



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 02:53 pm BST

PDB ID : 9S7B / pdb_00009s7b
EMDB ID : EMD-54637
Title : Structure of human mitochondrial COX1-translating ribosome nascent chain complex with tRNAs in intermediate state (AP*)
Authors : Schoendorf, T.; Petrychenko, V.; Kotan, I.; Cruz-Zaragoza, L.D.; Dahal, D.; Wang, C.; Gal, T.; Dennerlein, S.; Kramer, G.; Fischer, N.; Rehling, P.
Deposited on : 2025-08-04
Resolution : 3.70 Å (reported)
Based on initial model : 7QI5

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 Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

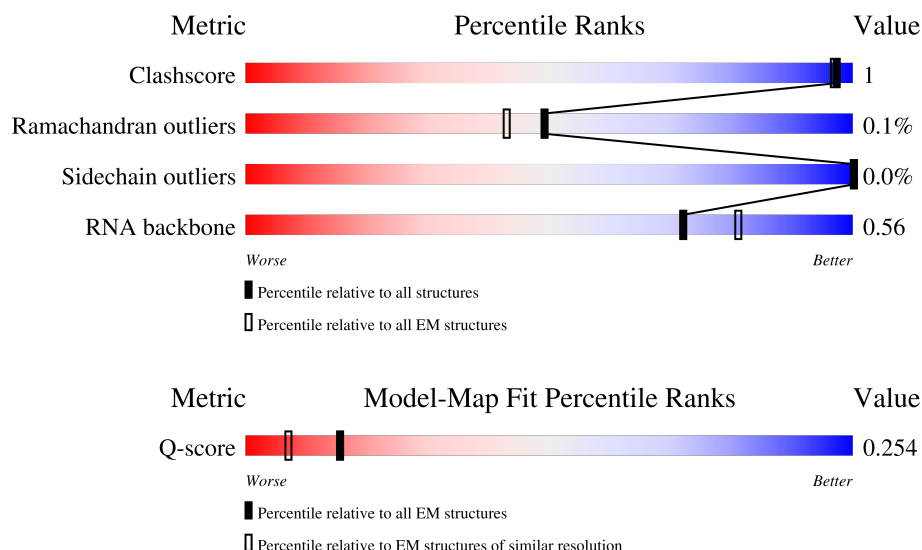
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	1561	
2	B	72	

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Mol	Chain	Length	Quality of chain
3	D	305	
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	

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Mol	Chain	Length	Quality of chain
28	3	188	
29	4	103	
30	z	325	
31	t	198	
31	u	198	
31	v	198	
31	w	198	
31	x	198	
31	y	198	
32	5	423	
33	6	380	
34	7	338	
35	8	206	
36	9	137	
37	a	142	
38	b	215	
39	c	332	
40	d	306	
41	e	279	
42	f	212	
43	g	166	
44	h	158	
45	i	128	
46	j	123	
47	k	112	

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Mol	Chain	Length	Quality of chain
48	l	138	
49	m	128	
50	o	102	
51	p	206	
52	q	222	
53	r	196	
54	s	439	
55	AA	954	
56	AB	296	
57	AC	167	
58	AD	430	
59	AE	125	
60	AF	242	
61	AG	396	
62	AH	201	
63	AI	194	
64	AJ	138	
65	AK	128	
66	AL	257	
67	AM	137	
68	AN	130	
69	AO	258	
70	AP	142	
71	AQ	87	
72	AR	360	

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Mol	Chain	Length	Quality of chain
73	AS	190	
74	AT	173	
75	AU	205	
76	AV	414	
77	AW	187	
78	AX	398	
79	AY	395	
80	AZ	106	
81	A0	217	
82	A1	323	
83	A2	118	
84	A3	199	
85	A4	689	
86	Az	33	
87	Av	23	
88	Aw	68	
89	Ax	71	

2 Entry composition

There are 97 unique types of molecules in this entry. The entry contains 179948 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 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	212	Total	C	N	O	S	0	0
			1695	1088	304	292	11		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	178	Total	C	N	O	S	0	0
			1455	936	259	253	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP Q9BYD1

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	239	Total	C	N	O	S	0	0
			1990	1277	353	351	9		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	153	Total	C	N	O	S	0	0
			1251	788	234	226	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	ACE	-	acetylation	UNP Q16540

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	113	Total	C	N	O	S	0	0
			880	562	166	149	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	z	252	Total	C	N	O	S	0	0
			2027	1304	336	381	6		

- Molecule 31 is a protein called Large ribosomal subunit protein bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	w	31	Total	C	N	O	0	0
			245	159	39	47		
31	x	31	Total	C	N	O	0	0
			245	159	39	47		
31	t	46	Total	C	N	O	0	0
			354	228	56	70		
31	u	32	Total	C	N	O	0	0
			257	168	40	49		
31	v	32	Total	C	N	O	0	0
			257	168	40	49		
31	y	31	Total	C	N	O	0	0
			245	159	39	47		

- Molecule 32 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	393	Total	C	N	O	S	0	0
			3200	2067	557	565	11		

- Molecule 33 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 34 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 35 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	144	Total	C	N	O	S	0	0
			1219	775	214	228	2		

- Molecule 36 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 37 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 38 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	151	Total	C	N	O	S	0	0
			1196	744	231	218	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	1	ACE	-	acetylation	UNP Q8N983

- Molecule 39 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 40 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	221	Total	C	N	O	S	0	0
			1807	1153	311	330	13		

- Molecule 41 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	230	Total	C	N	O	S	0	0
			1866	1185	329	346	6		

- Molecule 42 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 43 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 44 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 45 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 46 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 47 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	k	102	Total	C	N	O	S	0	0
			774	479	148	142	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	1	ACE	-	acetylation	UNP Q96EL3

- Molecule 48 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 49 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	m	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 50 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 51 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 52 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	q	166	Total	C	N	O	S	0	0
			1398	870	272	251	5		

- Molecule 53 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 54 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	s	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 55 is a RNA chain called Large ribosomal subunit protein mL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AA	954	Total	C	N	O	P	0	0
			20260	9088	3647	6571	954		

- Molecule 56 is a protein called Small ribosomal subunit protein uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AB	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 57 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 58 is a protein called Small ribosomal subunit protein uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AD	339	Total	C	N	O	S	0	0
			2700	1695	510	482	13		

- Molecule 59 is a protein called Small ribosomal subunit protein bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 60 is a protein called Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 61 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AG	328	Total	C	N	O	S	0	0
			2695	1714	478	489	14		

- Molecule 62 is a protein called Small ribosomal subunit protein uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 63 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AI	137	Total	C	N	O	S	0	0
			1020	642	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 64 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 65 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 67 is a protein called Small ribosomal subunit protein bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 68 is a protein called Small ribosomal subunit protein uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 69 is a protein called Small ribosomal subunit protein mS40.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 70 is a protein called Small ribosomal subunit protein bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 71 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AQ	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP P82921
AQ	50	ARG	CYS	conflict	UNP P82921

- Molecule 72 is a protein called Small ribosomal subunit protein mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 73 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 74 is a protein called Small ribosomal subunit protein mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 75 is a protein called Small ribosomal subunit protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 76 is a protein called Small ribosomal subunit protein mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 77 is a protein called Small ribosomal subunit protein bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 78 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 79 is a protein called Small ribosomal subunit protein mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AY	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 80 is a protein called Small ribosomal subunit protein mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 81 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	A0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 82 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	A1	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 83 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	A2	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 84 is a protein called Small ribosomal subunit protein bS22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	A3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 85 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	A4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 86 is a RNA chain called mRNA (Visualization example).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Az	33	Total	C	N	O	P	0	0
			701	316	124	228	33		

- Molecule 87 is a protein called COX1 nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
87	Av	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 88 is a RNA chain called A-site tRNA (Visualisation example).

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Aw	68	Total	C	N	O	P	0	0
			1435	646	249	472	68		

- Molecule 89 is a RNA chain called P-site tRNA (Visualisation example).

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Ax	67	Total	C	N	O	P	0	0
			1415	634	244	470	67		

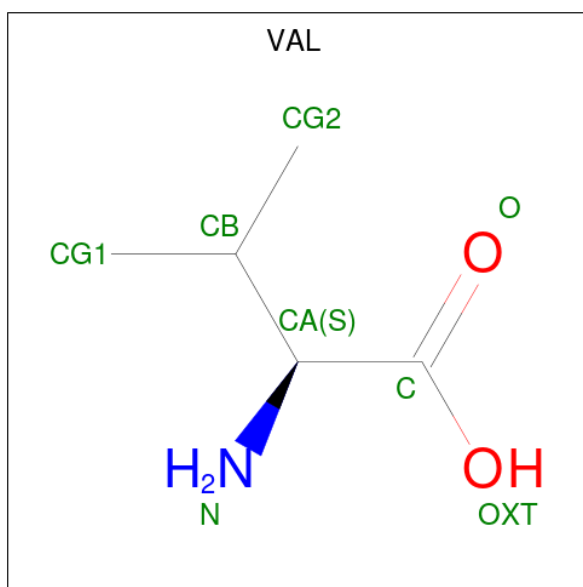
- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	A	28	Total 28	K 28	0
90	D	1	Total 1	K 1	0
90	M	1	Total 1	K 1	0
90	N	1	Total 1	K 1	0
90	3	1	Total 1	K 1	0
90	6	1	Total 1	K 1	0
90	o	1	Total 1	K 1	0
90	AA	19	Total 19	K 19	0
90	AJ	1	Total 1	K 1	0

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

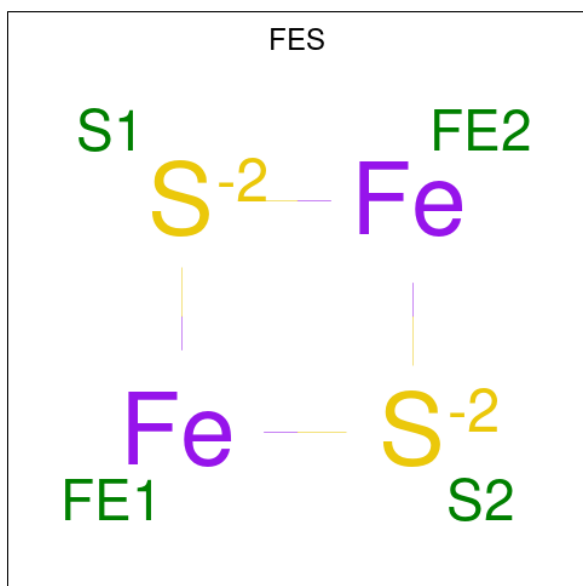
Mol	Chain	Residues	Atoms		AltConf
91	A	130	Total 130	Mg 130	0
91	D	2	Total 2	Mg 2	0
91	E	1	Total 1	Mg 1	0
91	g	1	Total 1	Mg 1	0
91	AA	55	Total 55	Mg 55	0
91	AB	1	Total 1	Mg 1	0
91	AX	1	Total 1	Mg 1	0
91	A3	1	Total 1	Mg 1	0

- Molecule 92 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
92	B	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 93 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

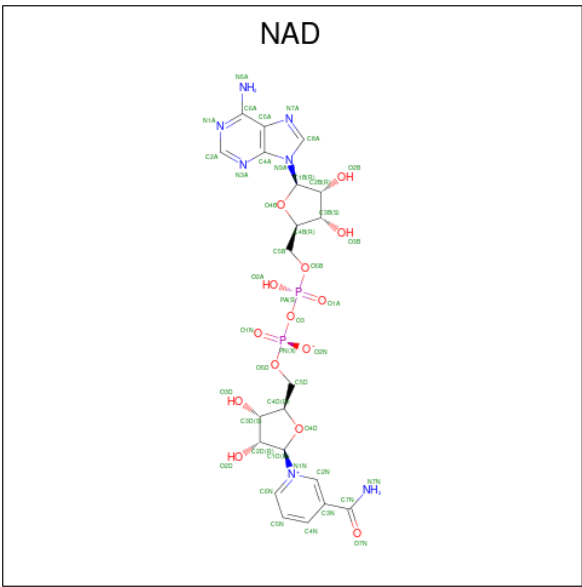


Mol	Chain	Residues	Atoms			AltConf
93	I	1	Total	Fe	S	0
			4	2	2	
93	AE	1	Total	Fe	S	0
			4	2	2	
93	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

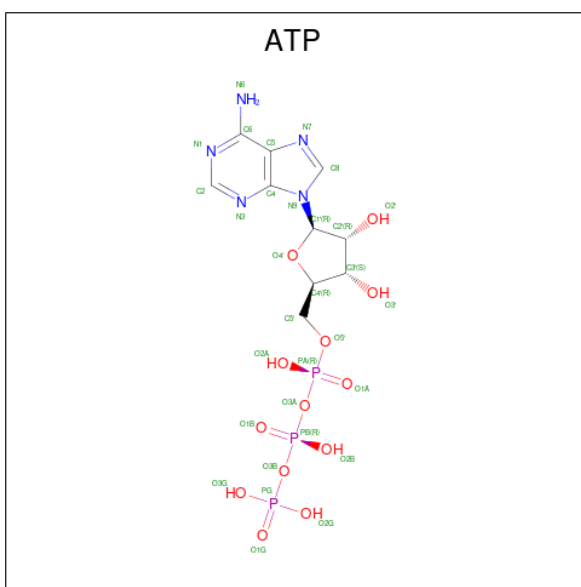
Mol	Chain	Residues	Atoms		AltConf
94	0	1	Total	Zn	0
			1	1	
94	4	1	Total	Zn	0
			1	1	
94	AO	1	Total	Zn	0
			1	1	

- Molecule 95 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



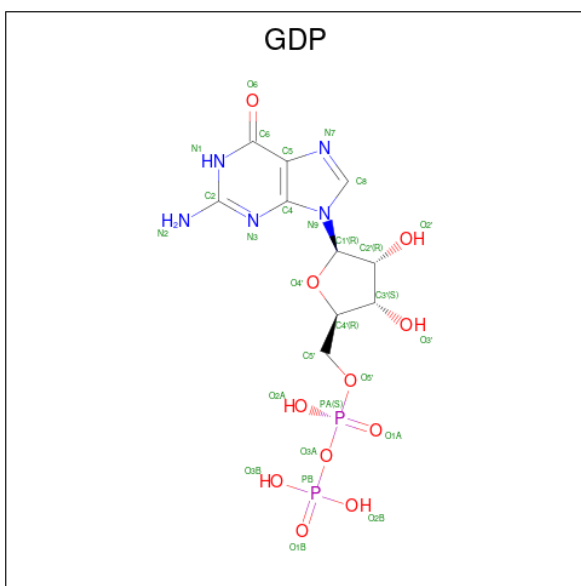
Mol	Chain	Residues	Atoms					AltConf
95	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 96 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 97 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

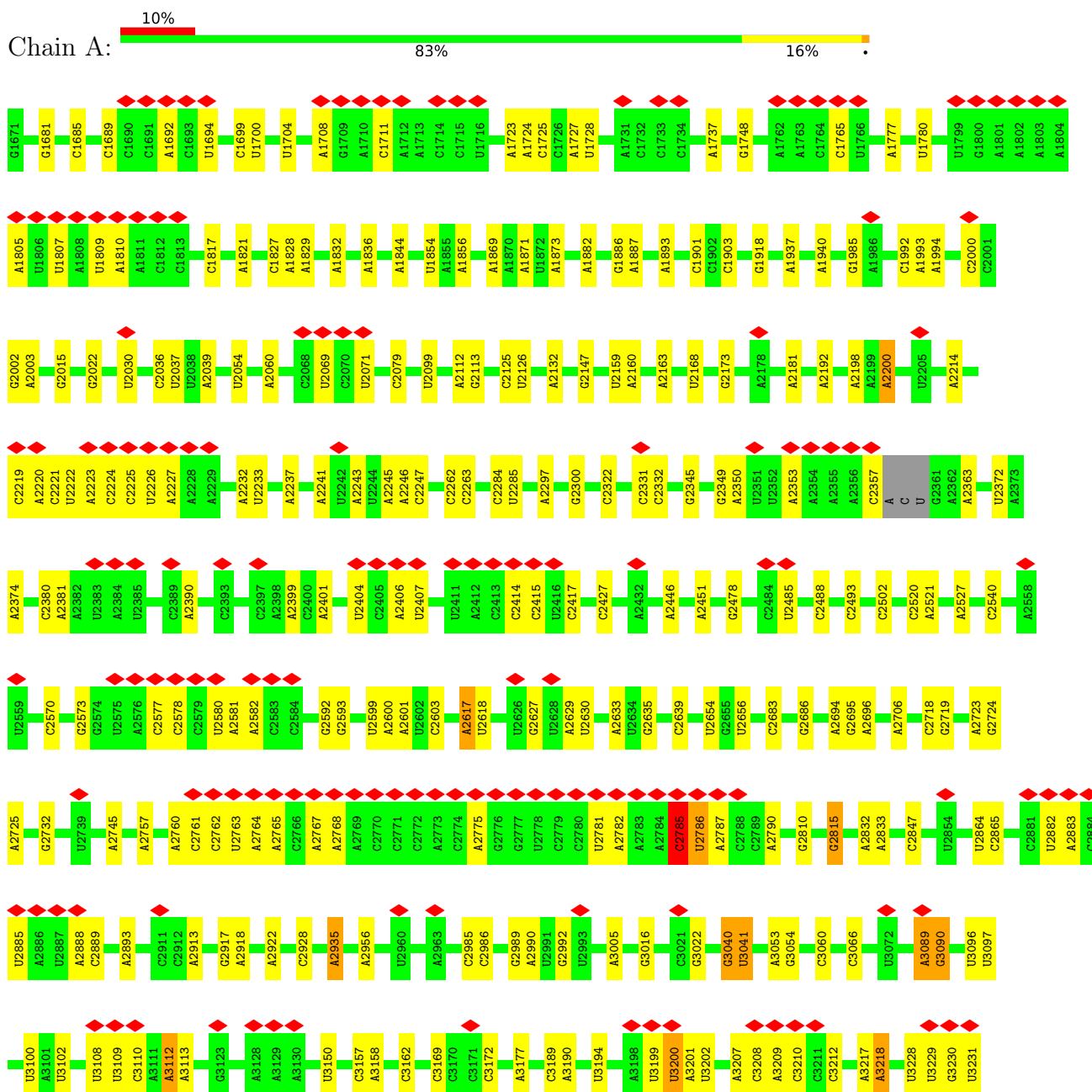


Mol	Chain	Residues	Atoms					AltConf
97	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots

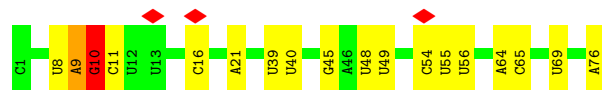
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S mitochondrial rRNA



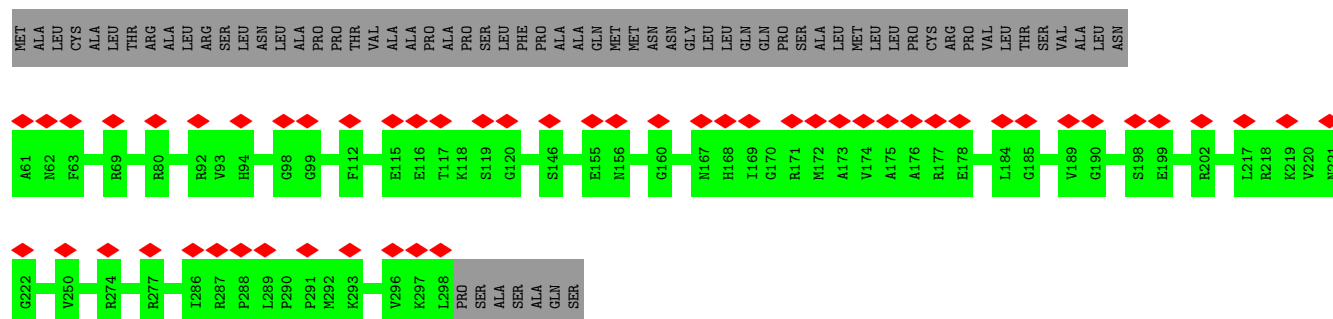
- Molecule 2: mitochondrial tRNA^{Val}

Chain B: 



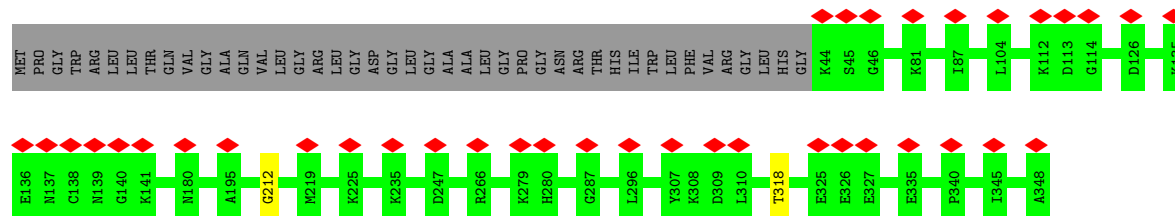
- Molecule 3: Large ribosomal subunit protein uL2m

Chain D: 



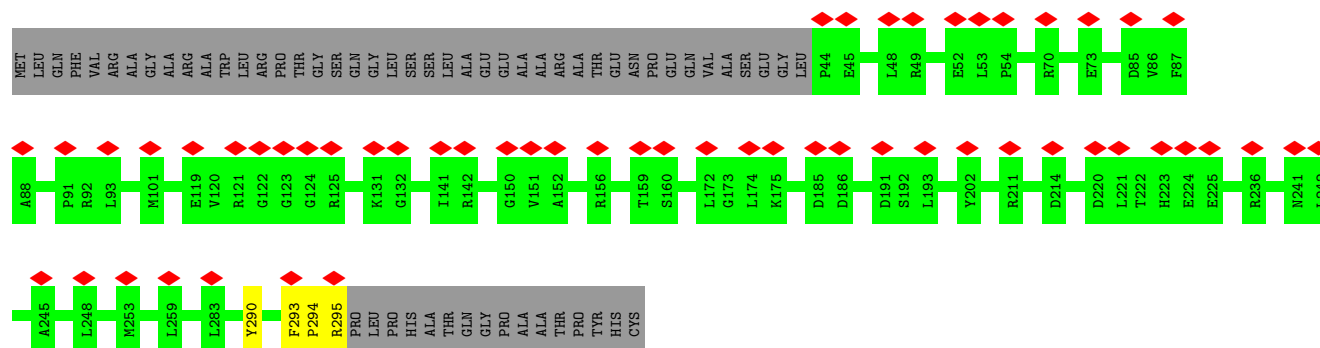
- Molecule 4: Large ribosomal subunit protein uL3m

Chain E: 



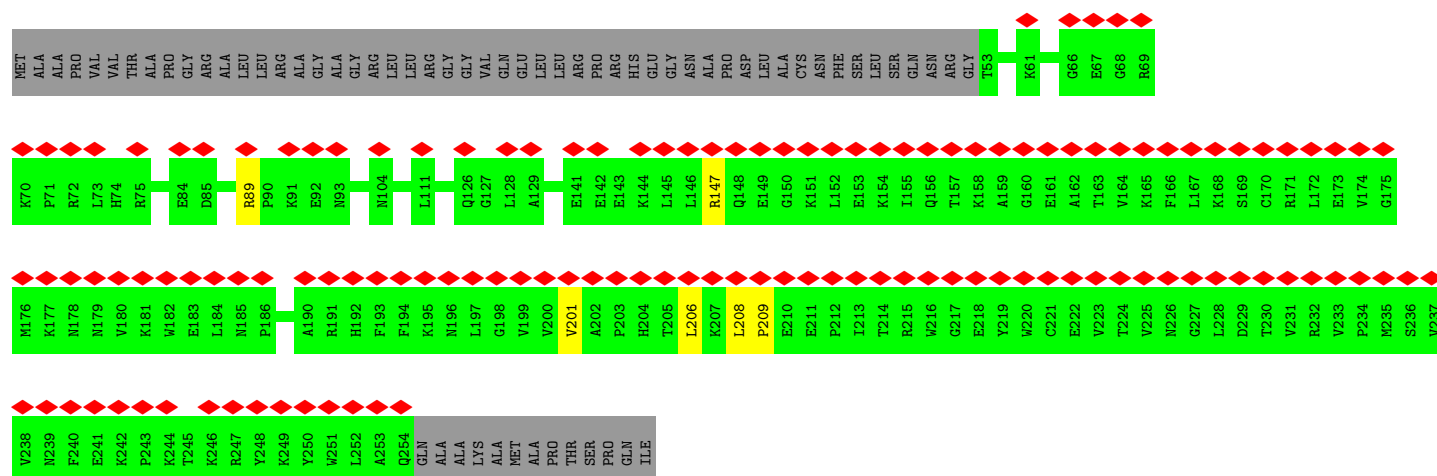
- Molecule 5: Large ribosomal subunit protein uL4m

Chain F: 



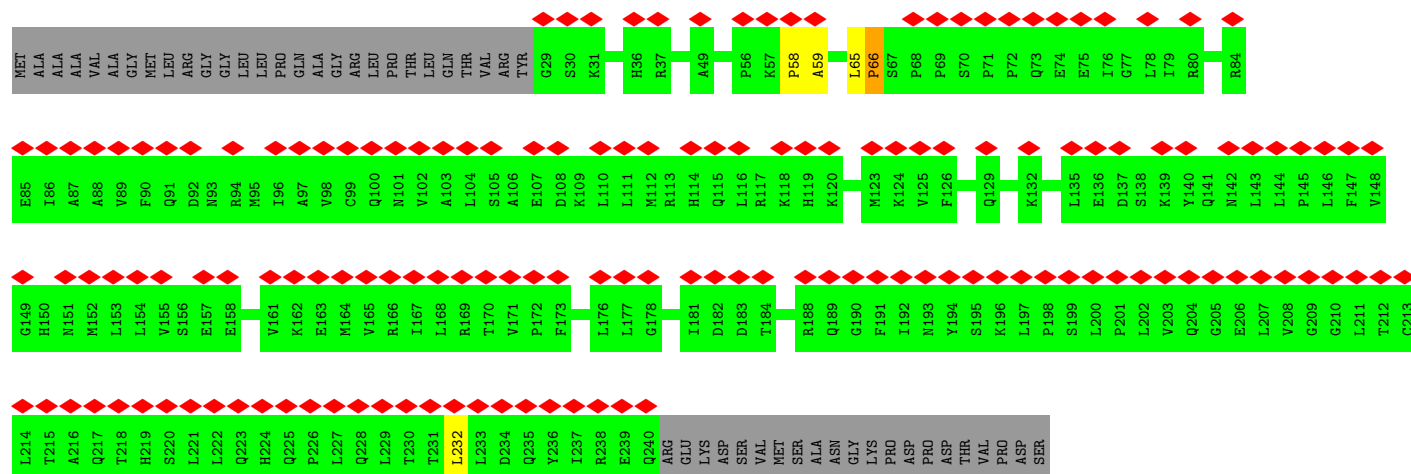
- Molecule 6: Large ribosomal subunit protein bL9m

