



## wwPDB EM Validation Summary Report ⓘ

Dec 1, 2025 – 04:54 PM JST

PDB ID : 9UWH / pdb\_00009uwh  
EMDB ID : EMD-64554  
Title : human mitoribosome trapped by retapamulin  
Authors : Ando, Y.; Nureki, O.; Itoh, Y.  
Deposited on : 2025-05-12  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

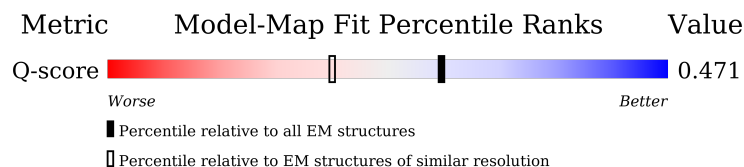
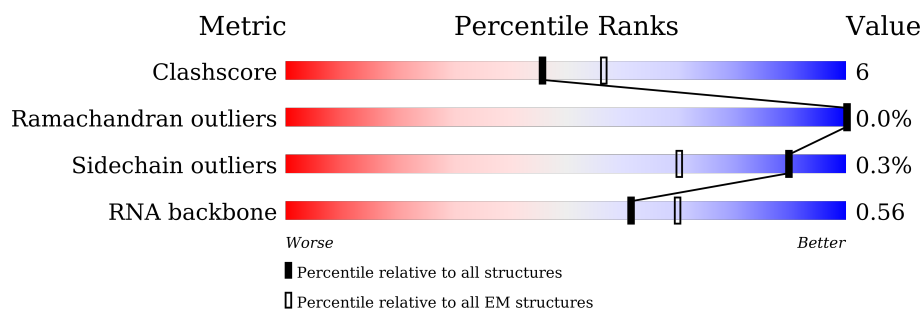
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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  $\geq 3$ , 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	
3	D	305	



















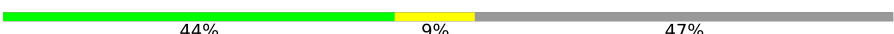






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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	AA	954	
26	AB	296	
27	AC	167	
28	AD	430	







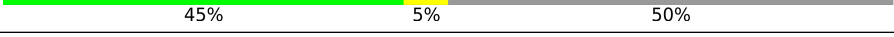

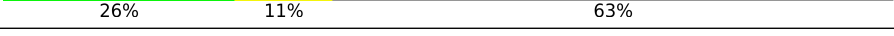

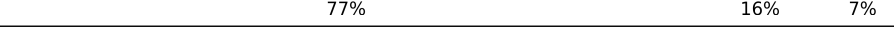
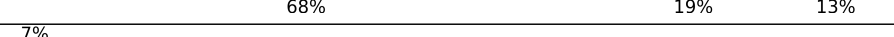

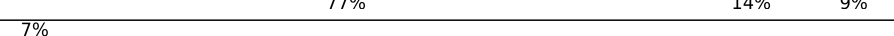


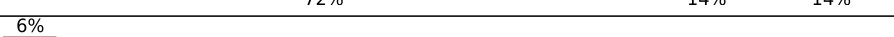

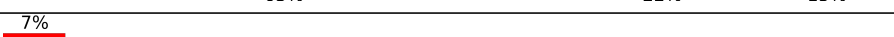






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Mol	Chain	Length	Quality of chain
29	AE	125	
30	AF	242	
31	AG	396	
32	AH	201	
33	AI	194	
34	AJ	138	
35	AK	128	
36	AL	257	
37	AM	137	
38	AN	130	
39	AO	258	
40	AP	142	
41	AQ	87	
42	AR	360	
43	AS	190	
44	AT	173	
45	AU	205	
46	AV	414	
47	AW	187	
48	AX	398	
49	AY	395	
50	AZ	106	
51	A0	217	
52	A1	323	
53	A2	118	

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Mol	Chain	Length	Quality of chain
54	A3	199	
55	A4	689	
56	Ax	71	
57	Az	8	
58	0	188	
59	1	65	
60	2	92	
61	3	188	
62	4	103	
63	5	423	
64	6	380	
65	7	338	
66	8	206	
67	9	137	
68	a	142	
69	b	215	
70	c	332	
71	d	306	
72	e	279	
73	f	212	
74	g	166	
75	h	158	
76	i	128	
77	j	123	
78	k	112	

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Mol	Chain	Length	Quality of chain
79	l	138	
80	m	128	
81	o	102	
82	p	206	
83	q	222	
84	r	196	
85	s	439	
86	t	198	

## 2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 171472 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	1523	Total	C	N	O	P	0	0
			32331	14510	5827	10471	1523		

- 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	100	Total	C	N	O		0	0
			823	522	159	142			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	169	Total	C	N	O	S	0	0
			1362	877	247	228	10		

- 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	289	Total	C	N	O	S	0	0
			2314	1476	427	405	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	116	Total	C	N	O	S	0	0
			904	577	171	153	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 RNA chain called 12S mitochondrial rRNA.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS2m.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS3m.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 29 is a protein called Small ribosomal subunit protein bS6m.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS7m.

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

- Molecule 31 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AG	311	Total	C	N	O	S	0	0
			2561	1627	454	466	14		

- Molecule 32 is a protein called Small ribosomal subunit protein uS10m.

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

- Molecule 33 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	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 34 is a protein called Small ribosomal subunit protein uS12m.

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS14m.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS15m.

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

- Molecule 37 is a protein called Small ribosomal subunit protein bS16m.

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS17m.

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

- Molecule 39 is a protein called Small ribosomal subunit protein mS40.

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

- Molecule 40 is a protein called Small ribosomal subunit protein bS18m.

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

- Molecule 41 is a protein called MRPS21 isoform 1.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP A0A2J8VEN6

- Molecule 42 is a protein called Small ribosomal subunit protein mS22.

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

- Molecule 43 is a protein called Small ribosomal subunit protein mS23.

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

- Molecule 44 is a protein called Small ribosomal subunit protein mS25.

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

- Molecule 45 is a protein called Small ribosomal subunit protein mS26.

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

- Molecule 46 is a protein called Small ribosomal subunit protein mS27.

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

- Molecule 47 is a protein called Small ribosomal subunit protein bS1m.

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

- Molecule 48 is a protein called Small ribosomal subunit protein mS29.

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

- Molecule 49 is a protein called Small ribosomal subunit protein mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AY	120	Total	C	N	O	S	0	0
			1016	657	167	190	2		

- Molecule 50 is a protein called Small ribosomal subunit protein mS33.

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

- Molecule 51 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 52 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A1	277	Total	C	N	O	S	0	0
			2245	1424	382	428	11		

- Molecule 53 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	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 54 is a protein called Small ribosomal subunit protein mS38.

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

- Molecule 55 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	A4	533	Total	C	N	O	S	0	0
			4329	2780	730	793	26		

- Molecule 56 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Ax	65	Total	C	N	O	P	0	0
			1378	617	242	454	65		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Az	8	Total	C	N	O	P	0	0
			167	75	25	59	8		

- Molecule 58 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 59 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	1	53	Total	C	N	O	S	0	0
			440	281	84	73	2		

- Molecule 60 is a protein called Large ribosomal subunit protein bL34m.

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

- Molecule 61 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 62 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 63 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 64 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 65 is a protein called Large ribosomal subunit protein mL39.



Mol	Chain	Residues	Atoms					AltConf	Trace
65	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 66 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	8	140	Total	C	N	O	S	0	0
			1184	755	208	219	2		

- Molecule 67 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 68 is a protein called Large ribosomal subunit protein mL42.

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

- Molecule 69 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	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 70 is a protein called Large ribosomal subunit protein mL44.

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

- Molecule 71 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	d	241	Total	C	N	O	S	0	0
			1985	1273	340	359	13		

- Molecule 72 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	e	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 73 is a protein called Large ribosomal subunit protein mL48.

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

- Molecule 74 is a protein called Large ribosomal subunit protein mL49.

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

- Molecule 75 is a protein called Large ribosomal subunit protein mL50.

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

- Molecule 76 is a protein called Large ribosomal subunit protein mL51.

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

- Molecule 77 is a protein called Large ribosomal subunit protein mL52.

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

- Molecule 78 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	k	95	Total	C	N	O	S	0	0
			738	459	142	132	5		

- Molecule 79 is a protein called Large ribosomal subunit protein mL54.

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

- Molecule 80 is a protein called Large ribosomal subunit protein mL55.

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

- Molecule 81 is a protein called Large ribosomal subunit protein mL63.

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

- Molecule 82 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	p	143	Total	C	N	O	S	0	0
			1179	735	222	218	4		

- Molecule 83 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	q	133	Total	C	N	O	S	0	0
			1120	697	220	198	5		

- Molecule 84 is a protein called Large ribosomal subunit protein mL66.

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

- Molecule 85 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	s	383	Total	C	N	O	S	0	0
			3134	2010	556	554	14		

- Molecule 86 is a protein called Large ribosomal subunit protein bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	t	11	Total	C	N	O	0	0
			72	44	12	16		

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

Mol	Chain	Residues	Atoms		AltConf
87	A	138	Total	Mg	0
			138	138	
87	D	2	Total	Mg	0
			2	2	
87	E	1	Total	Mg	0
			1	1	
87	AA	63	Total	Mg	0
			63	63	
87	AB	1	Total	Mg	0
			1	1	
87	AX	1	Total	Mg	0
			1	1	
87	A3	1	Total	Mg	0
			1	1	
87	g	1	Total	Mg	0
			1	1	

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

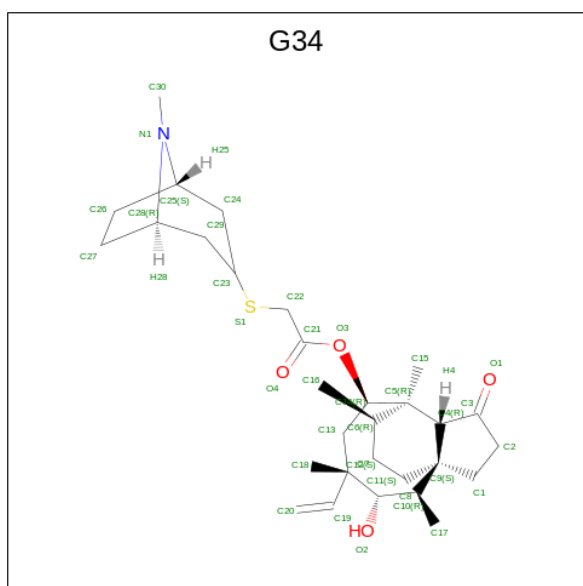
Mol	Chain	Residues	Atoms		AltConf
88	A	29	Total	K	0
			29	29	
88	D	1	Total	K	0
			1	1	
88	M	1	Total	K	0
			1	1	
88	W	1	Total	K	0
			1	1	
88	AA	18	Total	K	0
			18	18	

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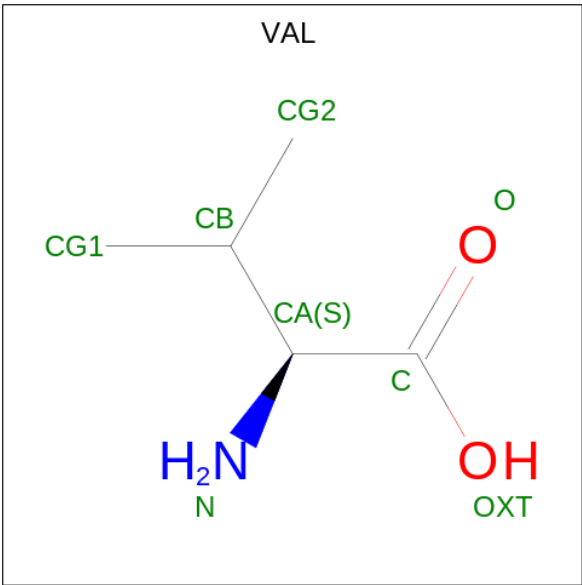
Mol	Chain	Residues	Atoms		AltConf
88	6	1	Total	K	0
			1	1	
88	i	1	Total	K	0
			1	1	
88	o	1	Total	K	0
			1	1	

- Molecule 89 is Retapamulin (CCD ID: G34) (formula:  $C_{30}H_{47}NO_4S$ ) (labeled as "Ligand of Interest" by depositor).



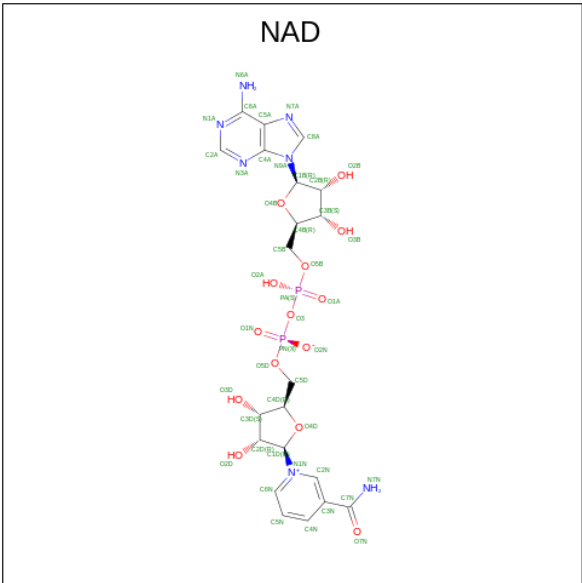
Mol	Chain	Residues	Atoms					AltConf
89	A	1	Total	C	N	O	S	0
			36	30	1	4	1	

- Molecule 90 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).



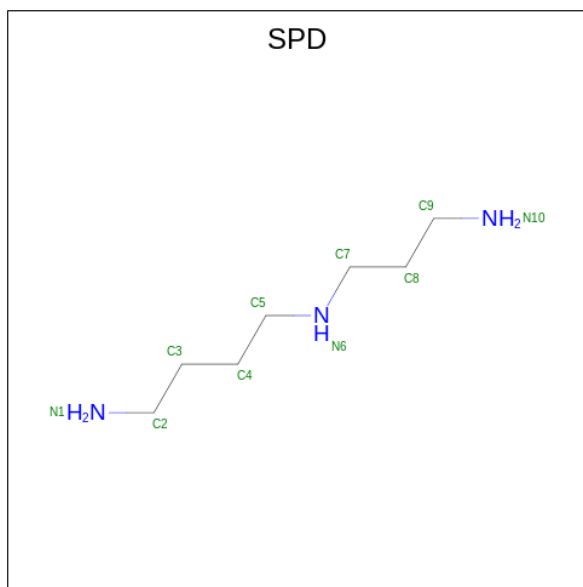
Mol	Chain	Residues	Atoms				AltConf
90	B	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 91 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).

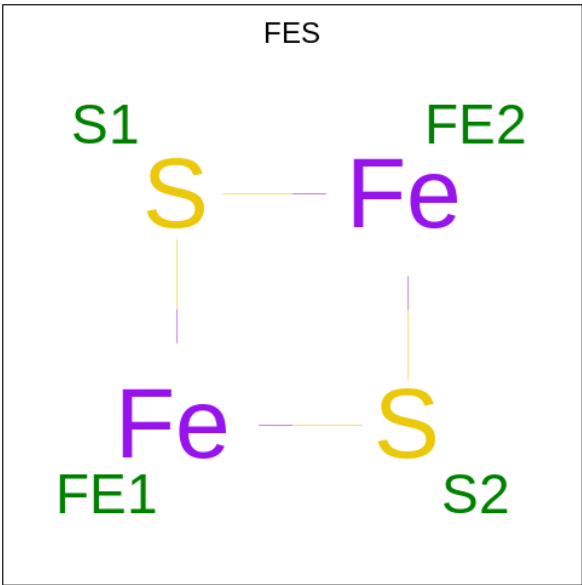


Mol	Chain	Residues	Atoms			AltConf
92	AA	1	Total	C	N	0
			10	7	3	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

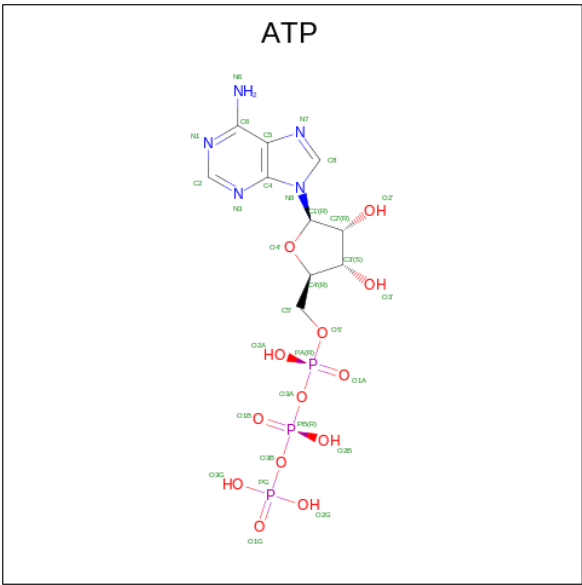
Mol	Chain	Residues	Atoms		AltConf
93	AO	1	Total	Zn	0
			1	1	
93	0	1	Total	Zn	0
			1	1	
93	4	1	Total	Zn	0
			1	1	

- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	
94	r	1	Total	Fe	S	0
			4	2	2	

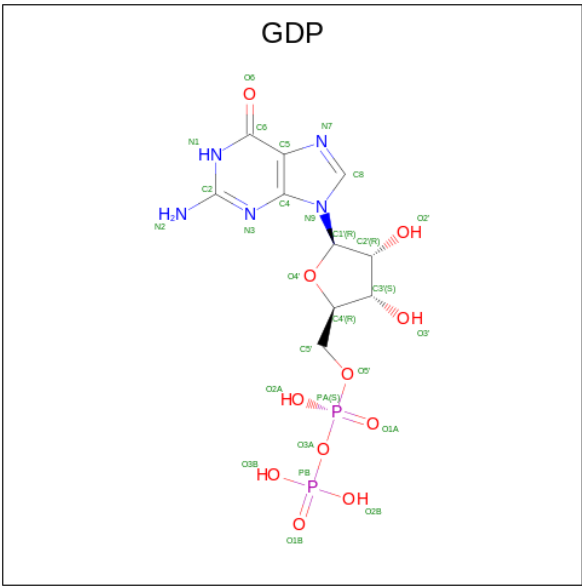
- Molecule 95 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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



