wwPDB EM Validation Summary Report

Oct 24, 2026 – 11:24 am BST

PDB ID	:	9TS7 / pdb_00009ts7
EMDB ID	:	EMD-56210
Title	:	Structure of the Plant mitochondrial initiation complex, (SSU, LSU, initiator tRNA, mRNA)
Authors	:	Skaltsogiannis, V.; Giege, P.; Soufari, H.
Deposited on	:	2025-12-29
Resolution	:	2.92 Å(reported)

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

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

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

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

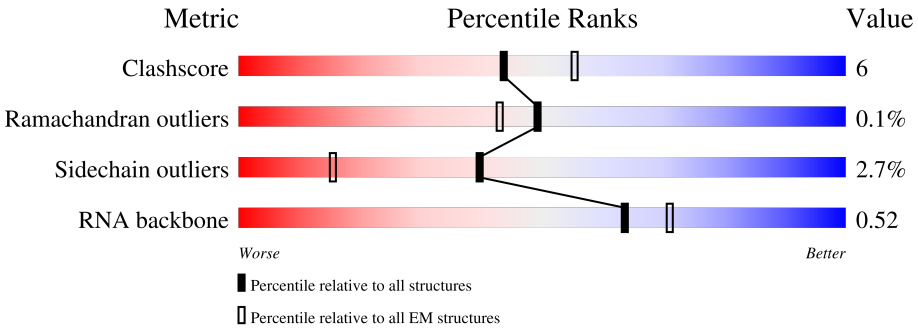
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

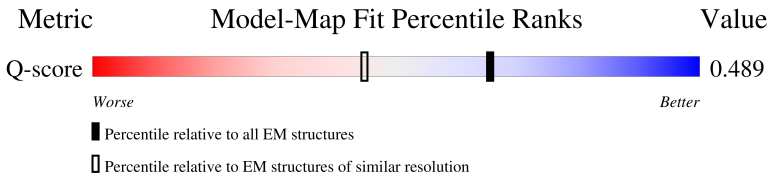
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.92 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	1	2923	17% 64% 32% 5%
2	1B	217	6% 73% 7% • 18%
3	1C	286	40% 64% 10% 25%

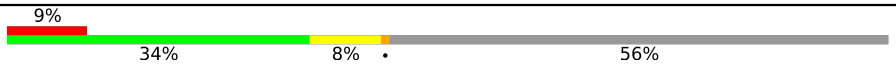
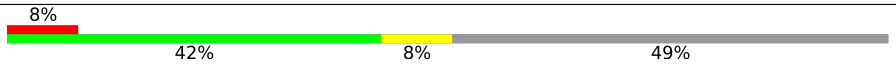
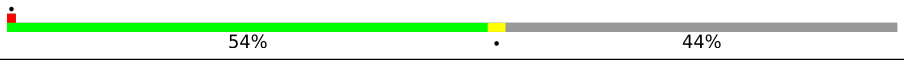
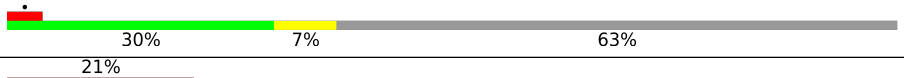
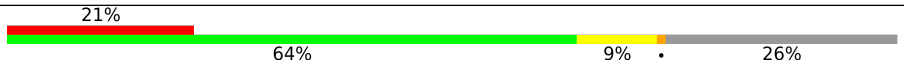
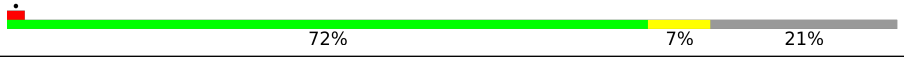
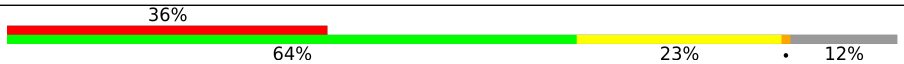
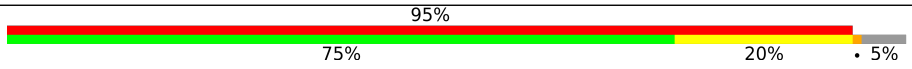
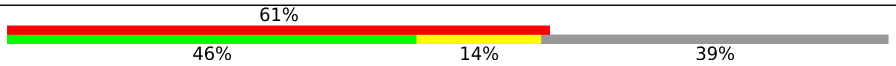
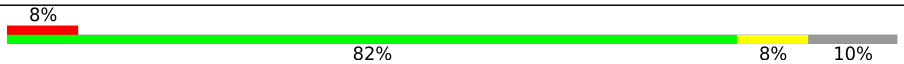
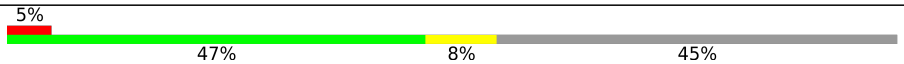
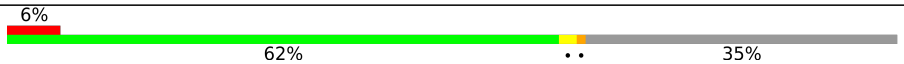
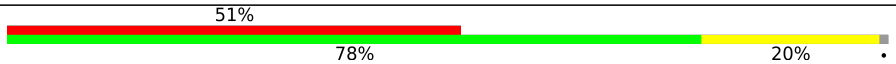
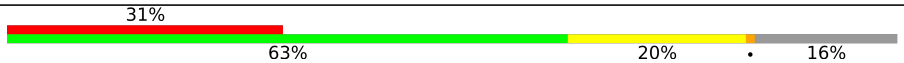
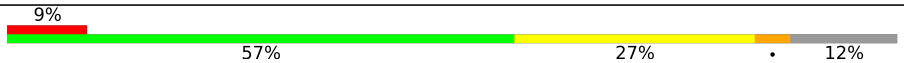
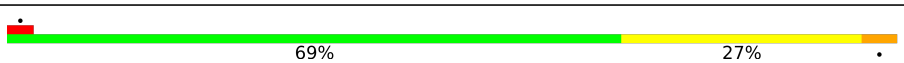
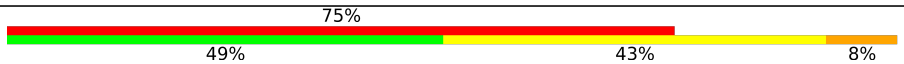
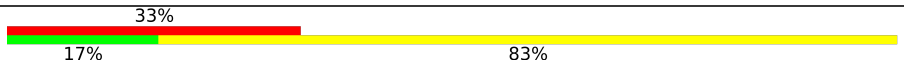
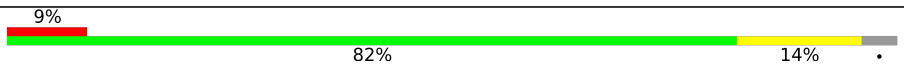
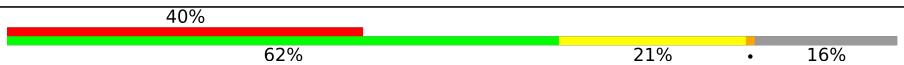
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Mol	Chain	Length	Quality of chain
4	1D	319	73% 10% 17%
5	1E	296	69% 6% 25%
6	1F	185	14% 66% 18% 15%
7	1G	102	88% 87% 9%
8	1H	220	6% 24% 6% 70%
9	1I	170	76% 53% 22% 24%
10	1J	156	94% 69% 26% 6%
11	1K	204	10% 83% 10% 7%
12	1L	176	62% 10% 28%
13	1M	281	66% 8% 25%
14	1N	179	21% 69% 13% 17%
15	1O	160	84% 10% 6%
16	1P	114	82% 17%
17	1Q	233	46% 6% 48%
18	1R	126	78% 10% 13%
19	1S	270	49% 5% 46%
20	1T	264	53% 5% 41%
21	1U	180	7% 64% 8% 28%
22	1V	159	89% 11%
23	1W	238	85% 63% 23% 14%
24	1X	271	18% 68% 11% 20%
25	1Y	156	8% 54% 8% 37%
26	1Z	215	32% 70% 12% 18%
27	1a	144	65% 11% 24%
28	1b	109	85% 6% 8%

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Mol	Chain	Length	Quality of chain
29	1c	135	
30	1d	139	
31	1e	106	
32	1f	146	
33	1g	162	
34	1h	103	
35	1i	247	
36	1j	90	
37	1k	119	
38	1l	239	
39	1m	128	
40	1o	125	
41	1p	130	
42	1q	78	
43	1r	167	
44	1s	181	
45	1t	491	
46	1u	751	
47	1v	514	
48	2	1766	
49	3	118	
50	5	77	
51	6	6	
52	A	212	
53	B	554	

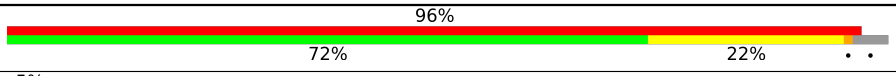
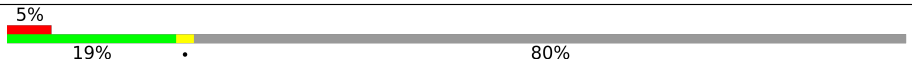
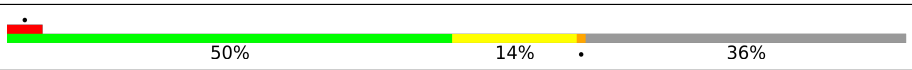
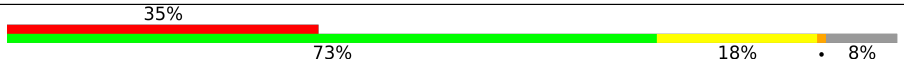
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Mol	Chain	Length	Quality of chain
54	C	362	11% 69% 22% 8%
55	D	501	26% 68% 14% 17%
56	E	138	63% 10% 27%
57	F	157	96% 78% 22%
58	G	129	88% 11%
59	H	383	16% 43% 12% 44%
60	I	228	36% 13% 50%
61	J	304	7% 34% 8% 58%
62	K	125	7% 78% 21%
63	L	154	10% 64% 13% 23%
64	M	155	55% 9% 35%
65	N	414	24% 72%
66	O	136	65% 15% 19%
67	P	110	10% 76% 6% 17%
68	Q	237	33% 5% 62%
69	R	212	50% 65% 13% 22%
70	S	100	20% 57% 18% 25%
71	T	94	46% 7% 47%
72	U	192	43% 51% 15% 34%
73	V	193	13% 68% 16% 15%
74	W	483	24% 63% 16% 21%
75	X	496	18% 30% 10% 59%
76	Y	102	21% 74% 20%
77	Z	153	20% 39% 13% 48%
78	a	424	40% 57% 16% 26%

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Mol	Chain	Length	Quality of chain
79	b	80	
80	c	128	
81	d	110	
82	e	383	
83	f	410	
84	h	384	
85	i	725	
86	k	153	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 207751 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2922	62518	27942	11365	20289	2922	5	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL2 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	177	1325	819	259	233	14	0	0

- Molecule 3 is a protein called uL2m N-ter mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	215	1696	1078	316	296	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	264	2045	1309	367	358	11	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1E	221	1753	1104	334	308	7	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1F	158	1286	829	212	236	9	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1F	12	LEU	SER	conflict	UNP A0A068BF07
1F	16	LEU	PRO	conflict	UNP A0A068BF07
1F	20	LEU	PRO	conflict	UNP A0A068BF07
1F	22	TYR	HIS	conflict	UNP A0A068BF07
1F	31	LEU	SER	conflict	UNP A0A068BF07
1F	57	CYS	ARG	conflict	UNP A0A068BF07
1F	106	LEU	SER	conflict	UNP A0A068BF07
1F	110	LEU	SER	conflict	UNP A0A068BF07
1F	160	ILE	VAL	conflict	UNP A0A068BF07
1F	171	LEU	PRO	conflict	UNP A0A068BF07

- Molecule 7 is a protein called Large ribosomal subunit protein uL6 alpha-beta domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	98	Total	C	N	O	S	0	0
			779	508	136	130	5		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	66	Total	C	N	O	S	0	0
			539	345	98	94	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	19	THR	LYS	conflict	UNP A0A0D3EAI8
1H	24	THR	SER	conflict	UNP A0A0D3EAI8
1H	69	PHE	LEU	conflict	UNP A0A0D3EAI8
1H	99	TYR	PHE	conflict	UNP A0A0D3EAI8
1H	104	GLU	VAL	conflict	UNP A0A0D3EAI8
1H	105	GLU	VAL	conflict	UNP A0A0D3EAI8
1H	106	VAL	HIS	conflict	UNP A0A0D3EAI8
1H	108	SER	THR	conflict	UNP A0A0D3EAI8
1H	160	ILE	LEU	conflict	UNP A0A0D3EAI8
1H	173	ASP	ASN	conflict	UNP A0A0D3EAI8
1H	184	ALA	THR	conflict	UNP A0A0D3EAI8
1H	212	VAL	LEU	conflict	UNP A0A0D3EAI8

- Molecule 9 is a protein called Large ribosomal subunit protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	130	Total	C	N	O	S	0	0
			1036	669	178	184	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1I	118	LYS	GLU	conflict	UNP A0A0D3AE97
1I	124	GLN	LYS	conflict	UNP A0A0D3AE97

- Molecule 10 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	147	Total	C	N	O	S	0	0
			1129	722	193	205	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1J	78	SER	THR	conflict	UNP A0A3P6F9L4
1J	79	VAL	PHE	conflict	UNP A0A3P6F9L4
1J	83	THR	SER	conflict	UNP A0A3P6F9L4

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	189	Total	C	N	O	S	0	0
			1526	955	299	265	7		

- Molecule 12 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	127	Total	C	N	O	S	0	0
			966	609	184	168	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL15/eL18 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	210	Total	C	N	O	S	0	0
			1649	1052	321	273	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1M	46	SER	PRO	conflict	UNP A0A0D3BF13
1M	58	ILE	MET	conflict	UNP A0A0D3BF13
1M	127	LYS	ASN	conflict	UNP A0A0D3BF13
1M	249	LEU	GLN	conflict	UNP A0A0D3BF13
1M	280	GLU	GLY	conflict	UNP A0A0D3BF13

- Molecule 14 is a protein called Large ribosomal subunit protein uL16m|.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	148	Total	C	N	O	S	0	0
			1160	731	230	192	7		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	151	Total	C	N	O	S	0	0
			1231	767	244	214	6		

- Molecule 16 is a protein called Ribosomal protein L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	113	Total	C	N	O	S	0	0
			878	564	160	149	5		

- Molecule 17 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	122	Total	C	N	O	S	0	0
			1008	641	198	166	3		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	110	Total	C	N	O	S	0	0
			915	572	184	154	5		

- Molecule 19 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	145	Total	C	N	O	S	0	0
			1170	750	207	211	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	155	Total	C	N	O	S	0	0
			1241	782	249	205	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1U	130	Total	C	N	O	S	0	0
			1048	675	190	181	2		

- Molecule 22 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1V	158	Total	C	N	O	S	0	0
			1223	770	229	220	4		

- Molecule 23 is a protein called bL25-2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1W	205	Total	C	N	O	S	0	0
			1588	1006	284	294	4		

- Molecule 24 is a protein called bL25m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1X	216	Total	C	N	O	S	0	0
			1670	1069	298	302	1		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Y	98	Total	C	N	O	S	0	0
			768	484	152	131	1		

- Molecule 26 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1Z	177	Total	C	N	O	S	0	0
			1441	911	266	255	9		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1Z	20	ASN	THR	conflict	UNP A0A3P6BNQ4
1Z	21	ILE	LEU	conflict	UNP A0A3P6BNQ4
1Z	27	GLU	GLY	conflict	UNP A0A3P6BNQ4
1Z	36	THR	SER	conflict	UNP A0A3P6BNQ4
1Z	87	SER	ARG	conflict	UNP A0A3P6BNQ4
1Z	126	TYR	PHE	conflict	UNP A0A3P6BNQ4
1Z	133	ALA	GLN	conflict	UNP A0A3P6BNQ4
1Z	148	PRO	ALA	conflict	UNP A0A3P6BNQ4
1Z	154	LEU	PHE	conflict	UNP A0A3P6BNQ4
1Z	174	ARG	LYS	conflict	UNP A0A3P6BNQ4
1Z	175	THR	GLU	conflict	UNP A0A3P6BNQ4
1Z	176	PHE	ALA	conflict	UNP A0A3P6BNQ4
1Z	178	LYS	ARG	conflict	UNP A0A3P6BNQ4

- Molecule 27 is a protein called Cation-transporting P-type ATPase N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1a	110	Total	C	N	O	S	0	0
			928	588	172	158	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1a	24	THR	ALA	conflict	UNP A0A3P6EWC5
1a	143	GLY	ALA	conflict	UNP A0A3P6EWC5

- Molecule 28 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1b	100	Total	C	N	O	S	0	0
			803	504	160	134	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1b	17	GLN	GLU	conflict	UNP A0A0D3EB87

- Molecule 29 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1c	59	Total	C	N	O	S	0	0
			489	313	98	73	5		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1d	49	Total	C	N	O	S	0	0
			379	240	80	55	4		

- Molecule 31 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1e	54	Total	C	N	O	S	0	0
			459	300	85	72	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	1f	44	Total	C	N	O	0	0
			364	224	88	52		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1g	91	Total	C	N	O	S	0	0
			770	496	152	119	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1g	30	ILE	LEU	conflict	UNP A0A0D3AUD0
1g	54	ARG	THR	conflict	UNP A0A0D3AUD0
1g	127	ASP	TYR	conflict	UNP A0A0D3AUD0

- Molecule 34 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1h	38	Total	C	N	O	S	0	0
			309	190	65	49	5		

- Molecule 35 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1i	183	Total	C	N	O	S	0	0
			1424	885	255	274	10		

- Molecule 36 is a protein called 39S ribosomal protein L41-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1j	71	Total	C	N	O	S	0	0
			570	369	102	97	2		

- Molecule 37 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1k	118	Total	C	N	O	S	0	0
			952	599	184	165	4		

- Molecule 38 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1l	211	Total	C	N	O	S	0	0
			1741	1131	286	316	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1l	25	ASP	GLU	conflict	UNP A0A0D3B6Y5
1l	126	LYS	GLU	conflict	UNP A0A0D3B6Y5
1l	154	VAL	LEU	conflict	UNP A0A0D3B6Y5
1l	179	MET	THR	conflict	UNP A0A0D3B6Y5
1l	201	ASP	ASN	conflict	UNP A0A0D3B6Y5
1l	220	PHE	LEU	conflict	UNP A0A0D3B6Y5

- Molecule 39 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1m	122	Total	C	N	O	S	0	0
			970	610	170	184	6		

- Molecule 40 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	1o	76	Total	C	N	O	0	0
			626	397	114	115		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	4	CYS	TYR	conflict	UNP A0A3P6AZ01
1o	63	ARG	GLY	conflict	UNP A0A3P6AZ01

- Molecule 41 is a protein called MRPL25 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	117	Total	C	N	O	S	0	0
			992	626	189	169	8		

- Molecule 42 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	50	Total	C	N	O	S	0	0
			390	243	79	67	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1q	63	ALA	SER	conflict	UNP A0A0D3BIE3

- Molecule 43 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	92	Total	C	N	O	S	0	0
			735	469	139	122	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1r	5	GLY	-	insertion	UNP A0A0D3D0H7
1r	6	VAL	-	insertion	UNP A0A0D3D0H7
1r	20	LEU	PHE	conflict	UNP A0A0D3D0H7
1r	22	LYS	ASN	conflict	UNP A0A0D3D0H7
1r	63	ASP	GLU	conflict	UNP A0A0D3D0H7
1r	130	PRO	ILE	conflict	UNP A0A0D3D0H7
1r	136	PRO	-	insertion	UNP A0A0D3D0H7
1r	137	VAL	-	insertion	UNP A0A0D3D0H7
1r	138	ALA	-	insertion	UNP A0A0D3D0H7
1r	139	ALA	-	insertion	UNP A0A0D3D0H7
1r	140	ALA	-	insertion	UNP A0A0D3D0H7
1r	141	ALA	LEU	conflict	UNP A0A0D3D0H7

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Chain	Residue	Modelled	Actual	Comment	Reference
1r	144	ALA	THR	conflict	UNP A0A0D3D0H7
1r	145	ALA	PRO	conflict	UNP A0A0D3D0H7
1r	149	THR	-	insertion	UNP A0A0D3D0H7
1r	150	THR	-	insertion	UNP A0A0D3D0H7
1r	151	ASP	-	insertion	UNP A0A0D3D0H7
1r	152	LYS	GLU	conflict	UNP A0A0D3D0H7
1r	156	ALA	GLN	conflict	UNP A0A0D3D0H7
1r	157	PHE	THR	conflict	UNP A0A0D3D0H7

- Molecule 44 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	118	Total	C	N	O	S	0	0
			985	617	203	163	2		

- Molecule 45 is a protein called Pentacotripeptide-repeat region of PRORP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1t	484	Total	C	N	O	S	0	0
			3856	2433	665	733	25		

- Molecule 46 is a protein called mL102.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1u	666	Total	C	N	O	S	0	0
			5264	3316	915	991	42		

- Molecule 47 is a protein called mL104.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1v	433	Total	C	N	O	S	0	0
			3440	2173	599	640	28		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	1560	Total	C	N	O	P	0	0
			33425	14925	6097	10843	1560		

- Molecule 49 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	118	Total	C	N	O	P	0	0
			2513	1124	453	819	117		

- Molecule 50 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5	77	Total	C	N	O	P	0	0
			1641	733	294	537	77		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 52 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A	204	Total	C	N	O	S	0	0
			1611	1032	284	285	10		

- Molecule 53 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B	467	Total	C	N	O	S	0	0
			3877	2520	701	643	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 54 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	C	333	Total	C	N	O	S	0	0
			2811	1798	540	462	11		

- Molecule 55 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	D	417	Total	C	N	O	S	0	0
			3425	2146	603	664	12		

- Molecule 56 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 57 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 58 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 59 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	H	213	Total	C	N	O	S	0	0
			1682	1054	312	311	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	50	SER	PRO	conflict	UNP A0A3P6FWE0
H	94	SER	ASN	conflict	UNP A0A3P6FWE0

- Molecule 60 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 61 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	J	127	Total	C	N	O	S	0	0
			988	608	195	181	4		

- Molecule 62 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	K	124	Total	C	N	O	S	0	0
			992	613	208	167	4		

- Molecule 63 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	L	119	Total	C	N	O	S	0	0
			940	572	200	163	5		

- Molecule 64 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	M	101	Total	C	N	O	S	0	0
			843	524	174	140	5		

- Molecule 65 is a protein called Small ribosomal subunit protein uS15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	N	116	Total	C	N	O	S	0	0
			941	593	170	171	7		

- Molecule 66 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	O	110	Total	C	N	O	S	0	0
			869	550	169	144	6		

- Molecule 67 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	P	91	Total	C	N	O	S	0	0
			717	455	135	124	3		

- Molecule 68 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

- Molecule 69 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 70 is a protein called Ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 71 is a protein called 30S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 72 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	127	Total	C	N	O	S	0	0
			1014	647	184	178	5		

- Molecule 73 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 74 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 75 is a protein called mS31/mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 76 is a protein called MOSC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 77 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Z	80	Total	C	N	O	S	0	0
			649	422	121	104	2		

- Molecule 78 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	a	315	Total	C	N	O	S	0	0
			2487	1547	448	482	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	186	GLU	ASP	conflict	UNP A0A3P6FE97
a	239	ALA	PRO	conflict	UNP A0A3P6FE97

- Molecule 79 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	b	77	Total	C	N	O	S	0	0
			610	378	116	108	8		

- Molecule 80 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 81 is a protein called Small ribosomal subunit protein mS41 SAM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 82 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 83 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	f	377	Total	C	N	O	S	0	0
			2922	1843	486	573	20		

- Molecule 84 is a protein called Adenylyl cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	h	310	Total	C	N	O	S	0	0
			2460	1551	436	458	15		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	?	-	THR	deletion	UNP A0A3P6FIH7
h	?	-	ILE	deletion	UNP A0A3P6FIH7
h	?	-	SER	deletion	UNP A0A3P6FIH7
h	?	-	SER	deletion	UNP A0A3P6FIH7
h	?	-	PHE	deletion	UNP A0A3P6FIH7
h	?	-	HIS	deletion	UNP A0A3P6FIH7
h	?	-	ALA	deletion	UNP A0A3P6FIH7
h	?	-	PHE	deletion	UNP A0A3P6FIH7
h	?	-	LEU	deletion	UNP A0A3P6FIH7
h	?	-	GLN	deletion	UNP A0A3P6FIH7
h	?	-	TRP	deletion	UNP A0A3P6FIH7
h	?	-	VAL	deletion	UNP A0A3P6FIH7
h	?	-	PHE	deletion	UNP A0A3P6FIH7
h	?	-	LEU	deletion	UNP A0A3P6FIH7
h	?	-	TYR	deletion	UNP A0A3P6FIH7
h	?	-	ALA	deletion	UNP A0A3P6FIH7
h	152	GLN	ARG	conflict	UNP A0A3P6FIH7
h	189	MET	LEU	conflict	UNP A0A3P6FIH7
h	190	MET	LEU	conflict	UNP A0A3P6FIH7

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Chain	Residue	Modelled	Actual	Comment	Reference
h	203	GLU	ASP	conflict	UNP A0A3P6FIH7
h	330	LYS	PHE	conflict	UNP A0A3P6FIH7
h	331	GLU	LYS	conflict	UNP A0A3P6FIH7

- Molecule 85 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	i	306	Total 2487	C 1567	N 419	O 487	S 14	0	0

- Molecule 86 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	k	47	Total 314	C 194	N 61	O 55	S 4	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	23	SER	ALA	conflict	UNP A0A3P6FEP3
k	38	ILE	LEU	conflict	UNP A0A3P6FEP3
k	46	SER	THR	conflict	UNP A0A3P6FEP3
k	50	GLU	ASP	conflict	UNP A0A3P6FEP3
k	51	LEU	ILE	conflict	UNP A0A3P6FEP3

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	1	251	Total 251	Mg 251	0
87	1D	1	Total 1	Mg 1	0
87	1j	1	Total 1	Mg 1	0
87	1q	1	Total 1	Mg 1	0
87	2	97	Total 97	Mg 97	0
87	3	3	Total 3	Mg 3	0
87	D	1	Total 1	Mg 1	0

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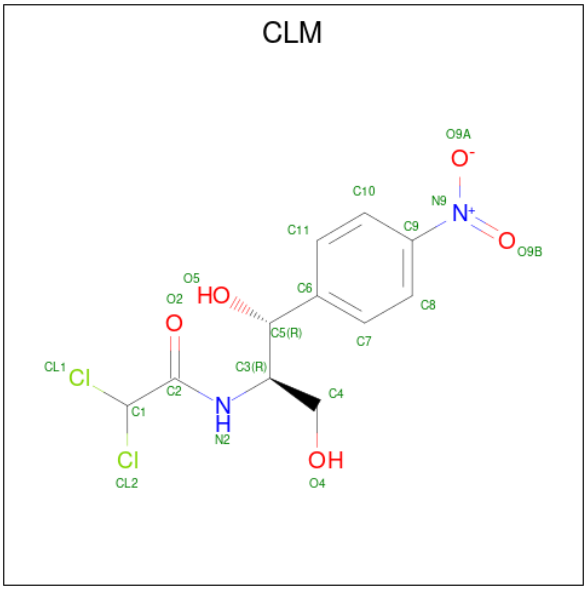
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Mol	Chain	Residues	Atoms	AltConf
87	T	1	Total Mg 1 1	0
87	W	1	Total Mg 1 1	0

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
88	1	57	Total K 57 57	0
88	1B	2	Total K 2 2	0
88	1E	1	Total K 1 1	0
88	2	14	Total K 14 14	0

- Molecule 89 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).

