0	100	100
All	All	15380/21346 (72%)	15140 (98%)	235 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
67	XX	181	VAL
67	XX	180	ARG
67	XX	182	THR

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Mol	Chain	Res	Type
76	88	205	VAL
76	88	203	PRO

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	B	257/312 (82%)	253 (98%)	4 (2%)	62	83
3	C	242/303 (80%)	242 (100%)	0	100	100
4	D	216/274 (79%)	216 (100%)	0	100	100
5	E	267/296 (90%)	266 (100%)	1 (0%)	91	95
6	F	173/216 (80%)	172 (99%)	1 (1%)	86	93
7	G	64/254 (25%)	64 (100%)	0	100	100
8	f	206/287 (72%)	205 (100%)	1 (0%)	88	94
9	g	120/124 (97%)	119 (99%)	1 (1%)	81	91
10	H	149/149 (100%)	149 (100%)	0	100	100
11	I	100/105 (95%)	99 (99%)	1 (1%)	76	89
12	J	198/255 (78%)	196 (99%)	2 (1%)	76	89
13	K	142/205 (69%)	142 (100%)	0	100	100
14	L	164/165 (99%)	163 (99%)	1 (1%)	86	93
15	M	164/209 (78%)	162 (99%)	2 (1%)	71	87
16	N	119/188 (63%)	119 (100%)	0	100	100
17	O	235/315 (75%)	235 (100%)	0	100	100
18	P	158/196 (81%)	157 (99%)	1 (1%)	86	93
19	Q	312/347 (90%)	311 (100%)	1 (0%)	92	96
20	R	212/359 (59%)	211 (100%)	1 (0%)	88	94
21	S	159/242 (66%)	158 (99%)	1 (1%)	86	93
22	T	161/224 (72%)	161 (100%)	0	100	100
23	U	118/138 (86%)	117 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	V	80/170 (47%)	80 (100%)	0	100	100
25	W	50/102 (49%)	50 (100%)	0	100	100
26	X	46/54 (85%)	46 (100%)	0	100	100
27	Y	38/116 (33%)	38 (100%)	0	100	100
28	0	41/108 (38%)	40 (98%)	1 (2%)	49	74
29	1	316/384 (82%)	313 (99%)	3 (1%)	78	90
30	2	109/317 (34%)	108 (99%)	1 (1%)	78	90
31	3	83/91 (91%)	82 (99%)	1 (1%)	71	87
32	4	113/114 (99%)	113 (100%)	0	100	100
33	5	279/351 (80%)	279 (100%)	0	100	100
34	6	238/310 (77%)	235 (99%)	3 (1%)	69	86
35	7	69/136 (51%)	68 (99%)	1 (1%)	67	84
36	8	285/378 (75%)	280 (98%)	5 (2%)	59	80
37	h	88/88 (100%)	88 (100%)	0	100	100
38	i	101/162 (62%)	101 (100%)	0	100	100
39	9	176/225 (78%)	175 (99%)	1 (1%)	86	93
40	a	146/196 (74%)	146 (100%)	0	100	100
41	b	141/141 (100%)	140 (99%)	1 (1%)	84	92
42	c	86/96 (90%)	84 (98%)	2 (2%)	50	75
43	d	201/243 (83%)	200 (100%)	1 (0%)	88	94
44	AA	314/393 (80%)	313 (100%)	1 (0%)	92	96
45	BB	237/347 (68%)	235 (99%)	2 (1%)	81	91
46	CC	405/461 (88%)	403 (100%)	2 (0%)	88	94
47	DD	242/377 (64%)	235 (97%)	7 (3%)	42	70
48	EE	308/392 (79%)	307 (100%)	1 (0%)	92	96
49	FF	99/99 (100%)	97 (98%)	2 (2%)	55	78
50	GG	186/260 (72%)	183 (98%)	3 (2%)	62	83
51	HH	134/135 (99%)	131 (98%)	3 (2%)	52	76
52	II	206/263 (78%)	206 (100%)	0	100	100
53	JJ	166/227 (73%)	165 (99%)	1 (1%)	86	93
54	KK	108/324 (33%)	107 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	LL	103/142 (72%)	103 (100%)	0	100	100
56	MM	98/99 (99%)	98 (100%)	0	100	100
57	NN	96/97 (99%)	96 (100%)	0	100	100
58	OO	230/265 (87%)	230 (100%)	0	100	100
59	PP	85/92 (92%)	85 (100%)	0	100	100
60	QQ	132/138 (96%)	132 (100%)	0	100	100
61	RR	118/218 (54%)	118 (100%)	0	100	100
62	SS	70/80 (88%)	70 (100%)	0	100	100
63	TT	75/191 (39%)	75 (100%)	0	100	100
64	UU	193/218 (88%)	192 (100%)	1 (0%)	88	94
65	VV	224/268 (84%)	224 (100%)	0	100	100
66	WW	300/333 (90%)	299 (100%)	1 (0%)	92	96
67	XX	345/391 (88%)	341 (99%)	4 (1%)	71	87
68	YY	83/89 (93%)	82 (99%)	1 (1%)	71	87
69	ZZ	278/328 (85%)	277 (100%)	1 (0%)	91	95
70	11	73/75 (97%)	73 (100%)	0	100	100
71	22	33/293 (11%)	33 (100%)	0	100	100
72	33	162/195 (83%)	159 (98%)	3 (2%)	57	79
73	44	215/250 (86%)	215 (100%)	0	100	100
73	55	195/250 (78%)	194 (100%)	1 (0%)	88	94
74	66	245/303 (81%)	245 (100%)	0	100	100
75	77	153/304 (50%)	153 (100%)	0	100	100
76	88	388/419 (93%)	386 (100%)	2 (0%)	88	94
77	00	43/78 (55%)	43 (100%)	0	100	100
77	99	34/78 (44%)	34 (100%)	0	100	100
82	e	132/256 (52%)	131 (99%)	1 (1%)	81	91
83	j	168/171 (98%)	163 (97%)	5 (3%)	41	69
All	All	13298/17844 (74%)	13216 (99%)	82 (1%)	86	93

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	109	HIS

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Mol	Chain	Res	Type
2	B	215	LEU
2	B	298	HIS
2	B	326	ASP
5	E	333	THR
6	F	167	ASP
8	f	245	LYS
9	g	47	LYS
11	I	73	ARG
12	J	57	ARG
12	J	130	TRP
14	L	8	TYR
15	M	145	ARG
15	M	203	ARG
18	P	53	PHE
19	Q	198	ARG
20	R	74	LYS
21	S	126	LYS
23	U	68	LEU
28	0	106	TYR
29	1	271	ARG
29	1	427	ARG
29	1	447	ARG
30	2	253	ASN
31	3	41	TYR
34	6	165	ARG
34	6	311	LEU
34	6	334	ASN
35	7	111	GLN
36	8	273	LEU
36	8	283	LYS
36	8	296	LEU
36	8	322	TRP
36	8	362	PHE
39	9	123	LEU
41	b	155	ARG
42	c	18	LYS
42	c	57	LYS
43	d	69	LEU
44	AA	230	LYS
45	BB	177	TRP
45	BB	287	ARG
46	CC	45	ARG

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Mol	Chain	Res	Type
46	CC	227	LEU
47	DD	35	GLU
47	DD	51	LYS
47	DD	123	ASN
47	DD	134	GLN
47	DD	162	GLN
47	DD	170	THR
47	DD	407	ARG
48	EE	378	ARG
49	FF	89	ARG
49	FF	93	VAL
50	GG	165	ASN
50	GG	190	HIS
50	GG	198	TYR
51	HH	31	TYR
51	HH	78	ARG
51	HH	132	CYS
53	JJ	121	ILE
54	KK	273	LYS
64	UU	80	GLU
66	WW	192	ASN
67	XX	66	LYS
67	XX	157	ASP
67	XX	174	MET
67	XX	307	PHE
68	YY	38	ARG
69	ZZ	75	ASP
72	33	138	SER
72	33	229	LEU
72	33	230	ARG
73	55	299	GLU
76	88	255	ARG
76	88	404	PRO
82	e	64	PHE
83	j	46	MET
83	j	90	LYS
83	j	185	MET
83	j	188	LYS
83	j	194	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	64	ASN
43	d	120	ASN
57	NN	95	ASN
83	j	39	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2826/3464 (81%)	350 (12%)	6 (0%)
78	aa	1430/1864 (76%)	183 (12%)	0
79	bb	71/73 (97%)	13 (18%)	0
80	ee	10/11 (90%)	0	0
All	All	4337/5412 (80%)	546 (12%)	6 (0%)