Chain H: 



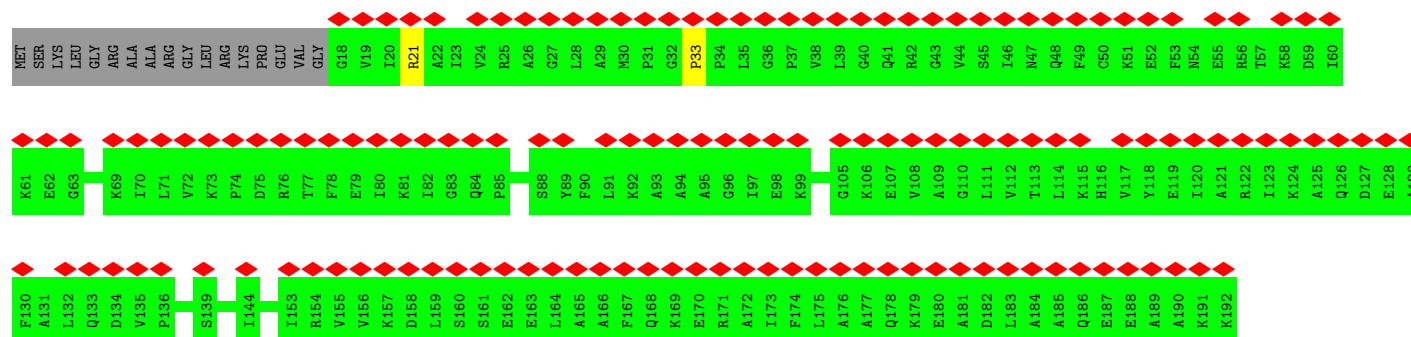
• Molecule 7: Large ribosomal subunit protein uL10m

Chain I: 58% 79% 19%

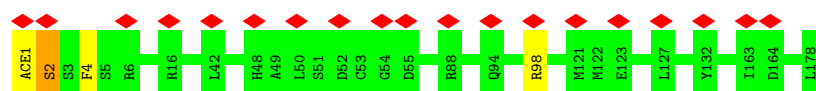


• Molecule 8: Large ribosomal subunit protein uL11m

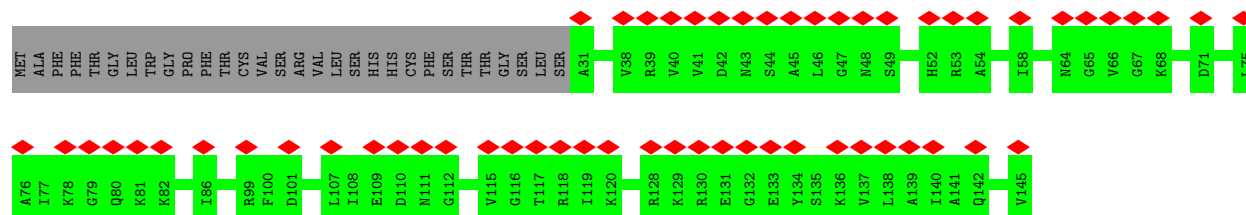
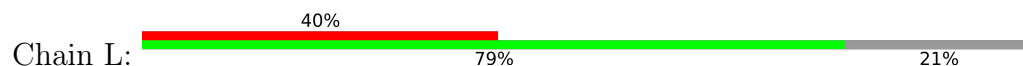
Chain J: 74% 90% 9%



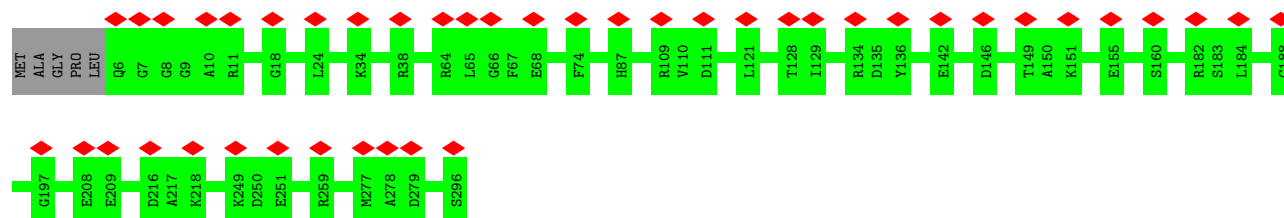
• Molecule 9: Large ribosomal subunit protein uL13m



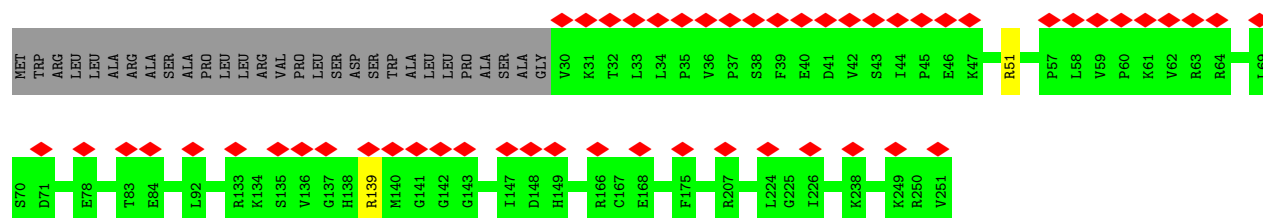
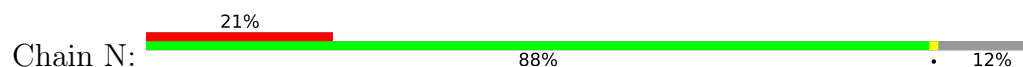
- Molecule 10: Large ribosomal subunit protein uL14m



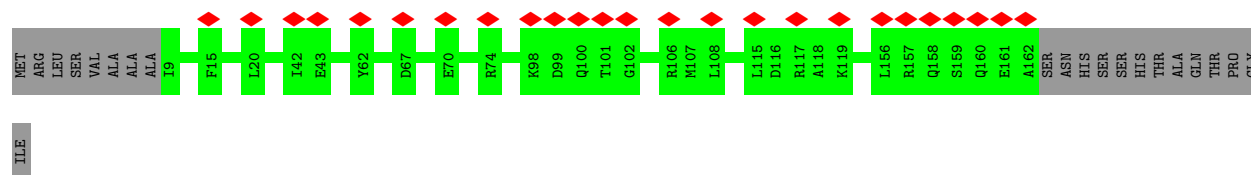
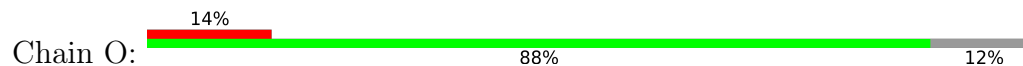
- Molecule 11: Large ribosomal subunit protein uL15m



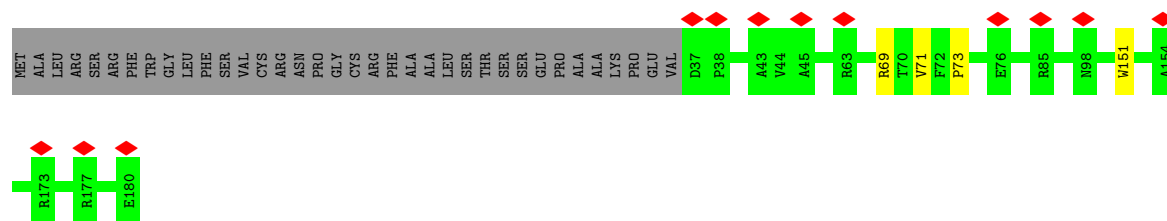
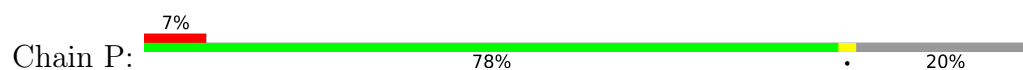
- Molecule 12: Large ribosomal subunit protein uL16m



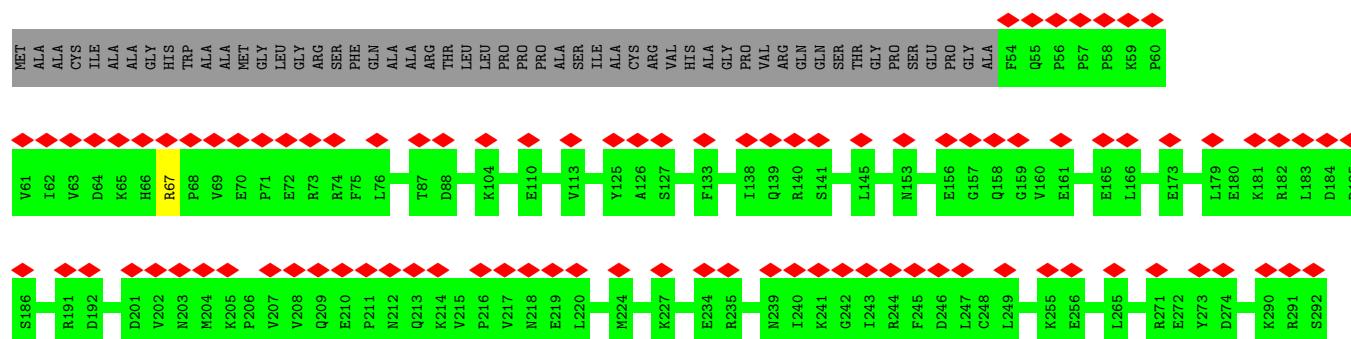
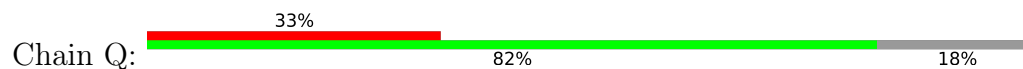
- Molecule 13: Large ribosomal subunit protein bL17m



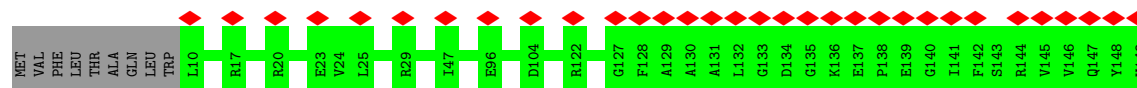
- Molecule 14: Large ribosomal subunit protein uL18m



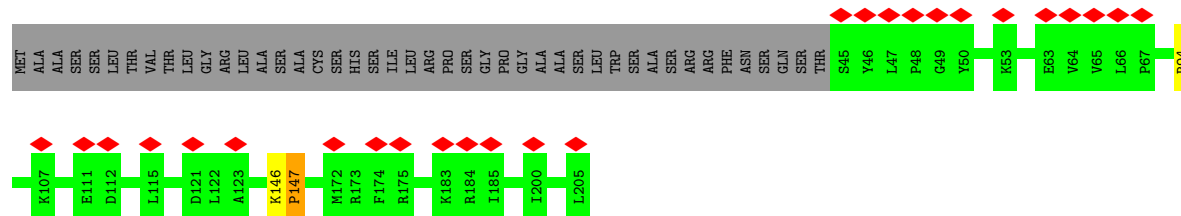
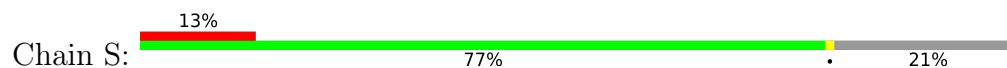
- Molecule 15: Large ribosomal subunit protein bL19m



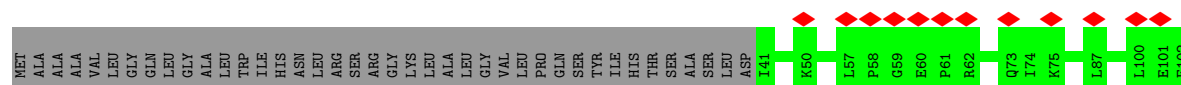
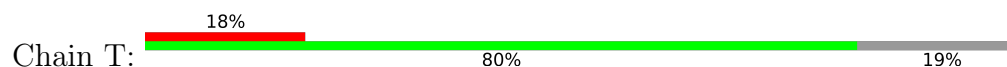
- Molecule 16: Large ribosomal subunit protein bL20m

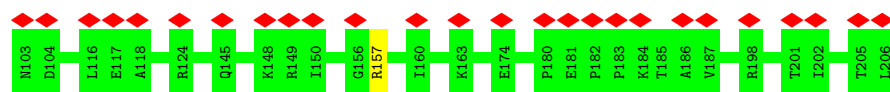


- Molecule 17: Large ribosomal subunit protein bL21m

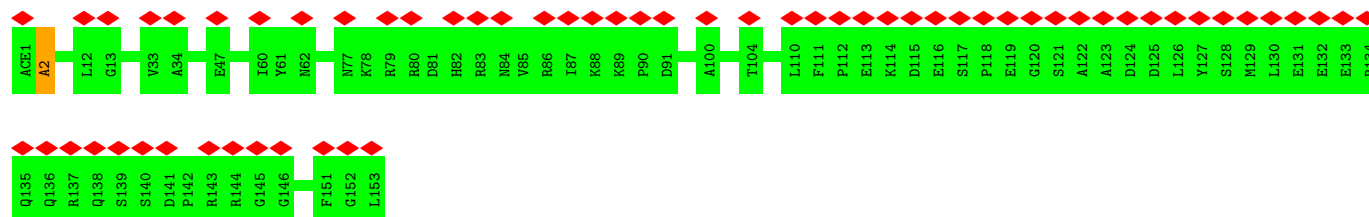
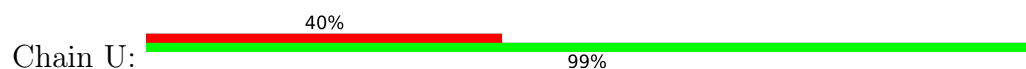


- Molecule 18: Large ribosomal subunit protein uL22m

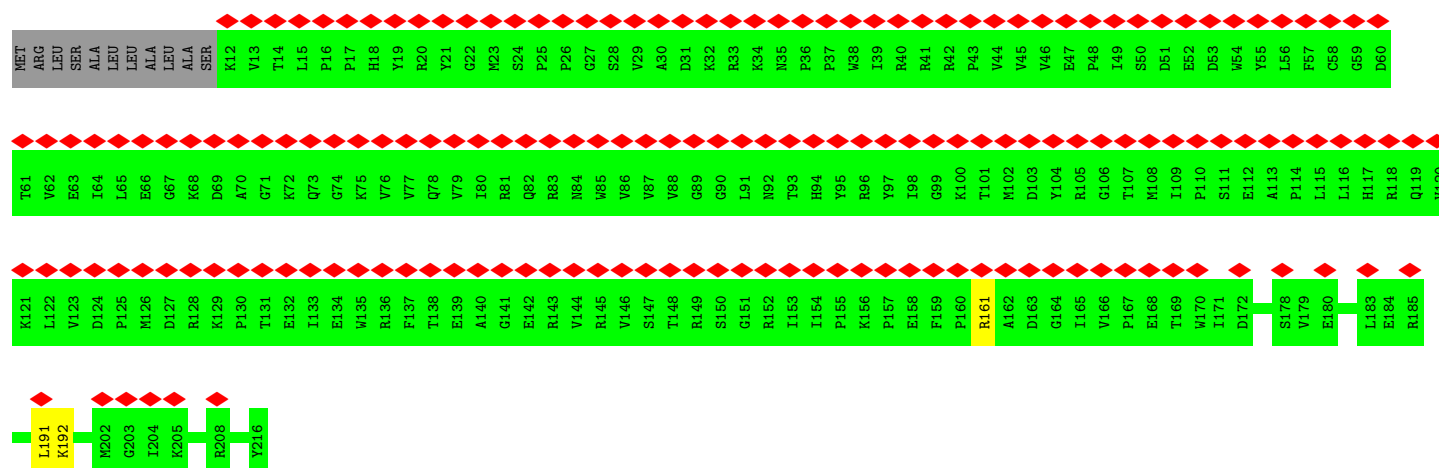
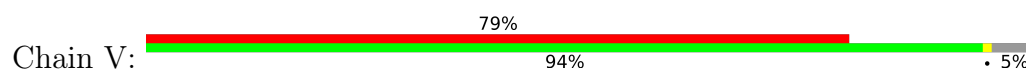




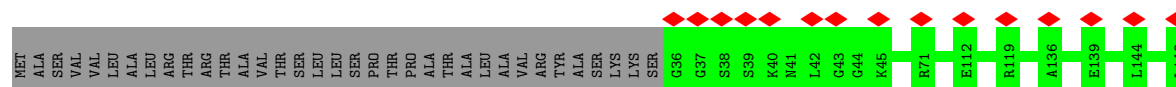
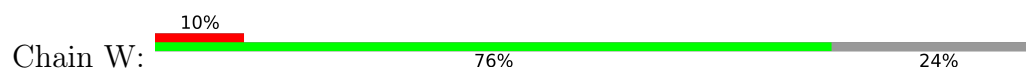
- Molecule 19: Large ribosomal subunit protein uL23m



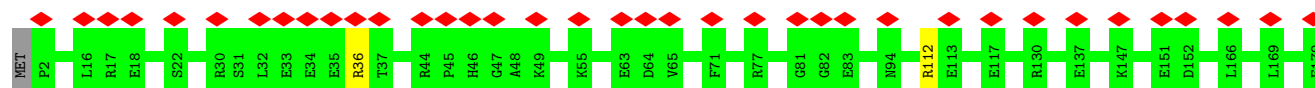
- Molecule 20: Large ribosomal subunit protein uL24m

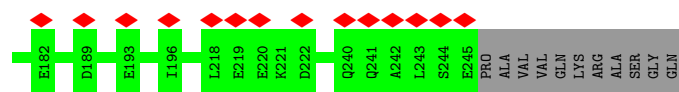


- Molecule 21: Large ribosomal subunit protein bL27m



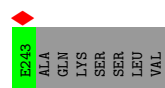
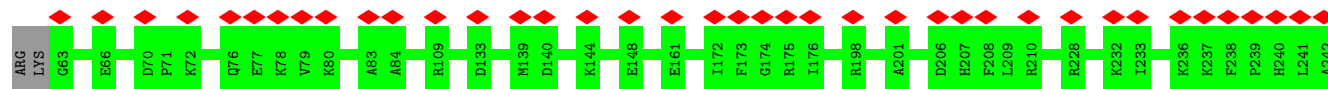
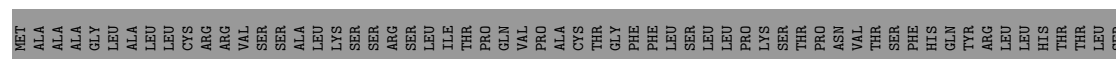
- Molecule 22: Large ribosomal subunit protein bL28m





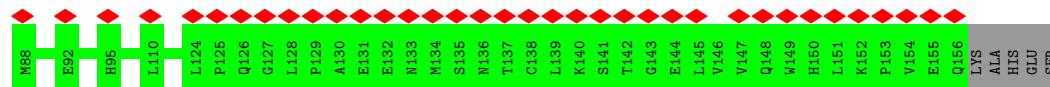
- Molecule 23: Large ribosomal subunit protein uL29m

Chain Y: 16% 72% 28%



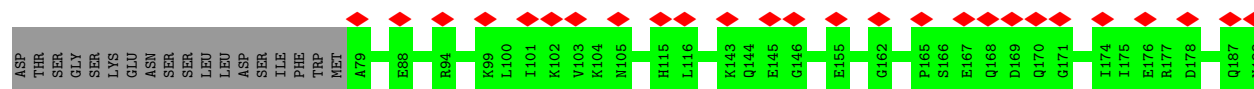
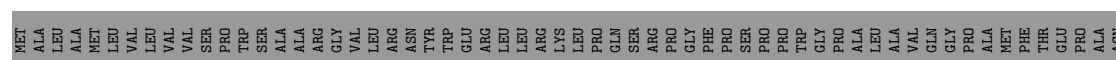
- Molecule 24: Large ribosomal subunit protein uL30m

Chain Z: 32% 76% 24%



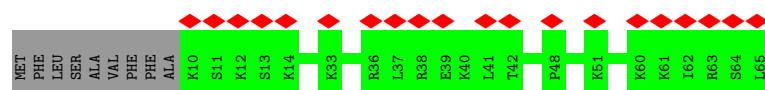
- Molecule 25: Large ribosomal subunit protein bL32m

Chain 0: 14% 59% 41%



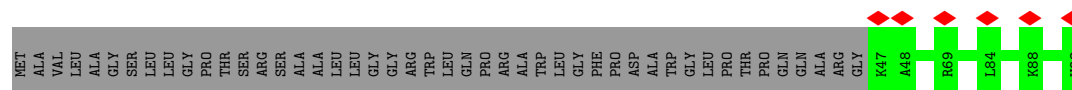
- Molecule 26: Large ribosomal subunit protein bL33m

Chain 1: 31% 86% 14%

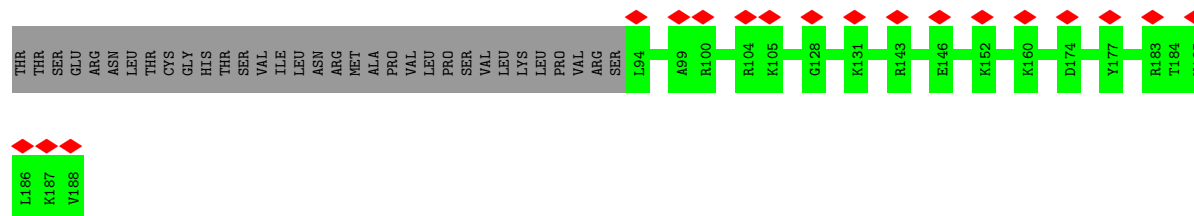


- Molecule 27: Large ribosomal subunit protein bL34m

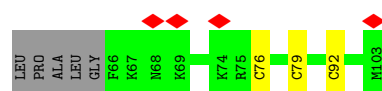
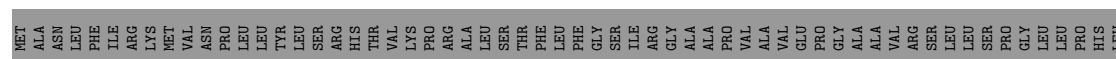
Chain 2: 7% 50% 50%



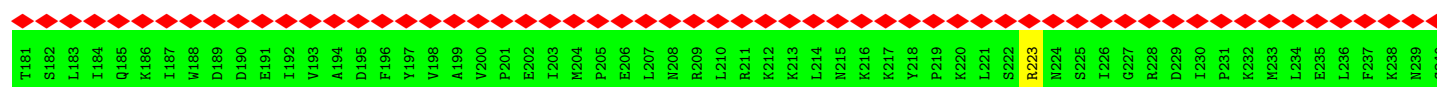
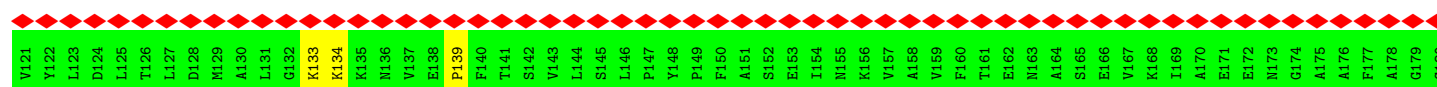
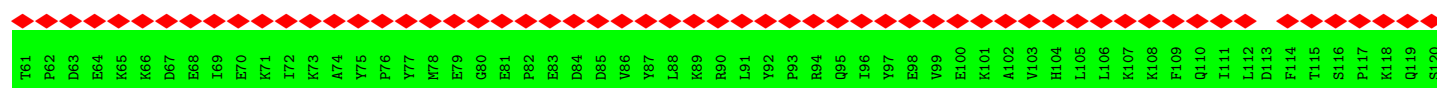
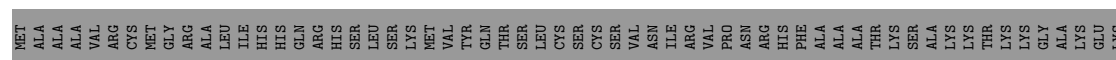
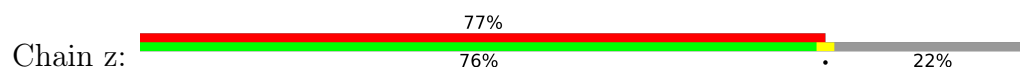
- Molecule 28: Large ribosomal subunit protein bL35m