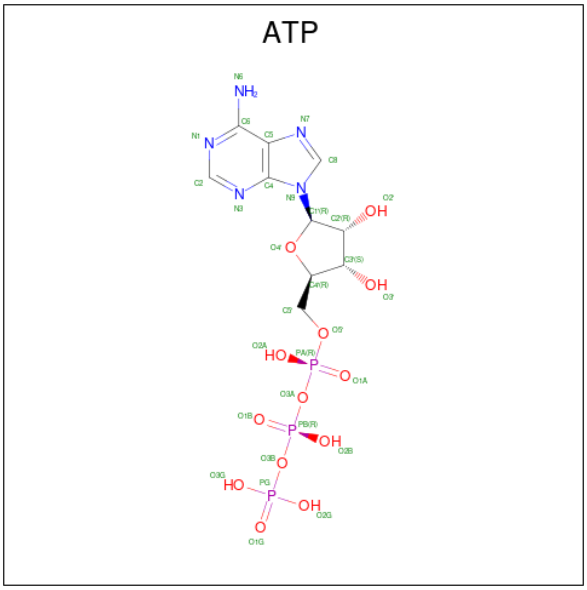


Mol	Chain	Residues	Atoms	AltConf
89	1	1	Total C Cl N O 20 11 2 2 5	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
90	1d	1	Total Zn 1 1	0
90	1h	1	Total Zn 1 1	0

- Molecule 91 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
91	W	1	Total C N O P 31 10 5 13 3	0

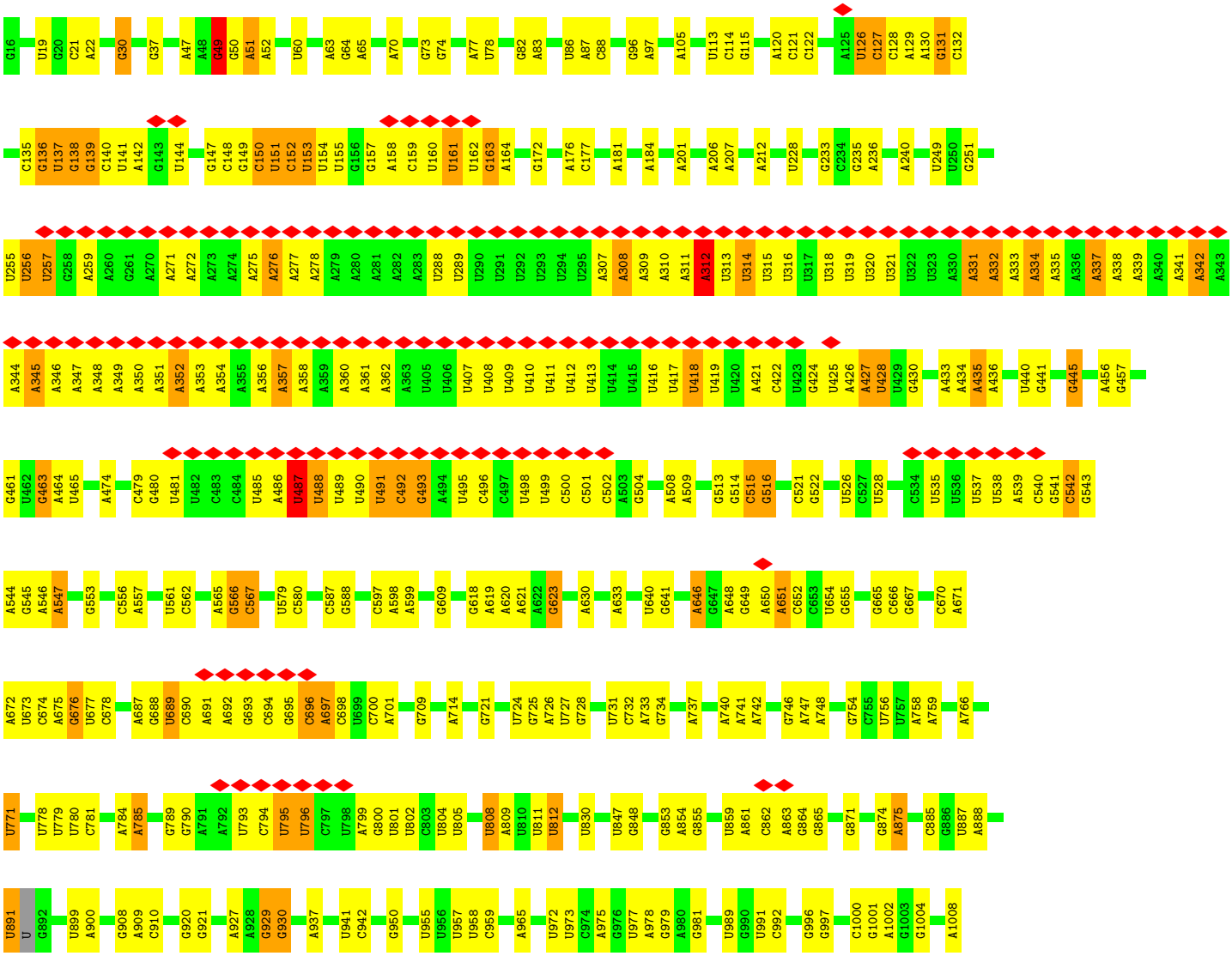
3 Residue-property plots (i)

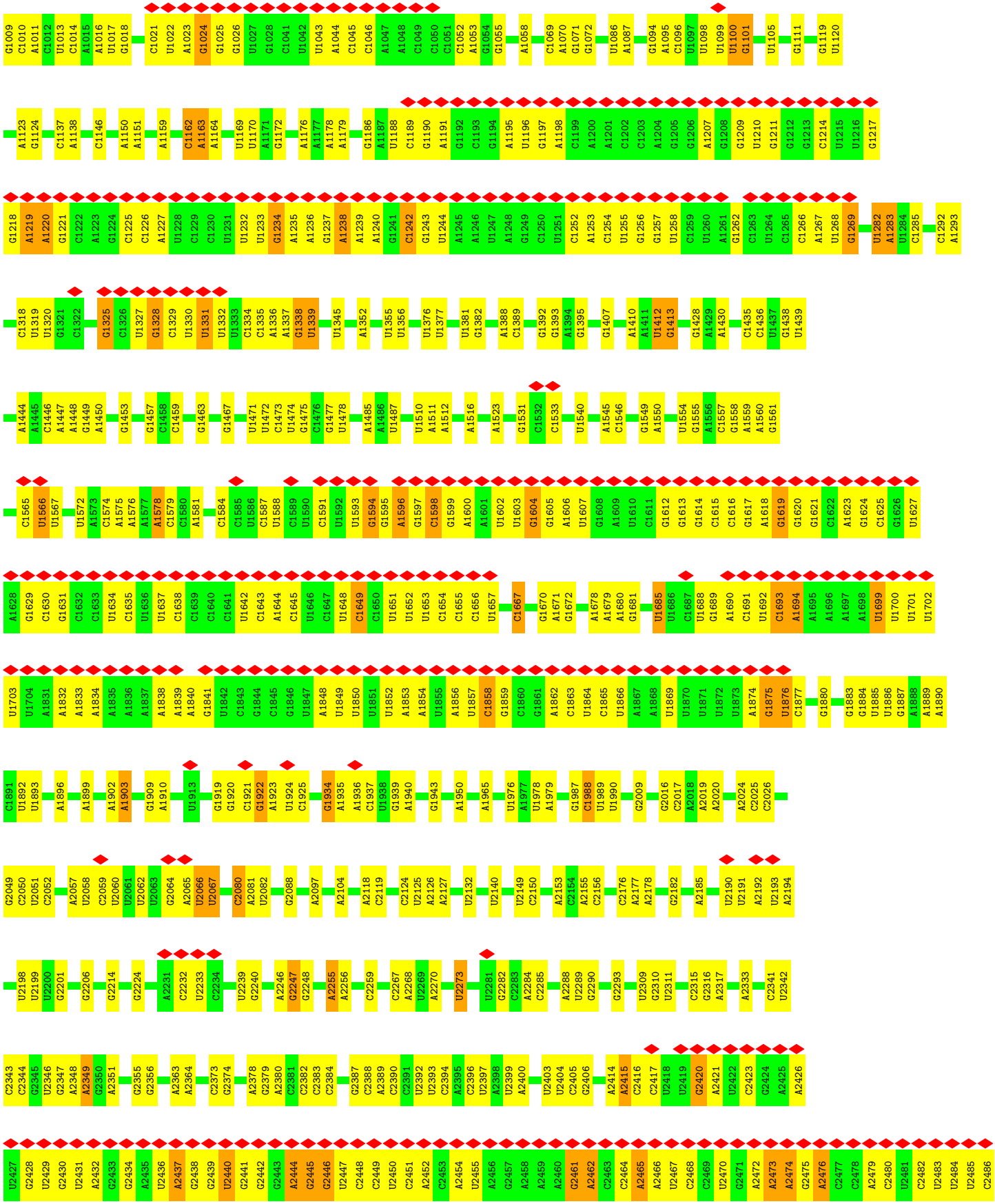
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

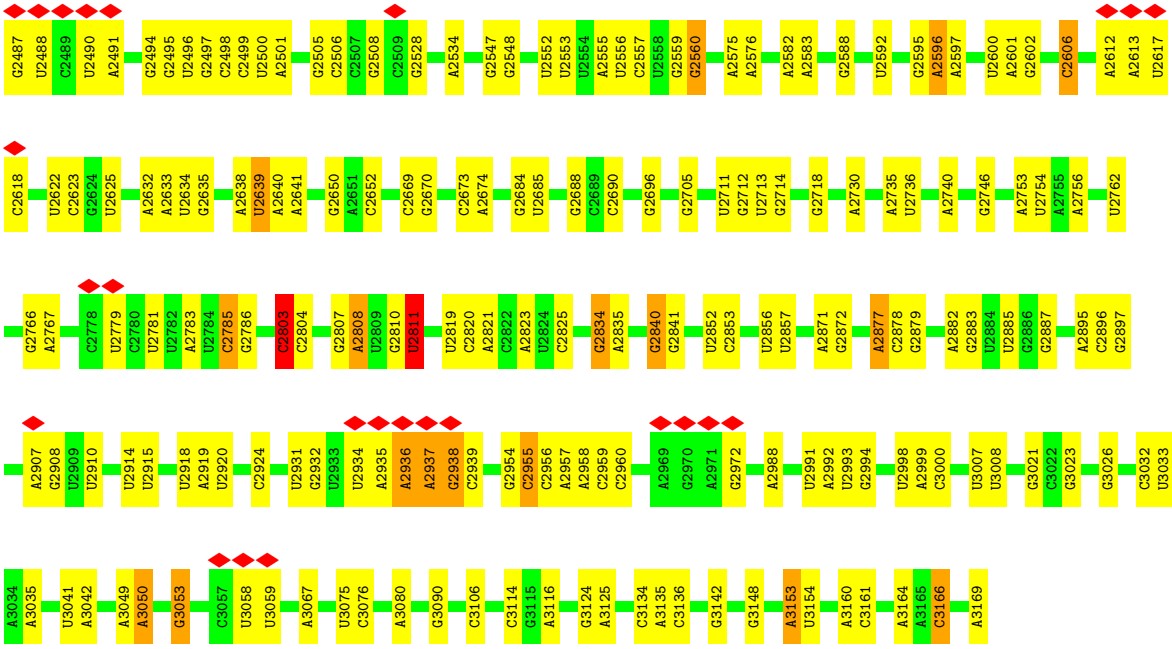
- Molecule 1: 26S rRNA

Chain 1:





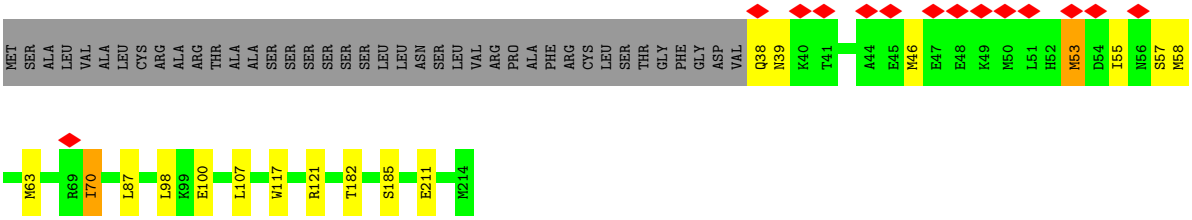

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A1628 G1629 C1630 G1631 C1632 C1633 U1634 C1635 U1636 U1637 C1638 C1639 C1640 C1641 U1642 C1643 A1644 C1645 U1646 C1647 U1648 C1649 C1650 U1651 U1652 U1653 C1654 C1655 C1656 U1657 C1687 G1670 A1671 G1672 A1678 A1679 A1680 G1681 U1685 U1686 C1687 U1688 G1689 A1690 C1691 U1692 C1693 A1694 A1695 A1696 A1697 A1698 U1699 U1700 U1701 U1702
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U2198 U2199 U2200 G2201 G2206 G2214 G2224 A2231 C2232 U2233 C2234 U2239 G2240 A2246 G2247 G2248 A2255 A2256 C2259 C2267 A2268 U2269 A2270 U2273 U2281 G2282 C2283 A2284 C2285 A2288 U2289 G2290 G2293 U2309 G2310 U2311 C2315 G2316 A2317 A2333 C2341 U2342
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• Molecule 2: Large ribosomal subunit protein uL2 C-terminal domain-containing protein

Chain 1B:

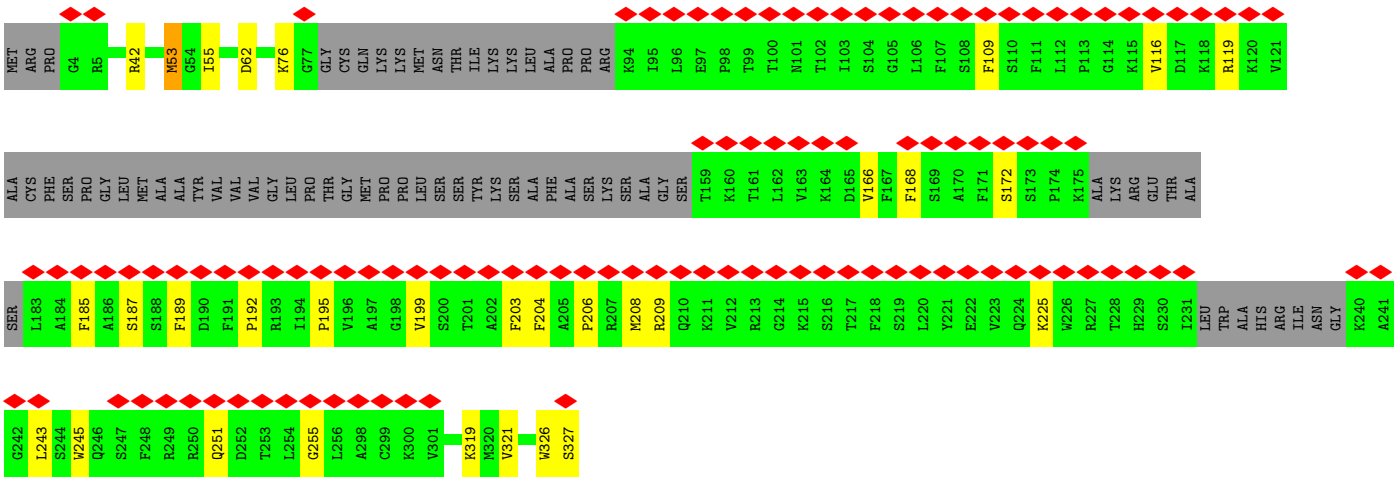




• Molecule 3: uL2m N-ter mitochondrial

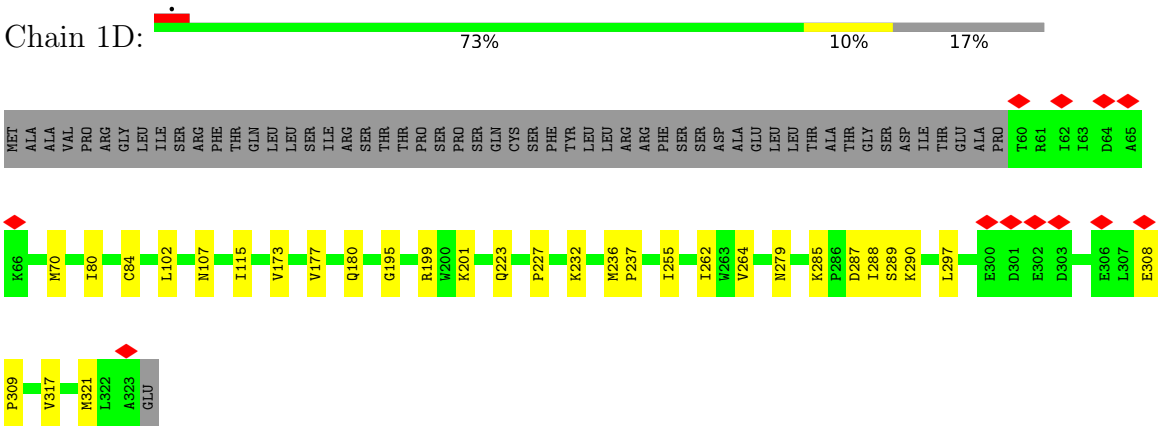
Chain 1C:





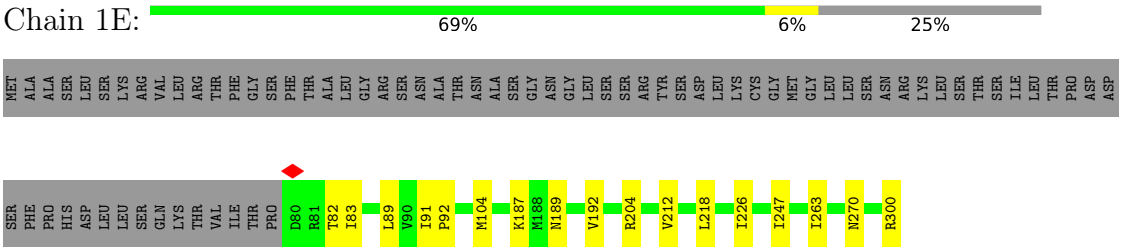
• Molecule 4: 50S ribosomal protein L3-2, chloroplastic

Chain 1D:



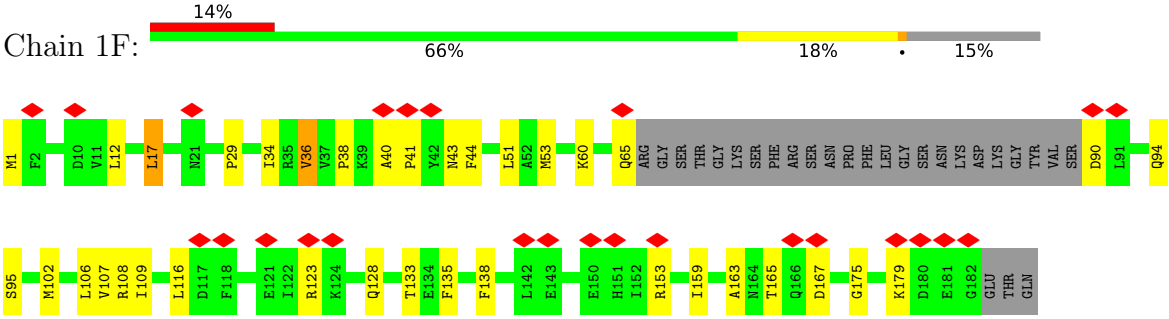
• Molecule 5: Large ribosomal subunit protein uL4m

Chain 1E:



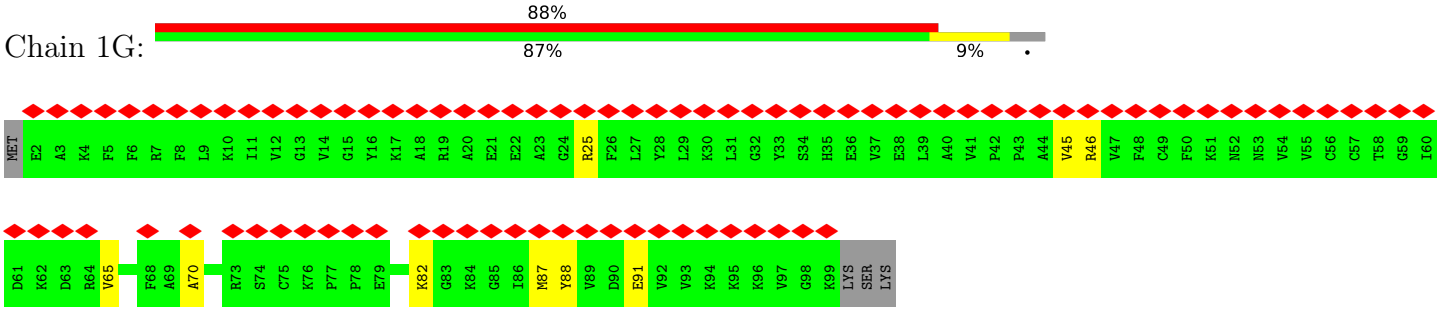
• Molecule 6: Large ribosomal subunit protein uL5m

Chain 1F:



• Molecule 7: Large ribosomal subunit protein uL6 alpha-beta domain-containing protein

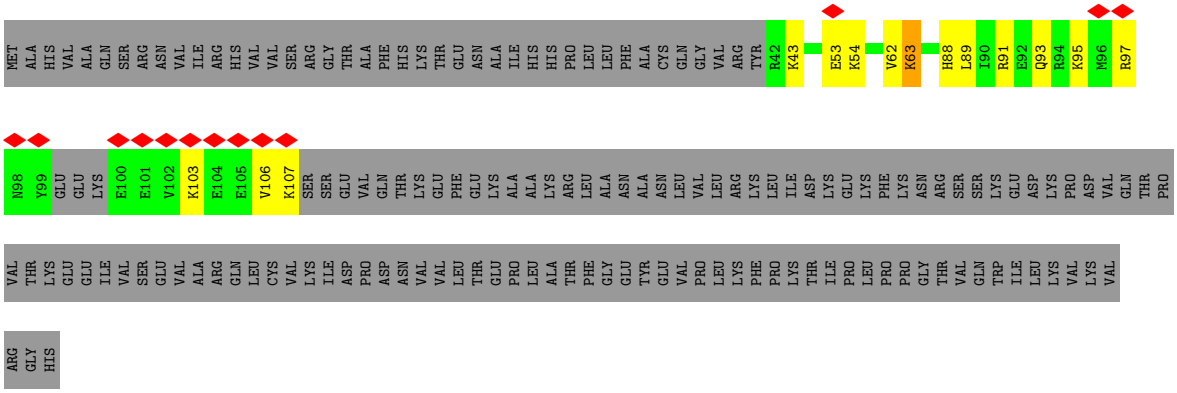
Chain 1G:



• Molecule 8: Large ribosomal subunit protein bL9c

Chain 1H:

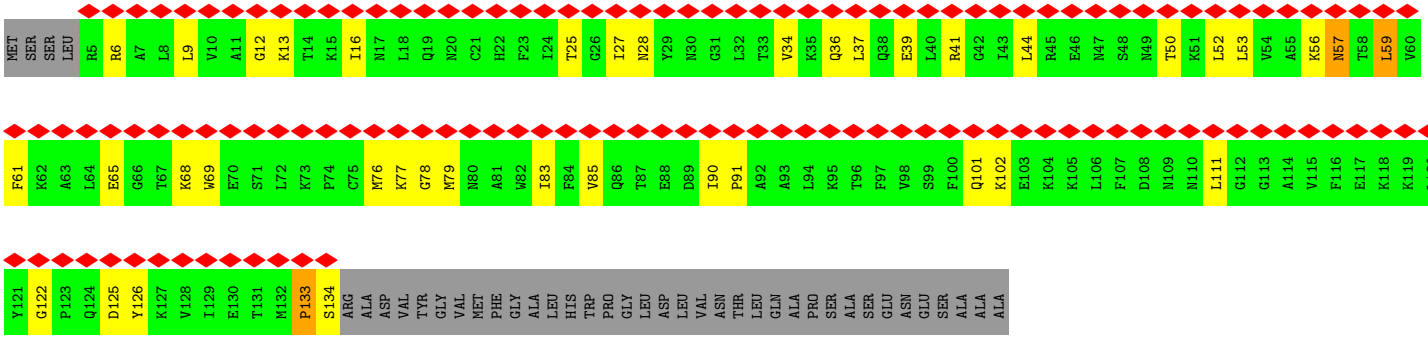




• Molecule 9: Large ribosomal subunit protein uL10c

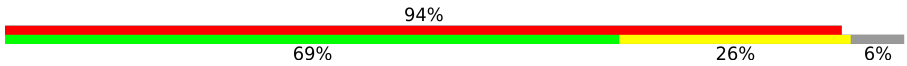
Chain 1I:

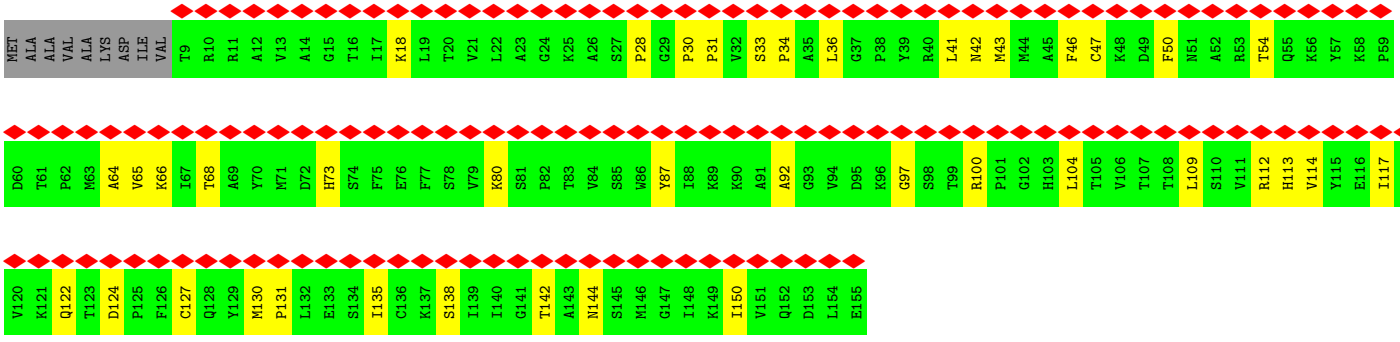




• Molecule 10: Large ribosomal subunit protein uL11m

Chain 1J:

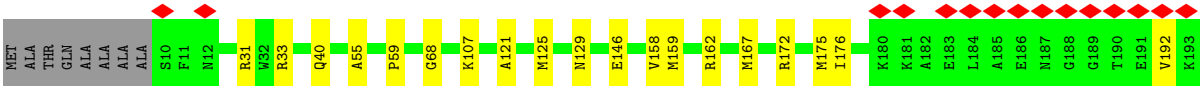


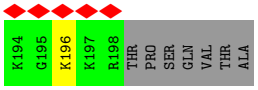


• Molecule 11: 50S ribosomal protein L13

Chain 1K:





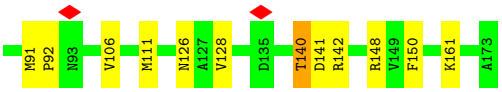


• Molecule 12: uL14m

Chain 1L:



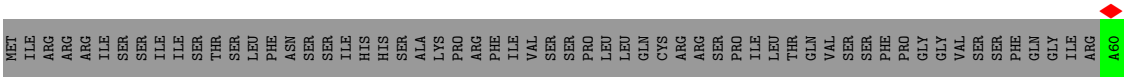


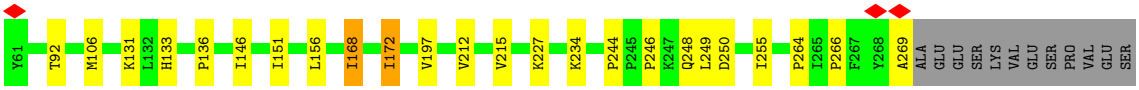


• Molecule 13: Large ribosomal subunit protein uL15/eL18 domain-containing protein