All (546) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U
1	A	47	A
1	A	52	U
1	A	58	G
1	A	79	A
1	A	90	A
1	A	98	A
1	A	99	U
1	A	104	U
1	A	106	A
1	A	107	U
1	A	118	G
1	A	311	G
1	A	317	A
1	A	319	C
1	A	334	U
1	A	347	U
1	A	348	A
1	A	350	U
1	A	351	A
1	A	353	A

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Mol	Chain	Res	Type
1	A	367	A
1	A	370	A
1	A	376	U
1	A	387	A
1	A	392	A
1	A	393	A
1	A	395	U
1	A	414	U
1	A	419	U
1	A	433	G
1	A	435	A
1	A	440	A
1	A	441	U
1	A	443	A
1	A	462	U
1	A	477	A
1	A	478	U
1	A	486	A
1	A	522	C
1	A	525	A
1	A	569	G
1	A	571	A
1	A	583	A
1	A	584	A
1	A	587	A
1	A	599	A
1	A	608	A
1	A	609	U
1	A	611	A
1	A	639	A
1	A	829	A
1	A	839	A
1	A	840	U
1	A	845	A
1	A	846	A
1	A	849	U
1	A	888	U
1	A	910	A
1	A	914	U
1	A	931	U
1	A	958	A
1	A	960	C

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Mol	Chain	Res	Type
1	A	967	A
1	A	969	G
1	A	977	U
1	A	988	G
1	A	994	U
1	A	995	U
1	A	1010	A
1	A	1011	A
1	A	1042	G
1	A	1070	A
1	A	1071	G
1	A	1081	C
1	A	1107	U
1	A	1108	U
1	A	1109	U
1	A	1118	C
1	A	1119	A
1	A	1125	G
1	A	1134	A
1	A	1136	A
1	A	1137	U
1	A	1141	A
1	A	1160	C
1	A	1190	A
1	A	1191	G
1	A	1206	G
1	A	1219	A
1	A	1235	A
1	A	1242	G
1	A	1248	G
1	A	1257	U
1	A	1258	U
1	A	1267	G
1	A	1271	A
1	A	1280	A
1	A	1307	G
1	A	1316	A
1	A	1331	A
1	A	1333	G
1	A	1334	A
1	A	1358	A
1	A	1376	A

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Mol	Chain	Res	Type
1	A	1377	U
1	A	1379	U
1	A	1380	A
1	A	1381	A
1	A	1382	C
1	A	1389	A
1	A	1417	G
1	A	1431	A
1	A	1452	G
1	A	1453	A
1	A	1457	G
1	A	1487	U
1	A	1494	U
1	A	1495	A
1	A	1496	U
1	A	1497	A
1	A	1509	A
1	A	1522	U
1	A	1526	A
1	A	1528	U
1	A	1529	G
1	A	1565	A
1	A	1566	A
1	A	1567	A
1	A	1568	A
1	A	1578	G
1	A	1589	A
1	A	1590	A
1	A	1591	A
1	A	1604	G
1	A	1605	U
1	A	1613	C
1	A	1620	U
1	A	1626	U
1	A	1627	A
1	A	1634	G
1	A	1648	U
1	A	1703	A
1	A	1719	A
1	A	1722	A
1	A	1726	A
1	A	1842	A

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Mol	Chain	Res	Type
1	A	1844	U
1	A	1880	U
1	A	1881	G
1	A	1882	A
1	A	1884	U
1	A	1910	G
1	A	1921	A
1	A	1922	C
1	A	1951	A
1	A	1970	A
1	A	1971	A
1	A	1985	U
1	A	1988	A
1	A	1991	A
1	A	1993	U
1	A	2002	A
1	A	2029	C
1	A	2030	A
1	A	2032	A
1	A	2039	A
1	A	2041	A
1	A	2048	A
1	A	2051	A
1	A	2052	U
1	A	2091	U
1	A	2105	A
1	A	2108	A
1	A	2136	A
1	A	2142	G
1	A	2145	C
1	A	2148	A
1	A	2149	G
1	A	2150	C
1	A	2158	U
1	A	2164	G
1	A	2165	G
1	A	2172	A
1	A	2173	A
1	A	2189	A
1	A	2190	U
1	A	2198	U
1	A	2199	G

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Mol	Chain	Res	Type
1	A	2202	U
1	A	2205	A
1	A	2206	U
1	A	2207	G
1	A	2226	U
1	A	2228	U
1	A	2256	A
1	A	2258	A
1	A	2265	C
1	A	2266	A
1	A	2268	A
1	A	2278	C
1	A	2287	A
1	A	2290	C
1	A	2291	G
1	A	2295	A
1	A	2296	G
1	A	2297	A
1	A	2304	G
1	A	2328	G
1	A	2330	A
1	A	2332	A
1	A	2333	C
1	A	2337	U
1	A	2347	U
1	A	2367	A
1	A	2370	A
1	A	2371	G
1	A	2384	C
1	A	2402	G
1	A	2409	U
1	A	2411	A
1	A	2418	A
1	A	2419	A
1	A	2420	U
1	A	2427	A
1	A	2439	A
1	A	2440	G
1	A	2441	A
1	A	2477	A
1	A	2486	U
1	A	2491	A

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Mol	Chain	Res	Type
1	A	2509	U
1	A	2511	C
1	A	2541	A
1	A	2543	C
1	A	2547	A
1	A	2548	U
1	A	2558	A
1	A	2559	G
1	A	2581	G
1	A	2582	G
1	A	2592	A
1	A	2595	A
1	A	2596	A
1	A	2611	A
1	A	2612	U
1	A	2621	A
1	A	2626	U
1	A	2631	A
1	A	2632	G
1	A	2636	U
1	A	2637	U
1	A	2638	A
1	A	2656	A
1	A	2658	A
1	A	2659	G
1	A	2685	A
1	A	2686	U
1	A	2690	G
1	A	2694	G
1	A	2706	C
1	A	2710	U
1	A	2711	U
1	A	2719	U
1	A	2720	U
1	A	2721	U
1	A	2722	U
1	A	2723	U
1	A	2757	G
1	A	2758	U
1	A	2775	U
1	A	2784	U
1	A	2786	A

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Mol	Chain	Res	Type
1	A	2795	U
1	A	2797	C
1	A	2806	U
1	A	2808	A
1	A	2810	A
1	A	2811	A
1	A	2836	G
1	A	2838	C
1	A	2843	G
1	A	2852	A
1	A	2858	A
1	A	2875	U
1	A	2881	G
1	A	2882	A
1	A	2883	A
1	A	2884	A
1	A	2891	G
1	A	2897	G
1	A	2898	A
1	A	2909	A
1	A	2912	U
1	A	2927	A
1	A	2942	U
1	A	2945	G
1	A	2953	G
1	A	2955	U
1	A	2956	G
1	A	2957	U
1	A	2958	C
1	A	2969	A
1	A	2971	C
1	A	2980	U
1	A	2981	G
1	A	3006	U
1	A	3018	A
1	A	3019	A
1	A	3025	C
1	A	3030	G
1	A	3034	G
1	A	3038	A
1	A	3054	A
1	A	3061	U

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Mol	Chain	Res	Type
1	A	3065	U
1	A	3067	U
1	A	3081	U
1	A	3082	U
1	A	3124	G
1	A	3125	G
1	A	3156	U
1	A	3166	U
1	A	3259	A
1	A	3260	C
1	A	3261	A
1	A	3262	A
1	A	3263	U
1	A	3276	G
1	A	3288	A
1	A	3296	A
1	A	3310	A
1	A	3349	A
1	A	3359	A
1	A	3391	A
1	A	3399	A
1	A	3407	U
1	A	3408	A
1	A	3413	A
1	A	3420	A
1	A	3424	A
1	A	3425	U
1	A	3428	U
1	A	3429	A
1	A	3447	A
1	A	3449	U
78	aa	51	G
78	aa	52	A
78	aa	54	G
78	aa	77	A
78	aa	84	U
78	aa	90	U
78	aa	92	C
78	aa	93	U
78	aa	96	A
78	aa	106	A
78	aa	113	G

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Mol	Chain	Res	Type
78	aa	115	U
78	aa	118	A
78	aa	122	U
78	aa	242	A
78	aa	255	U
78	aa	256	A
78	aa	266	A
78	aa	268	A
78	aa	269	A
78	aa	270	U
78	aa	271	A
78	aa	273	U
78	aa	278	C
78	aa	282	U
78	aa	302	U
78	aa	314	C
78	aa	318	A
78	aa	376	A
78	aa	380	G
78	aa	388	U
78	aa	389	C
78	aa	390	A
78	aa	401	G
78	aa	416	G
78	aa	417	C
78	aa	430	U
78	aa	431	A
78	aa	441	G
78	aa	445	A
78	aa	446	A
78	aa	454	A
78	aa	455	G
78	aa	482	A
78	aa	483	A
78	aa	497	U
78	aa	518	U
78	aa	540	A
78	aa	556	G
78	aa	561	A
78	aa	669	C
78	aa	670	G
78	aa	675	U