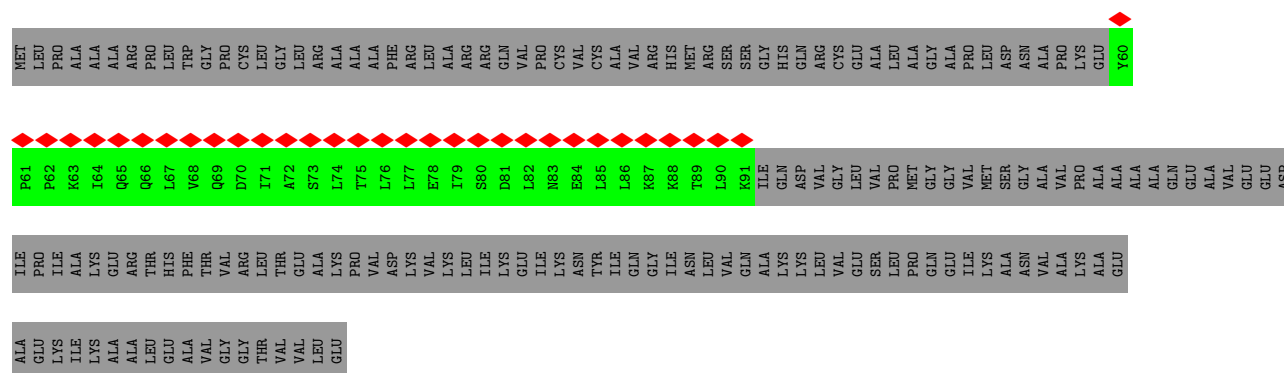


- Molecule 29: Large ribosomal subunit protein bL36m

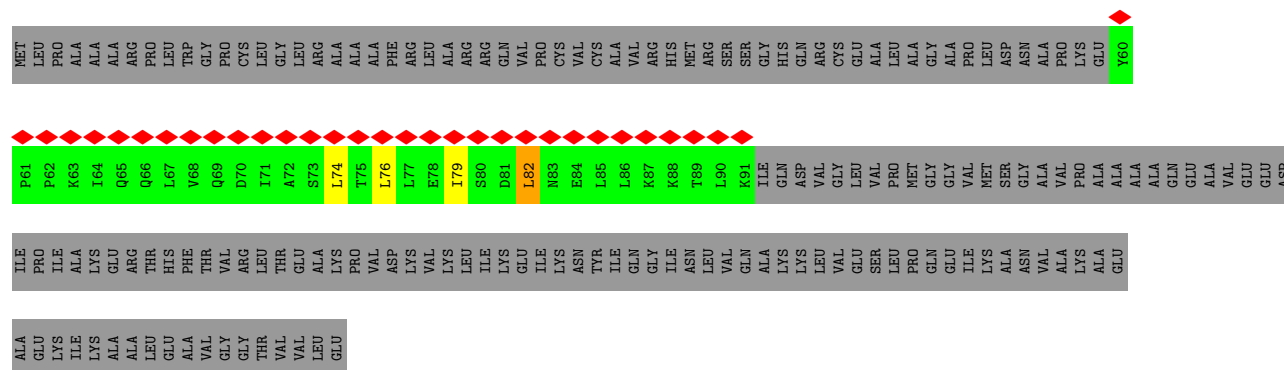


- Molecule 30: Large ribosomal subunit protein uL1m

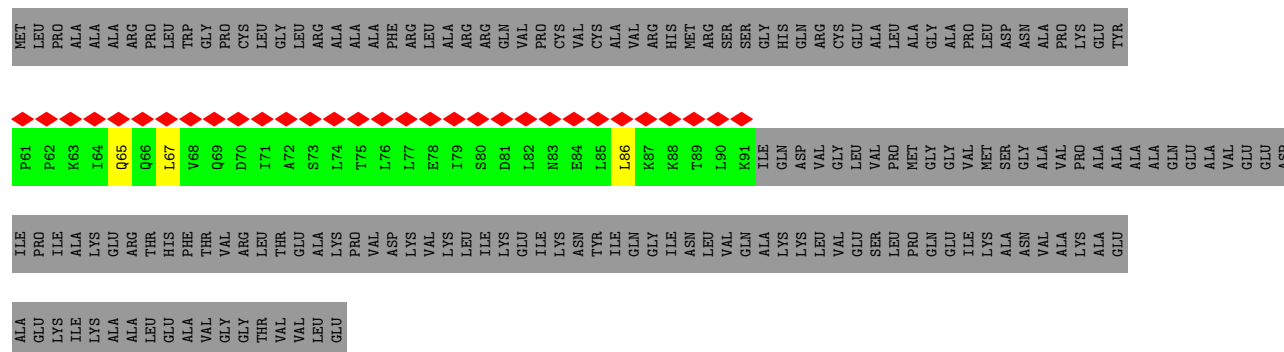




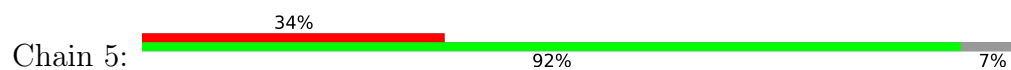
• Molecule 31: Large ribosomal subunit protein bL12m

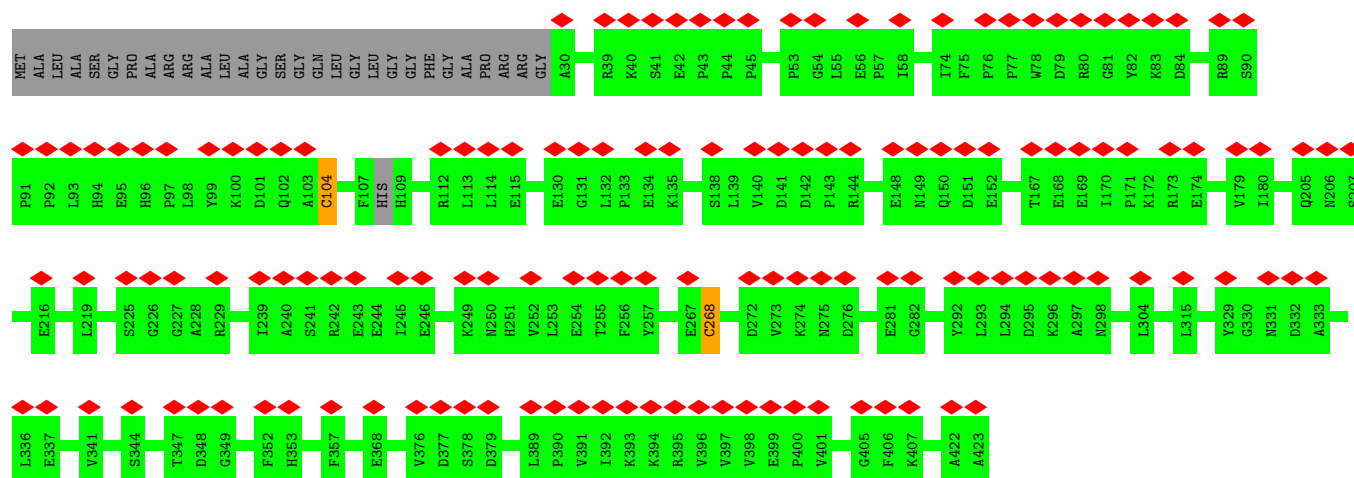


• Molecule 31: Large ribosomal subunit protein bL12m

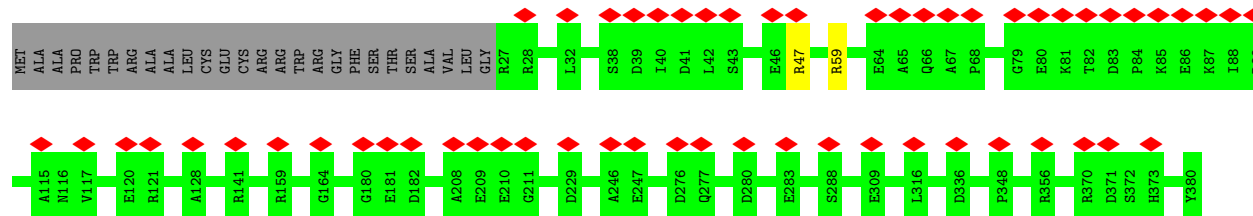
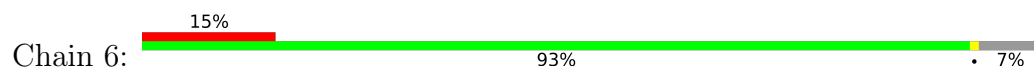


• Molecule 32: Large ribosomal subunit protein mL37

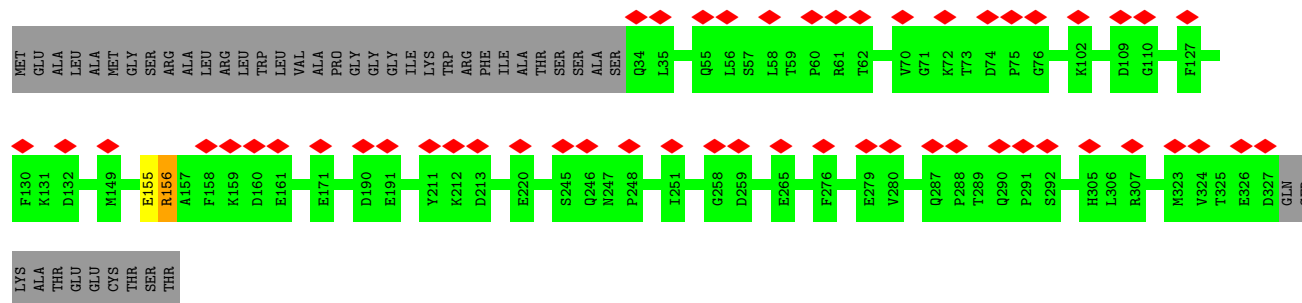
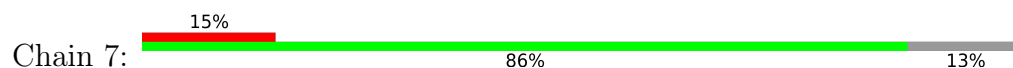




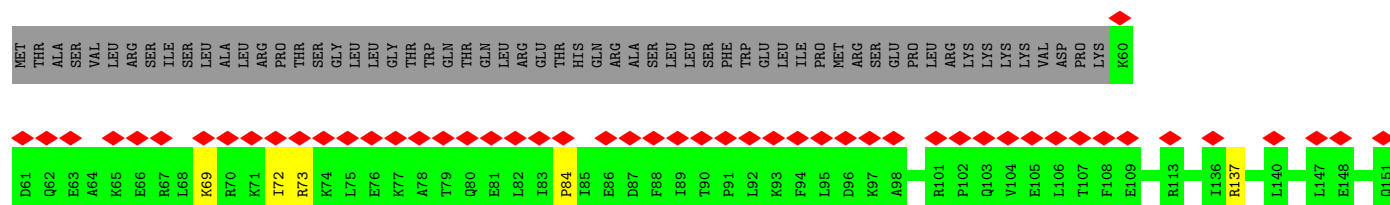
- Molecule 33: Large ribosomal subunit protein mL38

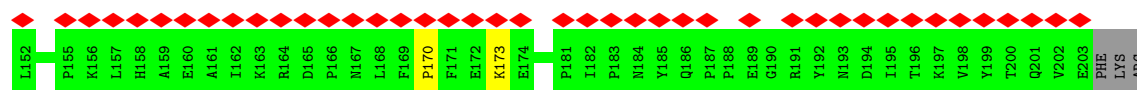


- Molecule 34: Large ribosomal subunit protein mL39

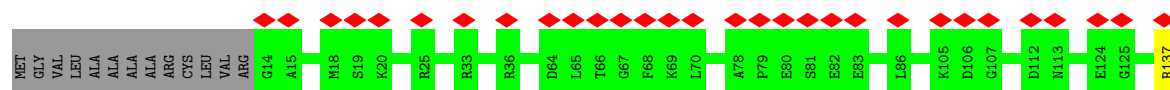
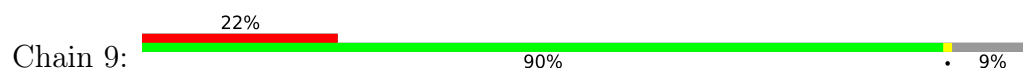


- Molecule 35: Large ribosomal subunit protein mL40

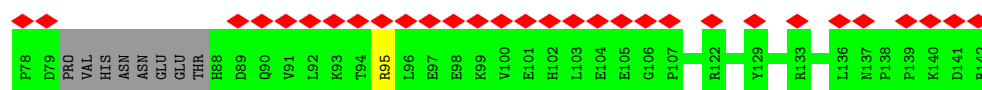
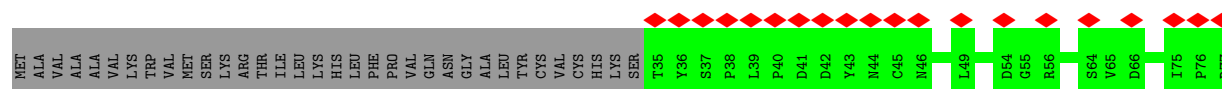




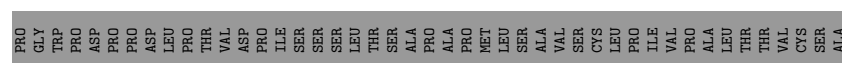
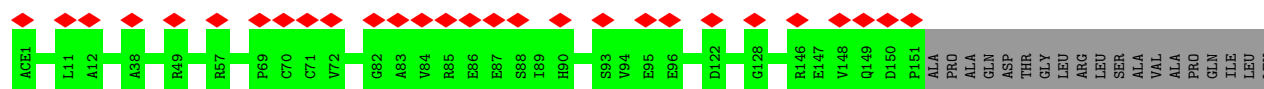
- Molecule 36: Large ribosomal subunit protein mL41



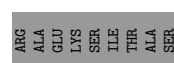
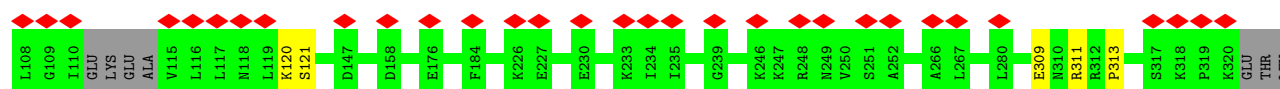
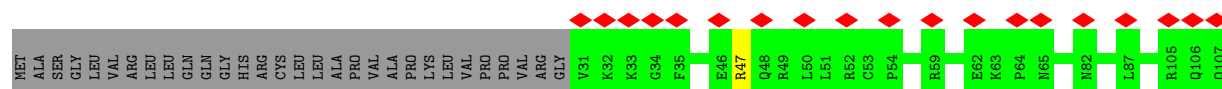
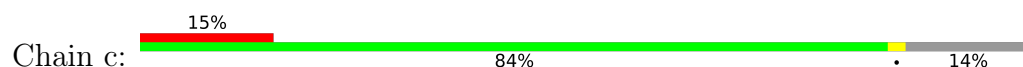
- Molecule 37: Large ribosomal subunit protein mL42



- Molecule 38: Large ribosomal subunit protein mL43



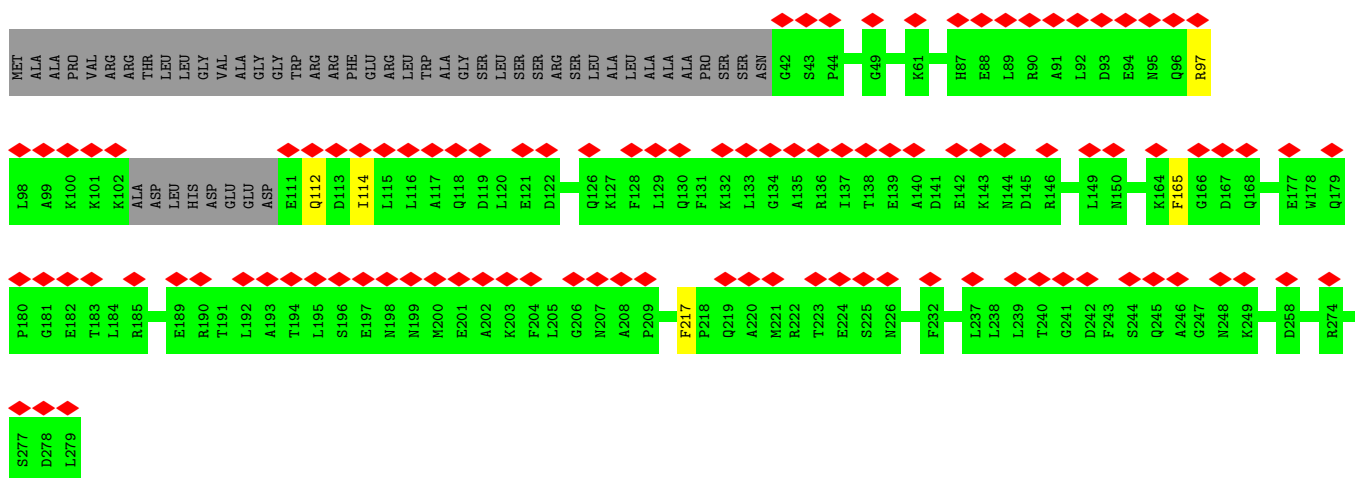
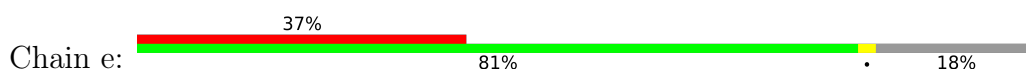
- Molecule 39: Large ribosomal subunit protein mL44



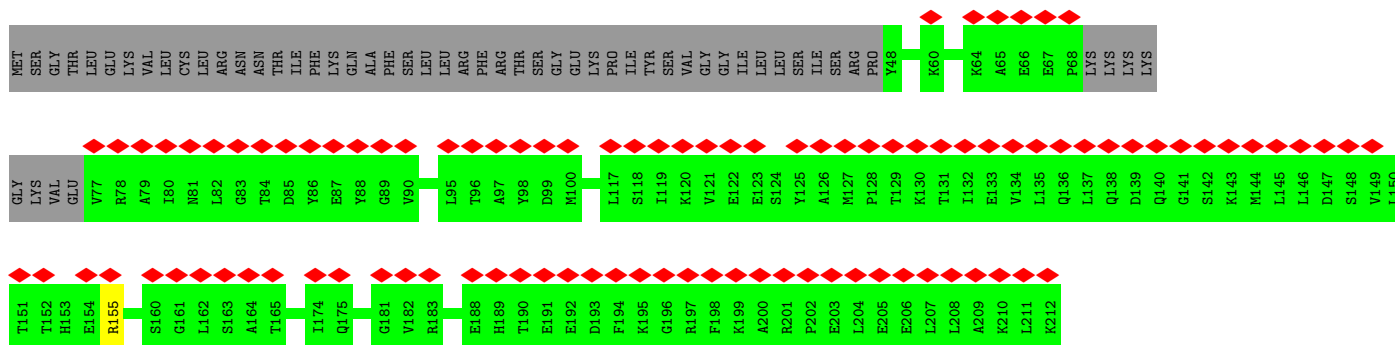
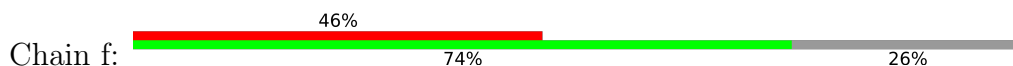
- Molecule 40: Large ribosomal subunit protein mL45



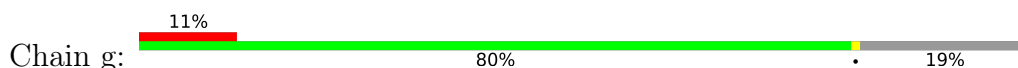
- Molecule 41: Large ribosomal subunit protein mL46

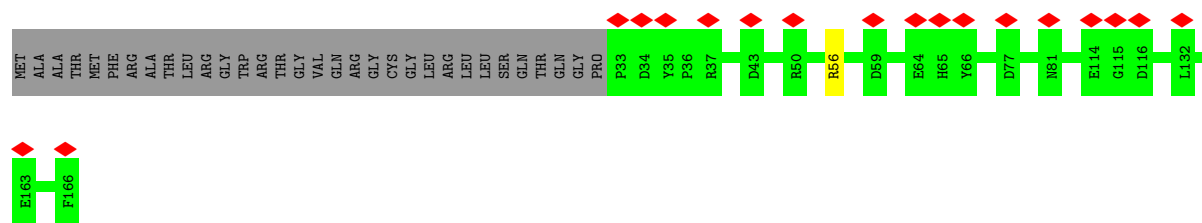


- Molecule 42: Large ribosomal subunit protein mL48

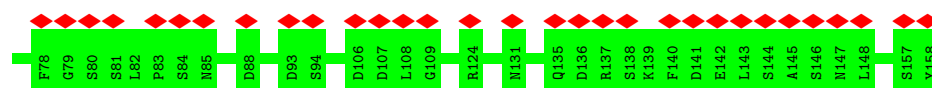
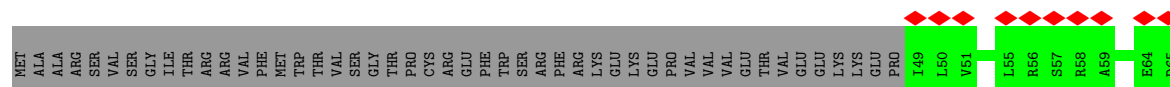


- Molecule 43: Large ribosomal subunit protein mL49

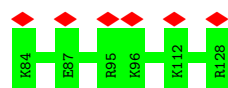
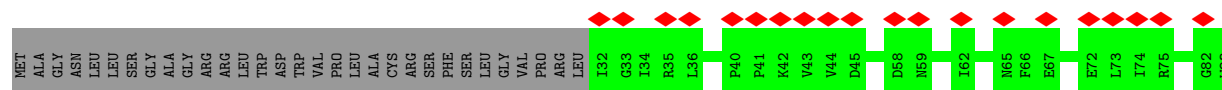
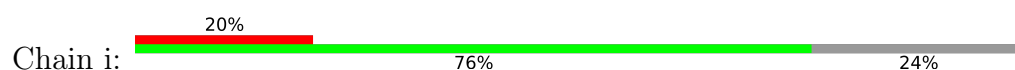




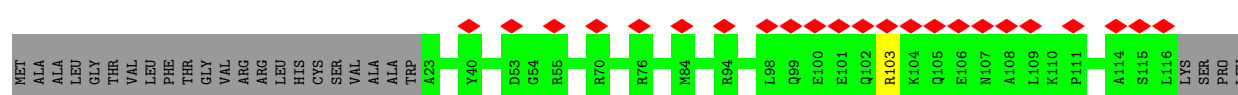
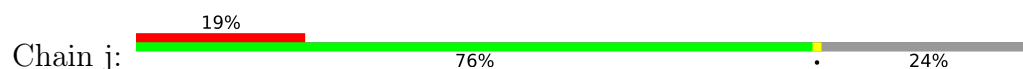
- Molecule 44: Large ribosomal subunit protein mL50



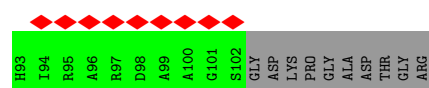
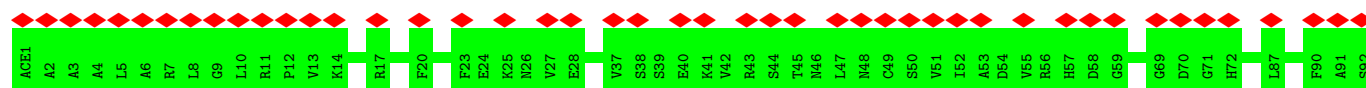
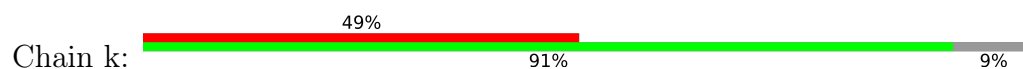
- Molecule 45: Large ribosomal subunit protein mL51



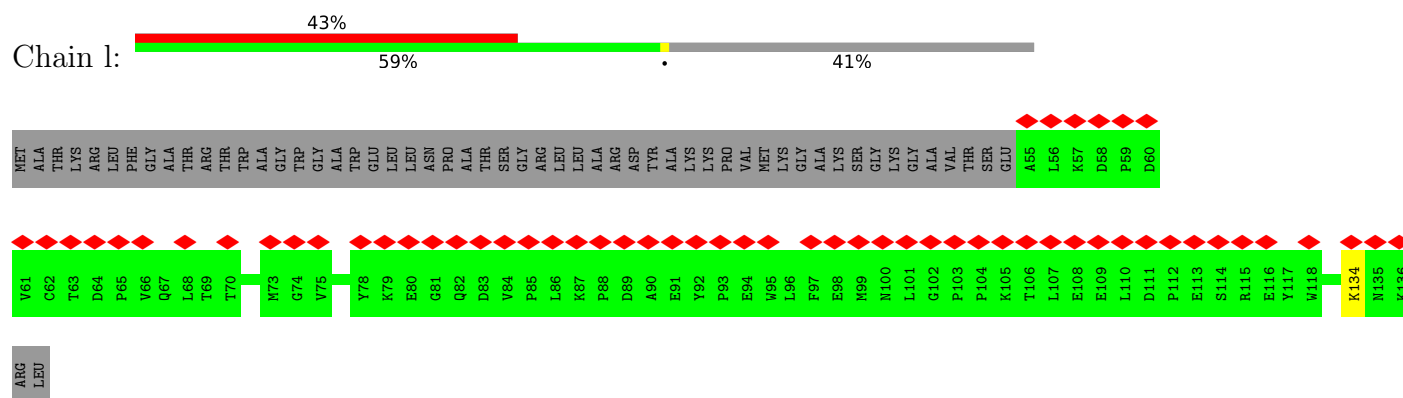
- Molecule 46: Large ribosomal subunit protein mL52



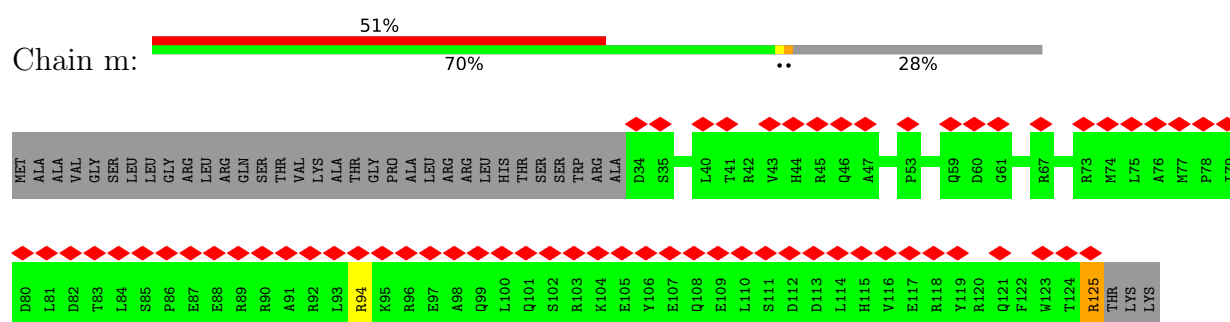
- Molecule 47: Large ribosomal subunit protein mL53



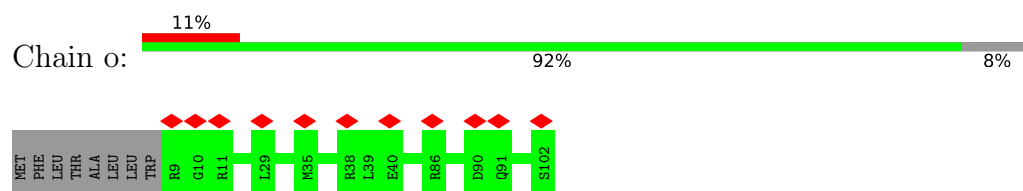
• Molecule 48: Large ribosomal subunit protein mL54



