



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:06 pm BST

PDB ID : 9S7E / pdb_00009s7e
EMDB ID : EMD-54640
Title : Structure of human mitochondrial COX1-translating ribosome nascent chain-OXA1L/MITRAC complex in closed state (closed COX1-mtRNC-OXA1L/MITRAC)
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 : 3.10 Å(reported)
Based on initial model : 7QI5

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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)

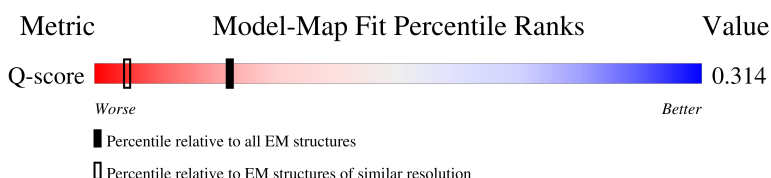
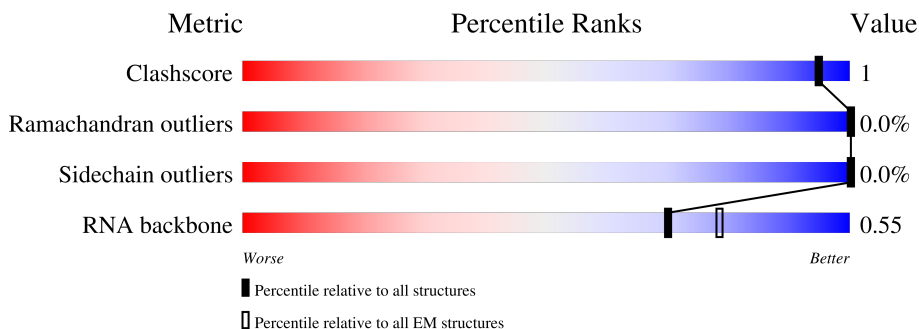
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



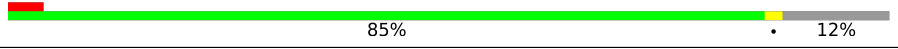
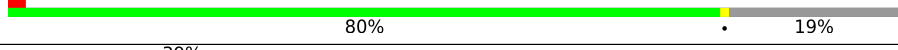
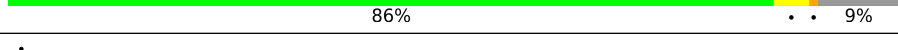
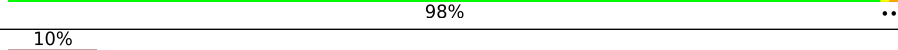
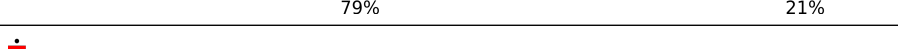
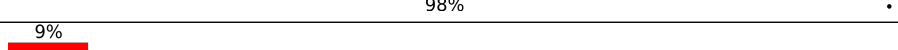
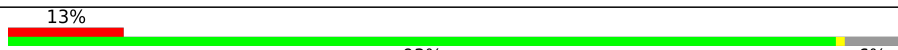
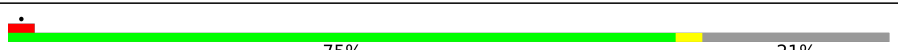
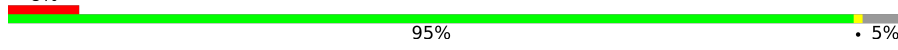
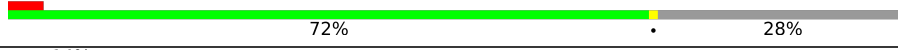
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	72	
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	AA	954	
26	AB	296	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	AC	167	
28	0	188	
29	1	65	
30	2	92	
31	3	188	
32	4	103	
33	z	325	
34	t	198	
34	u	198	
34	v	198	
34	w	198	
34	x	198	
34	y	198	
35	5	423	
36	6	380	
37	7	338	
38	8	206	
39	9	137	
40	a	142	
41	b	215	
42	c	332	
43	e	279	
44	f	212	
45	g	166	
46	h	158	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
47	i	128	
48	j	123	
49	k	112	
50	l	138	
51	m	128	
52	o	102	
53	p	206	
54	q	222	
55	r	196	
56	s	439	
57	AD	430	
58	AE	125	
59	AF	242	
60	AG	396	
61	AH	201	
62	AI	194	
63	AJ	138	
64	AK	128	
65	AL	257	
66	AM	137	
67	AN	130	
68	AO	258	
69	AP	142	
70	AQ	87	
71	AR	360	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
72	AS	190	
73	AT	173	
74	AU	205	
75	AV	414	
76	AW	187	
77	AX	398	
78	AY	395	
79	AZ	106	
80	A0	217	
81	A1	323	
82	A2	118	
83	A3	199	
84	A4	689	
85	Az	33	
86	Av	23	
87	Aw	68	
88	Ax	71	
89	d	306	
90	Au	435	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
96	FES	r	201	-	-	X	-

2 Entry composition

There are 99 unique types of molecules in this entry. The entry contains 180448 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 tRNA-Val.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	C	G	conflict	GB NC_012920.1
B	76	A	U	conflict	GB NC_012920.1

- 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	128	Total	C	N	O	S	0	0
			1049	670	200	177	2		

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 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 Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 29 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 31 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 32 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL1m.

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

- Molecule 34 is a protein called Large ribosomal subunit protein bL12m.

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

- Molecule 35 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5	393	Total	C	N	O	S	0	0
			3200	2067	557	565	11		

- Molecule 36 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 37 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 38 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	144	Total	C	N	O	S	0	0
			1219	775	214	228	2		

- Molecule 39 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 40 is a protein called Large ribosomal subunit protein mL42.

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

- Molecule 41 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	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	2	ACE	-	acetylation	UNP Q8N983

- Molecule 42 is a protein called Large ribosomal subunit protein mL44.

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

- Molecule 43 is a protein called Large ribosomal subunit protein mL46.

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

- Molecule 44 is a protein called Large ribosomal subunit protein mL48.

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

- Molecule 45 is a protein called Large ribosomal subunit protein mL49.

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

- Molecule 46 is a protein called Large ribosomal subunit protein mL50.

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

- Molecule 47 is a protein called Large ribosomal subunit protein mL51.

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

- Molecule 48 is a protein called Large ribosomal subunit protein mL52.

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

- Molecule 49 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a protein called Large ribosomal subunit protein mL54.

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

- Molecule 51 is a protein called Large ribosomal subunit protein mL55.

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

- Molecule 52 is a protein called Large ribosomal subunit protein mL63.

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

- Molecule 53 is a protein called Large ribosomal subunit protein mL62.

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

- Molecule 54 is a protein called Large ribosomal subunit protein mL64.

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

- Molecule 55 is a protein called Large ribosomal subunit protein mL66.

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

- Molecule 56 is a protein called Large ribosomal subunit protein mL65.

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

- Molecule 57 is a protein called Small ribosomal subunit protein uS5m.

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

- Molecule 58 is a protein called Small ribosomal subunit protein bS6m.

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

- Molecule 59 is a protein called Small ribosomal subunit protein uS7m.

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

- Molecule 60 is a protein called Small ribosomal subunit protein uS9m.

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

- Molecule 61 is a protein called Small ribosomal subunit protein uS10m.

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

- Molecule 62 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	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 63 is a protein called Small ribosomal subunit protein uS12m.

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

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

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

- Molecule 65 is a protein called Small ribosomal subunit protein uS15m.

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

- Molecule 66 is a protein called Small ribosomal subunit protein bS16m.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS17m.

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

- Molecule 68 is a protein called Small ribosomal subunit protein mS40.

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

- Molecule 69 is a protein called Small ribosomal subunit protein bS18m.

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

- Molecule 70 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	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 71 is a protein called Small ribosomal subunit protein mS22.

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

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

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

- Molecule 73 is a protein called Small ribosomal subunit protein mS25.

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

- Molecule 74 is a protein called Small ribosomal subunit protein mS26.

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

- Molecule 75 is a protein called Small ribosomal subunit protein mS27.

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

- Molecule 76 is a protein called Small ribosomal subunit protein bS1m.

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

- Molecule 77 is a protein called Small ribosomal subunit protein mS29.

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

- Molecule 78 is a protein called Small ribosomal subunit protein mS31.

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

- Molecule 79 is a protein called Small ribosomal subunit protein mS33.

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

- Molecule 80 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 81 is a protein called Small ribosomal subunit protein mS35.

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

- Molecule 82 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	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 83 is a protein called Small ribosomal subunit protein bS22, mitochondrial.

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

- Molecule 84 is a protein called Small ribosomal subunit protein mS39.

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

- Molecule 85 is a RNA chain called mRNA (Visualization example).

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

- Molecule 86 is a protein called COX1 nascent chain.

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

- Molecule 87 is a RNA chain called A-site tRNA (Visualisation example).

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aw	35	A	C	conflict	GB 1896813690
Aw	36	C	G	conflict	GB 1896813690
Aw	44	C	A	conflict	GB 1896813690

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

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ax	71	Total	C	N	O	P	0	0
			1499	672	260	496	71		

- Molecule 89 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	d	242	Total	C	N	O	S	0	0
			1988	1275	343	358	12		

- Molecule 90 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Au	51	Total	C	N	O	S	0	0
			431	265	87	77	2		

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
91	A	28	Total	K	0
			28	28	
91	D	1	Total	K	0
			1	1	
91	M	1	Total	K	0
			1	1	
91	N	1	Total	K	0
			1	1	
91	AA	20	Total	K	0
			20	20	
91	3	1	Total	K	0
			1	1	
91	6	1	Total	K	0
			1	1	
91	o	1	Total	K	0
			1	1	

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

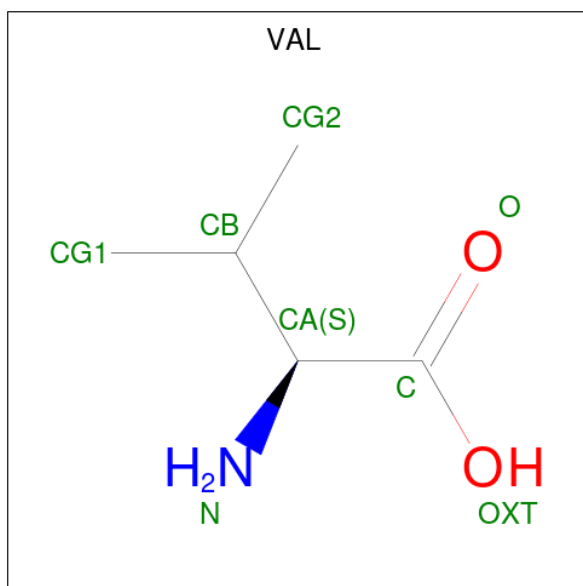
Mol	Chain	Residues	Atoms		AltConf
92	A	135	Total	Mg	0
			135	135	
92	D	2	Total	Mg	0
			2	2	

Continued on next page...

Continued from previous page...

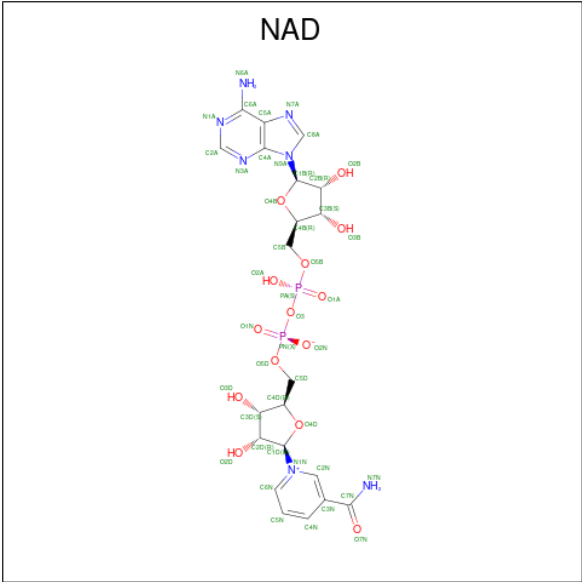
Mol	Chain	Residues	Atoms		AltConf
92	E	1	Total	Mg	0
			1	1	
92	O	1	Total	Mg	0
			1	1	
92	AA	54	Total	Mg	0
			54	54	
92	AB	1	Total	Mg	0
			1	1	
92	g	1	Total	Mg	0
			1	1	
92	AX	1	Total	Mg	0
			1	1	
92	A3	1	Total	Mg	0
			1	1	

- Molecule 93 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



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

- Molecule 94 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

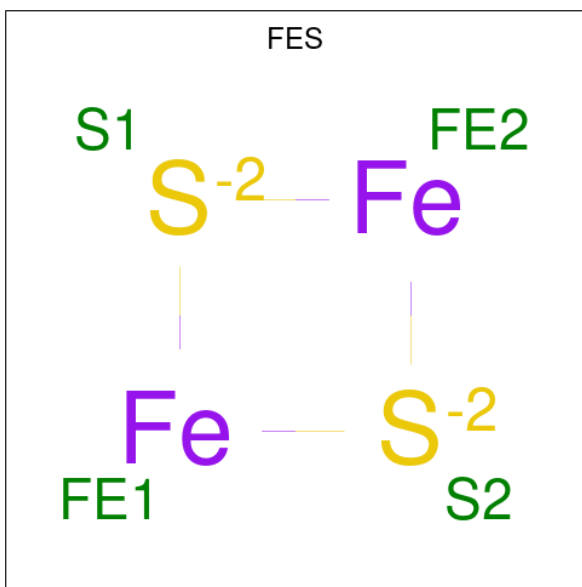


Mol	Chain	Residues	Atoms					AltConf
94	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 95 is ZINC ION (CCD ID: ZN) (formula: Zn).

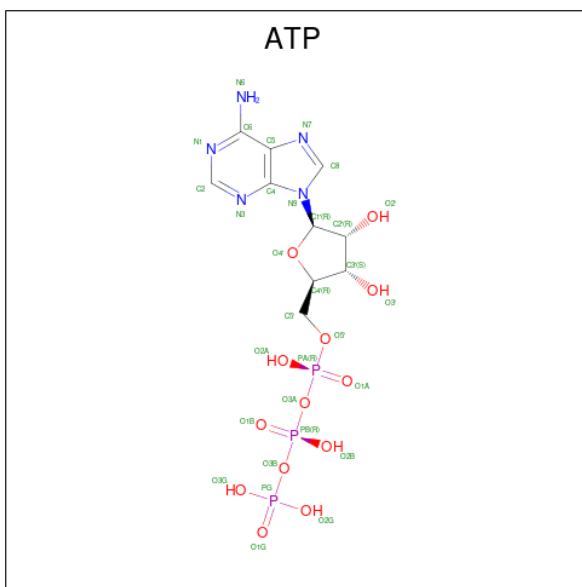
Mol	Chain	Residues	Atoms		AltConf
95	0	1	Total	Zn	0
			1	1	
95	4	1	Total	Zn	0
			1	1	
95	AO	1	Total	Zn	0
			1	1	

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



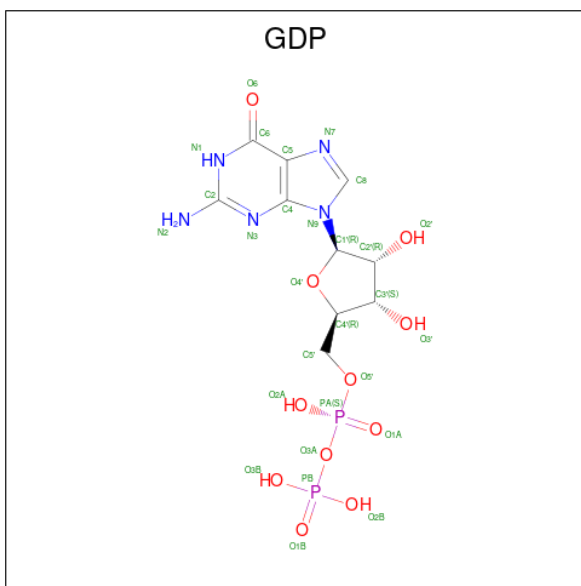
Mol	Chain	Residues	Atoms			AltConf
96	r	1	Total 4	Fe 2	S 2	0
96	AE	1	Total 4	Fe 2	S 2	0
96	AT	1	Total 4	Fe 2	S 2	0

- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 98 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 99 is water.

Mol	Chain	Residues	Atoms		AltConf
99	A	1	Total	O	0
			1	1	

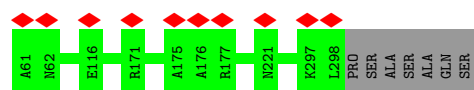
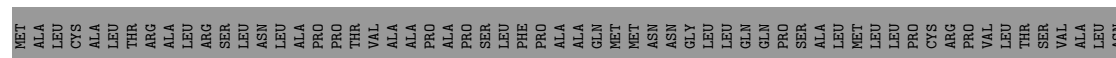
- Molecule 2: mitochondrial tRNA-Val

Chain B:  76% 19%



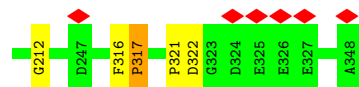
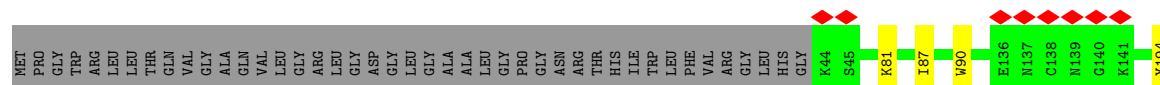
- Molecule 3: Large ribosomal subunit protein uL2m

Chain D:  78% 22%



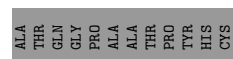
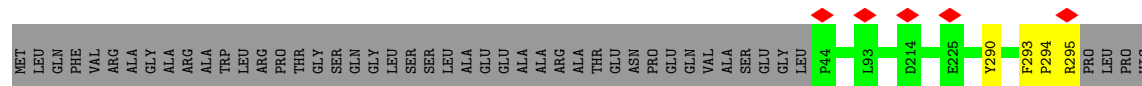
- Molecule 4: Large ribosomal subunit protein uL3m

Chain E:  85% 12%



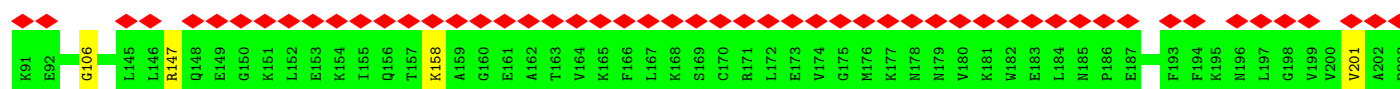
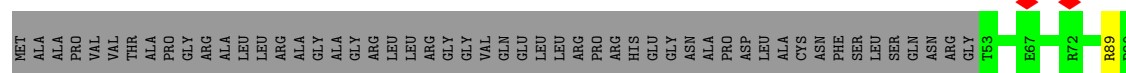
- Molecule 5: Large ribosomal subunit protein uL4m

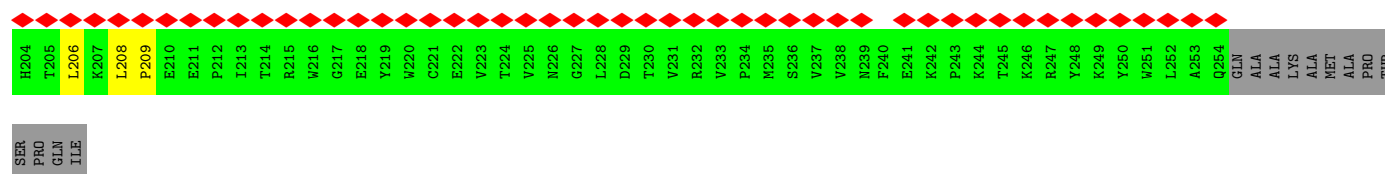
Chain F:  80% 19%



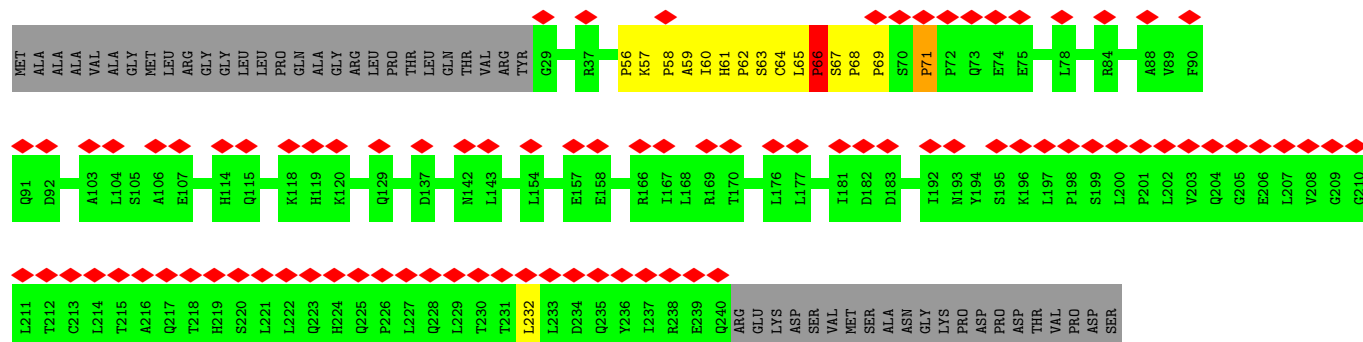
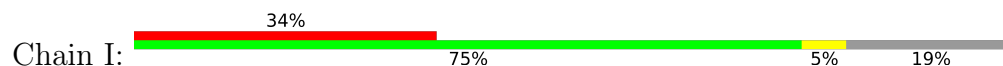
- Molecule 6: Large ribosomal subunit protein bL9m

Chain H:  73% 24%

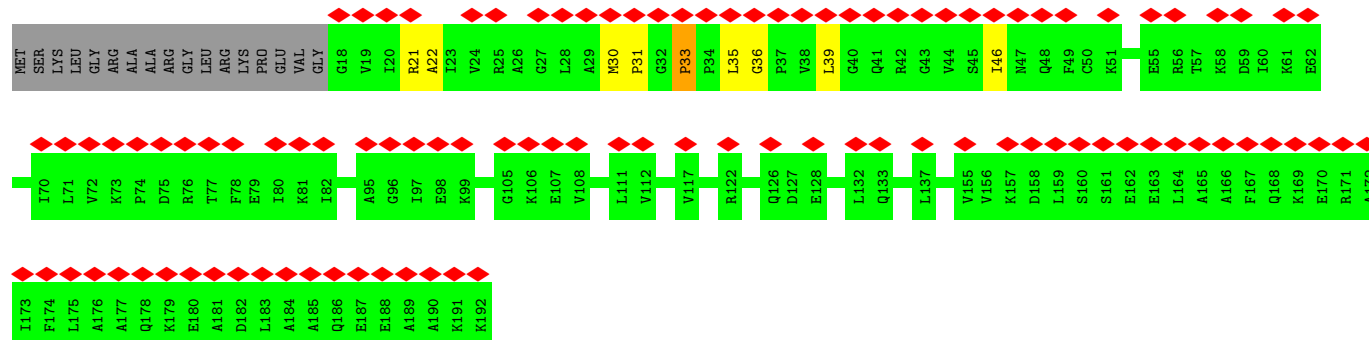
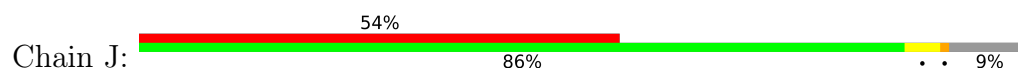




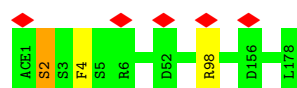
- Molecule 7: Large ribosomal subunit protein uL10m



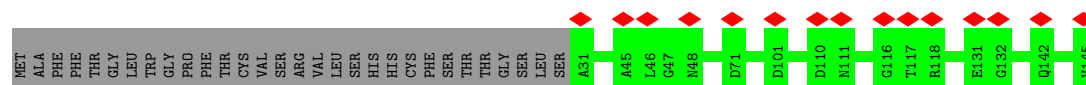
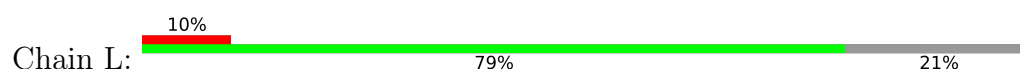
- Molecule 8: Large ribosomal subunit protein uL11m