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Mol	Chain	Res	Type
78	aa	676	U
78	aa	677	U
78	aa	680	C
78	aa	684	U
78	aa	722	A
78	aa	725	U
78	aa	737	U
78	aa	744	C
78	aa	756	G
78	aa	759	A
78	aa	773	A
78	aa	790	A
78	aa	799	A
78	aa	802	G
78	aa	803	G
78	aa	811	A
78	aa	828	A
78	aa	830	U
78	aa	838	A
78	aa	849	A
78	aa	856	U
78	aa	861	A
78	aa	862	A
78	aa	867	G
78	aa	871	U
78	aa	879	A
78	aa	880	G
78	aa	911	G
78	aa	913	C
78	aa	921	G
78	aa	924	G
78	aa	944	A
78	aa	945	A
78	aa	952	G
78	aa	978	A
78	aa	990	U
78	aa	991	A
78	aa	1012	A
78	aa	1014	U
78	aa	1024	C
78	aa	1038	U
78	aa	1039	U

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Mol	Chain	Res	Type
78	aa	1040	A
78	aa	1063	U
78	aa	1064	A
78	aa	1106	A
78	aa	1118	G
78	aa	1119	U
78	aa	1126	C
78	aa	1127	A
78	aa	1138	A
78	aa	1152	U
78	aa	1158	G
78	aa	1161	C
78	aa	1164	C
78	aa	1167	A
78	aa	1168	A
78	aa	1169	A
78	aa	1184	U
78	aa	1185	G
78	aa	1348	C
78	aa	1357	U
78	aa	1358	C
78	aa	1385	U
78	aa	1386	U
78	aa	1392	G
78	aa	1417	U
78	aa	1425	A
78	aa	1426	U
78	aa	1437	U
78	aa	1445	U
78	aa	1450	A
78	aa	1457	G
78	aa	1475	A
78	aa	1476	A
78	aa	1480	A
78	aa	1492	A
78	aa	1493	U
78	aa	1504	A
78	aa	1505	U
78	aa	1506	A
78	aa	1511	U
78	aa	1518	U
78	aa	1526	A

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Mol	Chain	Res	Type
78	aa	1527	A
78	aa	1529	A
78	aa	1537	G
78	aa	1553	U
78	aa	1559	A
78	aa	1566	A
78	aa	1579	A
78	aa	1580	A
78	aa	1581	U
78	aa	1582	A
78	aa	1583	U
78	aa	1584	A
78	aa	1585	C
78	aa	1601	A
78	aa	1630	A
78	aa	1643	C
78	aa	1654	G
78	aa	1655	G
78	aa	1658	A
78	aa	1664	C
78	aa	1677	A
78	aa	1680	A
78	aa	1707	G
78	aa	1731	U
78	aa	1735	A
78	aa	1741	G
78	aa	1751	A
78	aa	1753	G
78	aa	1758	G
78	aa	1803	A
78	aa	1805	G
78	aa	1810	A
78	aa	1817	U
78	aa	1818	U
78	aa	1828	G
78	aa	1840	G
78	aa	1841	A
78	aa	1843	U
78	aa	1844	U
78	aa	1845	A
78	aa	1847	C
78	aa	1848	A

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Mol	Chain	Res	Type
78	aa	1849	A
78	aa	1853	U
78	aa	1854	G
78	aa	1864	A
79	bb	12	U
79	bb	13	C
79	bb	14	A
79	bb	19	G
79	bb	20	U
79	bb	21	A
79	bb	45	U
79	bb	47	A
79	bb	49	U
79	bb	65	C
79	bb	68	A
79	bb	73	C
79	bb	75	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	909	A
1	A	1205	A
1	A	2051	A
1	A	2332	A
1	A	2720	U
1	A	2883	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 304 ligands modelled in this entry, 301 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
89	ATP	XX	501	84	26,33,33	3.44	1 (3%)	31,52,52	1.10	1 (3%)
88	NAD	2	4301	86	42,48,48	0.75	1 (2%)	50,73,73	0.82	2 (4%)
85	SPM	A	3645	-	13,13,13	0.33	0	12,12,12	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	ATP	XX	501	84	-	2/18/38/38	0/3/3/3
88	NAD	2	4301	86	-	1/26/62/62	0/5/5/5
85	SPM	A	3645	-	-	2/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XX	501	ATP	C2'-C1'	-16.90	1.28	1.53
88	2	4301	NAD	C2N-N1N	-2.38	1.32	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	XX	501	ATP	C3'-C2'-C1'	4.76	108.14	100.98
88	2	4301	NAD	N3A-C2A-N1A	-2.67	124.50	128.68
88	2	4301	NAD	O4B-C1B-C2B	-2.51	103.25	106.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	A	3645	SPM	N10-C11-C12-C13
85	A	3645	SPM	N5-C6-C7-C8

Continued on next page...

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Mol	Chain	Res	Type	Atoms
89	XX	501	ATP	PA-O3A-PB-O2B
88	2	4301	NAD	O4D-C4D-C5D-O5D
89	XX	501	ATP	PA-O3A-PB-O1B

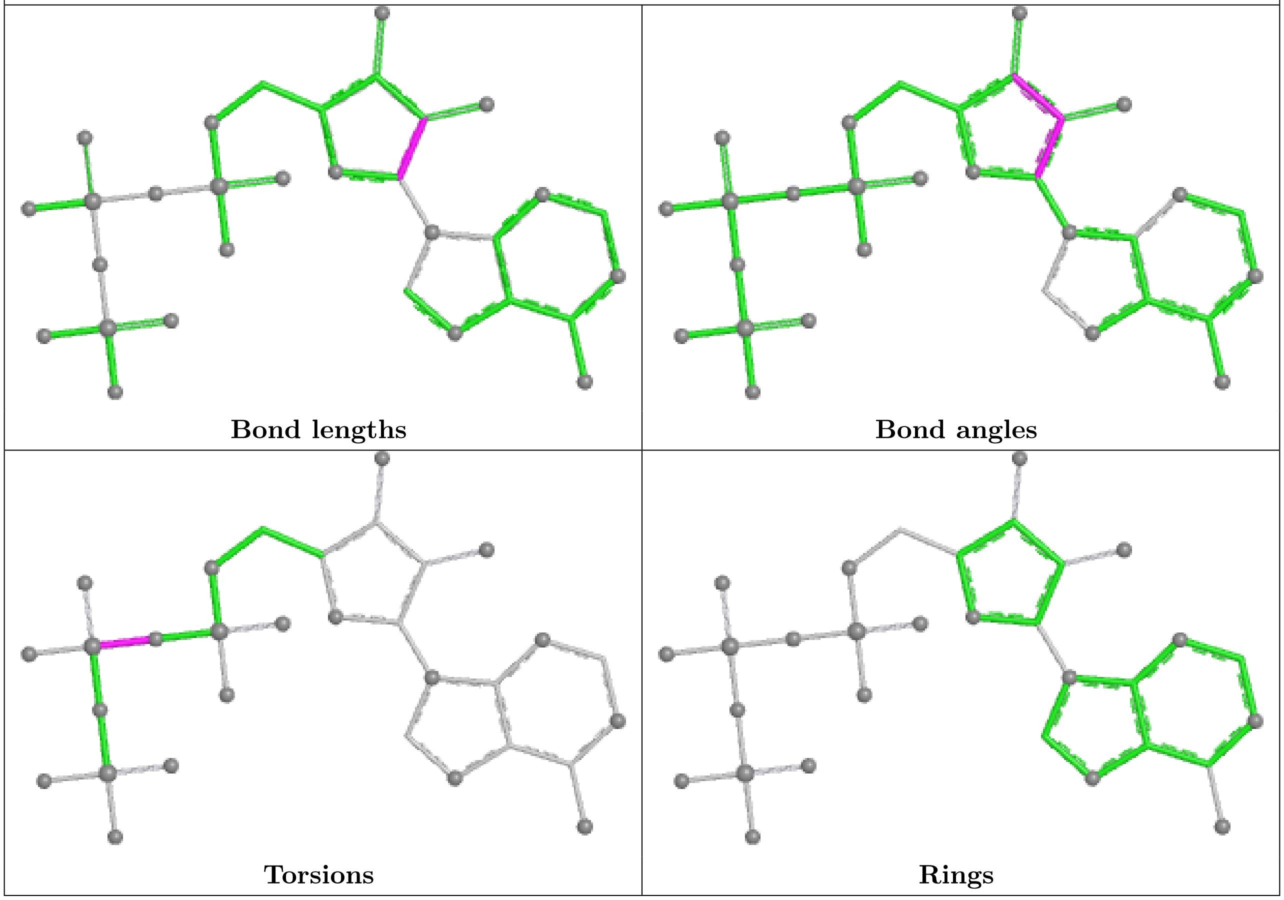
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	XX	501	ATP	2	0
88	2	4301	NAD	3	0