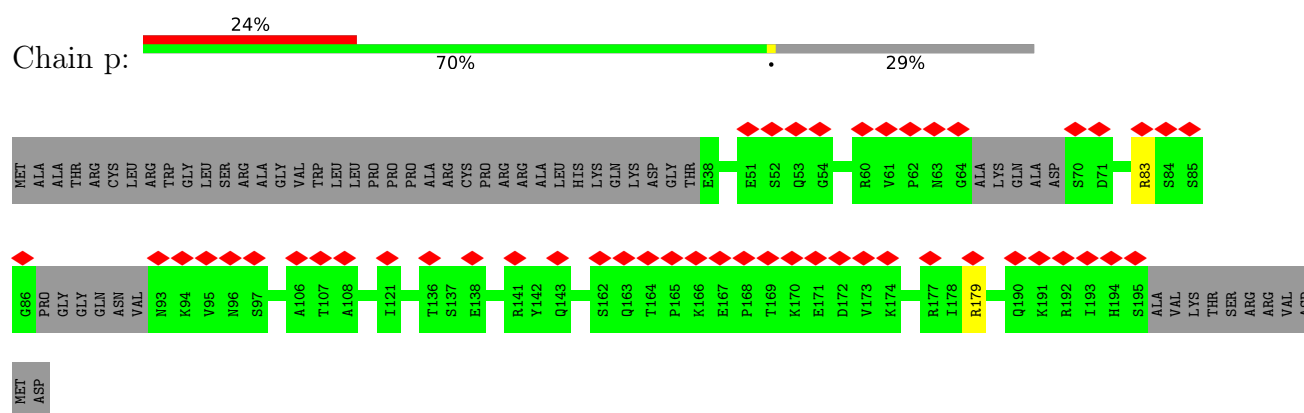
• Molecule 49: Large ribosomal subunit protein mL55



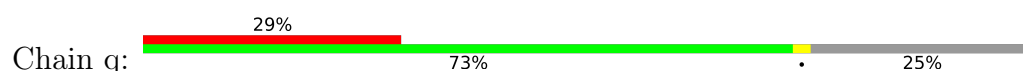
• Molecule 50: Large ribosomal subunit protein mL63

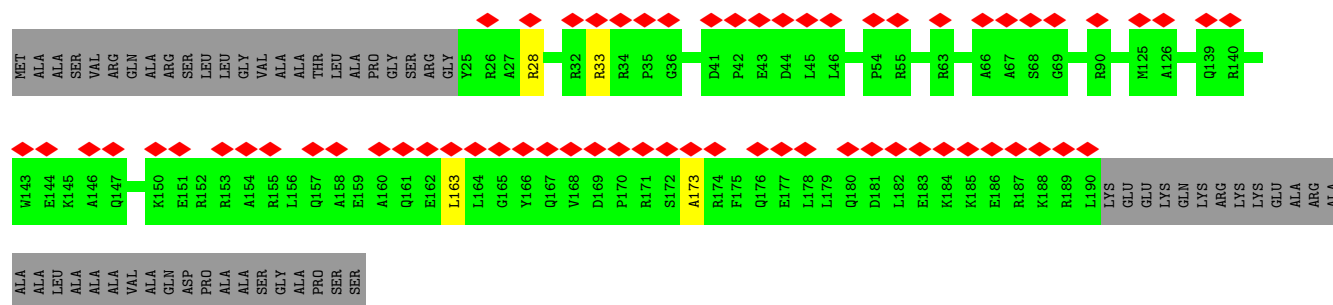


• Molecule 51: Large ribosomal subunit protein mL62

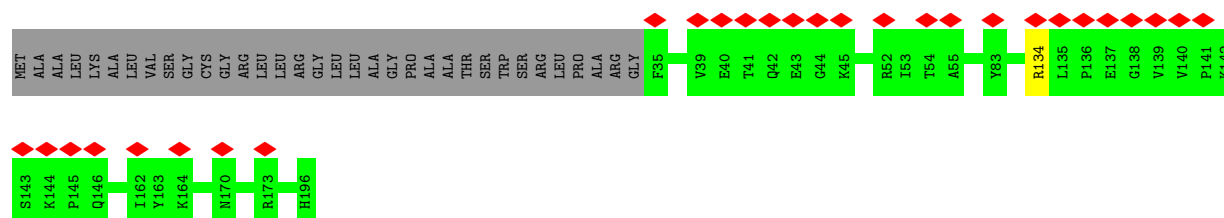
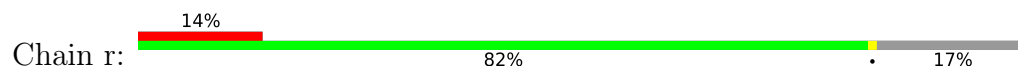


• Molecule 52: Large ribosomal subunit protein mL64

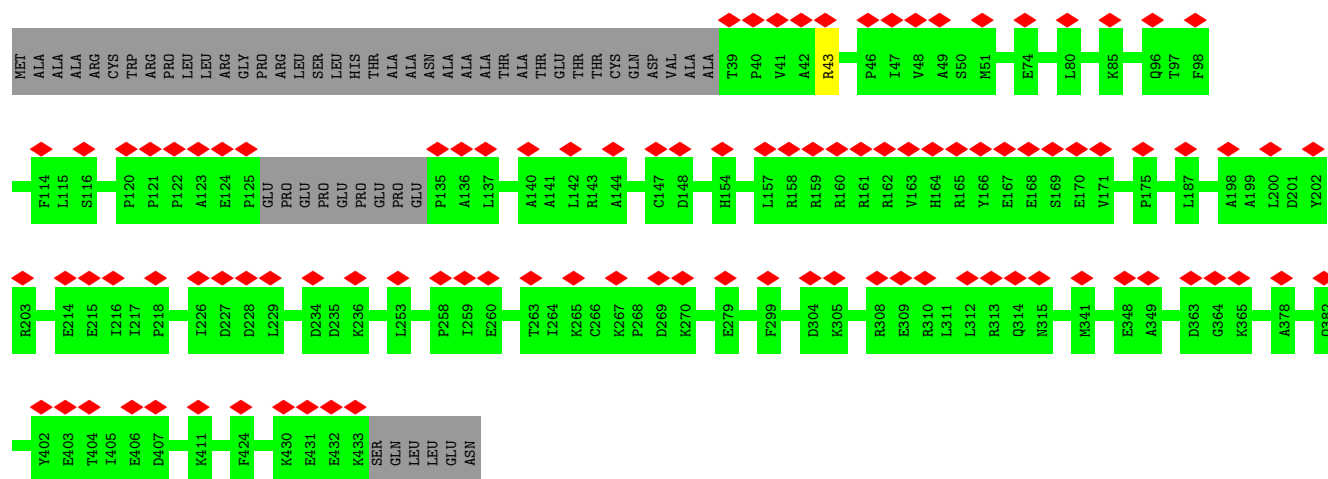
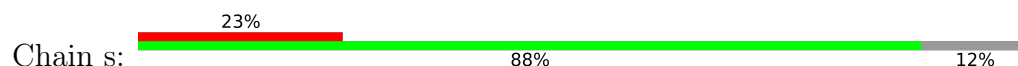




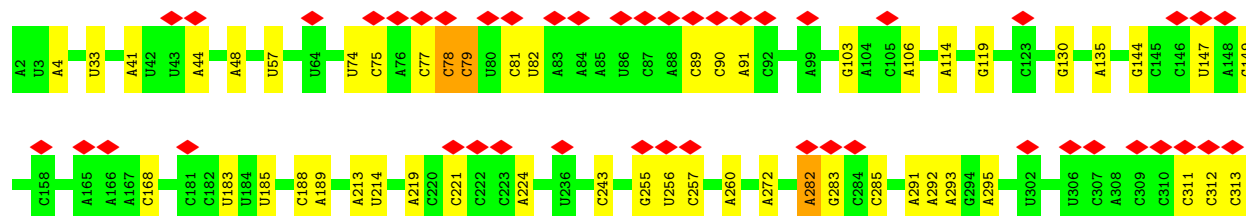
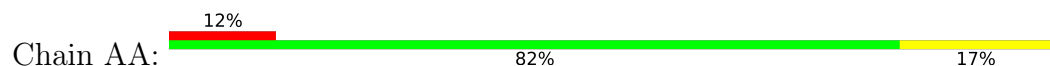
• Molecule 53: Large ribosomal subunit protein mL66

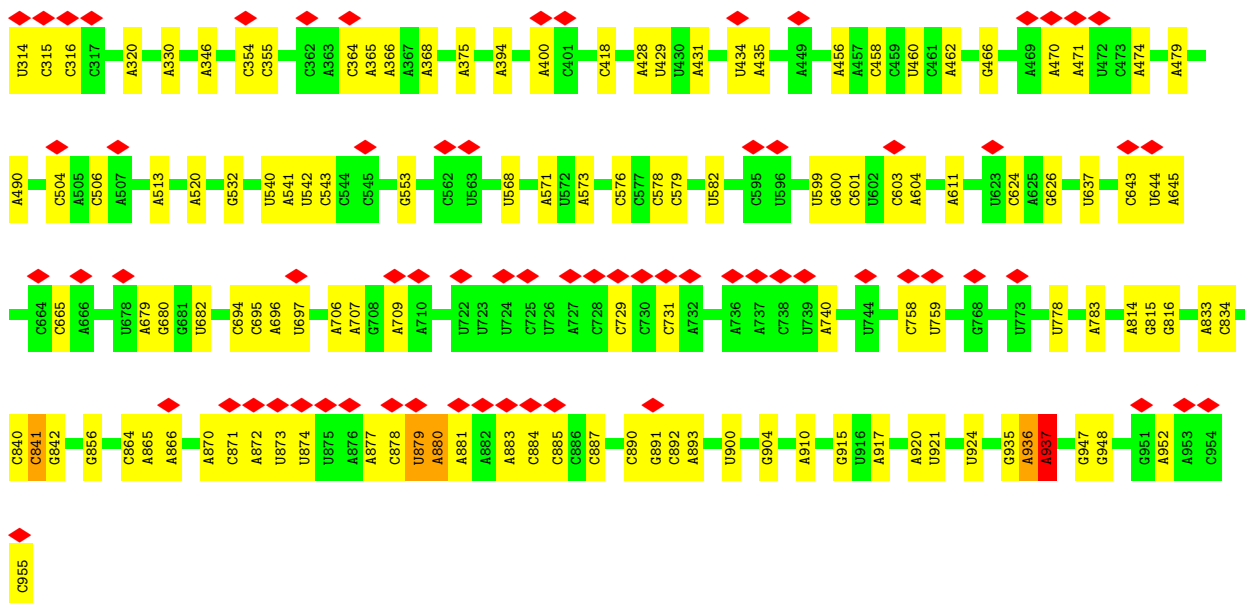


• Molecule 54: Large ribosomal subunit protein mL65

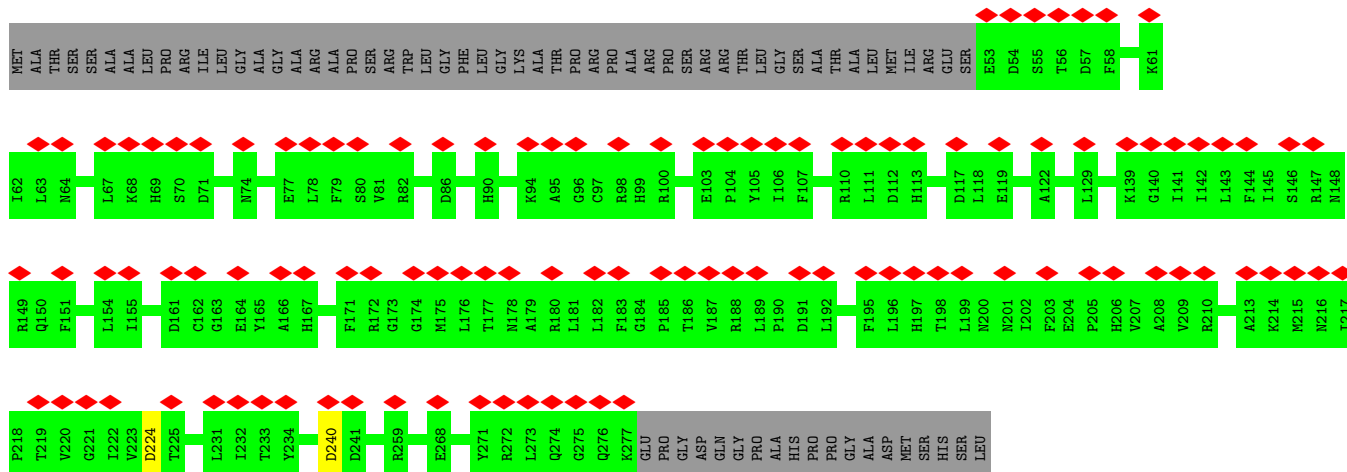
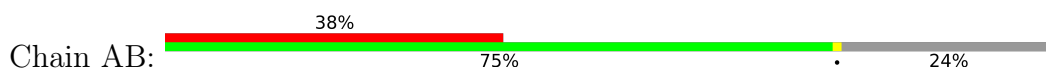


• Molecule 55: Large ribosomal subunit protein mL32

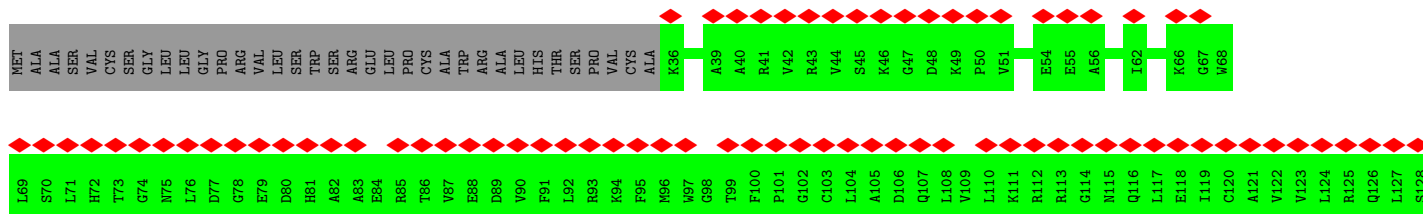
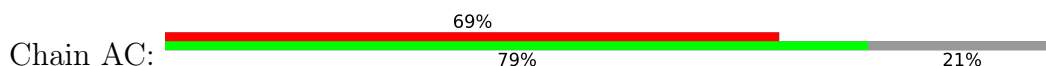


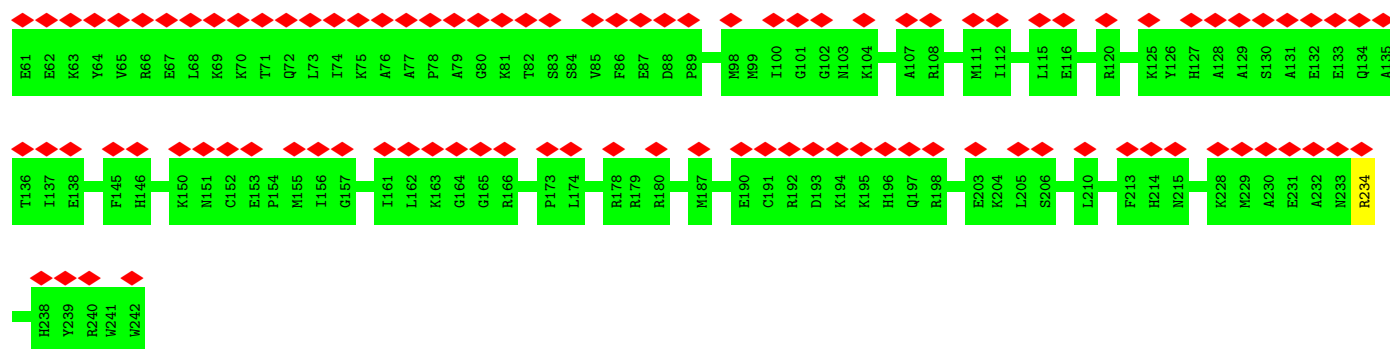


- Molecule 56: Small ribosomal subunit protein uS2m

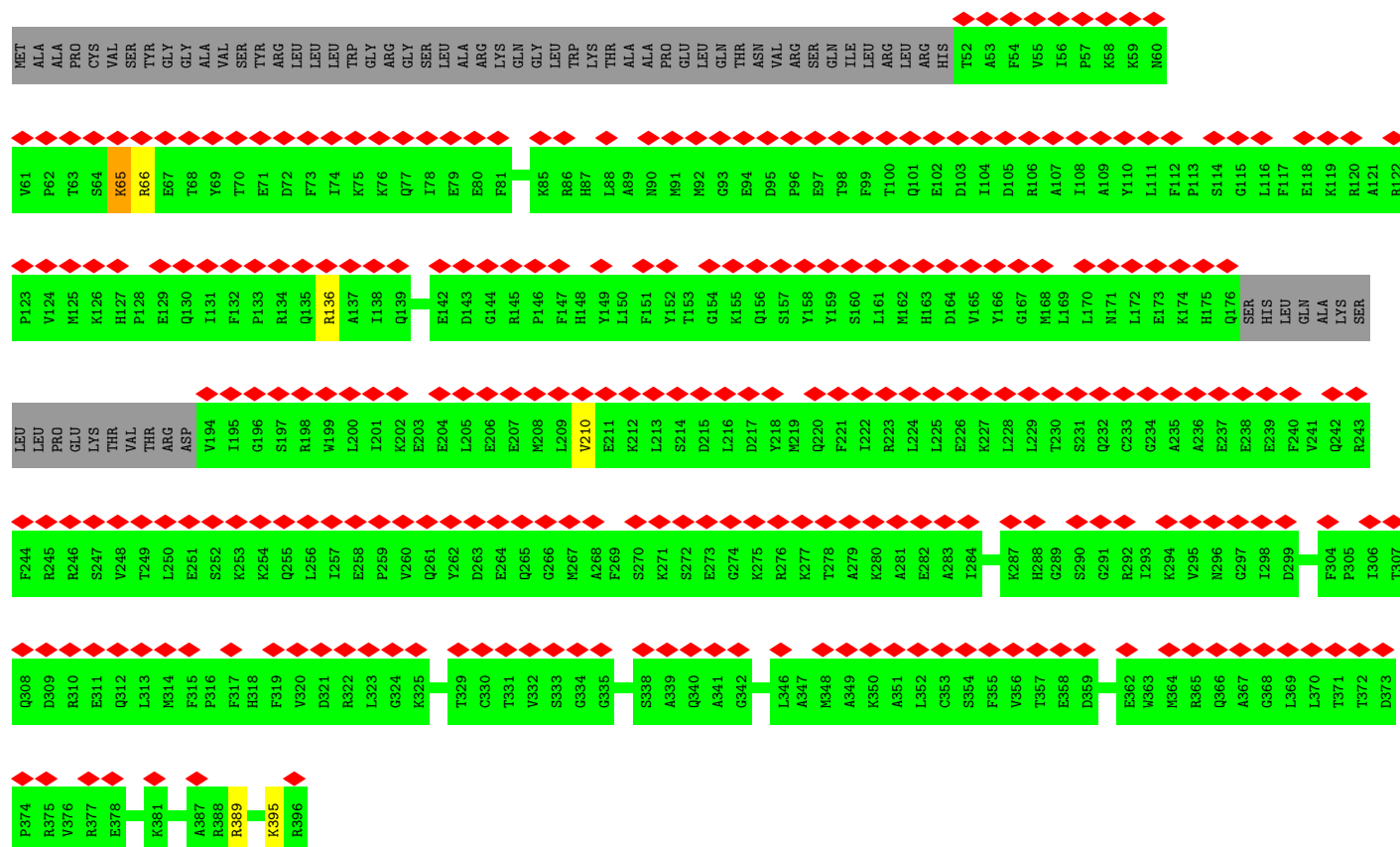
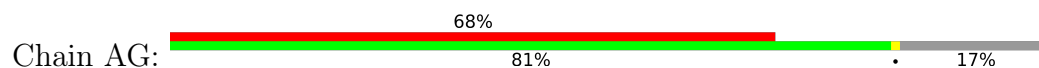


- Molecule 57: Small ribosomal subunit protein uS3m

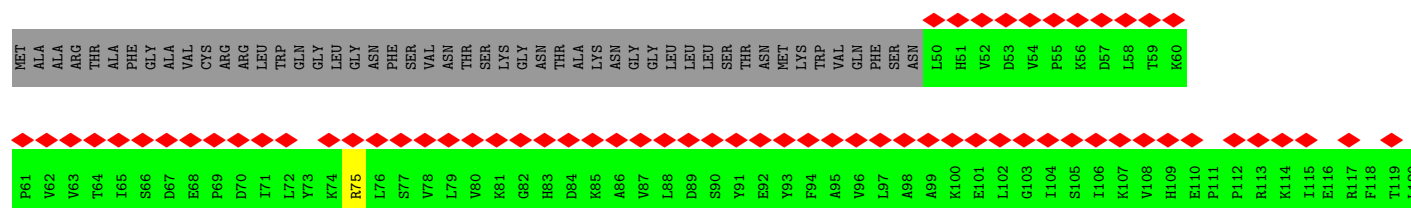


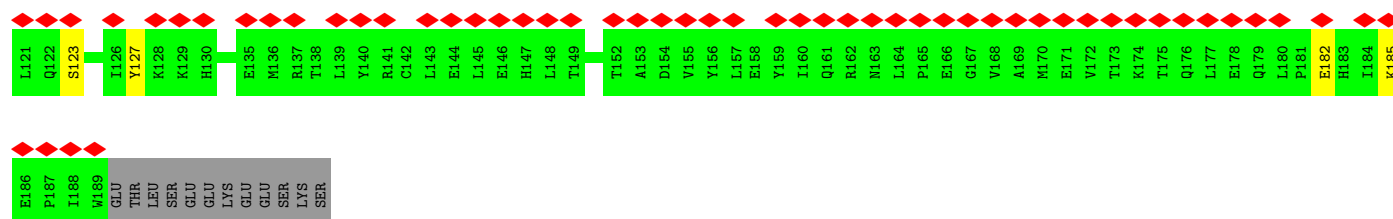


• Molecule 61: Small ribosomal subunit protein uS9m

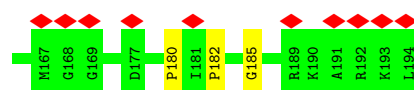
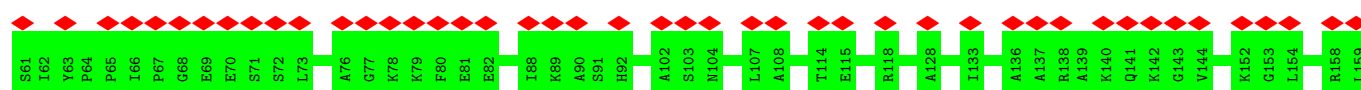
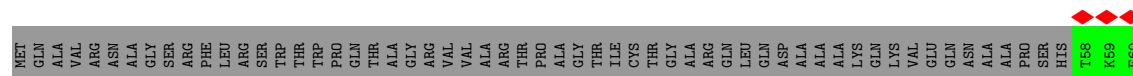


• Molecule 62: Small ribosomal subunit protein uS10m

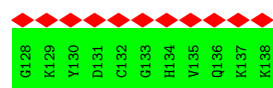
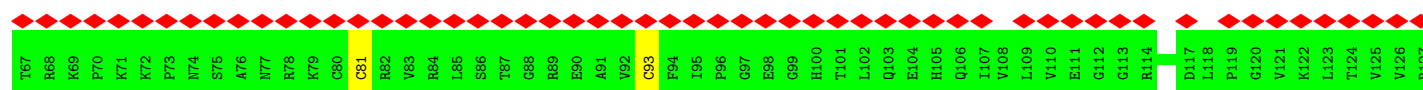
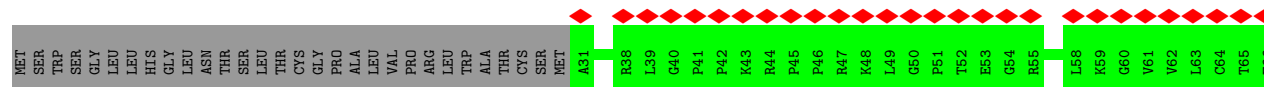
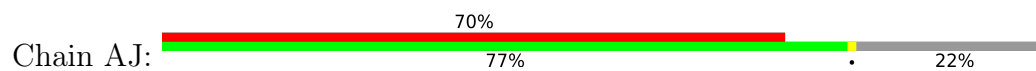




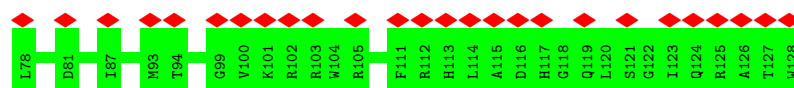
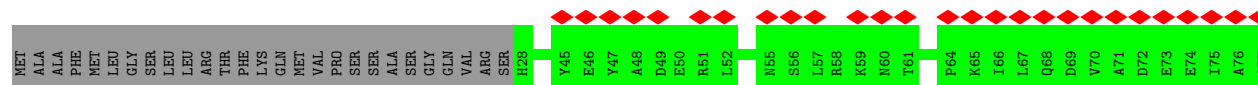
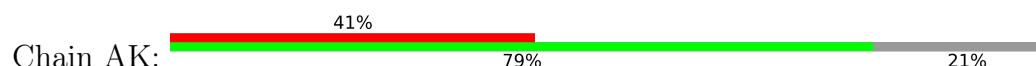
- Molecule 63: Small ribosomal subunit protein uS11m



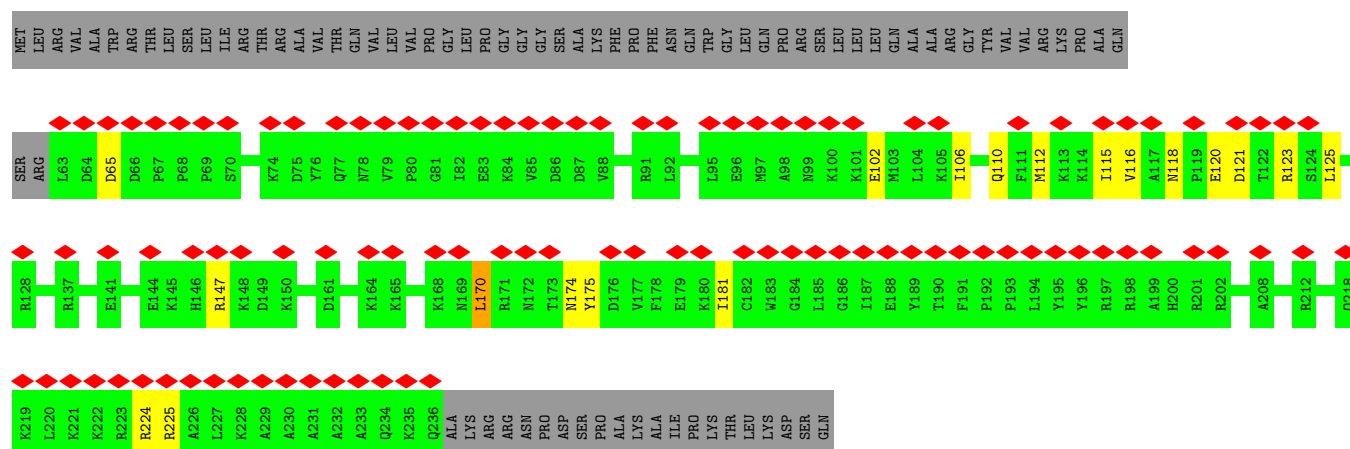
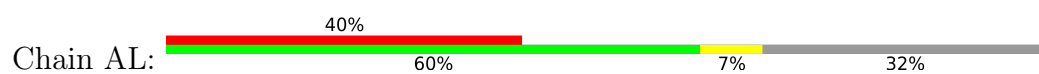
- Molecule 64: Small ribosomal subunit protein uS12m