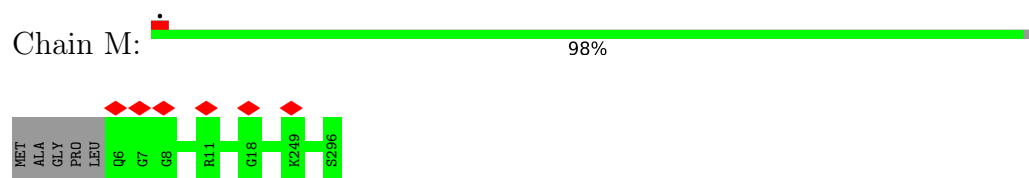
- Molecule 9: Large ribosomal subunit protein uL13m



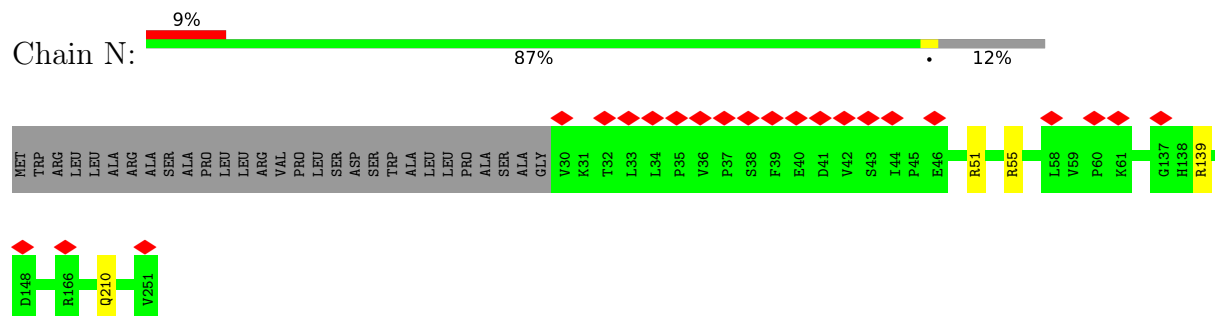
- Molecule 10: Large ribosomal subunit protein uL14m



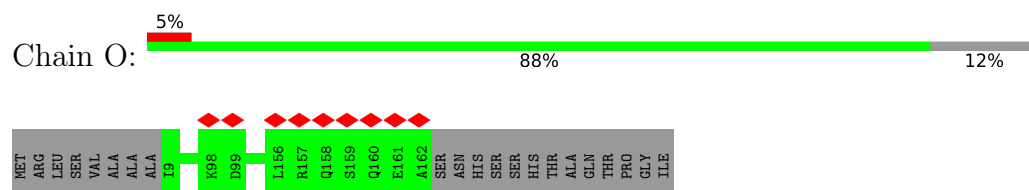
- Molecule 11: Large ribosomal subunit protein uL15m



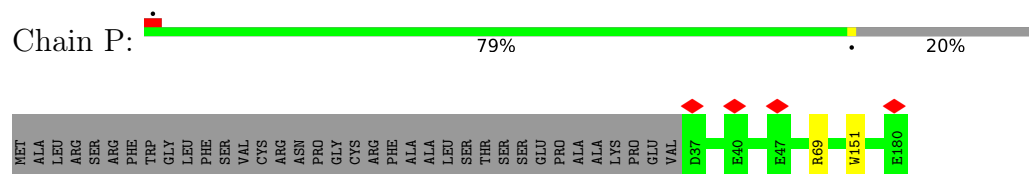
- Molecule 12: Large ribosomal subunit protein uL16m



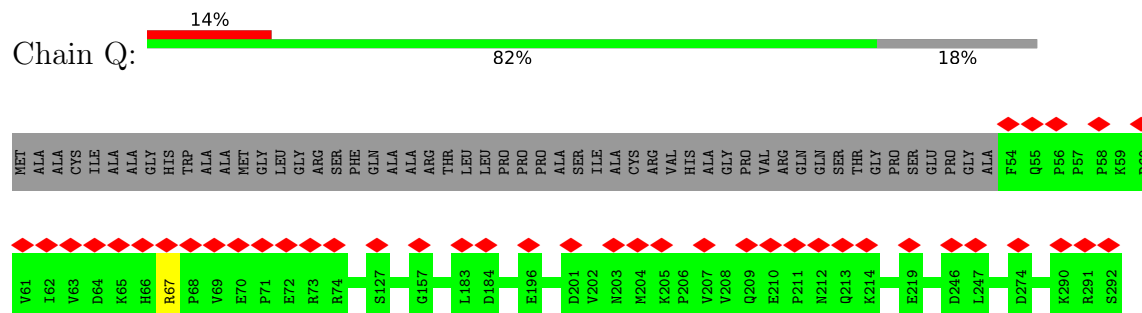
- Molecule 13: Large ribosomal subunit protein bL17m



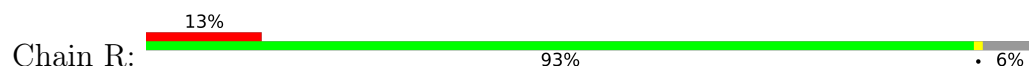
- Molecule 14: Large ribosomal subunit protein uL18m

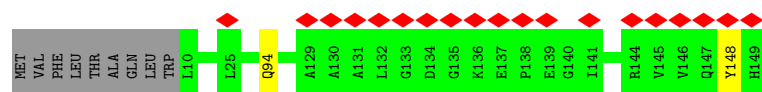


- Molecule 15: Large ribosomal subunit protein bL19m

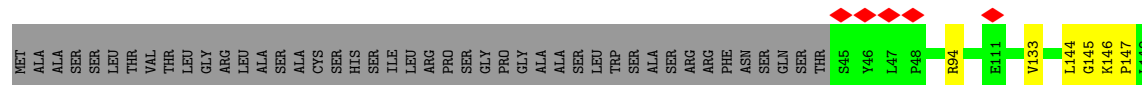
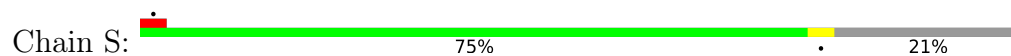


- Molecule 16: Large ribosomal subunit protein bL20m

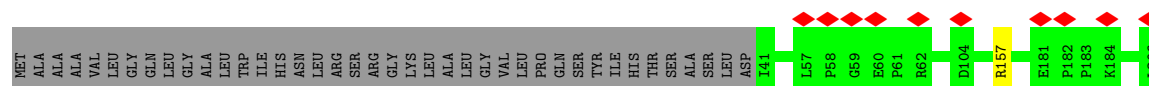
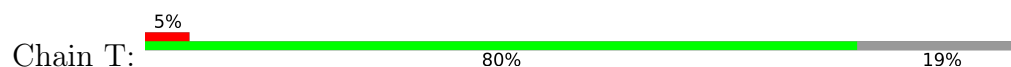




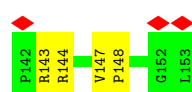
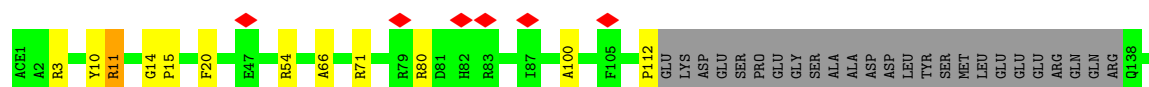
- Molecule 17: Large ribosomal subunit protein bL21m



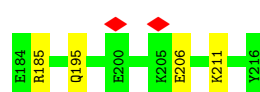
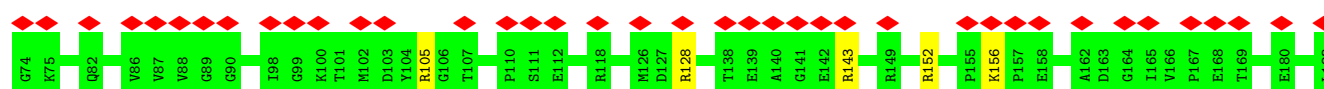
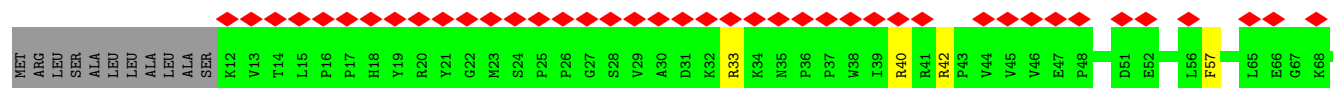
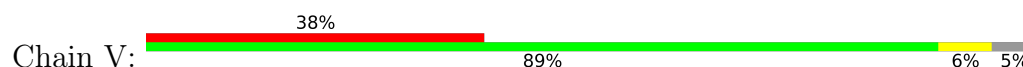
- Molecule 18: Large ribosomal subunit protein uL22m



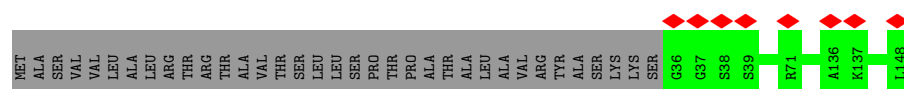
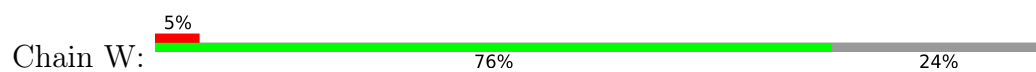
- Molecule 19: Large ribosomal subunit protein uL23m



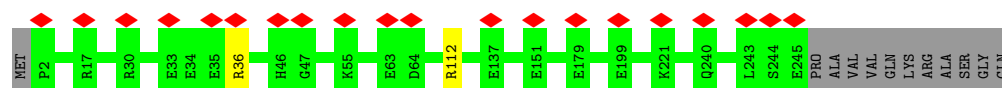
- Molecule 20: Large ribosomal subunit protein uL24m



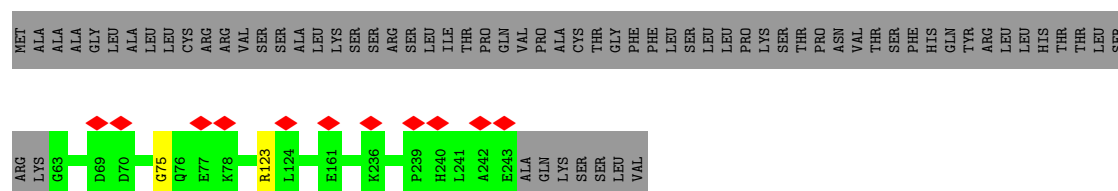
- Molecule 21: Large ribosomal subunit protein bL27m



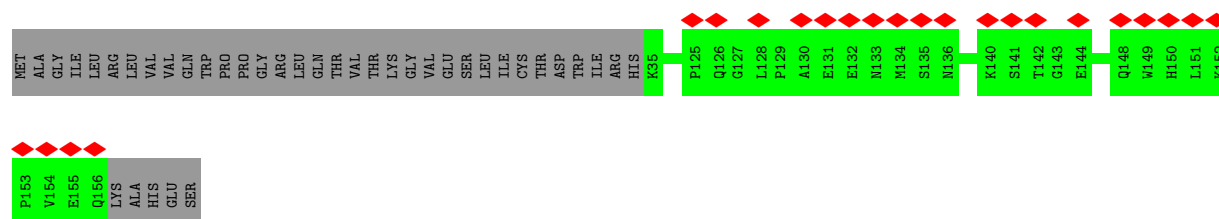
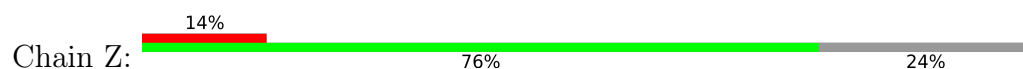
- Molecule 22: Large ribosomal subunit protein bL28m



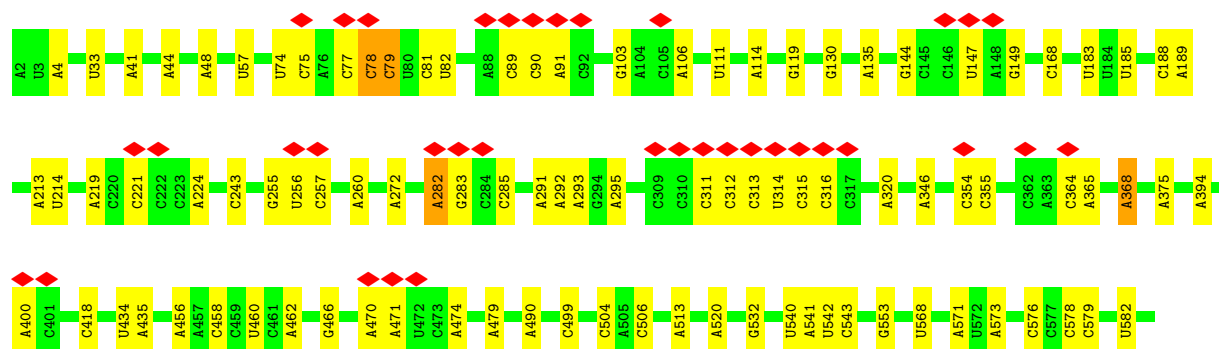
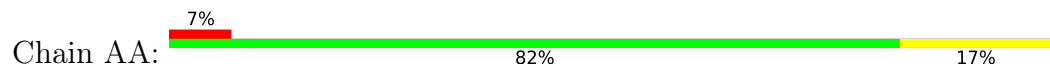
- Molecule 23: Large ribosomal subunit protein uL29m

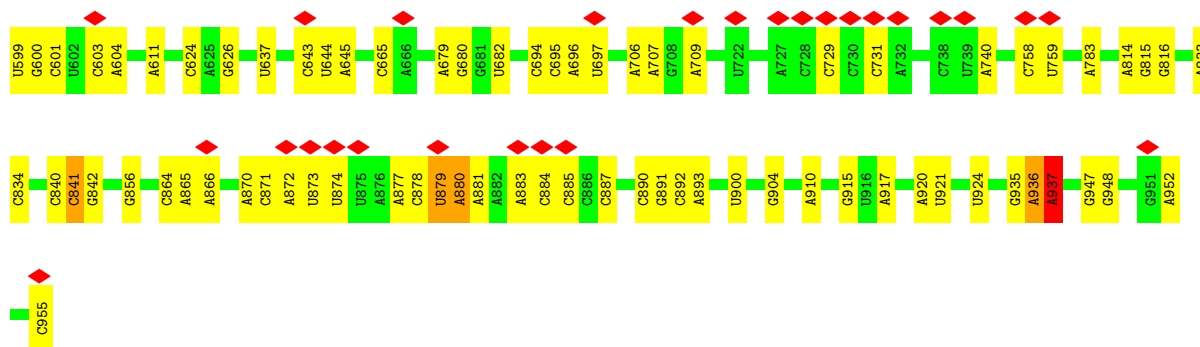


- Molecule 24: Large ribosomal subunit protein uL30m

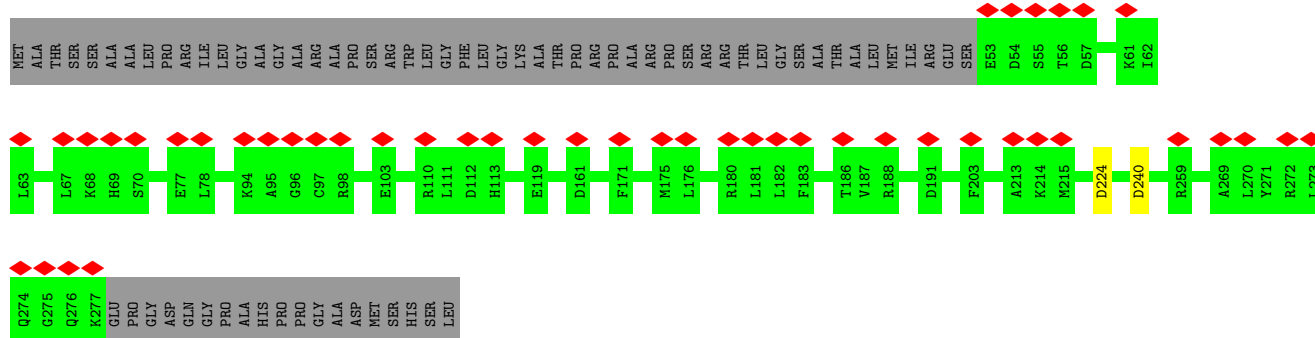
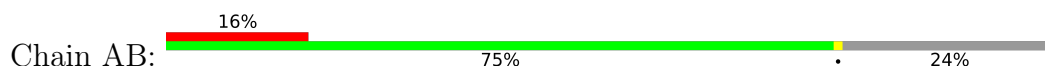


- Molecule 25: 12S mitochondrial rRNA

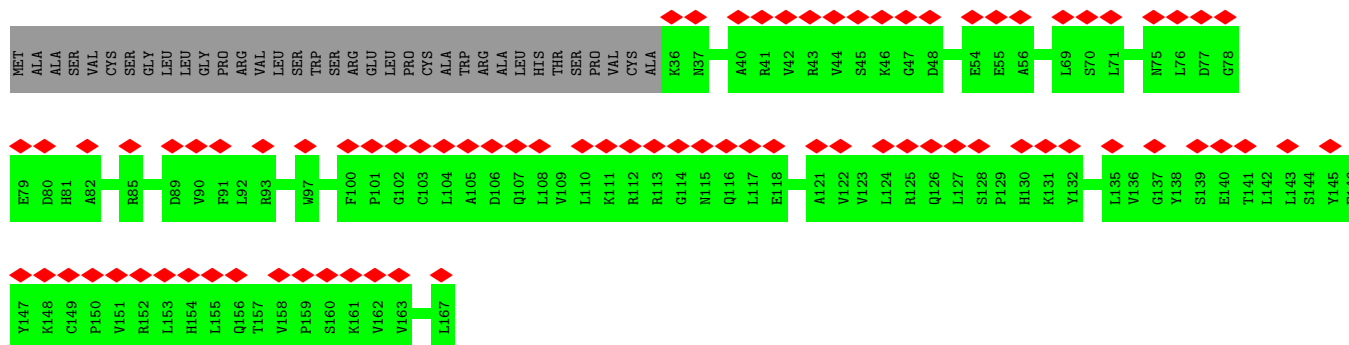
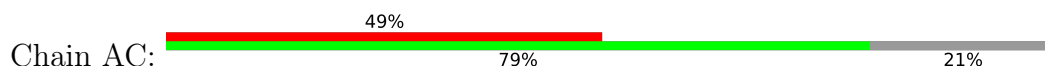




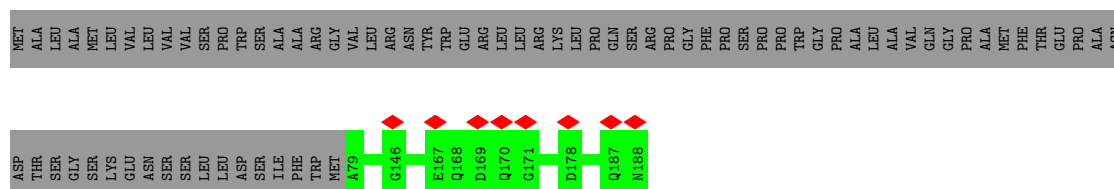
- Molecule 26: Small ribosomal subunit protein uS2m



- Molecule 27: Small ribosomal subunit protein uS3m



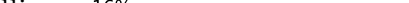
- Molecule 28: Large ribosomal subunit protein bL32m



- | |
|------|
| Y122 | L123 | D124 | L125 | T126 | L127 | M128 | M129 | A130 | L131 | G132 | K133 | K134 | K135 | N136 | V137 | E138 | P139 | F140 | T141 | S142 | V143 | L144 | S145 | L146 | P147 | P148 | P149 | F150 | A151 | S152 | E153 | I154 | N155 | K156 | V157 | A158 | V159 | F160 | F161 | E162 | N163 | A164 | S165 | E166 | V167 | K168 | I169 | A170 | E171 | E172 | N173 | G174 | A175 | A176 | F177 | A178 | G179 | G180 | T181 |
|------|

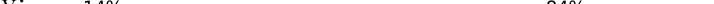
[illegible]

- Molecule 34: Large ribosomal subunit protein bL12m

Chain u:  16% 84%

[illegible]

- Molecule 34: Large ribosomal subunit protein bL12m

Chain v:  16% 14% .. 84%

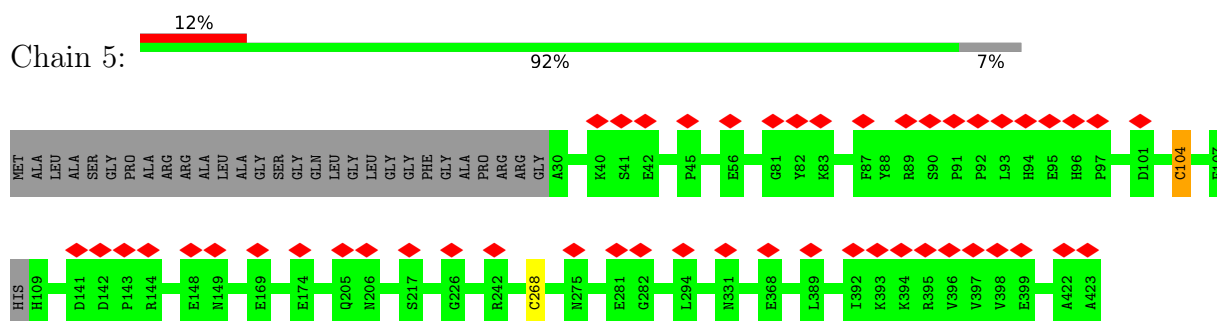
ALA	GLU	ILE	PRO	P61	WET
LYS	ILE	PRO	P62	LEU	PRO
LYS	ALA	ALA	K63	ALA	ALA
ALA	GLU	LYS	T64	ARG	ARG
LEU	THR	ARG	Q65	PRO	PRO
GLU	HIS	PHE	Q66	LEU	TRP
ALA	PHE	THR	L67	GLY	GLY
VAL	THR	VAL	Q69	PRO	PRO
GLY	ARG	ARG	D70	CYS	CYS
THR	LEU	LEU	T71	LEU	LEU
VAL	THR	THR	A72	GLY	GLY
LEU	GLU	ALA	S73	LEU	LEU
VAL	ALA	LYS	L74	ARG	ARG
GLU	PRO	PRO	T75	ALA	ALA
GLU	ASP	ASP	L76	ALA	ALA
VAL	LYS	VAL	L77	PHE	PHE
LYS	VAL	VAL	E78	LEU	LEU
LYS	LYS	LYS	I79	ALA	ALA
LEU	LEU	LEU	S80	ARG	ARG
ILE	ILE	LYS	D81	GLN	GLN
GLU	GLU	GLU	L82	VAL	VAL
ILE	ILE	ILE	N83	PRO	PRO
ASN	ASN	ASN	E84	CYS	CYS
TYR	TYR	ILE	L85	VAL	VAL
ILE	ILE	ILE	L86	CYS	CYS
GLN	GLN	GLN	K87	ALA	ALA
GLY	GLY	GLY	K88	VAL	VAL
ILE	ILE	ILE	T89	ARG	ARG
ASN	ASN	ASN	L90	WET	WET
LEU	LEU	LEU	K91	ARG	ARG
VAL	VAL	VAL	ILE	SER	SER
GLN	GLN	ALA	ALA	SER	SER
ALA	ALA	LYS	GLN	GLY	GLY
LYS	LYS	LYS	ASP	HIS	HIS
LEU	LEU	LEU	VAL	GLN	GLN
LEU	LEU	LEU	GLY	ARG	ARG
GLU	GLU	GLU	VAL	CYS	CYS
SER	SER	SER	LEU	GLU	GLU
PRO	PRO	PRO	VAL	ALA	ALA
PRO	PRO	PRO	MET	LEU	LEU
GLN	GLN	GLN	GLY	ALA	ALA
GLY	GLY	GLY	VAL	GLY	GLY
ILE	ILE	ILE	VAL	ALA	ALA
LYS	LYS	LYS	NET	PRO	PRO
ALA	ALA	ALA	GLY	LEU	LEU
ASN	ASN	ASN	SER	LEU	LEU
VAL	VAL	VAL	GLY	ASN	ASN
VAL	VAL	VAL	ALA	ALA	ALA
LYS	LYS	LYS	VAL	PRO	PRO
ALA	ALA	ALA	PRO	LYS	LYS
ALA	ALA	ALA	ALA	GLU	GLU
ALA	ALA	ALA	ALA	760	760