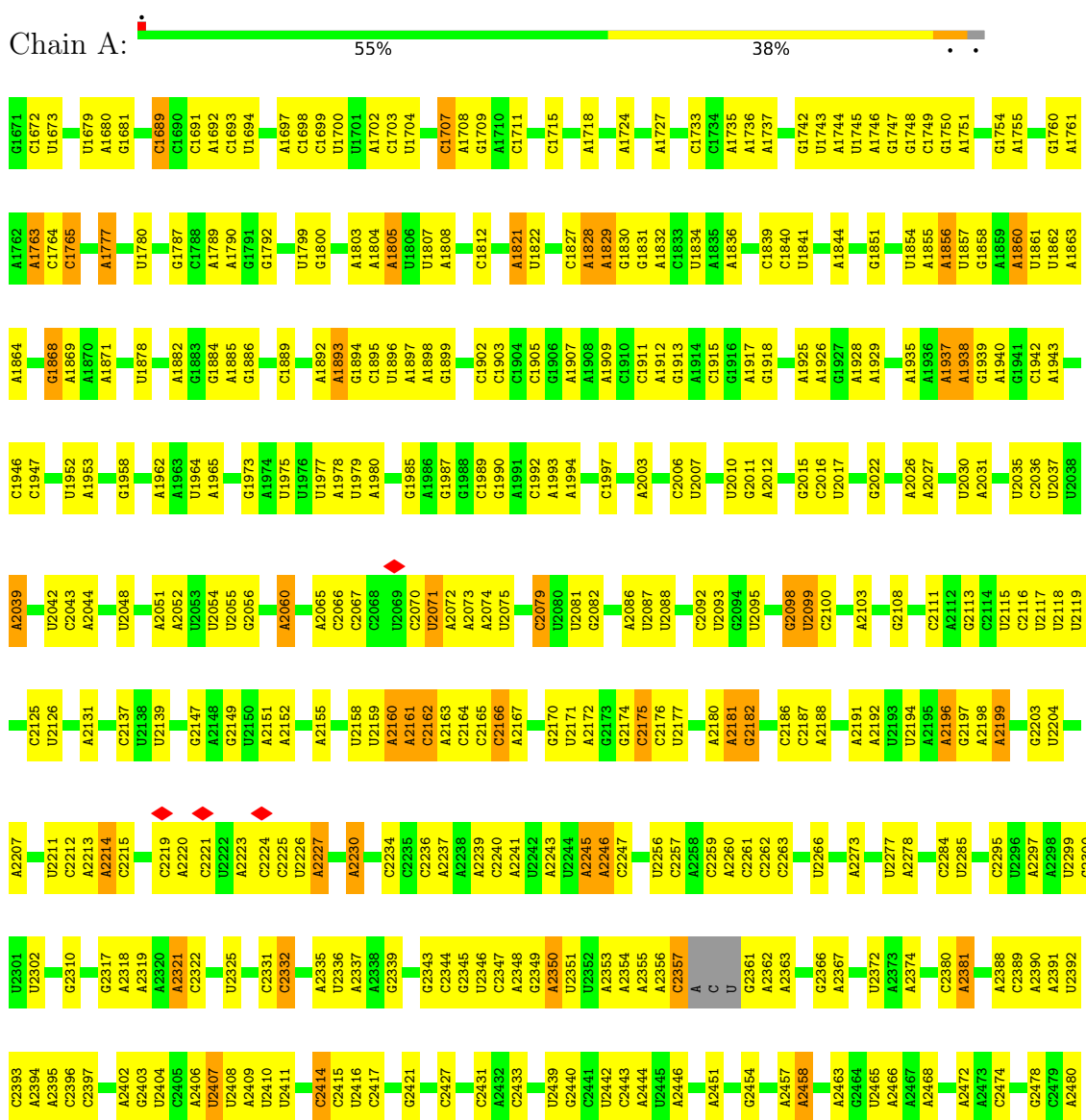
- Molecule 96 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



### 3 Residue-property plots

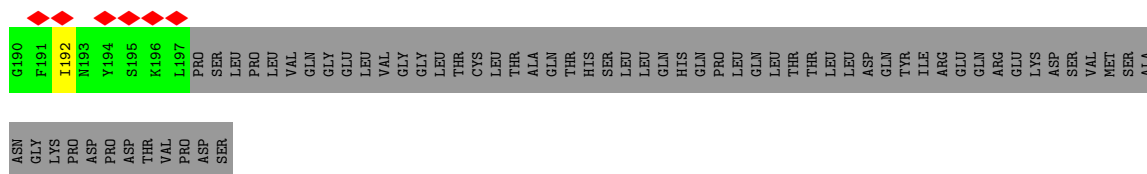
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

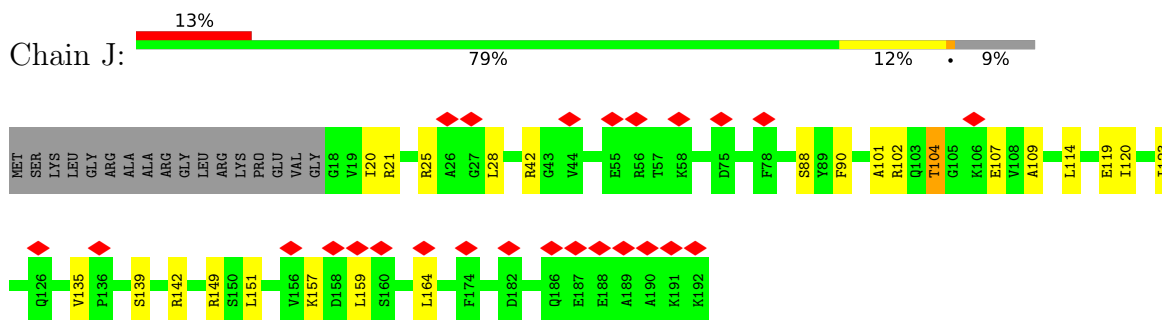




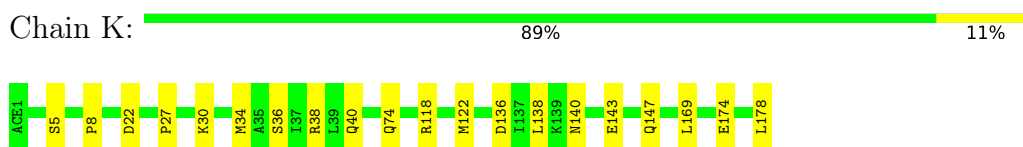




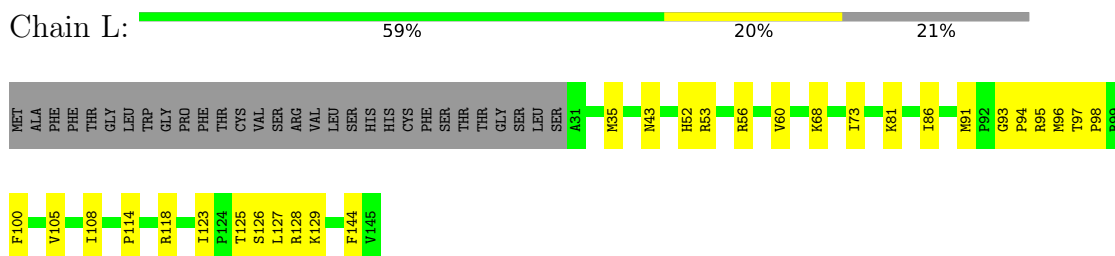
- Molecule 8: Large ribosomal subunit protein uL11m



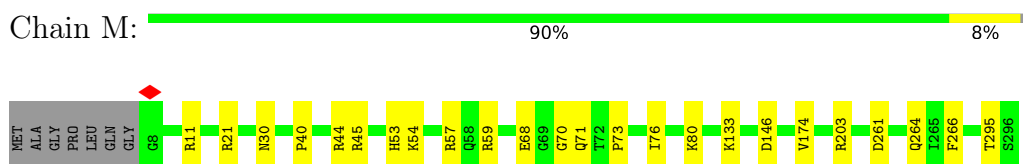
- Molecule 9: Large ribosomal subunit protein uL13m



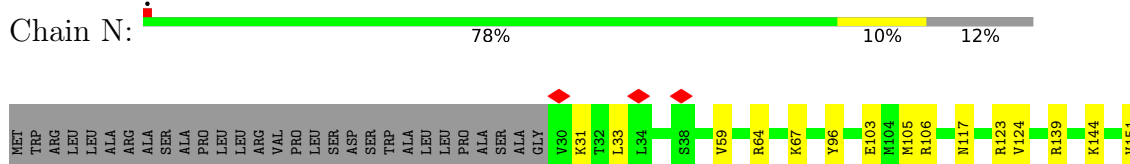
- Molecule 10: Large ribosomal subunit protein uL14m



- Molecule 11: Large ribosomal subunit protein uL15m

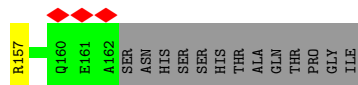


- Molecule 12: Large ribosomal subunit protein uL16m

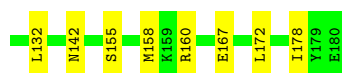
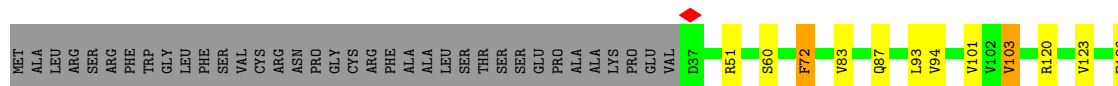




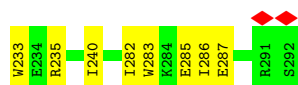
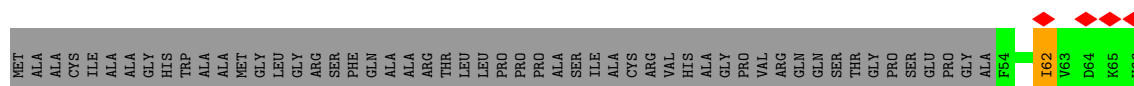
- Molecule 13: Large ribosomal subunit protein bL17m



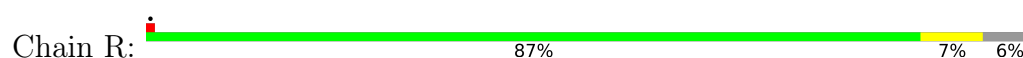
- Molecule 14: Large ribosomal subunit protein uL18m



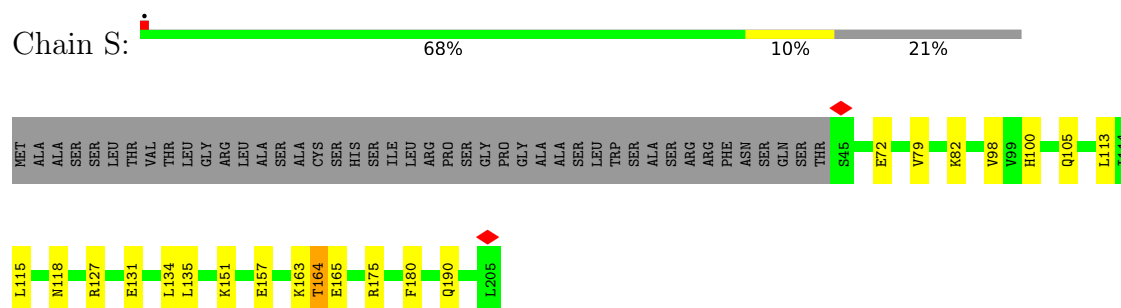
- Molecule 15: Large ribosomal subunit protein bL19m



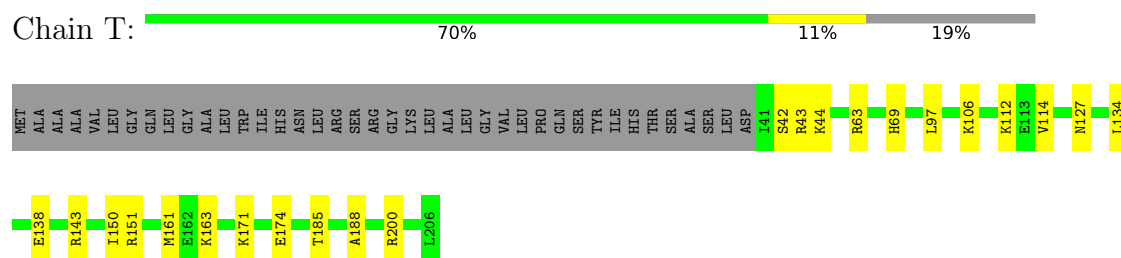
- Molecule 16: Large ribosomal subunit protein bL20m



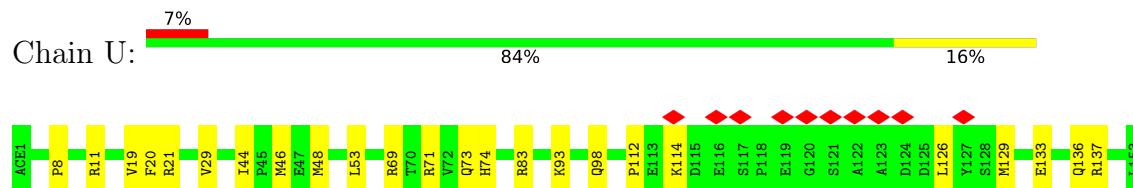
- Molecule 17: Large ribosomal subunit protein bL21m



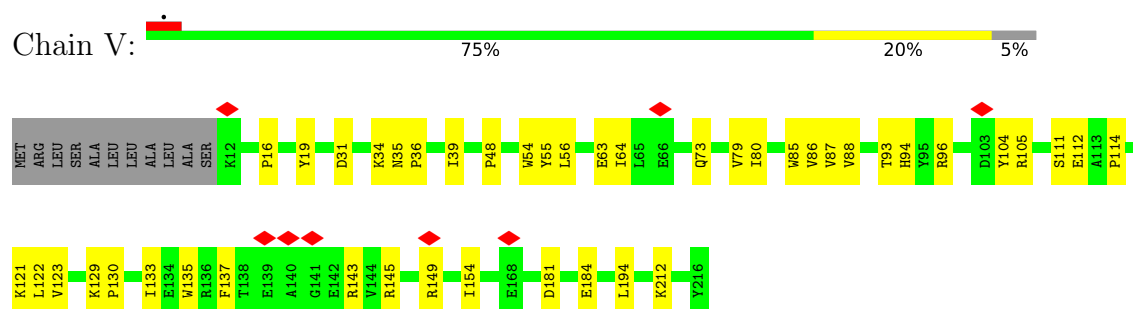
- Molecule 18: Large ribosomal subunit protein uL22m



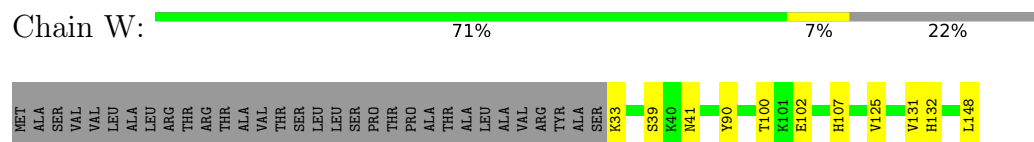
- Molecule 19: Large ribosomal subunit protein uL23m



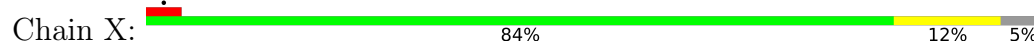
- Molecule 20: Large ribosomal subunit protein uL24m



- Molecule 21: Large ribosomal subunit protein bL27m

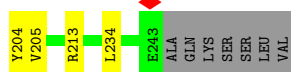


- Molecule 22: Large ribosomal subunit protein bL28m

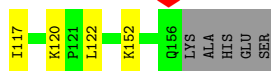




- Chain Y:  58% 14% 28%



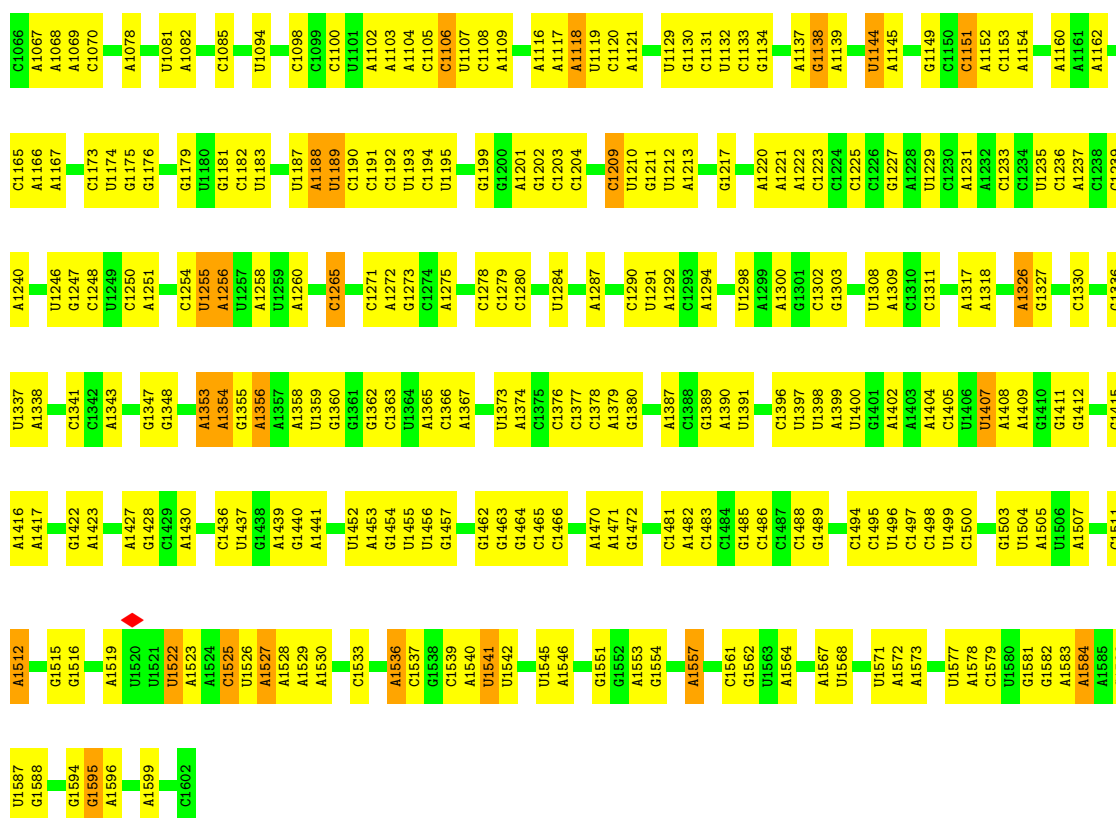
- Chain Z:  64% 11% 24%



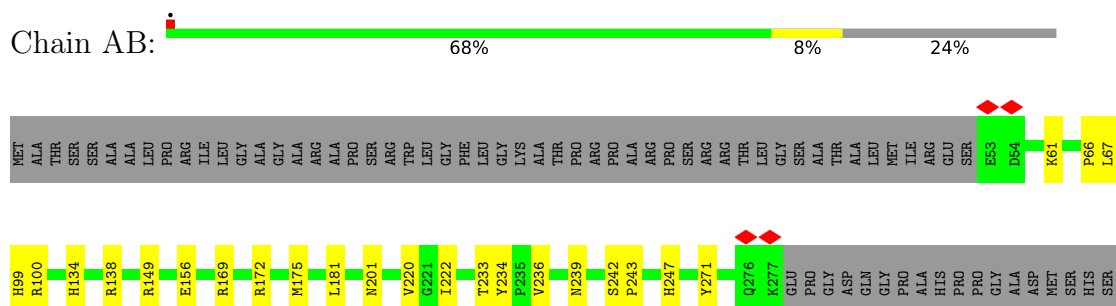
- Chain AA:  56% 40% .