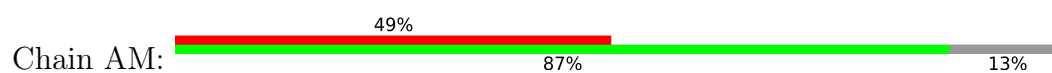
- Molecule 65: Small ribosomal subunit protein uS14m



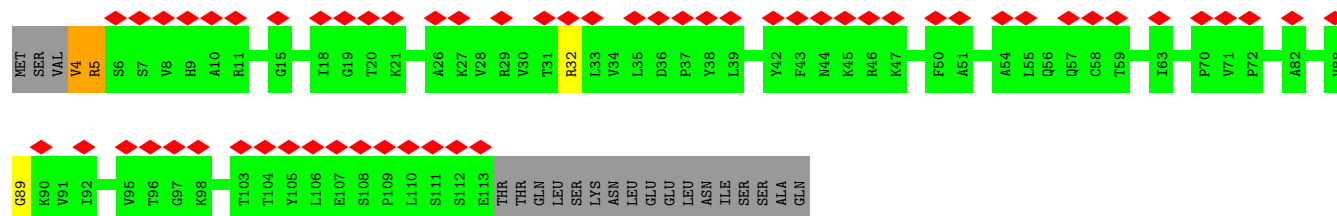
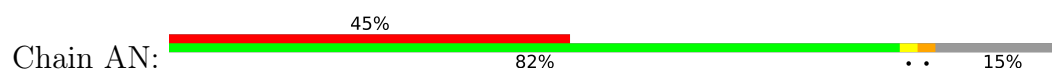
- Molecule 66: Small ribosomal subunit protein uS15m



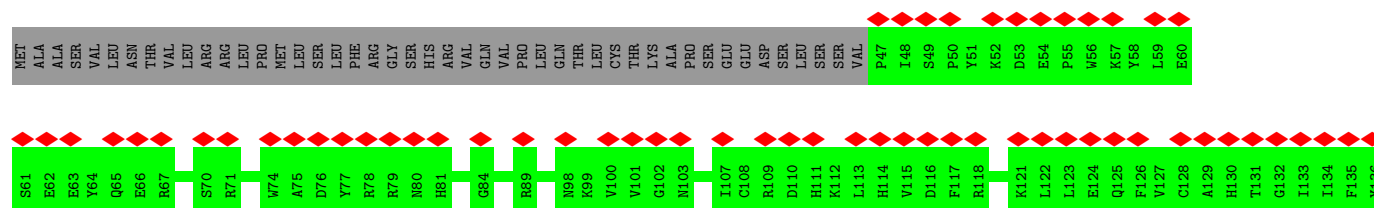
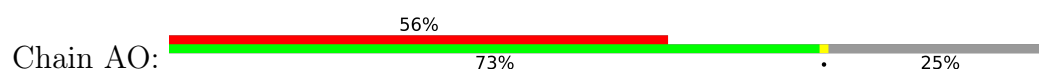
- Molecule 67: Small ribosomal subunit protein bS16m

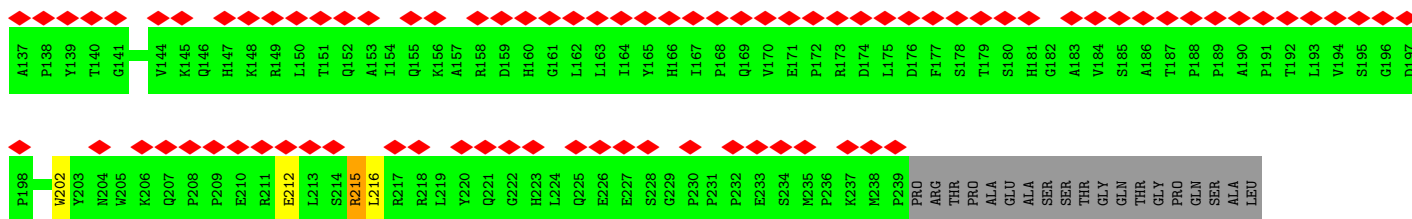


- Molecule 68: Small ribosomal subunit protein uS17m

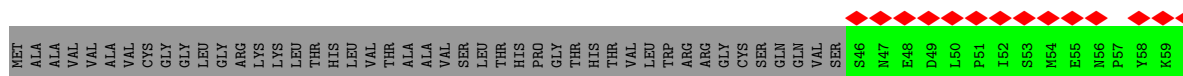


- Molecule 69: Small ribosomal subunit protein mS40

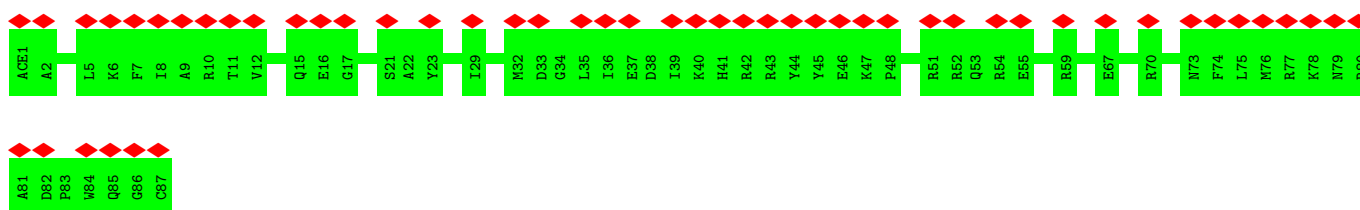




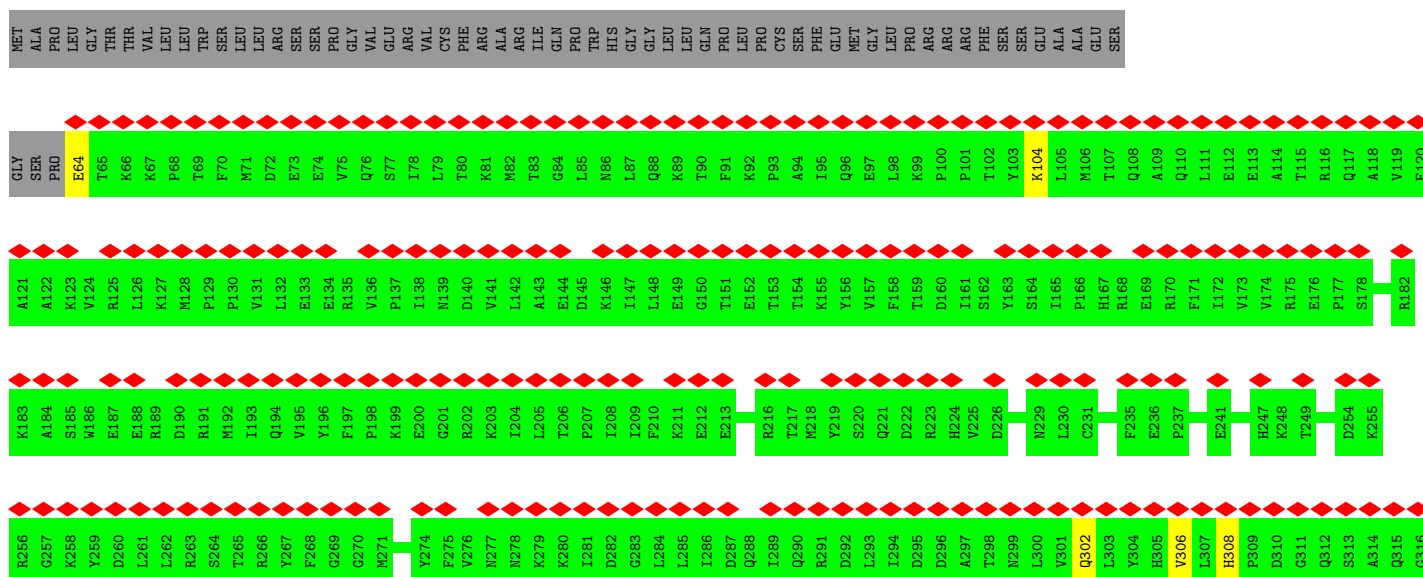
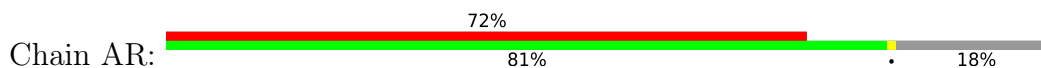
- Molecule 70: Small ribosomal subunit protein bS18m

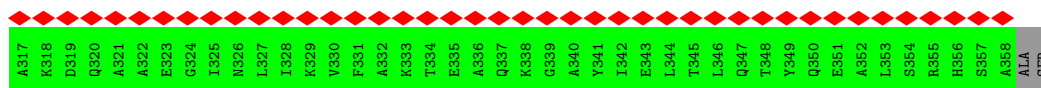


- Molecule 71: Small ribosomal subunit protein bS21m

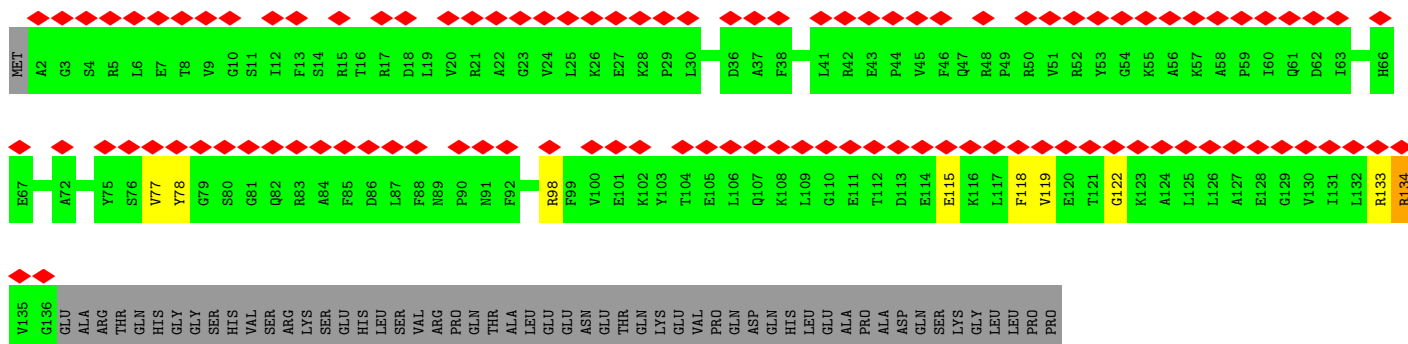


- Molecule 72: Small ribosomal subunit protein mS22

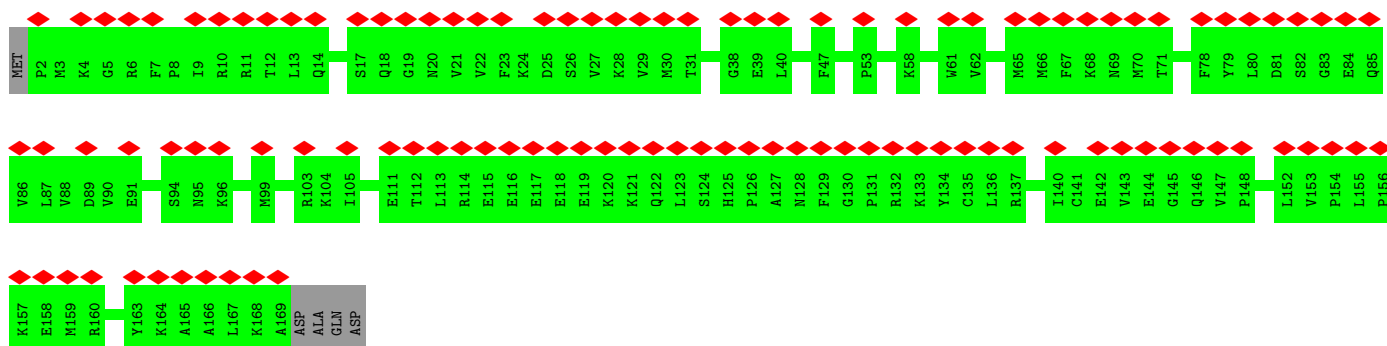




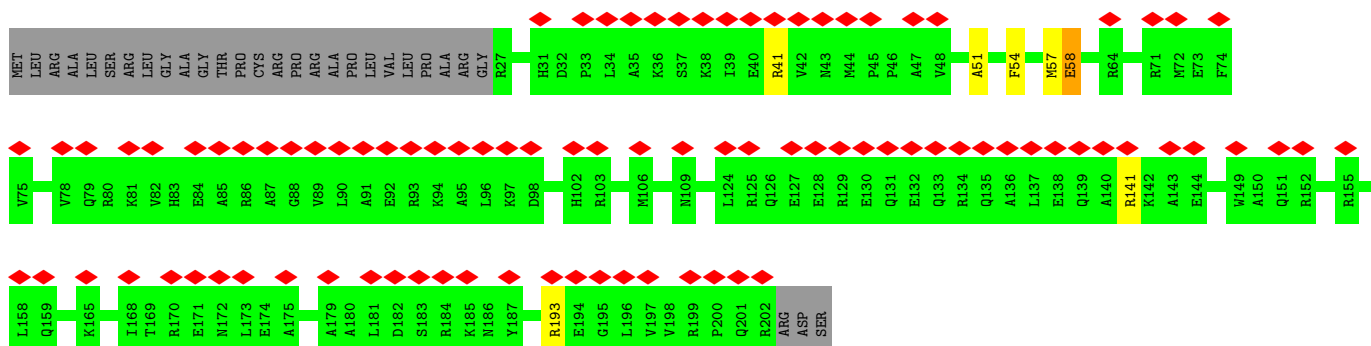
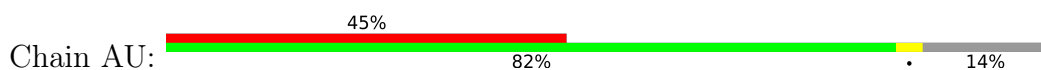
• Molecule 73: Small ribosomal subunit protein mS23



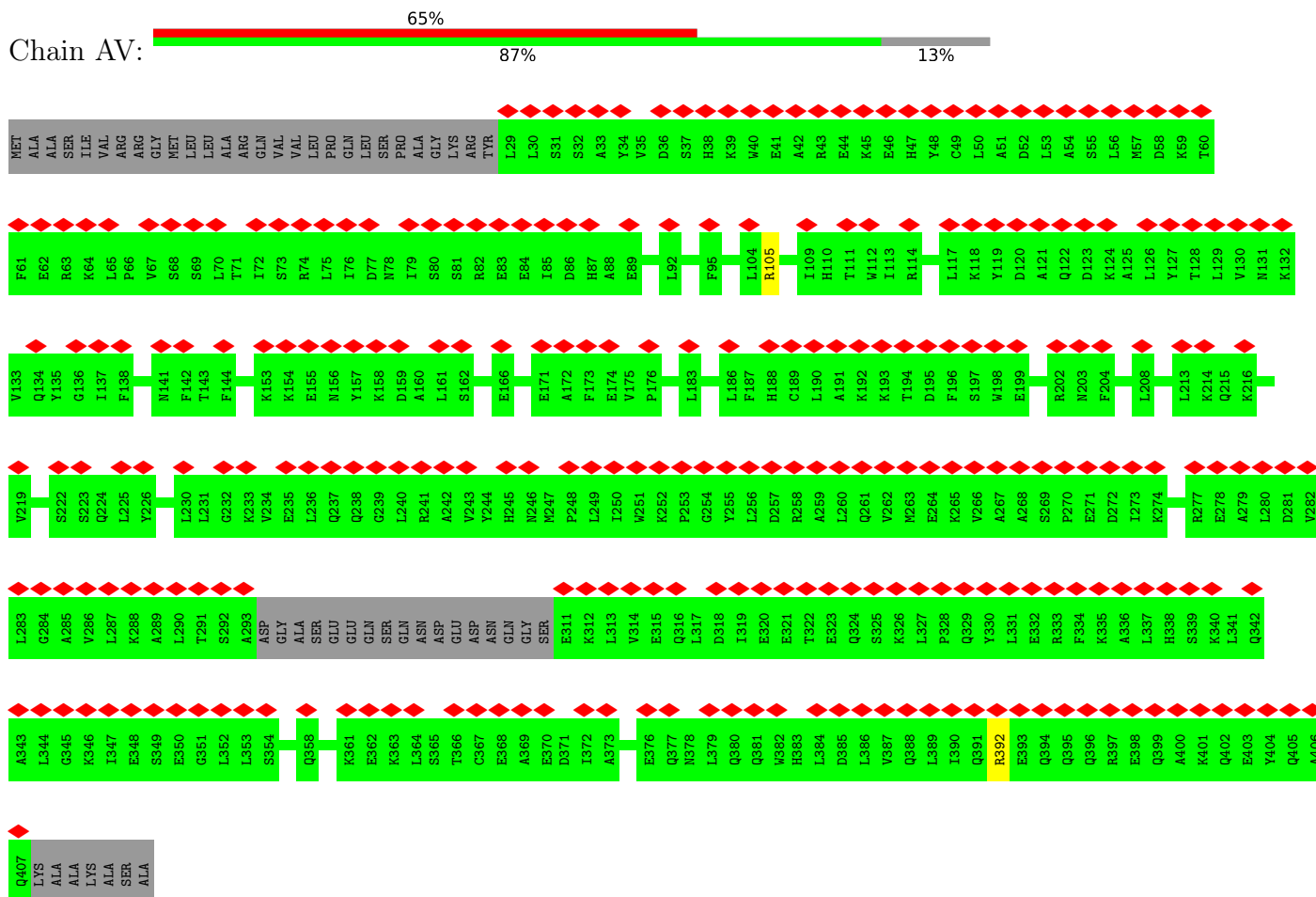
• Molecule 74: Small ribosomal subunit protein mS25



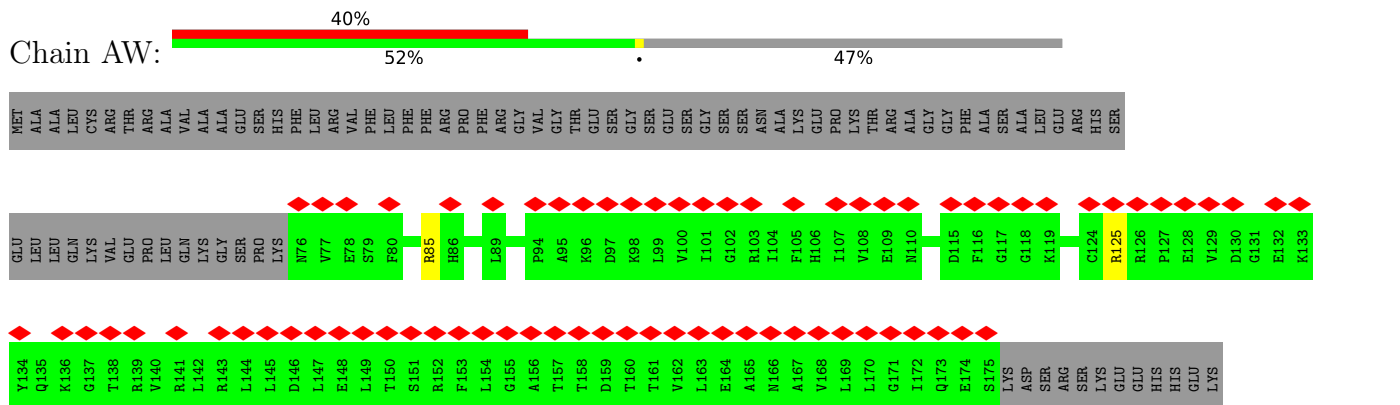
• Molecule 75: Small ribosomal subunit protein mS26



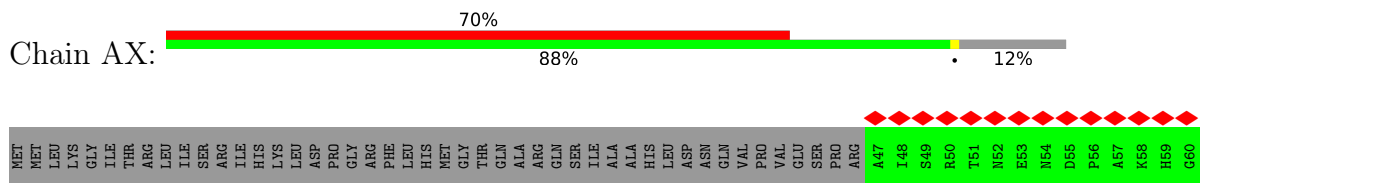
• Molecule 76: Small ribosomal subunit protein mS27

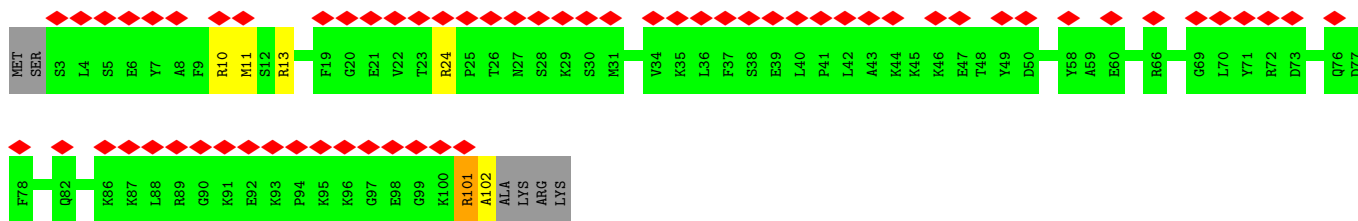


- Molecule 77: Small ribosomal subunit protein bS1m



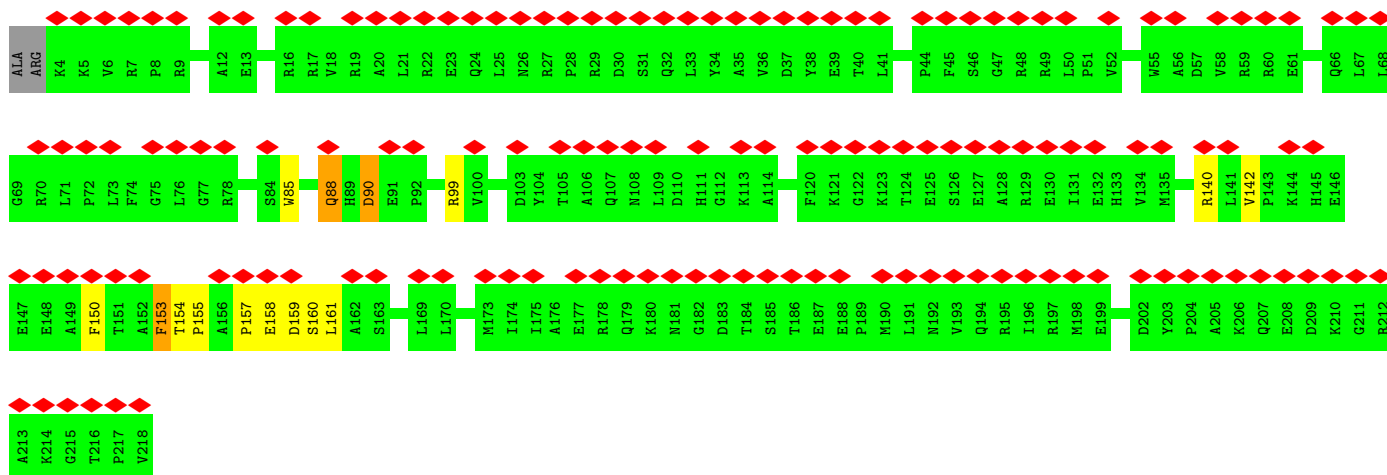
- Molecule 78: Small ribosomal subunit protein mS29





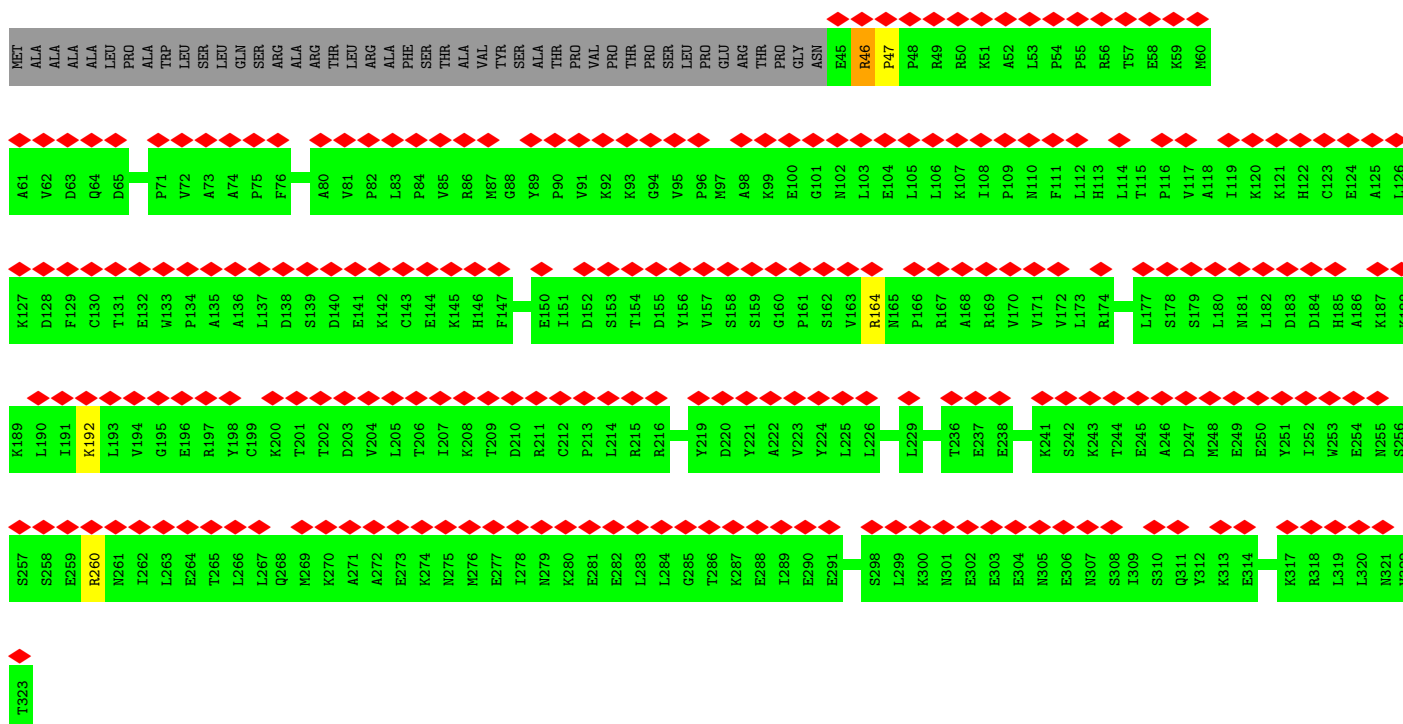
• Molecule 81: Small ribosomal subunit protein mS34

Chain A0: 68% 92% 6% ..