- Molecule 34: Large ribosomal subunit protein bL12m

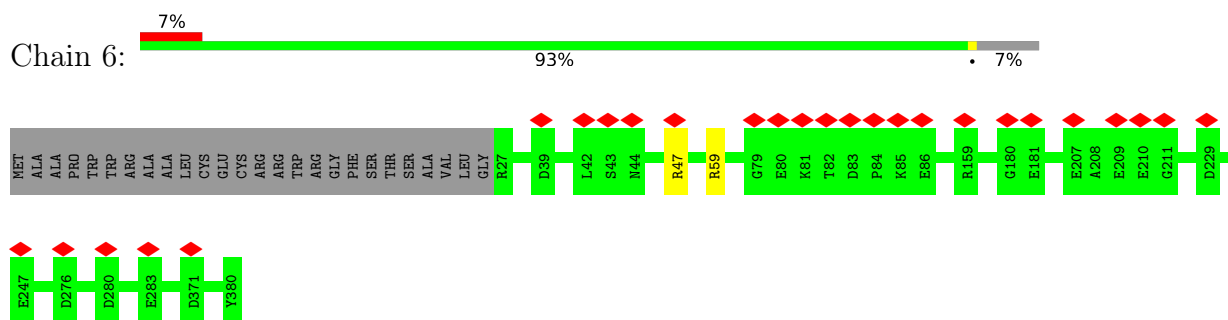
Chain y : 16% 14% 84%

[illegible]

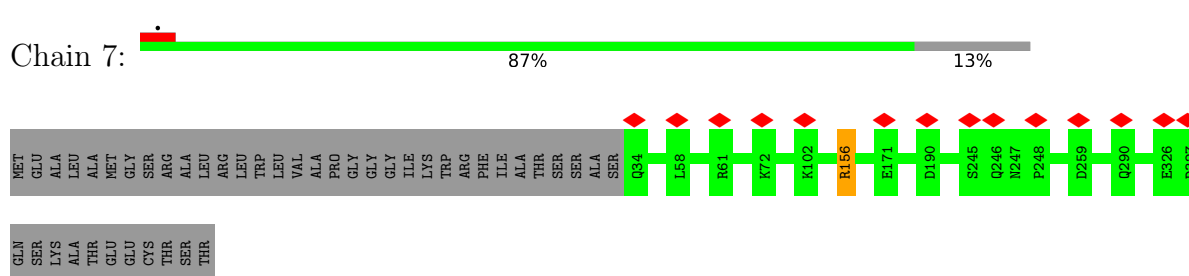
- Molecule 35: Large ribosomal subunit protein mL37



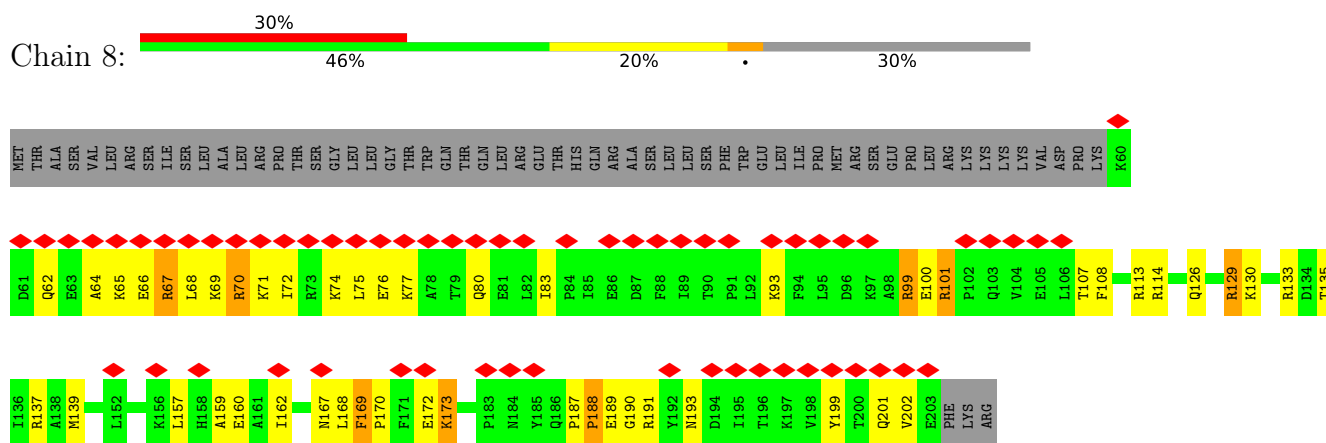
- Molecule 36: Large ribosomal subunit protein mL38



- Molecule 37: Large ribosomal subunit protein mL39

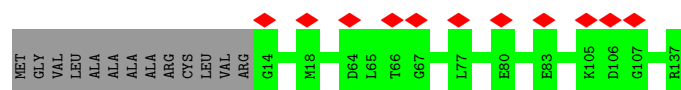


- Molecule 38: Large ribosomal subunit protein mL40

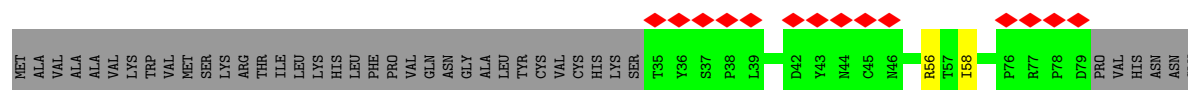


- Molecule 39: Large ribosomal subunit protein mL41

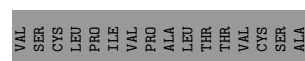
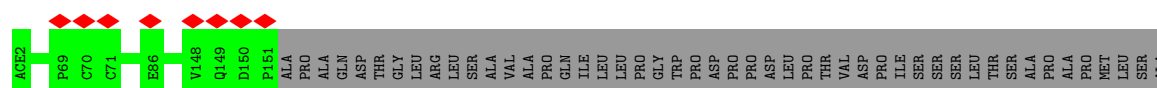




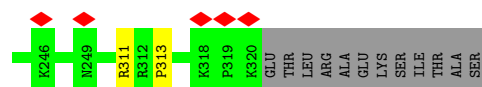
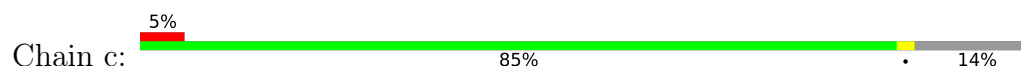
- Molecule 40: Large ribosomal subunit protein mL42



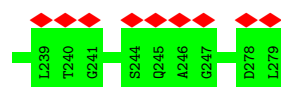
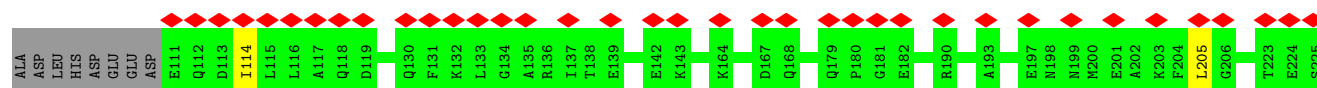
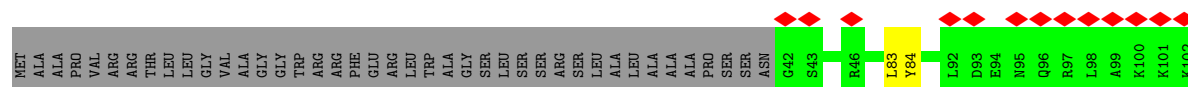
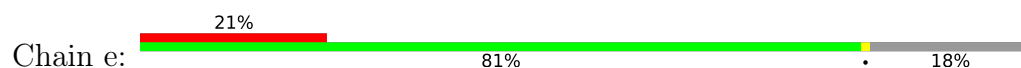
- Molecule 41: Large ribosomal subunit protein mL43



- Molecule 42: Large ribosomal subunit protein mL44



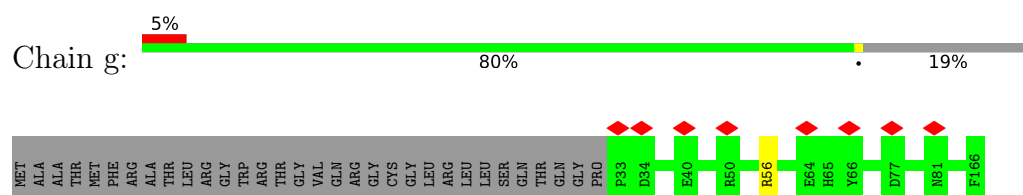
- Molecule 43: Large ribosomal subunit protein mL46



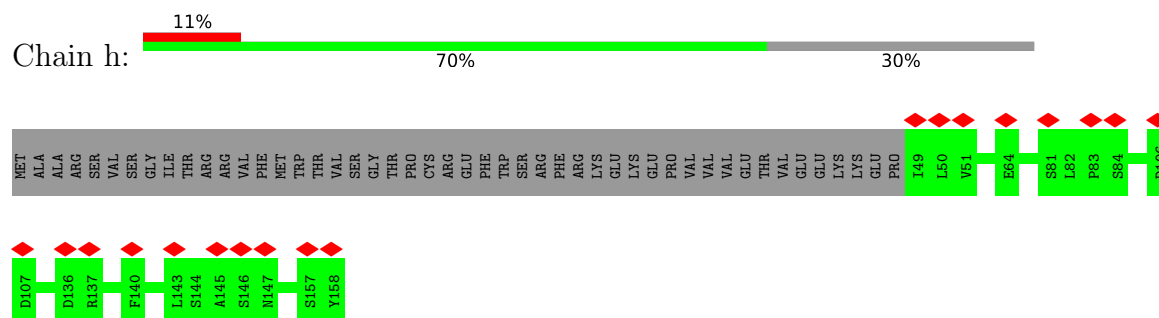
- Molecule 44: Large ribosomal subunit protein mL48



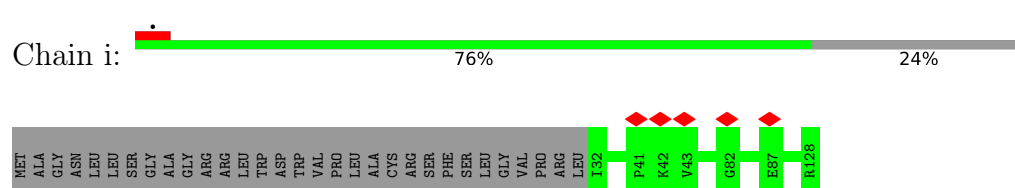
- Molecule 45: Large ribosomal subunit protein mL49



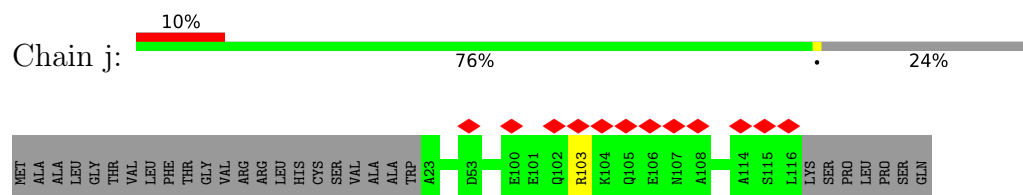
- Molecule 46: Large ribosomal subunit protein mL50



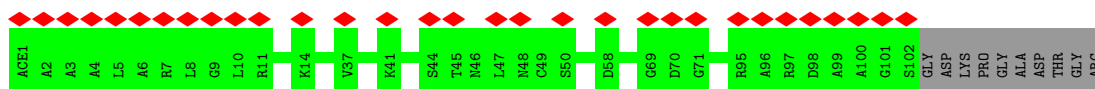
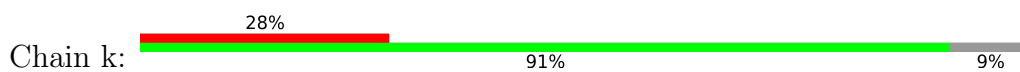
- Molecule 47: Large ribosomal subunit protein mL51



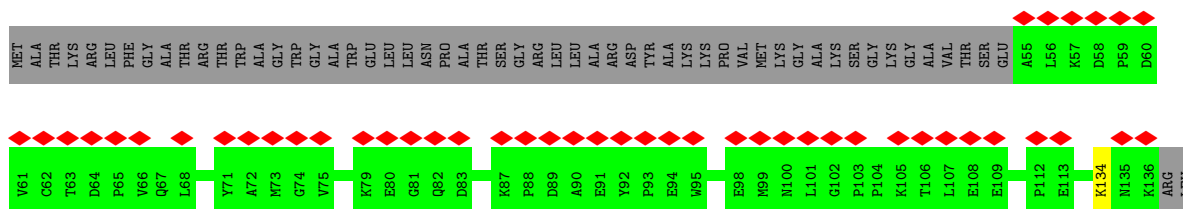
- Molecule 48: Large ribosomal subunit protein mL52



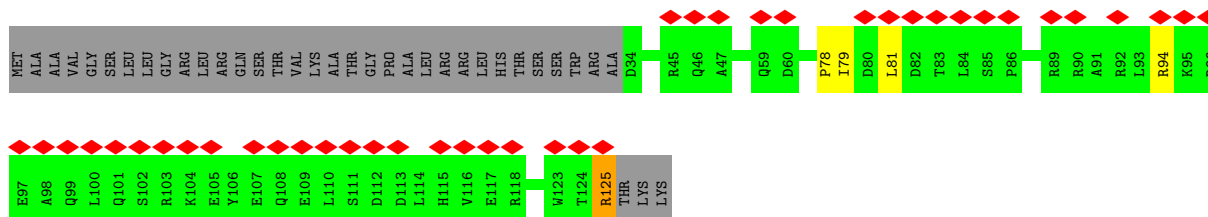
- Molecule 49: Large ribosomal subunit protein mL53



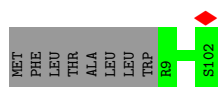
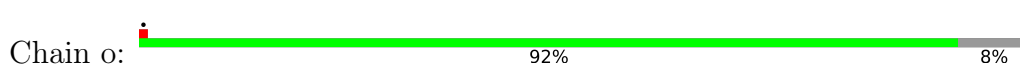
- Molecule 50: Large ribosomal subunit protein mL54



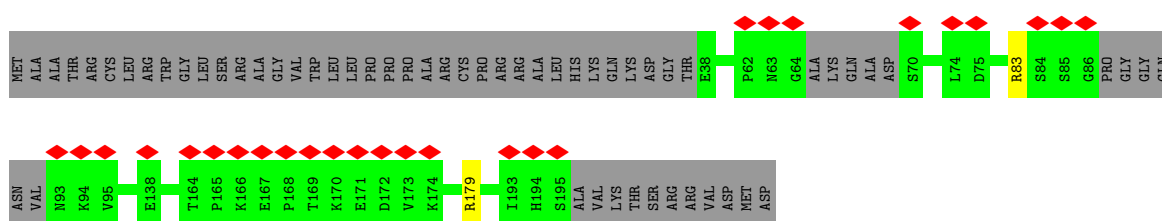
- Molecule 51: Large ribosomal subunit protein mL55



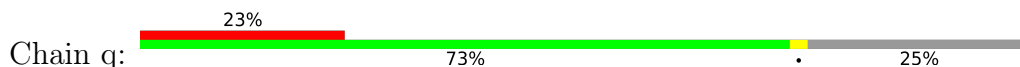
- Molecule 52: Large ribosomal subunit protein mL63



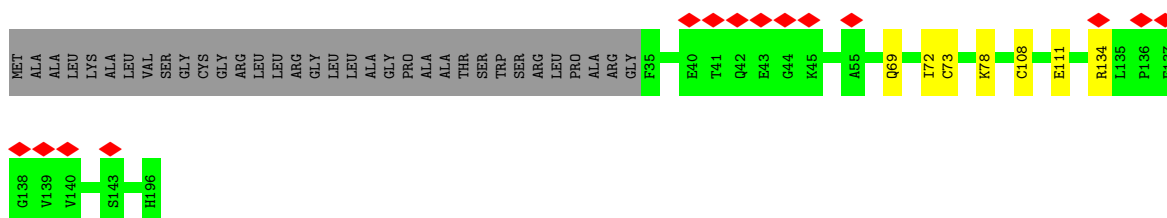
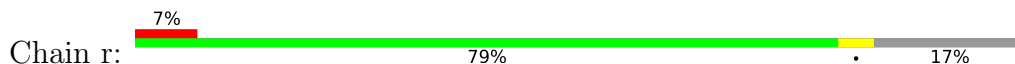
- Molecule 53: Large ribosomal subunit protein mL62



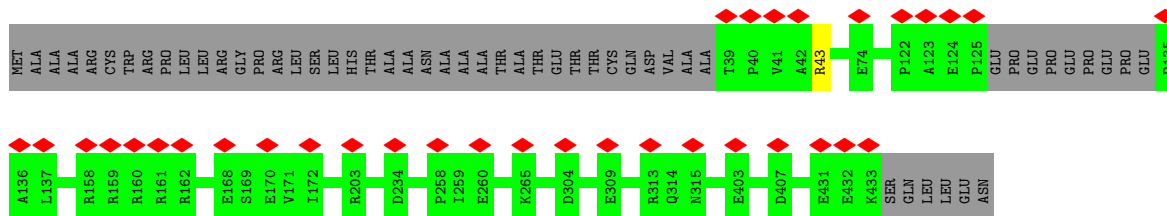
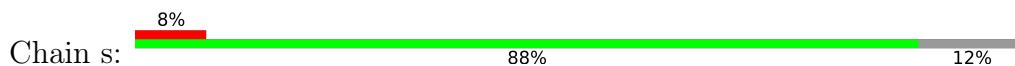
- Molecule 54: Large ribosomal subunit protein mL64



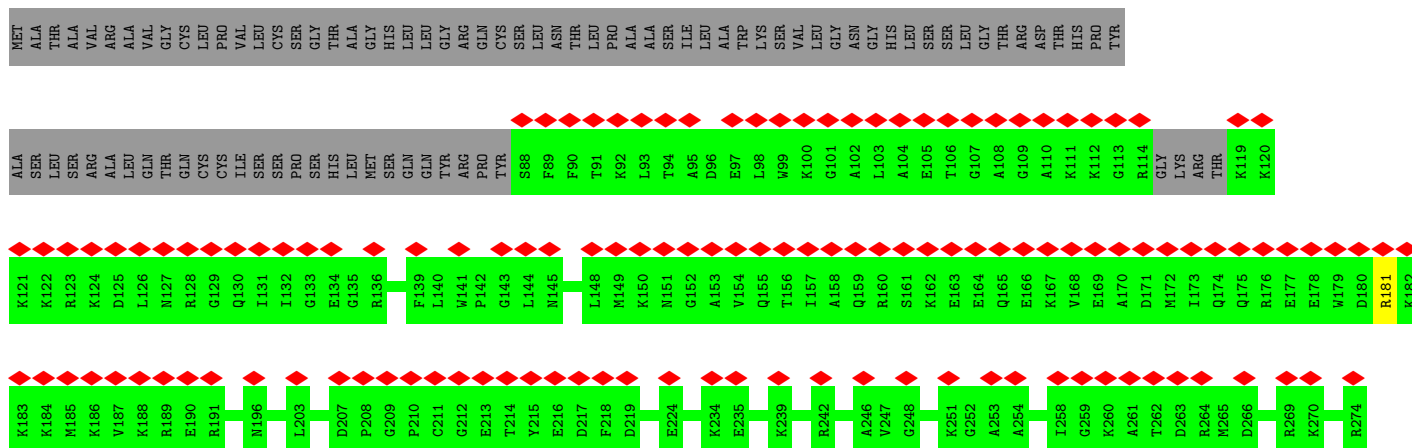
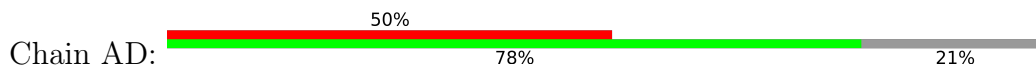
- Molecule 55: Large ribosomal subunit protein mL66

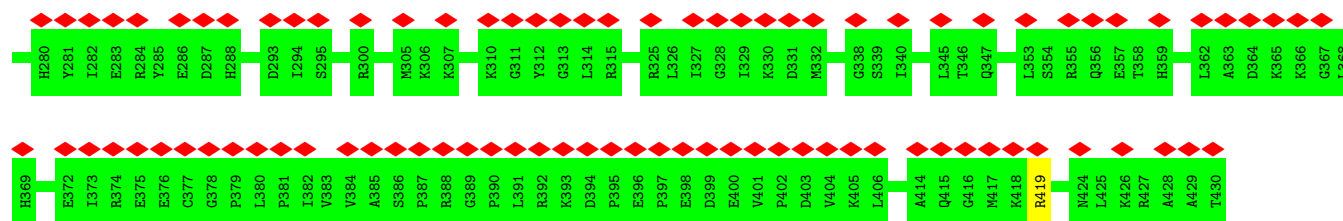


- Molecule 56: Large ribosomal subunit protein mL65



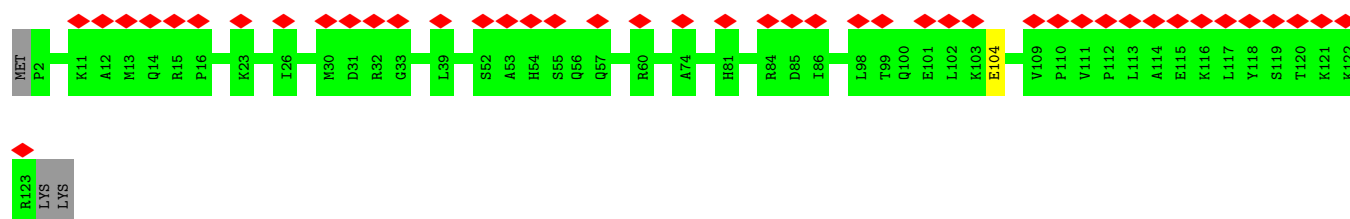
- Molecule 57: Small ribosomal subunit protein uS5m





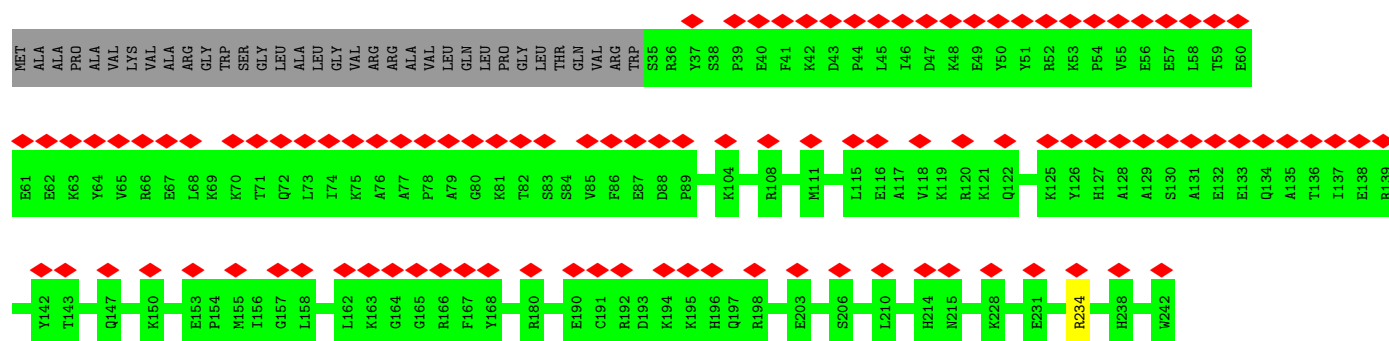
- Molecule 58: Small ribosomal subunit protein bS6m

Chain AE: 35% 97%



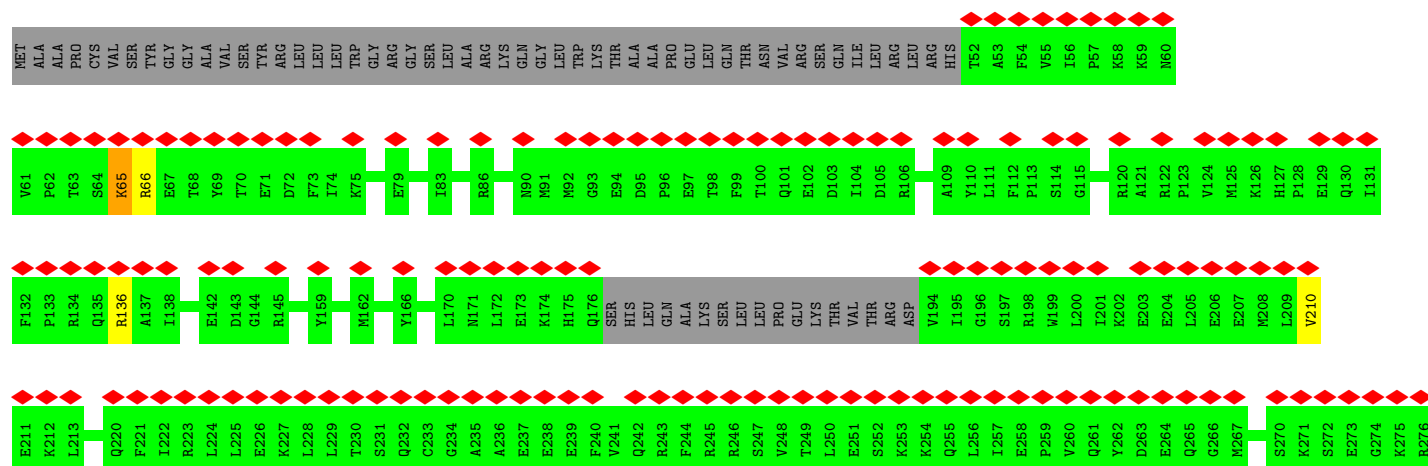
- Molecule 59: Small ribosomal subunit protein uS7m