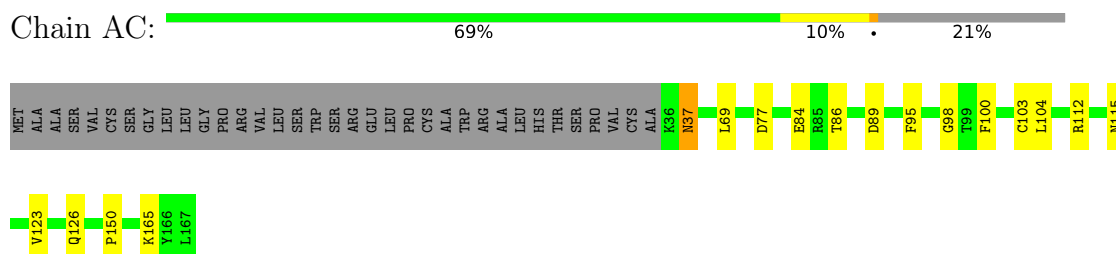




- Molecule 26: Small ribosomal subunit protein uS2m



- Molecule 27: Small ribosomal subunit protein uS3m



- Molecule 28: Small ribosomal subunit protein uS5m





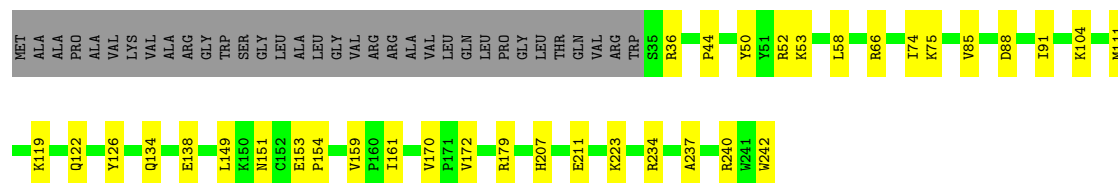
- Molecule 29: Small ribosomal subunit protein bS6m

Chain AE: 85% 13% .



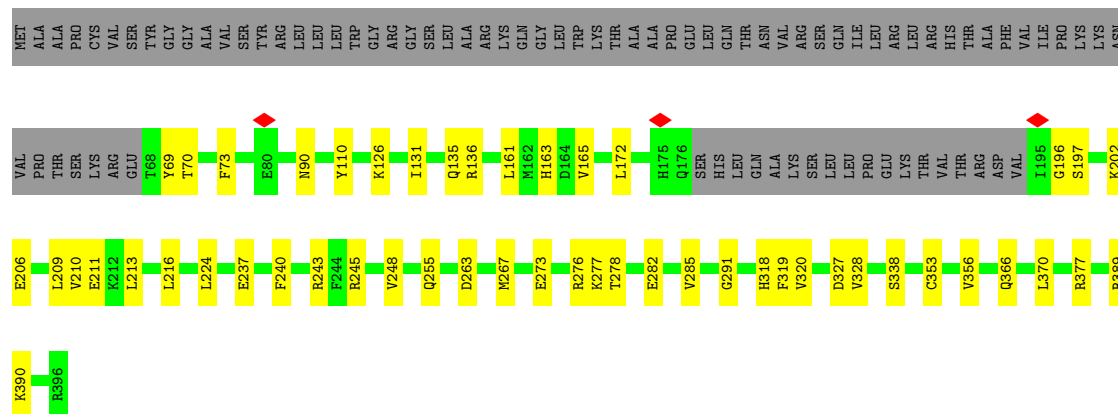
- Molecule 30: Small ribosomal subunit protein uS7m

Chain AF: 71% 14% 14%



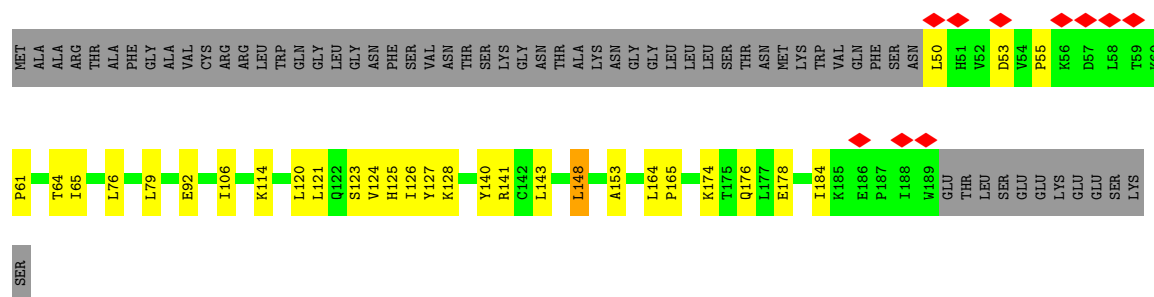
- Molecule 31: Small ribosomal subunit protein uS9m

Chain AG: 66% 13% 21%

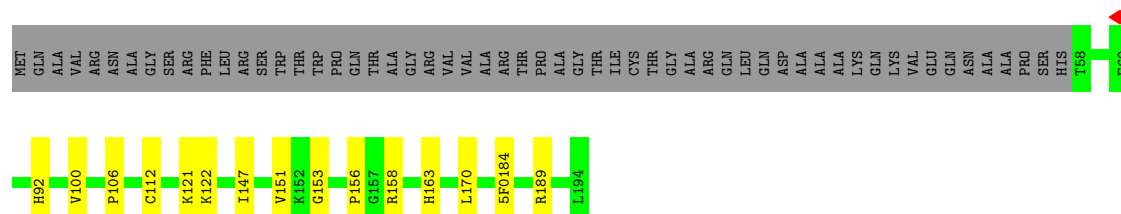


- Molecule 32: Small ribosomal subunit protein uS10m

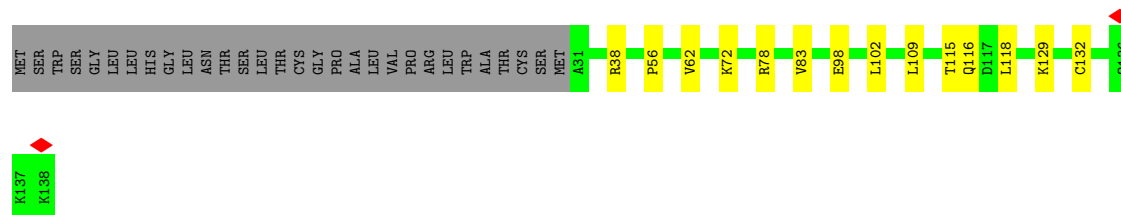
Chain AH: 5% 55% 14% 30%



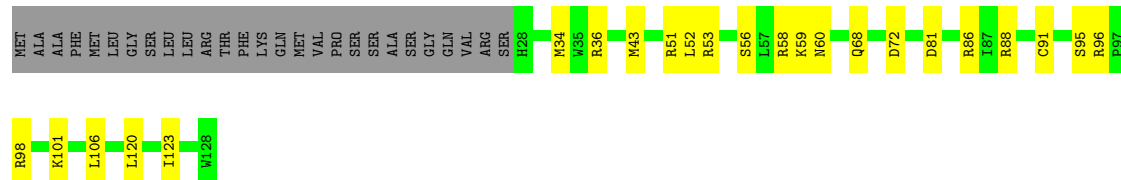
- Molecule 33: Small ribosomal subunit protein uS11m



- Molecule 34: Small ribosomal subunit protein uS12m



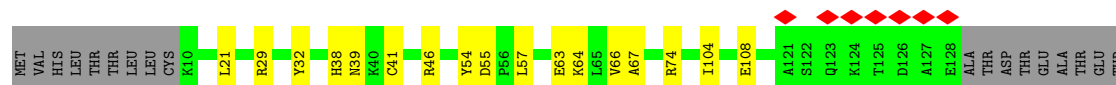
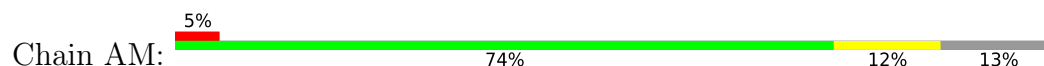
- Molecule 35: Small ribosomal subunit protein uS14m



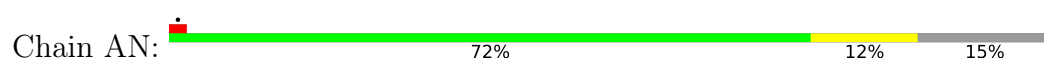
- Molecule 36: Small ribosomal subunit protein uS15m



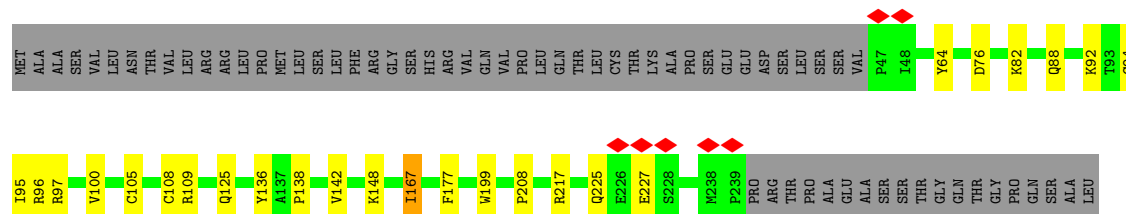
- Molecule 37: Small ribosomal subunit protein bS16m



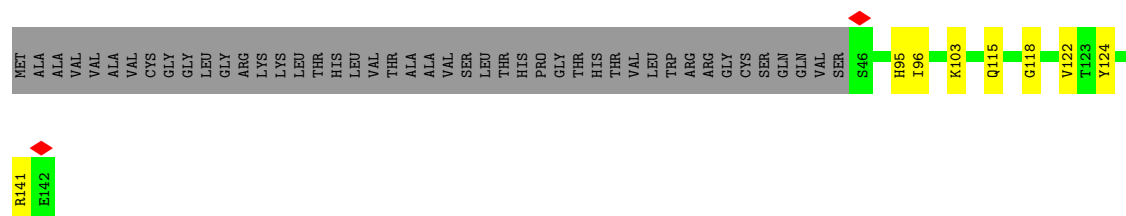
- Molecule 38: Small ribosomal subunit protein uS17m



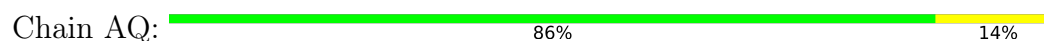
- Molecule 39: Small ribosomal subunit protein mS40



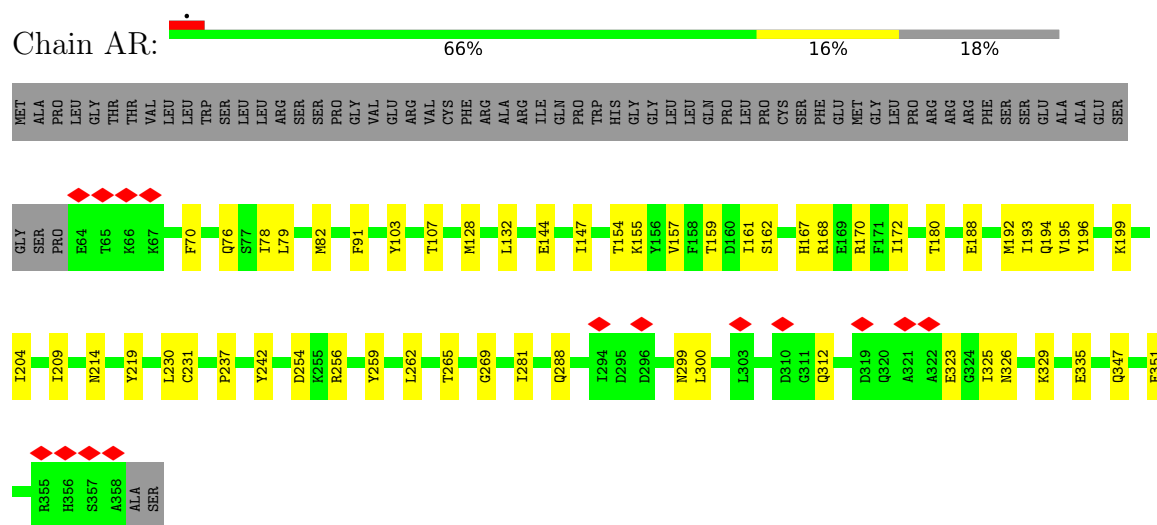
- Molecule 40: Small ribosomal subunit protein bS18m



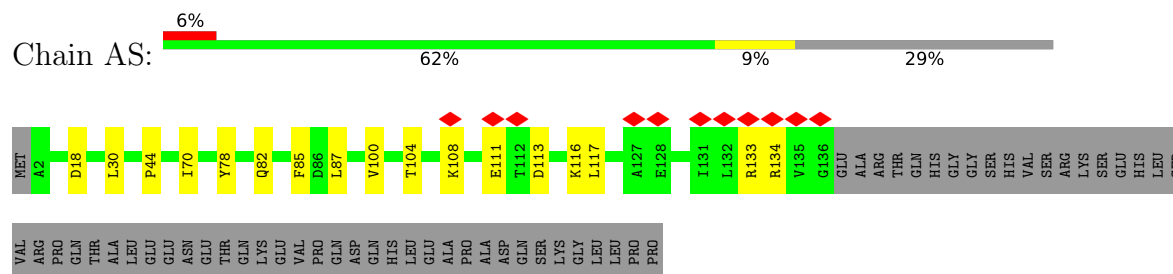
- Molecule 41: MRPS21 isoform 1



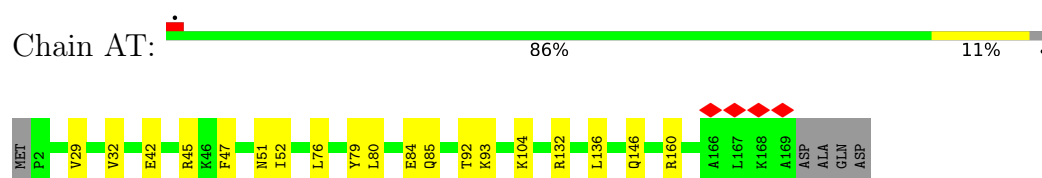
- Molecule 42: Small ribosomal subunit protein mS22



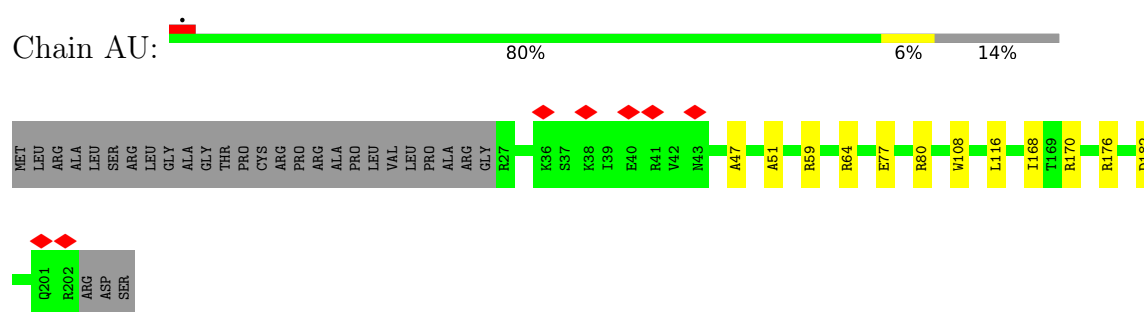
- Molecule 43: Small ribosomal subunit protein mS23



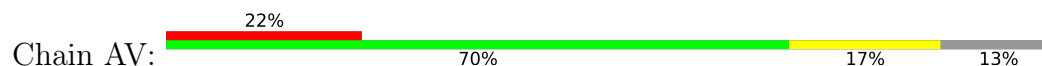
- Molecule 44: Small ribosomal subunit protein mS25

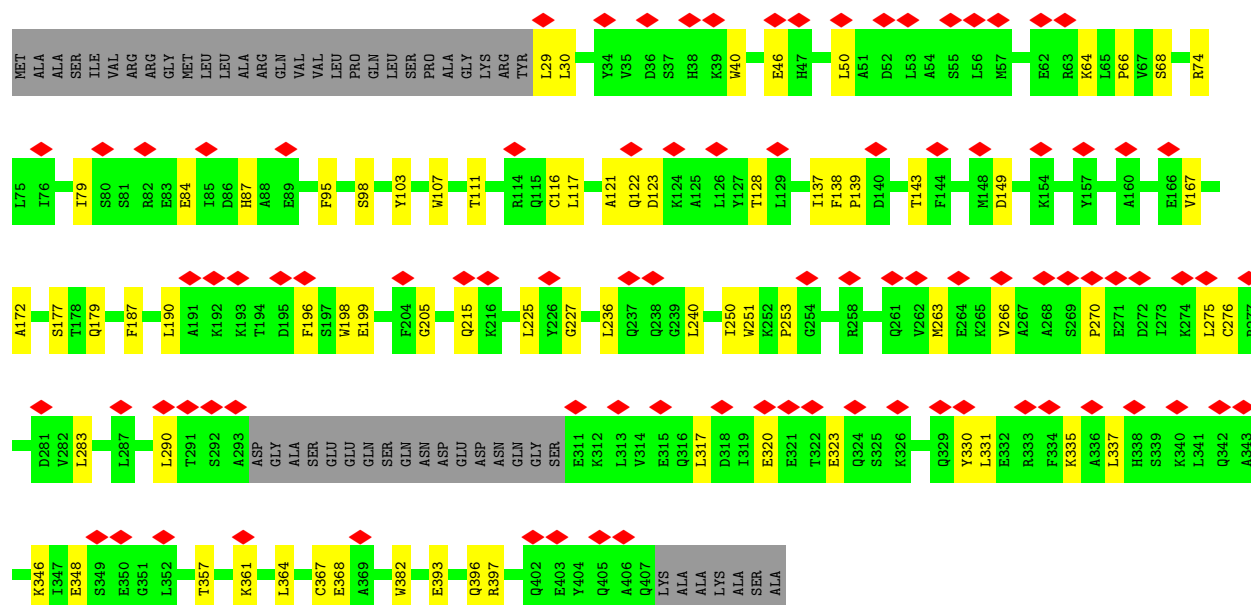


- Molecule 45: Small ribosomal subunit protein mS26



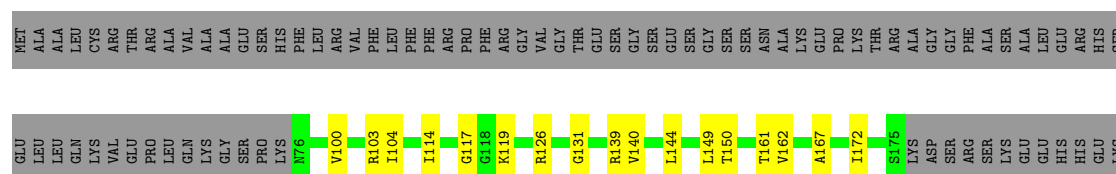
- Molecule 46: Small ribosomal subunit protein mS27