Chain 1M:



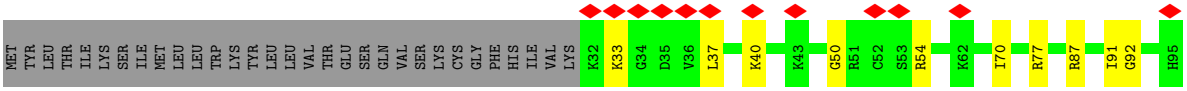


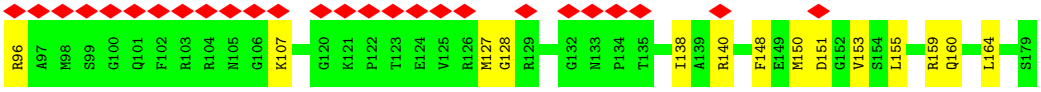


• Molecule 14: Large ribosomal subunit protein uL16m|

Chain 1N:



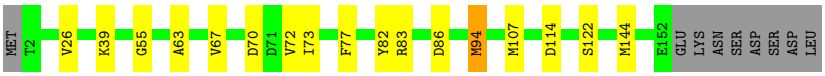




• Molecule 15: 50S ribosomal protein L17

Chain 1O:

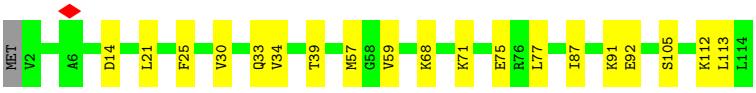




• Molecule 16: Ribosomal protein L18e/L15P domain-containing protein

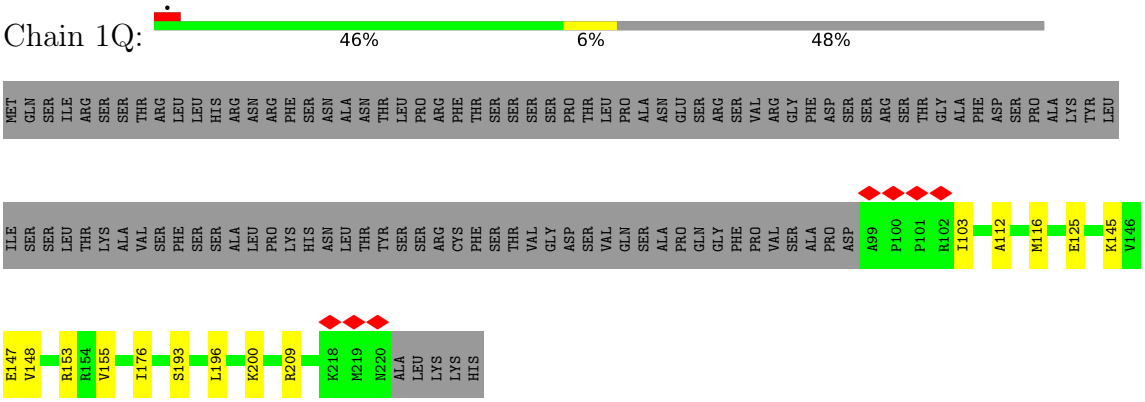
Chain 1P:





• Molecule 17: bL19m

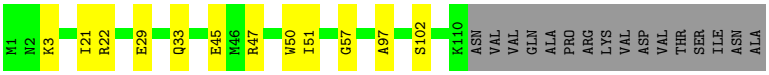
Chain 1Q:



• Molecule 18: 50S ribosomal protein L20

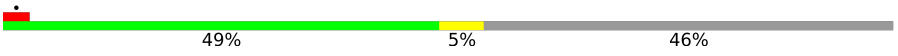
Chain 1R:

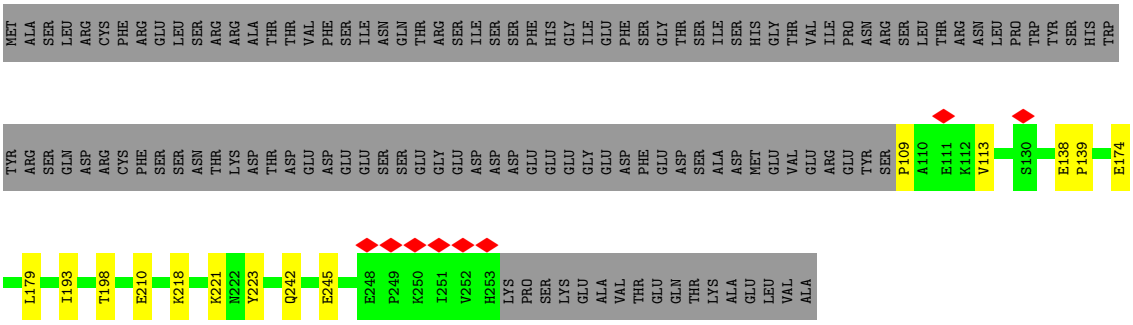




• Molecule 19: bL21m

Chain 1S:

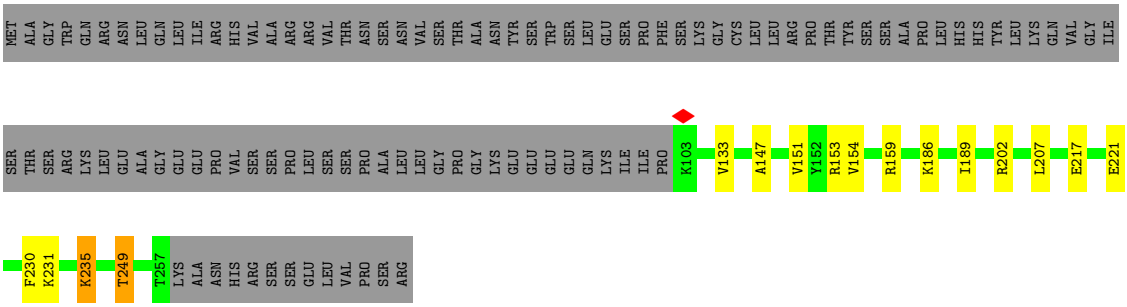




• Molecule 20: Large ribosomal subunit protein uL22c

Chain 1T:

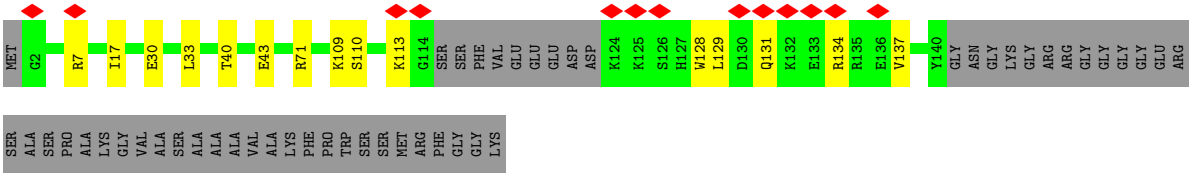




• Molecule 21: Large ribosomal subunit protein uL23m

Chain 1U:

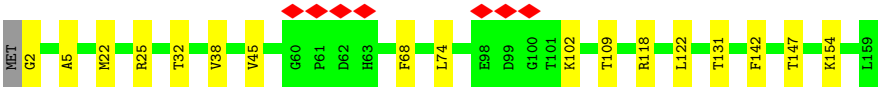




• Molecule 22: KOW domain-containing protein

Chain 1V:



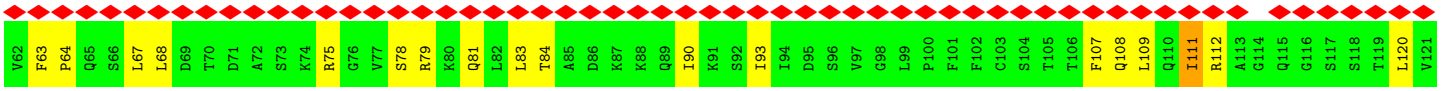


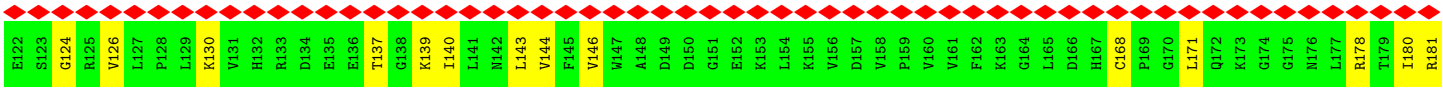
• Molecule 23: bL25-2m

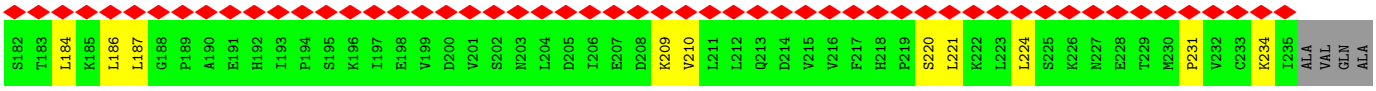
Chain 1W:







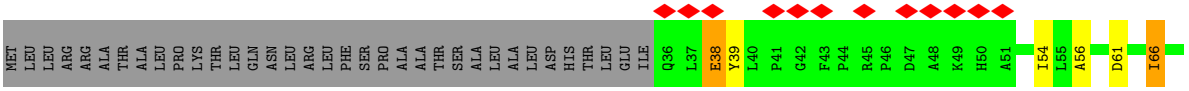


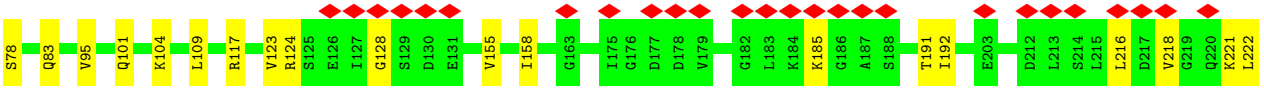


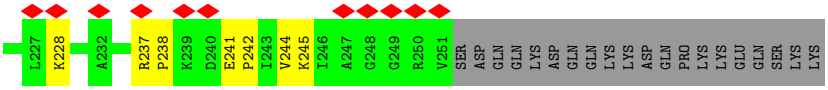
• Molecule 24: bL25m

Chain 1X:





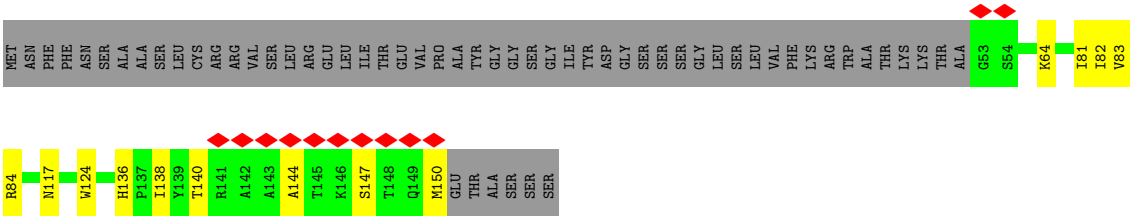




• Molecule 25: 50S ribosomal protein L27

Chain 1Y:

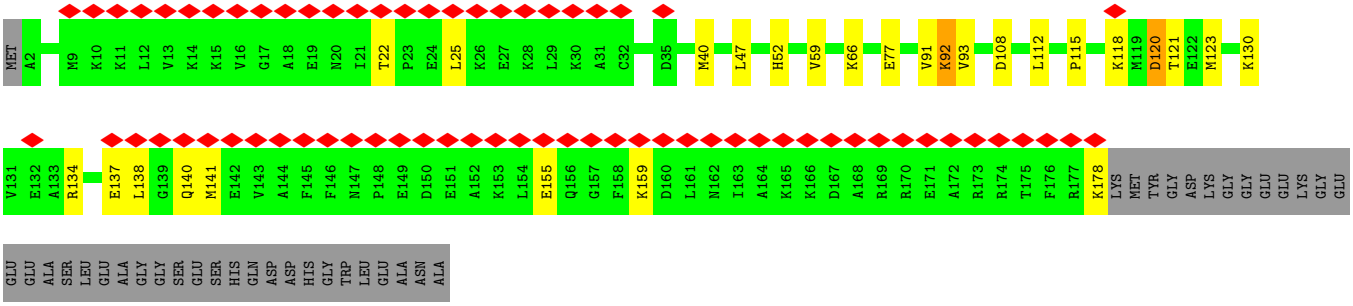




• Molecule 26: Large ribosomal subunit protein bL28m

Chain 1Z:

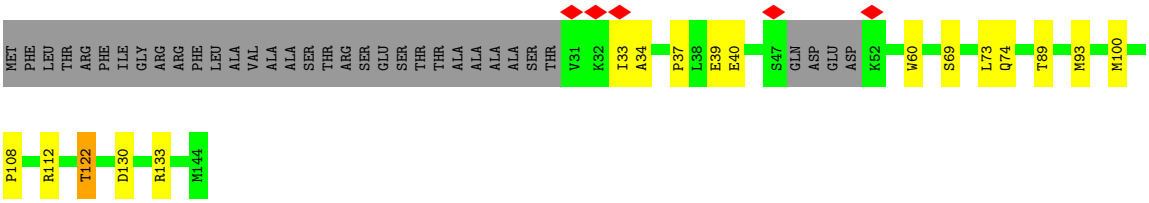




• Molecule 27: Cation-transporting P-type ATPase N-terminal domain-containing protein

Chain 1a:

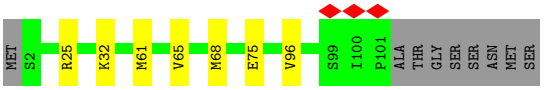




• Molecule 28: Large ribosomal subunit protein uL30m

Chain 1b:

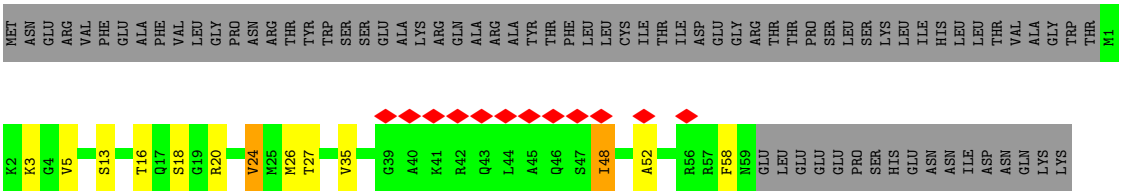




• Molecule 29: bL31m

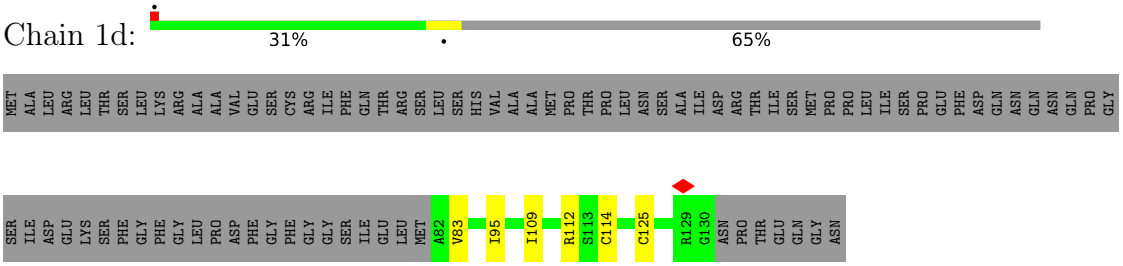
Chain 1c:





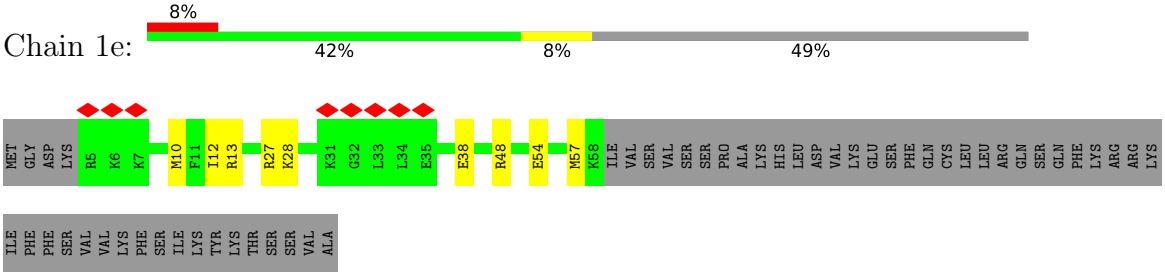
• Molecule 30: Large ribosomal subunit protein bL32m

Chain 1d:



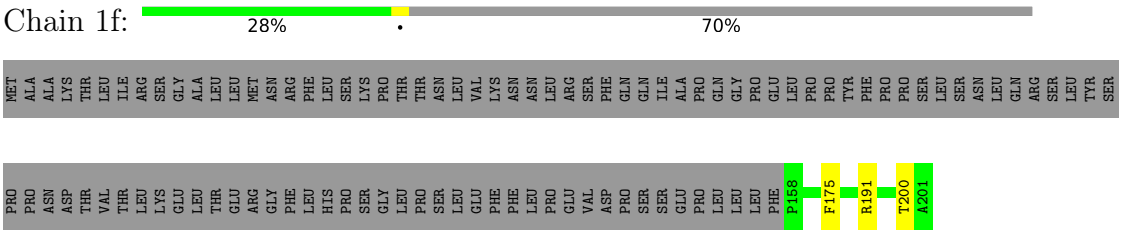
• Molecule 31: bL33m

Chain 1e:



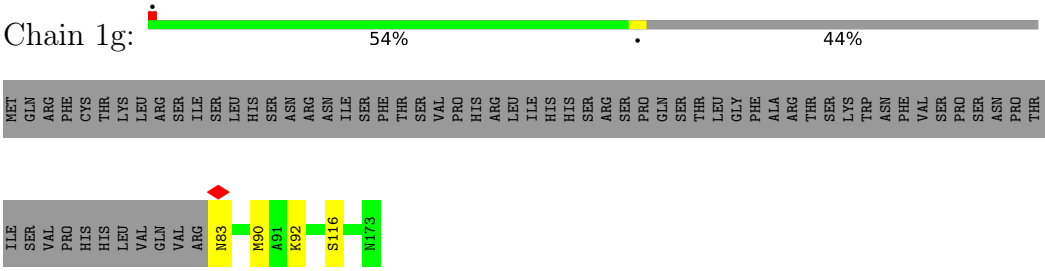
• Molecule 32: Large ribosomal subunit protein bL34m

Chain 1f:



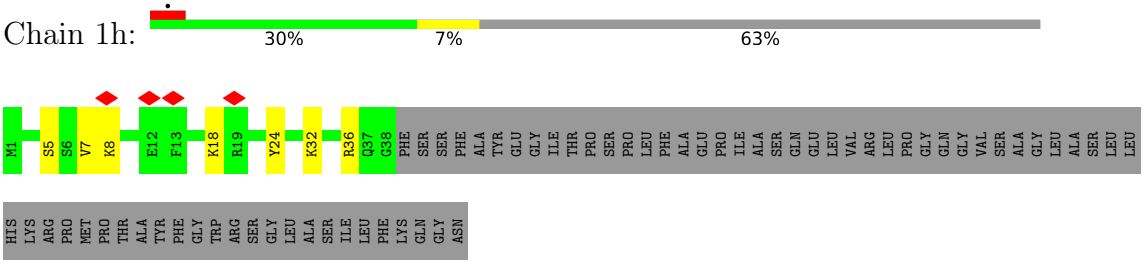
• Molecule 33: 50S ribosomal protein L35

Chain 1g:



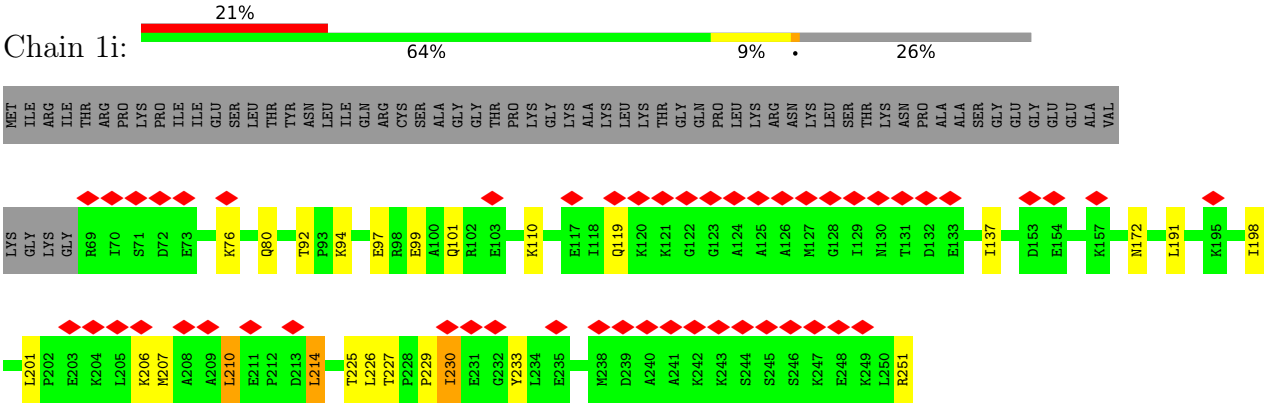
• Molecule 34: Ribosomal protein

Chain 1h:



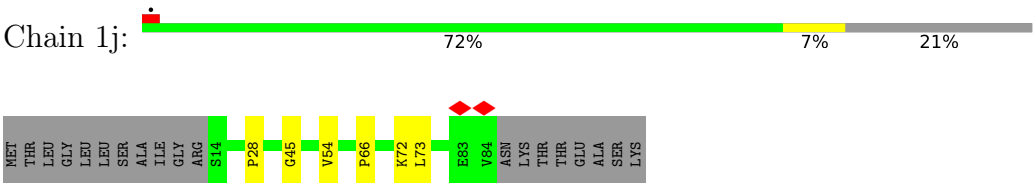
• Molecule 35: mL40

Chain 1i:



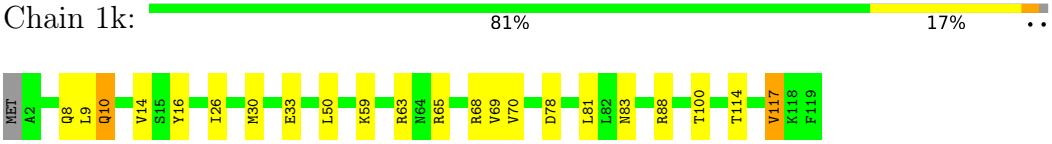
• Molecule 36: 39S ribosomal protein L41-A, mitochondrial

Chain 1j:



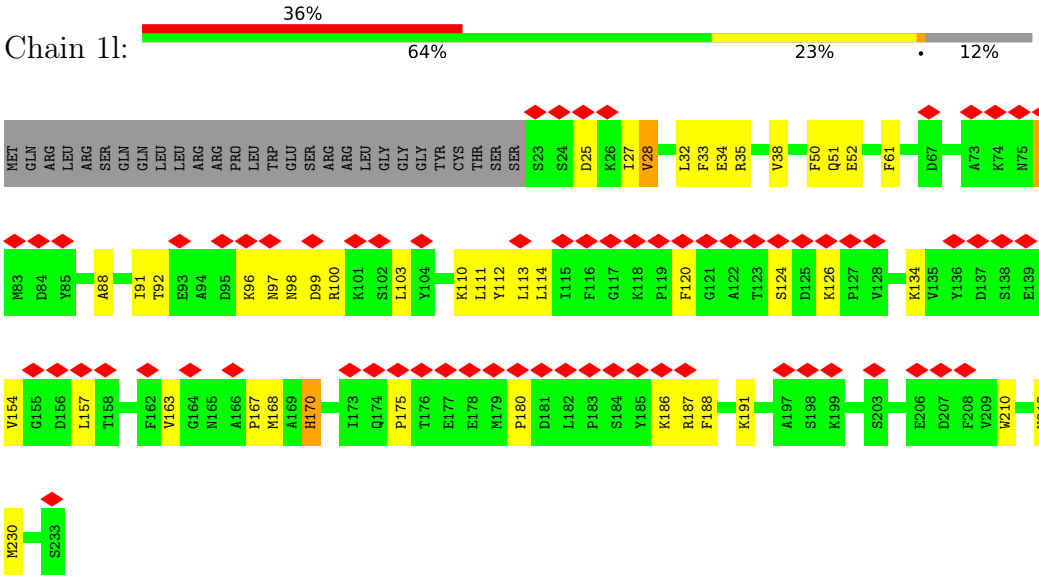
• Molecule 37: Large ribosomal subunit protein mL43

Chain 1k:



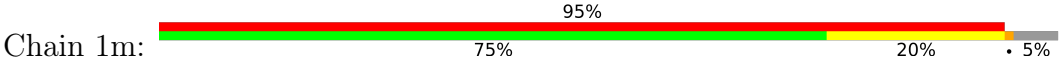
• Molecule 38: Large ribosomal subunit protein mL46

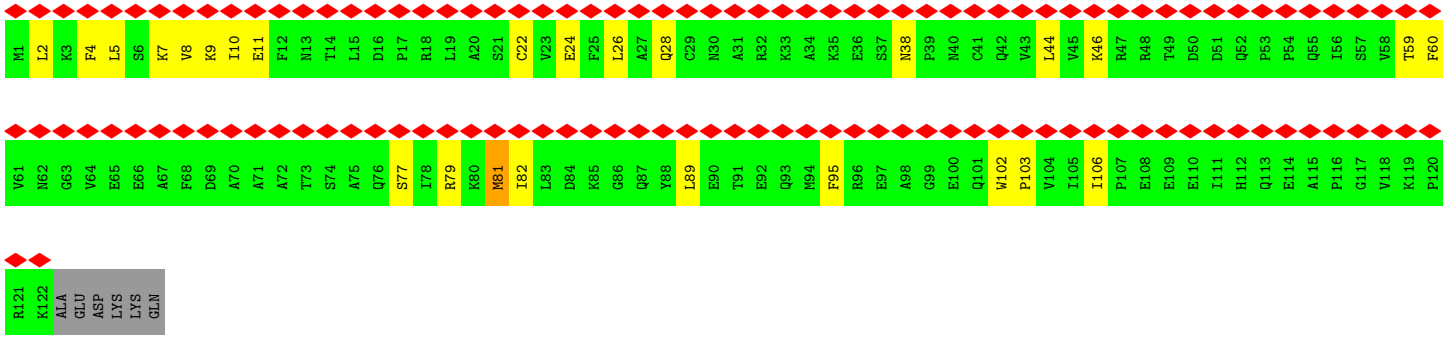
Chain 1l:



• Molecule 39: Large ribosomal subunit protein mL53

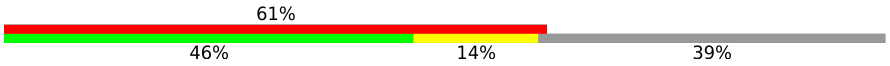
Chain 1m:

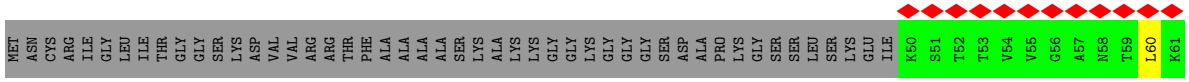


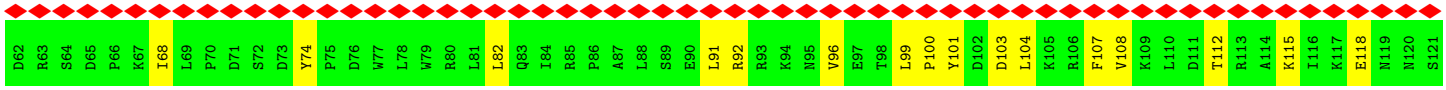


• Molecule 40: Large ribosomal subunit protein mL54

Chain 1o:







• Molecule 41: MRPL25 domain-containing protein

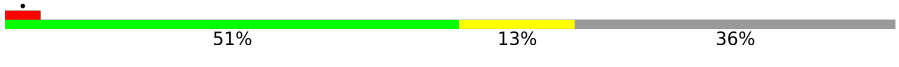
Chain 1p:

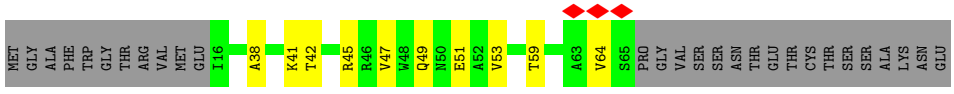




• Molecule 42: mL60

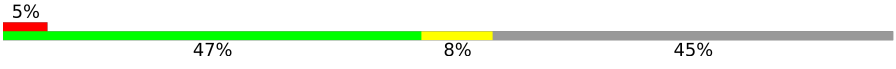
Chain 1q:

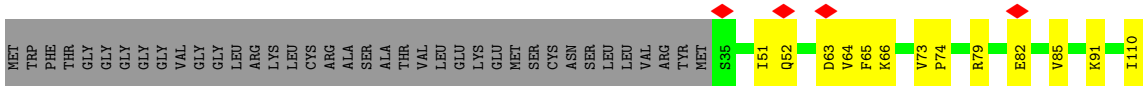


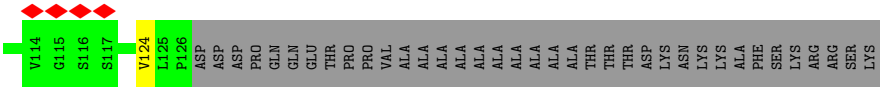


• Molecule 43: mL80

Chain 1r:



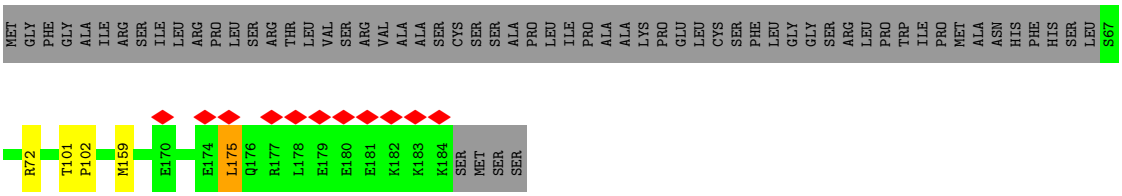




• Molecule 44: mL87

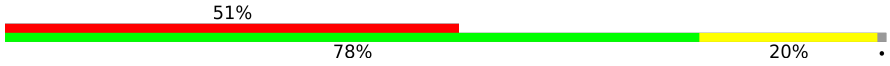
Chain 1s:



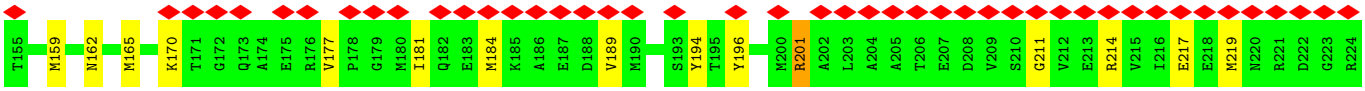


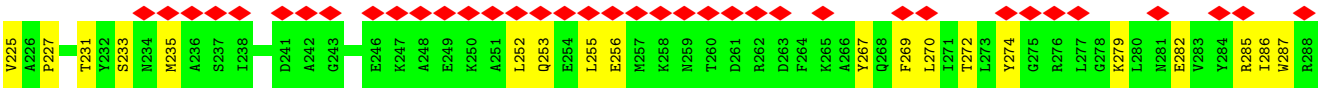
• Molecule 45: Pentacotripeptide-repeat region of PRORP domain-containing protein

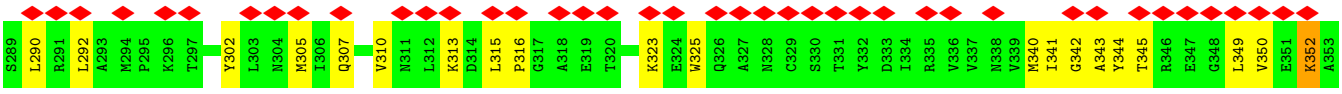
Chain 1t:

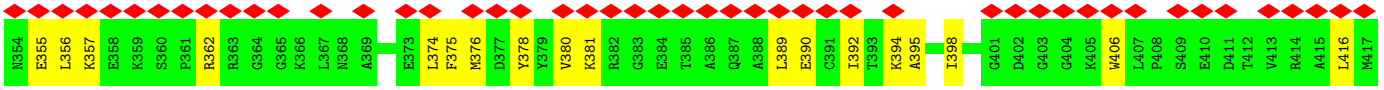


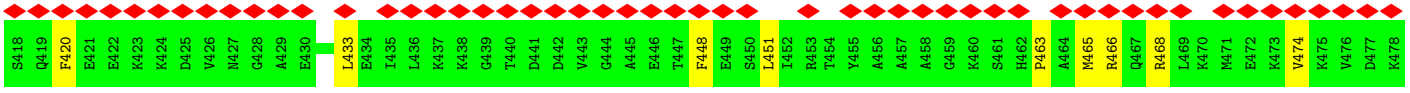


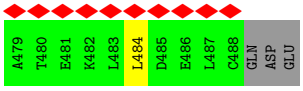










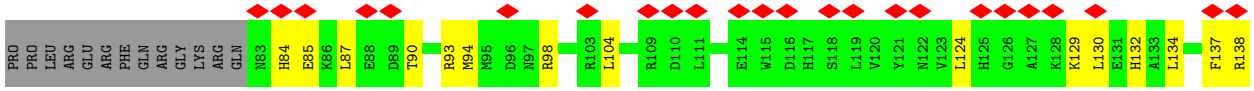


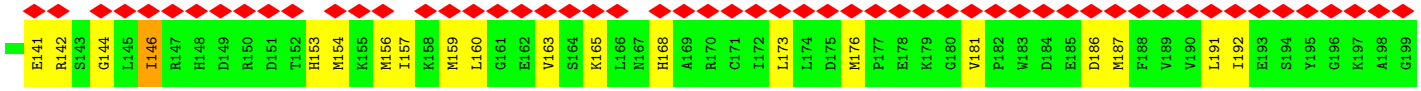
• Molecule 46: mL102

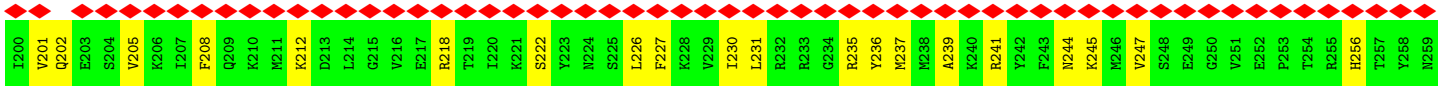
Chain 1u:

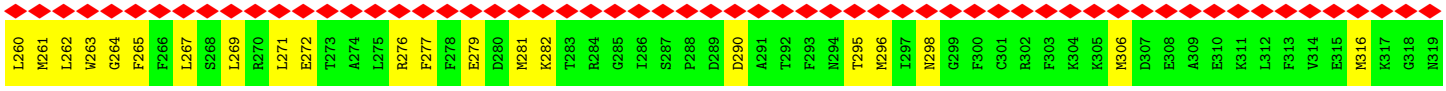


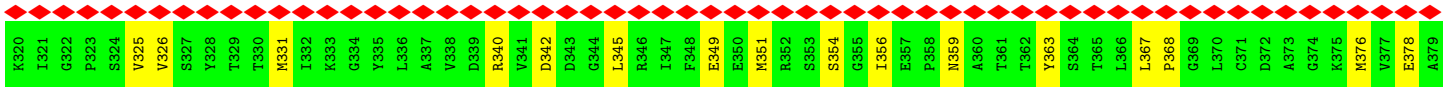


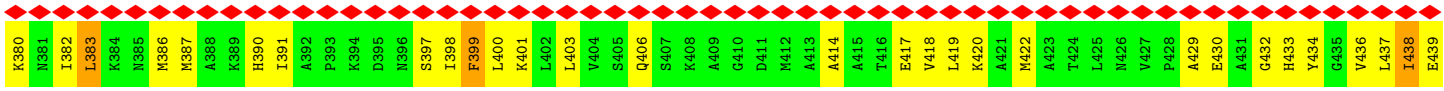


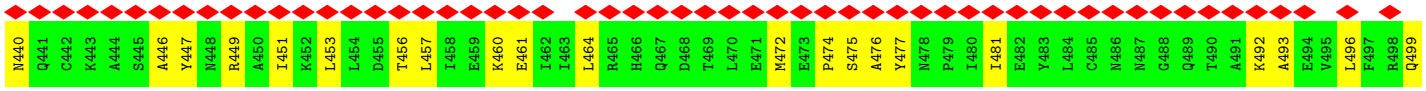


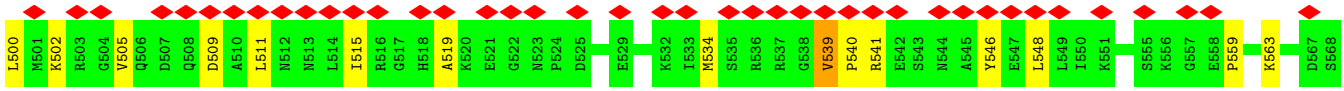


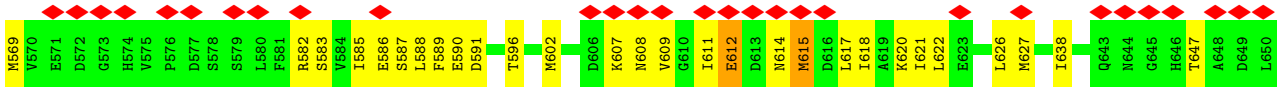


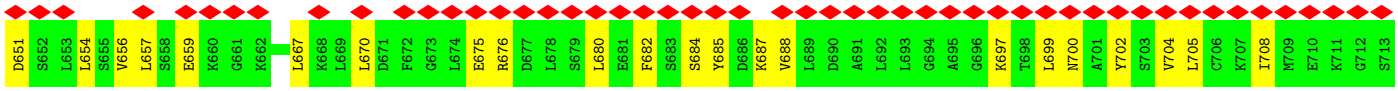


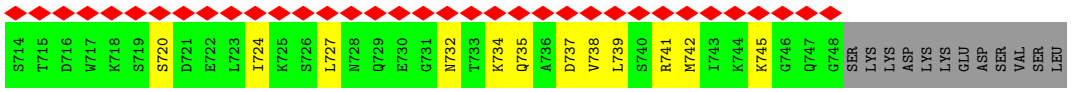








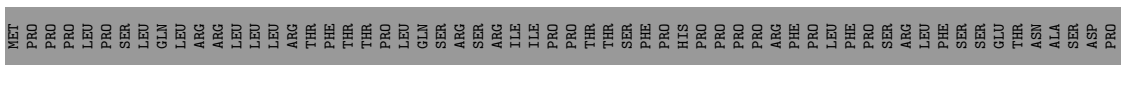


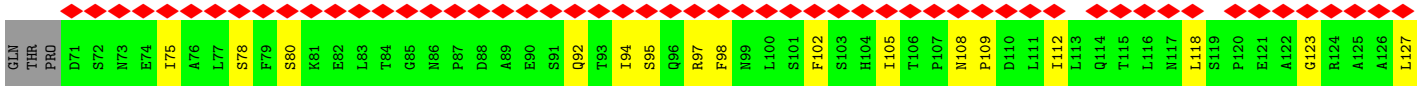


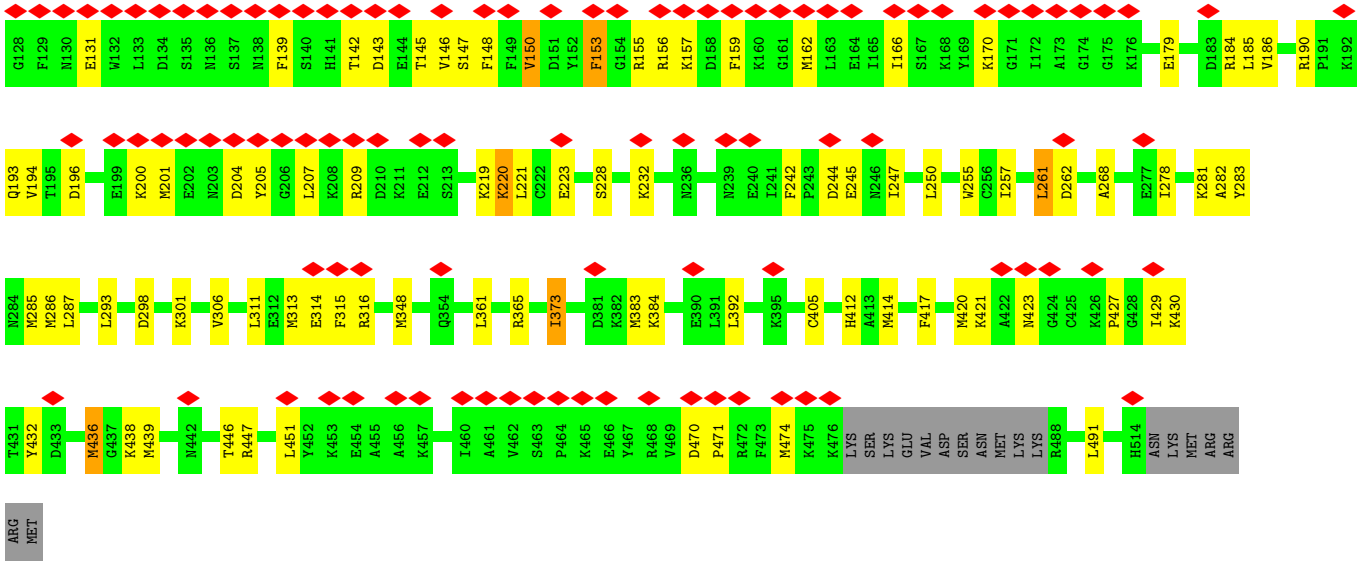
• Molecule 47: mL104

Chain 1v:





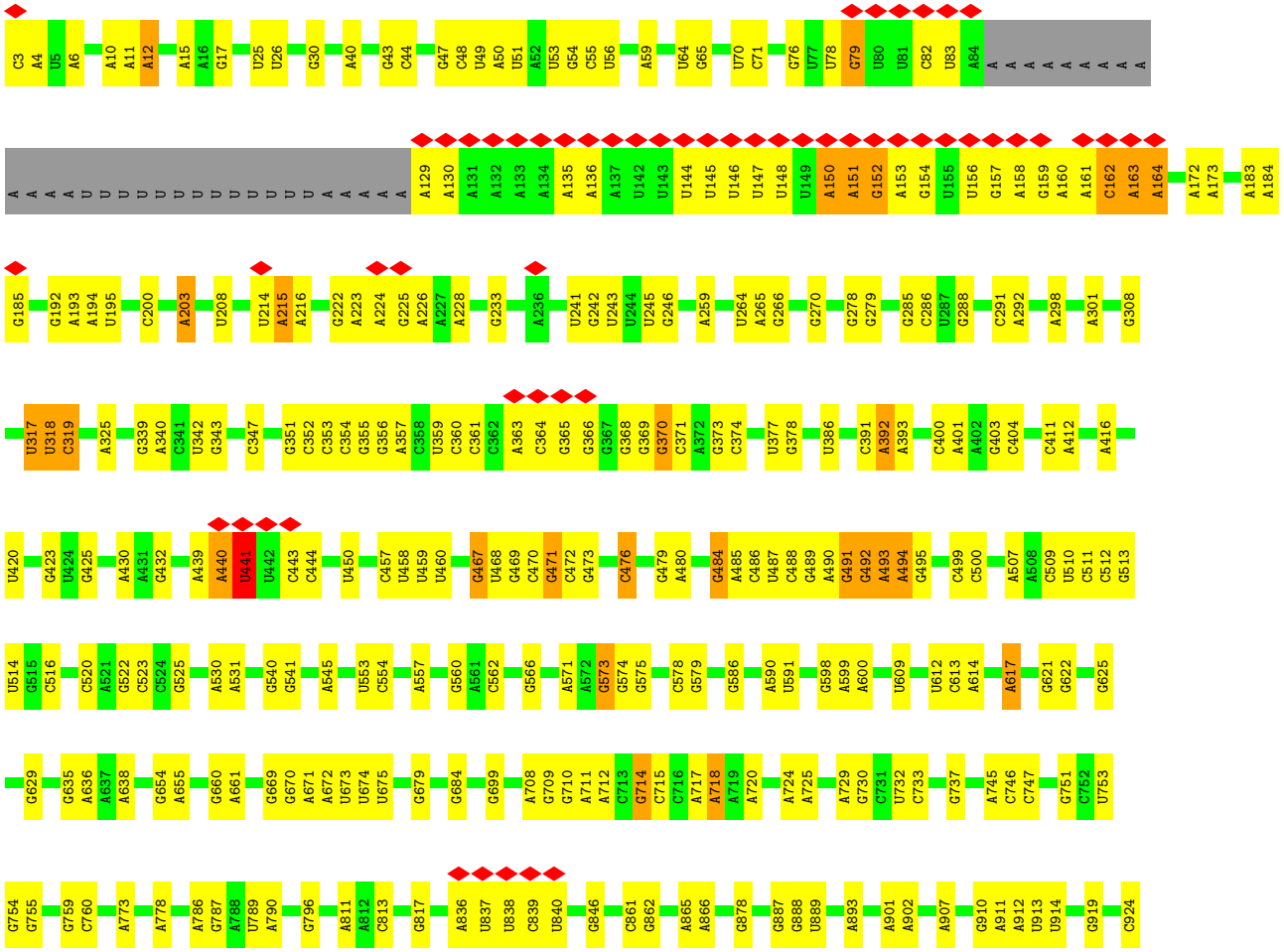


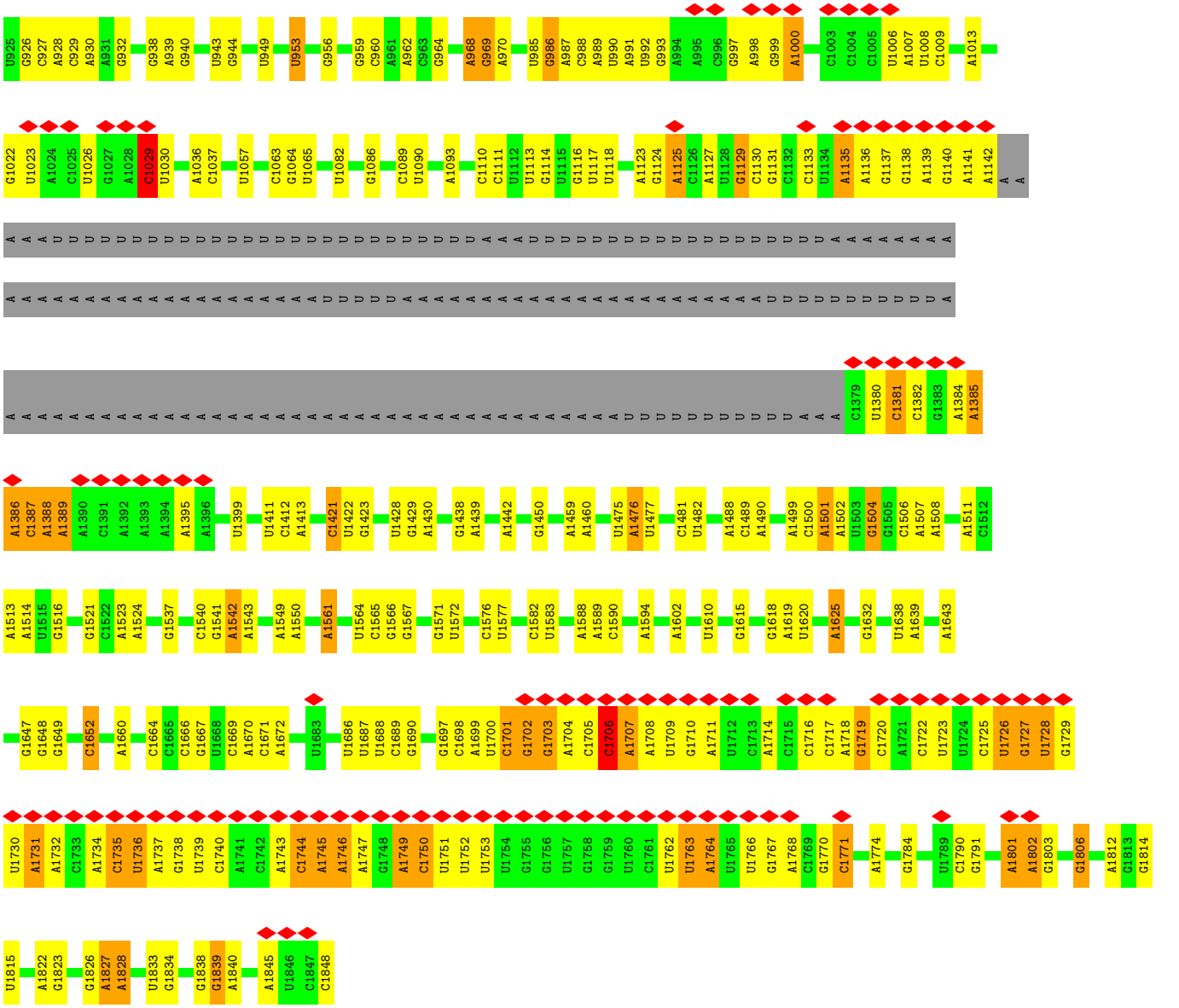


• Molecule 48: 18S rRNA

Chain 2:



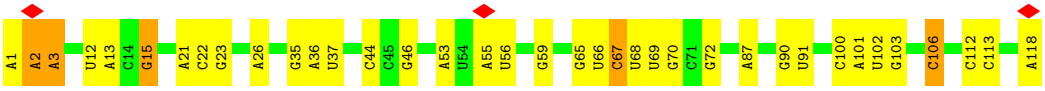




• Molecule 49: 5S rRNA

Chain 3:

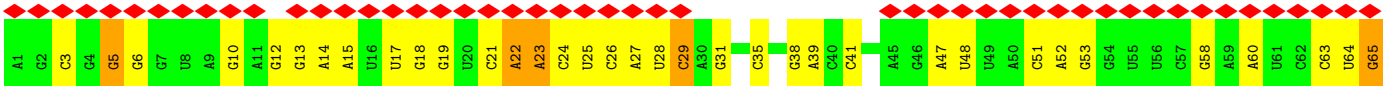


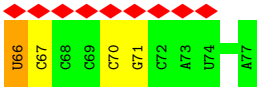


• Molecule 50: tRNA

Chain 5:



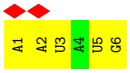




• Molecule 51: mRNA

Chain 6:

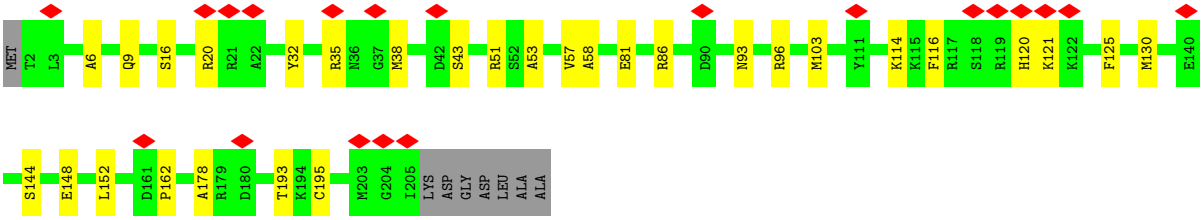




• Molecule 52: Ribosomal protein S2

Chain A:

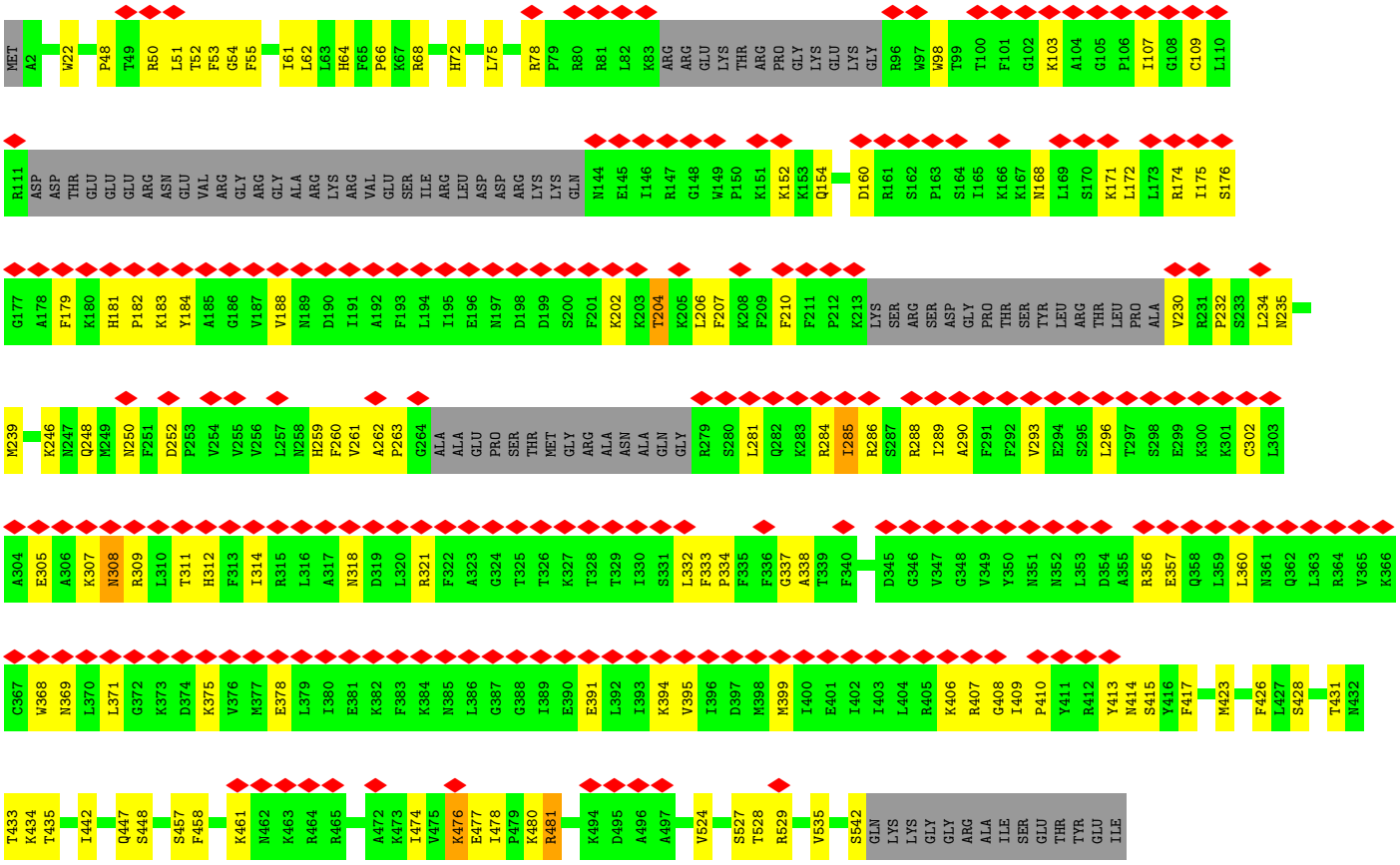




• Molecule 53: Small ribosomal subunit protein uS3m

Chain B:

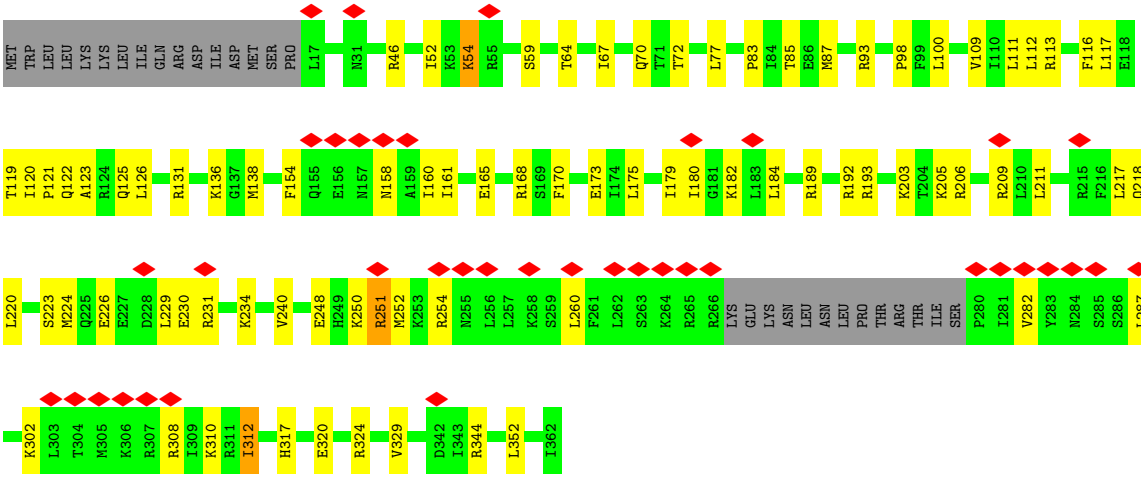




• Molecule 54: uS4m

Chain C:

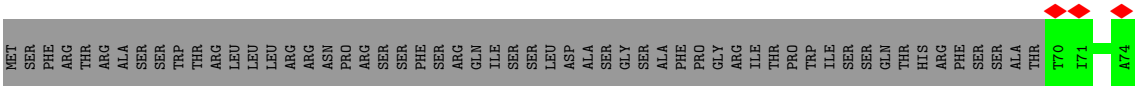


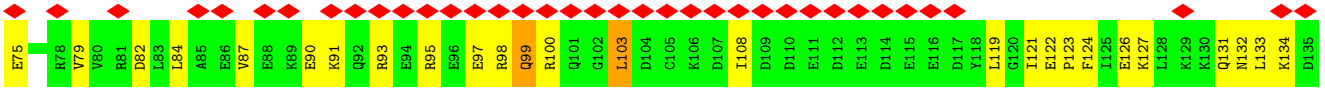


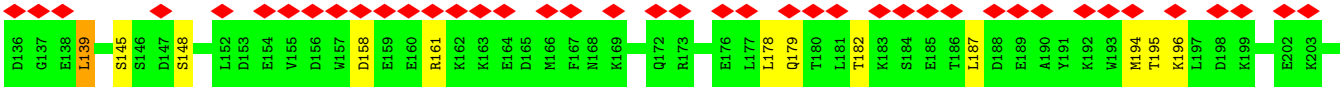
• Molecule 55: S5 DRBM domain-containing protein

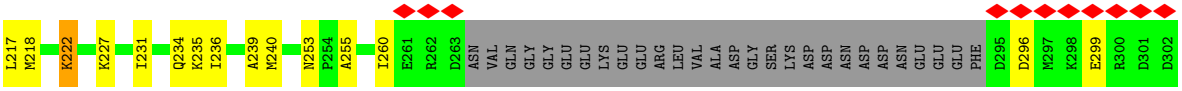
Chain D:

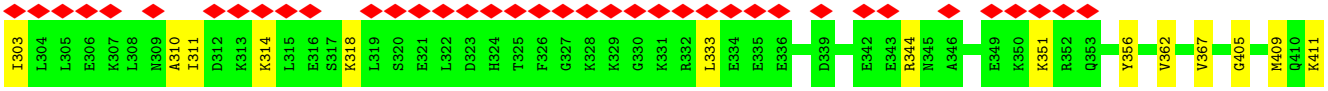










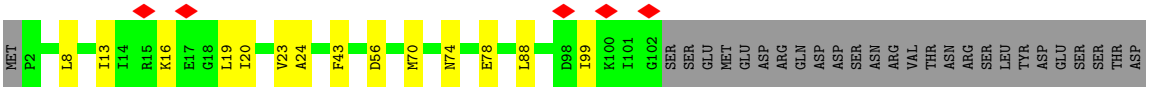




• Molecule 56: bS6m

Chain E:

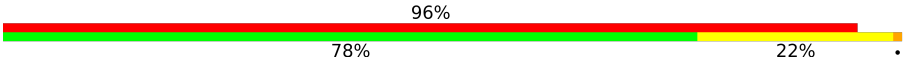


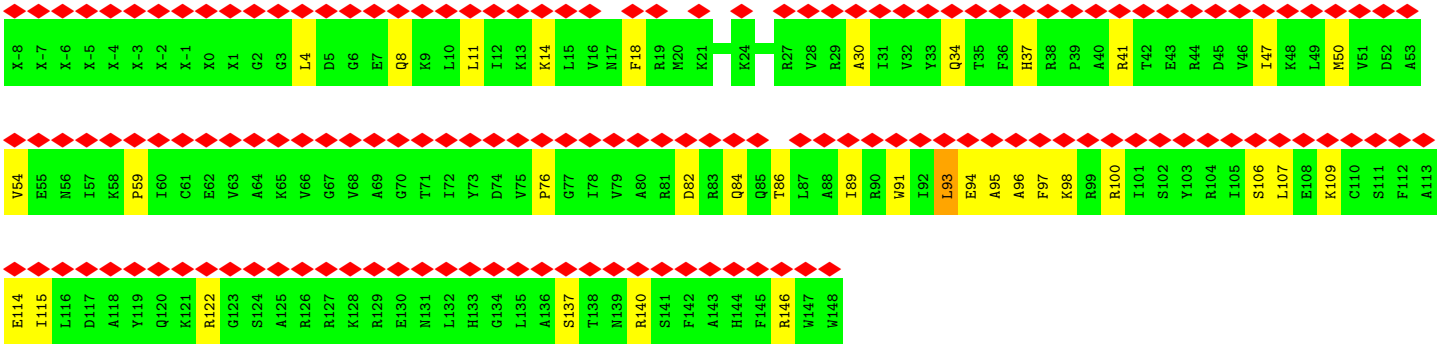




- Molecule 57: uS7m

Chain F:





- Molecule 58: uS8m

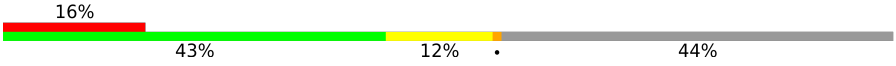
Chain G:

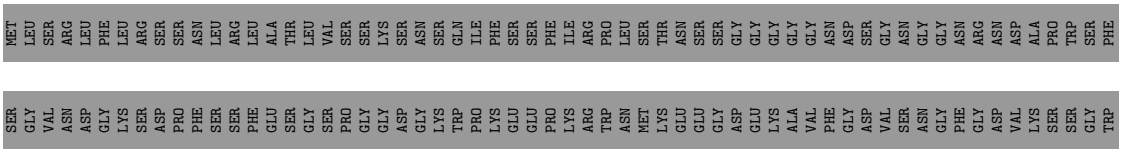


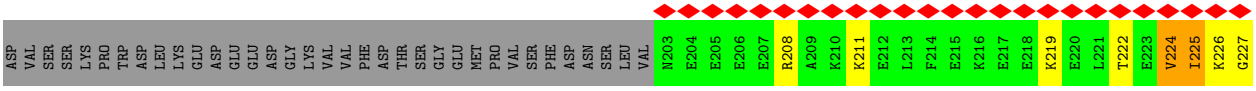


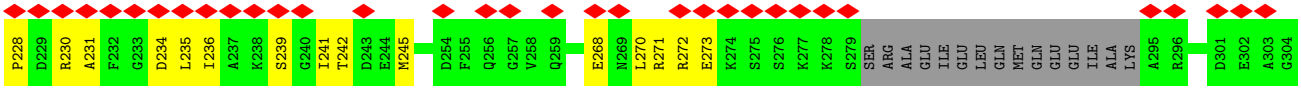
- Molecule 59: 30S ribosomal protein S9

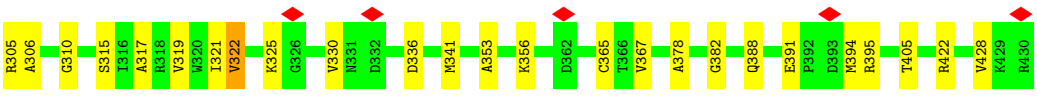
Chain H:









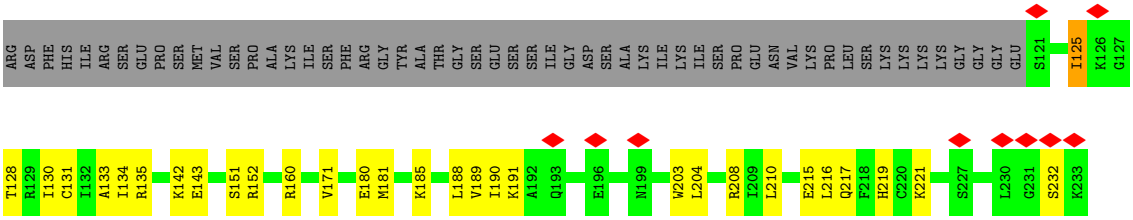


- Molecule 60: Small ribosomal subunit protein uS10 domain-containing protein

Chain I:



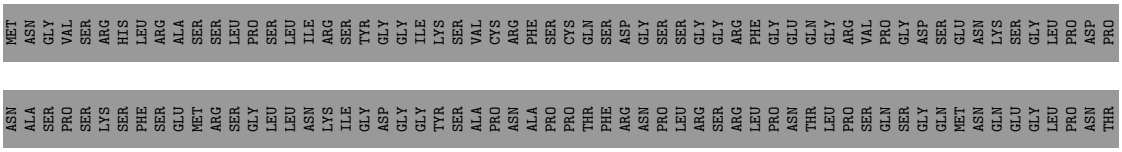


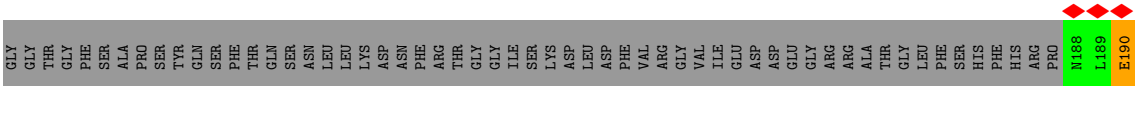


• Molecule 61: Ribosomal protein S11

Chain J:





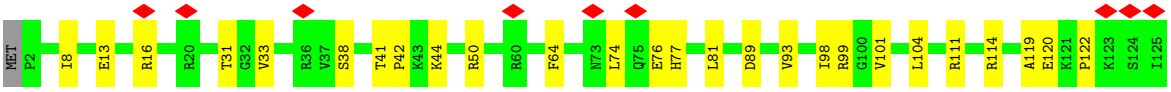




• Molecule 62: uS12m

Chain K:

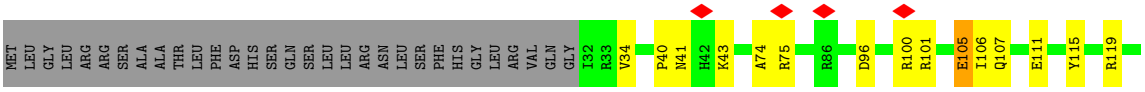


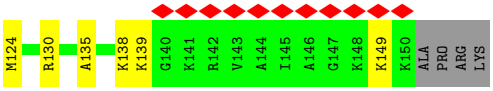


• Molecule 63: uS13m

Chain L:



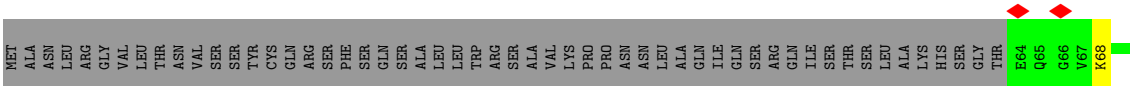


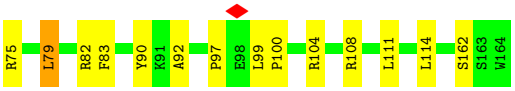


• Molecule 64: Small ribosomal subunit protein uS14m

Chain M:



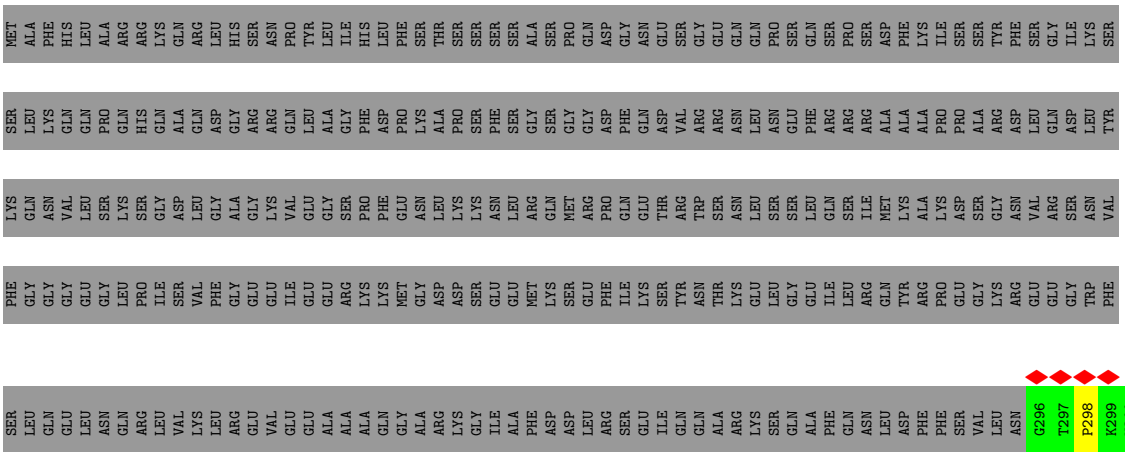




• Molecule 65: Small ribosomal subunit protein uS15c

Chain N:

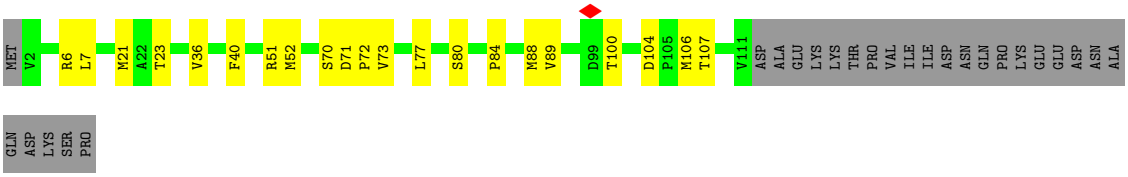




• Molecule 66: 30S ribosomal protein S16

Chain O:

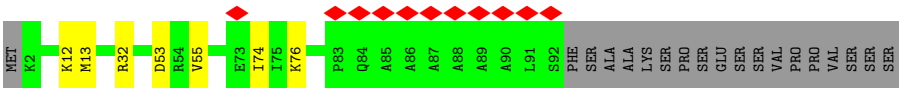




• Molecule 67: Small ribosomal subunit protein uS17c

Chain P:

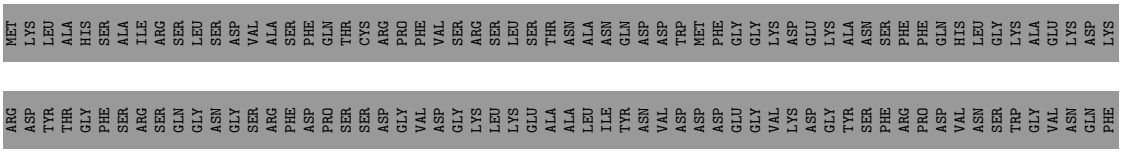




• Molecule 68: bS18m

Chain Q:

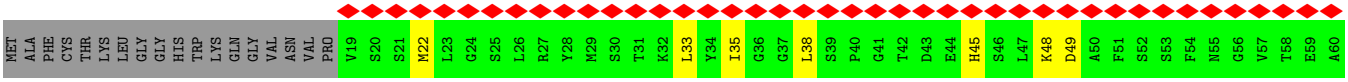


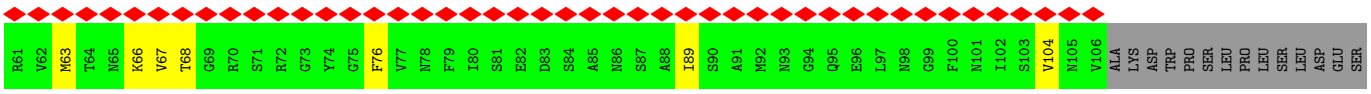


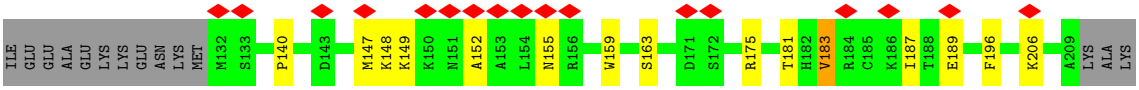


• Molecule 69: uS19m



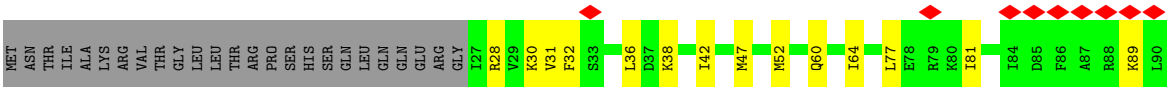


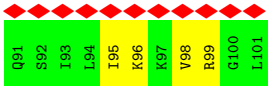




• Molecule 70: Ribosomal protein S21

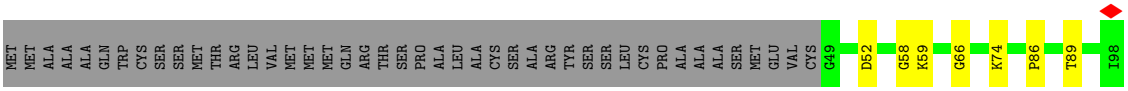






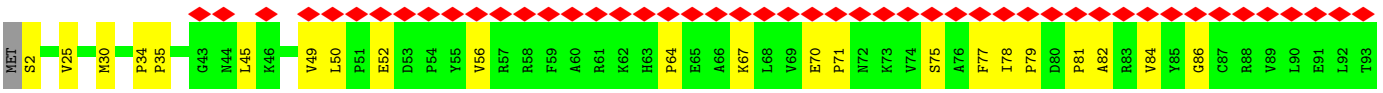
• Molecule 71: 30S ribosomal protein S31, mitochondrial

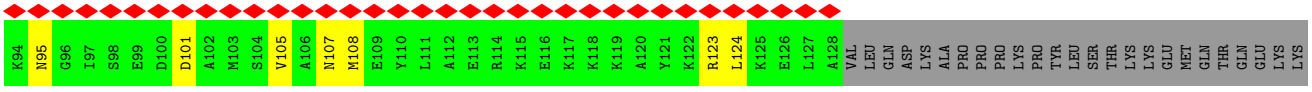




• Molecule 72: Small ribosomal subunit protein mS23

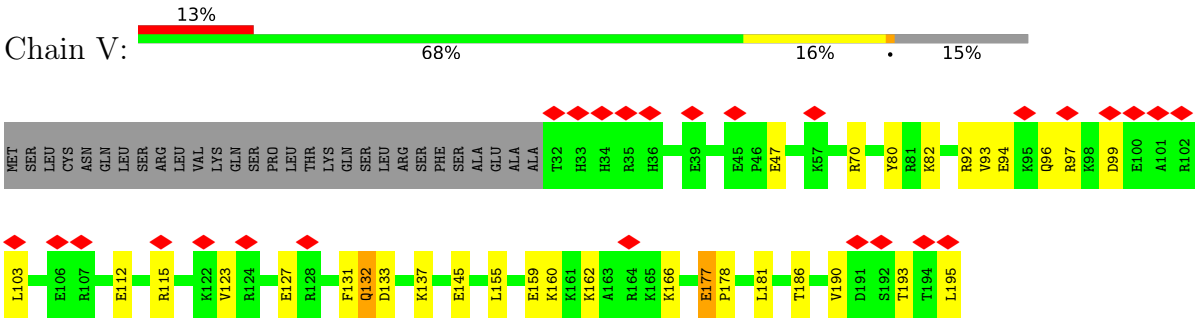




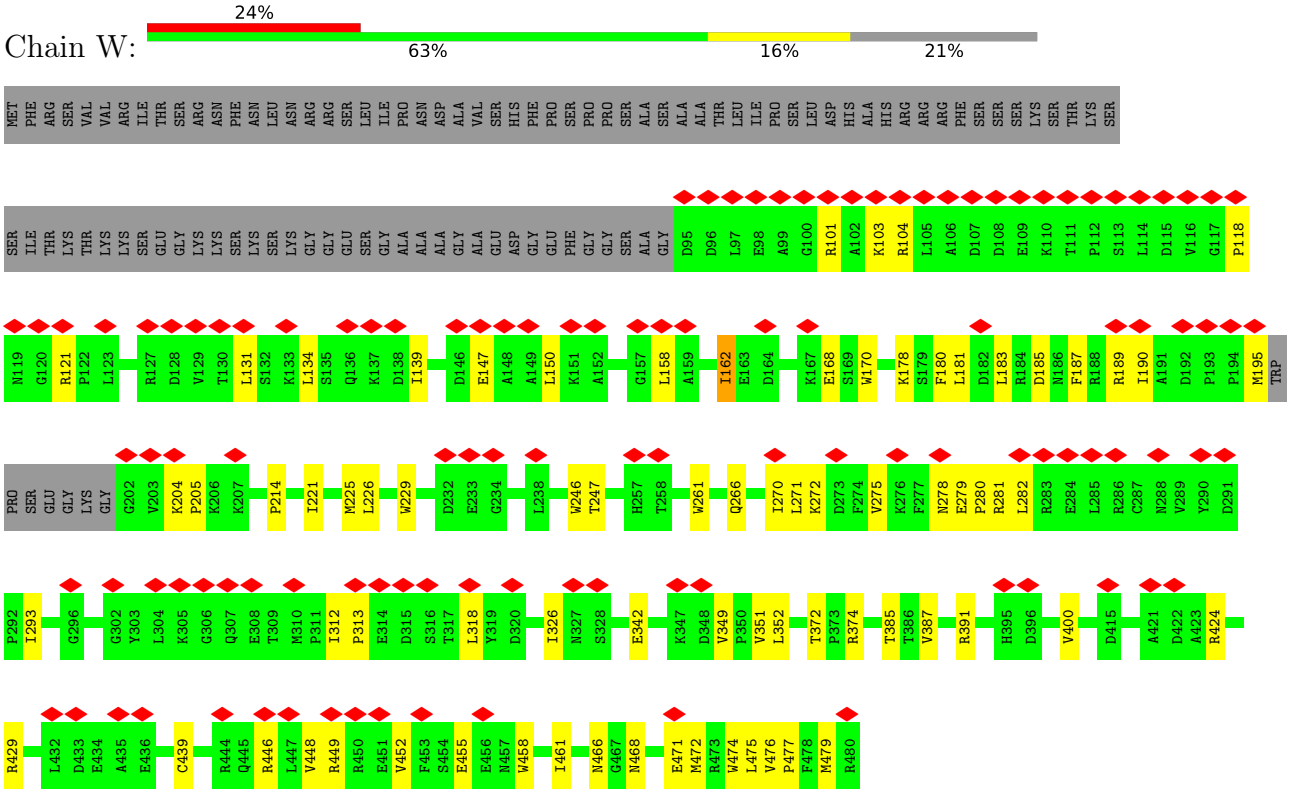




• Molecule 73: mS26

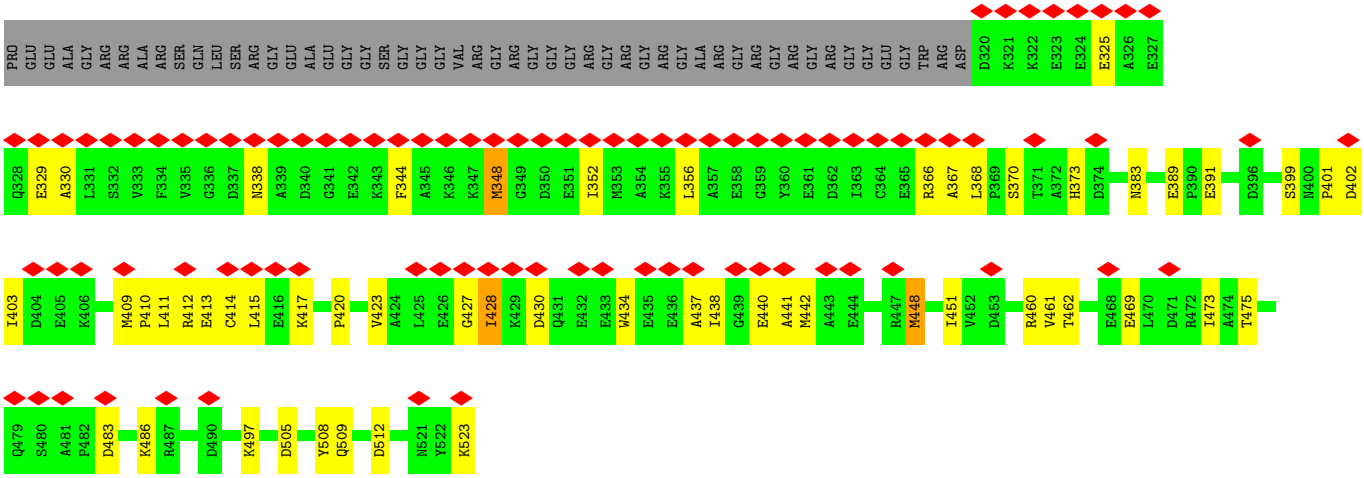


• Molecule 74: Small ribosomal subunit protein mS29



• Molecule 75: mS31/mS46

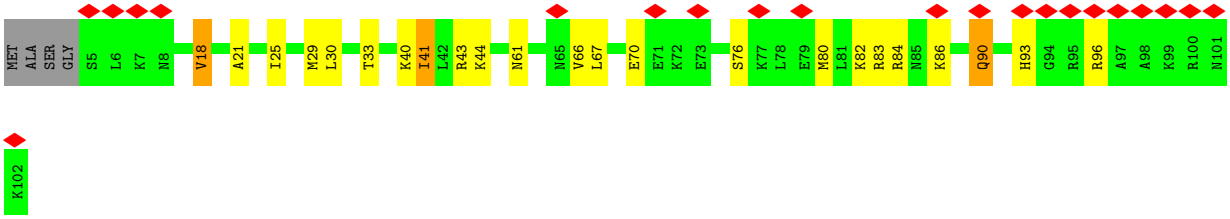




• Molecule 76: MOSC domain-containing protein

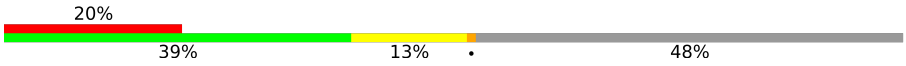
Chain Y:

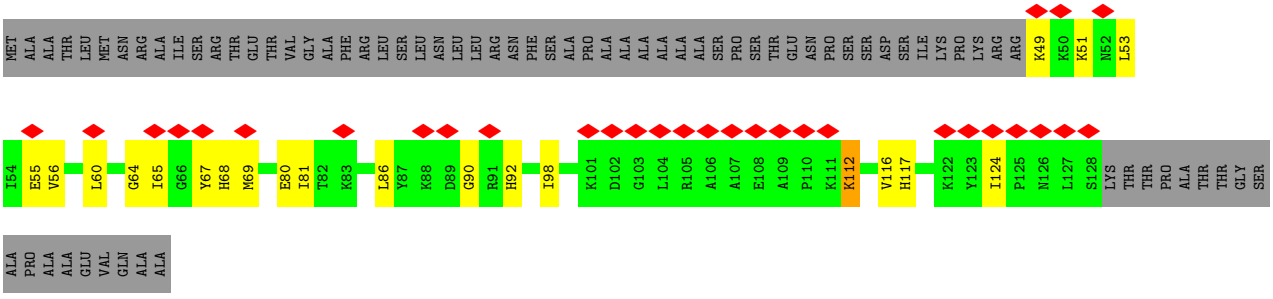




• Molecule 77: mS34

Chain Z:

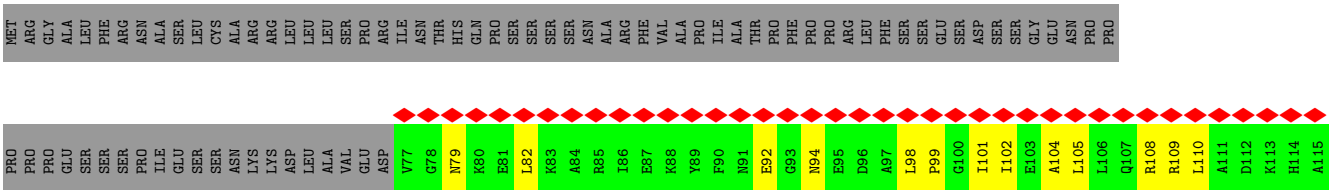


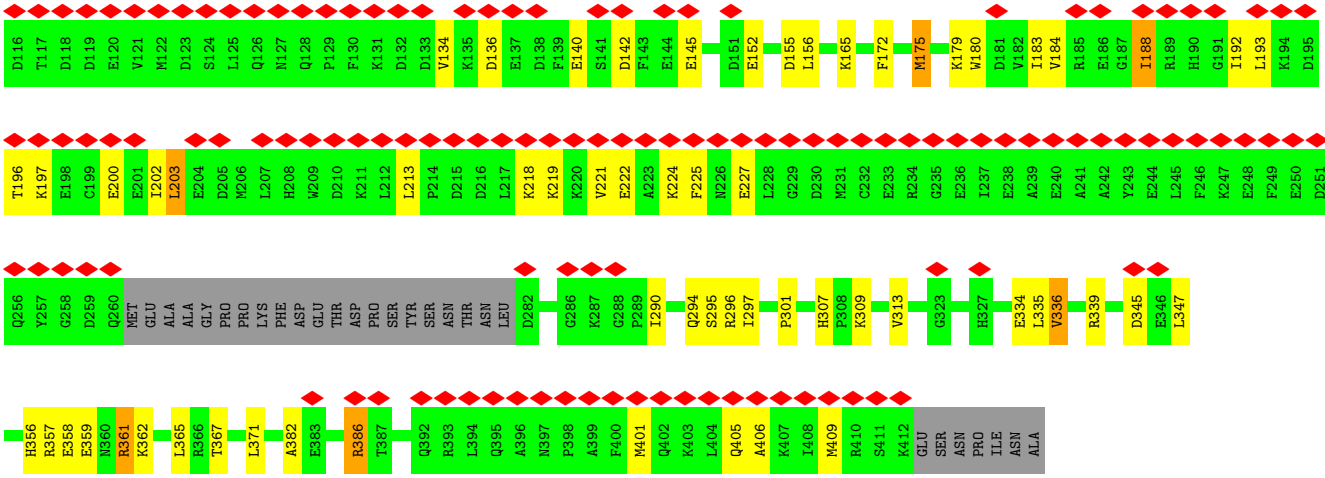


• Molecule 78: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

Chain a:

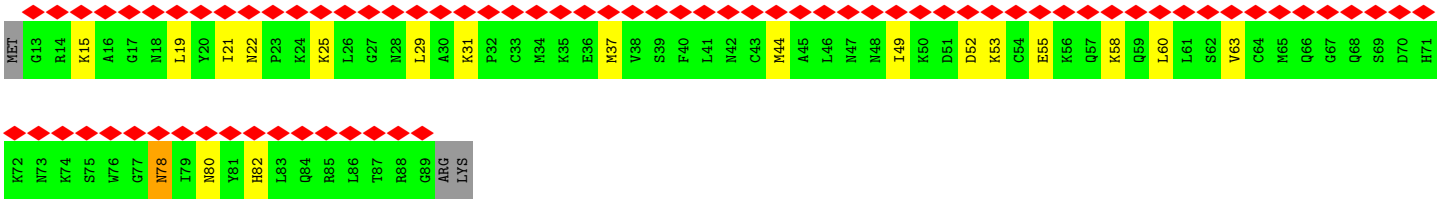






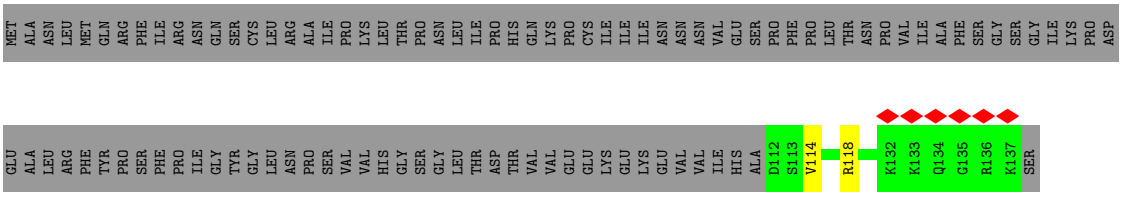
• Molecule 79: mS37





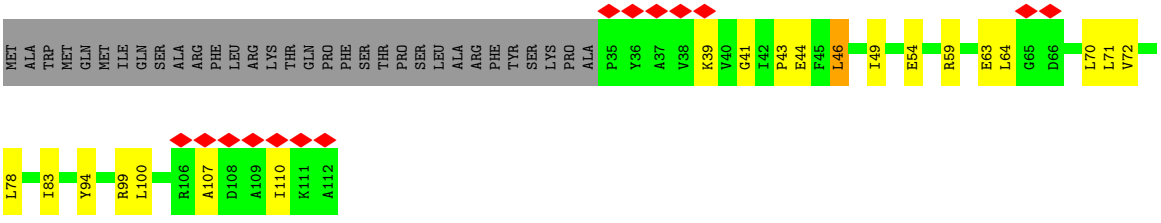
• Molecule 80: Small ribosomal subunit protein mS38





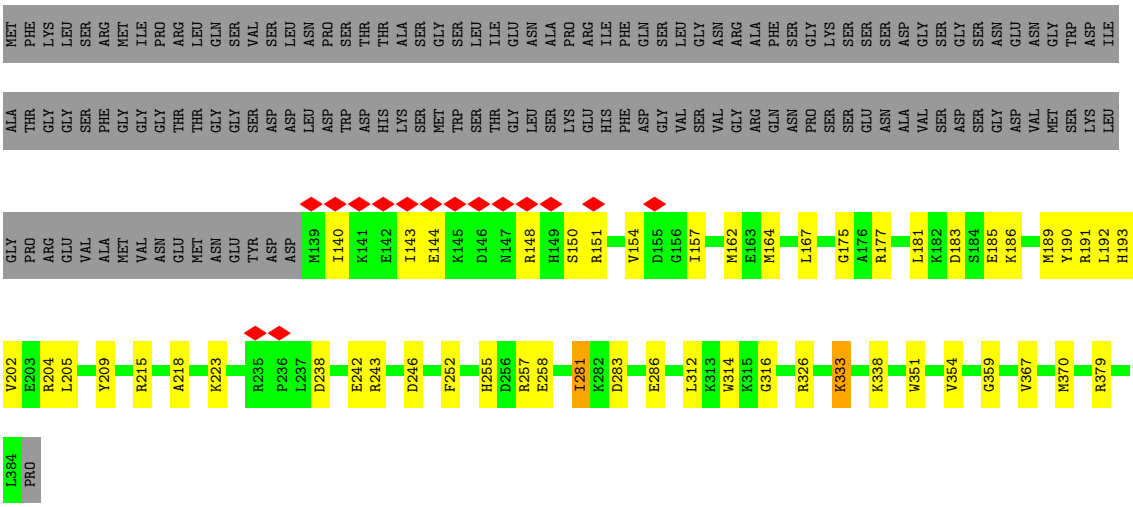
• Molecule 81: Small ribosomal subunit protein mS41 SAM domain-containing protein





• Molecule 82: mS45

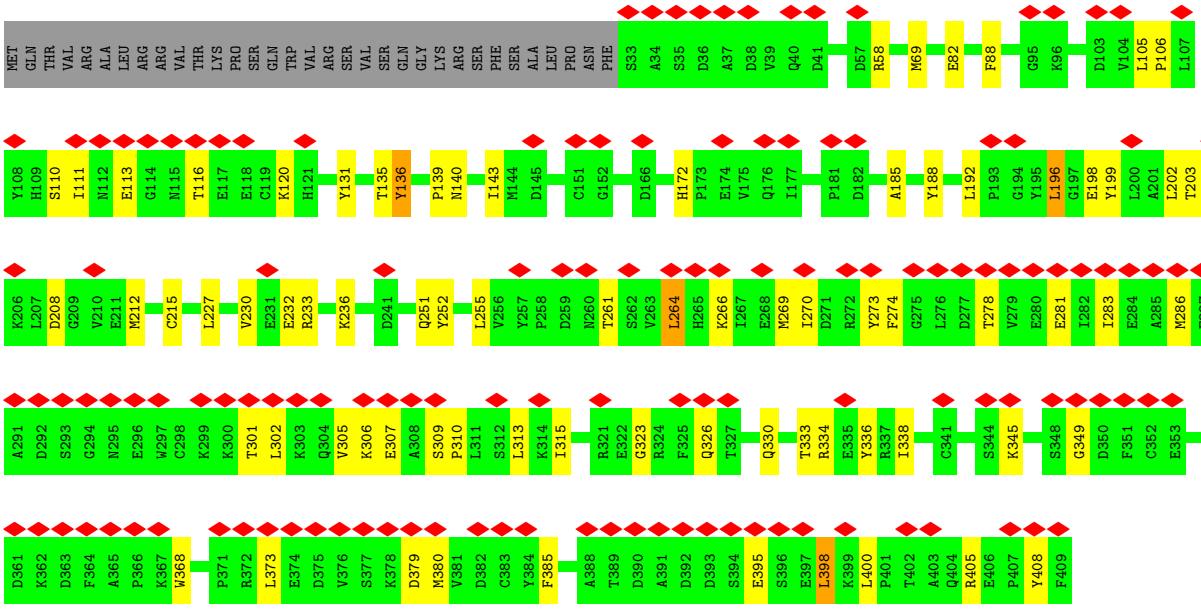




• Molecule 83: mS47

Chain f:

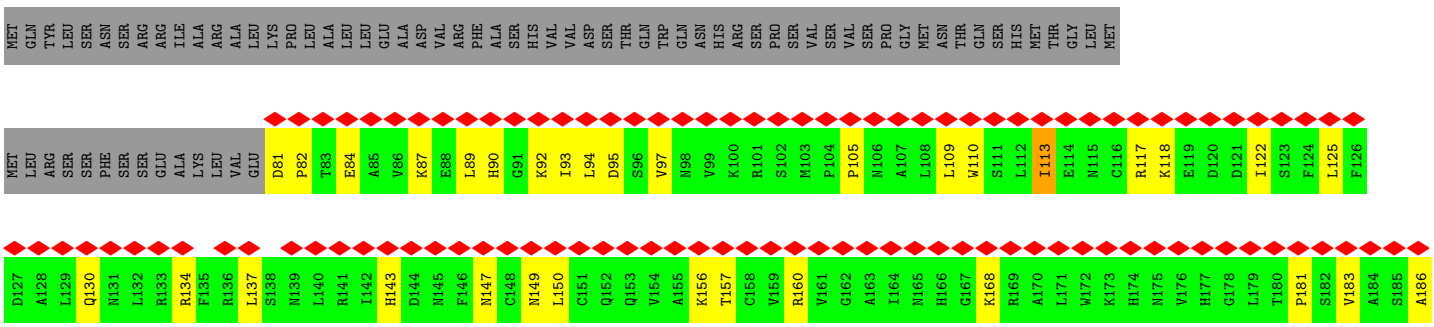


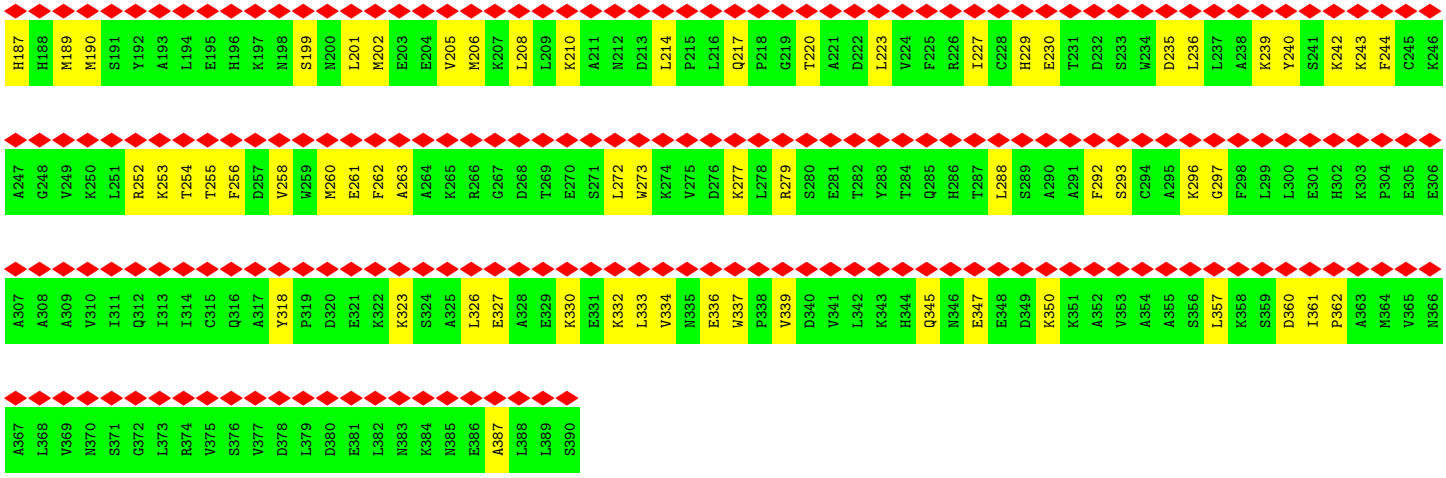


• Molecule 84: Adenylyl cyclase

Chain h:

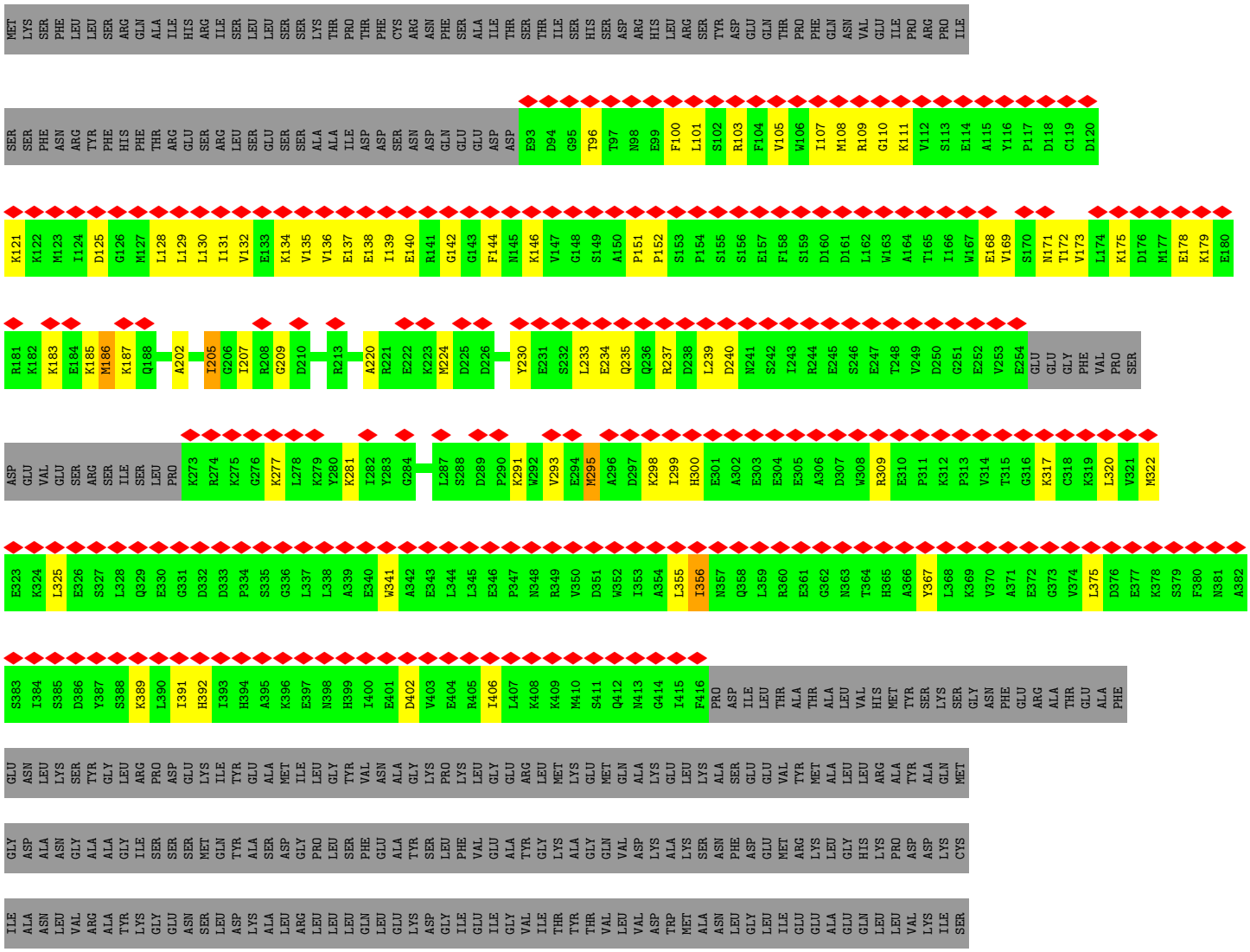


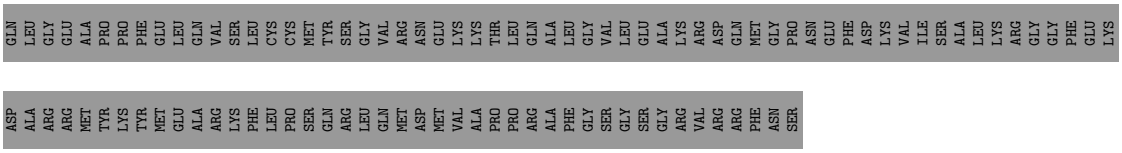




- Molecule 85: PROP1-like PPR domain-containing protein



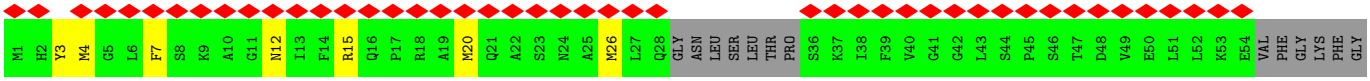




• Molecule 86: RRM domain-containing protein

Chain k:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.011	Depositor
Minimum map value	-0.579	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	730.296, 730.296, 730.296	wwPDB
Map dimensions	756, 756, 756	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, OMG, ZN, 5MU, 4OC, PSU, CLM, H2U, OMC, 2MA, OMU, MA6, UR3, K, 2MG, G7M

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	1	0.35	0/69733	0.77	33/108691 (0.0%)
2	1B	0.16	0/1347	0.37	0/1797
3	1C	0.16	0/1727	0.36	0/2311
4	1D	0.17	0/2099	0.34	0/2836
5	1E	0.15	0/1786	0.30	0/2412
6	1F	0.15	0/1313	0.37	0/1772
7	1G	0.15	0/796	0.39	0/1067
8	1H	0.14	0/547	0.37	0/731
9	1I	0.14	0/1054	0.39	0/1417
10	1J	0.17	0/1155	0.47	0/1563
11	1K	0.17	0/1553	0.32	0/2080
12	1L	0.15	0/976	0.35	0/1304
13	1M	0.17	0/1682	0.37	0/2248
14	1N	0.16	0/1184	0.35	0/1580
15	1O	0.16	0/1255	0.33	0/1687
16	1P	0.15	0/895	0.38	0/1206
17	1Q	0.15	0/1022	0.31	0/1368
18	1R	0.17	0/930	0.30	0/1234
19	1S	0.17	0/1192	0.33	0/1602
20	1T	0.18	0/1259	0.36	0/1687
21	1U	0.16	0/1065	0.37	0/1421
22	1V	0.16	0/1247	0.34	0/1681
23	1W	0.15	0/1613	0.41	0/2180
24	1X	0.14	0/1703	0.36	0/2307
25	1Y	0.16	0/785	0.31	0/1051
26	1Z	0.15	0/1466	0.39	1/1954 (0.1%)
27	1a	0.16	0/946	0.36	0/1262
28	1b	0.17	0/818	0.40	0/1099
29	1c	0.13	0/501	0.33	0/666
30	1d	0.17	0/387	0.30	0/514
31	1e	0.16	0/468	0.30	0/618

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1f	0.17	0/370	0.29	0/486
33	1g	0.17	0/789	0.34	0/1048
34	1h	0.12	0/312	0.28	0/409
35	1i	0.13	0/1440	0.32	0/1927
36	1j	0.17	0/586	0.33	0/789
37	1k	0.16	0/970	0.35	0/1309
38	1l	0.16	0/1792	0.44	1/2423 (0.0%)
39	1m	0.12	0/987	0.35	0/1331
40	1o	0.15	0/637	0.44	0/860
41	1p	0.15	0/1014	0.35	0/1349
42	1q	0.16	0/394	0.31	0/527
43	1r	0.17	0/750	0.40	0/1005
44	1s	0.17	0/1001	0.35	0/1327
45	1t	0.15	0/3919	0.41	0/5272
46	1u	0.17	0/5345	0.48	1/7180 (0.0%)
47	1v	0.15	0/3497	0.38	0/4681
48	2	0.31	0/37259	0.74	13/58092 (0.0%)
49	3	0.31	0/2810	0.79	1/4378 (0.0%)
50	5	0.31	0/1834	0.80	1/2854 (0.0%)
51	6	0.80	0/144	1.06	0/222
52	A	0.16	0/1647	0.36	0/2227
53	B	0.16	0/3969	0.41	0/5320
54	C	0.15	0/2865	0.38	0/3836
55	D	0.19	0/3474	0.45	3/4647 (0.1%)
56	E	0.16	0/838	0.37	0/1121
57	F	0.16	0/1225	0.45	0/1641
58	G	0.15	0/1054	0.33	0/1418
59	H	0.18	0/1707	0.44	0/2287
60	I	0.16	0/964	0.40	0/1293
61	J	0.15	0/1000	0.36	0/1340
62	K	0.17	0/1009	0.38	0/1345
63	L	0.15	0/950	0.44	0/1263
64	M	0.17	0/856	0.39	0/1134
65	N	0.15	0/958	0.34	0/1280
66	O	0.18	0/890	0.41	0/1196
67	P	0.14	0/730	0.33	0/984
68	Q	0.15	0/733	0.38	0/978
69	R	0.14	0/1323	0.43	0/1772
70	S	0.15	0/614	0.34	0/809
71	T	0.15	0/416	0.29	0/547
72	U	0.17	0/1036	0.44	0/1395
73	V	0.14	0/1423	0.37	0/1895
74	W	0.15	0/3139	0.37	0/4250

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	X	0.17	0/1644	0.44	0/2216
76	Y	0.15	0/807	0.37	0/1077
77	Z	0.14	0/669	0.42	0/900
78	a	0.17	0/2524	0.42	0/3387
79	b	0.15	0/618	0.41	0/822
80	c	0.13	0/233	0.24	0/296
81	d	0.14	0/628	0.43	0/840
82	e	0.16	0/2118	0.40	0/2828
83	f	0.16	0/2981	0.42	0/4033
84	h	0.15	0/2507	0.42	0/3384
85	i	0.14	0/2532	0.39	0/3400
86	k	0.15	0/317	0.43	0/424
All	All	0.26	0/220752	0.62	54/320400 (0.0%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3166[A]	C	N1-C2-O2	8.46	123.98	118.90
1	1	2811	U	C2-N1-C1'	8.19	127.52	117.70
1	1	3166[A]	C	C2-N1-C1'	8.14	127.75	118.80
48	2	1706	C	C2-N1-C1'	7.32	126.86	118.80
48	2	1387	C	C2-N1-C1'	7.32	126.85	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62518	0	31502	513	0
2	1B	1325	0	1398	11	0
3	1C	1696	0	1745	22	0
4	1D	2045	0	2080	15	0
5	1E	1753	0	1815	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1F	1286	0	1280	24	0
7	1G	779	0	810	8	0
8	1H	539	0	574	9	0
9	1I	1036	0	1084	26	0
10	1J	1129	0	1166	30	0
11	1K	1526	0	1586	12	0
12	1L	966	0	1048	13	0
13	1M	1649	0	1765	11	0
14	1N	1160	0	1206	16	0
15	1O	1231	0	1262	9	0
16	1P	878	0	939	10	0
17	1Q	1008	0	1101	7	0
18	1R	915	0	946	7	0
19	1S	1170	0	1226	8	0
20	1T	1241	0	1346	12	0
21	1U	1048	0	1123	10	0
22	1V	1223	0	1277	16	0
23	1W	1588	0	1663	35	0
24	1X	1670	0	1751	17	0
25	1Y	768	0	792	7	0
26	1Z	1441	0	1485	20	0
27	1a	928	0	959	11	0
28	1b	803	0	845	5	0
29	1c	489	0	511	11	0
30	1d	379	0	416	3	0
31	1e	459	0	491	3	0
32	1f	364	0	398	2	0
33	1g	770	0	841	3	0
34	1h	309	0	337	3	0
35	1i	1424	0	1482	19	0
36	1j	570	0	593	7	0
37	1k	952	0	987	11	0
38	1l	1741	0	1707	34	0
39	1m	970	0	979	16	0
40	1o	626	0	657	17	0
41	1p	992	0	1027	8	0
42	1q	390	0	421	4	0
43	1r	735	0	781	8	0
44	1s	985	0	1072	4	0
45	1t	3856	0	3912	79	0
46	1u	5264	0	5353	154	0
47	1v	3440	0	3497	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	2	33425	0	16848	294	0
49	3	2513	0	1275	11	0
50	5	1641	0	831	22	0
51	6	129	0	65	3	0
52	A	1611	0	1633	19	0
53	B	3877	0	4008	91	0
54	C	2811	0	2986	63	0
55	D	3425	0	3453	62	0
56	E	823	0	879	9	0
57	F	1254	0	1268	25	0
58	G	1037	0	1058	8	0
59	H	1682	0	1726	43	0
60	I	941	0	970	21	0
61	J	988	0	1022	17	0
62	K	992	0	1051	15	0
63	L	940	0	989	17	0
64	M	843	0	884	10	0
65	N	941	0	978	8	0
66	O	869	0	898	14	0
67	P	717	0	755	4	0
68	Q	724	0	744	10	0
69	R	1299	0	1307	20	0
70	S	611	0	687	14	0
71	T	408	0	444	4	0
72	U	1014	0	1061	23	0
73	V	1399	0	1427	26	0
74	W	3062	0	3030	48	0
75	X	1613	0	1559	42	0
76	Y	793	0	834	16	0
77	Z	649	0	662	14	0
78	a	2487	0	2382	62	0
79	b	610	0	626	17	0
80	c	232	0	278	1	0
81	d	616	0	674	12	0
82	e	2074	0	2074	46	0
83	f	2922	0	2870	52	0
84	h	2460	0	2478	73	0
85	i	2487	0	2450	61	0
86	k	314	0	261	8	0
87	1	251	0	0	0	0
87	1D	1	0	0	0	0
87	1j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	1q	1	0	0	0	0
87	2	97	0	0	0	0
87	3	3	0	0	0	0
87	D	1	0	0	0	0
87	T	1	0	0	0	0
87	W	1	0	0	0	0
88	1	57	0	0	0	0
88	1B	2	0	0	0	0
88	1E	1	0	0	0	0
88	2	14	0	0	0	0
89	1	20	0	11	1	0
90	1d	1	0	0	0	0
90	1h	1	0	0	0	0
91	W	31	0	12	0	0
All	All	207751	0	160684	2384	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 6.