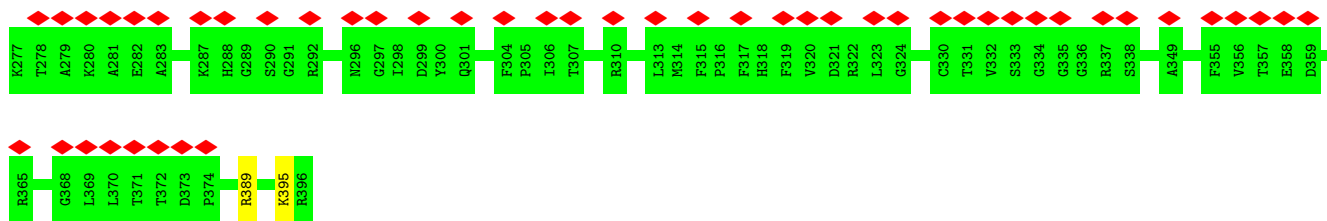
Chain AF: 44% 86% 14%



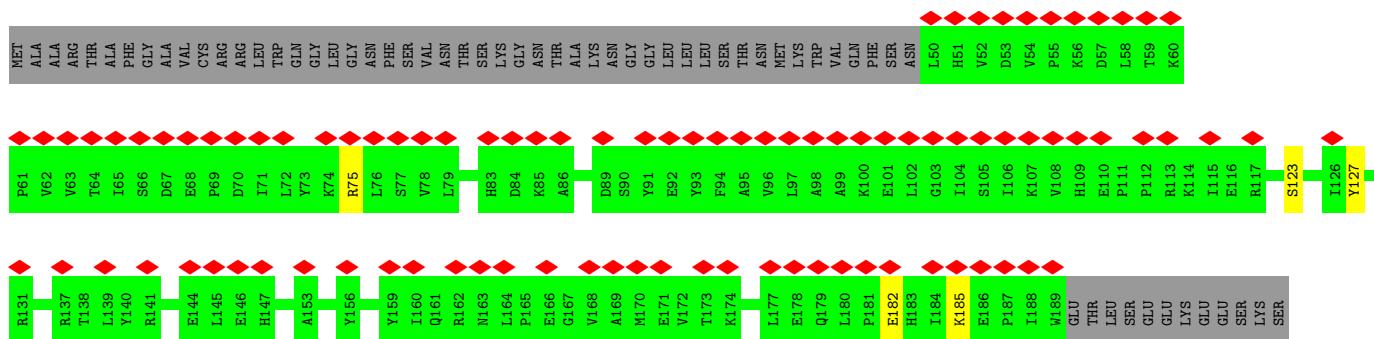
- Molecule 60: Small ribosomal subunit protein uS9m

Chain AG: 50% 81% 17%

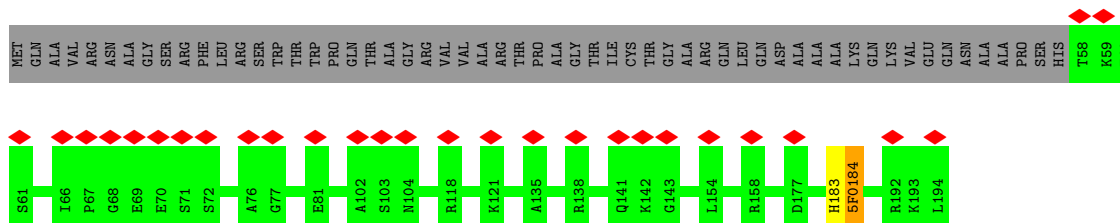




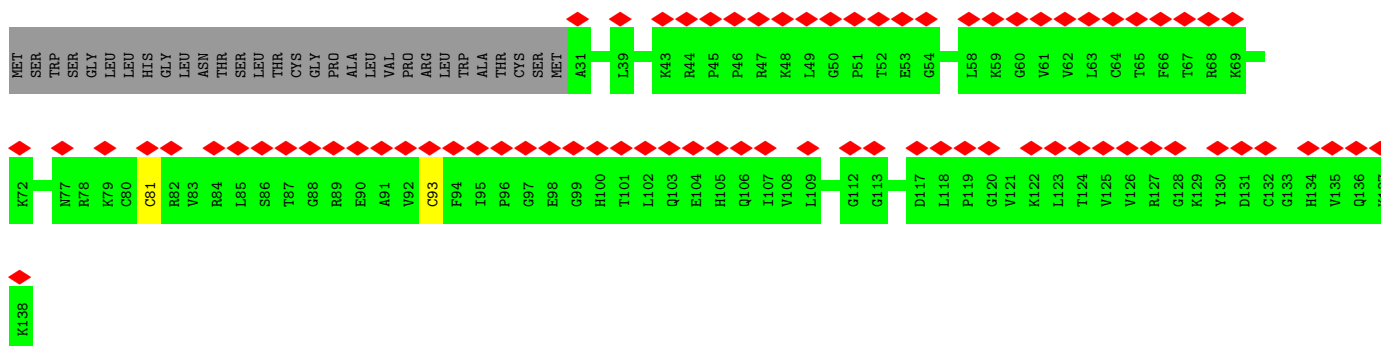
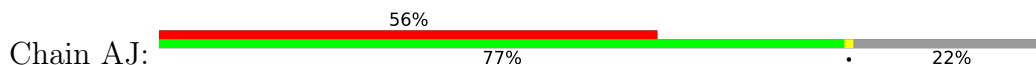
- Molecule 61: Small ribosomal subunit protein uS10m



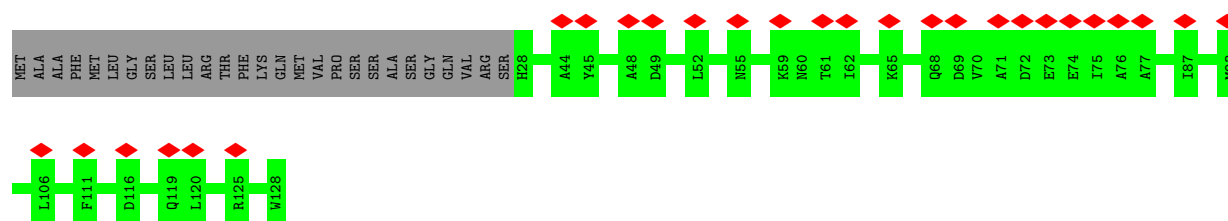
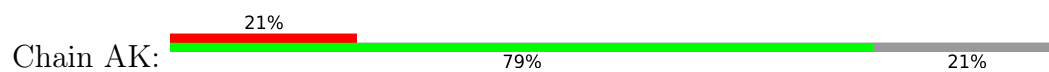
- Molecule 62: Small ribosomal subunit protein uS11m



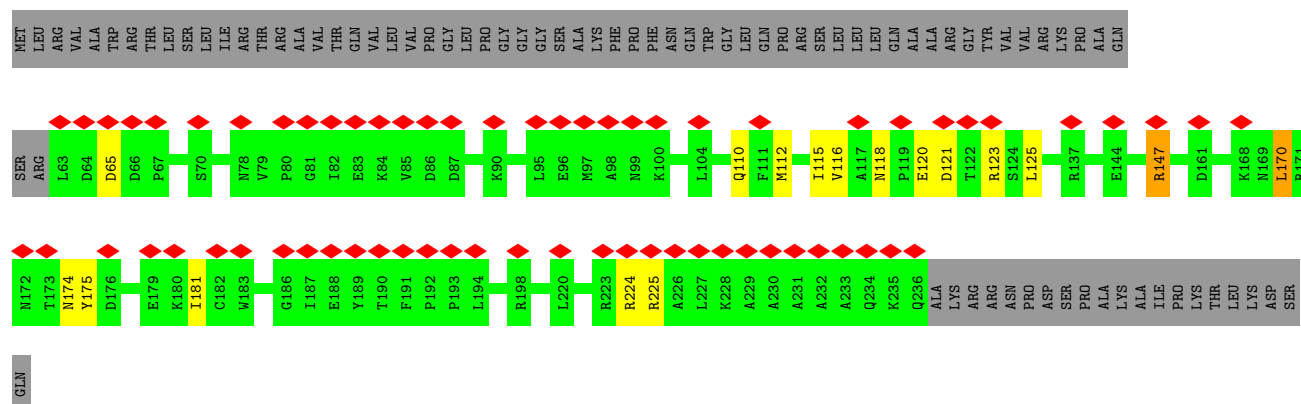
- Molecule 63: Small ribosomal subunit protein uS12m



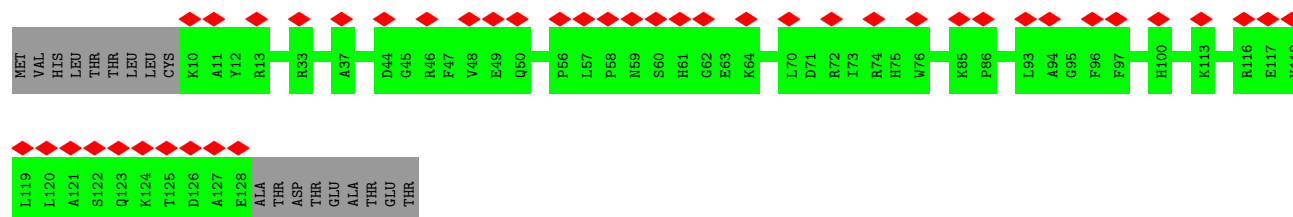
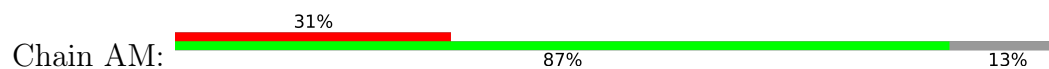
- Molecule 64: Small ribosomal subunit protein uS14m



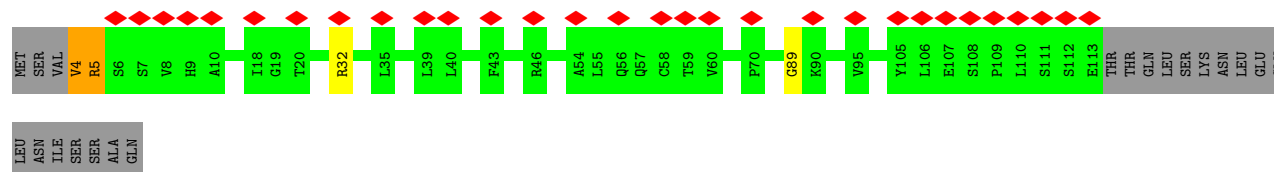
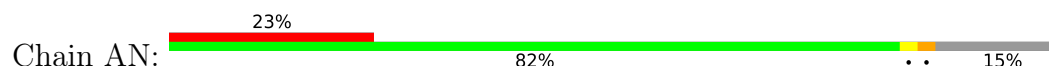
- Molecule 65: Small ribosomal subunit protein uS15m



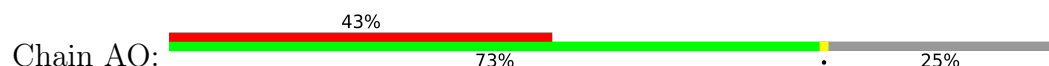
- Molecule 66: Small ribosomal subunit protein bS16m

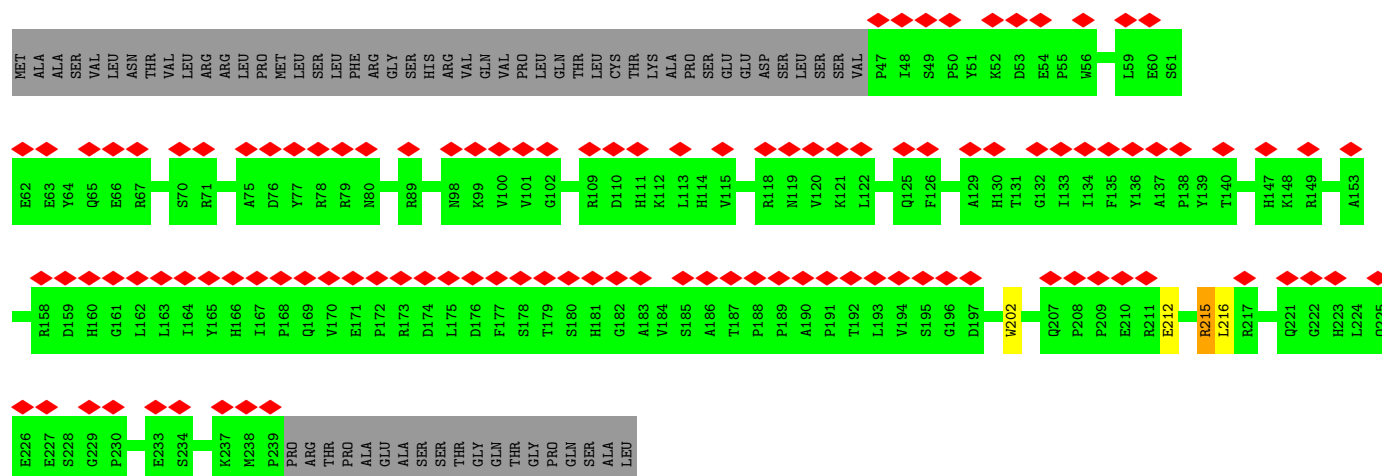


- Molecule 67: Small ribosomal subunit protein uS17m

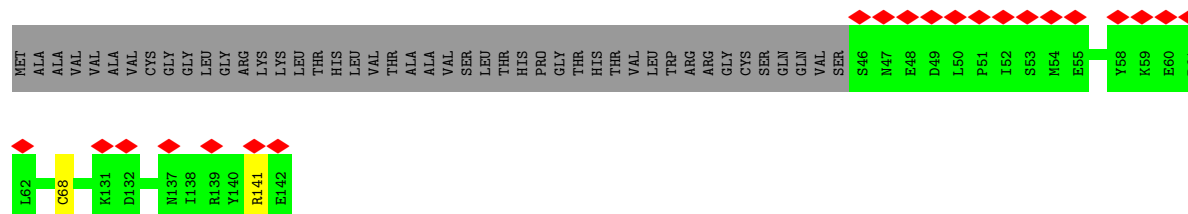


- Molecule 68: Small ribosomal subunit protein mS40

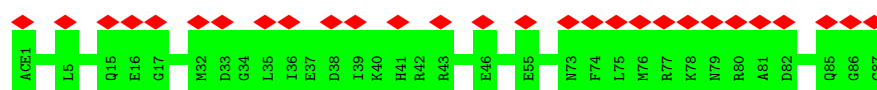




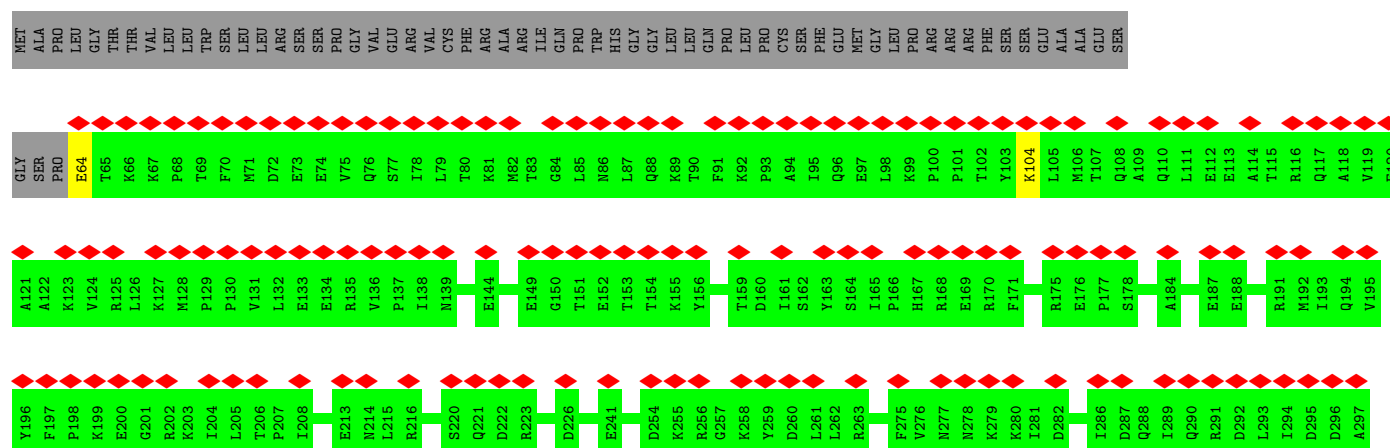
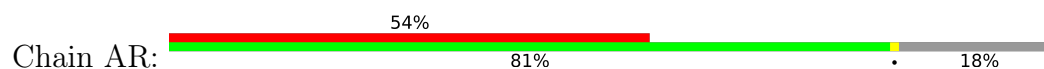
- Molecule 69: Small ribosomal subunit protein bS18m



- Molecule 70: Small ribosomal subunit protein bS21m



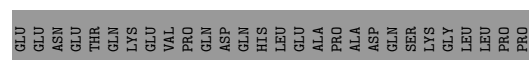
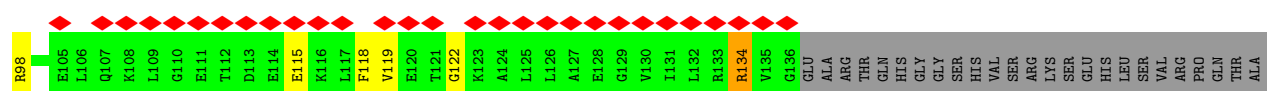
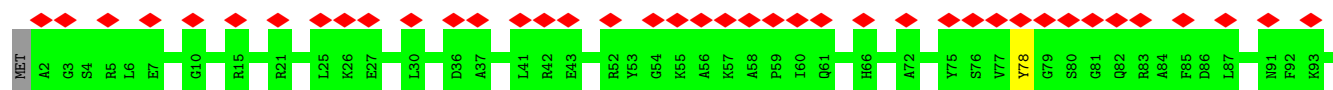
- Molecule 71: Small ribosomal subunit protein mS22





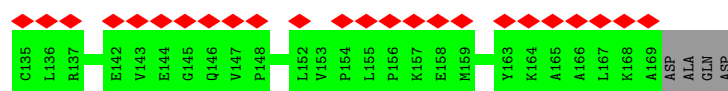
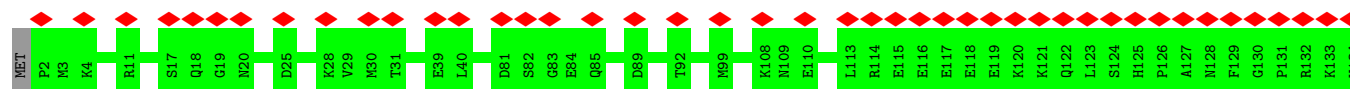
- Molecule 72: Small ribosomal subunit protein mS23

Chain AS:



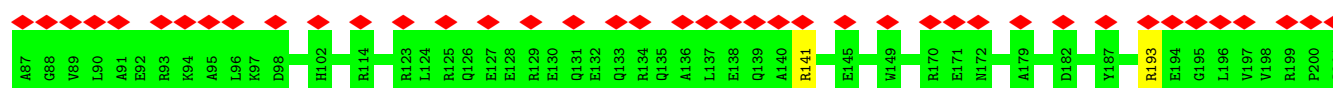
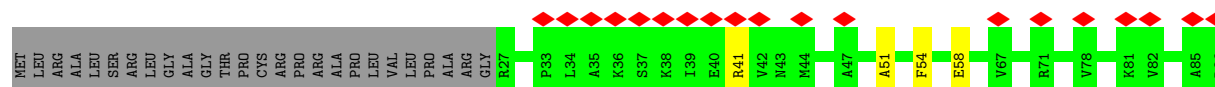
- Molecule 73: Small ribosomal subunit protein mS25

Chain AT:



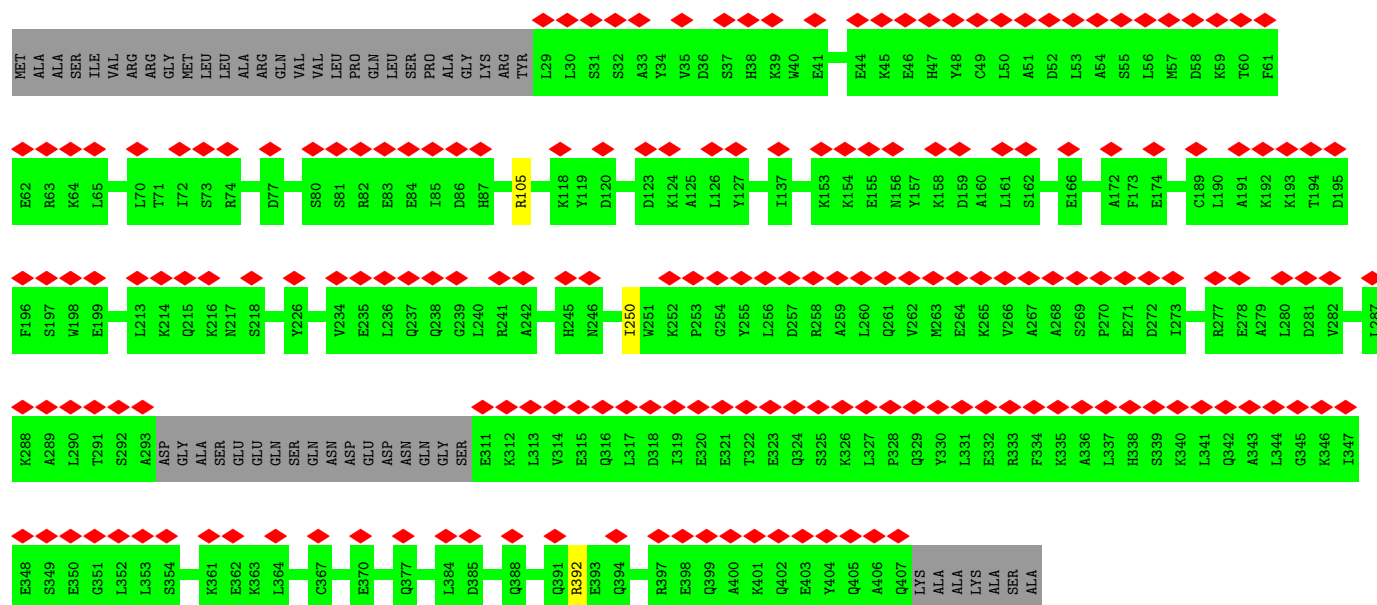
- Molecule 74: Small ribosomal subunit protein mS26

Chain AU:

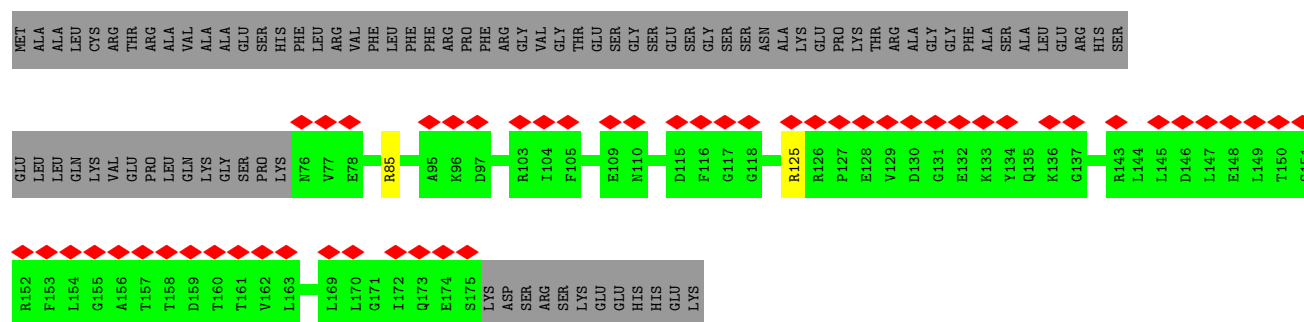


- Molecule 75: Small ribosomal subunit protein mS27

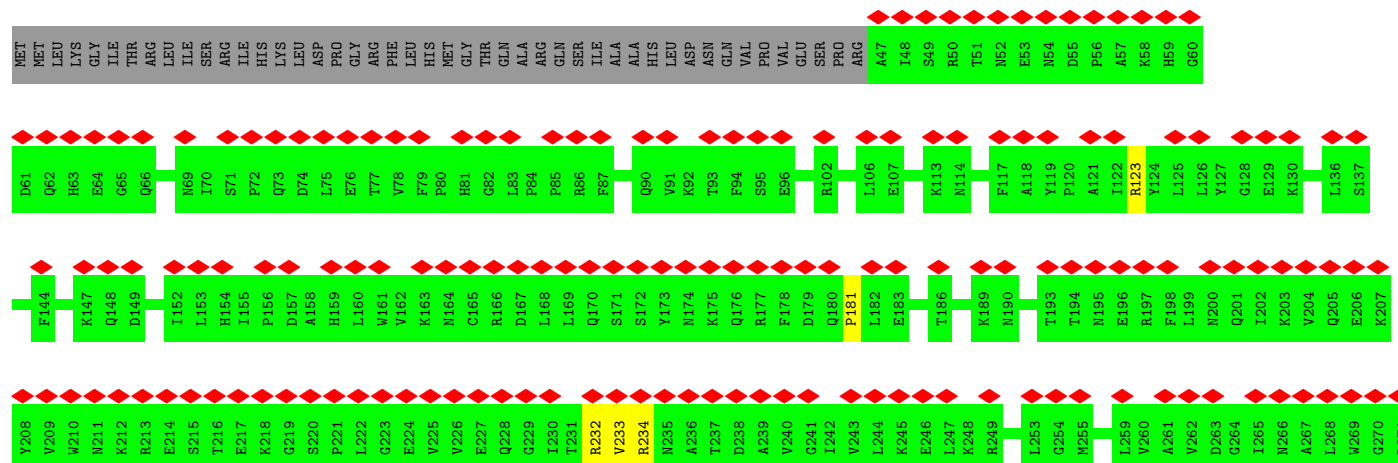
Chain AV:

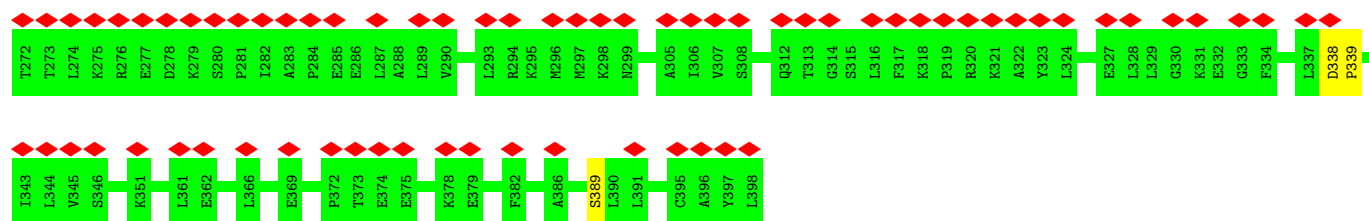


• Molecule 76: Small ribosomal subunit protein bS1m



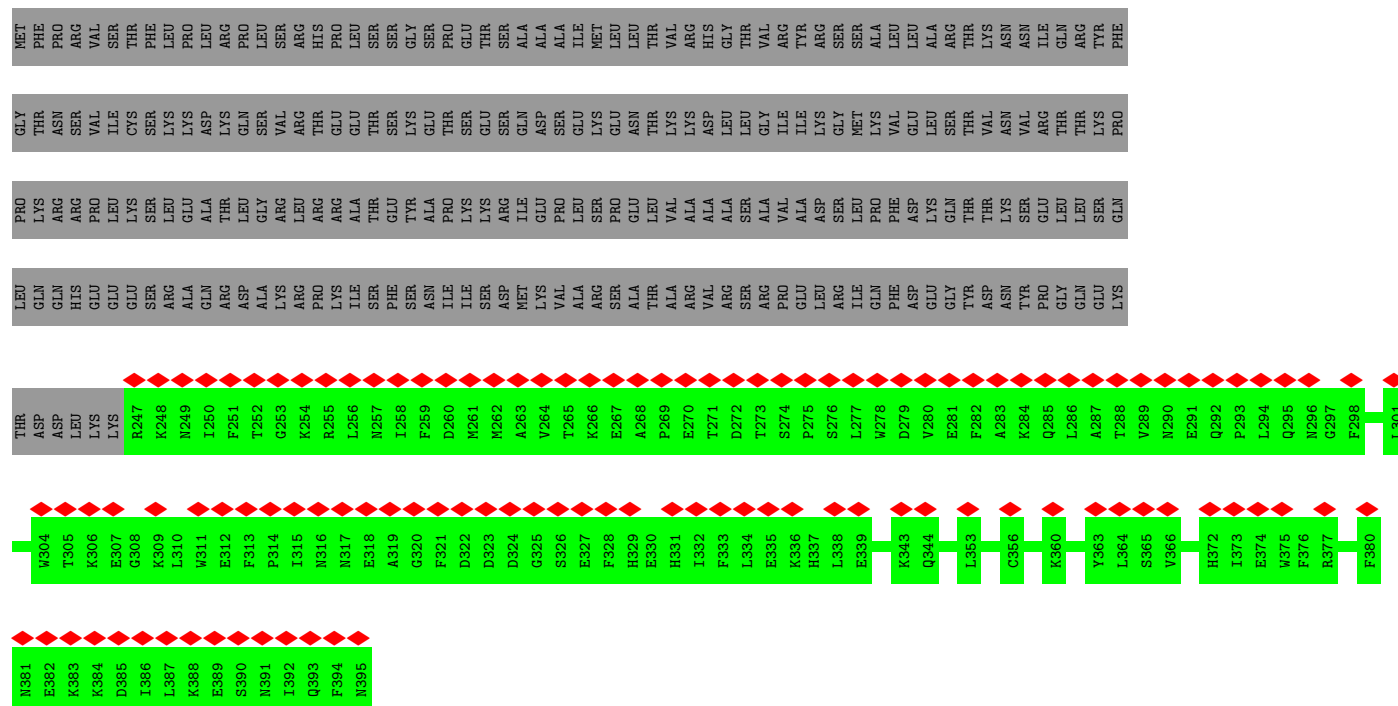
• Molecule 77: Small ribosomal subunit protein mS29





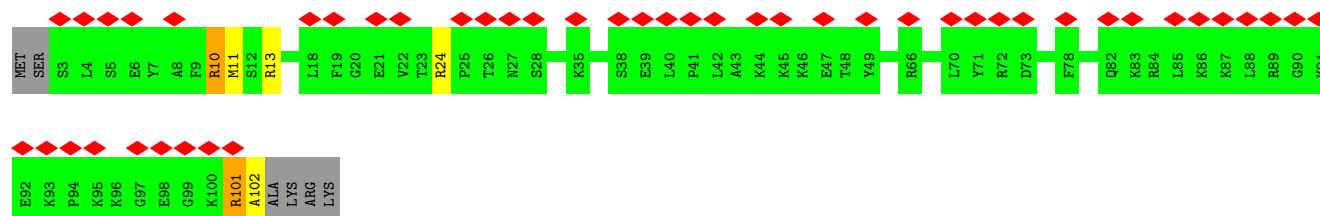
• Molecule 78: Small ribosomal subunit protein mS31

Chain AY: 29% 38% 62%



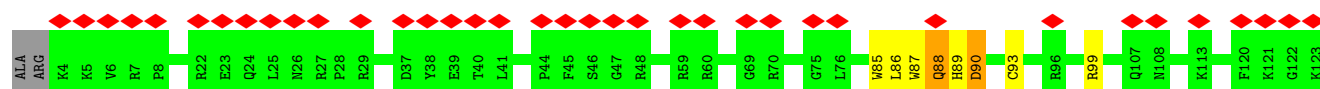
• Molecule 79: Small ribosomal subunit protein mS33

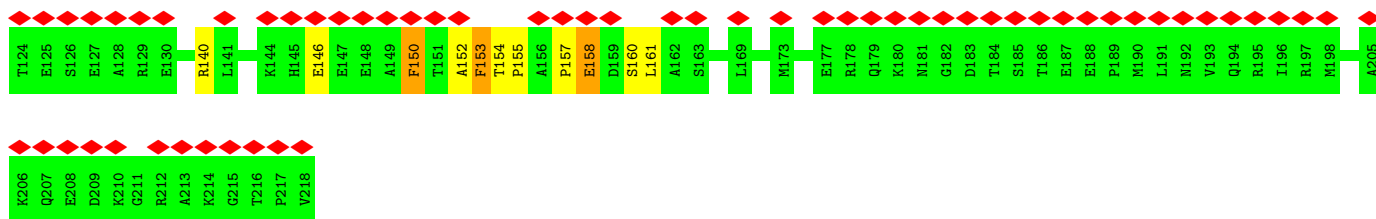
Chain AZ: 44% 89% 6%



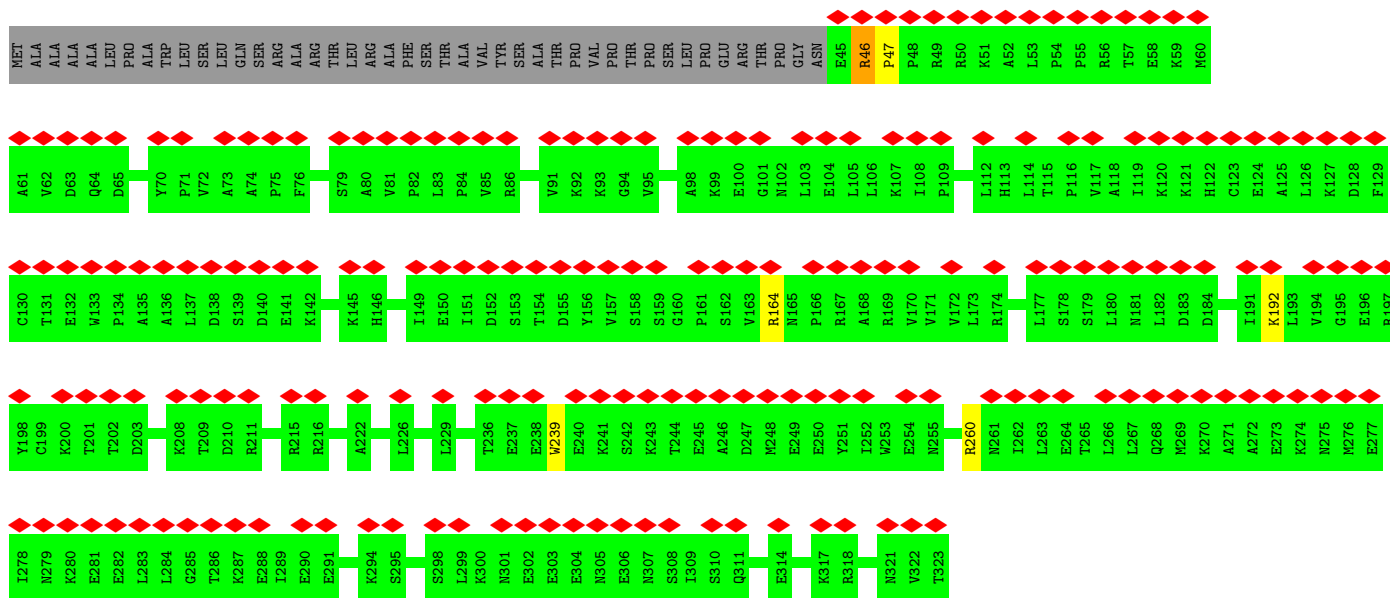
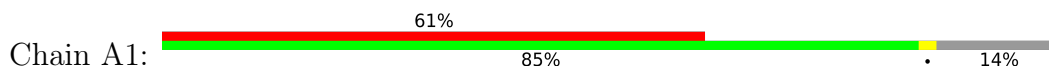
• Molecule 80: Small ribosomal subunit protein mS34

Chain A0: 45% 90% 6%

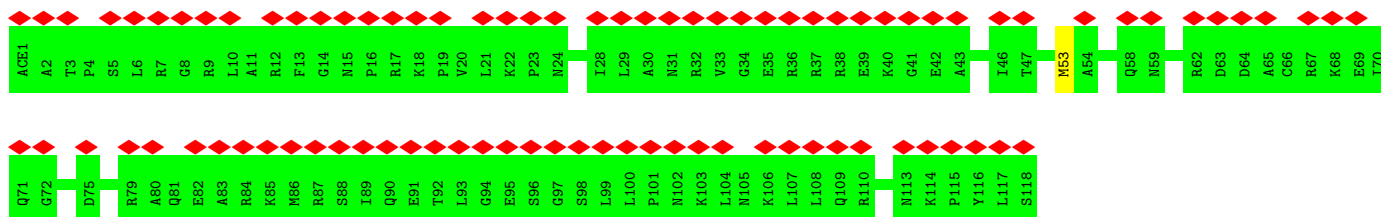
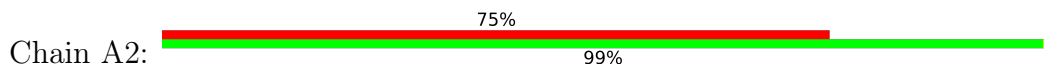




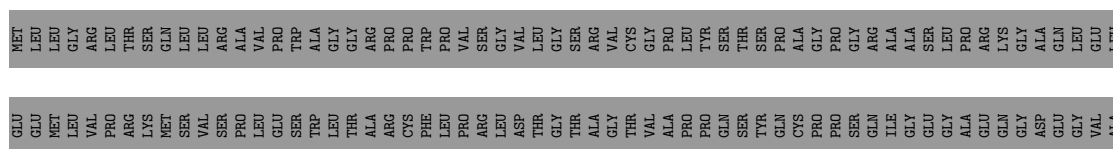
• Molecule 81: Small ribosomal subunit protein mS35

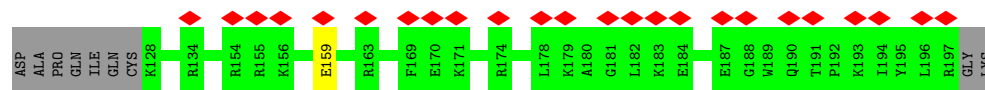


• Molecule 82: Small ribosomal subunit protein mS37



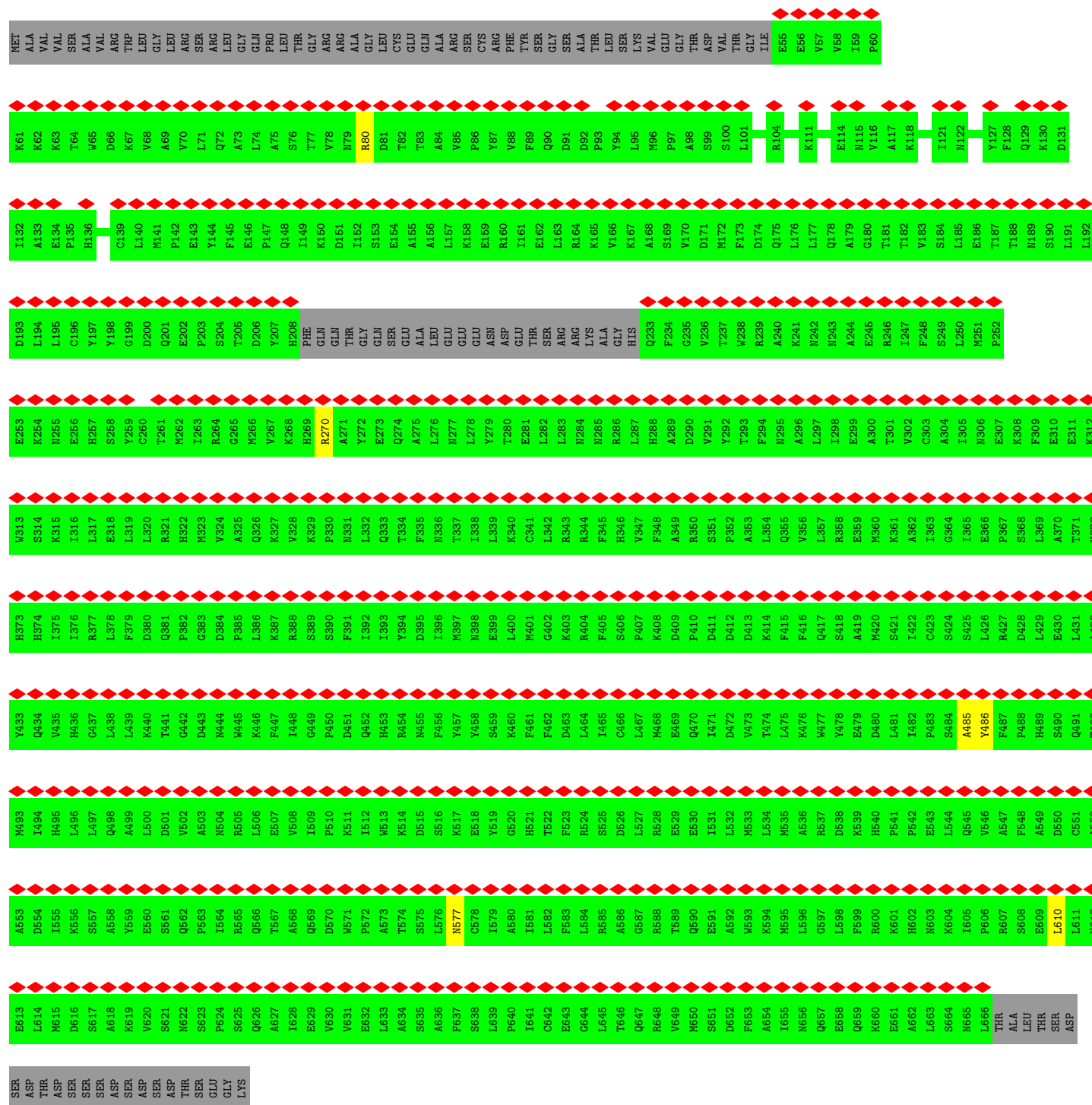
• Molecule 83: Small ribosomal subunit protein bS22, mitochondrial



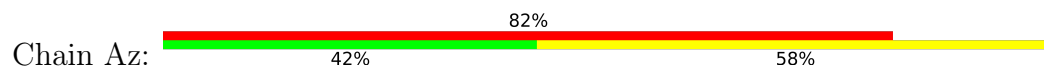


• Molecule 84: Small ribosomal subunit protein mS39

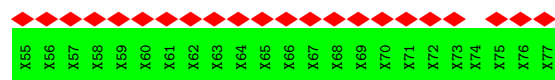
Chain A4: 82%
84% 15%



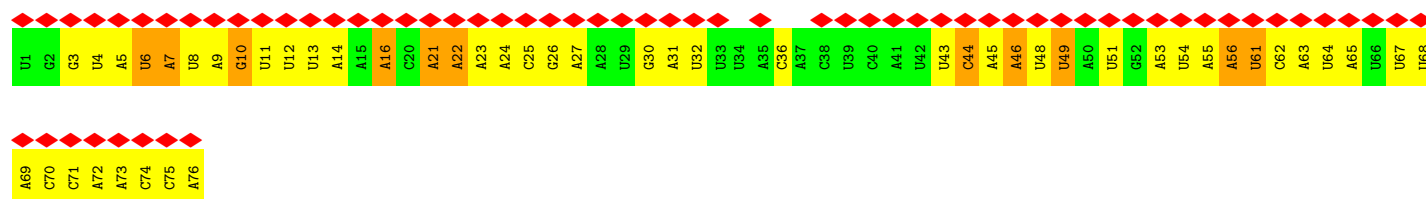
- Molecule 85: mRNA (Visualization example)



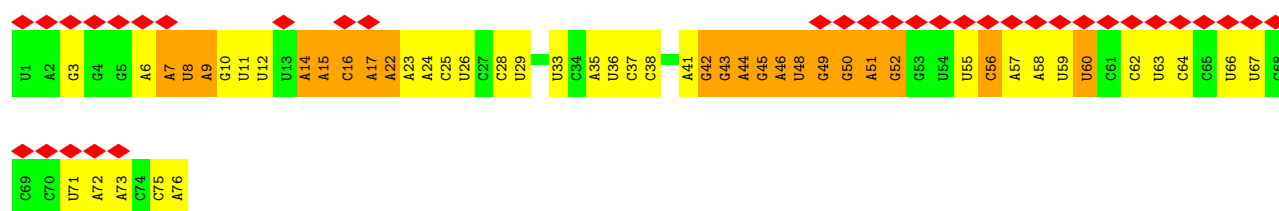
- Molecule 86: COX1 nascent chain



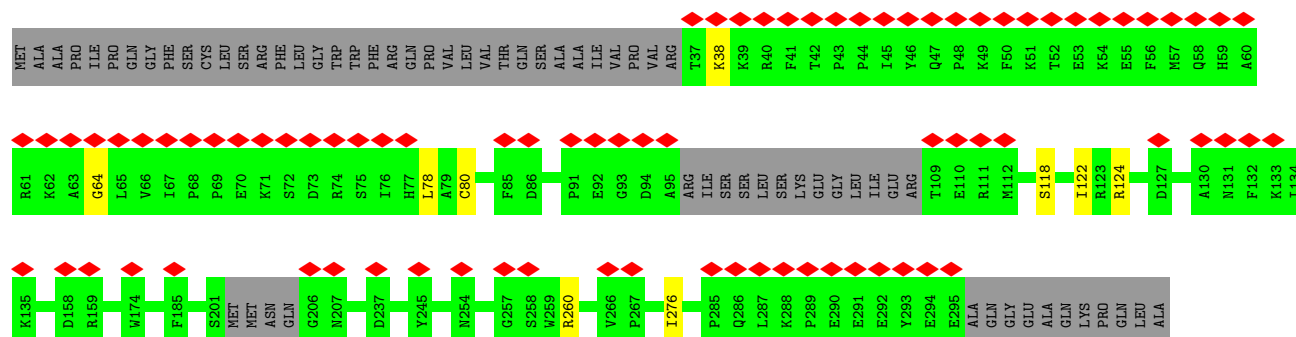
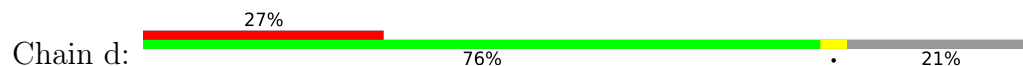
- Molecule 87: A-site tRNA (Visualisation example)



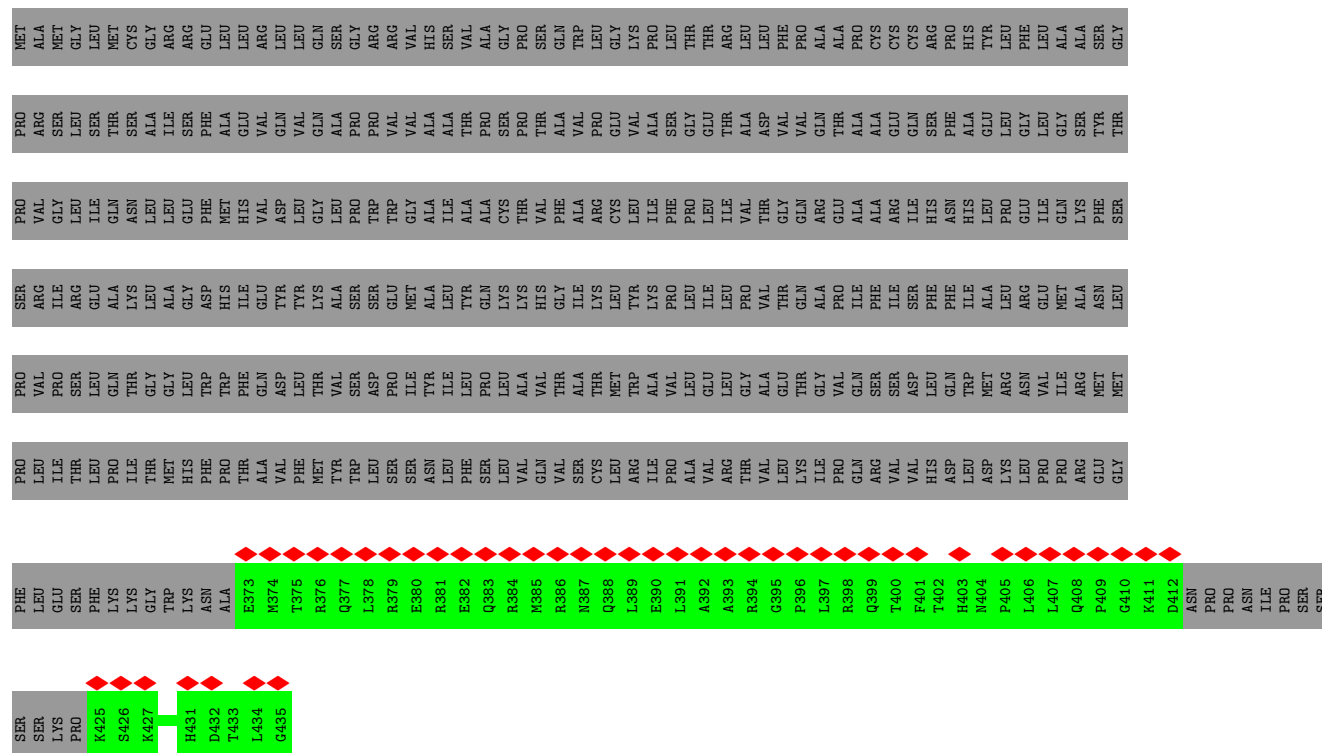
- Molecule 88: P-site tRNA (Visualisation example)