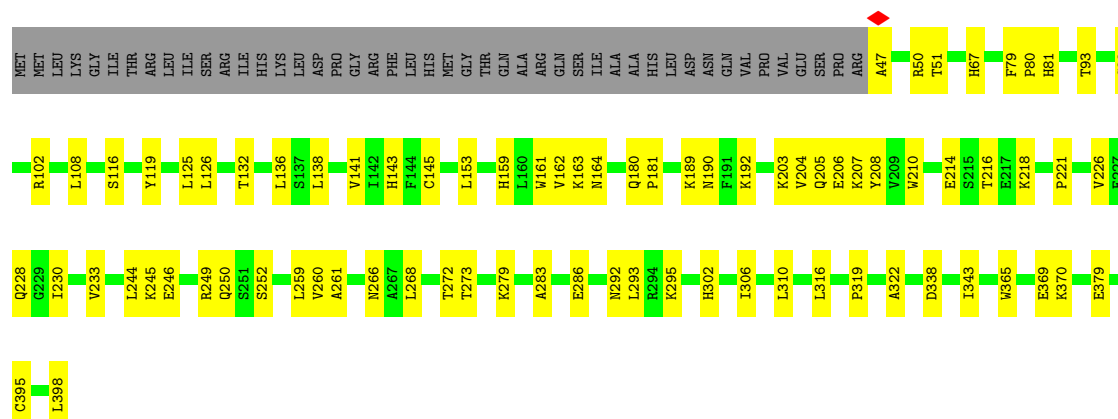
• Molecule 47: Small ribosomal subunit protein bS1m

Chain AW: 44% 9% 47%



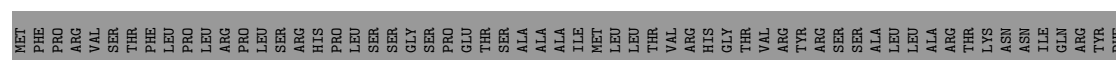
• Molecule 48: Small ribosomal subunit protein mS29

Chain AX: 68% 20% 12%

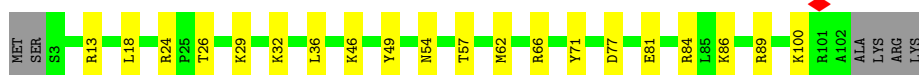
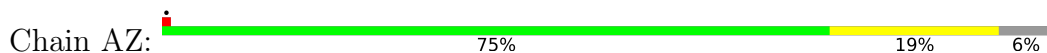


• Molecule 49: Small ribosomal subunit protein mS31

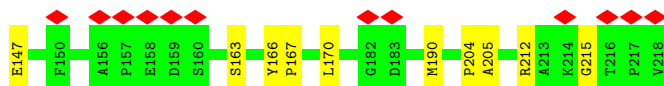
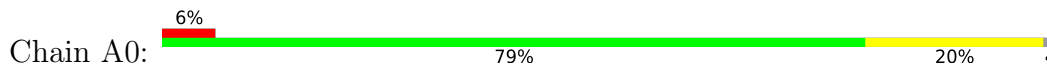
Chain AY: 29% 70%



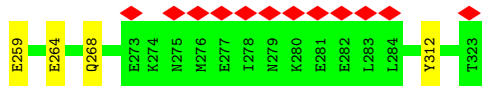
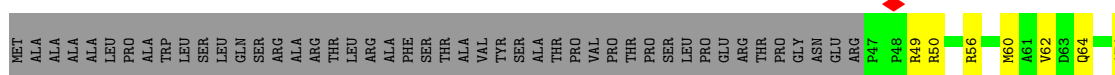
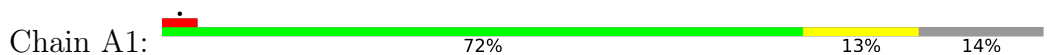
- Molecule 50: Small ribosomal subunit protein mS33



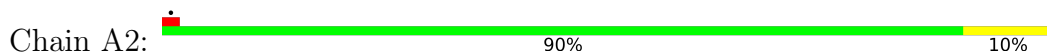
- Molecule 51: Small ribosomal subunit protein mS34



- Molecule 52: Small ribosomal subunit protein mS35

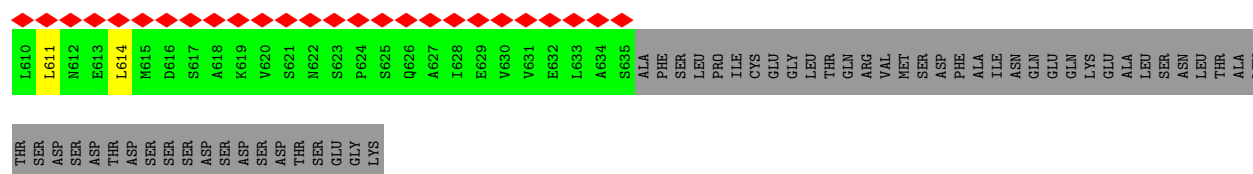


- Molecule 53: Small ribosomal subunit protein mS37



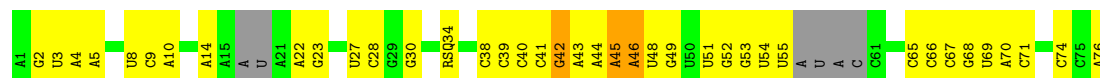






- Molecule 56: P/P-tRNA

Chain Ax: 37% 51% 8%



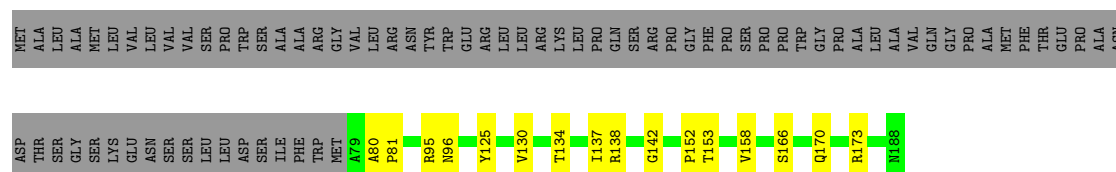
- Molecule 57: mRNA

Chain Az: 75% 25%



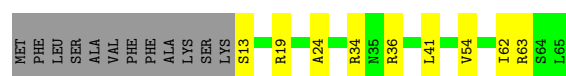
- Molecule 58: Large ribosomal subunit protein bL32m

Chain 0: 50% 9% 41%



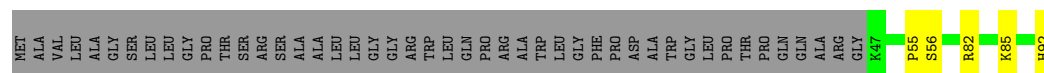
- Molecule 59: Large ribosomal subunit protein bL33m

Chain 1: 68% 14% 18%



- Molecule 60: Large ribosomal subunit protein bL34m

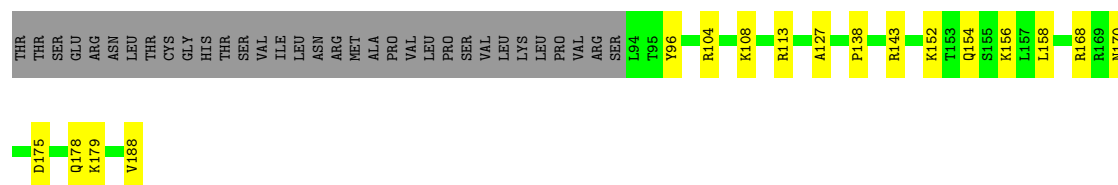
Chain 2: 45% 5% 50%



- Molecule 61: Large ribosomal subunit protein bL35m

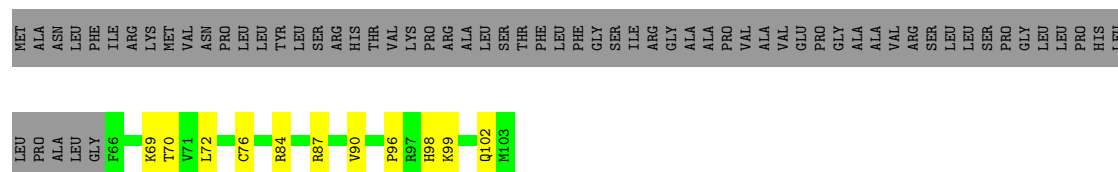
Chain 3: 41% 9% 49%





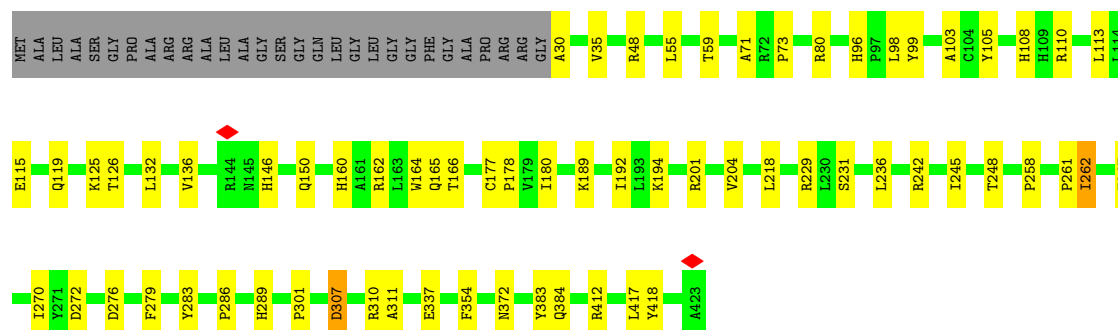
- Molecule 62: Large ribosomal subunit protein bL36m

Chain 4: 26% 11% 63%



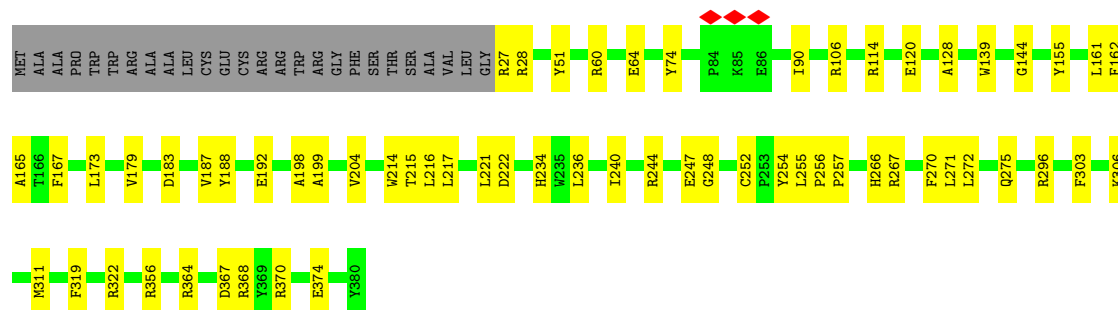
- Molecule 63: Large ribosomal subunit protein mL37

Chain 5: 77% 15% 7%



- Molecule 64: Large ribosomal subunit protein mL38

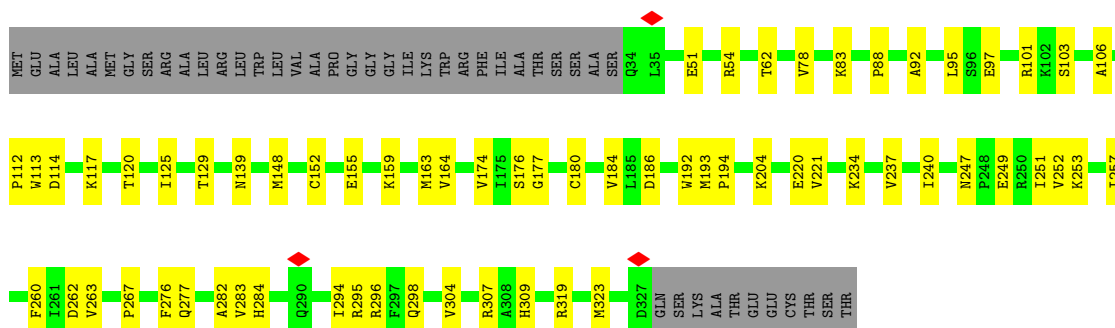
Chain 6: 77% 16% 7%



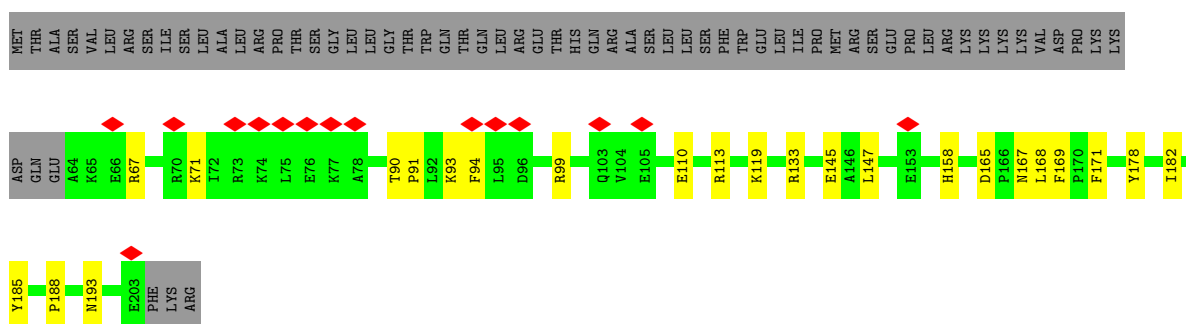
- Molecule 65: Large ribosomal subunit protein mL39

Chain 7: 68% 19% 13%

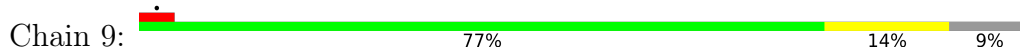




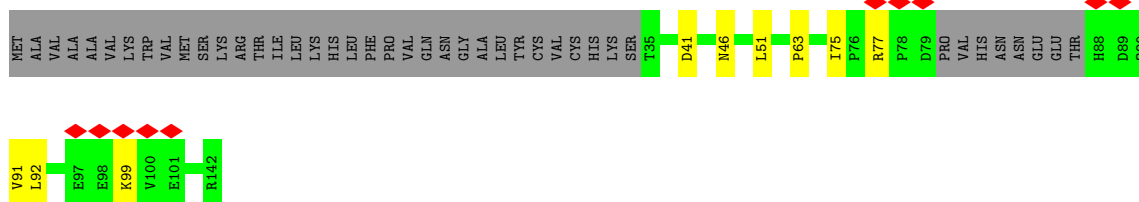
• Molecule 66: Large ribosomal subunit protein mL40



• Molecule 67: Large ribosomal subunit protein mL41



• Molecule 68: Large ribosomal subunit protein mL42



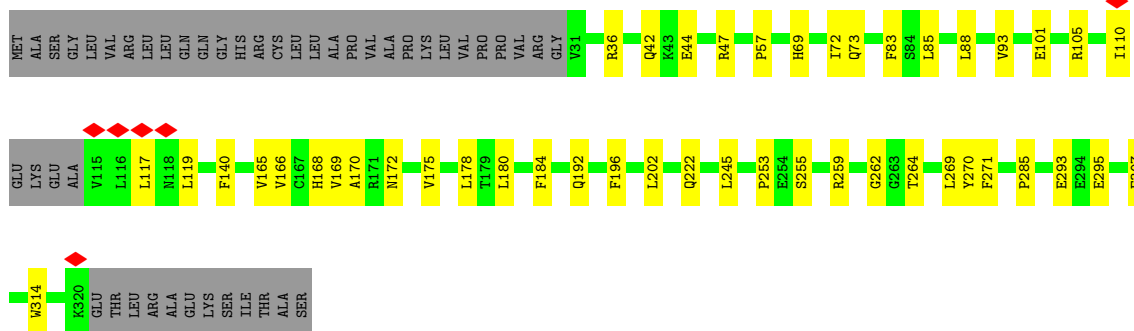
• Molecule 69: Large ribosomal subunit protein mL43



PRO ASP PRO PRO ASP PRO ASP PRO THR VAL ASP PRO ILE SER SER SER THR THR VAL THR THR VAL CYS SER ALA

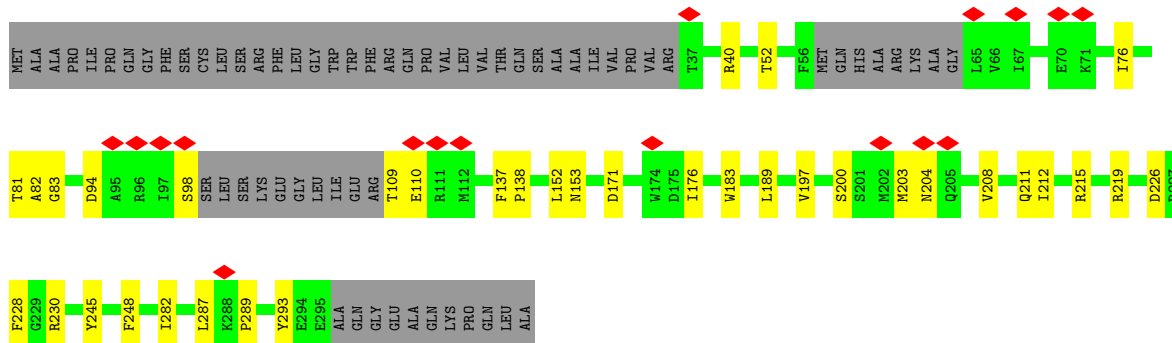
• Molecule 70: Large ribosomal subunit protein mL44

Chain c:



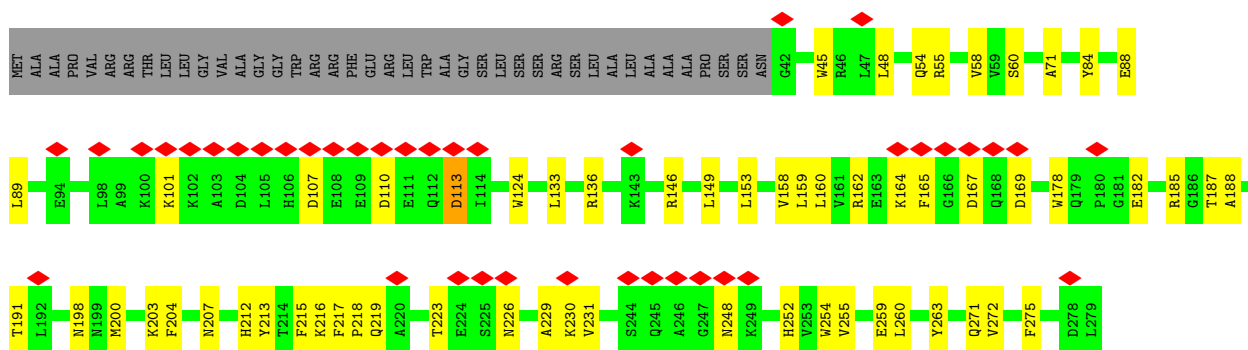
• Molecule 71: Large ribosomal subunit protein mL45

Chain d:



• Molecule 72: Large ribosomal subunit protein mL46

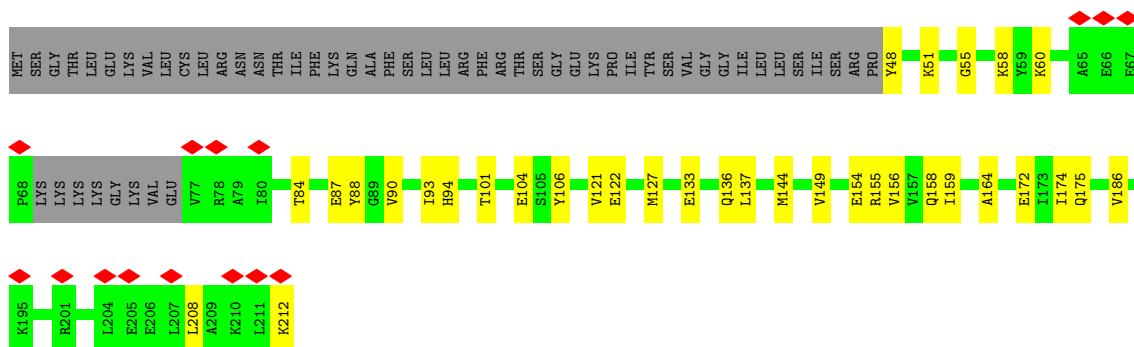
Chain e:



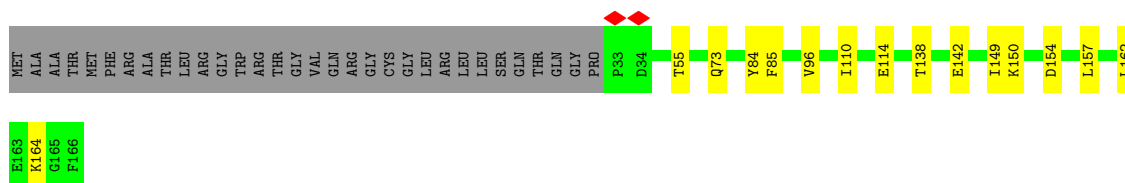
• Molecule 73: Large ribosomal subunit protein mL48

Chain f:

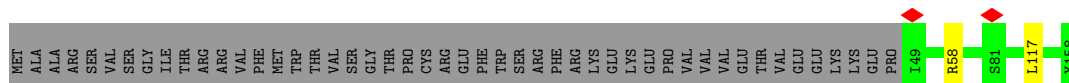




- Molecule 74: Large ribosomal subunit protein mL49



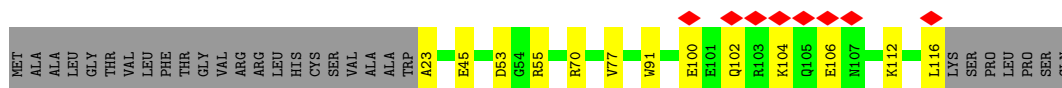
- Molecule 75: Large ribosomal subunit protein mL50



- Molecule 76: Large ribosomal subunit protein mL51



- Molecule 77: Large ribosomal subunit protein mL52



- Molecule 78: Large ribosomal subunit protein mL53

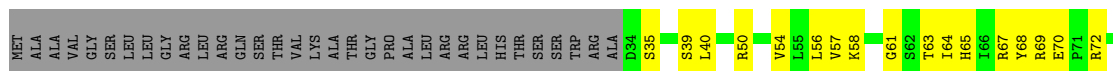




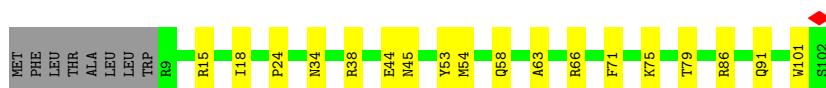
- Molecule 79: Large ribosomal subunit protein mL54



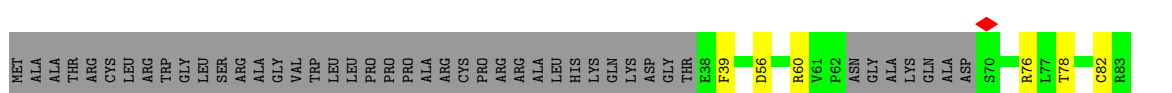
- Molecule 80: Large ribosomal subunit protein mL55



- Molecule 81: Large ribosomal subunit protein mL63

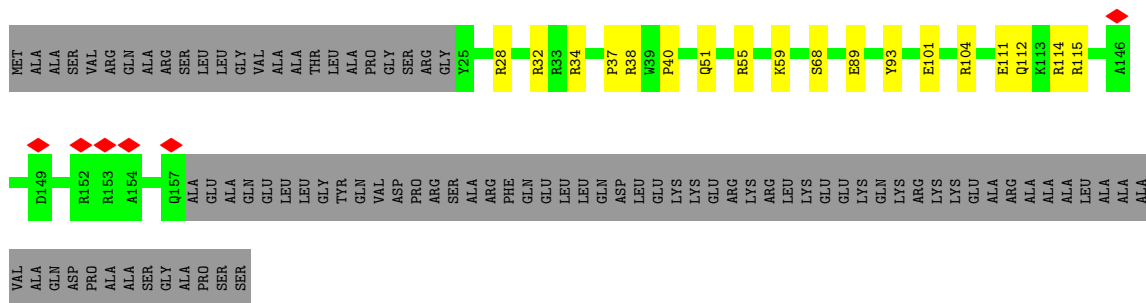


- Molecule 82: Large ribosomal subunit protein mL62

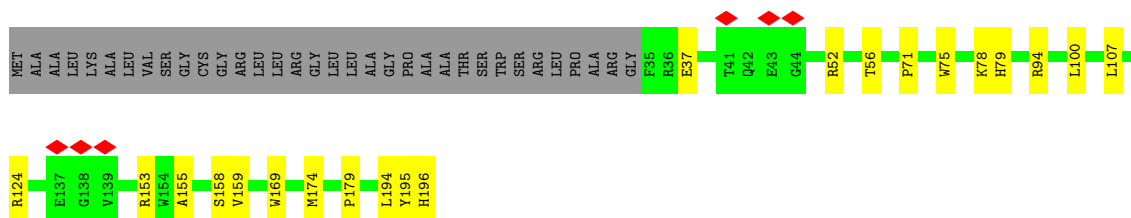


- Molecule 83: Large ribosomal subunit protein mL64

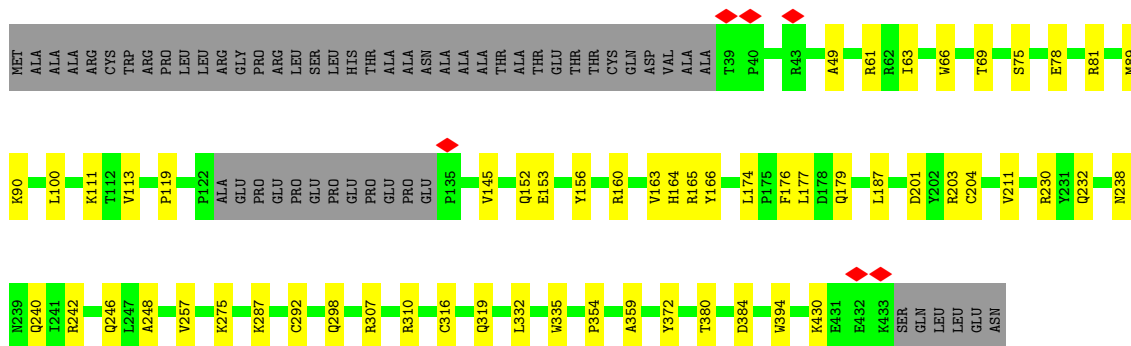




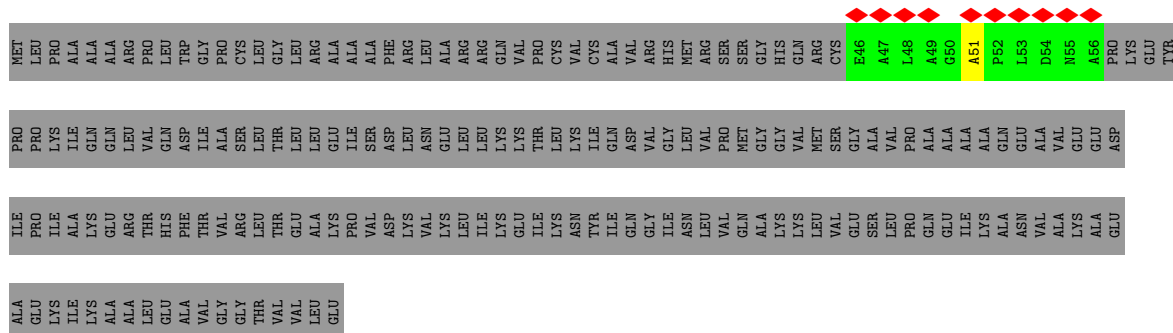
- Molecule 84: Large ribosomal subunit protein mL66



- Molecule 85: Large ribosomal subunit protein mL65



- Molecule 86: Large ribosomal subunit protein bL12m



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114776	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.321	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, GDP, ZN, 1MA, K, NAD, 5F0, G34, ACE, B8T, OMU, PSU, 5MU, RSQ, FES, 2MG, 5MC, OMG, MG, MA6, ATP

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	0.09	0/36048	0.21	0/56112
2	B	0.08	0/1627	0.20	0/2527
3	D	0.09	0/1896	0.24	0/2549
4	E	0.08	0/2475	0.22	0/3355
5	F	0.08	0/2090	0.23	0/2842
6	H	0.07	0/837	0.19	0/1124
7	I	0.08	0/1392	0.23	0/1880
8	J	0.08	0/1348	0.19	0/1813
9	K	0.09	0/1497	0.23	0/2031
10	L	0.08	0/905	0.23	0/1218
11	M	0.09	0/2368	0.24	0/3195
12	N	0.09	0/1833	0.24	0/2468
13	O	0.09	0/1283	0.22	0/1727
14	P	0.09	0/1199	0.24	0/1623
15	Q	0.09	0/2039	0.23	0/2750
16	R	0.09	0/1175	0.19	0/1572
17	S	0.09	0/1320	0.25	0/1789
18	T	0.09	0/1403	0.23	0/1886
19	U	0.11	0/1280	0.25	0/1732
20	V	0.07	0/1721	0.22	0/2333
21	W	0.08	0/926	0.21	0/1244
22	X	0.08	0/2099	0.19	0/2837
23	Y	0.08	0/1593	0.18	0/2136
24	Z	0.08	0/1021	0.25	0/1378
25	AA	0.08	0/22537	0.20	0/35085
26	AB	0.07	0/1871	0.22	0/2531
27	AC	0.07	0/1113	0.20	0/1505
28	AD	0.07	0/2783	0.19	0/3724
29	AE	0.07	0/989	0.19	0/1335
30	AF	0.07	0/1767	0.19	0/2373
31	AG	0.06	0/2616	0.18	0/3505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	AH	0.08	0/1178	0.23	0/1598
33	AI	0.08	0/1030	0.23	0/1386
34	AJ	0.07	0/855	0.21	0/1148
35	AK	0.06	0/880	0.18	0/1182
36	AL	0.06	0/1477	0.17	0/1974
37	AM	0.06	0/963	0.19	0/1295
38	AN	0.07	0/886	0.20	0/1199
39	AO	0.06	0/1648	0.19	0/2243
40	AP	0.07	0/798	0.18	0/1070
41	AQ	0.12	0/754	0.20	0/1003
42	AR	0.06	0/2456	0.18	0/3317
43	AS	0.06	0/1138	0.18	0/1533
44	AT	0.07	0/1402	0.20	0/1883
45	AU	0.05	0/1510	0.16	0/2025
46	AV	0.06	0/3030	0.17	0/4093
47	AW	0.08	0/801	0.20	0/1079
48	AX	0.06	0/2921	0.19	0/3954
49	AY	0.07	0/1046	0.18	0/1410
50	AZ	0.05	0/857	0.16	0/1141
51	A0	0.07	0/1834	0.20	0/2484
52	A1	0.06	0/2293	0.19	0/3102
53	A2	0.12	0/947	0.22	0/1266
54	A3	0.07	0/636	0.19	0/839
55	A4	0.07	0/4427	0.19	0/5987
56	Ax	0.08	0/1511	0.21	0/2341
57	Az	0.06	0/185	0.16	0/285
58	0	0.08	0/913	0.18	0/1224
59	1	0.07	0/445	0.20	0/591
60	2	0.07	0/383	0.18	0/507
61	3	0.08	0/853	0.21	0/1136
62	4	0.07	0/350	0.18	0/461
63	5	0.09	0/3305	0.23	0/4502
64	6	0.07	0/3043	0.21	0/4140
65	7	0.08	0/2447	0.22	0/3310
66	8	0.08	0/1209	0.20	0/1628
67	9	0.07	0/1025	0.20	0/1379
68	a	0.08	0/866	0.22	0/1174
69	b	0.07	0/1219	0.23	0/1651
70	c	0.08	0/2347	0.20	0/3171
71	d	0.07	0/2039	0.21	0/2759
72	e	0.07	0/1970	0.22	0/2658
73	f	0.07	0/1273	0.21	0/1716
74	g	0.08	0/1151	0.21	0/1569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	h	0.07	0/918	0.18	0/1249
76	i	0.08	0/850	0.20	0/1135
77	j	0.08	0/760	0.18	0/1023
78	k	0.07	0/749	0.18	0/1010
79	l	0.06	0/707	0.19	0/960
80	m	0.06	0/805	0.19	0/1081
81	o	0.08	0/819	0.22	0/1097
82	p	0.07	0/1197	0.18	0/1606
83	q	0.09	0/1151	0.19	0/1556
84	r	0.07	0/1362	0.20	0/1846
85	s	0.09	0/3217	0.22	0/4369
86	t	0.04	0/72	0.17	0/98
All	All	0.08	0/179959	0.21	0/255622

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
14	P	0	1
66	8	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	8	169	PHE	Peptide
14	P	72	PHE	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	32331	0	16416	412	0
2	B	1524	0	779	21	0
3	D	1859	0	1920	30	0
4	E	2406	0	2415	27	0
5	F	2031	0	2065	24	0
6	H	823	0	873	12	0
7	I	1362	0	1442	29	0
8	J	1330	0	1407	23	0
9	K	1455	0	1452	16	0
10	L	890	0	941	18	0
11	M	2314	0	2384	18	0
12	N	1786	0	1817	19	0
13	O	1259	0	1294	20	0
14	P	1173	0	1165	16	0
15	Q	1990	0	2031	28	0
16	R	1154	0	1214	11	0
17	S	1293	0	1365	16	0
18	T	1369	0	1410	17	0
19	U	1251	0	1232	20	0
20	V	1676	0	1687	35	0
21	W	904	0	935	9	0
22	X	2044	0	2060	21	0
23	Y	1556	0	1597	27	0
24	Z	996	0	1044	15	0
25	AA	20260	0	10285	269	0
26	AB	1828	0	1815	18	0
27	AC	1083	0	1088	14	0
28	AD	2731	0	2804	35	0
29	AE	972	0	1000	13	0
30	AF	1725	0	1769	24	0
31	AG	2561	0	2545	34	0
32	AH	1152	0	1183	24	0
33	AI	1020	0	1053	9	0
34	AJ	839	0	887	11	0
35	AK	862	0	885	18	0
36	AL	1453	0	1540	12	0
37	AM	942	0	965	14	0
38	AN	868	0	928	11	0
39	AO	1592	0	1557	19	0
40	AP	781	0	806	7	0
41	AQ	744	0	758	11	0
42	AR	2409	0	2428	36	0
43	AS	1111	0	1115	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	AT	1371	0	1393	12	0
45	AU	1488	0	1499	11	0
46	AV	2969	0	2961	45	0
47	AW	789	0	802	11	0
48	AX	2849	0	2844	54	0
49	AY	1016	0	962	6	0
50	AZ	839	0	858	16	0
51	A0	1787	0	1796	32	0
52	A1	2245	0	2276	27	0
53	A2	935	0	971	10	0
54	A3	625	0	699	5	0
55	A4	4329	0	4350	59	0
56	Ax	1378	0	703	26	0
57	Az	167	0	83	1	0
58	0	898	0	916	14	0
59	1	440	0	480	5	0
60	2	377	0	406	4	0
61	3	832	0	883	13	0
62	4	342	0	361	7	0
63	5	3210	0	3206	45	0
64	6	2948	0	2841	42	0
65	7	2390	0	2397	40	0
66	8	1184	0	1210	18	0
67	9	997	0	987	17	0
68	a	840	0	810	8	0
69	b	1196	0	1195	16	0
70	c	2299	0	2320	31	0
71	d	1985	0	1976	25	0
72	e	1931	0	1916	42	0
73	f	1252	0	1269	22	0
74	g	1113	0	1097	10	0
75	h	895	0	881	2	0
76	i	828	0	857	14	0
77	j	745	0	746	10	0
78	k	738	0	753	12	0
79	l	688	0	674	14	0
80	m	791	0	796	25	0
81	o	798	0	804	17	0
82	p	1179	0	1203	21	0
83	q	1120	0	1099	12	0
84	r	1322	0	1348	18	0
85	s	3134	0	3121	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	t	72	0	67	1	0
87	A	138	0	0	0	0
87	A3	1	0	0	0	0
87	AA	63	0	0	0	0
87	AB	1	0	0	0	0
87	AX	1	0	0	0	0
87	D	2	0	0	0	0
87	E	1	0	0	0	0
87	g	1	0	0	0	0
88	6	1	0	0	0	0
88	A	29	0	0	0	0
88	AA	18	0	0	0	0
88	D	1	0	0	0	0
88	M	1	0	0	0	0
88	W	1	0	0	0	0
88	i	1	0	0	0	0
88	o	1	0	0	0	0
89	A	36	0	47	3	0
90	B	7	0	8	2	0
91	AA	44	0	26	1	0
92	AA	10	0	19	0	0
93	0	1	0	0	0	0
93	4	1	0	0	0	0
93	AO	1	0	0	0	0
94	AP	4	0	0	0	0
94	AT	4	0	0	0	0
94	r	4	0	0	0	0
95	AX	31	0	12	1	0
96	AX	28	0	12	1	0
All	All	171472	0	145296	1877	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1877 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)
1:A:2485:U:H3	1:A:2650:C:N4	1.52	1.06
1:A:2234:C:HO2'	1:A:2688:C:HO2'	1.30	0.80
64:6:179:VAL:O	64:6:183:ASP:HB2	1.82	0.78
9:K:74:GLN:HE21	84:r:159:VAL:HG21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:p:84:SER:HB3	82:p:98:LYS:HB2	1.65	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%)	227 (96%)	9 (4%)	0	100	100
4	E	303/348 (87%)	299 (99%)	4 (1%)	0	100	100
5	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
6	H	98/267 (37%)	97 (99%)	1 (1%)	0	100	100
7	I	167/261 (64%)	162 (97%)	5 (3%)	0	100	100
8	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
9	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
10	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
11	M	287/296 (97%)	280 (98%)	7 (2%)	0	100	100
12	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
13	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
14	P	142/180 (79%)	136 (96%)	6 (4%)	0	100	100
15	Q	237/292 (81%)	232 (98%)	4 (2%)	1 (0%)	30	66
16	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
18	T	164/206 (80%)	160 (98%)	4 (2%)	0	100	100
19	U	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
20	V	203/216 (94%)	196 (97%)	7 (3%)	0	100	100
21	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	X	242/256 (94%)	236 (98%)	6 (2%)	0	100	100
23	Y	179/250 (72%)	179 (100%)	0	0	100	100
24	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
26	AB	223/296 (75%)	217 (97%)	6 (3%)	0	100	100
27	AC	130/167 (78%)	129 (99%)	1 (1%)	0	100	100
28	AD	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
29	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
30	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
31	AG	307/396 (78%)	300 (98%)	7 (2%)	0	100	100
32	AH	138/201 (69%)	135 (98%)	3 (2%)	0	100	100
33	AI	134/194 (69%)	130 (97%)	4 (3%)	0	100	100
34	AJ	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
35	AK	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
36	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
37	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
38	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
39	AO	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
40	AP	95/142 (67%)	95 (100%)	0	0	100	100
41	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
42	AR	293/360 (81%)	288 (98%)	5 (2%)	0	100	100
43	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
44	AT	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
45	AU	174/205 (85%)	174 (100%)	0	0	100	100
46	AV	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
47	AW	98/187 (52%)	98 (100%)	0	0	100	100
48	AX	350/398 (88%)	348 (99%)	2 (1%)	0	100	100
49	AY	118/395 (30%)	116 (98%)	2 (2%)	0	100	100
50	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
51	A0	213/217 (98%)	207 (97%)	6 (3%)	0	100	100
52	A1	275/323 (85%)	272 (99%)	3 (1%)	0	100	100
53	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
55	A4	527/689 (76%)	520 (99%)	7 (1%)	0	100	100
58	0	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
59	1	51/65 (78%)	50 (98%)	1 (2%)	0	100	100
60	2	44/92 (48%)	44 (100%)	0	0	100	100
61	3	93/188 (50%)	93 (100%)	0	0	100	100
62	4	36/103 (35%)	36 (100%)	0	0	100	100
63	5	392/423 (93%)	386 (98%)	6 (2%)	0	100	100
64	6	352/380 (93%)	347 (99%)	5 (1%)	0	100	100
65	7	292/338 (86%)	282 (97%)	10 (3%)	0	100	100
66	8	138/206 (67%)	136 (99%)	2 (1%)	0	100	100
67	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
68	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
69	b	149/215 (69%)	145 (97%)	4 (3%)	0	100	100
70	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
71	d	235/306 (77%)	232 (99%)	3 (1%)	0	100	100
72	e	236/279 (85%)	229 (97%)	7 (3%)	0	100	100
73	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
74	g	132/166 (80%)	132 (100%)	0	0	100	100
75	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
76	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
77	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
78	k	93/112 (83%)	93 (100%)	0	0	100	100
79	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
80	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
81	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
82	p	137/206 (66%)	137 (100%)	0	0	100	100
83	q	131/222 (59%)	131 (100%)	0	0	100	100
84	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
85	s	379/439 (86%)	372 (98%)	7 (2%)	0	100	100
86	t	9/198 (4%)	9 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13960/18169 (77%)	13735 (98%)	224 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Q	62	ILE