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

Ligand ATP XX 501



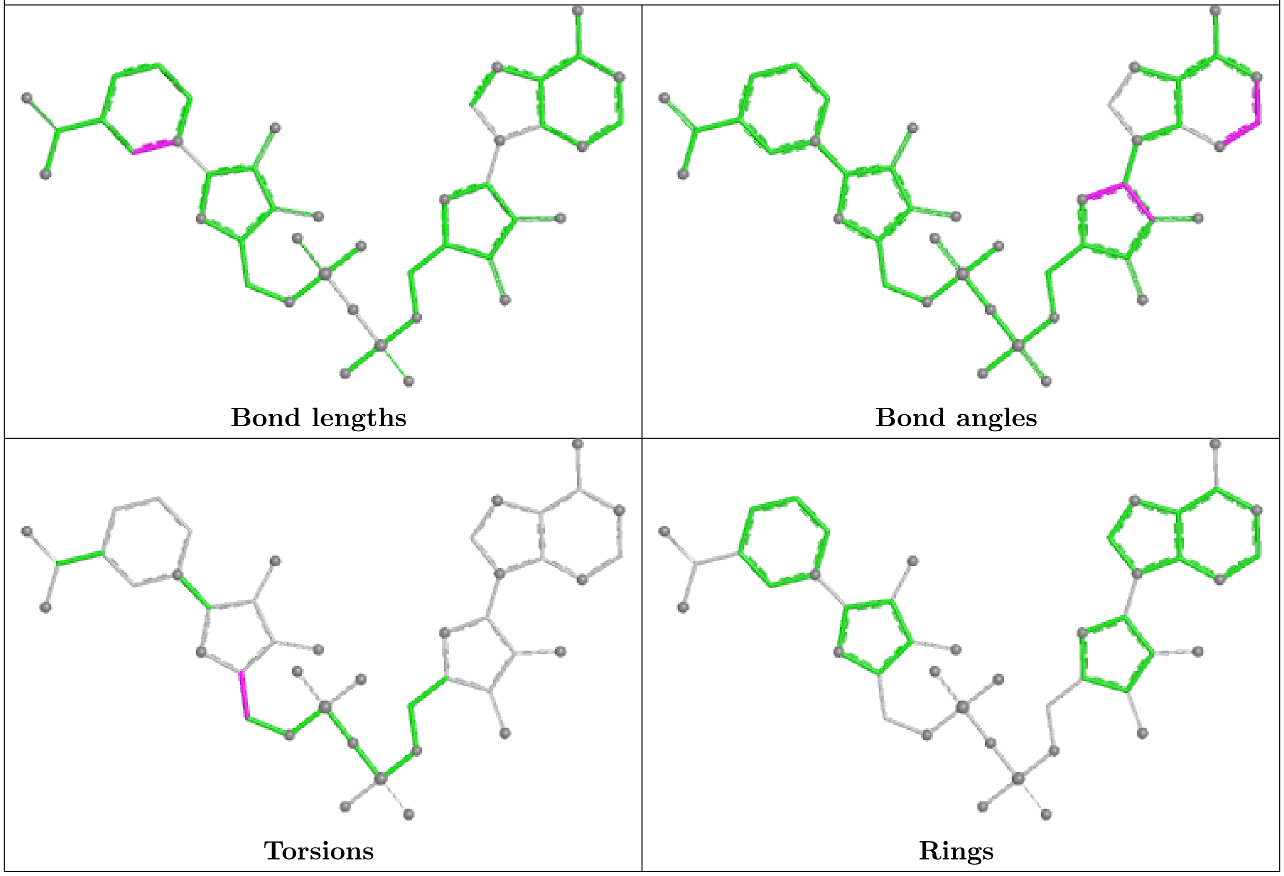
Bond lengths

Bond angles

Torsions

Rings

Ligand NAD 2 4301



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	bb	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	bb	15:A	O3’	18:A	P	9.12

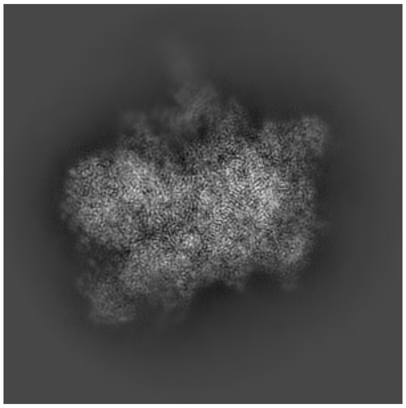
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10985. These allow visual inspection of the internal detail of the map and identification of artifacts.

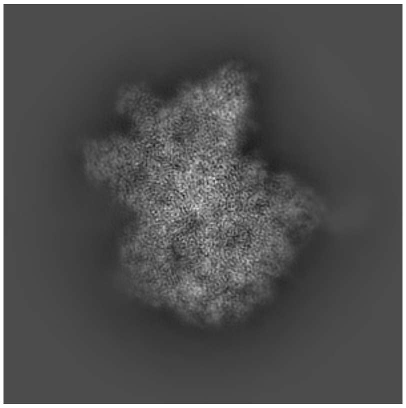
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

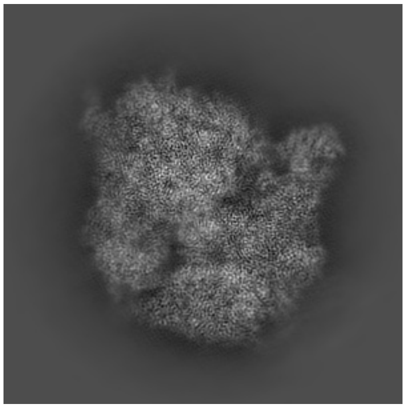
6.1.1 Primary map



X

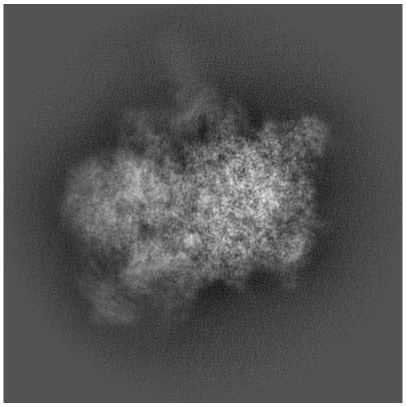


Y

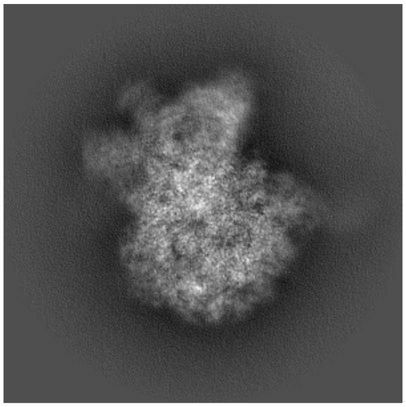


Z

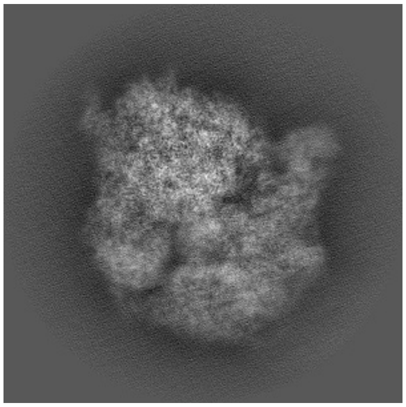
6.1.2 Raw map



X



Y

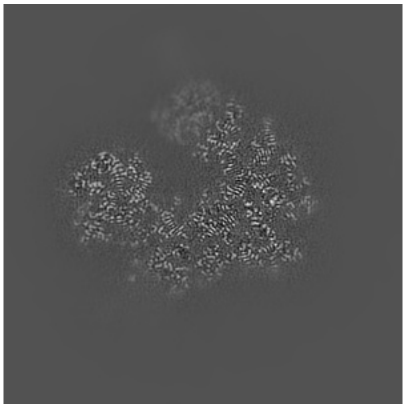


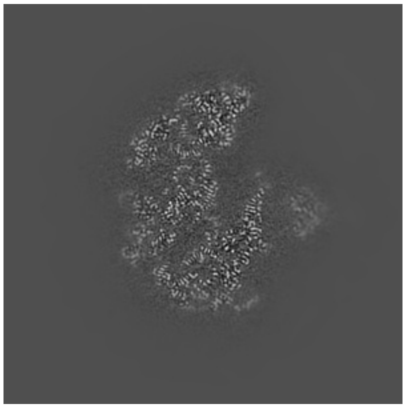
Z

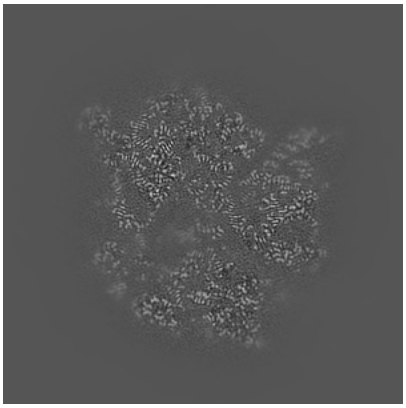
The images above show the map projected in three orthogonal directions.