The worst 5 of 2384 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)
48:2:1726:U:H3	48:2:1744:C:N4	1.66	0.94
48:2:1726:U:H3	48:2:1744:C:H42	0.90	0.88
37:1k:10:GLN:HE22	37:1k:63:ARG:HG2	1.38	0.88
53:B:234:LEU:HD21	75:X:441:ALA:HB2	1.57	0.85
1:1:1257:G:H5”	9:1I:57:ASN:HD21	1.42	0.85

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1B	175/217 (81%)	171 (98%)	4 (2%)	0	100	100
3	1C	203/286 (71%)	194 (96%)	8 (4%)	1 (0%)	24	53
4	1D	262/319 (82%)	256 (98%)	6 (2%)	0	100	100
5	1E	219/296 (74%)	215 (98%)	4 (2%)	0	100	100
6	1F	154/185 (83%)	147 (96%)	7 (4%)	0	100	100
7	1G	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
8	1H	64/220 (29%)	63 (98%)	1 (2%)	0	100	100
9	1I	128/170 (75%)	125 (98%)	2 (2%)	1 (1%)	16	43
10	1J	145/156 (93%)	132 (91%)	13 (9%)	0	100	100
11	1K	187/204 (92%)	185 (99%)	2 (1%)	0	100	100
12	1L	125/176 (71%)	119 (95%)	6 (5%)	0	100	100
13	1M	208/281 (74%)	199 (96%)	9 (4%)	0	100	100
14	1N	146/179 (82%)	141 (97%)	5 (3%)	0	100	100
15	1O	149/160 (93%)	141 (95%)	8 (5%)	0	100	100
16	1P	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
17	1Q	120/233 (52%)	115 (96%)	5 (4%)	0	100	100
18	1R	108/126 (86%)	106 (98%)	2 (2%)	0	100	100
19	1S	143/270 (53%)	140 (98%)	3 (2%)	0	100	100
20	1T	153/264 (58%)	148 (97%)	5 (3%)	0	100	100
21	1U	126/180 (70%)	123 (98%)	3 (2%)	0	100	100
22	1V	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
23	1W	203/238 (85%)	198 (98%)	5 (2%)	0	100	100
24	1X	214/271 (79%)	208 (97%)	6 (3%)	0	100	100
25	1Y	96/156 (62%)	94 (98%)	2 (2%)	0	100	100
26	1Z	175/215 (81%)	173 (99%)	2 (1%)	0	100	100
27	1a	106/144 (74%)	106 (100%)	0	0	100	100
28	1b	98/109 (90%)	93 (95%)	5 (5%)	0	100	100
29	1c	57/135 (42%)	53 (93%)	4 (7%)	0	100	100
30	1d	47/139 (34%)	46 (98%)	1 (2%)	0	100	100
31	1e	52/106 (49%)	52 (100%)	0	0	100	100
32	1f	42/146 (29%)	42 (100%)	0	0	100	100
33	1g	89/162 (55%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	1h	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
35	1i	181/247 (73%)	178 (98%)	3 (2%)	0	100	100
36	1j	69/90 (77%)	67 (97%)	2 (3%)	0	100	100
37	1k	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
38	1l	209/239 (87%)	200 (96%)	9 (4%)	0	100	100
39	1m	120/128 (94%)	116 (97%)	4 (3%)	0	100	100
40	1o	74/125 (59%)	70 (95%)	4 (5%)	0	100	100
41	1p	115/130 (88%)	115 (100%)	0	0	100	100
42	1q	48/78 (62%)	47 (98%)	0	1 (2%)	5	20
43	1r	90/167 (54%)	85 (94%)	5 (6%)	0	100	100
44	1s	116/181 (64%)	114 (98%)	2 (2%)	0	100	100
45	1t	482/491 (98%)	466 (97%)	16 (3%)	0	100	100
46	1u	664/751 (88%)	627 (94%)	36 (5%)	1 (0%)	43	71
47	1v	429/514 (84%)	417 (97%)	12 (3%)	0	100	100
52	A	202/212 (95%)	192 (95%)	10 (5%)	0	100	100
53	B	457/554 (82%)	429 (94%)	28 (6%)	0	100	100
54	C	329/362 (91%)	322 (98%)	7 (2%)	0	100	100
55	D	413/501 (82%)	398 (96%)	15 (4%)	0	100	100
56	E	99/138 (72%)	96 (97%)	3 (3%)	0	100	100
57	F	146/157 (93%)	141 (97%)	5 (3%)	0	100	100
58	G	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
59	H	209/383 (55%)	196 (94%)	12 (6%)	1 (0%)	24	53
60	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
61	J	125/304 (41%)	123 (98%)	2 (2%)	0	100	100
62	K	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
63	L	117/154 (76%)	110 (94%)	7 (6%)	0	100	100
64	M	99/155 (64%)	99 (100%)	0	0	100	100
65	N	114/414 (28%)	113 (99%)	1 (1%)	0	100	100
66	O	108/136 (79%)	104 (96%)	4 (4%)	0	100	100
67	P	89/110 (81%)	86 (97%)	3 (3%)	0	100	100
68	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
69	R	162/212 (76%)	155 (96%)	7 (4%)	0	100 100
70	S	73/100 (73%)	72 (99%)	1 (1%)	0	100 100
71	T	48/94 (51%)	46 (96%)	2 (4%)	0	100 100
72	U	125/192 (65%)	120 (96%)	4 (3%)	1 (1%)	16 43
73	V	162/193 (84%)	158 (98%)	4 (2%)	0	100 100
74	W	376/483 (78%)	368 (98%)	8 (2%)	0	100 100
75	X	202/496 (41%)	190 (94%)	10 (5%)	2 (1%)	12 37
76	Y	96/102 (94%)	92 (96%)	4 (4%)	0	100 100
77	Z	78/153 (51%)	75 (96%)	3 (4%)	0	100 100
78	a	311/424 (73%)	305 (98%)	6 (2%)	0	100 100
79	b	75/80 (94%)	66 (88%)	9 (12%)	0	100 100
80	c	24/128 (19%)	24 (100%)	0	0	100 100
81	d	76/110 (69%)	75 (99%)	1 (1%)	0	100 100
82	e	244/383 (64%)	234 (96%)	10 (4%)	0	100 100
83	f	375/410 (92%)	362 (96%)	13 (4%)	0	100 100
84	h	308/384 (80%)	300 (97%)	8 (3%)	0	100 100
85	i	302/725 (42%)	292 (97%)	10 (3%)	0	100 100
86	k	43/153 (28%)	40 (93%)	3 (7%)	0	100 100
All	All	13140/18602 (71%)	12693 (97%)	439 (3%)	8 (0%)	49 76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	H	225	ILE
72	U	64	PRO
9	1I	133	PRO
46	1u	84	HIS
75	X	428	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1B	141/173 (82%)	137 (97%)	4 (3%)	38	70
3	1C	184/239 (77%)	179 (97%)	5 (3%)	39	71
4	1D	216/264 (82%)	208 (96%)	8 (4%)	30	63
5	1E	192/256 (75%)	189 (98%)	3 (2%)	55	81
6	1F	145/168 (86%)	139 (96%)	6 (4%)	27	60
7	1G	82/86 (95%)	82 (100%)	0	100	100
8	1H	58/196 (30%)	56 (97%)	2 (3%)	32	65
9	1I	113/143 (79%)	111 (98%)	2 (2%)	51	79
10	1J	125/131 (95%)	124 (99%)	1 (1%)	73	89
11	1K	161/170 (95%)	159 (99%)	2 (1%)	63	85
12	1L	103/140 (74%)	101 (98%)	2 (2%)	50	78
13	1M	169/235 (72%)	161 (95%)	8 (5%)	23	55
14	1N	116/146 (80%)	115 (99%)	1 (1%)	70	88
15	1O	129/139 (93%)	126 (98%)	3 (2%)	44	74
16	1P	94/95 (99%)	88 (94%)	6 (6%)	16	43
17	1Q	110/208 (53%)	105 (96%)	5 (4%)	24	56
18	1R	96/110 (87%)	94 (98%)	2 (2%)	47	76
19	1S	130/244 (53%)	128 (98%)	2 (2%)	57	82
20	1T	133/229 (58%)	131 (98%)	2 (2%)	57	82
21	1U	114/147 (78%)	114 (100%)	0	100	100
22	1V	132/133 (99%)	130 (98%)	2 (2%)	57	82
23	1W	181/204 (89%)	176 (97%)	5 (3%)	38	70
24	1X	186/235 (79%)	181 (97%)	5 (3%)	39	71
25	1Y	80/127 (63%)	80 (100%)	0	100	100
26	1Z	150/177 (85%)	148 (99%)	2 (1%)	61	84
27	1a	102/128 (80%)	99 (97%)	3 (3%)	37	69
28	1b	88/95 (93%)	88 (100%)	0	100	100
29	1c	51/119 (43%)	49 (96%)	2 (4%)	28	61
30	1d	42/119 (35%)	40 (95%)	2 (5%)	23	54
31	1e	49/98 (50%)	45 (92%)	4 (8%)	10	31
32	1f	35/129 (27%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	1g	84/152 (55%)	83 (99%)	1 (1%)	63 85
34	1h	36/87 (41%)	34 (94%)	2 (6%)	19 48
35	1i	152/203 (75%)	145 (95%)	7 (5%)	24 56
36	1j	64/79 (81%)	64 (100%)	0	100 100
37	1k	105/106 (99%)	99 (94%)	6 (6%)	18 48
38	1l	189/214 (88%)	184 (97%)	5 (3%)	40 72
39	1m	107/112 (96%)	104 (97%)	3 (3%)	38 70
40	1o	71/105 (68%)	71 (100%)	0	100 100
41	1p	101/108 (94%)	101 (100%)	0	100 100
42	1q	41/64 (64%)	40 (98%)	1 (2%)	43 73
43	1r	83/138 (60%)	82 (99%)	1 (1%)	63 85
44	1s	103/155 (66%)	101 (98%)	2 (2%)	50 78
45	1t	417/423 (99%)	411 (99%)	6 (1%)	59 83
46	1u	578/659 (88%)	558 (96%)	20 (4%)	32 64
47	1v	374/454 (82%)	357 (96%)	17 (4%)	24 56
52	A	177/182 (97%)	174 (98%)	3 (2%)	53 80
53	B	421/492 (86%)	406 (96%)	15 (4%)	31 63
54	C	314/343 (92%)	297 (95%)	17 (5%)	20 49
55	D	370/444 (83%)	363 (98%)	7 (2%)	50 78
56	E	90/126 (71%)	88 (98%)	2 (2%)	45 75
57	F	124/124 (100%)	122 (98%)	2 (2%)	55 81
58	G	112/113 (99%)	111 (99%)	1 (1%)	70 88
59	H	176/320 (55%)	169 (96%)	7 (4%)	28 61
60	I	104/197 (53%)	98 (94%)	6 (6%)	18 47
61	J	108/256 (42%)	105 (97%)	3 (3%)	38 70
62	K	107/108 (99%)	101 (94%)	6 (6%)	19 48
63	L	99/128 (77%)	97 (98%)	2 (2%)	48 77
64	M	90/137 (66%)	88 (98%)	2 (2%)	45 75
65	N	107/362 (30%)	106 (99%)	1 (1%)	70 88
66	O	93/117 (80%)	88 (95%)	5 (5%)	20 49
67	P	78/95 (82%)	77 (99%)	1 (1%)	61 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Q	75/203 (37%)	75 (100%)	0	100	100
69	R	141/180 (78%)	139 (99%)	2 (1%)	59	83
70	S	68/90 (76%)	68 (100%)	0	100	100
71	T	44/79 (56%)	44 (100%)	0	100	100
72	U	109/170 (64%)	106 (97%)	3 (3%)	38	70
73	V	147/173 (85%)	142 (97%)	5 (3%)	32	65
74	W	328/410 (80%)	322 (98%)	6 (2%)	51	79
75	X	174/395 (44%)	166 (95%)	8 (5%)	24	56
76	Y	84/86 (98%)	77 (92%)	7 (8%)	10	30
77	Z	65/119 (55%)	63 (97%)	2 (3%)	35	67
78	a	252/374 (67%)	243 (96%)	9 (4%)	31	63
79	b	68/71 (96%)	67 (98%)	1 (2%)	57	82
80	c	25/116 (22%)	25 (100%)	0	100	100
81	d	65/93 (70%)	63 (97%)	2 (3%)	35	67
82	e	226/339 (67%)	222 (98%)	4 (2%)	51	79
83	f	321/351 (92%)	313 (98%)	8 (2%)	42	73
84	h	271/337 (80%)	266 (98%)	5 (2%)	51	79
85	i	272/629 (43%)	263 (97%)	9 (3%)	33	65
86	k	22/110 (20%)	21 (96%)	1 (4%)	24	56
All	All	11539/16011 (72%)	11227 (97%)	312 (3%)	40	71

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
64	M	68	LYS
82	e	281	ILE
66	O	100	THR
75	X	448	MET
84	h	122	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
53	B	516	ASN

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Mol	Chain	Res	Type
67	P	47	ASN
54	C	186	GLN
61	J	263	ASN
70	S	62	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2910/2923 (99%)	542 (18%)	29 (0%)
48	2	1555/1766 (88%)	248 (15%)	11 (0%)
49	3	117/118 (99%)	25 (21%)	1 (0%)
50	5	76/77 (98%)	19 (25%)	0
51	6	5/6 (83%)	2 (40%)	1 (20%)
All	All	4663/4890 (95%)	836 (17%)	42 (0%)

5 of 836 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	30	G
1	1	37	G
1	1	47	A
1	1	49	G
1	1	50	G

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2998	U
48	2	1705	C
48	2	225	G
48	2	998	A
48	2	1726	U

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	OMG	1	2560	88,50,1	23,26,27	2.71	8 (34%)	33,38,41	3.05	12 (36%)
1	PSU	1	2762	1	18,21,22	4.23	7 (38%)	22,30,33	1.88	6 (27%)
1	2MA	1	2808	87,1	22,25,26	3.80	7 (31%)	33,37,40	2.18	10 (30%)
1	H2U	1	2754	1	18,21,22	0.50	0	21,30,33	1.00	1 (4%)
1	OMU	1	2857	87,1	19,22,23	2.99	8 (42%)	26,31,34	1.69	5 (19%)
1	PSU	1	891	87,1	18,21,22	4.35	8 (44%)	22,30,33	1.88	5 (22%)
48	G7M	2	525	48	23,26,27	2.60	9 (39%)	35,39,42	1.74	9 (25%)
48	2MG	2	1825	48	23,26,27	0.50	0	32,38,41	0.61	0
48	UR3	2	1807	48	19,22,23	0.28	0	26,32,35	0.64	0
1	PSU	1	2885	88,1	18,21,22	4.27	8 (44%)	22,30,33	1.89	6 (27%)
48	MA6	2	1827	48	23,26,27	1.34	3 (13%)	34,38,41	3.59	11 (32%)
1	PSU	1	2910	1	18,21,22	4.28	7 (38%)	22,30,33	1.80	5 (22%)
1	PSU	1	1105	1	18,21,22	4.27	7 (38%)	22,30,33	1.83	5 (22%)
1	OMC	1	2803	87,1	19,22,23	3.67	8 (42%)	26,31,34	0.81	0
48	MA6	2	1828	48	23,26,27	1.34	3 (13%)	34,38,41	3.57	11 (32%)
48	4OC	2	1664	48	20,23,24	0.35	0	26,32,35	0.48	0
1	5MU	1	2257	88,1	19,22,23	0.46	0	28,32,35	0.49	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
1	OMG	1	2560	88,50,1	-	1/9/27/28	0/3/3/3
1	PSU	1	2762	1	-	0/7/25/26	0/2/2/2
1	2MA	1	2808	87,1	-	2/7/25/26	0/3/3/3
1	H2U	1	2754	1	-	0/7/38/39	0/2/2/2
1	OMU	1	2857	87,1	-	0/9/27/28	0/2/2/2
1	PSU	1	891	87,1	-	3/7/25/26	0/2/2/2
48	G7M	2	525	48	-	1/7/25/26	0/3/3/3
48	2MG	2	1825	48	-	0/9/27/28	0/3/3/3
48	UR3	2	1807	48	-	0/7/25/26	0/2/2/2
1	PSU	1	2885	88,1	-	2/7/25/26	0/2/2/2
48	MA6	2	1827	48	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2910	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1105	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2803	87,1	-	2/9/27/28	0/2/2/2
48	MA6	2	1828	48	-	1/11/29/30	0/3/3/3
48	4OC	2	1664	48	-	0/9/29/30	0/2/2/2
1	5MU	1	2257	88,1	-	0/7/25/26	0/2/2/2

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2808	2MA	C4-N3	12.19	1.49	1.34
1	1	891	PSU	C6-C5	11.29	1.48	1.35
1	1	1105	PSU	C6-C5	11.07	1.48	1.35
1	1	2910	PSU	C6-C5	11.04	1.48	1.35
1	1	2885	PSU	C6-C5	10.93	1.48	1.35

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	2	1827	MA6	N1-C6-N6	-14.80	100.90	117.08
48	2	1828	MA6	N1-C6-N6	-14.63	101.08	117.08
1	1	2560	OMG	C1'-N9-C8	-10.46	96.92	126.70
1	1	2560	OMG	C1'-N9-C4	9.45	154.57	126.50
48	2	1827	MA6	C5-C6-N6	7.56	138.47	125.30

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	891	PSU	C2'-C1'-C5-C6
1	1	2560	OMG	C1'-C2'-O2'-CM2
1	1	2808	2MA	O4'-C4'-C5'-O5'
1	1	2808	2MA	C3'-C4'-C5'-O5'
1	1	2885	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2560	OMG	1	0
48	2	1827	MA6	1	0

Continued on next page...

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2803	OMC	1	0
48	2	1664	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 435 ligands modelled in this entry, 433 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
91	ATP	W	502	87	29,33,33	0.33	0	44,52,52	0.54	1 (2%)
89	CLM	1	3238	-	19,20,20	0.54	0	23,27,27	0.86	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	ATP	W	502	87	-	1/22/38/38	0/3/3/3
89	CLM	1	3238	-	-	4/20/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	1	3238	CLM	O5-C5-C3	2.18	113.83	107.99
91	W	502	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	1	3238	CLM	CL1-C1-C2-N2
89	1	3238	CLM	CL2-C1-C2-O2
89	1	3238	CLM	CL2-C1-C2-N2
89	1	3238	CLM	CL1-C1-C2-O2
91	W	502	ATP	PA-O3A-PB-O2B

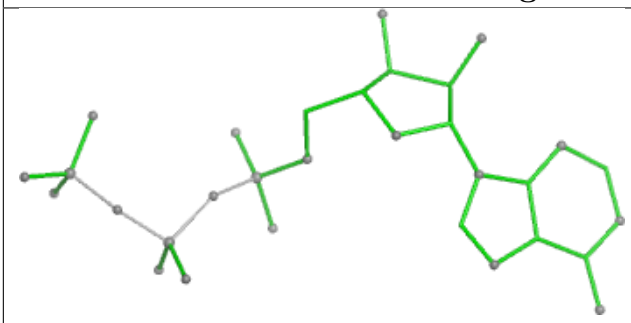
There are no ring outliers.

1 monomer is involved in 1 short contact:

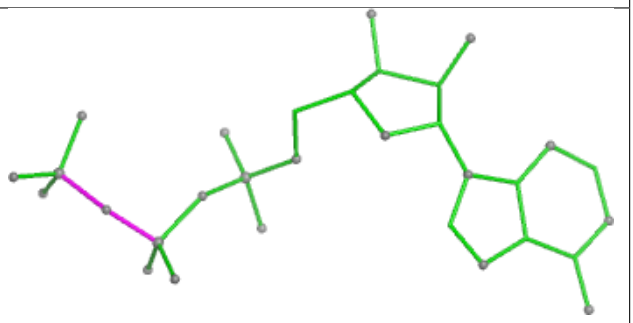
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	1	3238	CLM	1	0

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.

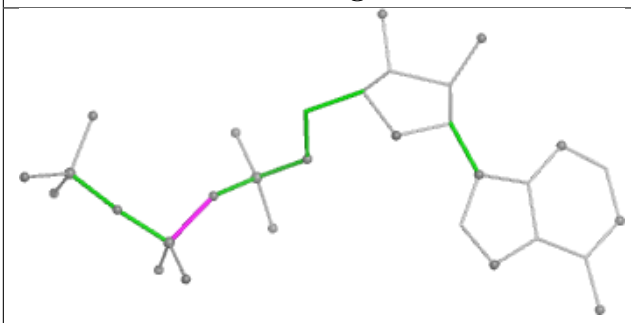
Ligand ATP W 502



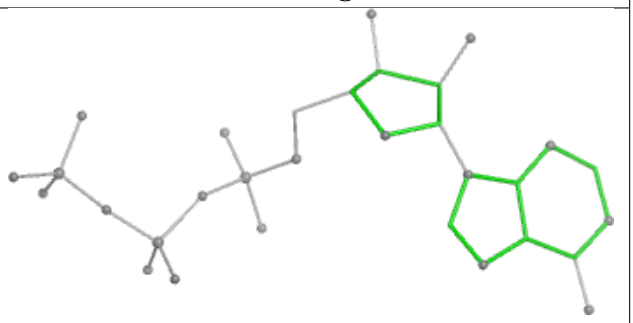
Bond lengths



Bond angles

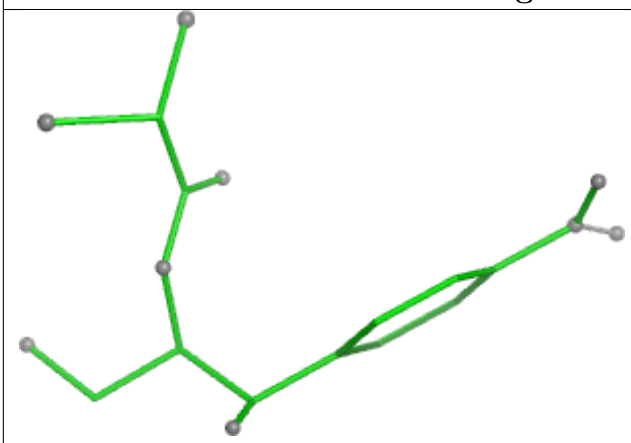


Torsions

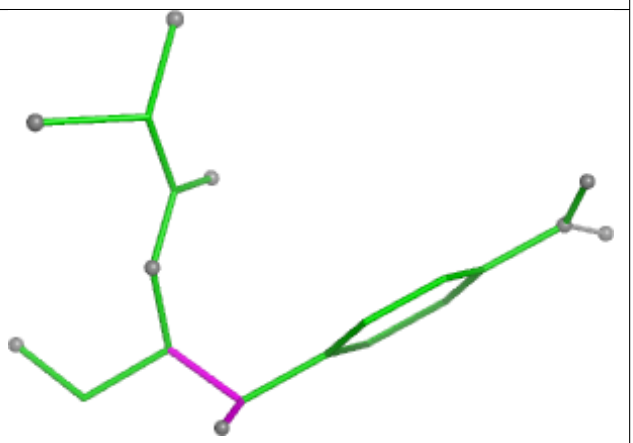


Rings

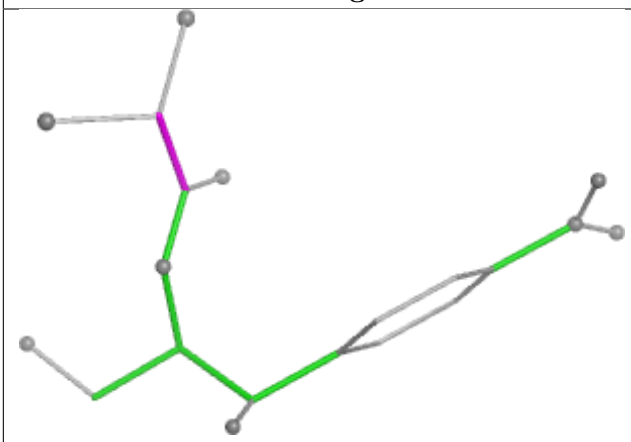
Ligand CLM 1 3238



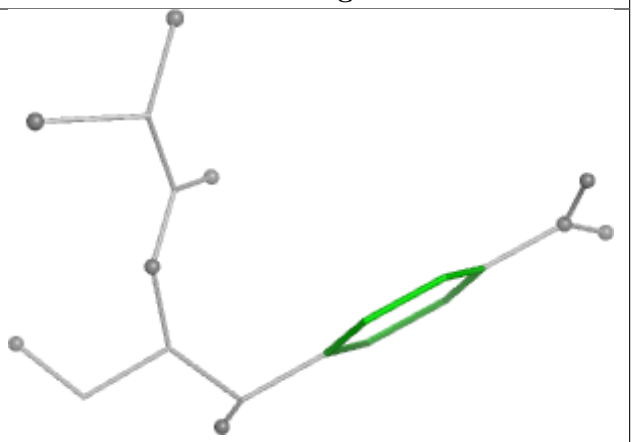
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	11
48	2	2
3	1C	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1C	256:LEU	C	298:ALA	N	38.94
1	1	261:G	O3'	270:A	P	27.38
1	1	295:U	O3'	307:A	P	27.27
1	1	1704:U	O3'	1831:A	P	17.63
1	1	363:A	O3'	405:U	P	17.03

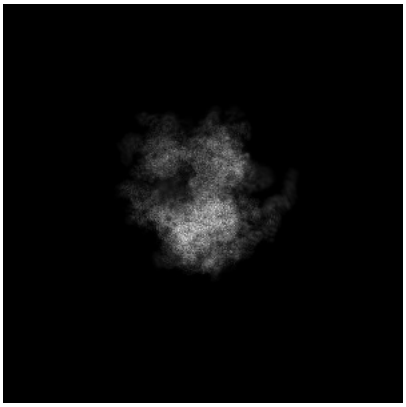
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56210. These allow visual inspection of the internal detail of the map and identification of artifacts.

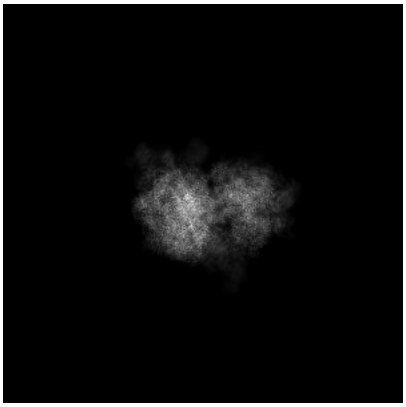
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

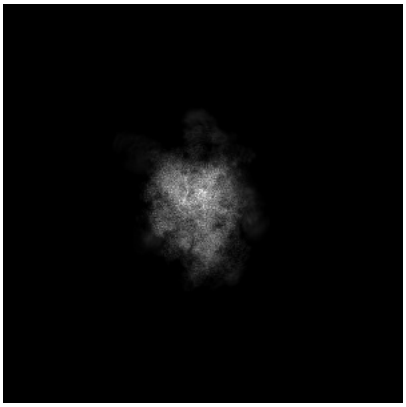
6.1.1 Primary map



X



Y



Z

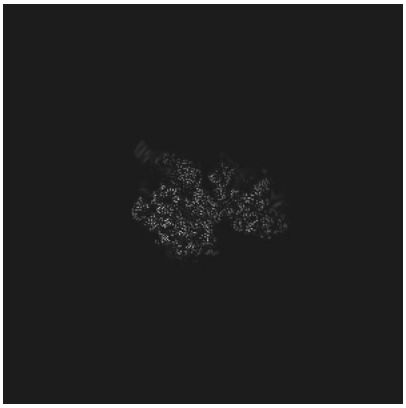
The images above show the map projected in three orthogonal directions.