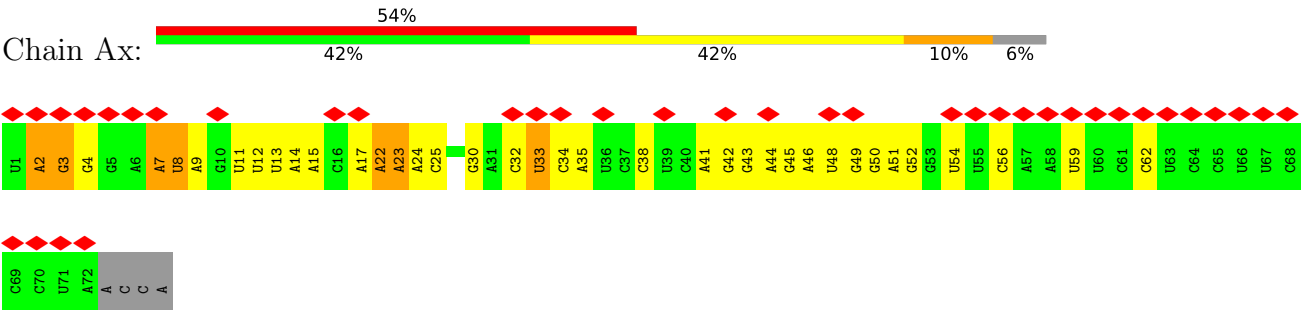


• Molecule 82: Small ribosomal subunit protein mS35

Chain A1: 72% 85% 14%



● Molecule 89: P-site tRNA (Visualisation example)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.639	Depositor
Minimum map value	-0.996	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	464.0, 464.0, 464.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, 5MU, OMG, PSU, ATP, NAD, MG, MA6, ZN, 5F0, FES, 1MA, 5MC, OMU, K, 2MG, B8T, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/36876	0.42	1/57402 (0.0%)
2	B	0.23	0/1627	0.45	0/2527
3	D	0.24	0/1896	0.46	0/2549
4	E	0.26	0/2475	0.49	0/3355
5	F	0.28	0/2090	0.49	0/2842
6	H	0.25	0/1698	0.54	0/2292
7	I	0.28	0/1731	0.56	0/2345
8	J	0.22	0/1348	0.47	0/1813
9	K	0.28	0/1497	0.44	0/2031
10	L	0.22	0/905	0.46	0/1218
11	M	0.27	0/2381	0.49	0/3212
12	N	0.28	0/1833	0.49	0/2468
13	O	0.26	0/1283	0.48	0/1727
14	P	0.27	0/1199	0.47	0/1623
15	Q	0.26	0/2039	0.51	0/2750
16	R	0.28	0/1175	0.50	0/1572
17	S	0.28	0/1320	0.54	0/1789
18	T	0.28	0/1403	0.48	0/1886
19	U	0.24	0/1280	0.45	0/1732
20	V	0.23	0/1721	0.51	0/2333
21	W	0.30	0/902	0.53	0/1214
22	X	0.25	0/2099	0.45	0/2837
23	Y	0.26	0/1593	0.43	0/2136
24	Z	0.27	0/1021	0.48	0/1378
25	0	0.26	0/913	0.46	0/1224
26	1	0.23	0/469	0.49	0/621
27	2	0.31	0/383	0.44	0/507
28	3	0.29	0/853	0.47	0/1136
29	4	0.24	0/350	0.41	0/461
30	z	0.27	0/2067	0.57	0/2793
31	t	0.24	0/358	0.47	0/486

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	u	0.26	0/259	0.56	0/350
31	v	0.32	0/259	0.72	1/350 (0.3%)
31	w	0.33	0/246	0.67	0/331
31	x	0.27	0/246	0.67	0/331
31	y	0.30	0/246	0.61	0/331
32	5	0.26	1/3293 (0.0%)	0.51	1/4484 (0.0%)
33	6	0.24	0/3043	0.47	0/4140
34	7	0.29	0/2447	0.55	0/3310
35	8	0.31	0/1244	0.68	0/1674
36	9	0.23	0/1025	0.46	0/1379
37	a	0.24	0/866	0.54	0/1174
38	b	0.25	0/1219	0.45	0/1651
39	c	0.26	0/2347	0.49	0/3171
40	d	0.21	0/1855	0.43	0/2514
41	e	0.26	0/1903	0.60	0/2565
42	f	0.26	0/1273	0.50	0/1716
43	g	0.27	0/1151	0.49	0/1569
44	h	0.21	0/918	0.41	0/1249
45	i	0.29	0/850	0.46	0/1135
46	j	0.26	0/760	0.50	0/1023
47	k	0.20	0/783	0.43	0/1057
48	l	0.20	0/707	0.47	0/960
49	m	0.24	0/805	0.55	0/1081
50	o	0.27	0/819	0.48	0/1097
51	p	0.24	0/1223	0.45	0/1641
52	q	0.28	0/1432	0.56	0/1931
53	r	0.26	0/1362	0.49	0/1846
54	s	0.25	0/3239	0.47	0/4400
55	AA	0.23	0/22537	0.44	6/35085 (0.0%)
56	AB	0.22	0/1871	0.46	0/2531
57	AC	0.21	0/1113	0.46	0/1505
58	AD	0.19	0/2751	0.42	0/3681
59	AE	0.24	0/989	0.52	0/1335
60	AF	0.23	0/1767	0.49	0/2373
61	AG	0.23	0/2753	0.50	1/3691 (0.0%)
62	AH	0.25	0/1178	0.53	0/1598
63	AI	0.30	0/1030	0.44	0/1386
64	AJ	0.30	0/855	0.62	2/1148 (0.2%)
65	AK	0.21	0/880	0.46	0/1182
66	AL	0.37	0/1477	0.79	1/1974 (0.1%)
67	AM	0.22	0/963	0.47	0/1295
68	AN	0.33	0/886	0.64	2/1199 (0.2%)
69	AO	0.22	0/1648	0.49	0/2243

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AP	0.26	0/798	0.55	0/1070
71	AQ	0.21	0/754	0.39	0/1003
72	AR	0.24	0/2456	0.50	0/3317
73	AS	0.29	0/1138	0.71	1/1533 (0.1%)
74	AT	0.22	0/1402	0.48	0/1883
75	AU	0.28	0/1510	0.64	3/2025 (0.1%)
76	AV	0.22	0/3030	0.45	0/4093
77	AW	0.22	0/801	0.46	0/1079
78	AX	0.22	0/2921	0.47	0/3954
79	AY	0.23	0/1280	0.51	0/1725
80	AZ	0.25	0/857	0.61	0/1141
81	A0	0.43	0/1834	0.84	7/2484 (0.3%)
82	A1	0.24	0/2313	0.53	0/3129
83	A2	0.21	0/947	0.49	0/1266
84	A3	0.27	0/636	0.55	0/839
85	A4	0.25	0/4877	0.50	1/6598 (0.0%)
86	Az	0.23	0/785	0.51	0/1219
88	Aw	0.72	0/1604	0.98	2/2490 (0.1%)
89	Ax	0.33	0/1579	0.71	0/2453
All	All	0.27	1/188825 (0.0%)	0.49	29/268246 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	1
6	H	0	2
8	J	0	2
9	K	0	1
12	N	0	2
14	P	0	1
15	Q	0	1
18	T	0	1
20	V	0	1
22	X	0	2
30	z	0	1
33	6	0	2
34	7	0	1
35	8	0	2
37	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	c	0	2
40	d	0	1
42	f	0	1
43	g	0	1
46	j	0	1
49	m	0	2
51	p	0	2
52	q	0	2
53	r	0	1
54	s	0	1
58	AD	0	1
61	AG	0	2
62	AH	0	1
66	AL	0	4
68	AN	0	1
69	AO	0	1
70	AP	0	1
73	AS	0	2
75	AU	0	3
76	AV	0	2
77	AW	0	2
78	AX	0	1
80	AZ	0	4
81	A0	0	2
82	A1	0	3
85	A4	0	3
All	All	0	68

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	268	CYS	CB-SG	-5.25	1.64	1.81

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	883	A	OP1-P-O3'	-11.85	72.45	108.00
81	A0	153	PHE	CB-CA-C	11.00	127.43	109.72
81	A0	153	PHE	CA-CB-CG	9.77	123.57	113.80
81	A0	88	GLN	N-CA-C	9.04	122.90	111.24
55	AA	883	A	OP2-P-O3'	-8.88	81.37	108.00

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	295	ARG	Sidechain
6	H	147	ARG	Sidechain
6	H	89	ARG	Sidechain
8	J	21	ARG	Sidechain
8	J	33	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33070	0	16792	14	0
2	B	1524	0	777	5	0
3	D	1859	0	1920	0	0
4	E	2406	0	2415	1	0
5	F	2031	0	2065	2	0
6	H	1661	0	1734	2	0
7	I	1695	0	1785	2	0
8	J	1330	0	1407	0	0
9	K	1455	0	1452	2	0
10	L	890	0	941	0	0
11	M	2327	0	2395	0	0
12	N	1786	0	1817	0	0
13	O	1259	0	1294	0	0
14	P	1173	0	1165	2	0
15	Q	1990	0	2031	0	0
16	R	1154	0	1214	0	0
17	S	1293	0	1365	2	0
18	T	1369	0	1410	0	0
19	U	1251	0	1232	1	0
20	V	1676	0	1687	1	0
21	W	880	0	904	0	0
22	X	2044	0	2060	0	0
23	Y	1556	0	1597	0	0
24	Z	996	0	1044	0	0
25	0	898	0	916	0	0
26	1	464	0	511	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	2	377	0	406	0	0
28	3	832	0	883	0	0
29	4	342	0	361	2	0
30	z	2027	0	2076	2	0
31	t	354	0	377	0	0
31	u	257	0	283	0	0
31	v	257	0	283	4	0
31	w	245	0	275	3	0
31	x	245	0	275	1	0
31	y	245	0	275	3	0
32	5	3200	0	3196	2	0
33	6	2948	0	2841	0	0
34	7	2390	0	2397	1	0
35	8	1219	0	1241	2	0
36	9	997	0	987	1	0
37	a	840	0	810	0	0
38	b	1196	0	1195	0	0
39	c	2299	0	2320	3	0
40	d	1807	0	1790	1	0
41	e	1866	0	1868	4	0
42	f	1252	0	1269	0	0
43	g	1113	0	1097	0	0
44	h	895	0	881	0	0
45	i	828	0	857	0	0
46	j	745	0	746	0	0
47	k	774	0	784	0	0
48	l	688	0	674	1	0
49	m	791	0	796	1	0
50	o	798	0	804	0	0
51	p	1205	0	1223	0	0
52	q	1398	0	1383	2	0
53	r	1322	0	1348	0	0
54	s	3155	0	3139	0	0
55	AA	20260	0	10284	28	0
56	AB	1828	0	1815	1	0
57	AC	1083	0	1088	0	0
58	AD	2700	0	2767	1	0
59	AE	972	0	1001	1	0
60	AF	1725	0	1769	1	0
61	AG	2695	0	2694	3	0
62	AH	1152	0	1183	3	0
63	AI	1020	0	1053	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	AJ	839	0	885	0	0
65	AK	862	0	885	0	0
66	AL	1453	0	1540	14	0
67	AM	942	0	965	0	0
68	AN	868	0	928	9	0
69	AO	1592	0	1557	5	0
70	AP	781	0	806	1	0
71	AQ	744	0	758	0	0
72	AR	2409	0	2428	3	0
73	AS	1111	0	1115	5	0
74	AT	1371	0	1393	0	0
75	AU	1488	0	1499	7	0
76	AV	2969	0	2961	0	0
77	AW	789	0	802	0	0
78	AX	2849	0	2843	2	0
79	AY	1246	0	1197	0	0
80	AZ	839	0	858	3	0
81	A0	1787	0	1796	18	0
82	A1	2265	0	2294	2	0
83	A2	935	0	971	1	0
84	A3	625	0	699	1	0
85	A4	4768	0	4766	3	0
86	Az	701	0	351	2	0
87	Av	115	0	38	0	0
88	Aw	1435	0	725	46	0
89	Ax	1415	0	719	8	0
90	3	1	0	0	0	0
90	6	1	0	0	0	0
90	A	28	0	0	0	0
90	AA	19	0	0	0	0
90	AJ	1	0	0	0	0
90	D	1	0	0	0	0
90	M	1	0	0	0	0
90	N	1	0	0	0	0
90	o	1	0	0	0	0
91	A	130	0	0	0	0
91	A3	1	0	0	0	0
91	AA	55	0	0	0	0
91	AB	1	0	0	0	0
91	AX	1	0	0	0	0
91	D	2	0	0	0	0
91	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	g	1	0	0	0	0
92	B	7	0	8	2	0
93	AE	4	0	0	0	0
93	AT	4	0	0	0	0
93	I	4	0	0	0	0
94	0	1	0	0	0	0
94	4	1	0	0	0	0
94	AO	1	0	0	0	0
95	AA	44	0	26	1	0
96	AX	31	0	12	1	0
97	AX	28	0	12	0	0
All	All	179948	0	152561	190	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 1.

The worst 5 of 190 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)
29:4:76:CYS:SG	29:4:92:CYS:SG	2.45	1.13
88:Aw:21:A:H61	88:Aw:46:A:H2'	1.46	0.80
1:A:3112:A:N7	1:A:3200:U:O2	2.14	0.80
88:Aw:14:A:H3'	88:Aw:15:A:H8	1.49	0.76
55:AA:330:A:H1'	63:AI:182:PRO:HB3	1.68	0.76

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
3	D	236/305 (77%)	231 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	303/348 (87%)	297 (98%)	5 (2%)	1 (0%)	36	65
5	F	250/311 (80%)	245 (98%)	5 (2%)	0	100	100
6	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
7	I	210/261 (80%)	202 (96%)	5 (2%)	3 (1%)	9	37
8	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
9	K	176/178 (99%)	176 (100%)	0	0	100	100
10	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
11	M	289/296 (98%)	284 (98%)	5 (2%)	0	100	100
12	N	220/251 (88%)	220 (100%)	0	0	100	100
13	O	152/175 (87%)	151 (99%)	1 (1%)	0	100	100
14	P	142/180 (79%)	140 (99%)	2 (1%)	0	100	100
15	Q	237/292 (81%)	234 (99%)	3 (1%)	0	100	100
16	R	138/149 (93%)	138 (100%)	0	0	100	100
17	S	159/205 (78%)	156 (98%)	2 (1%)	1 (1%)	21	52
18	T	164/206 (80%)	164 (100%)	0	0	100	100
19	U	151/153 (99%)	147 (97%)	3 (2%)	1 (1%)	18	50
20	V	203/216 (94%)	198 (98%)	5 (2%)	0	100	100
21	W	111/148 (75%)	110 (99%)	1 (1%)	0	100	100
22	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
23	Y	179/250 (72%)	177 (99%)	2 (1%)	0	100	100
24	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
25	0	108/188 (57%)	108 (100%)	0	0	100	100
26	1	54/65 (83%)	54 (100%)	0	0	100	100
27	2	44/92 (48%)	44 (100%)	0	0	100	100
28	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	4	36/103 (35%)	36 (100%)	0	0	100	100
30	z	250/325 (77%)	240 (96%)	10 (4%)	0	100	100
31	t	44/198 (22%)	44 (100%)	0	0	100	100
31	u	30/198 (15%)	30 (100%)	0	0	100	100
31	v	30/198 (15%)	30 (100%)	0	0	100	100
31	w	29/198 (15%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	x	29/198 (15%)	29 (100%)	0	0	100	100
31	y	29/198 (15%)	29 (100%)	0	0	100	100
32	5	389/423 (92%)	384 (99%)	5 (1%)	0	100	100
33	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
34	7	292/338 (86%)	281 (96%)	11 (4%)	0	100	100
35	8	142/206 (69%)	136 (96%)	4 (3%)	2 (1%)	9	37
36	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
37	a	96/142 (68%)	88 (92%)	8 (8%)	0	100	100
38	b	149/215 (69%)	145 (97%)	4 (3%)	0	100	100
39	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
40	d	217/306 (71%)	214 (99%)	3 (1%)	0	100	100
41	e	226/279 (81%)	221 (98%)	5 (2%)	0	100	100
42	f	153/212 (72%)	150 (98%)	3 (2%)	0	100	100
43	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
44	h	108/158 (68%)	108 (100%)	0	0	100	100
45	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
46	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
47	k	100/112 (89%)	100 (100%)	0	0	100	100
48	l	80/138 (58%)	80 (100%)	0	0	100	100
49	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
50	o	92/102 (90%)	92 (100%)	0	0	100	100
51	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
52	q	164/222 (74%)	160 (98%)	4 (2%)	0	100	100
53	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
54	s	382/439 (87%)	372 (97%)	10 (3%)	0	100	100
56	AB	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
57	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
58	AD	335/430 (78%)	326 (97%)	9 (3%)	0	100	100
59	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
60	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
61	AG	324/396 (82%)	320 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	AH	138/201 (69%)	135 (98%)	3 (2%)	0	100	100
63	AI	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
64	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
65	AK	99/128 (77%)	99 (100%)	0	0	100	100
66	AL	172/257 (67%)	161 (94%)	11 (6%)	0	100	100
67	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
68	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
69	AO	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
70	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
71	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
72	AR	293/360 (81%)	283 (97%)	10 (3%)	0	100	100
73	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
74	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
75	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
76	AV	358/414 (86%)	351 (98%)	7 (2%)	0	100	100
77	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
78	AX	350/398 (88%)	343 (98%)	7 (2%)	0	100	100
79	AY	147/395 (37%)	144 (98%)	3 (2%)	0	100	100
80	AZ	98/106 (92%)	92 (94%)	6 (6%)	0	100	100
81	A0	213/217 (98%)	205 (96%)	8 (4%)	0	100	100
82	A1	277/323 (86%)	275 (99%)	2 (1%)	0	100	100
83	A2	116/118 (98%)	116 (100%)	0	0	100	100
84	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
85	A4	584/689 (85%)	576 (99%)	8 (1%)	0	100	100
All	All	14658/19484 (75%)	14391 (98%)	259 (2%)	8 (0%)	49	78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	66	PRO
17	S	147	PRO
4	E	318	THR
7	I	59	ALA
7	I	58	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	192/245 (78%)	192 (100%)	0	100	100
4	E	260/290 (90%)	260 (100%)	0	100	100
5	F	219/262 (84%)	219 (100%)	0	100	100
6	H	182/228 (80%)	182 (100%)	0	100	100
7	I	194/232 (84%)	194 (100%)	0	100	100
8	J	138/150 (92%)	138 (100%)	0	100	100
9	K	155/155 (100%)	154 (99%)	1 (1%)	78	79
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	246/249 (99%)	246 (100%)	0	100	100
12	N	189/211 (90%)	189 (100%)	0	100	100
13	O	134/150 (89%)	134 (100%)	0	100	100
14	P	126/155 (81%)	126 (100%)	0	100	100
15	Q	221/256 (86%)	221 (100%)	0	100	100
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	146/180 (81%)	146 (100%)	0	100	100
18	T	146/176 (83%)	146 (100%)	0	100	100
19	U	134/134 (100%)	134 (100%)	0	100	100
20	V	183/191 (96%)	183 (100%)	0	100	100
21	W	91/119 (76%)	91 (100%)	0	100	100
22	X	220/229 (96%)	220 (100%)	0	100	100
23	Y	163/223 (73%)	163 (100%)	0	100	100
24	Z	113/147 (77%)	113 (100%)	0	100	100
25	0	99/164 (60%)	99 (100%)	0	100	100
26	1	53/60 (88%)	53 (100%)	0	100	100
27	2	40/72 (56%)	40 (100%)	0	100	100
28	3	88/166 (53%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	4	37/89 (42%)	37 (100%)	0	100	100
30	z	226/287 (79%)	226 (100%)	0	100	100
31	t	40/158 (25%)	40 (100%)	0	100	100
31	u	31/158 (20%)	31 (100%)	0	100	100
31	v	31/158 (20%)	31 (100%)	0	100	100
31	w	30/158 (19%)	30 (100%)	0	100	100
31	x	30/158 (19%)	30 (100%)	0	100	100
31	y	30/158 (19%)	30 (100%)	0	100	100
32	5	352/368 (96%)	352 (100%)	0	100	100
33	6	313/332 (94%)	313 (100%)	0	100	100
34	7	270/303 (89%)	270 (100%)	0	100	100
35	8	133/190 (70%)	133 (100%)	0	100	100
36	9	104/112 (93%)	104 (100%)	0	100	100
37	a	96/133 (72%)	96 (100%)	0	100	100
38	b	132/185 (71%)	132 (100%)	0	100	100
39	c	251/288 (87%)	251 (100%)	0	100	100
40	d	203/274 (74%)	203 (100%)	0	100	100
41	e	200/236 (85%)	200 (100%)	0	100	100
42	f	139/188 (74%)	139 (100%)	0	100	100
43	g	124/148 (84%)	124 (100%)	0	100	100
44	h	104/148 (70%)	104 (100%)	0	100	100
45	i	86/110 (78%)	86 (100%)	0	100	100
46	j	74/97 (76%)	74 (100%)	0	100	100
47	k	83/89 (93%)	83 (100%)	0	100	100
48	l	76/116 (66%)	76 (100%)	0	100	100
49	m	85/113 (75%)	85 (100%)	0	100	100
50	o	80/87 (92%)	80 (100%)	0	100	100
51	p	135/181 (75%)	135 (100%)	0	100	100
52	q	143/178 (80%)	143 (100%)	0	100	100
53	r	147/169 (87%)	147 (100%)	0	100	100
54	s	340/381 (89%)	340 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	AB	198/249 (80%)	198 (100%)	0	100	100
57	AC	115/143 (80%)	115 (100%)	0	100	100
58	AD	283/357 (79%)	283 (100%)	0	100	100
59	AE	104/107 (97%)	104 (100%)	0	100	100
60	AF	185/209 (88%)	185 (100%)	0	100	100
61	AG	286/342 (84%)	286 (100%)	0	100	100
62	AH	130/180 (72%)	130 (100%)	0	100	100
63	AI	104/146 (71%)	104 (100%)	0	100	100
64	AJ	93/118 (79%)	93 (100%)	0	100	100
65	AK	91/113 (80%)	91 (100%)	0	100	100
66	AL	158/226 (70%)	158 (100%)	0	100	100
67	AM	97/113 (86%)	97 (100%)	0	100	100
68	AN	96/115 (84%)	96 (100%)	0	100	100
69	AO	174/230 (76%)	174 (100%)	0	100	100
70	AP	88/123 (72%)	88 (100%)	0	100	100
71	AQ	78/78 (100%)	78 (100%)	0	100	100
72	AR	264/318 (83%)	264 (100%)	0	100	100
73	AS	116/164 (71%)	116 (100%)	0	100	100
74	AT	153/157 (98%)	153 (100%)	0	100	100
75	AU	152/174 (87%)	152 (100%)	0	100	100
76	AV	325/364 (89%)	325 (100%)	0	100	100
77	AW	87/158 (55%)	87 (100%)	0	100	100
78	AX	311/351 (89%)	311 (100%)	0	100	100
79	AY	137/357 (38%)	137 (100%)	0	100	100
80	AZ	90/95 (95%)	90 (100%)	0	100	100
81	A0	188/189 (100%)	188 (100%)	0	100	100
82	A1	257/291 (88%)	257 (100%)	0	100	100
83	A2	100/100 (100%)	100 (100%)	0	100	100
84	A3	65/166 (39%)	65 (100%)	0	100	100
85	A4	526/609 (86%)	526 (100%)	0	100	100
All	All	13124/16786 (78%)	13123 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	K	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
68	AN	52	HIS
78	AX	394	HIS
71	AQ	41	HIS
74	AT	37	HIS
85	A4	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1556/1561 (99%)	250 (16%)	1 (0%)
2	B	71/72 (98%)	13 (18%)	1 (1%)
55	AA	953/954 (99%)	149 (15%)	8 (0%)
86	Az	32/33 (96%)	19 (59%)	0
88	Aw	67/68 (98%)	35 (52%)	0
89	Ax	66/71 (92%)	32 (48%)	0
All	All	2745/2759 (99%)	498 (18%)	10 (0%)

5 of 498 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1681	G
1	A	1685	C
1	A	1689	C
1	A	1692	A
1	A	1694	U

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	AA	884	C
55	AA	890	C
55	AA	892	C
55	AA	865	A
55	AA	873	U

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

14 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
55	5MC	AA	841	55	18,22,23	0.44	0	26,32,35	1.03	3 (11%)
55	5MU	AA	429	55	19,22,23	0.39	0	28,32,35	0.30	0
55	B8T	AA	839	55	19,22,23	0.38	0	26,31,34	0.49	0
2	2MG	B	10	2	23,26,27	0.64	0	32,38,41	0.74	1 (3%)
55	MA6	AA	937	55	23,26,27	0.42	0	34,38,41	0.65	1 (2%)
1	OMG	A	2815	88,90,1	23,26,27	0.55	0	33,38,41	0.39	0
55	MA6	AA	936	55	23,26,27	0.33	0	34,38,41	0.61	1 (2%)
2	1MA	B	9	2	21,25,26	0.39	0	31,37,40	1.13	4 (12%)
2	PSU	B	39	2	18,21,22	0.54	0	22,30,33	0.49	0
1	1MA	A	2617	1	21,25,26	0.57	0	31,37,40	1.20	3 (9%)
1	OMU	A	3039	90,1	19,22,23	0.36	0	26,31,34	0.50	0
63	5F0	AI	184	63	8,8,9	0.35	0	7,9,11	0.53	0
1	OMG	A	3040	1	23,26,27	0.58	0	33,38,41	0.86	1 (3%)
1	PSU	A	3067	1	18,21,22	0.57	0	22,30,33	0.61	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
55	5MC	AA	841	55	-	0/7/25/26	0/2/2/2
55	5MU	AA	429	55	-	0/7/25/26	0/2/2/2
55	B8T	AA	839	55	-	2/7/27/28	0/2/2/2
2	2MG	B	10	2	-	2/9/27/28	0/3/3/3
55	MA6	AA	937	55	-	1/11/29/30	0/3/3/3
1	OMG	A	2815	88,90,1	-	1/9/27/28	0/3/3/3
55	MA6	AA	936	55	-	0/11/29/30	0/3/3/3
2	1MA	B	9	2	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
1	1MA	A	2617	1	-	2/7/25/26	0/3/3/3
1	OMU	A	3039	90,1	-	0/9/27/28	0/2/2/2
63	5F0	AI	184	63	-	3/9/9/10	-
1	OMG	A	3040	1	-	1/9/27/28	0/3/3/3
1	PSU	A	3067	1	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2617	1MA	O3'-C3'-C2'	3.88	124.38	111.82
2	B	9	1MA	O3'-C3'-C2'	3.19	122.16	111.82
2	B	9	1MA	O3'-C3'-C4'	2.89	119.41	111.05
1	A	3040	OMG	C2'-C1'-N9	-2.73	108.91	114.22
1	A	2617	1MA	O3'-C3'-C4'	2.55	118.41	111.05