6.2 Central slices

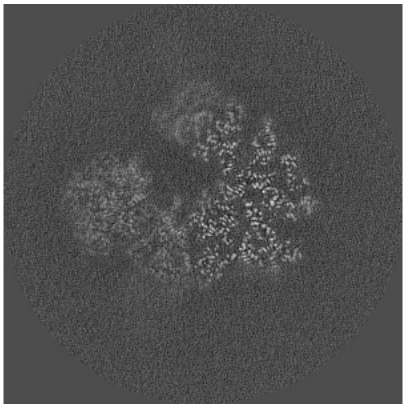
6.2.1 Primary map

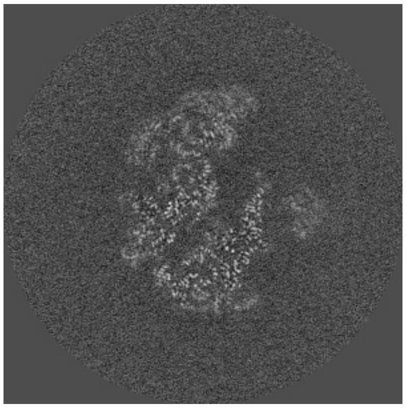

X Index: 200

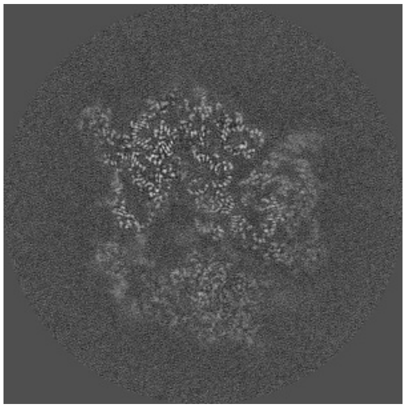

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

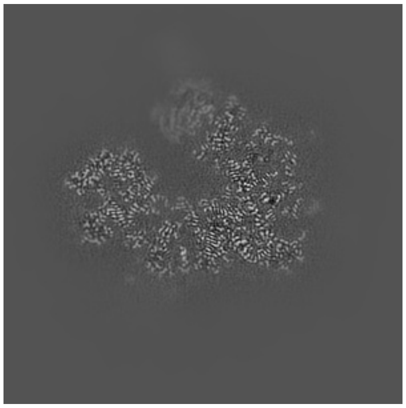

Y Index: 200


Z Index: 200

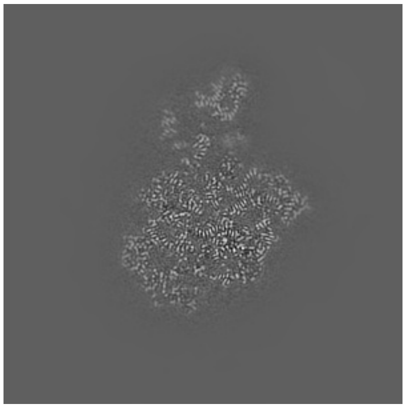
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

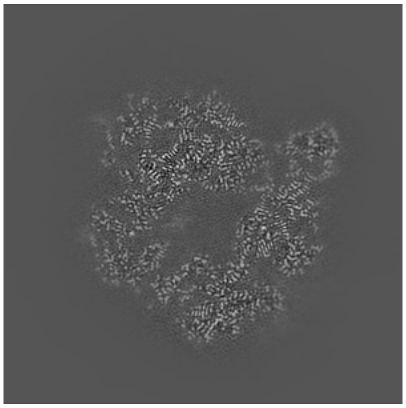
6.3.1 Primary map



X Index: 195

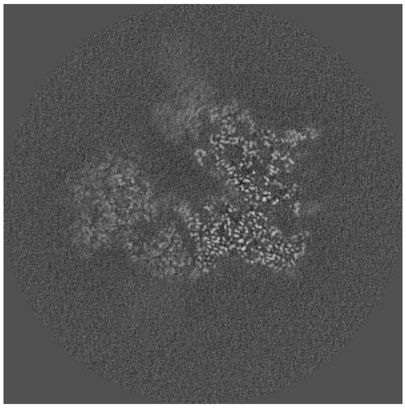


Y Index: 228

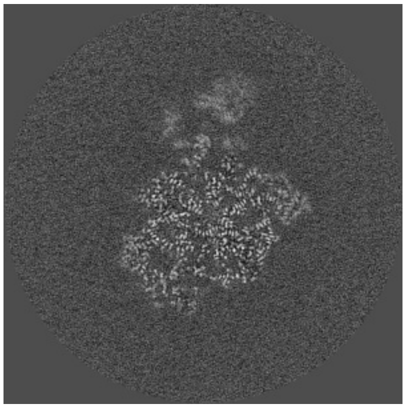


Z Index: 219

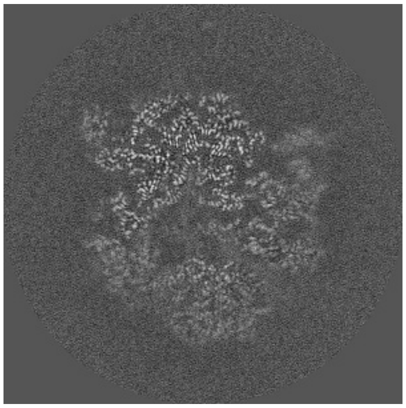
6.3.2 Raw map



X Index: 192



Y Index: 228



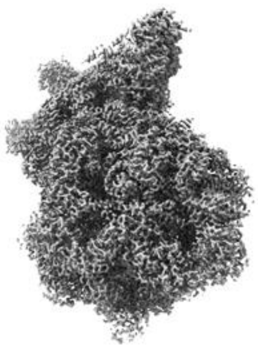
Z Index: 206

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

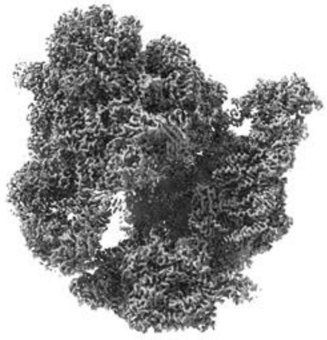
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



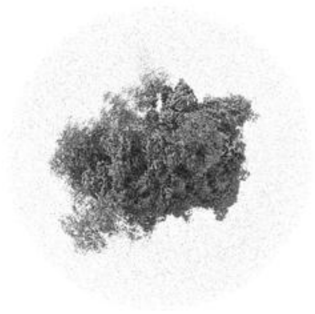
Y



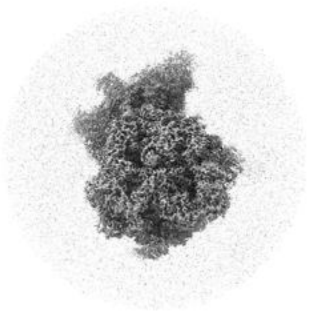
Z

The images above show the 3D surface view of the map at the recommended contour level 4.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