6.2 Central slices

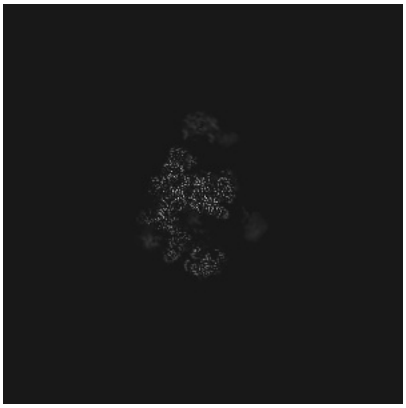
6.2.1 Primary map



X Index: 378



Y Index: 378

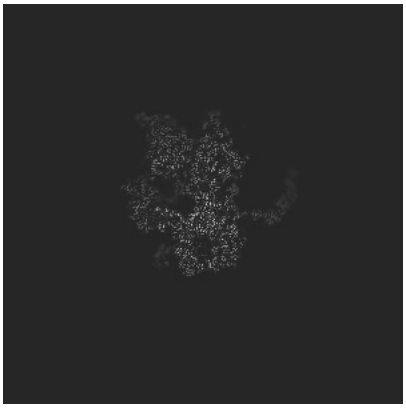


Z Index: 378

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

6.3 Largest variance slices (i)

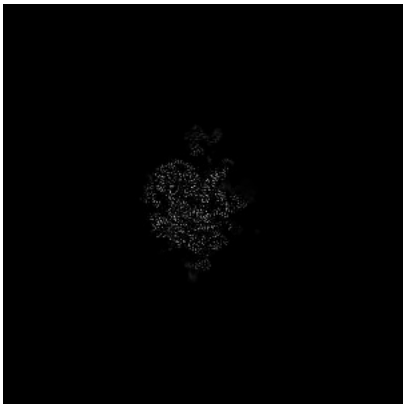
6.3.1 Primary map



X Index: 381



Y Index: 400

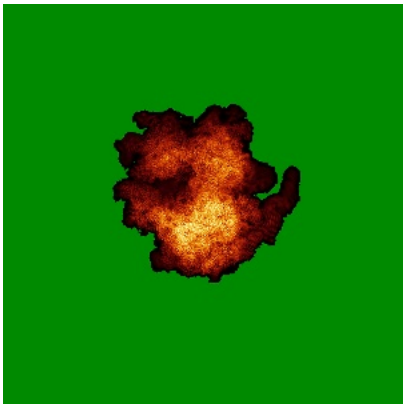


Z Index: 341

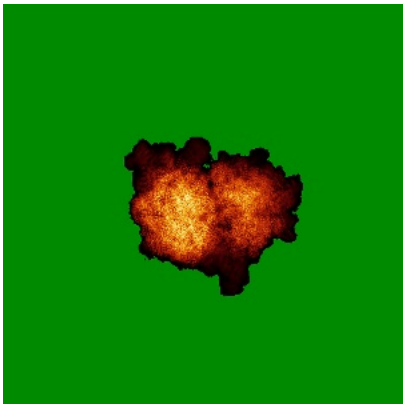
The images above show the largest variance slices of the map in three orthogonal directions.

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

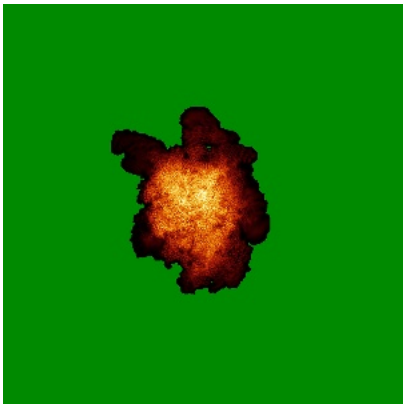
6.4.1 Primary map



X



Y

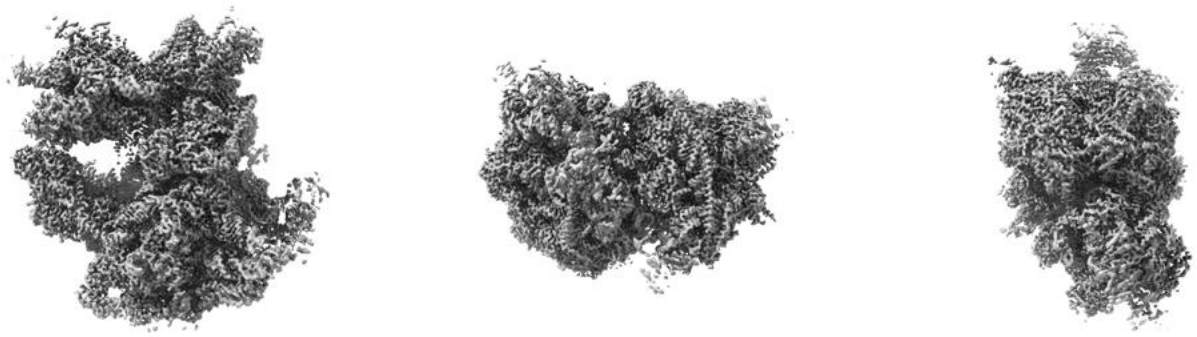


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

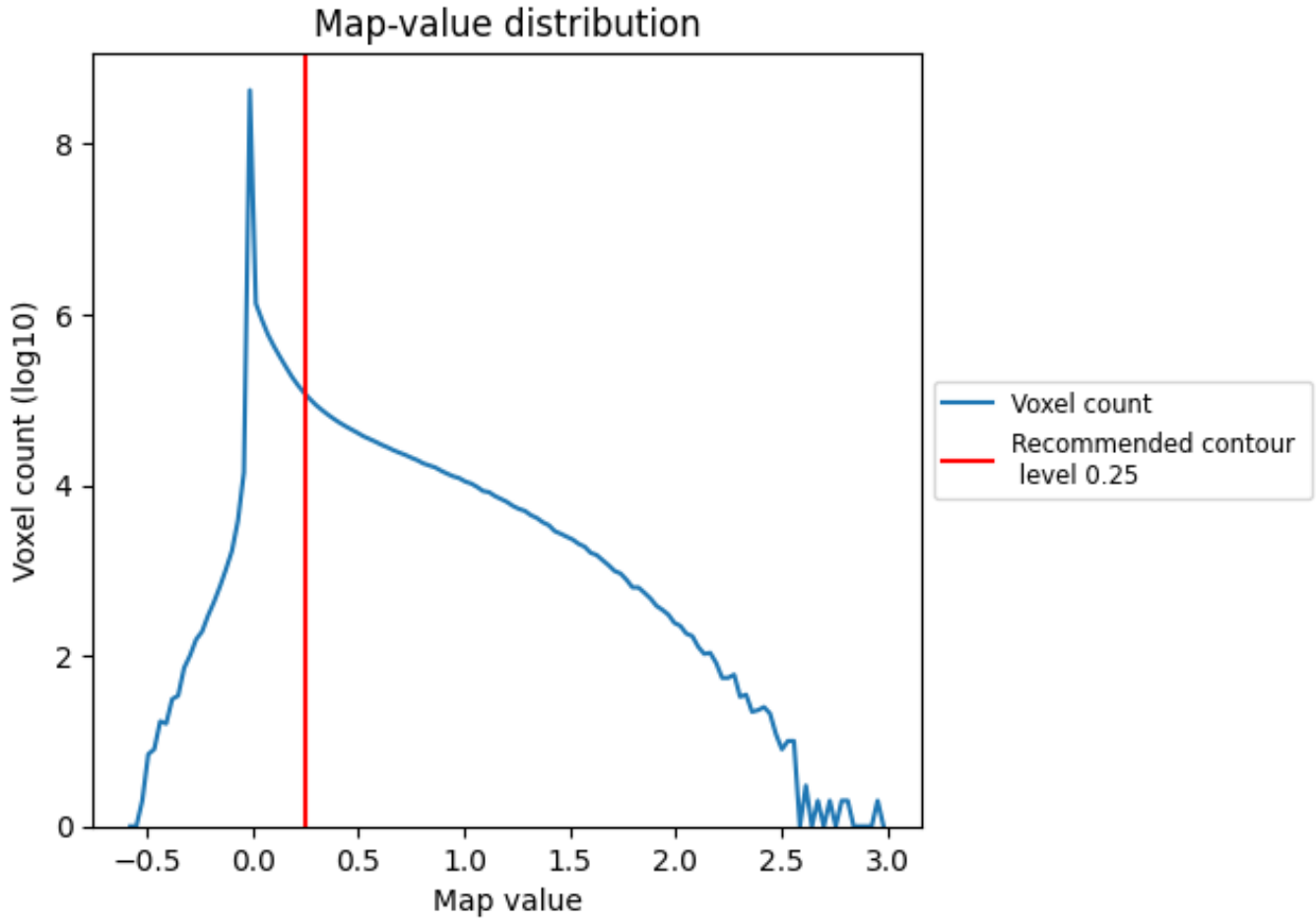
6.6 Mask visualisation (i)

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

7 Map analysis

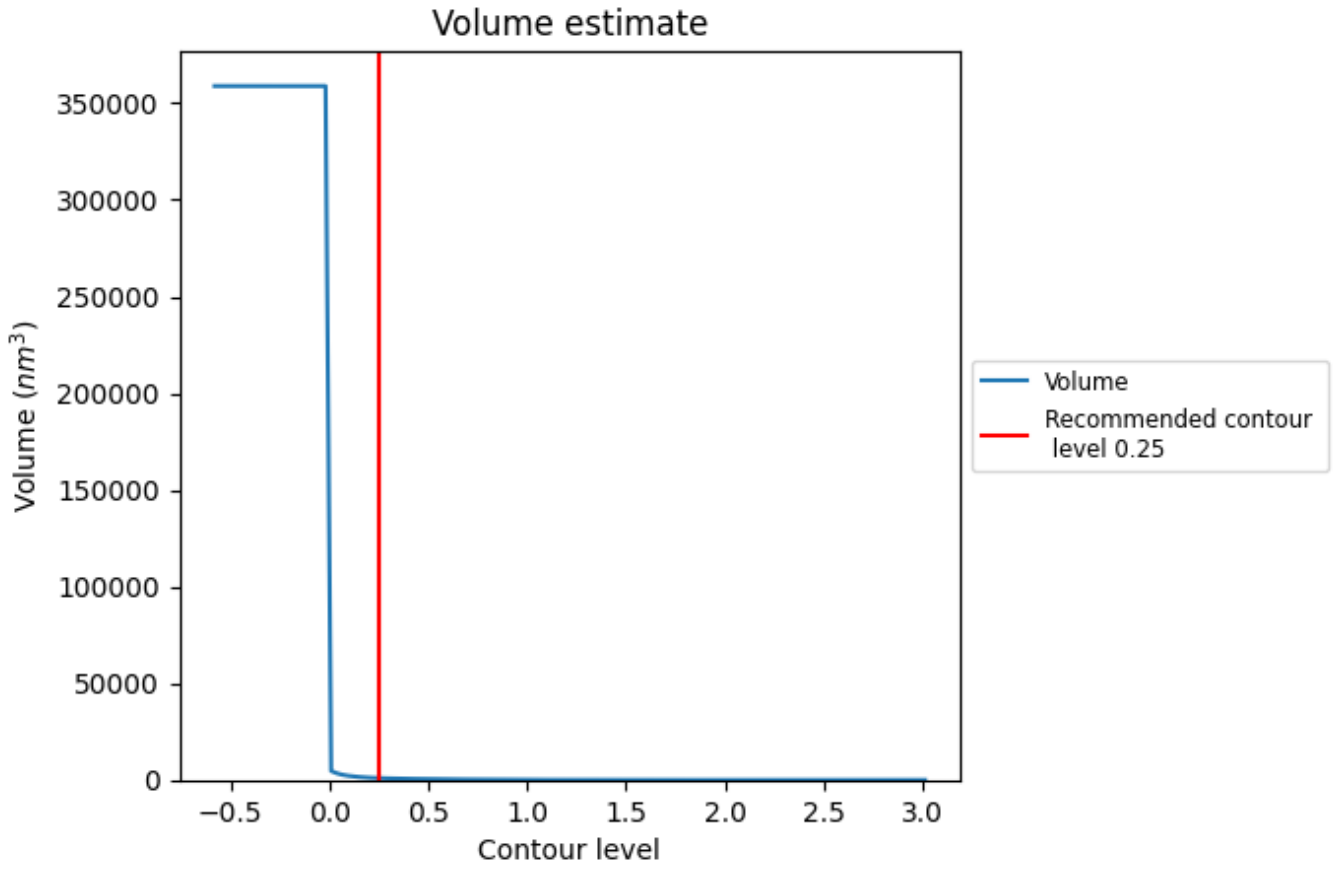
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

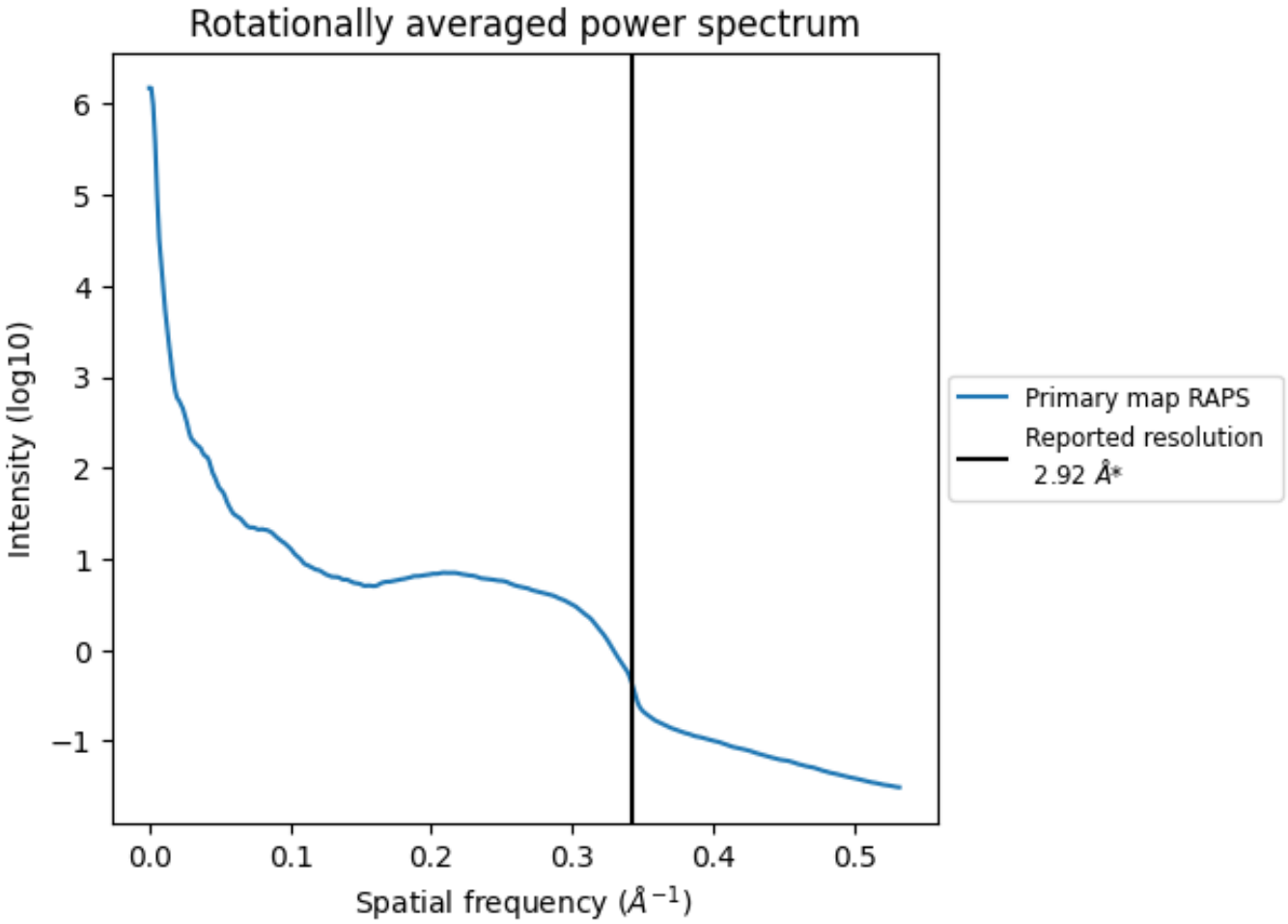
7.2 Volume estimate (i)



The volume at the recommended contour level is 973 nm^3; this corresponds to an approximate mass of 879 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

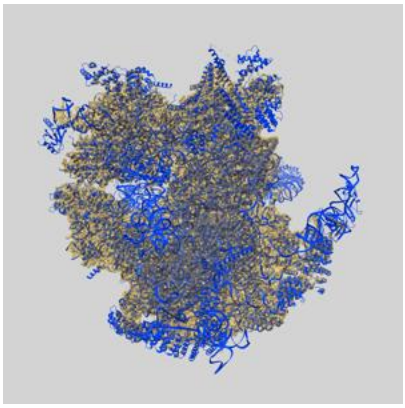
8 Fourier-Shell correlation (i)

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

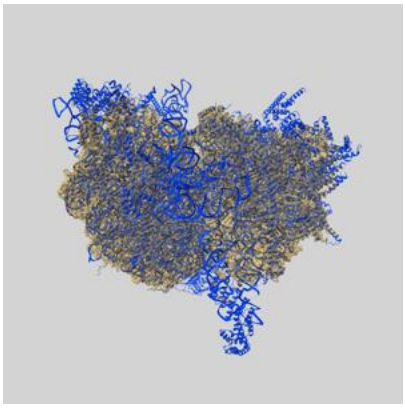
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56210 and PDB model 9TS7. Per-residue inclusion information can be found in section 3 on page 26.

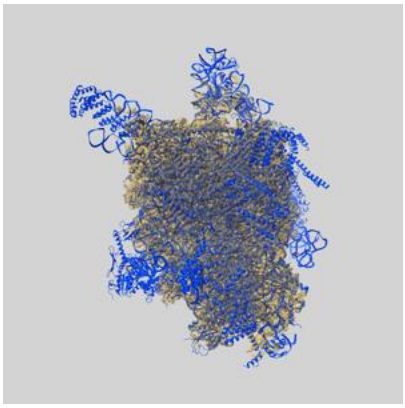
9.1 Map-model overlay



X



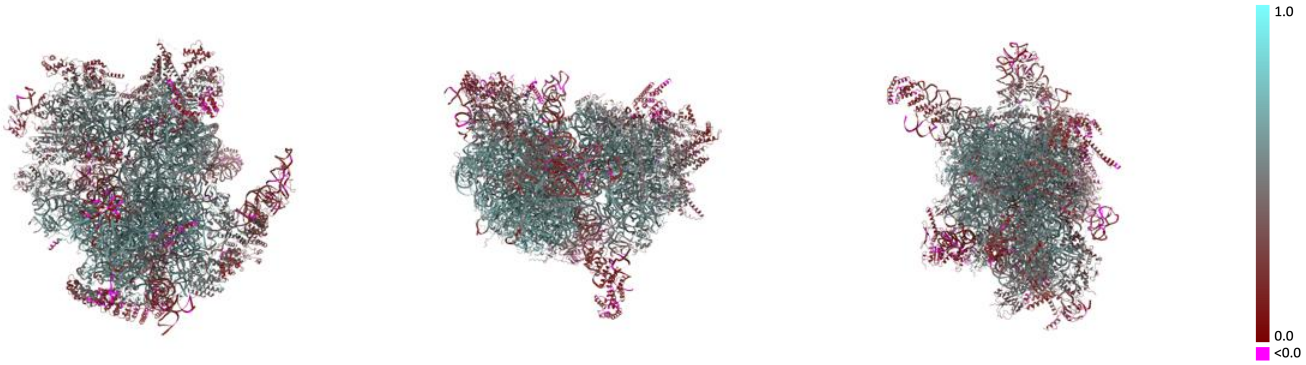
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

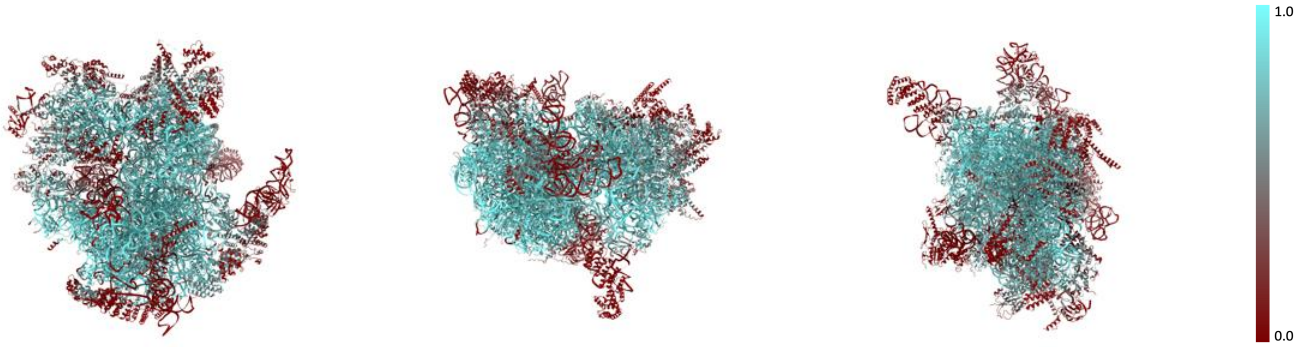
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

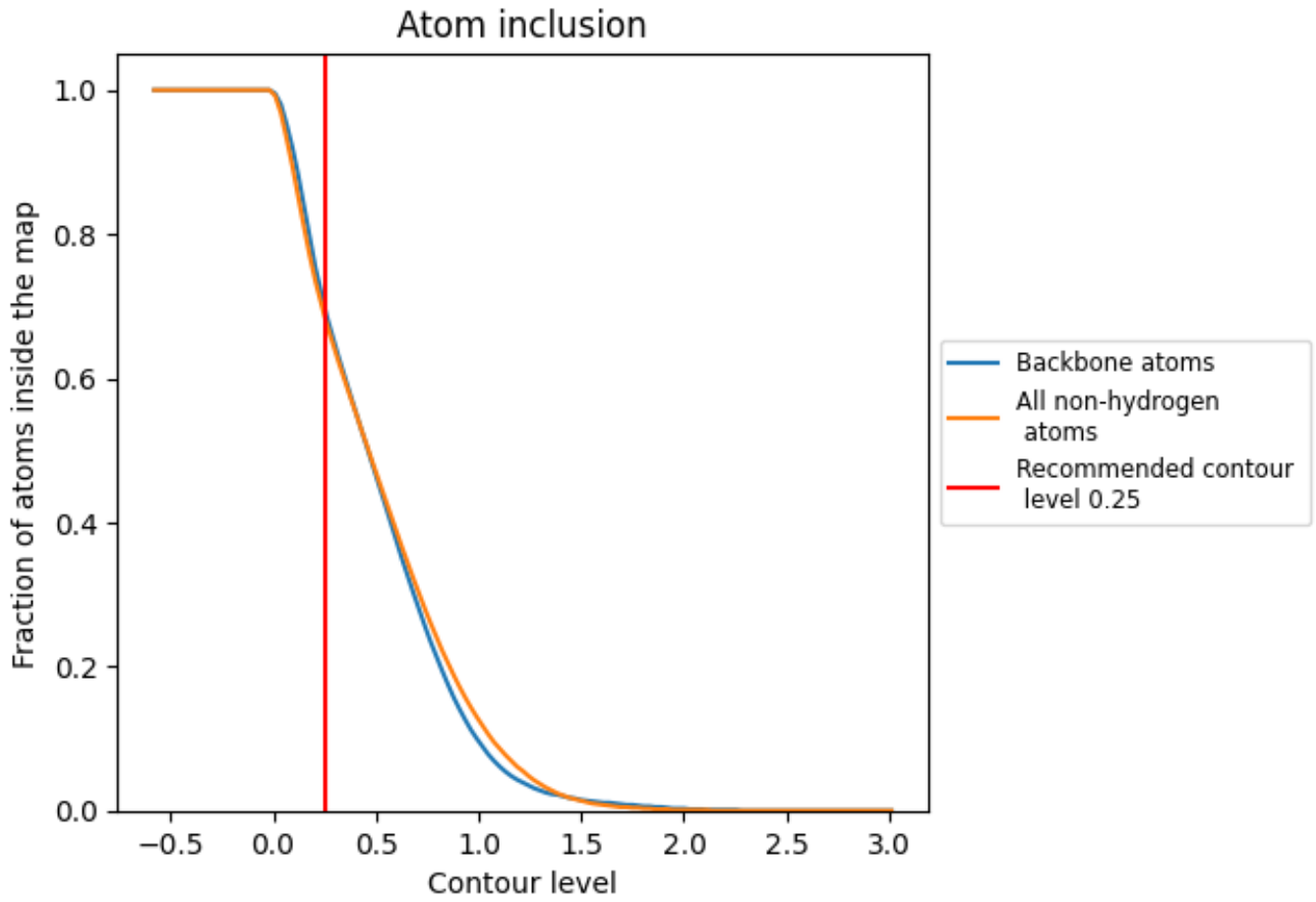
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4890
1	0.8060	0.5440
1B	0.8580	0.5940
1C	0.4200	0.3750
1D	0.9010	0.6180
1E	0.9120	0.6130
1F	0.6170	0.4810
1G	0.0930	0.3380
1H	0.6200	0.4290
1I	0.0000	0.0750
1J	0.0000	0.0820
1K	0.8380	0.5690
1L	0.8770	0.6100
1M	0.8990	0.5970
1N	0.5710	0.4800
1O	0.9390	0.6250
1P	0.8440	0.5730
1Q	0.8600	0.5920
1R	0.9600	0.6380
1S	0.8750	0.5900
1T	0.9070	0.6120
1U	0.8070	0.5730
1V	0.8590	0.5900
1W	0.0190	0.1730
1X	0.6140	0.4820
1Y	0.8290	0.5560
1Z	0.5330	0.4220
1a	0.8860	0.6010
1b	0.8920	0.6110
1c	0.6810	0.4920
1d	0.9510	0.6330
1e	0.8040	0.5760
1f	0.9830	0.6560
1g	0.9220	0.6190
1h	0.6690	0.5430



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Chain	Atom inclusion	Q-score
1i	0.5320	0.4340
1j	0.9120	0.6130
1k	0.9110	0.6090
1l	0.4690	0.4030
1m	0.0040	0.1270
1o	0.0000	0.1090
1p	0.7810	0.5550
1q	0.8840	0.5870
1r	0.7690	0.5380
1s	0.7720	0.5460
1t	0.4160	0.3660
1u	0.1810	0.2740
1v	0.5150	0.4140
2	0.8500	0.5440
3	0.9050	0.5630
5	0.1900	0.3050
6	0.4810	0.4520
A	0.7270	0.5180
B	0.4490	0.3910
C	0.7220	0.5010
D	0.5970	0.4490
E	0.8220	0.5630
F	0.0610	0.2700
G	0.8990	0.5920
H	0.5600	0.4210
I	0.7730	0.5460
J	0.6540	0.4790
K	0.7750	0.5430
L	0.6520	0.4760
M	0.8100	0.5500
N	0.7910	0.5410
O	0.9070	0.5880
P	0.7890	0.5520
Q	0.7420	0.5210
R	0.3080	0.3070
S	0.5310	0.4400
T	0.8510	0.5750
U	0.2830	0.2860
V	0.6070	0.4510
W	0.5350	0.4350
X	0.4240	0.3610
Y	0.5960	0.4680

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Chain	Atom inclusion	Q-score
Z	0.4660	0.4040
a	0.3900	0.3640
b	0.0050	0.1870
c	0.7180	0.5490
d	0.6480	0.4830
e	0.7550	0.5150
f	0.4800	0.3950
h	0.0130	0.1620
i	0.1520	0.2030
k	0.0420	0.2250