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2815	OMG	C1'-C2'-O2'-CM2
1	A	3040	OMG	C1'-C2'-O2'-CM2
2	B	10	2MG	O4'-C4'-C5'-O5'
63	AI	184	5F0	N-CA-CB-C
63	AI	184	5F0	C1-CA-CB-C

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	AA	841	5MC	2	0
55	AA	429	5MU	1	0
2	B	10	2MG	1	0
55	AA	937	MA6	1	0
1	A	2815	OMG	1	0
55	AA	936	MA6	2	0
2	B	39	PSU	3	0
1	A	3040	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 256 ligands modelled in this entry, 249 are monoatomic - leaving 7 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	$\# Z > 2$
92	VAL	B	101	2	4,6,7	0.74	0	6,7,9	1.07	1 (16%)
93	FES	I	301	-	0,4,4	-	-	-		
97	GDP	AX	503	-	28,30,30	0.40	0	44,47,47	0.40	0
93	FES	AE	201	-	0,4,4	-	-	-		
96	ATP	AX	501	91	29,33,33	0.38	0	44,52,52	0.66	0
95	NAD	AA	1002	-	45,48,48	0.40	0	63,73,73	0.64	1 (1%)
93	FES	AT	201	74,67	0,4,4	-	-	-		

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
92	VAL	B	101	2	-	4/5/6/8	-
93	FES	I	301	-	-	-	0/1/1/1
97	GDP	AX	503	-	-	1/16/32/32	0/3/3/3
93	FES	AE	201	-	-	-	0/1/1/1
96	ATP	AX	501	91	-	0/22/38/38	0/3/3/3
95	NAD	AA	1002	-	-	6/30/62/62	0/5/5/5
93	FES	AT	201	74,67	-	-	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(°)	Ideal(°)
95	AA	1002	NAD	PN-O3-PA	-2.76	123.36	132.83
92	B	101	VAL	O-C-CA	-2.21	118.99	124.78

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

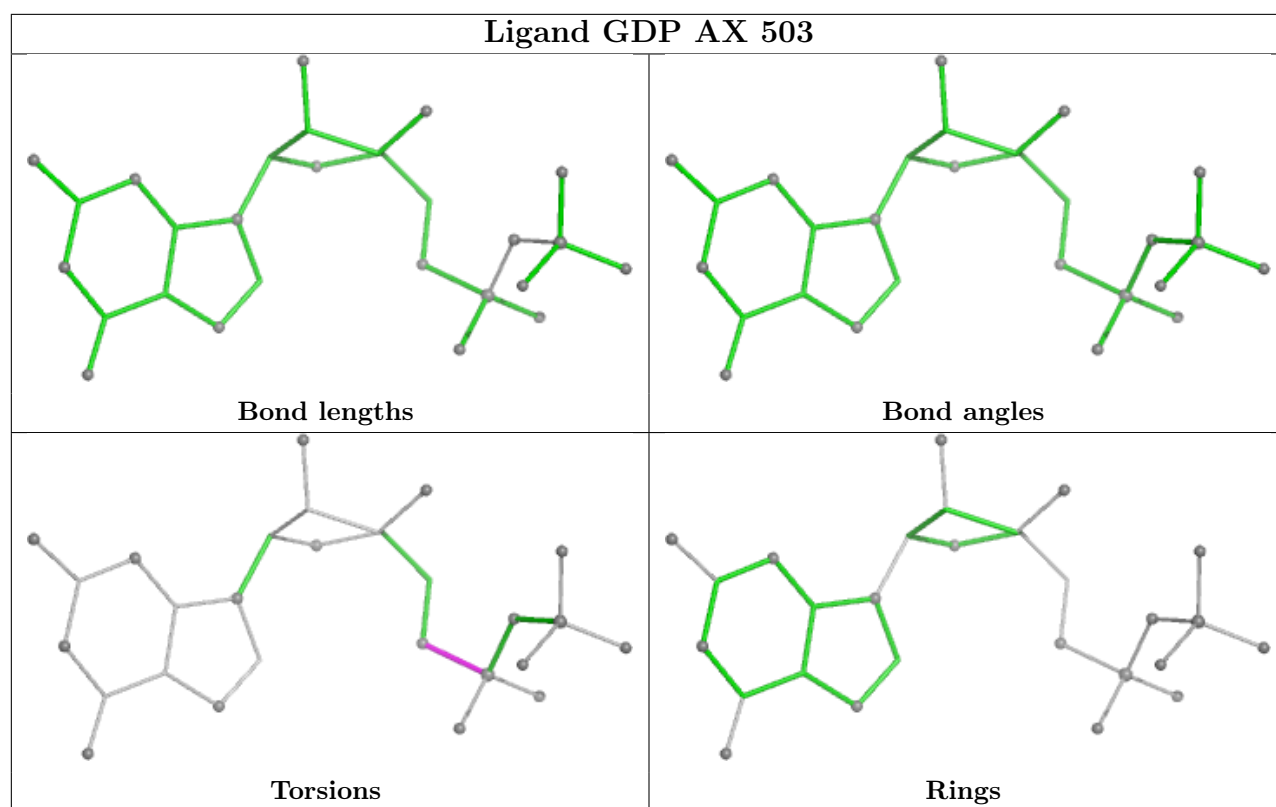
Mol	Chain	Res	Type	Atoms
92	B	101	VAL	N-CA-CB-CG1
92	B	101	VAL	N-CA-CB-CG2
92	B	101	VAL	C-CA-CB-CG1
92	B	101	VAL	C-CA-CB-CG2
95	AA	1002	NAD	C3D-C4D-C5D-O5D

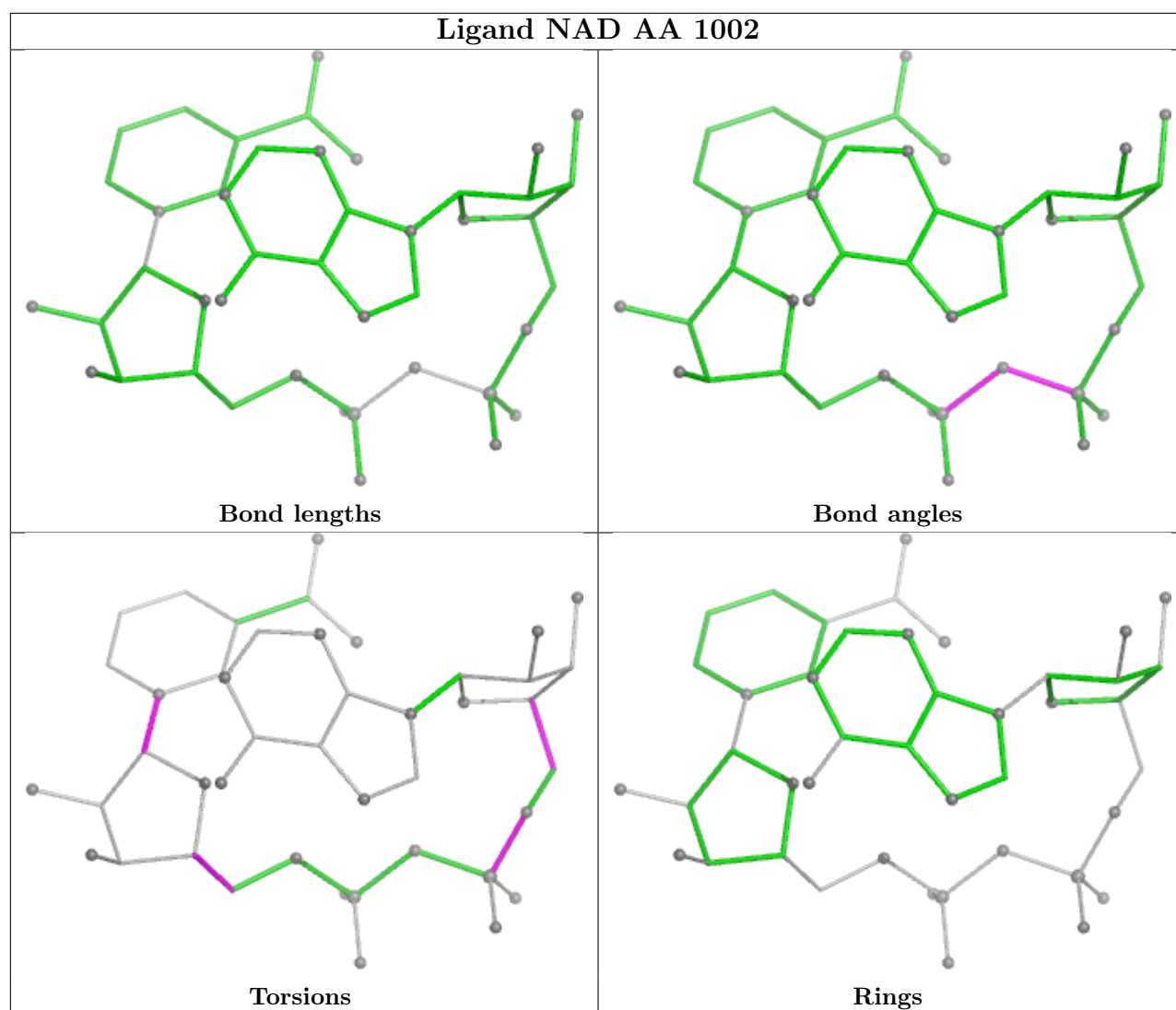
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	B	101	VAL	2	0
96	AX	501	ATP	1	0
95	AA	1002	NAD	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

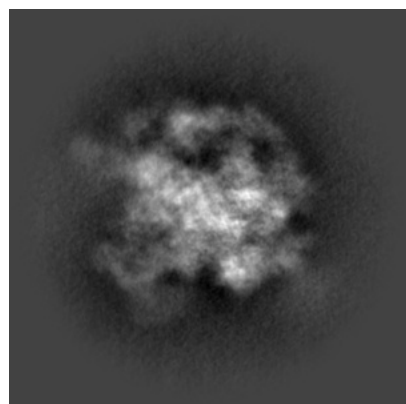
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54637. These allow visual inspection of the internal detail of the map and identification of artifacts.

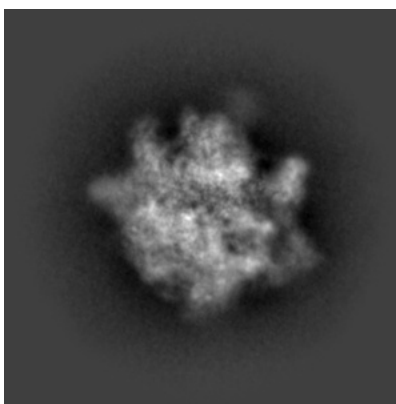
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

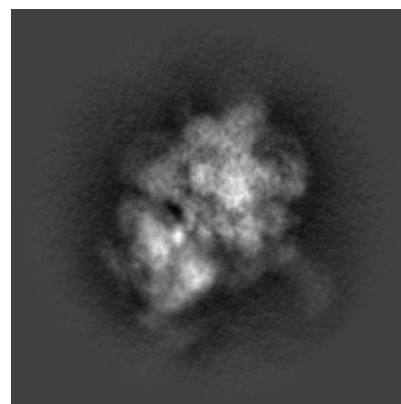
6.1.1 Primary map



X

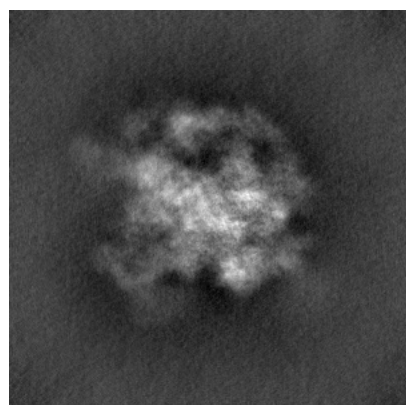


Y

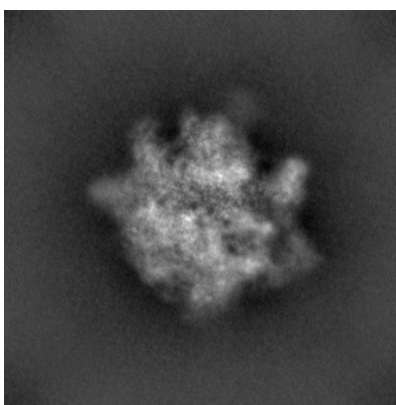


Z

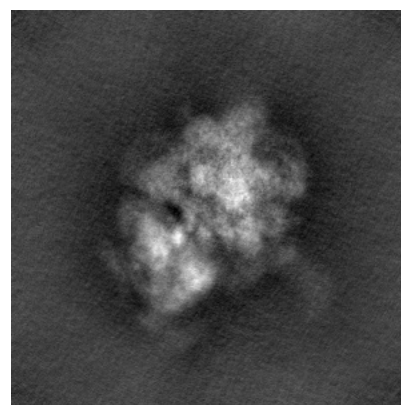
6.1.2 Raw map



X



Y

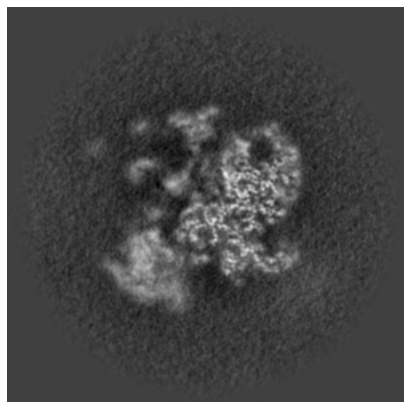


Z

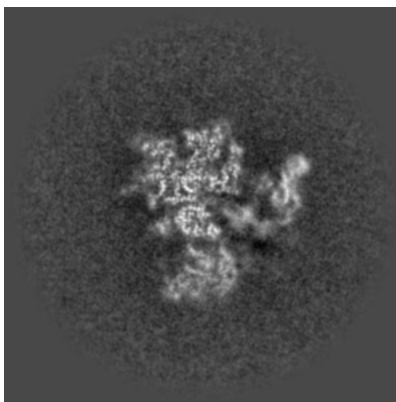
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

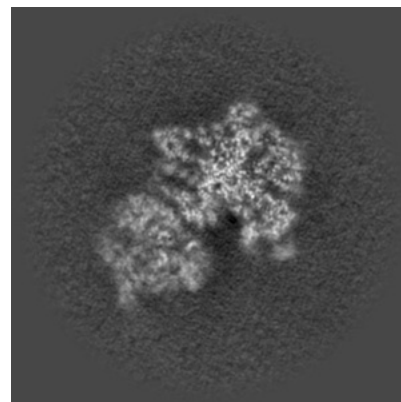
6.2.1 Primary map



X Index: 200

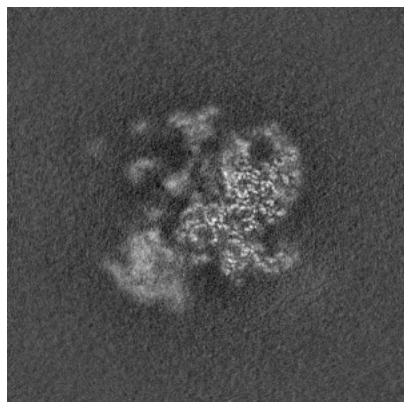


Y Index: 200

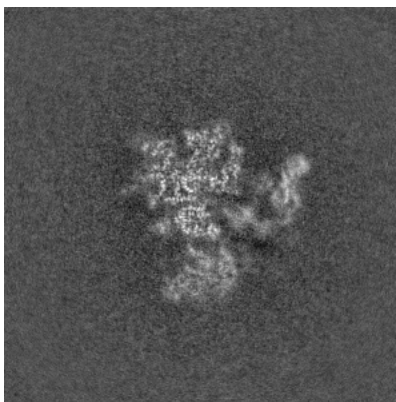


Z Index: 200

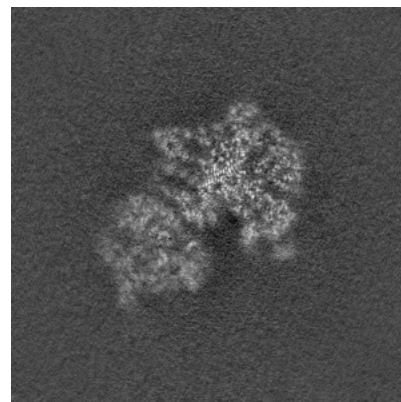
6.2.2 Raw map



X Index: 200



Y Index: 200

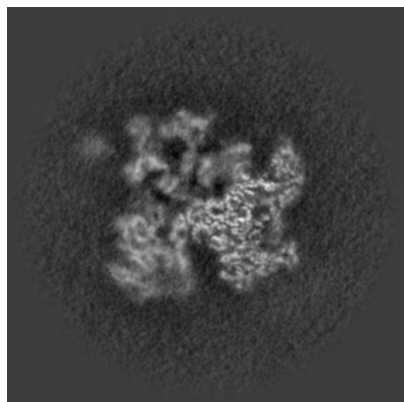


Z Index: 200

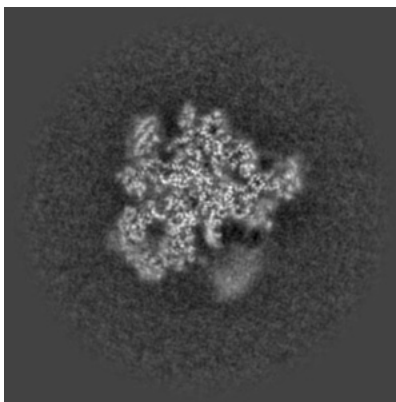
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

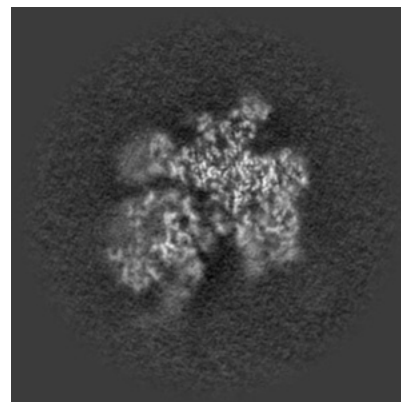
6.3.1 Primary map



X Index: 192

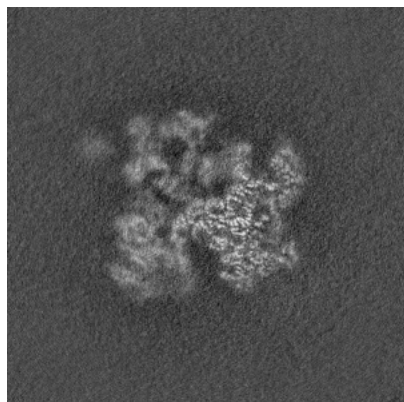


Y Index: 229

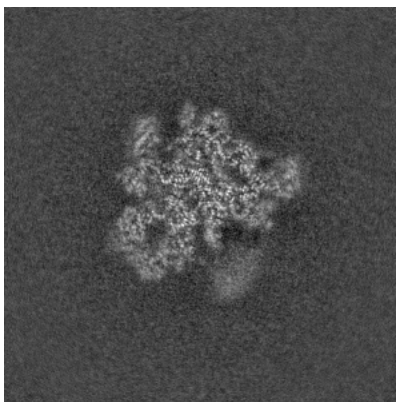


Z Index: 214

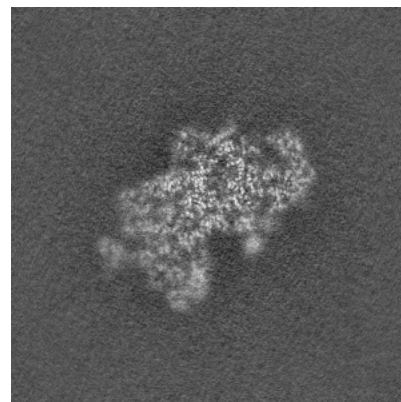
6.3.2 Raw map



X Index: 191



Y Index: 230

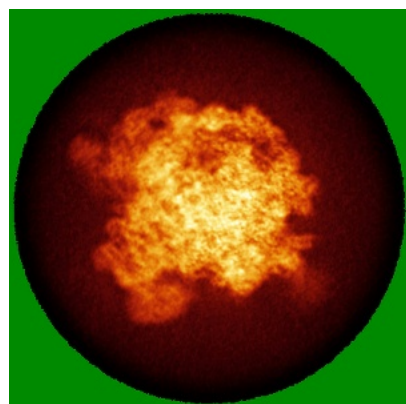


Z Index: 185

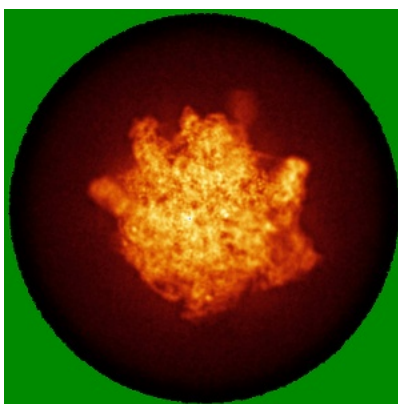
The images above show the largest variance slices of the map in three orthogonal directions.

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

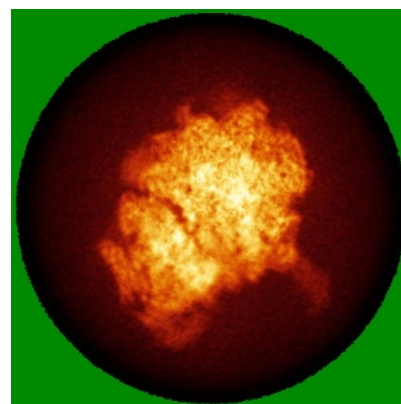
6.4.1 Primary map



X

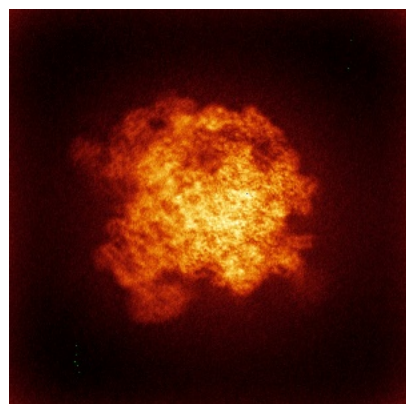


Y

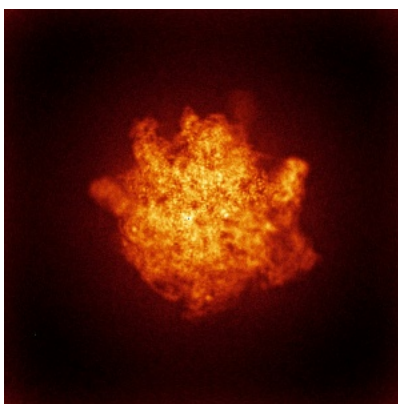


Z

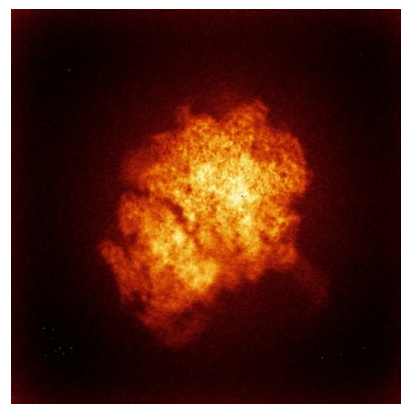
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

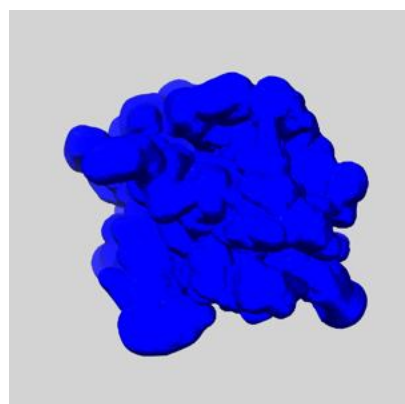
6.6 Mask visualisation [i](#)

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

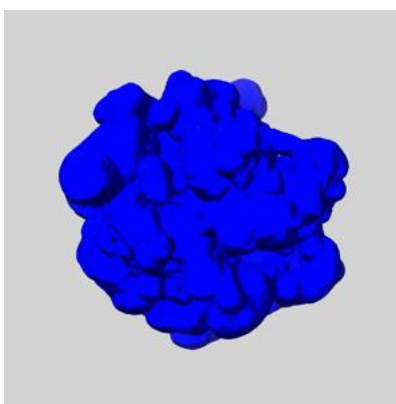
A mask typically either:

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

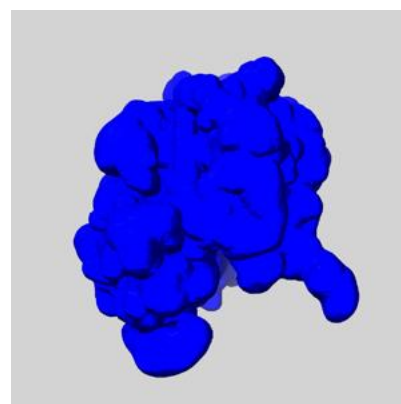
6.6.1 emd_54637_msk_1.map [i](#)