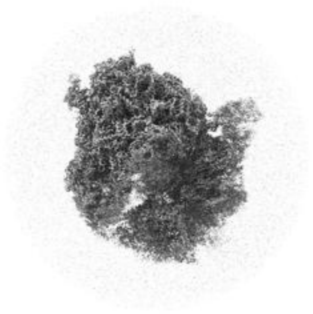
6.4.2 Raw map



X



Y



Z

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

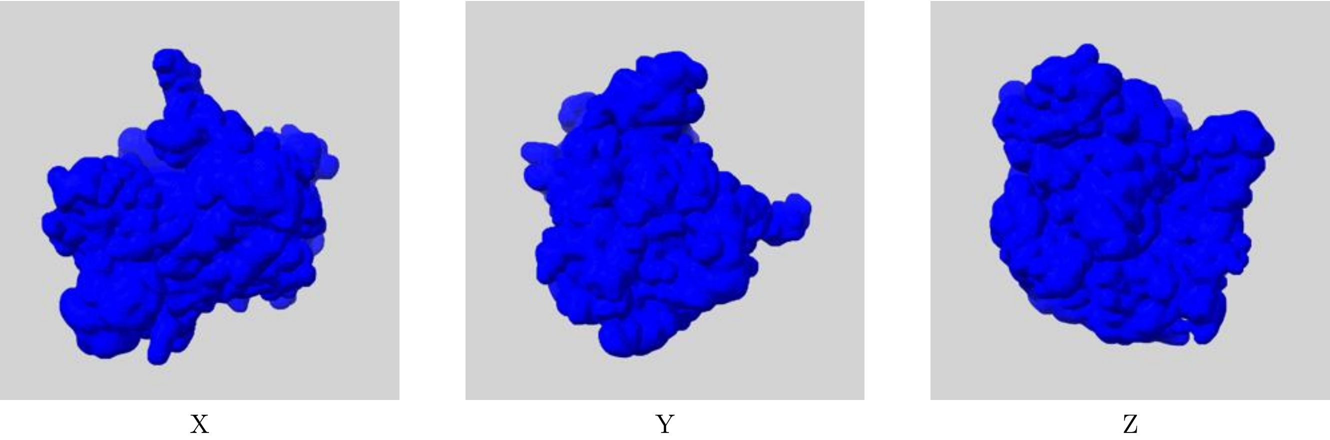
6.5 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

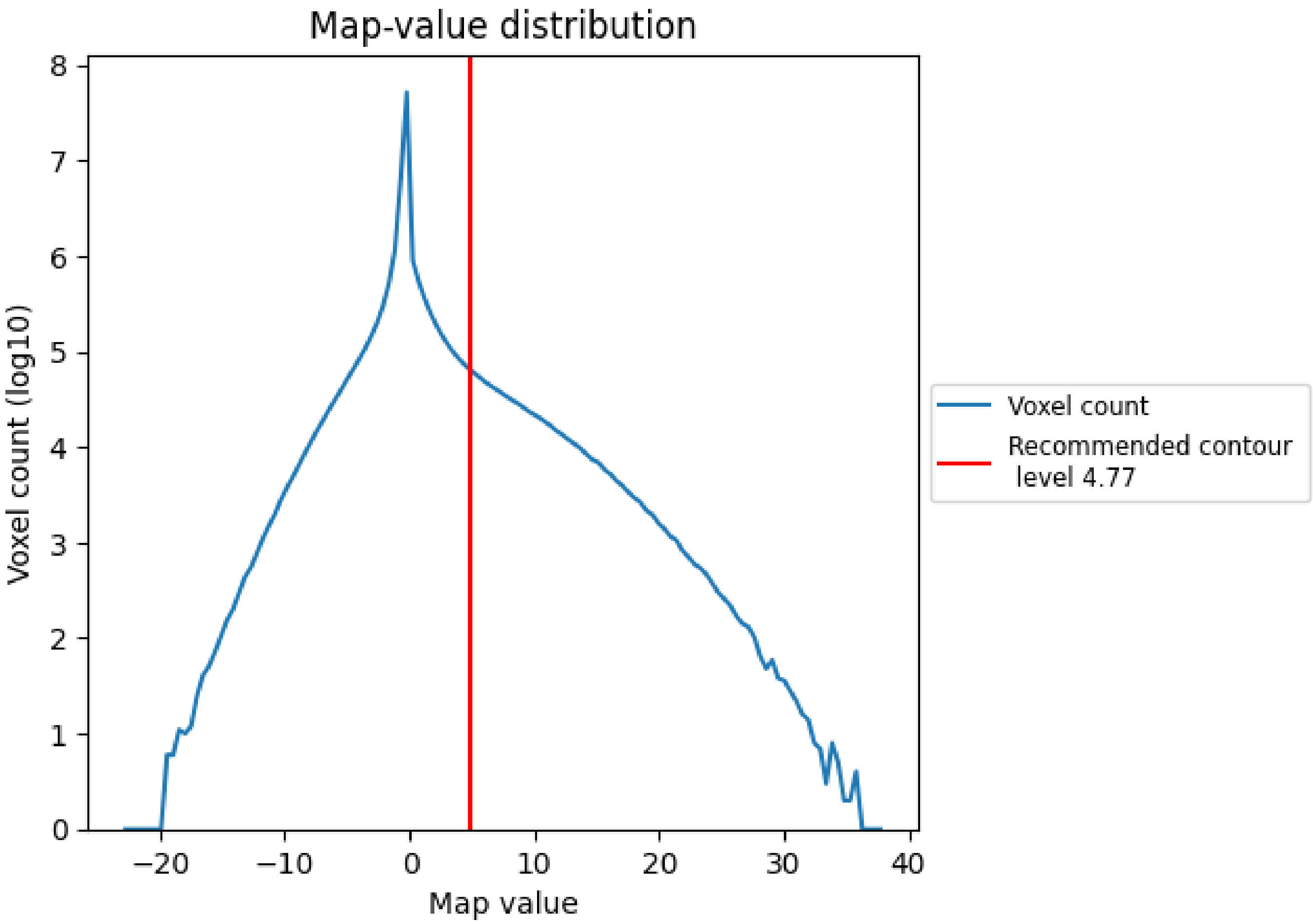
6.5.1 emd_10985_msk_1.map ⓘ



7 Map analysis ⓘ

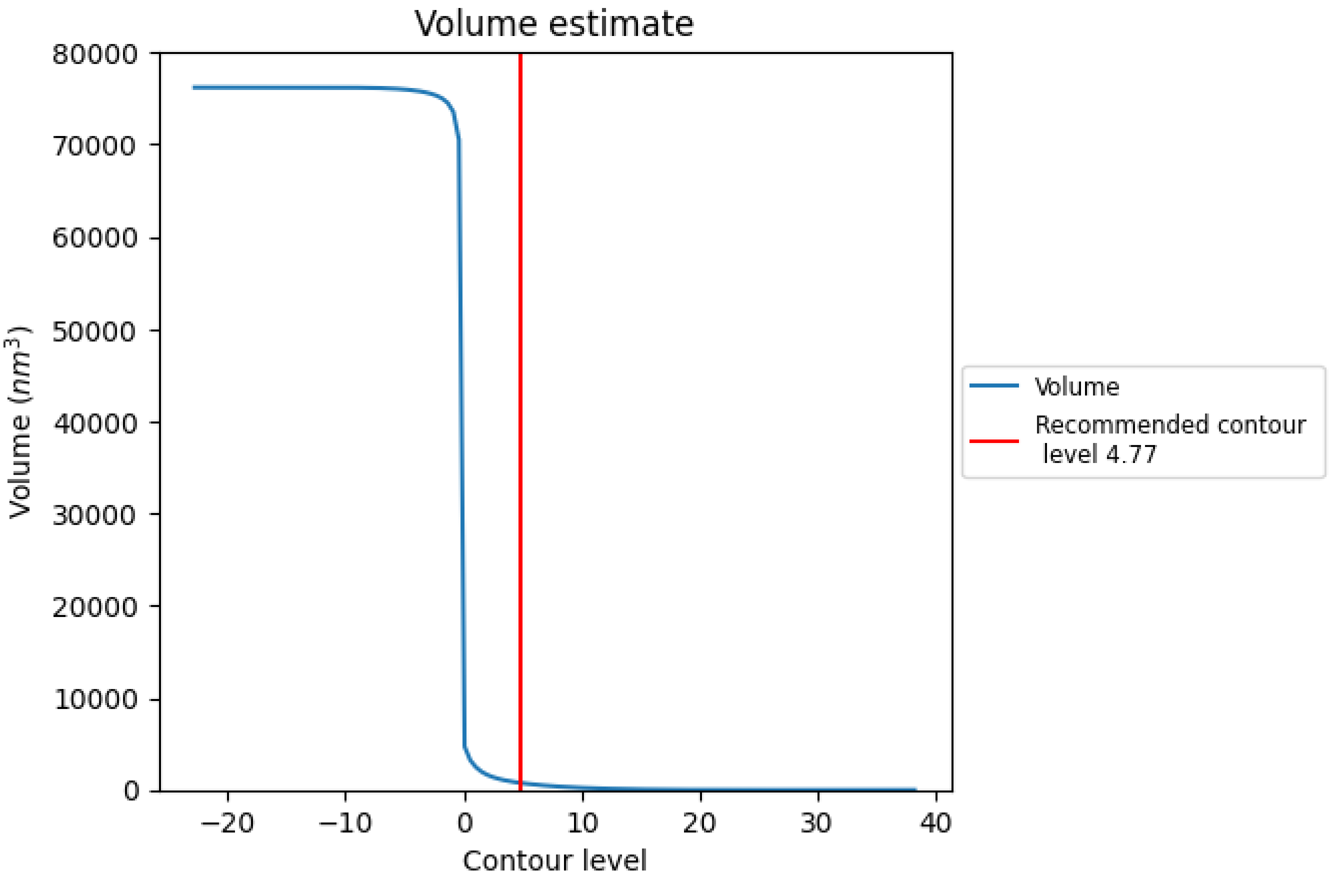
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