- Molecule 89: Large ribosomal subunit protein mL45



Chain Au: 10% 12% 88%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70865	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	2.958	Depositor
Minimum map value	-0.706	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.154	Depositor
Recommended contour level	0.7	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: 5MU, MA6, ACE, GDP, ATP, NAD, ZN, OMU, 1MA, PSU, B8T, 5MC, FES, K, 5F0, OMG, MG, 2MG

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	0.19	0/36876	0.41	1/57402 (0.0%)
2	B	0.18	0/1627	0.44	0/2527
3	D	0.19	0/1896	0.47	0/2549
4	E	0.27	0/2475	0.55	1/3355 (0.0%)
5	F	0.22	0/2090	0.49	0/2842
6	H	0.24	0/1698	0.54	0/2292
7	I	0.38	0/1731	0.65	3/2345 (0.1%)
8	J	0.33	0/1348	0.52	0/1813
9	K	0.21	0/1497	0.43	0/2031
10	L	0.18	0/905	0.46	0/1218
11	M	0.21	0/2381	0.48	0/3212
12	N	0.22	0/1833	0.47	0/2468
13	O	0.21	0/1283	0.47	0/1727
14	P	0.21	0/1199	0.48	0/1623
15	Q	0.22	0/2039	0.51	0/2750
16	R	0.22	0/1175	0.50	0/1572
17	S	0.31	0/1320	0.62	0/1789
18	T	0.22	0/1403	0.49	0/1886
19	U	0.50	0/1075	0.94	1/1456 (0.1%)
20	V	0.35	0/1721	0.73	0/2333
21	W	0.23	0/902	0.48	0/1214
22	X	0.20	0/2099	0.45	0/2837
23	Y	0.22	0/1593	0.45	0/2136
24	Z	0.21	0/1021	0.48	0/1378
25	AA	0.19	0/22537	0.43	5/35085 (0.0%)
26	AB	0.21	0/1871	0.46	0/2531
27	AC	0.19	0/1113	0.46	0/1505
28	0	0.21	0/913	0.47	0/1224
29	1	0.22	0/469	0.49	0/621
30	2	0.22	0/383	0.43	0/507
31	3	0.21	0/853	0.47	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	4	0.18	0/350	0.41	0/461
33	z	0.26	0/2067	0.57	0/2793
34	t	0.24	0/358	0.47	0/486
34	u	0.27	0/259	0.57	0/350
34	v	0.33	0/259	0.73	1/350 (0.3%)
34	w	0.33	0/246	0.67	0/331
34	x	0.28	0/246	0.68	0/331
34	y	0.30	0/246	0.61	0/331
35	5	0.24	0/3293	0.51	1/4484 (0.0%)
36	6	0.21	0/3043	0.48	0/4140
37	7	0.25	0/2447	0.56	1/3310 (0.0%)
38	8	0.70	1/1244 (0.1%)	1.10	4/1674 (0.2%)
39	9	0.21	0/1025	0.46	0/1379
40	a	0.21	0/866	0.55	0/1174
41	b	0.19	0/1219	0.45	0/1651
42	c	0.22	0/2347	0.49	0/3171
43	e	0.27	0/1903	0.64	0/2565
44	f	0.44	0/1273	0.82	0/1716
45	g	0.22	0/1151	0.50	0/1569
46	h	0.19	0/918	0.40	0/1249
47	i	0.21	0/850	0.45	0/1135
48	j	0.20	0/760	0.50	0/1023
49	k	0.19	0/783	0.42	0/1057
50	l	0.24	0/707	0.49	0/960
51	m	0.26	0/805	0.63	0/1081
52	o	0.22	0/819	0.48	0/1097
53	p	0.21	0/1223	0.45	0/1641
54	q	0.23	0/1432	0.51	0/1931
55	r	0.23	0/1362	0.49	0/1846
56	s	0.21	0/3239	0.47	0/4400
57	AD	0.18	0/2751	0.42	0/3681
58	AE	0.22	0/989	0.53	0/1335
59	AF	0.21	0/1767	0.49	0/2373
60	AG	0.21	0/2753	0.50	1/3691 (0.0%)
61	AH	0.24	0/1178	0.54	0/1598
62	AI	0.28	0/1030	0.46	0/1386
63	AJ	0.30	0/855	0.62	2/1148 (0.2%)
64	AK	0.20	0/880	0.45	0/1182
65	AL	0.37	0/1477	0.78	2/1974 (0.1%)
66	AM	0.21	0/963	0.48	0/1295
67	AN	0.33	0/886	0.65	2/1199 (0.2%)
68	AO	0.22	0/1648	0.49	0/2243
69	AP	0.24	0/798	0.55	0/1070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AQ	0.18	0/754	0.38	0/1003
71	AR	0.24	0/2456	0.51	0/3317
72	AS	0.29	0/1138	0.71	1/1533 (0.1%)
73	AT	0.20	0/1402	0.48	0/1883
74	AU	0.27	0/1510	0.60	0/2025
75	AV	0.22	0/3030	0.45	0/4093
76	AW	0.20	0/801	0.46	0/1079
77	AX	0.22	0/2921	0.47	0/3954
78	AY	0.23	0/1280	0.51	0/1725
79	AZ	0.25	0/857	0.62	0/1141
80	A0	0.41	0/1834	0.84	7/2484 (0.3%)
81	A1	0.23	0/2313	0.53	0/3129
82	A2	0.21	0/947	0.48	0/1266
83	A3	0.23	0/636	0.54	0/839
84	A4	0.26	0/4877	0.50	0/6598
85	Az	0.20	0/785	0.47	0/1219
87	Aw	0.43	0/1604	0.73	0/2490
88	Ax	0.46	0/1673	0.87	0/2599
89	d	0.30	0/2043	0.65	0/2764
90	Au	0.26	0/439	0.61	0/586
All	All	0.24	1/189341 (0.0%)	0.51	33/268952 (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
19	U	0	5
20	V	0	8
22	X	0	2
33	z	0	1
36	6	0	2
37	7	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
38	8	0	8
40	a	0	1
42	c	0	2
44	f	0	5
45	g	0	1
48	j	0	1
51	m	0	2
53	p	0	2
54	q	0	2
55	r	0	1
56	s	0	1
57	AD	0	1
60	AG	0	2
61	AH	0	1
65	AL	0	4
67	AN	0	1
68	AO	0	1
69	AP	0	1
72	AS	0	2
74	AU	0	3
75	AV	0	2
76	AW	0	2
77	AX	0	1
79	AZ	0	4
80	A0	0	2
81	A1	0	3
84	A4	0	3
89	d	0	2
All	All	0	91

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	74	LYS	C-N	9.30	1.47	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AA	883	A	OP1-P-O3'	-11.92	72.24	108.00
80	A0	153	PHE	N-CA-CB	-11.00	91.90	110.49
80	A0	153	PHE	CA-CB-CG	10.73	124.53	113.80
80	A0	88	GLN	N-CA-C	9.24	123.16	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	74	LYS	O-C-N	9.24	131.59	122.07
25	AA	883	A	OP2-P-O3'	-8.93	81.22	108.00
35	5	104	CYS	CA-CB-SG	8.74	134.51	114.40
38	8	169	PHE	CA-CB-CG	-8.64	105.16	113.80
80	A0	153	PHE	CB-CA-C	8.53	127.40	110.42
25	AA	78	C	O3'-P-O5'	7.90	115.86	104.00
65	AL	170	LEU	CA-CB-CG	7.27	141.74	116.30
7	I	66	PRO	N-CA-CB	-7.24	95.65	103.25
4	E	317	PRO	N-CA-C	-7.16	98.28	111.03
63	AJ	81	CYS	CA-CB-SG	6.85	130.15	114.40
67	AN	5	ARG	CG-CD-NE	6.74	126.82	112.00
7	I	71	PRO	N-CA-C	6.36	118.46	110.70
1	A	2785	C	O3'-P-O5'	6.29	113.44	104.00
63	AJ	93	CYS	CA-CB-SG	6.21	128.69	114.40
7	I	71	PRO	N-CA-CB	-6.07	97.19	103.08
38	8	129	ARG	CB-CG-CD	5.93	124.93	111.30
72	AS	78	TYR	CA-CB-CG	5.86	124.45	113.90
38	8	188	PRO	N-CA-C	-5.82	102.07	111.03
80	A0	90	ASP	N-CA-C	5.68	117.47	111.28
60	AG	65	LYS	CA-CB-CG	5.32	124.74	114.10
25	AA	79	C	C5'-C4'-C3'	5.26	123.89	116.00
25	AA	695	C	P-O3'-C3'	5.19	127.98	120.20
65	AL	147	ARG	CA-CB-CG	5.15	124.40	114.10
37	7	156	ARG	N-CA-CB	5.11	118.98	110.91
19	U	148	PRO	N-CA-C	-5.09	102.50	110.50
80	A0	158	GLU	CA-CB-CG	5.09	124.27	114.10
34	v	82	LEU	N-CA-CB	5.07	117.57	110.12
67	AN	4	VAL	N-CA-C	-5.04	96.90	111.00
80	A0	158	GLU	N-CA-CB	-5.02	102.01	110.49

There are no chirality outliers.

All (91) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	6	47	ARG	Sidechain
36	6	59	ARG	Sidechain
37	7	156	ARG	Sidechain
38	8	101	ARG	Sidechain
38	8	113	ARG	Sidechain
38	8	114	ARG	Sidechain
38	8	133	ARG	Sidechain
38	8	137	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
38	8	67	ARG	Sidechain
38	8	70	ARG	Sidechain
38	8	99	ARG	Sidechain
80	A0	140	ARG	Sidechain
80	A0	99	ARG	Sidechain
81	A1	164	ARG	Sidechain
81	A1	260	ARG	Sidechain
81	A1	46	ARG	Sidechain
84	A4	270	ARG	Sidechain
84	A4	485	ALA	Mainchain
84	A4	80	ARG	Sidechain
57	AD	181	ARG	Sidechain
60	AG	136	ARG	Sidechain
60	AG	389	ARG	Sidechain
61	AH	75	ARG	Sidechain
65	AL	123	ARG	Sidechain
65	AL	147	ARG	Sidechain
65	AL	224	ARG	Sidechain
65	AL	225	ARG	Sidechain
67	AN	32	ARG	Sidechain
68	AO	215	ARG	Sidechain
69	AP	141	ARG	Sidechain
72	AS	134	ARG	Sidechain
72	AS	98	ARG	Sidechain
74	AU	141	ARG	Sidechain
74	AU	193	ARG	Sidechain
74	AU	41	ARG	Sidechain
75	AV	105	ARG	Sidechain
75	AV	392	ARG	Sidechain
76	AW	125	ARG	Sidechain
76	AW	85	ARG	Sidechain
77	AX	123	ARG	Sidechain
79	AZ	10	ARG	Sidechain
79	AZ	101	ARG	Sidechain
79	AZ	13	ARG	Sidechain
79	AZ	24	ARG	Sidechain
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
9	K	98	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	N	139	ARG	Sidechain
12	N	51	ARG	Sidechain
14	P	69	ARG	Sidechain
15	Q	67	ARG	Sidechain
18	T	157	ARG	Sidechain
19	U	11	ARG	Sidechain
19	U	3	ARG	Sidechain
19	U	54	ARG	Sidechain
19	U	71	ARG	Sidechain
19	U	80	ARG	Sidechain
20	V	105	ARG	Sidechain
20	V	128	ARG	Sidechain
20	V	143	ARG	Sidechain
20	V	152	ARG	Sidechain
20	V	185	ARG	Sidechain
20	V	33	ARG	Sidechain
20	V	40	ARG	Sidechain
20	V	42	ARG	Sidechain
22	X	112	ARG	Sidechain
22	X	36	ARG	Sidechain
40	a	95	ARG	Sidechain
42	c	311	ARG	Sidechain
42	c	47	ARG	Sidechain
89	d	124	ARG	Sidechain
89	d	260	ARG	Sidechain
44	f	155	ARG	Sidechain
44	f	183	ARG	Sidechain
44	f	199	LYS	Mainchain
44	f	201	ARG	Sidechain
44	f	78	ARG	Sidechain
45	g	56	ARG	Sidechain
48	j	103	ARG	Sidechain
51	m	125	ARG	Sidechain
51	m	94	ARG	Sidechain
53	p	179	ARG	Sidechain
53	p	83	ARG	Sidechain
54	q	28	ARG	Sidechain
54	q	33	ARG	Sidechain
55	r	134	ARG	Sidechain
56	s	43	ARG	Sidechain
33	z	223	ARG	Sidechain

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	15	0
2	B	1524	0	778	5	0
3	D	1859	0	1920	0	0
4	E	2406	0	2415	7	0
5	F	2031	0	2065	2	0
6	H	1661	0	1734	3	0
7	I	1695	0	1785	30	0
8	J	1330	0	1407	7	0
9	K	1455	0	1452	1	0
10	L	890	0	941	0	0
11	M	2327	0	2395	0	0
12	N	1786	0	1817	4	0
13	O	1259	0	1294	0	0
14	P	1173	0	1165	1	0
15	Q	1990	0	2031	0	0
16	R	1154	0	1214	5	0
17	S	1293	0	1365	15	0
18	T	1369	0	1410	0	0
19	U	1049	0	1053	12	0
20	V	1676	0	1687	4	0
21	W	880	0	904	0	0
22	X	2044	0	2060	0	0
23	Y	1556	0	1597	2	0
24	Z	996	0	1044	0	0
25	AA	20260	0	10285	24	0
26	AB	1828	0	1815	1	0
27	AC	1083	0	1088	0	0
28	0	898	0	916	0	0
29	1	464	0	511	0	0
30	2	377	0	406	0	0
31	3	832	0	883	0	0
32	4	342	0	361	2	0
33	z	2027	0	2076	3	0
34	t	354	0	377	0	0
34	u	257	0	283	0	0
34	v	257	0	283	4	0
34	w	245	0	275	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	x	245	0	275	1	0
34	y	245	0	275	3	0
35	5	3200	0	3196	2	0
36	6	2948	0	2841	0	0
37	7	2390	0	2397	0	0
38	8	1219	0	1241	62	0
39	9	997	0	987	0	0
40	a	840	0	810	2	0
41	b	1196	0	1195	0	0
42	c	2299	0	2320	2	0
43	e	1866	0	1868	10	0
44	f	1252	0	1269	32	0
45	g	1113	0	1097	0	0
46	h	895	0	881	0	0
47	i	828	0	857	0	0
48	j	745	0	746	0	0
49	k	774	0	784	0	0
50	l	688	0	674	1	0
51	m	791	0	796	6	0
52	o	798	0	804	0	0
53	p	1205	0	1223	0	0
54	q	1398	0	1383	2	0
55	r	1322	0	1348	15	0
56	s	3155	0	3139	0	0
57	AD	2700	0	2767	1	0
58	AE	972	0	1001	1	0
59	AF	1725	0	1769	1	0
60	AG	2695	0	2694	3	0
61	AH	1152	0	1183	3	0
62	AI	1020	0	1053	3	0
63	AJ	839	0	885	0	0
64	AK	862	0	885	0	0
65	AL	1453	0	1540	13	0
66	AM	942	0	965	0	0
67	AN	868	0	928	9	0
68	AO	1592	0	1557	6	0
69	AP	781	0	806	1	0
70	AQ	744	0	758	0	0
71	AR	2409	0	2428	3	0
72	AS	1111	0	1115	4	0
73	AT	1371	0	1393	0	0
74	AU	1488	0	1499	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	AV	2969	0	2961	2	0
76	AW	789	0	802	0	0
77	AX	2849	0	2843	6	0
78	AY	1246	0	1197	0	0
79	AZ	839	0	858	5	0
80	A0	1787	0	1796	31	0
81	A1	2265	0	2294	4	0
82	A2	935	0	971	1	0
83	A3	625	0	699	1	0
84	A4	4768	0	4766	1	0
85	Az	701	0	351	0	0
86	Av	115	0	38	0	0
87	Aw	1435	0	726	18	0
88	Ax	1499	0	762	43	0
89	d	1988	0	1978	6	0
90	Au	431	0	429	0	0
91	3	1	0	0	0	0
91	6	1	0	0	0	0
91	A	28	0	0	0	0
91	AA	20	0	0	0	0
91	D	1	0	0	0	0
91	M	1	0	0	0	0
91	N	1	0	0	0	0
91	o	1	0	0	0	0
92	A	135	0	0	0	0
92	A3	1	0	0	0	0
92	AA	54	0	0	0	0
92	AB	1	0	0	0	0
92	AX	1	0	0	0	0
92	D	2	0	0	0	0
92	E	1	0	0	0	0
92	O	1	0	0	0	0
92	g	1	0	0	0	0
93	B	7	0	8	0	0
94	AA	44	0	26	1	0
95	0	1	0	0	0	0
95	4	1	0	0	0	0
95	AO	1	0	0	0	0
96	AE	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	5	0
97	AX	31	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
98	AX	28	0	12	0	0
99	A	1	0	0	0	0
All	All	180448	0	153045	344	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.