X



Y

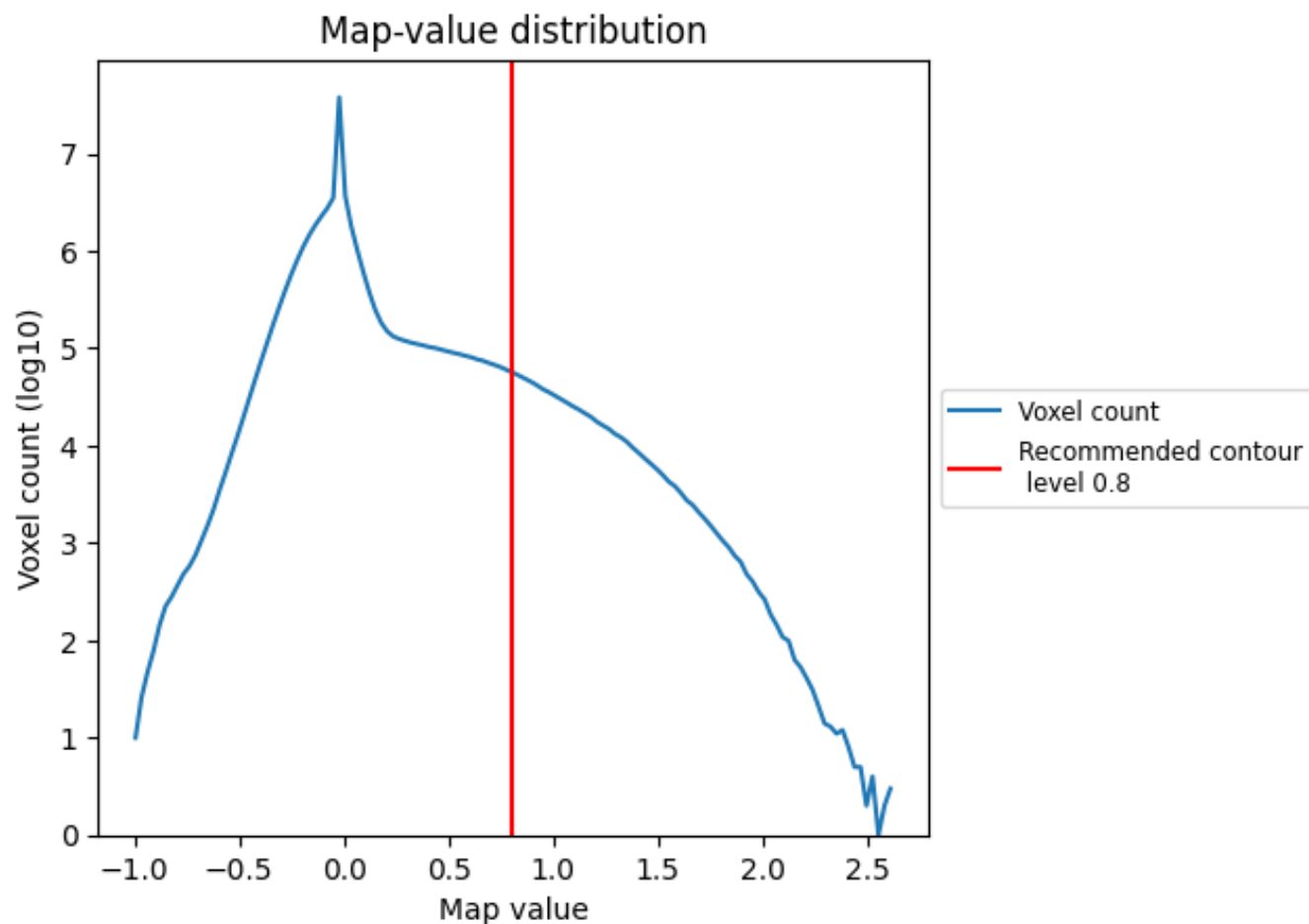


Z

7 Map analysis [i](#)

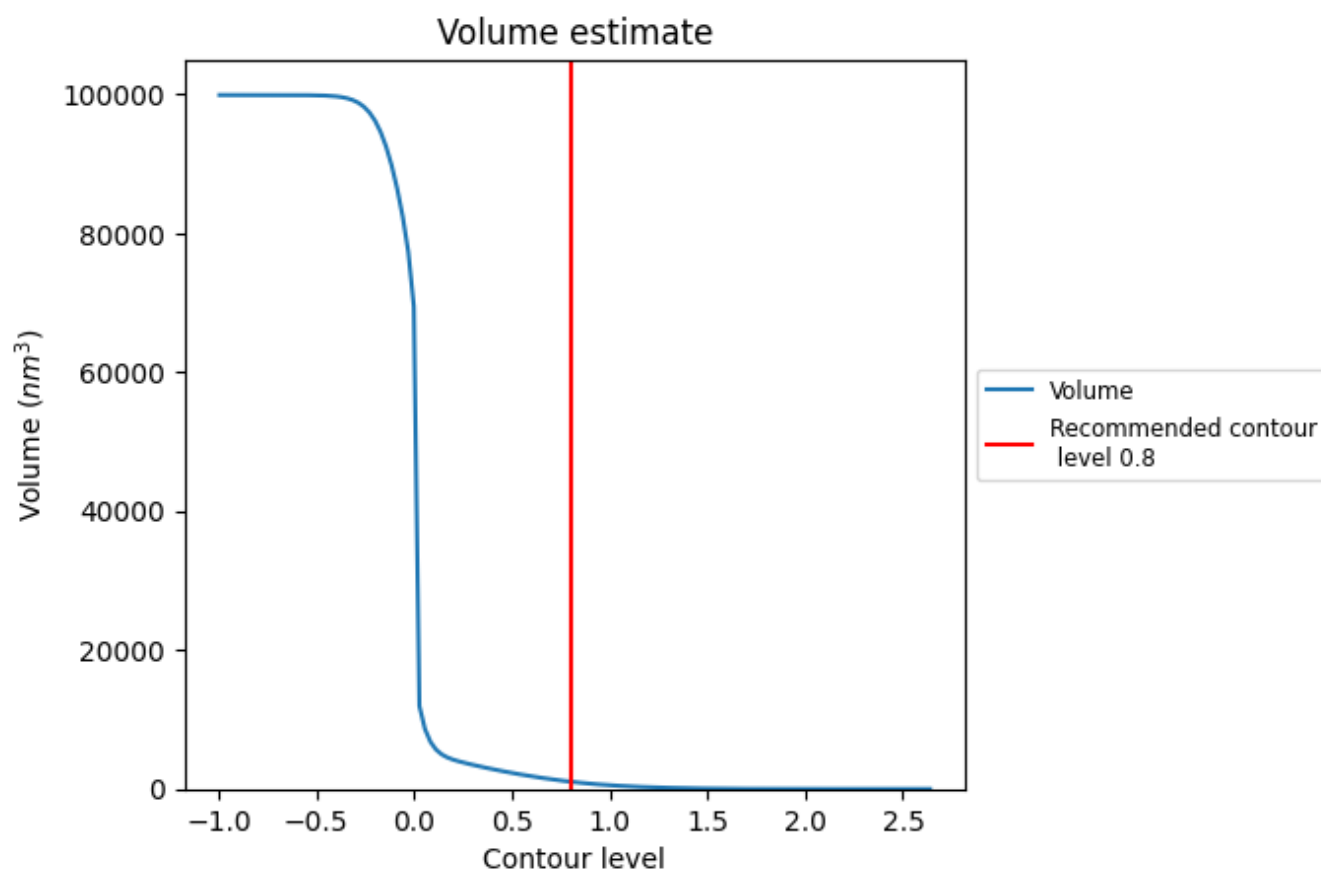
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

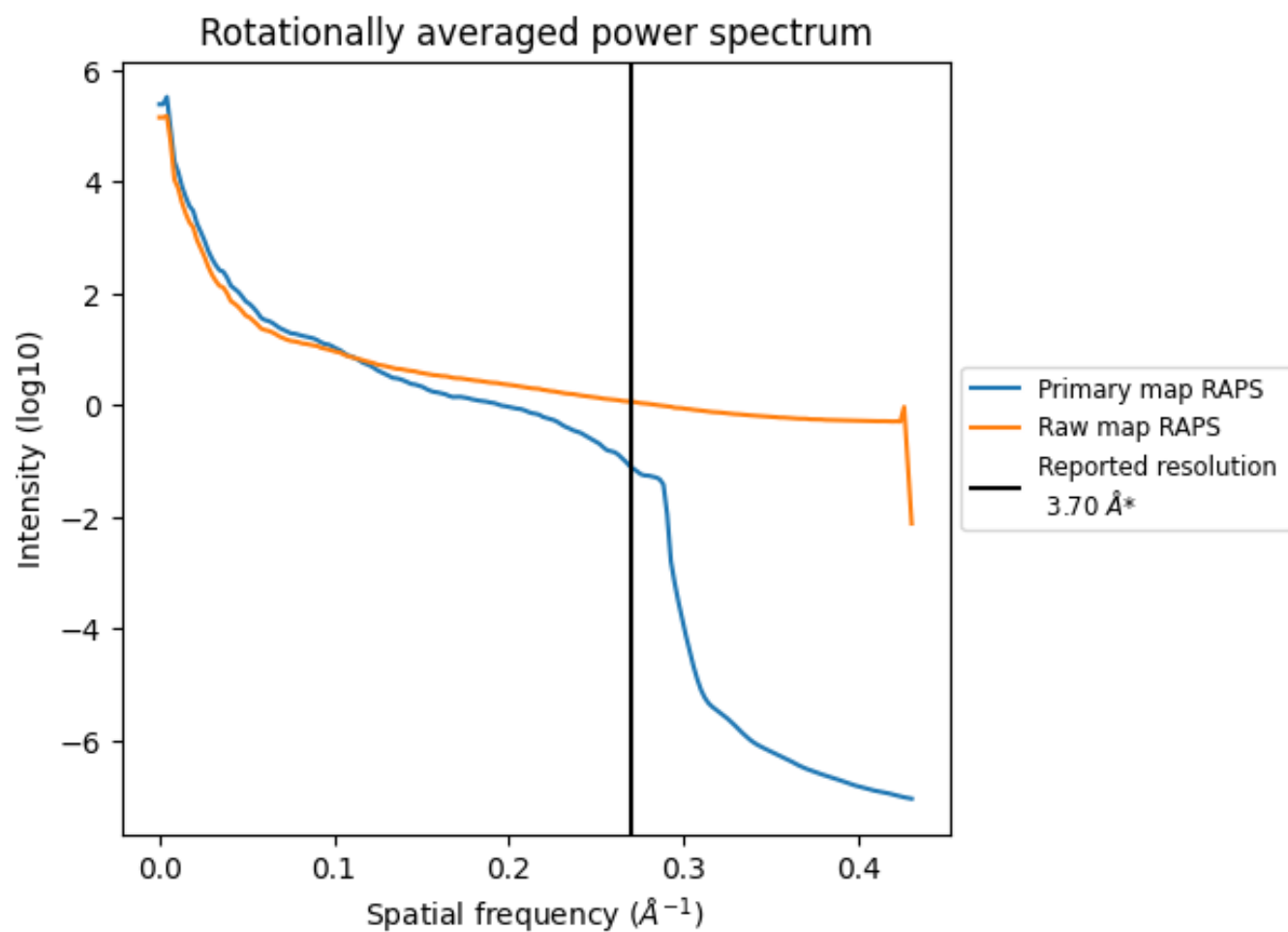
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1045 nm³; this corresponds to an approximate mass of 944 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

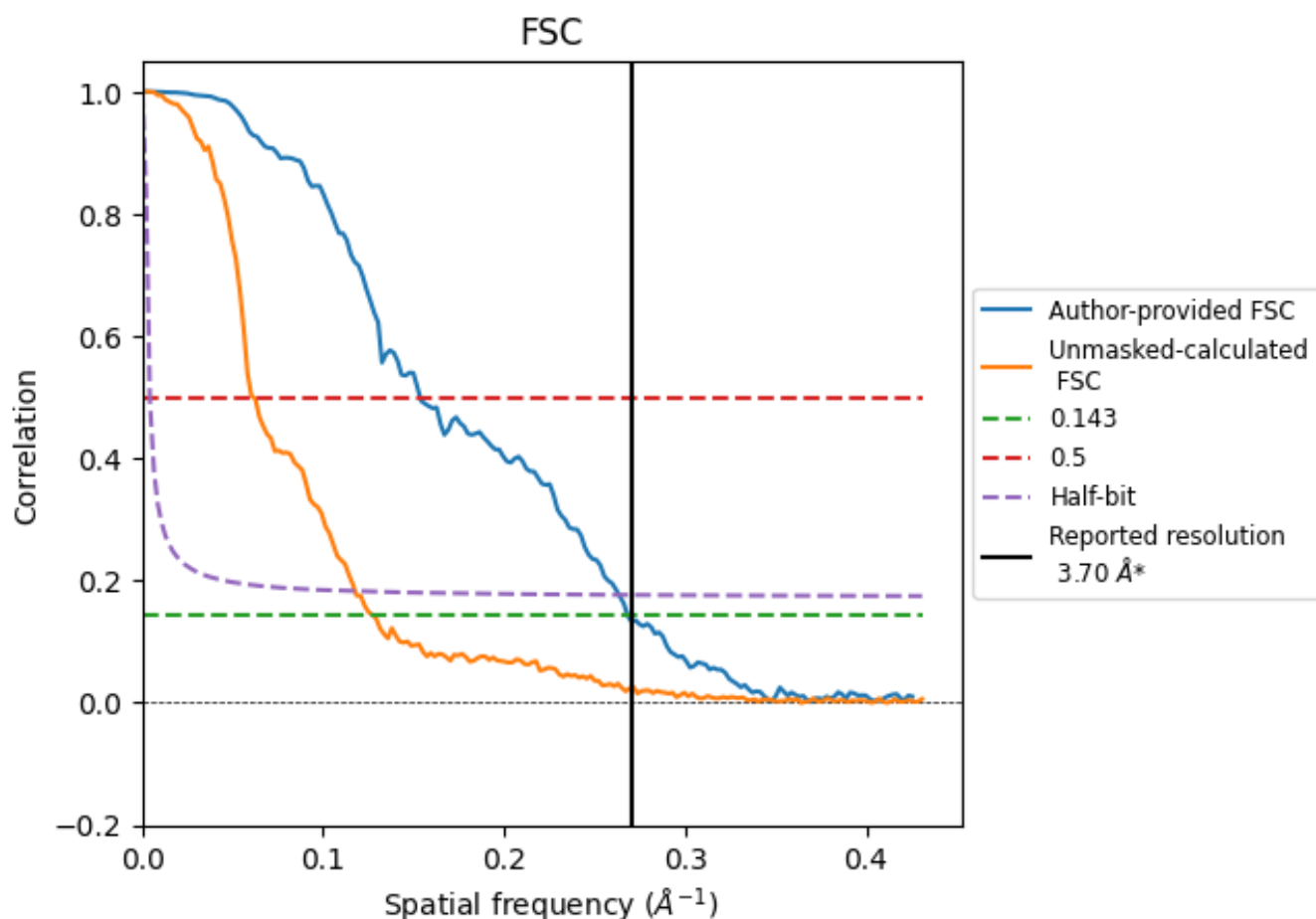


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

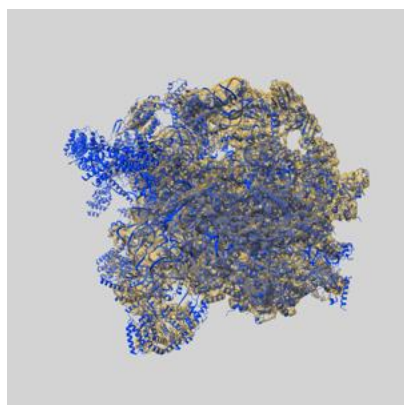
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	6.51	3.80
Unmasked-calculated*	7.85	16.31	8.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.85 differs from the reported value 3.7 by more than 10 %

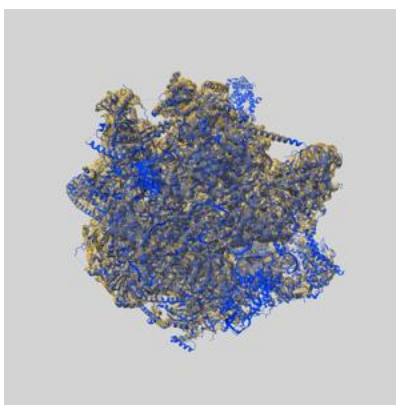
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54637 and PDB model 9S7B. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

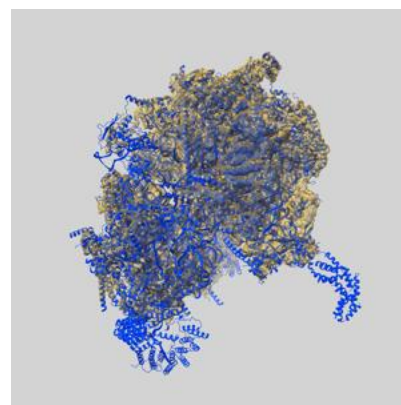
9.1 Map-model overlay [i](#)



X



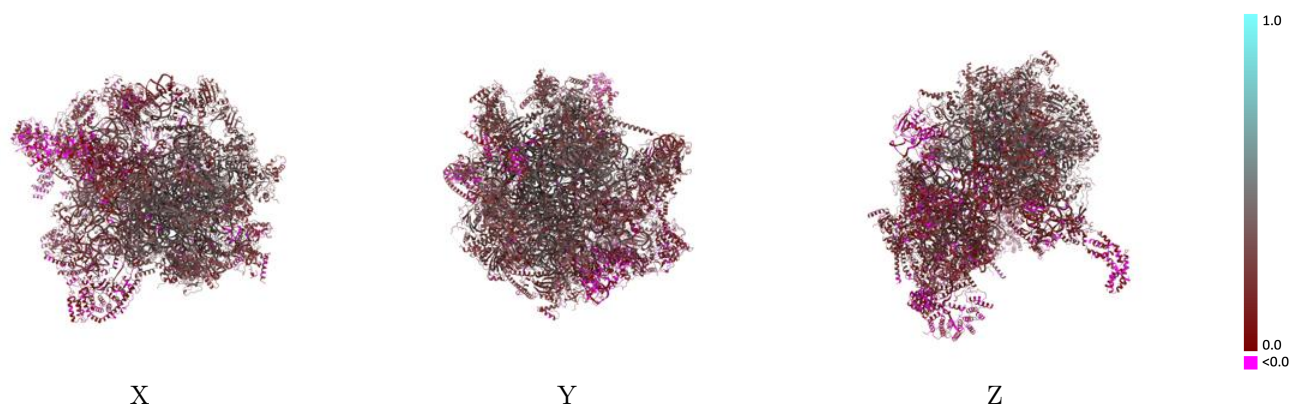
Y



Z

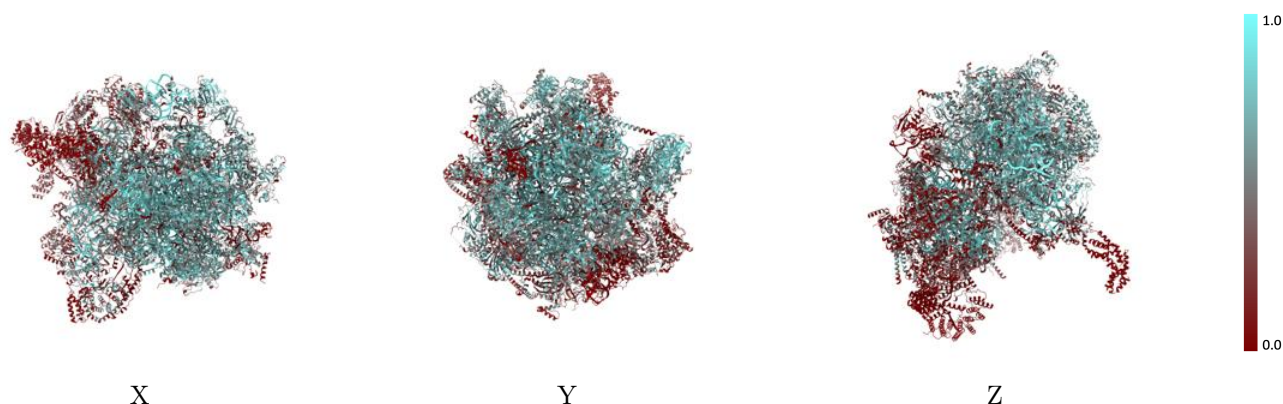
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



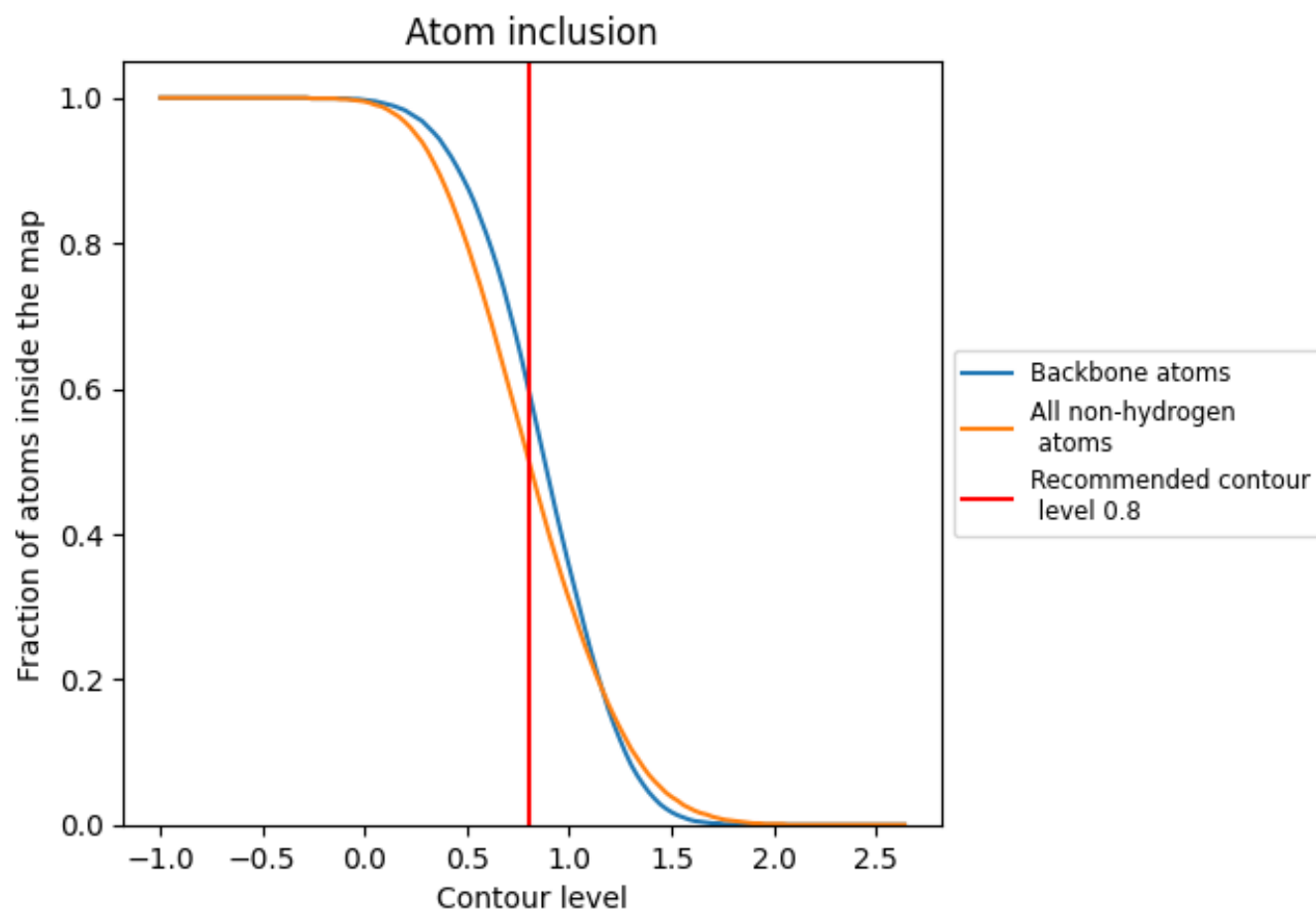
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5030	 0.2540
0	 0.5720	 0.3260
1	 0.4790	 0.2380
2	 0.6210	 0.3970
3	 0.5840	 0.3810
4	 0.6510	 0.2680
5	 0.4800	 0.2720
6	 0.6410	 0.2740
7	 0.5810	 0.2880
8	 0.3020	 0.1670
9	 0.5300	 0.3100
A	 0.8030	 0.3480
A0	 0.3060	 0.1240
A1	 0.1530	 0.1650
A2	 0.1020	 0.1950
A3	 0.3220	 0.2720
A4	 0.0190	 0.0780
AA	 0.7290	 0.2610
AB	 0.3970	 0.2090
AC	 0.1750	 0.2170
AD	 0.1580	 0.2160
AE	 0.2830	 0.2300
AF	 0.3130	 0.1910
AG	 0.1970	 0.1790
AH	 0.1650	 0.1790
AI	 0.4540	 0.2460
AJ	 0.1290	 0.2000
AK	 0.4170	 0.2020
AL	 0.3160	 0.1830
AM	 0.3430	 0.1570
AN	 0.3690	 0.2130
AO	 0.2540	 0.1800
AP	 0.4110	 0.2360
AQ	 0.3440	 0.2430
AR	 0.1540	 0.1480



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Chain	Atom inclusion	Q-score
AS	 0.2160	 0.1730
AT	 0.2940	 0.1950
AU	 0.3770	 0.1700
AV	 0.2400	 0.0920
AW	 0.2240	 0.1980
AX	 0.2000	 0.1160
AY	 0.1400	 0.1380
AZ	 0.2980	 0.1560
Av	 0.0170	 0.2510
Aw	 0.4330	 0.1900
Ax	 0.3510	 0.1190
Az	 0.2230	 0.1140
B	 0.8440	 0.2280
D	 0.5870	 0.3530
E	 0.6400	 0.3510
F	 0.5640	 0.3530
H	 0.2640	 0.1640
I	 0.2600	 0.1580
J	 0.1810	 0.1070
K	 0.6430	 0.3640
L	 0.4010	 0.3370
M	 0.6080	 0.3460
N	 0.5510	 0.3160
O	 0.6080	 0.3440
P	 0.6710	 0.3000
Q	 0.4270	 0.3100
R	 0.5440	 0.3250
S	 0.5800	 0.3350
T	 0.5520	 0.3480
U	 0.4630	 0.2840
V	 0.1340	 0.1570
W	 0.6340	 0.3710
X	 0.5680	 0.3190
Y	 0.5660	 0.3050
Z	 0.4450	 0.3360
a	 0.3890	 0.2840
b	 0.5660	 0.3380
c	 0.5770	 0.3000
d	 0.3730	 0.1970
e	 0.4480	 0.1630
f	 0.3030	 0.2160
g	 0.5970	 0.3350

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Chain	Atom inclusion	Q-score
h	 0.4810	 0.2640
i	 0.5380	 0.3700
j	 0.5230	 0.3170
k	 0.3880	 0.1830
l	 0.2530	 0.1110
m	 0.2700	 0.1470
o	 0.6450	 0.3560
p	 0.4860	 0.2650
q	 0.4310	 0.2170
r	 0.6440	 0.3050
s	 0.5510	 0.3040
t	 0.0060	 0.0810
u	 0.0000	 0.0560
v	 0.0000	 0.0730
w	 0.0000	 0.0220
x	 0.0000	 0.0080
y	 0.0000	 0.0440
z	 0.0130	 0.0430