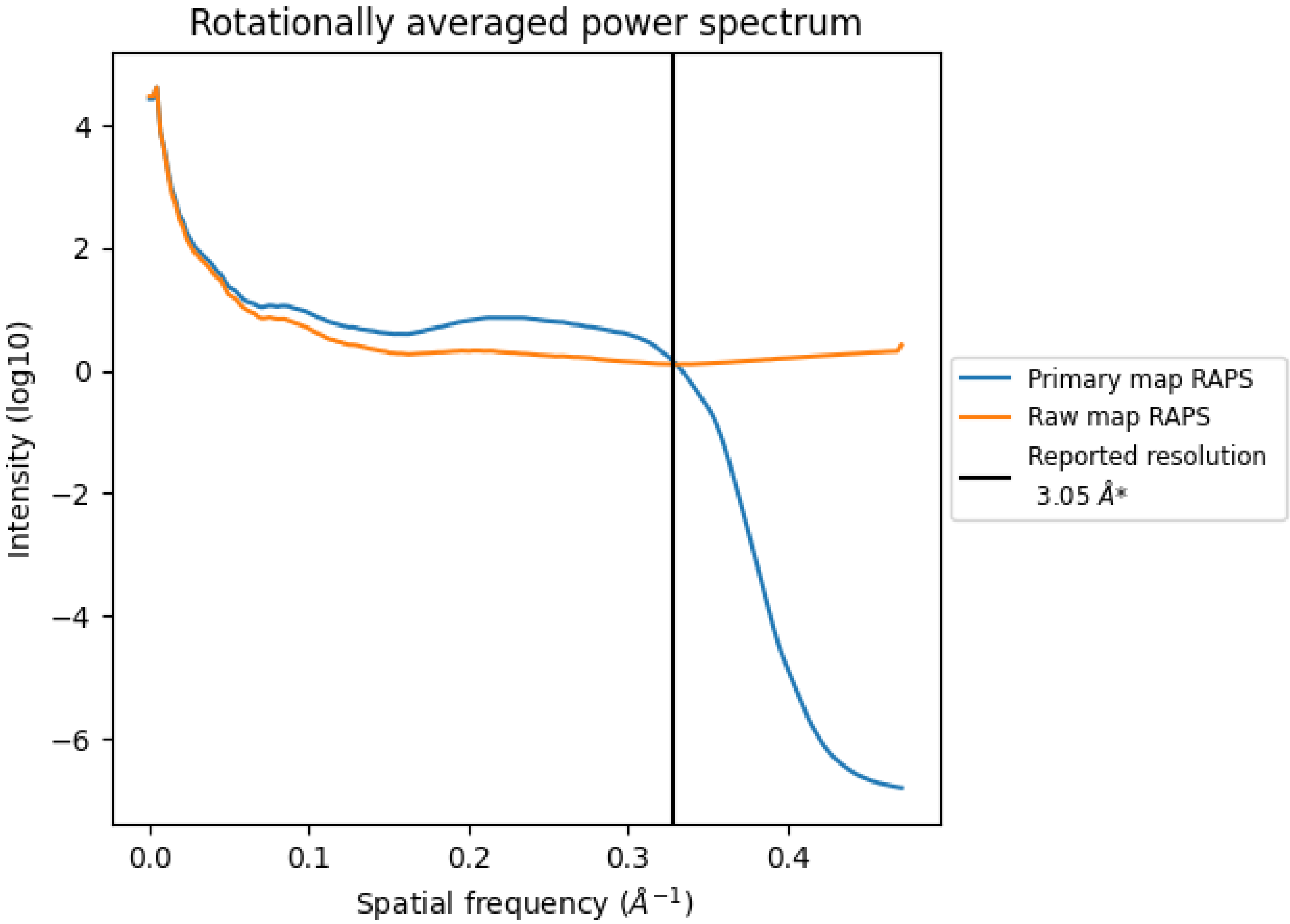
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 765 nm^3; this corresponds to an approximate mass of 691 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 ⓘ

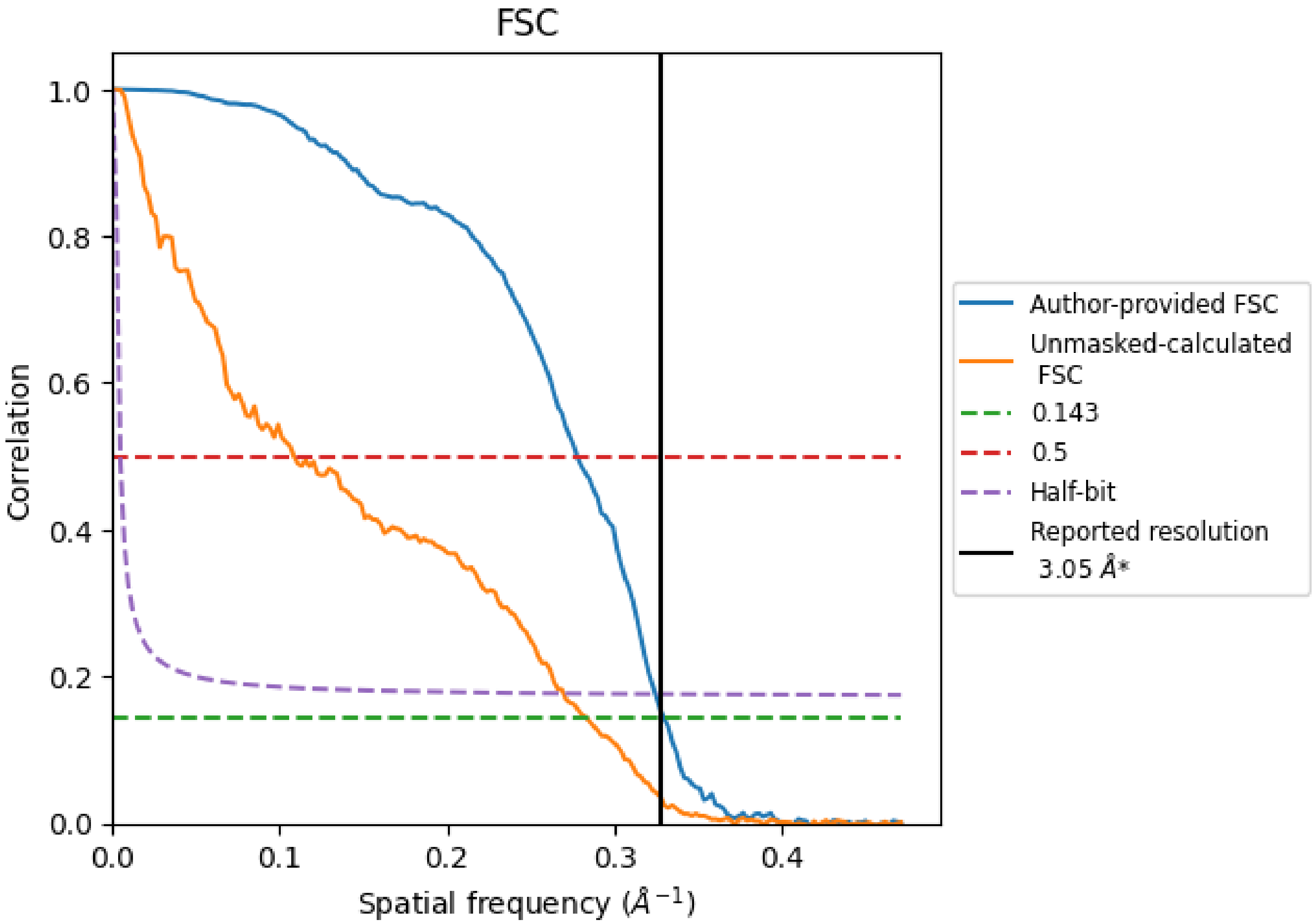


*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

8.2 Resolution estimates (i)

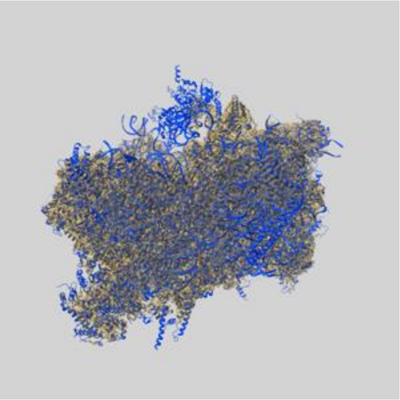
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.03	3.60	3.08
Unmasked-calculated*	3.52	9.22	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 3.05 by more than 10 %

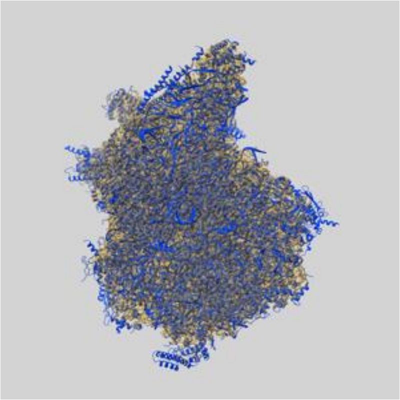
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10985 and PDB model 6YWY. Per-residue inclusion information can be found in section 3 on page 22.