### 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%)	191 (100%)	1 (0%)	86	94
4	E	260/290 (90%)	259 (100%)	1 (0%)	89	95
5	F	219/262 (84%)	218 (100%)	1 (0%)	86	94
6	H	90/228 (40%)	88 (98%)	2 (2%)	47	76
7	I	155/232 (67%)	155 (100%)	0	100	100
8	J	138/150 (92%)	137 (99%)	1 (1%)	81	91
9	K	155/155 (100%)	155 (100%)	0	100	100
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	245/249 (98%)	244 (100%)	1 (0%)	89	95
12	N	189/211 (90%)	188 (100%)	1 (0%)	86	94
13	O	134/150 (89%)	132 (98%)	2 (2%)	60	83
14	P	126/155 (81%)	125 (99%)	1 (1%)	79	90
15	Q	221/256 (86%)	220 (100%)	1 (0%)	86	94
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	146/180 (81%)	145 (99%)	1 (1%)	81	91
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	W	94/119 (79%)	93 (99%)	1 (1%)	70	87
22	X	220/229 (96%)	220 (100%)	0	100	100
23	Y	163/223 (73%)	162 (99%)	1 (1%)	84	93
24	Z	113/147 (77%)	112 (99%)	1 (1%)	75	89
26	AB	198/249 (80%)	198 (100%)	0	100	100
27	AC	115/143 (80%)	114 (99%)	1 (1%)	75	89
28	AD	286/357 (80%)	286 (100%)	0	100	100
29	AE	104/107 (97%)	104 (100%)	0	100	100
30	AF	185/209 (88%)	185 (100%)	0	100	100
31	AG	270/342 (79%)	270 (100%)	0	100	100
32	AH	130/180 (72%)	128 (98%)	2 (2%)	60	83
33	AI	104/146 (71%)	104 (100%)	0	100	100
34	AJ	93/118 (79%)	92 (99%)	1 (1%)	70	87
35	AK	91/113 (80%)	91 (100%)	0	100	100
36	AL	158/226 (70%)	156 (99%)	2 (1%)	65	85
37	AM	97/113 (86%)	97 (100%)	0	100	100
38	AN	96/115 (84%)	95 (99%)	1 (1%)	73	88
39	AO	174/230 (76%)	173 (99%)	1 (1%)	84	93
40	AP	88/123 (72%)	88 (100%)	0	100	100
41	AQ	78/78 (100%)	78 (100%)	0	100	100
42	AR	264/318 (83%)	263 (100%)	1 (0%)	89	95
43	AS	116/164 (71%)	116 (100%)	0	100	100
44	AT	153/157 (98%)	152 (99%)	1 (1%)	81	91
45	AU	152/174 (87%)	152 (100%)	0	100	100
46	AV	325/364 (89%)	325 (100%)	0	100	100
47	AW	87/158 (55%)	87 (100%)	0	100	100
48	AX	311/351 (89%)	310 (100%)	1 (0%)	91	96
49	AY	111/357 (31%)	111 (100%)	0	100	100
50	AZ	90/95 (95%)	90 (100%)	0	100	100
51	A0	188/189 (100%)	188 (100%)	0	100	100
52	A1	255/291 (88%)	255 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	A2	100/100 (100%)	100 (100%)	0	100	100
54	A3	65/166 (39%)	65 (100%)	0	100	100
55	A4	479/609 (79%)	475 (99%)	4 (1%)	79	90
58	0	99/164 (60%)	98 (99%)	1 (1%)	73	88
59	1	50/60 (83%)	50 (100%)	0	100	100
60	2	40/72 (56%)	39 (98%)	1 (2%)	42	73
61	3	88/166 (53%)	88 (100%)	0	100	100
62	4	37/89 (42%)	37 (100%)	0	100	100
63	5	353/368 (96%)	350 (99%)	3 (1%)	79	90
64	6	313/332 (94%)	313 (100%)	0	100	100
65	7	270/303 (89%)	269 (100%)	1 (0%)	89	95
66	8	129/190 (68%)	129 (100%)	0	100	100
67	9	104/112 (93%)	104 (100%)	0	100	100
68	a	96/133 (72%)	96 (100%)	0	100	100
69	b	132/185 (71%)	132 (100%)	0	100	100
70	c	251/288 (87%)	250 (100%)	1 (0%)	89	95
71	d	223/274 (81%)	222 (100%)	1 (0%)	89	95
72	e	207/236 (88%)	205 (99%)	2 (1%)	73	88
73	f	139/188 (74%)	139 (100%)	0	100	100
74	g	124/148 (84%)	124 (100%)	0	100	100
75	h	104/148 (70%)	104 (100%)	0	100	100
76	i	86/110 (78%)	86 (100%)	0	100	100
77	j	74/97 (76%)	74 (100%)	0	100	100
78	k	81/90 (90%)	81 (100%)	0	100	100
79	l	76/116 (66%)	76 (100%)	0	100	100
80	m	85/113 (75%)	85 (100%)	0	100	100
81	o	80/87 (92%)	80 (100%)	0	100	100
82	p	132/181 (73%)	132 (100%)	0	100	100
83	q	114/178 (64%)	114 (100%)	0	100	100
84	r	147/169 (87%)	147 (100%)	0	100	100
85	s	338/381 (89%)	338 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	t	6/158 (4%)	6 (100%)	0	100	100
All	All	12480/15710 (79%)	12439 (100%)	41 (0%)	90	96

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	A4	309	PHE
63	5	307	ASP
55	A4	379	PHE
60	2	92	HIS
70	c	307	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 151 such sidechains are listed below:

Mol	Chain	Res	Type
70	c	222	GLN
83	q	81	GLN
72	e	75	GLN
79	l	82	GLN
85	s	397	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1520/1561 (97%)	258 (16%)	3 (0%)
2	B	71/72 (98%)	16 (22%)	0
25	AA	953/954 (99%)	148 (15%)	2 (0%)
56	Ax	62/71 (87%)	11 (17%)	0
57	Az	7/8 (87%)	1 (14%)	0
All	All	2613/2666 (98%)	434 (16%)	5 (0%)

5 of 434 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1681	G
1	A	1689	C
1	A	1691	C
1	A	1693	C
1	A	1694	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1692	A
1	A	2245	A
1	A	2349	G
25	AA	1255	U
25	AA	1539	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMG	A	3040	1	18,26,27	0.91	1 (5%)	19,38,41	0.61	0
56	RSQ	Ax	34	56,57	20,23,24	0.31	0	26,33,36	0.34	0
1	1MA	A	2617	1	16,25,26	1.17	2 (12%)	18,37,40	0.87	1 (5%)
25	MA6	AA	1584	25	18,26,27	0.76	0	19,38,41	0.63	0
1	PSU	A	3067	1	18,21,22	0.51	0	22,30,33	0.62	1 (4%)
2	PSU	B	39	2	18,21,22	0.49	0	22,30,33	0.57	0
1	OMU	A	3039	1,88	19,22,23	0.28	0	26,31,34	0.42	0
25	MA6	AA	1583	25	18,26,27	0.74	0	19,38,41	0.62	0
33	5F0	AI	184	33	8,8,9	0.54	0	7,9,11	1.02	1 (14%)
2	2MG	B	10	2	18,26,27	0.91	1 (5%)	16,38,41	0.70	0
25	5MC	AA	1488	25	18,22,23	0.32	0	26,32,35	0.46	0
25	5MU	AA	1076	25	19,22,23	0.29	0	28,32,35	0.31	0
1	OMG	A	2815	1,88,56	18,26,27	0.92	1 (5%)	19,38,41	0.61	0
2	1MA	B	9	2	16,25,26	1.16	2 (12%)	18,37,40	0.85	1 (5%)
25	B8T	AA	1486	25,87	19,22,23	0.30	0	26,31,34	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	3040	1	-	0/5/27/28	0/3/3/3
56	RSQ	Ax	34	56,57	-	1/9/27/28	0/2/2/2
1	1MA	A	2617	1	-	0/3/25/26	0/3/3/3
25	MA6	AA	1584	25	-	4/7/29/30	0/3/3/3
1	PSU	A	3067	1	-	0/7/25/26	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
1	OMU	A	3039	1,88	-	0/9/27/28	0/2/2/2
25	MA6	AA	1583	25	-	3/7/29/30	0/3/3/3
33	5F0	AI	184	33	-	7/9/9/10	-
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
25	5MC	AA	1488	25	-	0/7/25/26	0/2/2/2
25	5MU	AA	1076	25	-	0/7/25/26	0/2/2/2
1	OMG	A	2815	1,88,56	-	0/5/27/28	0/3/3/3
2	1MA	B	9	2	-	0/3/25/26	0/3/3/3
25	B8T	AA	1486	25,87	-	0/7/27/28	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	1MA	C6-N6	3.20	1.35	1.27
1	A	2617	1MA	C6-N6	3.16	1.35	1.27
2	B	10	2MG	C5-C6	-2.30	1.42	1.47
1	A	2815	OMG	C5-C6	-2.27	1.42	1.47
1	A	3040	OMG	C5-C6	-2.19	1.43	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	AI	184	5F0	O-C-CB	-2.29	118.75	125.43
1	A	3067	PSU	O4'-C1'-C2'	2.13	108.14	105.14
2	B	9	1MA	N1-C6-N6	2.08	125.07	119.77
1	A	2617	1MA	N1-C6-N6	2.07	125.04	119.77

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AA	1583	MA6	C5-C6-N6-C9
25	AA	1584	MA6	C5-C6-N6-C9
25	AA	1584	MA6	C5-C6-N6-C10
33	AI	184	5F0	O1-C1-CA-CB
33	AI	184	5F0	OD1-C1-CA-CB

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AA	1584	MA6	1	0
25	AA	1583	MA6	3	0
25	AA	1488	5MC	2	0
1	A	2815	OMG	2	0
25	AA	1486	B8T	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 273 ligands modelled in this entry, 264 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
89	G34	A	6456	-	40,40,40	0.50	0	58,64,64	1.11	3 (5%)
90	VAL	B	101	2	4,6,7	0.51	0	6,7,9	0.95	0
94	FES	AP	201	29,40	0,4,4	-	-	-		
92	SPD	AA	1703	-	9,9,9	0.29	0	8,8,8	0.85	0
91	NAD	AA	1701	87	42,48,48	0.57	0	50,73,73	0.57	1 (2%)
96	GDP	AX	503	-	24,30,30	0.88	1 (4%)	30,47,47	0.62	0
94	FES	r	201	7,84	0,4,4	-	-	-		
95	ATP	AX	501	87	26,33,33	0.75	0	31,52,52	0.66	0
94	FES	AT	201	44,37	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
89	G34	A	6456	-	-	3/12/94/94	0/6/5/5
90	VAL	B	101	2	-	1/5/6/8	-
92	SPD	AA	1703	-	-	0/7/7/7	-
91	NAD	AA	1701	87	-	2/26/62/62	0/5/5/5
96	GDP	AX	503	-	-	0/12/32/32	0/3/3/3
94	FES	AP	201	29,40	-	-	0/1/1/1
94	FES	r	201	7,84	-	-	0/1/1/1
95	ATP	AX	501	87	-	0/18/38/38	0/3/3/3
94	FES	AT	201	44,37	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	AX	503	GDP	C5-C6	-2.15	1.43	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	A	6456	G34	O1-C3-C2	-3.28	120.80	125.56
89	A	6456	G34	C15-C5-C14	-3.22	105.77	108.95
89	A	6456	G34	C1-C9-C10	-2.64	107.44	110.58
91	AA	1701	NAD	C5A-C6A-N6A	2.32	123.88	120.35

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	A	6456	G34	C24-C23-S1-C22
91	AA	1701	NAD	O4B-C4B-C5B-O5B
91	AA	1701	NAD	C3B-C4B-C5B-O5B
89	A	6456	G34	C21-C22-S1-C23
89	A	6456	G34	C22-C21-O3-C14

There are no ring outliers.

5 monomers are involved in 8 short contacts:

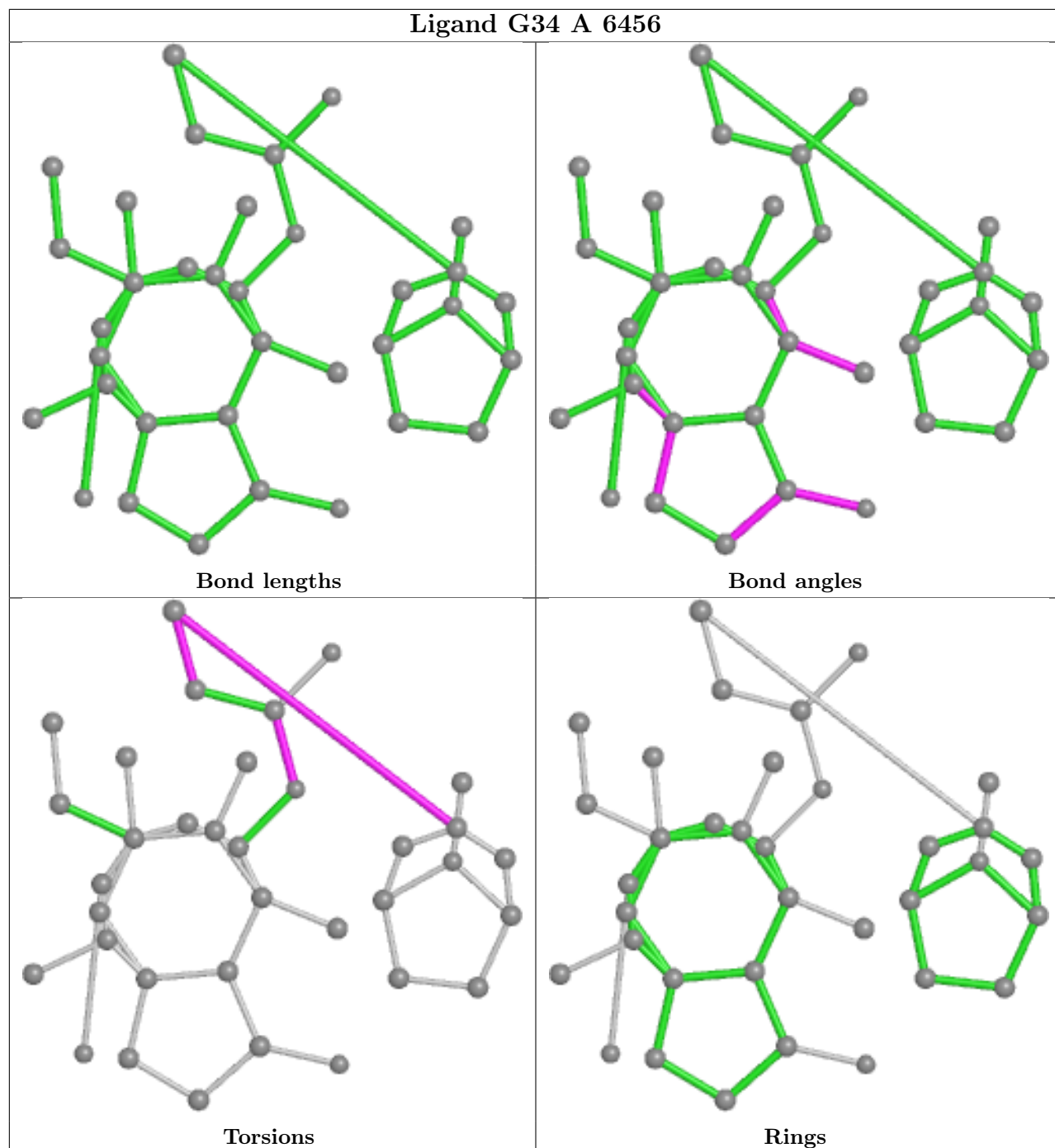
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	A	6456	G34	3	0
90	B	101	VAL	2	0
91	AA	1701	NAD	1	0
96	AX	503	GDP	1	0