All (344) 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)
17:S:144:LEU:HD12	17:S:144:LEU:O	1.41	1.18
16:R:94:GLN:HB2	17:S:146:LYS:HD3	1.13	1.12
32:4:76:CYS:SG	32:4:92:CYS:SG	2.52	1.06
87:Aw:9:A:H1'	87:Aw:45:A:H2'	1.37	1.05
1:A:2100:C:OP1	1:A:2114:C:OP1	1.80	1.00
7:I:67:SER:H	55:r:69:GLN:HG3	1.29	0.98
88:Ax:16:C:H2'	88:Ax:17:A:H2'	1.44	0.98
7:I:63:SER:HA	7:I:67:SER:HB3	1.45	0.95
17:S:146:LYS:CG	17:S:147:PRO:HD3	1.99	0.93
55:r:108:CYS:HB3	96:r:201:FES:S2	2.08	0.92
80:A0:89:HIS:H	80:A0:153:PHE:HD1	1.04	0.90
17:S:146:LYS:HG3	17:S:147:PRO:HD3	1.53	0.90
80:A0:93:CYS:HB2	80:A0:153:PHE:HE2	1.34	0.89
8:J:33:PRO:HA	8:J:36:GLY:H	1.37	0.88
16:R:94:GLN:HB2	17:S:146:LYS:CD	2.02	0.88
74:AU:58:GLU:HG3	80:A0:158:GLU:HG2	1.56	0.86
7:I:63:SER:H	7:I:67:SER:HA	1.39	0.86
80:A0:93:CYS:HB2	80:A0:153:PHE:CE2	2.16	0.81
1:A:3112:A:N7	1:A:3200:U:O2	2.16	0.77
7:I:66:PRO:HA	55:r:69:GLN:CG	2.16	0.76
88:Ax:23:A:H2'	88:Ax:24:A:C8	2.22	0.74
17:S:144:LEU:O	17:S:144:LEU:CD1	2.30	0.74
68:AO:215:ARG:HB3	80:A0:154:THR:HG22	1.69	0.73
4:E:90:TRP:HB2	4:E:316:PHE:HB2	1.70	0.72
38:8:187:PRO:HB2	51:m:78:PRO:HA	1.72	0.71
75:AV:250:ILE:HD11	80:A0:150:PHE:HA	1.72	0.71
38:8:100:GLU:HA	43:e:83:LEU:HD22	1.71	0.71
88:Ax:22:A:H2'	88:Ax:23:A:C8	2.25	0.71
88:Ax:8:U:O2	88:Ax:14:A:N7	2.24	0.70
55:r:73:CYS:N	96:r:201:FES:S1	2.64	0.70
38:8:99:ARG:HB3	43:e:83:LEU:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:8:66:GLU:HA	38:8:69:LYS:HE3	1.72	0.70
8:J:22:ALA:HB2	8:J:35:LEU:HD21	1.73	0.69
88:Ax:8:U:H1'	88:Ax:15:A:H62	1.57	0.69
80:A0:86:LEU:HA	80:A0:152:ALA:O	1.93	0.68
38:8:80:GLN:HB2	44:f:199:LYS:O	1.94	0.67
16:R:94:GLN:CB	17:S:146:LYS:HD3	2.08	0.67
17:S:146:LYS:HG3	17:S:147:PRO:CD	2.25	0.66
80:A0:89:HIS:O	80:A0:153:PHE:HB3	1.95	0.66
7:I:64:CYS:N	96:r:201:FES:S2	2.53	0.66
88:Ax:22:A:H2'	88:Ax:23:A:H8	1.62	0.66
88:Ax:46:A:H2'	88:Ax:48:U:H4'	1.78	0.66
80:A0:152:ALA:O	80:A0:153:PHE:HB2	1.97	0.65
38:8:75:LEU:HD23	44:f:204:LEU:HD12	1.77	0.65
17:S:146:LYS:HG2	17:S:147:PRO:HD3	1.76	0.65
26:AB:224:ASP:OD2	26:AB:240:ASP:OD1	2.14	0.65
38:8:189:GLU:HG2	51:m:81:LEU:HG	1.79	0.64
7:I:67:SER:N	55:r:69:GLN:HG3	2.06	0.64
7:I:66:PRO:HA	55:r:69:GLN:HG2	1.79	0.64
4:E:87:ILE:HG23	4:E:317:PRO:HG3	1.79	0.64
38:8:75:LEU:HD21	44:f:207:LEU:HD12	1.79	0.63
88:Ax:15:A:N1	88:Ax:48:U:H2'	2.14	0.63
87:Aw:9:A:H1'	87:Aw:45:A:C2'	2.24	0.62
38:8:80:GLN:HG2	44:f:198:PHE:HB3	1.81	0.62
80:A0:85:TRP:HB3	80:A0:153:PHE:CE2	2.34	0.62
7:I:66:PRO:HA	55:r:69:GLN:HE21	1.64	0.62
80:A0:86:LEU:HD23	80:A0:152:ALA:O	2.00	0.61
4:E:81:LYS:NZ	4:E:322:ASP:HB2	2.15	0.61
38:8:190:GLY:HA3	44:f:135:LEU:O	2.00	0.61
74:AU:58:GLU:HG3	80:A0:158:GLU:CG	2.30	0.61
2:B:39:PSU:H2'	2:B:40:U:C6	2.36	0.61
7:I:62:PRO:HB3	7:I:68:PRO:HD2	1.83	0.60
88:Ax:22:A:N7	88:Ax:46:A:H2	1.99	0.60
72:AS:122:GLY:HA3	72:AS:134:ARG:HG3	1.84	0.60
88:Ax:44:A:H3'	88:Ax:45:G:H8	1.67	0.60
19:U:11:ARG:H	19:U:11:ARG:HD3	1.66	0.60
55:r:108:CYS:CB	96:r:201:FES:S2	2.72	0.60
19:U:143:ARG:HH21	19:U:144:ARG:HD2	1.67	0.59
38:8:72:ILE:HA	44:f:211:LEU:HD13	1.83	0.59
38:8:191:ARG:HB2	44:f:144:MET:SD	2.43	0.58
1:A:3218:A:OP2	4:E:212:GLY:O	2.22	0.58
25:AA:840:C:H2'	25:AA:841:5MC:HM53	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:8:67:ARG:NH2	88:Ax:48:U:P	2.76	0.58
80:A0:88:GLN:O	80:A0:155:PRO:HA	2.04	0.58
88:Ax:8:U:H1'	88:Ax:15:A:N6	2.18	0.58
87:Aw:62:C:H2'	87:Aw:63:A:C8	2.39	0.57
87:Aw:44:C:H2'	87:Aw:45:A:C8	2.39	0.57
7:I:60:ILE:HB	7:I:65:LEU:HD22	1.85	0.57
35:5:104:CYS:O	35:5:268:CYS:HB3	2.04	0.57
4:E:81:LYS:HZ1	4:E:322:ASP:HB2	1.69	0.57
7:I:60:ILE:HB	7:I:65:LEU:HB2	1.87	0.57
80:A0:86:LEU:CD2	80:A0:152:ALA:HB3	2.34	0.57
7:I:68:PRO:N	7:I:69:PRO:HD2	2.20	0.56
88:Ax:15:A:N6	88:Ax:49:G:OP2	2.38	0.56
16:R:94:GLN:OE1	17:S:146:LYS:HD2	2.06	0.56
8:J:31:PRO:O	8:J:46:ILE:HG21	2.06	0.56
7:I:65:LEU:O	7:I:66:PRO:C	2.49	0.56
38:8:168:LEU:HD13	43:e:205:LEU:HA	1.88	0.56
88:Ax:44:A:H3'	88:Ax:45:G:C8	2.41	0.56
1:A:3112:A:N7	1:A:3200:U:C2	2.73	0.55
43:e:114:ILE:HD12	77:AX:234:ARG:HB3	1.87	0.55
17:S:145:GLY:HA2	40:a:56:ARG:O	2.07	0.55
1:A:2200:A:H5''	50:l:134:LYS:HD3	1.87	0.55
88:Ax:48:U:OP1	88:Ax:48:U:O3'	2.23	0.55
38:8:167:ASN:O	38:8:170:PRO:HD2	2.07	0.55
68:AO:202:TRP:CD1	80:A0:161:LEU:HB2	2.42	0.55
88:Ax:9:A:H2'	88:Ax:24:A:N6	2.22	0.55
12:N:55:ARG:HH21	87:Aw:63:A:H4'	1.70	0.55
25:AA:841:5MC:H2'	25:AA:842:G:C8	2.42	0.55
25:AA:103:G:C2	67:AN:4:VAL:HG22	2.42	0.55
38:8:66:GLU:O	38:8:69:LYS:HG2	2.08	0.54
38:8:67:ARG:HH21	88:Ax:48:U:P	2.30	0.54
2:B:39:PSU:H2'	2:B:40:U:H6	1.73	0.54
1:A:3089:A:H3'	1:A:3090:G:C5'	2.38	0.54
7:I:56:PRO:HA	12:N:210:GLN:CG	2.37	0.54
25:AA:936:MA6:H102	25:AA:937:MA6:H103	1.89	0.54
38:8:99:ARG:O	43:e:84:TYR:N	2.34	0.54
38:8:188:PRO:O	51:m:78:PRO:HB3	2.08	0.53
68:AO:212:GLU:HA	68:AO:215:ARG:HG2	1.90	0.53
25:AA:571:A:OP1	25:AA:682:U:OP1	2.27	0.53
38:8:75:LEU:CD2	44:f:207:LEU:HB2	2.39	0.53
25:AA:135:A:OP1	94:AA:1002:NAD:H2D	2.09	0.53
38:8:80:GLN:CG	44:f:198:PHE:HB3	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:63:SER:O	55:r:69:GLN:HB2	2.08	0.52
8:J:22:ALA:HB3	8:J:35:LEU:HD11	1.92	0.52
38:8:68:LEU:O	38:8:72:ILE:HG13	2.08	0.52
58:AE:104:GLU:OE2	69:AP:68:CYS:CB	2.58	0.52
38:8:191:ARG:HE	38:8:193:ASN:HB2	1.74	0.52
88:Ax:7:A:H3'	88:Ax:8:U:H5''	1.90	0.52
88:Ax:46:A:C4	88:Ax:48:U:H1'	2.43	0.52
87:Aw:63:A:H2'	87:Aw:64:U:C6	2.45	0.51
88:Ax:46:A:H3'	88:Ax:46:A:C8	2.45	0.51
38:8:75:LEU:HG	44:f:204:LEU:HD13	1.91	0.51
44:f:192:GLU:HA	44:f:195:LYS:HG2	1.92	0.51
2:B:10:2MG:H2'	2:B:11:C:C6	2.46	0.51
25:AA:79:C:C6	67:AN:5:ARG:HD2	2.45	0.51
87:Aw:56:A:H2'	87:Aw:61:U:C5	2.45	0.51
77:AX:389:SER:HB2	97:AX:501:ATP:H5'1	1.93	0.51
25:AA:78:C:N3	67:AN:4:VAL:HB	2.27	0.50
38:8:159:ALA:HA	38:8:162:ILE:HG12	1.93	0.50
68:AO:215:ARG:HH11	80:A0:155:PRO:HD2	1.75	0.50
25:AA:78:C:H2'	67:AN:5:ARG:HG3	1.93	0.50
87:Aw:49:U:OP1	87:Aw:49:U:H3'	2.11	0.50
87:Aw:55:A:H1'	87:Aw:56:A:H4'	1.93	0.50
38:8:172:GLU:HG2	44:f:185:SER:HA	1.94	0.50
68:AO:216:LEU:HD11	80:A0:157:PRO:HG3	1.94	0.50
25:AA:111:U:O2	25:AA:499:C:O2	2.30	0.50
65:AL:120:GLU:HB3	65:AL:174:ASN:HB3	1.93	0.50
19:U:144:ARG:HH21	19:U:147:VAL:HG11	1.76	0.50
87:Aw:54:U:H2'	87:Aw:55:A:O4'	2.11	0.50
2:B:39:PSU:H4'	14:P:151:TRP:CG	2.47	0.50
38:8:169:PHE:HZ	44:f:167:ALA:HB1	1.77	0.49
88:Ax:23:A:H2'	88:Ax:24:A:H8	1.74	0.49
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.92	0.49
25:AA:368:A:H1'	62:AI:183:HIS:HA	1.93	0.49
19:U:66:ALA:HB2	19:U:100:ALA:HB2	1.94	0.49
25:AA:79:C:O4'	67:AN:5:ARG:HD2	2.11	0.49
80:A0:90:ASP:OD1	80:A0:155:PRO:HD3	2.12	0.49
17:S:133:VAL:HG12	17:S:149:LEU:HD12	1.94	0.49
88:Ax:9:A:H8	88:Ax:23:A:N7	2.09	0.49
38:8:68:LEU:O	44:f:211:LEU:HD22	2.13	0.49
5:F:293:PHE:HB3	5:F:294:PRO:HD3	1.95	0.49
38:8:190:GLY:HA3	44:f:136:GLN:HA	1.94	0.49
7:I:62:PRO:HB3	7:I:68:PRO:CD	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:8:162:ILE:HD12	44:f:86:TYR:HE1	1.78	0.49
88:Ax:15:A:H2'	88:Ax:60:U:O2'	2.13	0.49
38:8:199:TYR:HB2	44:f:199:LYS:HE3	1.95	0.48
80:A0:86:LEU:HD22	80:A0:152:ALA:HB3	1.94	0.48
60:AG:65:LYS:HD3	60:AG:66:ARG:H	1.77	0.48
87:Aw:62:C:H2'	87:Aw:63:A:H8	1.77	0.48
38:8:83:ILE:HG23	44:f:199:LYS:HA	1.94	0.48
88:Ax:22:A:N7	88:Ax:46:A:C2	2.80	0.48
16:R:148:TYR:CE2	17:S:147:PRO:HG2	2.48	0.48
68:A0:216:LEU:HG	80:A0:157:PRO:HD3	1.95	0.48
80:A0:85:TRP:O	80:A0:153:PHE:HA	2.13	0.48
88:Ax:8:U:C2	88:Ax:14:A:N7	2.81	0.48
88:Ax:46:A:C5	88:Ax:48:U:H1'	2.48	0.48
38:8:80:GLN:HA	44:f:201:ARG:HD2	1.95	0.48
72:AS:118:PHE:CG	72:AS:134:ARG:HB3	2.49	0.48
25:AA:77:C:H2'	25:AA:78:C:C6	2.49	0.48
34:w:63:LYS:HD2	34:v:82:LEU:HB3	1.96	0.48
38:8:75:LEU:HD23	44:f:204:LEU:CD1	2.41	0.48
65:AL:175:TYR:HB2	67:AN:89:GLY:HA3	1.96	0.48
7:I:63:SER:HA	7:I:67:SER:CB	2.32	0.48
65:AL:120:GLU:CB	65:AL:174:ASN:HB3	2.44	0.48
7:I:63:SER:N	7:I:67:SER:HA	2.20	0.48
65:AL:112:MET:O	65:AL:116:VAL:HG13	2.14	0.48
88:Ax:46:A:H3'	88:Ax:46:A:H8	1.77	0.48
80:A0:87:TRP:C	80:A0:154:THR:H	2.22	0.47
25:AA:915:G:H1'	25:AA:936:MA6:H2	1.96	0.47
38:8:157:LEU:HD22	38:8:160:GLU:OE2	2.14	0.47
34:w:63:LYS:HE3	34:v:74:LEU:HD21	1.96	0.47
17:S:144:LEU:HD11	40:a:58:ILE:HD12	1.96	0.47
38:8:187:PRO:HG2	51:m:79:ILE:HG13	1.96	0.47
4:E:194:TYR:CE2	4:E:321:PRO:HG3	2.50	0.47
25:AA:81:C:H2'	25:AA:82:U:O4'	2.14	0.47
38:8:189:GLU:O	44:f:137:LEU:N	2.47	0.47
44:f:125:TYR:CD1	44:f:197:ARG:HD2	2.49	0.47
84:A4:577:ASN:OD1	84:A4:610:LEU:HB2	2.14	0.47
87:Aw:43:U:O2'	87:Aw:44:C:H5'	2.15	0.47
88:Ax:44:A:H2'	88:Ax:44:A:N3	2.29	0.47
89:d:78:LEU:HG	89:d:80:CYS:O	2.15	0.47
38:8:100:GLU:HA	43:e:83:LEU:CD2	2.44	0.47
25:AA:79:C:H1'	67:AN:5:ARG:O	2.14	0.46
38:8:72:ILE:CA	44:f:211:LEU:HD13	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:AR:104:LYS:HA	71:AR:104:LYS:HE3	1.96	0.46
87:Aw:21:A:N6	87:Aw:46:A:O2'	2.48	0.46
44:f:122:GLU:HB2	44:f:158:GLN:HG2	1.97	0.46
25:AA:879:U:H1'	25:AA:880:A:O5'	2.15	0.46
38:8:83:ILE:CD1	44:f:128:PRO:HG3	2.46	0.46
62:AI:183:HIS:O	62:AI:184:5F0:C	2.64	0.46
1:A:2935:A:OP1	1:A:2986:C:OP1	2.32	0.46
38:8:162:ILE:HD12	44:f:86:TYR:CE1	2.50	0.46
7:I:57:LYS:HD2	7:I:58:PRO:HD2	1.98	0.46
62:AI:183:HIS:C	62:AI:184:5F0:C	2.89	0.46
55:r:72:ILE:HB	96:r:201:FES:S1	2.56	0.46
59:AF:234:ARG:HB2	82:A2:53:MET:HE1	1.98	0.46
65:AL:121:ASP:CB	65:AL:125:LEU:HB3	2.46	0.46
88:Ax:46:A:C2'	88:Ax:48:U:H4'	2.43	0.46
77:AX:338:ASP:HB2	77:AX:339:PRO:HD3	1.97	0.45
65:AL:120:GLU:HA	65:AL:174:ASN:HB3	1.96	0.45
88:Ax:46:A:C8	88:Ax:46:A:C3'	2.99	0.45
65:AL:65:ASP:HB2	65:AL:110:GLN:HG3	1.98	0.45
87:Aw:16:A:H61	87:Aw:56:A:H2'	1.81	0.45
9:K:2:SER:HB3	9:K:4:PHE:CD2	2.51	0.45
38:8:157:LEU:O	38:8:160:GLU:HG2	2.17	0.45
88:Ax:17:A:O2'	88:Ax:22:A:OP2	2.35	0.45
7:I:56:PRO:HA	12:N:210:GLN:HG3	1.98	0.45
87:Aw:10:G:OP1	87:Aw:46:A:H5'	2.16	0.45
7:I:66:PRO:HA	55:r:69:GLN:HG3	1.95	0.45
7:I:64:CYS:SG	55:r:78:LYS:NZ	2.89	0.45
72:AS:115:GLU:O	72:AS:118:PHE:HB3	2.17	0.45
23:Y:123:ARG:HB3	89:d:64:GLY:HA2	1.99	0.44
65:AL:115:ILE:CG2	65:AL:181:ILE:HD13	2.47	0.44
38:8:67:ARG:NH2	88:Ax:46:A:O3'	2.51	0.44
38:8:101:ARG:HG2	43:e:84:TYR:CG	2.51	0.44
87:Aw:6:U:H2'	87:Aw:7:A:C8	2.53	0.44
8:J:39:LEU:HD12	8:J:46:ILE:HG23	1.98	0.44
17:S:94:ARG:HA	42:c:313:PRO:HD3	2.00	0.44
34:v:79:ILE:HA	34:v:82:LEU:CD2	2.48	0.44
65:AL:120:GLU:HG3	65:AL:170:LEU:HD12	1.98	0.44
88:Ax:15:A:O2'	88:Ax:60:U:O2	2.32	0.44
19:U:147:VAL:CG2	89:d:276:ILE:HG21	2.47	0.44
38:8:107:THR:O	38:8:108:PHE:C	2.61	0.44
75:AV:250:ILE:HD11	80:A0:150:PHE:CA	2.45	0.44
1:A:2639:C:H4'	83:A3:159:GLU:OE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:232:LEU:HD21	34:y:86:LEU:HD22	2.00	0.44
61:AH:182:GLU:HA	61:AH:185:LYS:HG2	2.00	0.44
88:Ax:15:A:H61	88:Ax:49:G:P	2.40	0.44
1:A:1798:A:N7	89:d:38:LYS:HE3	2.33	0.44
88:Ax:14:A:H2	88:Ax:17:A:O2'	2.00	0.44
19:U:144:ARG:O	19:U:147:VAL:HG23	2.17	0.44
38:8:70:ARG:CZ	88:Ax:48:U:OP2	2.65	0.44
88:Ax:9:A:C8	88:Ax:23:A:N7	2.85	0.44
8:J:30:MET:HB3	8:J:31:PRO:HD2	2.00	0.44
35:5:104:CYS:O	35:5:268:CYS:CB	2.64	0.43
88:Ax:17:A:H1'	88:Ax:22:A:O5'	2.18	0.43
6:H:201:VAL:HG11	6:H:206:LEU:HD21	2.01	0.43
7:I:56:PRO:HA	12:N:210:GLN:HG2	2.00	0.43
34:w:63:LYS:HG3	34:w:64:ILE:N	2.33	0.43
38:8:64:ALA:O	38:8:68:LEU:HG	2.18	0.43
38:8:93:LYS:HB2	38:8:99:ARG:HH21	1.83	0.43
61:AH:123:SER:HB3	61:AH:127:TYR:HB2	2.01	0.43
19:U:11:ARG:HH21	20:V:211:LYS:N	2.16	0.43
38:8:101:ARG:HH21	43:e:84:TYR:HA	1.83	0.43
1:A:2815:OMG:H1'	1:A:2815:OMG:HM23	1.58	0.43
7:I:66:PRO:HA	55:r:69:GLN:NE2	2.32	0.43
20:V:57:PHE:HB2	20:V:156:LYS:HE3	2.01	0.43
7:I:61:HIS:HA	7:I:62:PRO:HD3	1.91	0.43
7:I:66:PRO:CA	55:r:69:GLN:HG2	2.48	0.43
51:m:125:ARG:HH22	61:AH:182:GLU:HB2	1.83	0.43
74:AU:58:GLU:C	80:A0:160:SER:HG	2.27	0.43
79:AZ:11:MET:HE3	81:A1:192:LYS:HB2	2.00	0.43
74:AU:54:PHE:HD1	80:A0:157:PRO:CB	2.31	0.43
88:Ax:42:G:C2	88:Ax:43:G:H1'	2.54	0.43
80:A0:86:LEU:HD23	80:A0:152:ALA:HB3	1.99	0.43
1:A:2785:C:H3'	1:A:2786:U:C5'	2.49	0.42
44:f:80:ILE:HD11	44:f:191:GLU:HG3	2.00	0.42
81:A1:46:ARG:HB2	81:A1:47:PRO:HD3	2.00	0.42
34:x:67:LEU:HD22	34:y:67:LEU:HD22	2.01	0.42
65:AL:115:ILE:HG21	65:AL:181:ILE:HD13	2.01	0.42
38:8:201:GLN:HB3	44:f:201:ARG:HG2	2.01	0.42
38:8:202:VAL:HG11	54:q:171:ARG:HH12	1.85	0.42
88:Ax:50:G:N3	88:Ax:50:G:H2'	2.35	0.42
19:U:20:PHE:CD2	20:V:195:GLN:HG3	2.55	0.42
25:AA:78:C:H6	25:AA:78:C:O5'	2.02	0.42
80:A0:89:HIS:O	80:A0:153:PHE:CB	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:290:TYR:HB2	5:F:293:PHE:HB2	2.00	0.42
25:AA:694:C:H4'	79:AZ:102:ALA:HB2	2.02	0.42
44:f:111:HIS:CD2	44:f:121:VAL:HG11	2.54	0.42
60:AG:395:LYS:HD2	60:AG:395:LYS:O	2.19	0.42
74:AU:51:ALA:O	74:AU:54:PHE:HB3	2.19	0.42
38:8:62:GLN:HA	38:8:65:LYS:HD3	2.01	0.42
38:8:126:GLN:O	38:8:129:ARG:HG2	2.20	0.42
77:AX:338:ASP:CB	77:AX:339:PRO:HD3	2.49	0.42
80:A0:89:HIS:N	80:A0:153:PHE:CD1	2.69	0.42
32:4:76:CYS:SG	32:4:79:CYS:SG	3.17	0.42
33:z:139:PRO:HB2	33:z:245:VAL:HG21	2.02	0.42
71:AR:64:GLU:HB2	71:AR:308:HIS:H	1.85	0.42
43:e:114:ILE:HA	77:AX:232:ARG:HE	1.84	0.42
87:Aw:56:A:H2'	87:Aw:61:U:C6	2.55	0.42
80:A0:85:TRP:O	80:A0:153:PHE:CD1	2.73	0.41
44:f:137:LEU:HA	44:f:144:MET:HG2	2.01	0.41
54:q:170:PRO:HB3	88:Ax:56:C:H4'	2.02	0.41
89:d:118:SER:O	89:d:122:ILE:HG13	2.19	0.41
7:I:59:ALA:O	7:I:60:ILE:C	2.63	0.41
25:AA:814:A:H4'	25:AA:815:G:C8	2.56	0.41
34:v:76:LEU:HD11	34:y:65:GLN:HB3	2.02	0.41
65:AL:120:GLU:HG3	65:AL:170:LEU:HG	2.02	0.41
72:AS:119:VAL:HA	72:AS:134:ARG:HG2	2.02	0.41
6:H:106:GLY:H	6:H:158:LYS:HG3	1.86	0.41
71:AR:302:GLN:O	71:AR:306:VAL:HG23	2.20	0.41
77:AX:181:PRO:HB2	77:AX:233:VAL:HG12	2.02	0.41
87:Aw:22:A:OP2	87:Aw:46:A:N6	2.53	0.41
1:A:2380:C:H3'	1:A:2381:A:C5'	2.51	0.41
1:A:3040:OMG:H2'	1:A:3041:U:O4'	2.20	0.41
7:I:61:HIS:HD2	7:I:64:CYS:SG	2.44	0.41
38:8:67:ARG:HD2	38:8:71:LYS:HZ3	1.86	0.41
6:H:208:LEU:HB3	6:H:209:PRO:HD2	2.03	0.41
38:8:101:ARG:NH2	43:e:84:TYR:HA	2.35	0.41
60:AG:210:VAL:HG12	60:AG:210:VAL:O	2.20	0.41
8:J:31:PRO:HA	8:J:46:ILE:CG2	2.50	0.41
25:AA:282:A:H4'	57:AD:419:ARG:O	2.21	0.41
80:A0:146:GLU:O	80:A0:150:PHE:HB3	2.20	0.41
2:B:44:A:H2'	2:B:45:G:O4'	2.21	0.41
38:8:83:ILE:HD12	44:f:128:PRO:HG3	2.02	0.41
44:f:201:ARG:NH1	44:f:204:LEU:HD22	2.35	0.41
79:AZ:10:ARG:HD3	81:A1:239:TRP:CZ3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3040:OMG:HM22	1:A:3040:OMG:H1'	1.67	0.41
19:U:11:ARG:H	19:U:11:ARG:CD	2.34	0.41
19:U:15:PRO:HB3	20:V:206:GLU:HG2	2.02	0.41
25:AA:79:C:O4'	67:AN:5:ARG:HB3	2.21	0.41
25:AA:694:C:H5''	79:AZ:101:ARG:O	2.19	0.41
38:8:93:LYS:HE2	38:8:99:ARG:HH21	1.86	0.41
65:AL:118:ASN:HD22	65:AL:181:ILE:HG13	1.86	0.41
19:U:10:TYR:CE1	19:U:14:GLY:HA3	2.56	0.41
38:8:172:GLU:O	38:8:173:LYS:HB2	2.20	0.41
33:z:133:LYS:HG3	33:z:134:LYS:H	1.86	0.40
38:8:76:GLU:O	38:8:77:LYS:C	2.64	0.40
38:8:129:ARG:HG3	38:8:130:LYS:N	2.36	0.40
38:8:135:THR:O	38:8:139:MET:HG2	2.21	0.40
38:8:189:GLU:HG2	51:m:81:LEU:CG	2.50	0.40
42:c:120:LYS:HD3	42:c:121:SER:O	2.21	0.40
74:AU:58:GLU:HB3	80:A0:160:SER:OG	2.20	0.40
79:AZ:10:ARG:HD3	81:A1:239:TRP:HZ3	1.85	0.40
1:A:3040:OMG:HM22	1:A:3069:A:C2	2.57	0.40
7:I:64:CYS:SG	55:r:111:GLU:HG2	2.61	0.40
19:U:112:PRO:HD2	23:Y:75:GLY:HA3	2.03	0.40
25:AA:79:C:H6	67:AN:5:ARG:HH11	1.69	0.40
88:Ax:25:C:C5	88:Ax:26:U:C5	3.10	0.40
89:d:38:LYS:N	89:d:38:LYS:HD2	2.36	0.40
33:z:127:LEU:HD12	33:z:253:LEU:HD11	2.03	0.40
65:AL:120:GLU:HA	65:AL:174:ASN:CB	2.51	0.40
88:Ax:51:A:H3'	88:Ax:52:G:C8	2.57	0.40