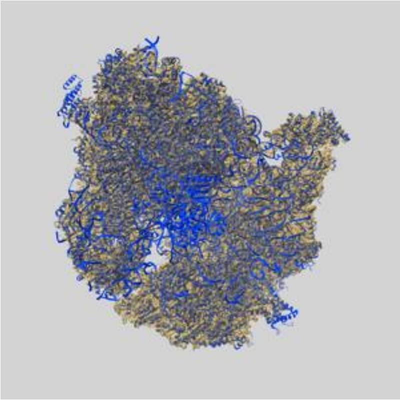
9.1 Map-model overlay ⓘ



X



Y



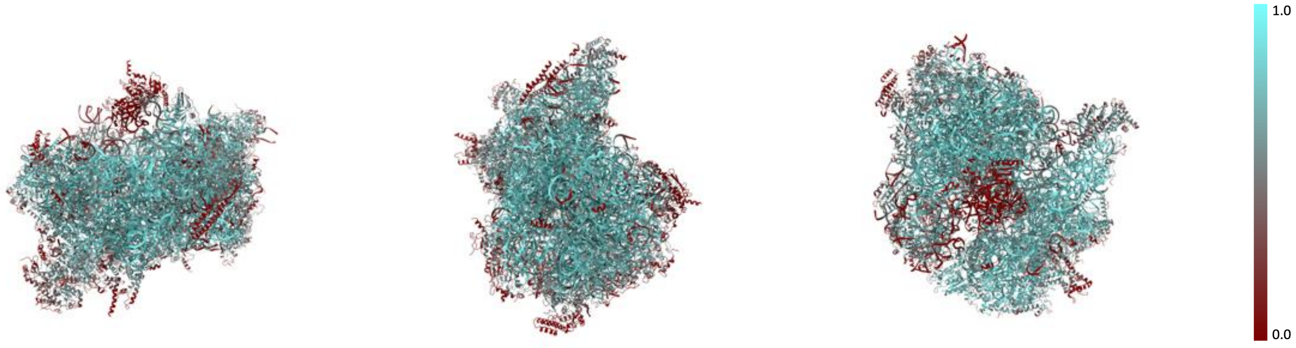
Z

The images above show the 3D surface view of the map at the recommended contour level 4.77 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 ⓘ

This section was not generated.

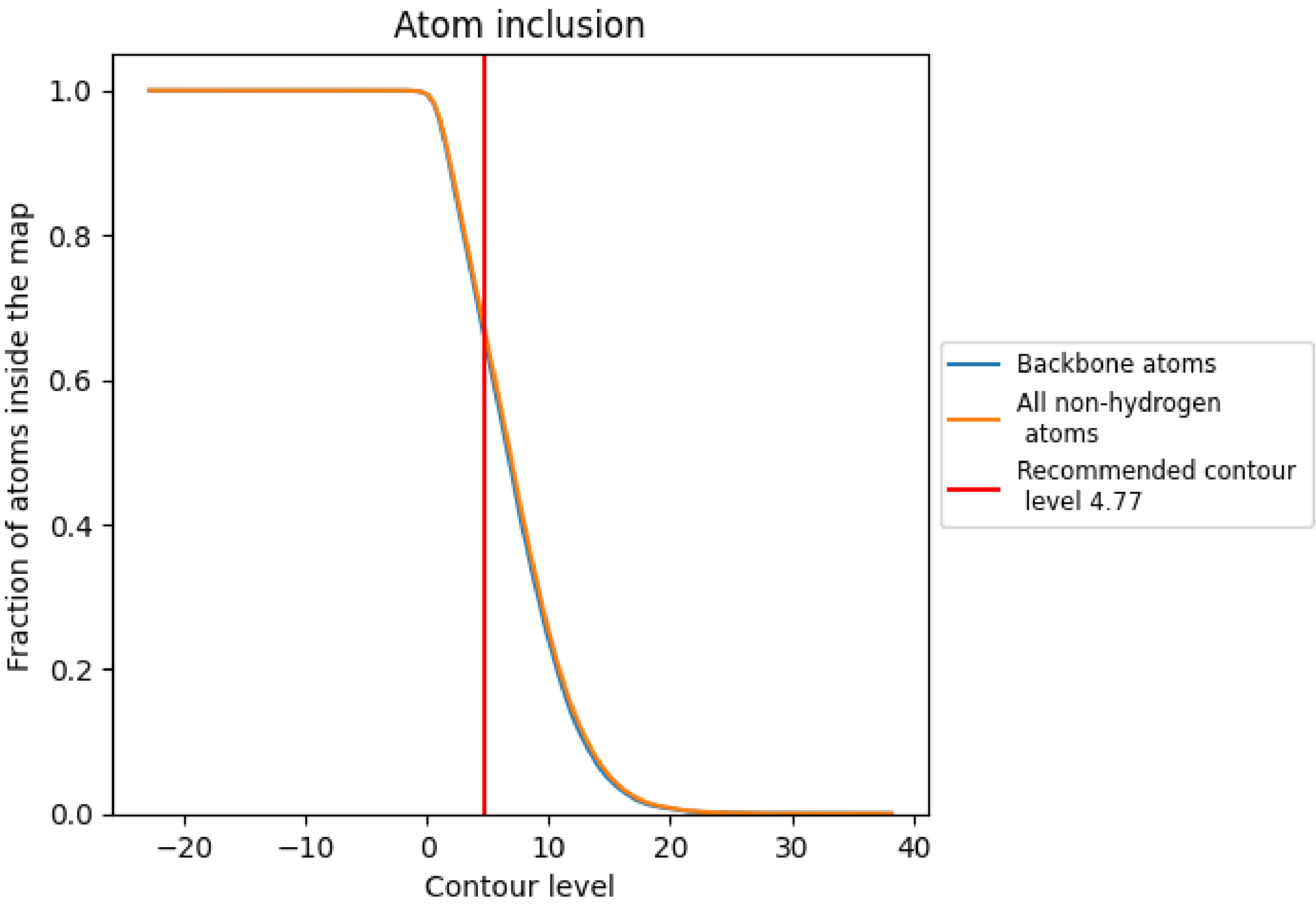
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.77).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 67% 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 (4.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6688
0	0.8737
00	0.1529
1	0.5981
11	0.6012
2	0.6724
22	0.7430
3	0.6519
33	0.6349
4	0.7628
44	0.3842
5	0.6072
55	0.3467
6	0.5429
66	0.6571
7	0.6458
77	0.6843
8	0.2851
88	0.5397
9	0.4167
99	0.0233
A	0.7653
AA	0.4306
B	0.7382
BB	0.6695
C	0.7705
CC	0.6451
D	0.6421
DD	0.7289
E	0.6246
EE	0.6582
F	0.5753
FF	0.6865
G	0.4428
GG	0.6570

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Chain	Atom inclusion
H	0.8081
HH	0.7510
I	0.6978
II	0.6484
J	0.6941
JJ	0.7984
K	0.7632
KK	0.7141
L	0.7154
LL	0.7565
M	0.5703
MM	0.6916
N	0.6909
NN	0.8474
O	0.6228
OO	0.6227
P	0.6987
PP	0.7922
Q	0.5457
QQ	0.5908
R	0.5587
RR	0.5673
S	0.6366
SS	0.6378
T	0.6398
TT	0.7217
U	0.6201
UU	0.6277
V	0.4931
VV	0.5288
W	0.7716
WW	0.5413
X	0.7371
XX	0.7222
Y	0.8386
YY	0.7372
ZZ	0.5565
a	0.5680
aa	0.8225
b	0.5680
bb	0.2730
c	0.8161

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Chain	Atom inclusion
cc	🟥 0.2571
d	🟩 0.6359
e	🟥 0.0000
ee	🟩 0.6391
f	🟥 0.0706
g	🟥 0.0000
h	🟥 0.0026
i	🟥 0.0241
j	🟥 0.0000