*Continued on next page...*

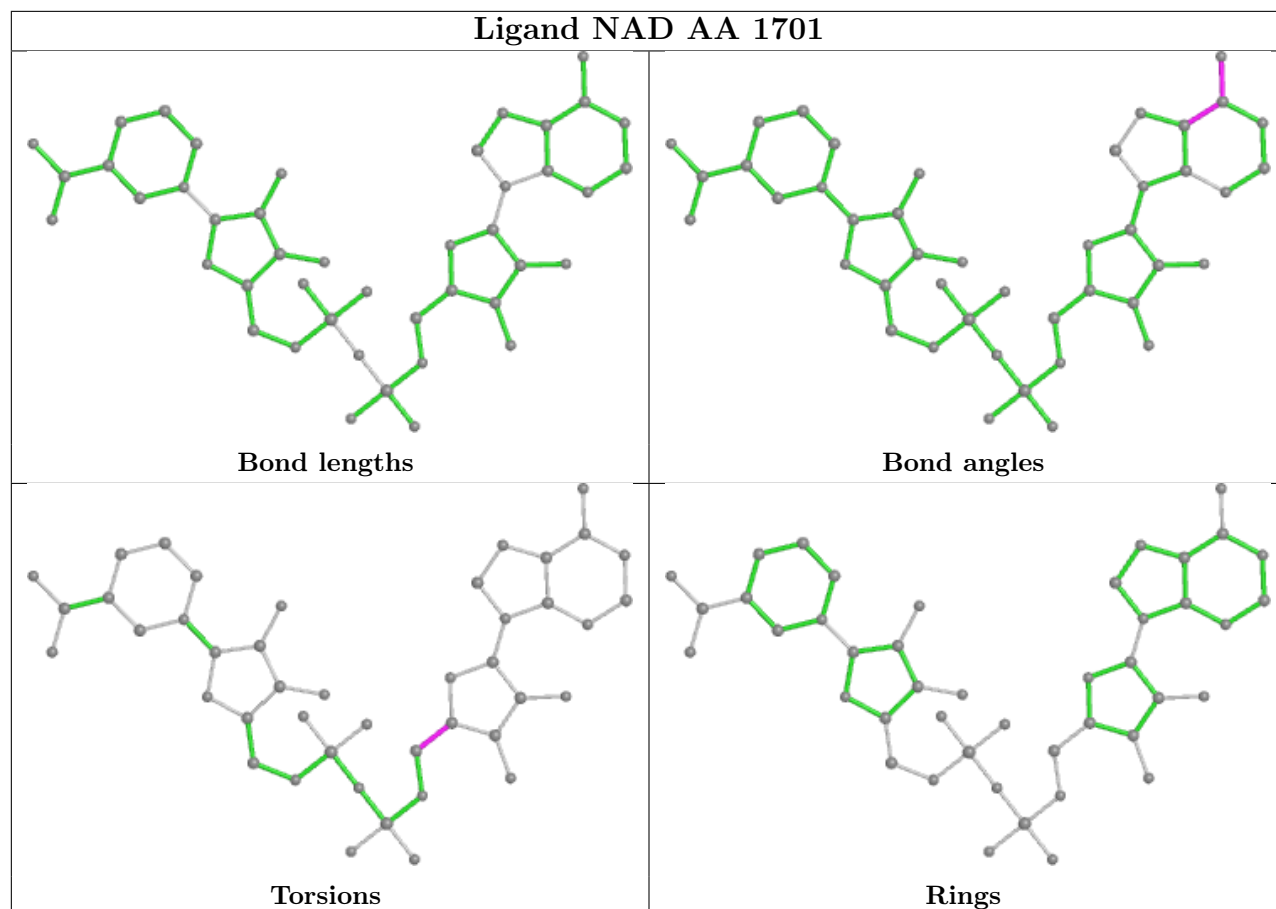
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
95	AX	501	ATP	1	0

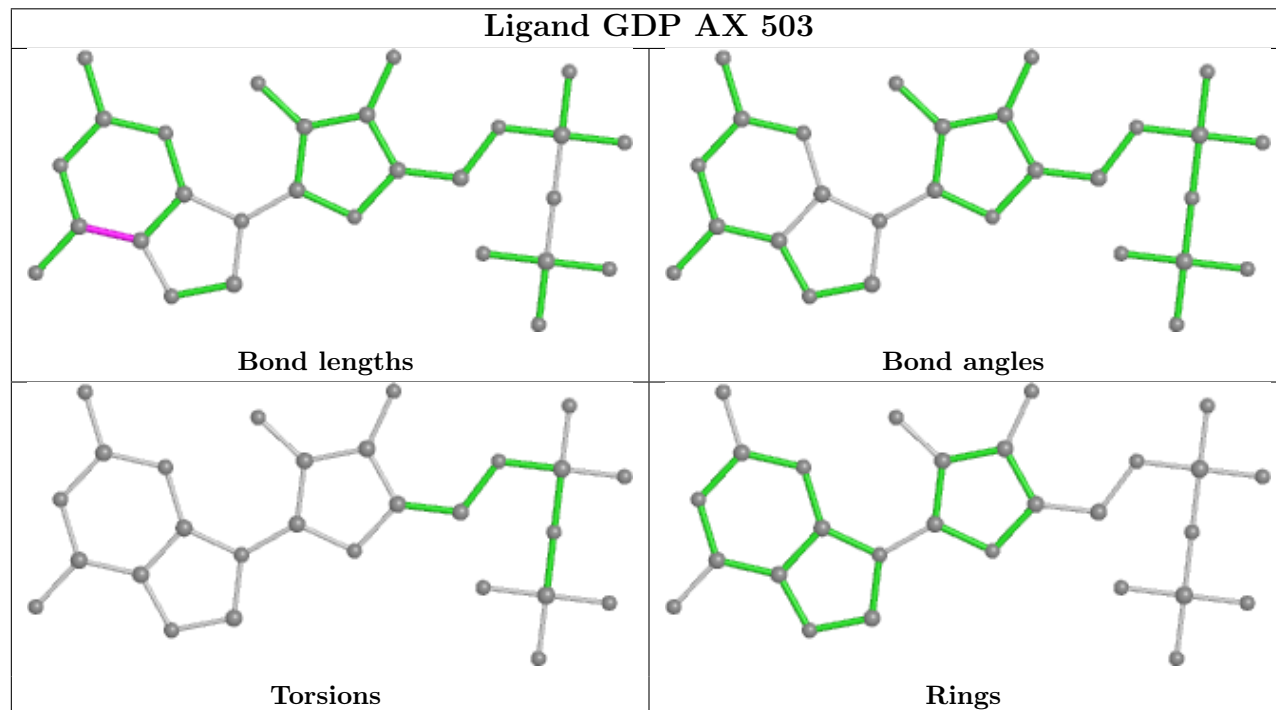
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



## Ligand NAD AA 1701



## Ligand GDP AX 503



## 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.

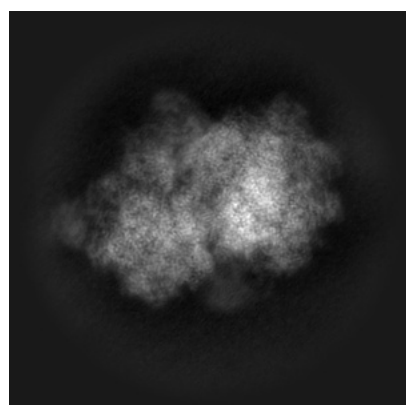
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64554. These allow visual inspection of the internal detail of the map and identification of artifacts.

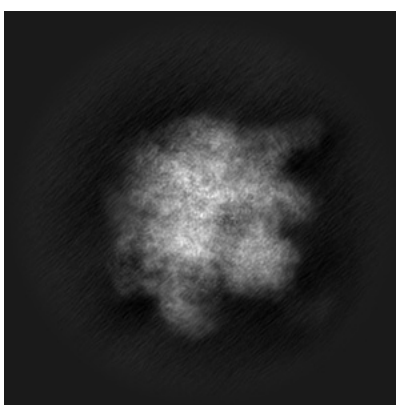
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

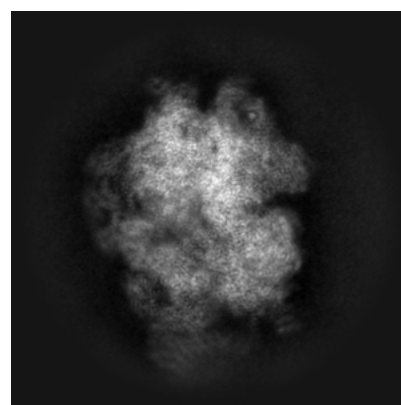
#### 6.1.1 Primary map



X



Y

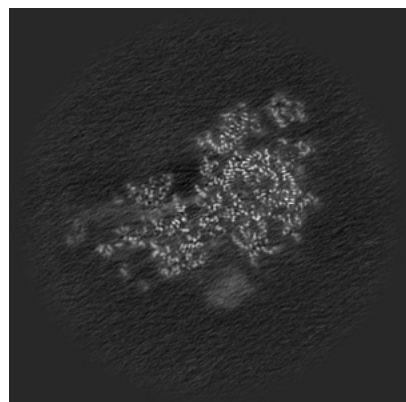


Z

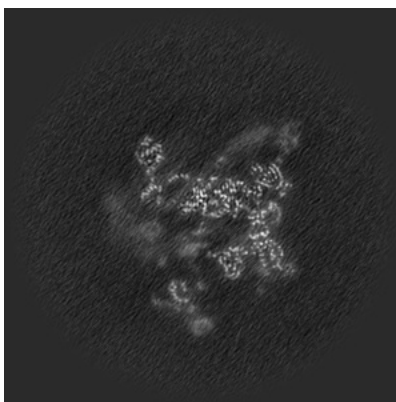
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

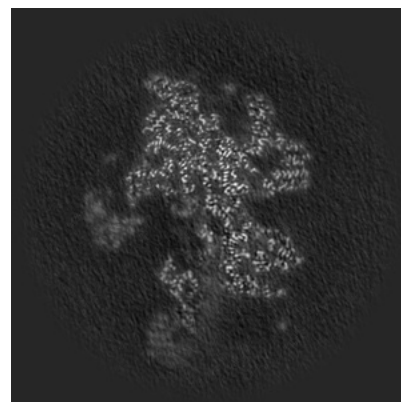
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

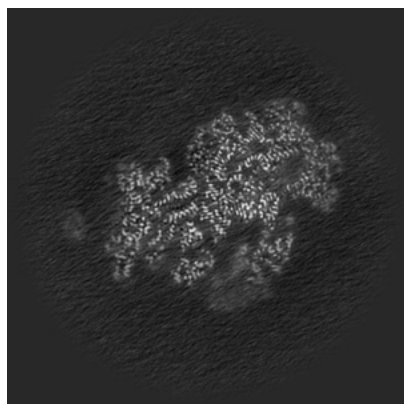


Z Index: 256

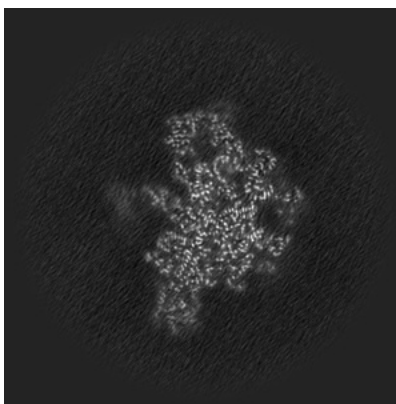
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

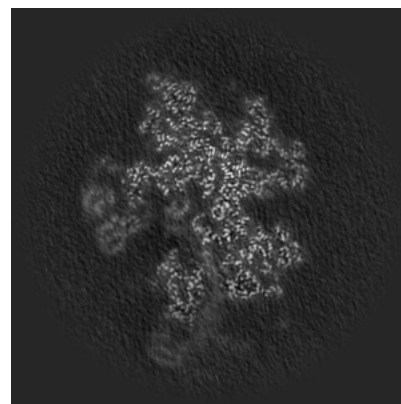
### 6.3.1 Primary map



X Index: 277



Y Index: 306

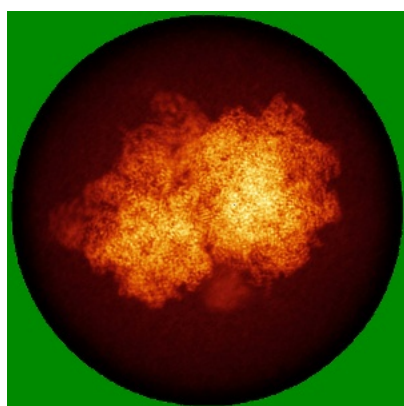


Z Index: 248

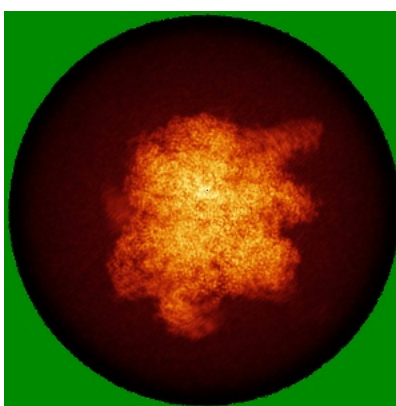
The images above show the largest variance slices of the map in three orthogonal directions.

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

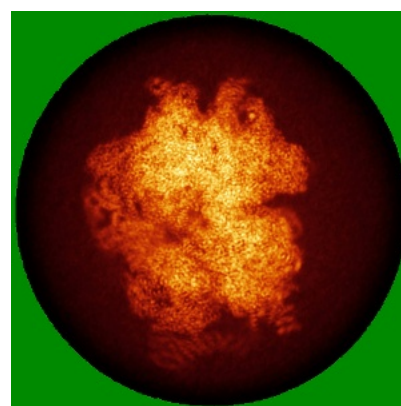
### 6.4.1 Primary map



X



Y

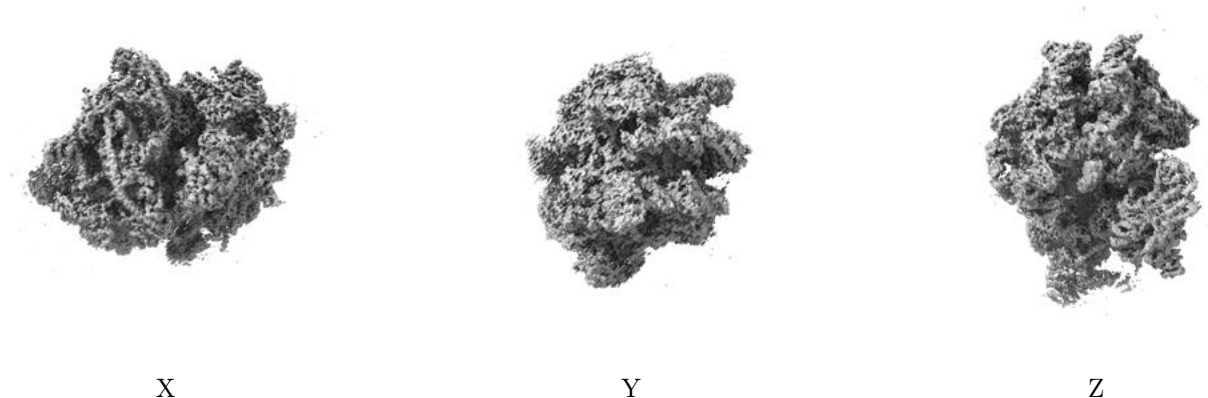


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

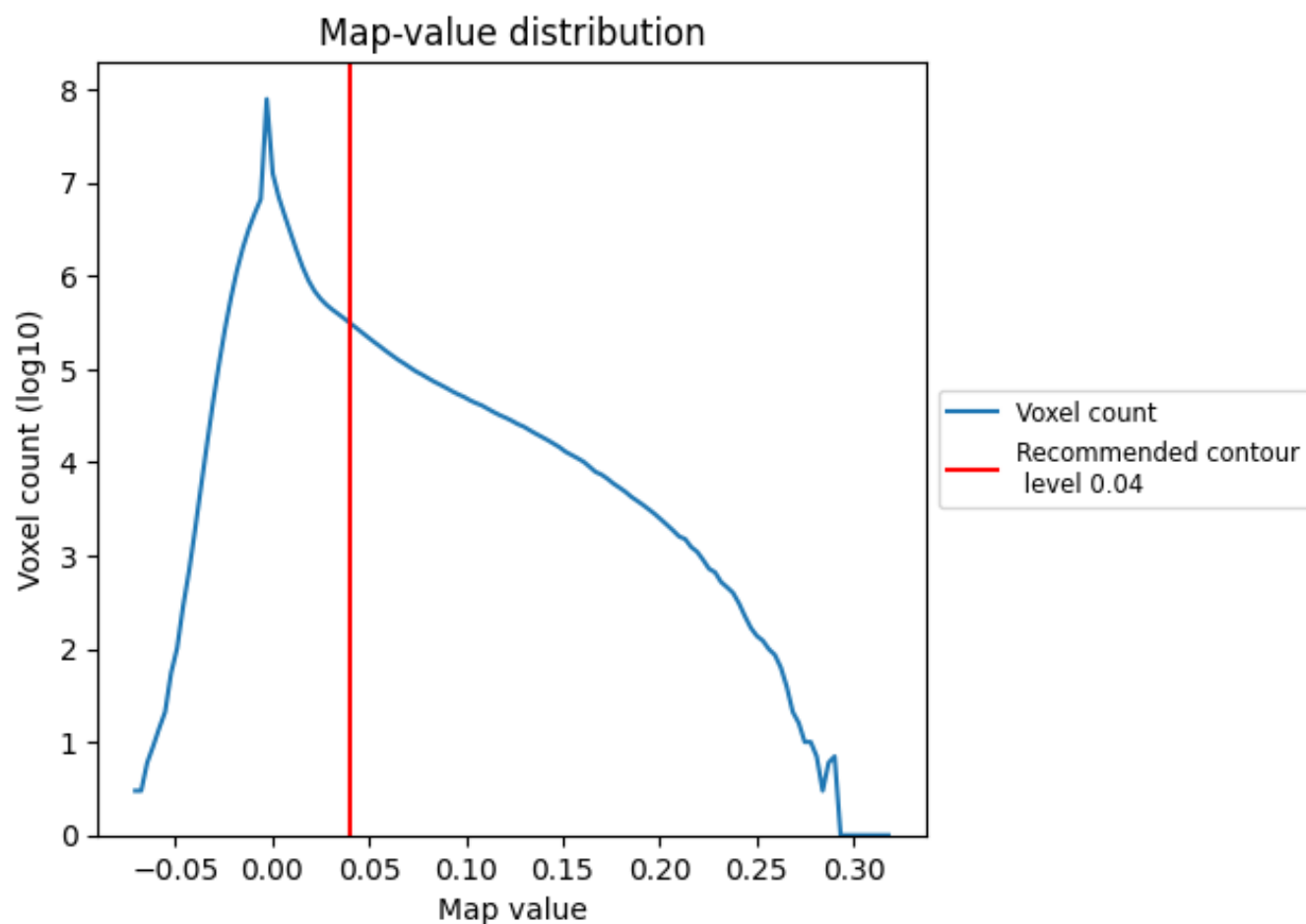
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

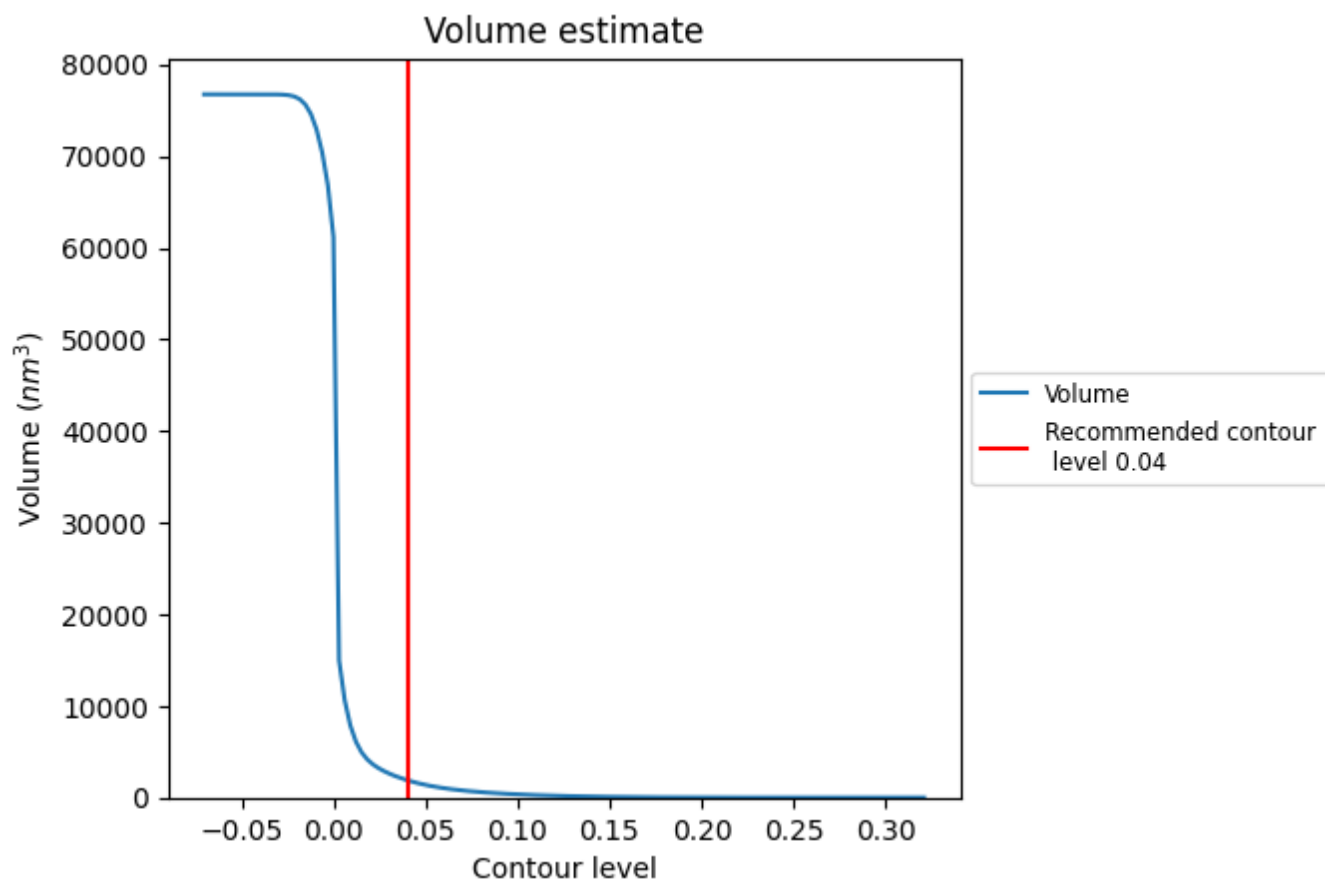
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

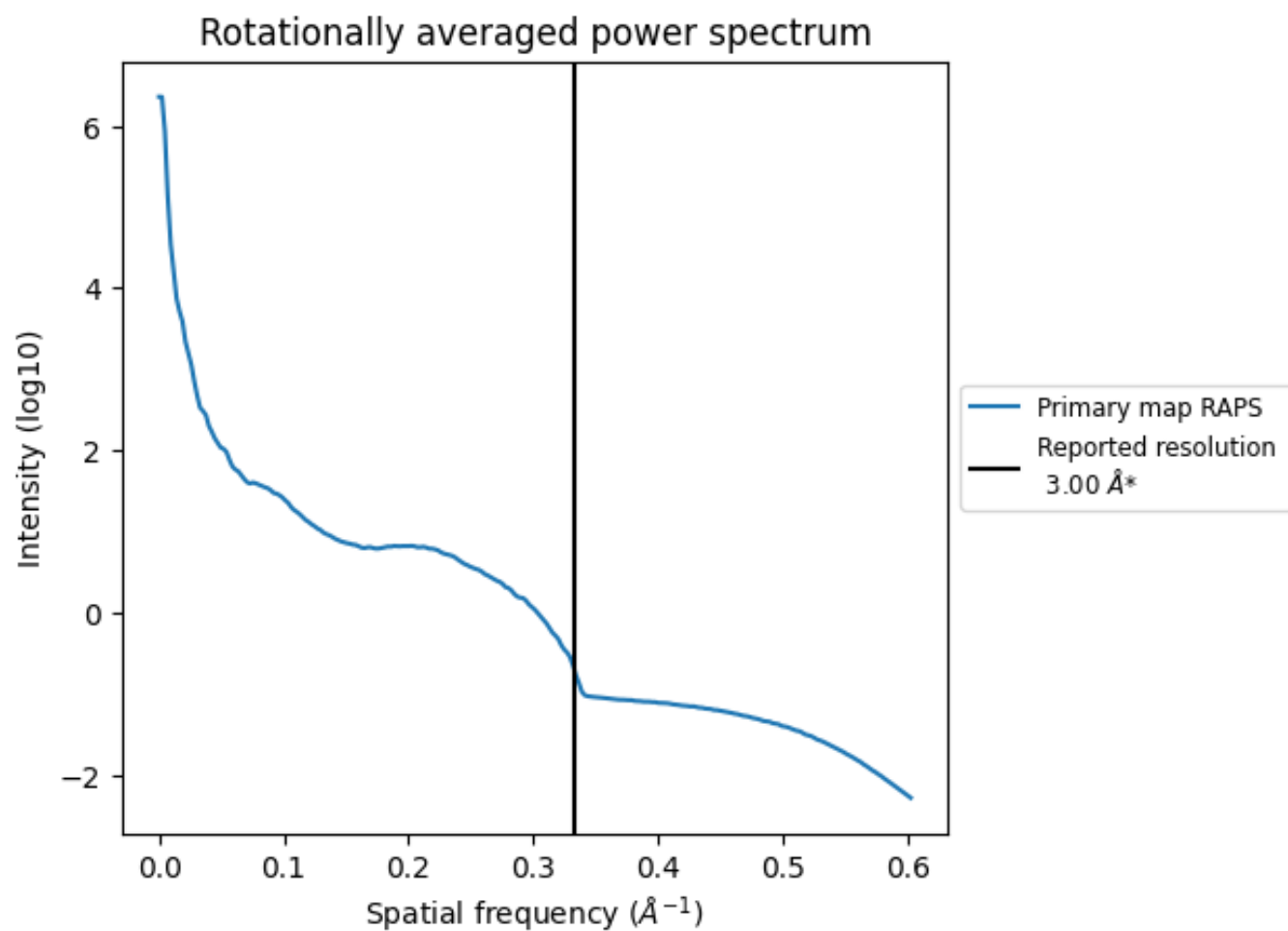
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1886 nm<sup>3</sup>; this corresponds to an approximate mass of 1704 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 0.333 Å<sup>-1</sup>

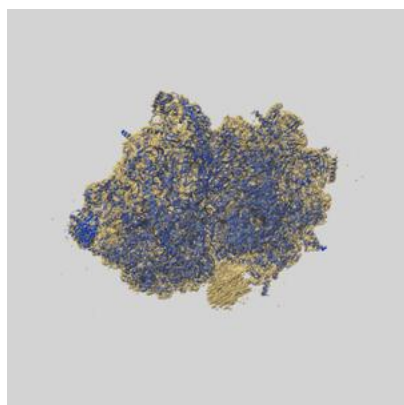
## 8 Fourier-Shell correlation

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

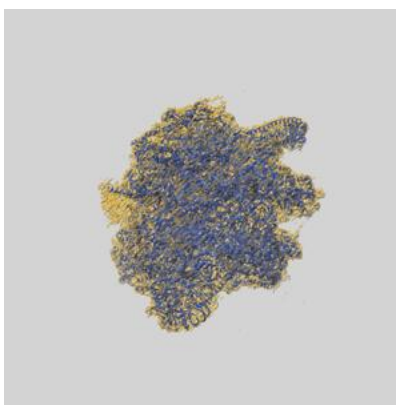
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64554 and PDB model 9UWH. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

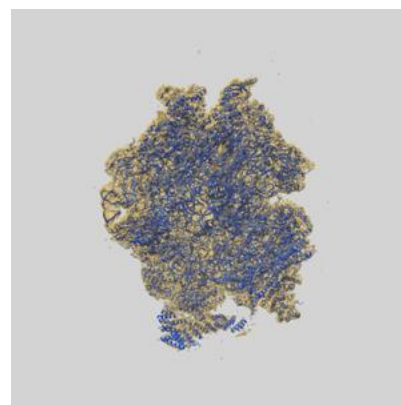
### 9.1 Map-model overlay [i](#)



X



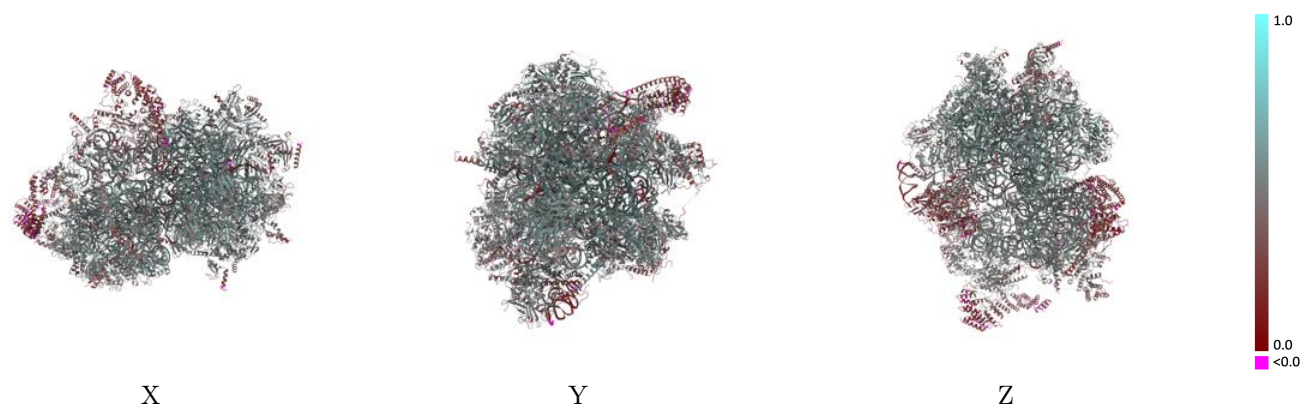
Y



Z

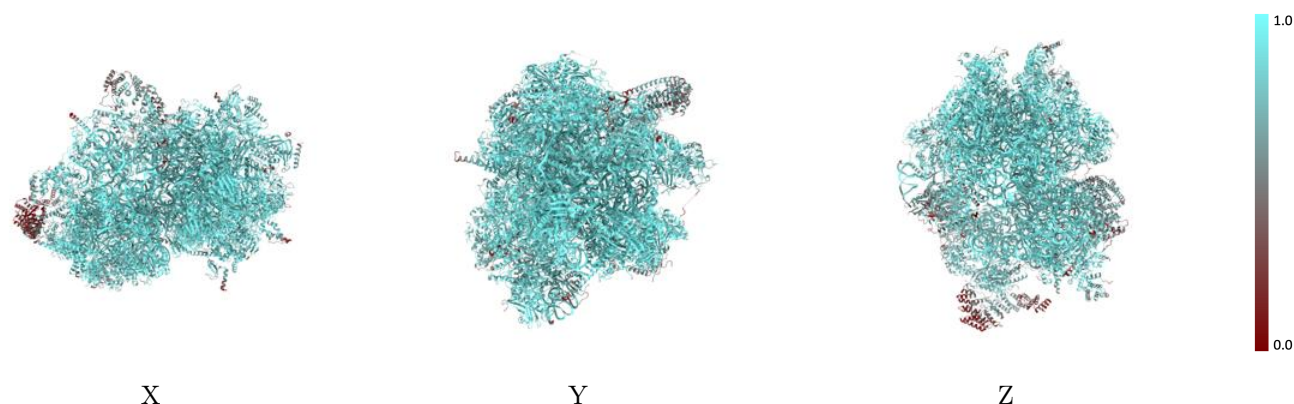
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



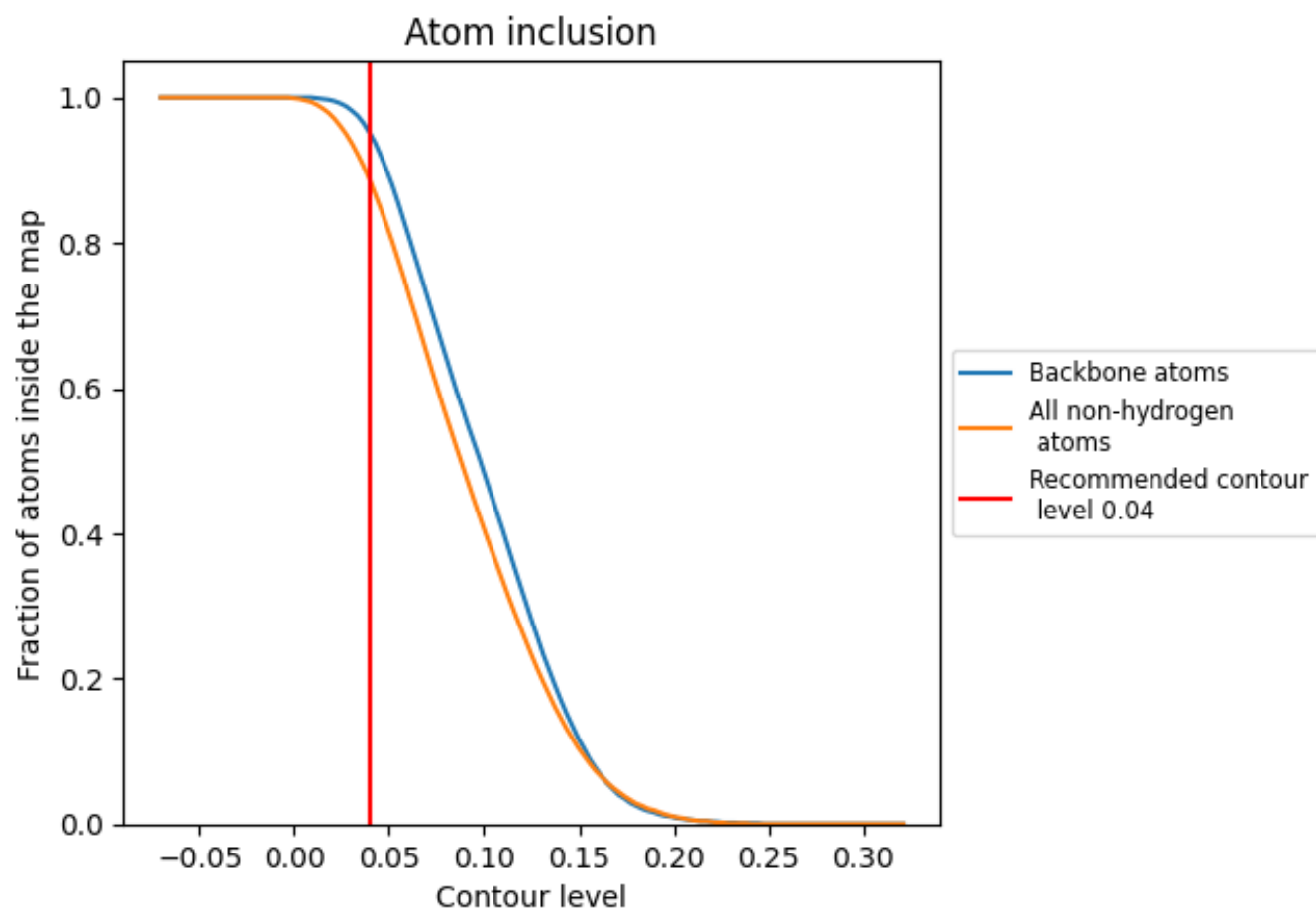
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.04) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.8850	 0.4710
0	 0.9130	 0.5220
1	 0.9390	 0.5290
2	 0.9950	 0.5750
3	 0.9830	 0.5750
4	 0.9630	 0.5360
5	 0.9120	 0.5090
6	 0.8890	 0.4600
7	 0.8380	 0.4390
8	 0.6930	 0.3330
9	 0.8590	 0.4890
A	 0.9840	 0.5220
A0	 0.7440	 0.3630
A1	 0.7760	 0.4220
A2	 0.8930	 0.4710
A3	 0.9510	 0.5140
A4	 0.3840	 0.2300
AA	 0.9750	 0.5010
AB	 0.9250	 0.5080
AC	 0.8980	 0.5060
AD	 0.8690	 0.4840
AE	 0.9110	 0.5110
AF	 0.8960	 0.4600
AG	 0.8890	 0.4680
AH	 0.8020	 0.4500
AI	 0.9280	 0.5200
AJ	 0.8580	 0.4970
AK	 0.9180	 0.5110
AL	 0.8720	 0.4610
AM	 0.8330	 0.4450
AN	 0.9380	 0.5270
AO	 0.8300	 0.4260
AP	 0.9300	 0.5160
AQ	 0.9600	 0.5350
AR	 0.8000	 0.4000



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













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Chain	Atom inclusion	Q-score
AS	 0.8130	 0.4450
AT	 0.8970	 0.4800
AU	 0.7840	 0.4010
AV	 0.5680	 0.2350
AW	 0.9090	 0.4910
AX	 0.8420	 0.4410
AY	 0.7300	 0.3870
AZ	 0.8270	 0.4580
Ax	 0.9190	 0.3980
Az	 0.9640	 0.4310
B	 0.8860	 0.3270
D	 0.9630	 0.5520
E	 0.9410	 0.5260
F	 0.9600	 0.5390
H	 0.7680	 0.4240
I	 0.6510	 0.3370
J	 0.6600	 0.2330
K	 0.9560	 0.5300
L	 0.9070	 0.5240
M	 0.9400	 0.5310
N	 0.9200	 0.5100
O	 0.9100	 0.5130
P	 0.9190	 0.4990
Q	 0.8410	 0.4960
R	 0.9580	 0.5450
S	 0.9290	 0.5290
T	 0.9510	 0.5470
U	 0.8750	 0.4760
V	 0.8330	 0.4480
W	 0.9340	 0.5430
X	 0.8840	 0.4920
Y	 0.9280	 0.5120
Z	 0.9280	 0.5360
a	 0.8240	 0.4500
b	 0.9390	 0.5380
c	 0.8880	 0.4800
d	 0.7980	 0.4060
e	 0.6400	 0.2670
f	 0.7210	 0.3980
g	 0.9180	 0.5160
h	 0.8560	 0.4380
i	 0.9710	 0.5660

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Chain	Atom inclusion	Q-score
j	 0.8410	 0.4670
k	 0.7410	 0.3440
l	 0.6820	 0.2940
m	 0.6660	 0.3170
o	 0.9630	 0.5300
p	 0.7720	 0.4120
q	 0.8010	 0.4080
r	 0.9000	 0.4930
s	 0.9340	 0.5140
t	 0.2360	 0.2580