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
4	E	303/348 (87%)	295 (97%)	8 (3%)	0	100	100
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%)	199 (95%)	9 (4%)	2 (1%)	12	41
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%)	285 (99%)	4 (1%)	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%)	3 (2%)	0	100	100
18	T	164/206 (80%)	164 (100%)	0	0	100	100
19	U	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
20	V	203/216 (94%)	197 (97%)	6 (3%)	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
26	AB	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
27	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
28	0	108/188 (57%)	108 (100%)	0	0	100	100
29	1	54/65 (83%)	54 (100%)	0	0	100	100
30	2	44/92 (48%)	44 (100%)	0	0	100	100
31	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
32	4	36/103 (35%)	36 (100%)	0	0	100	100
33	z	250/325 (77%)	240 (96%)	10 (4%)	0	100	100
34	t	44/198 (22%)	44 (100%)	0	0	100	100
34	u	30/198 (15%)	30 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	v	30/198 (15%)	30 (100%)	0	0	100	100
34	w	29/198 (15%)	28 (97%)	1 (3%)	0	100	100
34	x	29/198 (15%)	29 (100%)	0	0	100	100
34	y	29/198 (15%)	29 (100%)	0	0	100	100
35	5	389/423 (92%)	384 (99%)	5 (1%)	0	100	100
36	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
37	7	292/338 (86%)	281 (96%)	11 (4%)	0	100	100
38	8	142/206 (69%)	129 (91%)	12 (8%)	1 (1%)	18	49
39	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
40	a	96/142 (68%)	88 (92%)	8 (8%)	0	100	100
41	b	149/215 (69%)	145 (97%)	4 (3%)	0	100	100
42	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
43	e	226/279 (81%)	221 (98%)	5 (2%)	0	100	100
44	f	153/212 (72%)	138 (90%)	15 (10%)	0	100	100
45	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
46	h	108/158 (68%)	108 (100%)	0	0	100	100
47	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
48	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
49	k	100/112 (89%)	100 (100%)	0	0	100	100
50	l	80/138 (58%)	80 (100%)	0	0	100	100
51	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
52	o	92/102 (90%)	92 (100%)	0	0	100	100
53	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
54	q	164/222 (74%)	161 (98%)	3 (2%)	0	100	100
55	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
56	s	382/439 (87%)	373 (98%)	9 (2%)	0	100	100
57	AD	335/430 (78%)	326 (97%)	9 (3%)	0	100	100
58	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
59	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
60	AG	324/396 (82%)	320 (99%)	4 (1%)	0	100	100
61	AH	138/201 (69%)	135 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	AI	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
63	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
64	AK	99/128 (77%)	99 (100%)	0	0	100	100
65	AL	172/257 (67%)	161 (94%)	11 (6%)	0	100	100
66	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
67	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
68	AO	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
69	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
70	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
71	AR	293/360 (81%)	283 (97%)	10 (3%)	0	100	100
72	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
73	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
74	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
75	AV	358/414 (86%)	351 (98%)	7 (2%)	0	100	100
76	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
77	AX	350/398 (88%)	343 (98%)	7 (2%)	0	100	100
78	AY	147/395 (37%)	144 (98%)	3 (2%)	0	100	100
79	AZ	98/106 (92%)	92 (94%)	6 (6%)	0	100	100
80	A0	213/217 (98%)	205 (96%)	8 (4%)	0	100	100
81	A1	277/323 (86%)	275 (99%)	2 (1%)	0	100	100
82	A2	116/118 (98%)	116 (100%)	0	0	100	100
83	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
84	A4	584/689 (85%)	576 (99%)	8 (1%)	0	100	100
89	d	236/306 (77%)	234 (99%)	2 (1%)	0	100	100
90	Au	47/435 (11%)	47 (100%)	0	0	100	100
All	All	14697/19919 (74%)	14407 (98%)	287 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	66	PRO
7	I	71	PRO
38	8	173	LYS

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%)	193 (100%)	1 (0%)	81	85
8	J	138/150 (92%)	138 (100%)	0	100	100
9	K	155/155 (100%)	154 (99%)	1 (1%)	78	83
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	112/134 (84%)	112 (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
26	AB	198/249 (80%)	198 (100%)	0	100	100
27	AC	115/143 (80%)	115 (100%)	0	100	100
28	0	99/164 (60%)	99 (100%)	0	100	100
29	1	53/60 (88%)	53 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	2	40/72 (56%)	40 (100%)	0	100	100
31	3	88/166 (53%)	88 (100%)	0	100	100
32	4	37/89 (42%)	37 (100%)	0	100	100
33	z	226/287 (79%)	226 (100%)	0	100	100
34	t	40/158 (25%)	40 (100%)	0	100	100
34	u	31/158 (20%)	31 (100%)	0	100	100
34	v	31/158 (20%)	31 (100%)	0	100	100
34	w	30/158 (19%)	30 (100%)	0	100	100
34	x	30/158 (19%)	30 (100%)	0	100	100
34	y	30/158 (19%)	30 (100%)	0	100	100
35	5	352/368 (96%)	352 (100%)	0	100	100
36	6	313/332 (94%)	313 (100%)	0	100	100
37	7	270/303 (89%)	270 (100%)	0	100	100
38	8	133/190 (70%)	133 (100%)	0	100	100
39	9	104/112 (93%)	104 (100%)	0	100	100
40	a	96/133 (72%)	96 (100%)	0	100	100
41	b	132/185 (71%)	132 (100%)	0	100	100
42	c	251/288 (87%)	251 (100%)	0	100	100
43	e	200/236 (85%)	200 (100%)	0	100	100
44	f	139/188 (74%)	139 (100%)	0	100	100
45	g	124/148 (84%)	124 (100%)	0	100	100
46	h	104/148 (70%)	104 (100%)	0	100	100
47	i	86/110 (78%)	86 (100%)	0	100	100
48	j	74/97 (76%)	74 (100%)	0	100	100
49	k	83/89 (93%)	83 (100%)	0	100	100
50	l	76/116 (66%)	76 (100%)	0	100	100
51	m	85/113 (75%)	85 (100%)	0	100	100
52	o	80/87 (92%)	80 (100%)	0	100	100
53	p	135/181 (75%)	135 (100%)	0	100	100
54	q	143/178 (80%)	143 (100%)	0	100	100
55	r	147/169 (87%)	147 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	s	340/381 (89%)	340 (100%)	0	100	100
57	AD	283/357 (79%)	283 (100%)	0	100	100
58	AE	104/107 (97%)	104 (100%)	0	100	100
59	AF	185/209 (88%)	185 (100%)	0	100	100
60	AG	286/342 (84%)	286 (100%)	0	100	100
61	AH	130/180 (72%)	130 (100%)	0	100	100
62	AI	104/146 (71%)	104 (100%)	0	100	100
63	AJ	93/118 (79%)	93 (100%)	0	100	100
64	AK	91/113 (80%)	91 (100%)	0	100	100
65	AL	158/226 (70%)	158 (100%)	0	100	100
66	AM	97/113 (86%)	97 (100%)	0	100	100
67	AN	96/115 (84%)	96 (100%)	0	100	100
68	AO	174/230 (76%)	174 (100%)	0	100	100
69	AP	88/123 (72%)	88 (100%)	0	100	100
70	AQ	78/78 (100%)	78 (100%)	0	100	100
71	AR	264/318 (83%)	264 (100%)	0	100	100
72	AS	116/164 (71%)	116 (100%)	0	100	100
73	AT	153/157 (98%)	153 (100%)	0	100	100
74	AU	152/174 (87%)	152 (100%)	0	100	100
75	AV	325/364 (89%)	325 (100%)	0	100	100
76	AW	87/158 (55%)	87 (100%)	0	100	100
77	AX	311/351 (89%)	311 (100%)	0	100	100
78	AY	137/357 (38%)	137 (100%)	0	100	100
79	AZ	90/95 (95%)	90 (100%)	0	100	100
80	A0	188/189 (100%)	187 (100%)	1 (0%)	81	85
81	A1	257/291 (88%)	257 (100%)	0	100	100
82	A2	100/100 (100%)	100 (100%)	0	100	100
83	A3	65/166 (39%)	65 (100%)	0	100	100
84	A4	526/609 (86%)	525 (100%)	1 (0%)	87	89
89	d	221/274 (81%)	221 (100%)	0	100	100
90	Au	46/372 (12%)	46 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	13166/17158 (77%)	13162 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	I	66	PRO
9	K	2	SER
80	A0	150	PHE
84	A4	486	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	221	ASN
3	D	252	HIS
4	E	233	GLN
4	E	292	HIS
5	F	98	GLN
6	H	126	GLN
7	I	36	HIS
7	I	61	HIS
7	I	219	HIS
7	I	235	GLN
11	M	114	GLN
12	N	101	HIS
12	N	210	GLN
16	R	149	HIS
17	S	84	ASN
17	S	196	ASN
18	T	56	GLN
18	T	145	GLN
19	U	41	GLN
19	U	138	GLN
22	X	4	HIS
22	X	15	GLN
22	X	93	ASN
23	Y	88	GLN
23	Y	117	GLN
27	AC	81	HIS
27	AC	154	HIS
28	0	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	z	104	HIS
33	z	281	HIS
35	5	195	HIS
35	5	385	HIS
38	8	186	GLN
42	c	73	GLN
42	c	168	HIS
43	e	75	GLN
44	f	92	ASN
44	f	94	HIS
44	f	111	HIS
46	h	119	GLN
51	m	44	HIS
54	q	130	GLN
54	q	138	GLN
54	q	147	GLN
55	r	65	ASN
55	r	79	HIS
56	s	101	ASN
56	s	343	GLN
56	s	358	GLN
56	s	423	HIS
57	AD	356	GLN
57	AD	361	GLN
59	AF	113	GLN
59	AF	147	GLN
59	AF	214	HIS
59	AF	224	HIS
60	AG	175	HIS
60	AG	288	HIS
60	AG	308	GLN
61	AH	83	HIS
62	AI	119	ASN
64	AK	68	GLN
64	AK	117	HIS
66	AM	16	HIS
67	AN	52	HIS
67	AN	79	HIS
68	AO	160	HIS
70	AQ	41	HIS
71	AR	246	HIS
71	AR	305	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
71	AR	312	GLN
71	AR	320	GLN
73	AT	14	GLN
73	AT	37	HIS
74	AU	109	ASN
74	AU	117	HIS
75	AV	358	GLN
76	AW	110	ASN
77	AX	90	GLN
77	AX	250	GLN
77	AX	394	HIS
78	AY	257	ASN
83	A3	140	HIS
84	A4	175	GLN
84	A4	288	HIS
84	A4	326	GLN
84	A4	504	ASN
84	A4	540	HIS
90	Au	403	HIS
90	Au	431	HIS

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%)
25	AA	953/954 (99%)	149 (15%)	8 (0%)
85	Az	32/33 (96%)	19 (59%)	0
87	Aw	67/68 (98%)	42 (62%)	0
88	Ax	70/71 (98%)	47 (67%)	0
All	All	2749/2759 (99%)	520 (18%)	10 (0%)

All (520) 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
1	A	1699	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1700	U
1	A	1704	U
1	A	1708	A
1	A	1711	C
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1737	A
1	A	1748	G
1	A	1765	C
1	A	1777	A
1	A	1780	U
1	A	1805	A
1	A	1807	U
1	A	1809	U
1	A	1810	A
1	A	1817	C
1	A	1821	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1844	A
1	A	1854	U
1	A	1856	A
1	A	1869	A
1	A	1871	A
1	A	1873	A
1	A	1882	A
1	A	1886	G
1	A	1887	A
1	A	1893	A
1	A	1901	C
1	A	1903	C
1	A	1918	G
1	A	1937	A
1	A	1940	A
1	A	1985	G
1	A	1992	C
1	A	1993	A
1	A	1994	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2000	C
1	A	2002	G
1	A	2003	A
1	A	2015	G
1	A	2022	G
1	A	2030	U
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2054	U
1	A	2060	A
1	A	2069	U
1	A	2071	U
1	A	2079	C
1	A	2099	U
1	A	2113	G
1	A	2125	C
1	A	2126	U
1	A	2132	A
1	A	2147	G
1	A	2159	U
1	A	2160	A
1	A	2163	A
1	A	2168	U
1	A	2173	G
1	A	2181	A
1	A	2192	A
1	A	2198	A
1	A	2200	A
1	A	2214	A
1	A	2219	C
1	A	2220	A
1	A	2221	C
1	A	2222	U
1	A	2223	A
1	A	2224	C
1	A	2225	C
1	A	2226	U
1	A	2227	A
1	A	2232	A
1	A	2233	U
1	A	2237	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2241	A
1	A	2243	A
1	A	2245	A
1	A	2246	A
1	A	2247	C
1	A	2262	C
1	A	2263	C
1	A	2284	C
1	A	2285	U
1	A	2297	A
1	A	2300	G
1	A	2322	C
1	A	2331	C
1	A	2332	C
1	A	2345	G
1	A	2349	G
1	A	2350	A
1	A	2353	A
1	A	2357	C
1	A	2363	A
1	A	2372	U
1	A	2374	A
1	A	2390	A
1	A	2399	A
1	A	2401	A
1	A	2404	U
1	A	2406	A
1	A	2407	U
1	A	2414	C
1	A	2415	C
1	A	2417	C
1	A	2427	C
1	A	2446	A
1	A	2451	A
1	A	2478	G
1	A	2485	U
1	A	2488	C
1	A	2493	C
1	A	2502	C
1	A	2520	C
1	A	2521	A
1	A	2527	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2540	C
1	A	2570	C
1	A	2573	G
1	A	2577	C
1	A	2578	C
1	A	2580	U
1	A	2581	A
1	A	2582	A
1	A	2592	G
1	A	2593	G
1	A	2599	U
1	A	2600	A
1	A	2601	A
1	A	2603	C
1	A	2617	1MA
1	A	2618	U
1	A	2627	G
1	A	2629	A
1	A	2630	U
1	A	2633	A
1	A	2635	G
1	A	2654	U
1	A	2656	U
1	A	2683	C
1	A	2686	G
1	A	2694	A
1	A	2695	G
1	A	2696	A
1	A	2706	A
1	A	2718	C
1	A	2719	G
1	A	2723	A
1	A	2724	G
1	A	2725	A
1	A	2732	G
1	A	2745	A
1	A	2757	A
1	A	2760	A
1	A	2761	C
1	A	2762	C
1	A	2763	U
1	A	2764	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2765	A
1	A	2767	A
1	A	2768	A
1	A	2775	A
1	A	2781	U
1	A	2782	A
1	A	2785	C
1	A	2786	U
1	A	2787	A
1	A	2790	A
1	A	2810	G
1	A	2815	OMG
1	A	2832	A
1	A	2833	A
1	A	2847	C
1	A	2864	U
1	A	2865	C
1	A	2882	U
1	A	2883	A
1	A	2885	U
1	A	2888	A
1	A	2889	C
1	A	2893	A
1	A	2913	A
1	A	2917	G
1	A	2918	A
1	A	2922	A
1	A	2928	C
1	A	2935	A
1	A	2956	A
1	A	2985	C
1	A	2989	G
1	A	2990	A
1	A	2992	G
1	A	3005	A
1	A	3016	G
1	A	3022	G
1	A	3041	U
1	A	3053	A
1	A	3054	G
1	A	3060	C
1	A	3066	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3089	A
1	A	3090	G
1	A	3096	U
1	A	3097	U
1	A	3100	U
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3110	C
1	A	3112	A
1	A	3113	A
1	A	3150	U
1	A	3157	C
1	A	3158	A
1	A	3162	C
1	A	3169	C
1	A	3172	C
1	A	3177	A
1	A	3189	C
1	A	3190	A
1	A	3194	U
1	A	3199	U
1	A	3200	U
1	A	3207	A
1	A	3208	C
1	A	3209	A
1	A	3210	C
1	A	3212	C
1	A	3217	A
1	A	3218	A
1	A	3228	U
1	A	3229	U
1	A	3230	G
1	A	3231	U
2	B	8	U
2	B	9	1MA
2	B	10	2MG
2	B	16	C
2	B	21	A
2	B	45	G
2	B	48	U
2	B	54	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	55	U
2	B	56	U
2	B	64	A
2	B	69	U
2	B	76	A
25	AA	4	A
25	AA	33	U
25	AA	41	A
25	AA	44	A
25	AA	48	A
25	AA	57	U
25	AA	74	U
25	AA	75	C
25	AA	89	C
25	AA	90	C
25	AA	91	A
25	AA	106	A
25	AA	114	A
25	AA	119	G
25	AA	130	G
25	AA	144	G
25	AA	147	U
25	AA	149	G
25	AA	168	C
25	AA	183	U
25	AA	185	U
25	AA	188	C
25	AA	189	A
25	AA	213	A
25	AA	214	U
25	AA	219	A
25	AA	221	C
25	AA	224	A
25	AA	243	C
25	AA	255	G
25	AA	256	U
25	AA	257	C
25	AA	260	A
25	AA	272	A
25	AA	282	A
25	AA	283	G
25	AA	285	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	AA	291	A
25	AA	292	A
25	AA	293	A
25	AA	295	A
25	AA	311	C
25	AA	312	C
25	AA	313	C
25	AA	314	U
25	AA	315	C
25	AA	316	C
25	AA	320	A
25	AA	346	A
25	AA	354	C
25	AA	355	C
25	AA	364	C
25	AA	365	A
25	AA	368	A
25	AA	375	A
25	AA	394	A
25	AA	400	A
25	AA	418	C
25	AA	434	U
25	AA	435	A
25	AA	456	A
25	AA	458	C
25	AA	460	U
25	AA	462	A
25	AA	466	G
25	AA	470	A
25	AA	471	A
25	AA	474	A
25	AA	479	A
25	AA	490	A
25	AA	504	C
25	AA	506	C
25	AA	513	A
25	AA	520	A
25	AA	532	G
25	AA	540	U
25	AA	541	A
25	AA	542	U
25	AA	543	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	AA	553	G
25	AA	568	U
25	AA	573	A
25	AA	576	C
25	AA	578	C
25	AA	579	C
25	AA	582	U
25	AA	599	U
25	AA	600	G
25	AA	601	C
25	AA	603	C
25	AA	604	A
25	AA	611	A
25	AA	624	C
25	AA	626	G
25	AA	637	U
25	AA	643	C
25	AA	644	U
25	AA	645	A
25	AA	665	C
25	AA	679	A
25	AA	680	G
25	AA	696	A
25	AA	697	U
25	AA	706	A
25	AA	707	A
25	AA	709	A
25	AA	729	C
25	AA	731	C
25	AA	740	A
25	AA	758	C
25	AA	759	U
25	AA	783	A
25	AA	816	G
25	AA	833	A
25	AA	834	C
25	AA	856	G
25	AA	864	C
25	AA	865	A
25	AA	866	A
25	AA	870	A
25	AA	871	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	AA	872	A
25	AA	873	U
25	AA	874	U
25	AA	877	A
25	AA	878	C
25	AA	879	U
25	AA	880	A
25	AA	881	A
25	AA	884	C
25	AA	885	C
25	AA	887	C
25	AA	890	C
25	AA	891	G
25	AA	892	C
25	AA	893	A
25	AA	900	U
25	AA	904	G
25	AA	910	A
25	AA	917	A
25	AA	920	A
25	AA	921	U
25	AA	924	U
25	AA	935	G
25	AA	937	MA6
25	AA	947	G
25	AA	948	G
25	AA	952	A
25	AA	955	C
85	Az	1	U
85	Az	3	A
85	Az	4	A
85	Az	5	U
85	Az	6	G
85	Az	12	U
85	Az	13	U
85	Az	14	A
85	Az	15	U
85	Az	16	A
85	Az	18	A
85	Az	21	A
85	Az	22	A
85	Az	23	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	Az	24	U
85	Az	25	U
85	Az	26	A
85	Az	27	C
85	Az	32	A
87	Aw	3	G
87	Aw	4	U
87	Aw	5	A
87	Aw	6	U
87	Aw	7	A
87	Aw	8	U
87	Aw	10	G
87	Aw	11	U
87	Aw	12	U
87	Aw	13	U
87	Aw	14	A
87	Aw	16	A
87	Aw	21	A
87	Aw	22	A
87	Aw	23	A
87	Aw	24	A
87	Aw	25	C
87	Aw	26	G
87	Aw	27	A
87	Aw	30	G
87	Aw	31	A
87	Aw	32	U
87	Aw	36	C
87	Aw	44	C
87	Aw	46	A
87	Aw	48	U
87	Aw	49	U
87	Aw	51	U
87	Aw	53	A
87	Aw	56	A
87	Aw	61	U
87	Aw	65	A
87	Aw	67	U
87	Aw	68	U
87	Aw	69	A
87	Aw	70	C
87	Aw	71	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	Aw	72	A
87	Aw	73	A
87	Aw	74	C
87	Aw	75	C
87	Aw	76	A
88	Ax	3	G
88	Ax	6	A
88	Ax	7	A
88	Ax	8	U
88	Ax	9	A
88	Ax	10	G
88	Ax	11	U
88	Ax	12	U
88	Ax	14	A
88	Ax	15	A
88	Ax	16	C
88	Ax	17	A
88	Ax	22	A
88	Ax	28	C
88	Ax	29	U
88	Ax	33	U
88	Ax	35	A
88	Ax	36	U
88	Ax	37	C
88	Ax	38	C
88	Ax	41	A
88	Ax	42	G
88	Ax	43	G
88	Ax	44	A
88	Ax	45	G
88	Ax	46	A
88	Ax	48	U
88	Ax	49	G
88	Ax	50	G
88	Ax	51	A
88	Ax	52	G
88	Ax	55	U
88	Ax	56	C
88	Ax	57	A
88	Ax	58	A
88	Ax	59	U
88	Ax	60	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
88	Ax	62	C
88	Ax	63	U
88	Ax	64	C
88	Ax	66	U
88	Ax	67	U
88	Ax	71	U
88	Ax	72	A
88	Ax	73	A
88	Ax	75	C
88	Ax	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2112	A
2	B	9	1MA
25	AA	864	C
25	AA	865	A
25	AA	873	U
25	AA	878	C
25	AA	879	U
25	AA	884	C
25	AA	890	C
25	AA	892	C

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	$\# Z > 2$
25	MA6	AA	936	25	23,26,27	0.33	0	34,38,41	0.60	1 (2%)
1	OMG	A	2815	1,88,91	23,26,27	0.37	0	33,38,41	0.34	0
25	MA6	AA	937	25	23,26,27	0.38	0	34,38,41	0.61	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MU	AA	429	25	19,22,23	0.33	0	28,32,35	0.30	0
2	PSU	B	39	2	18,21,22	0.51	0	22,30,33	0.52	0
25	5MC	AA	841	25	18,22,23	0.36	0	26,32,35	1.03	3 (11%)
1	PSU	A	3067	1	18,21,22	0.48	0	22,30,33	0.61	0
2	1MA	B	9	2	21,25,26	0.36	0	31,37,40	1.15	4 (12%)
2	2MG	B	10	2	23,26,27	0.53	0	32,38,41	0.74	1 (3%)
1	OMU	A	3039	1,91	19,22,23	0.31	0	26,31,34	0.49	0
25	B8T	AA	839	25,92	19,22,23	0.36	0	26,31,34	0.57	0
62	5F0	AI	184	62	8,8,9	0.52	0	7,9,11	1.21	1 (14%)
1	1MA	A	2617	1	21,25,26	0.39	0	31,37,40	1.22	3 (9%)
1	OMG	A	3040	1,87	23,26,27	0.48	0	33,38,41	0.95	1 (3%)

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
25	MA6	AA	936	25	-	0/11/29/30	0/3/3/3
1	OMG	A	2815	1,88,91	-	1/9/27/28	0/3/3/3
25	MA6	AA	937	25	-	1/11/29/30	0/3/3/3
25	5MU	AA	429	25	-	0/7/25/26	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
25	5MC	AA	841	25	-	0/7/25/26	0/2/2/2
1	PSU	A	3067	1	-	0/7/25/26	0/2/2/2
2	1MA	B	9	2	-	1/7/25/26	0/3/3/3
2	2MG	B	10	2	-	2/9/27/28	0/3/3/3
1	OMU	A	3039	1,91	-	0/9/27/28	0/2/2/2
25	B8T	AA	839	25,92	-	2/7/27/28	0/2/2/2
62	5F0	AI	184	62	-	5/9/9/10	-
1	1MA	A	2617	1	-	2/7/25/26	0/3/3/3
1	OMG	A	3040	1,87	-	1/9/27/28	0/3/3/3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2617	1MA	O3'-C3'-C2'	3.90	124.45	111.82
2	B	9	1MA	O3'-C3'-C2'	3.21	122.20	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	1MA	O3'-C3'-C4'	2.95	119.58	111.05
62	AI	184	5F0	O-C-CB	-2.87	117.07	125.43
1	A	2617	1MA	O3'-C3'-C4'	2.66	118.73	111.05
1	A	3040	OMG	C2'-C1'-N9	-2.58	109.22	114.22
2	B	10	2MG	O3'-C3'-C4'	2.53	118.38	111.05
25	AA	936	MA6	C2-N1-C6	2.34	117.28	111.75
25	AA	841	5MC	O3'-C3'-C2'	2.31	119.30	111.82
25	AA	937	MA6	C2-N1-C6	2.28	117.15	111.75
25	AA	841	5MC	C2'-C3'-C4'	2.27	107.06	102.64
1	A	2617	1MA	C2'-C3'-C4'	2.26	107.03	102.64
25	AA	841	5MC	O3'-C3'-C4'	2.25	117.56	111.05
2	B	9	1MA	O4'-C4'-C5'	2.14	116.42	109.37
2	B	9	1MA	C5'-C4'-C3'	2.09	123.01	115.18

There are no chirality outliers.

All (15) 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'
62	AI	184	5F0	OD1-C1-CA-CB
62	AI	184	5F0	N-CA-CB-C
62	AI	184	5F0	C1-CA-CB-C
1	A	2617	1MA	C3'-C4'-C5'-O5'
2	B	10	2MG	C3'-C4'-C5'-O5'
1	A	2617	1MA	O4'-C4'-C5'-O5'
62	AI	184	5F0	O1-C1-CA-CB
62	AI	184	5F0	O-C-CB-CA
25	AA	839	B8T	O4'-C4'-C5'-O5'
25	AA	937	MA6	C4'-C5'-O5'-P
25	AA	839	B8T	C3'-C4'-C5'-O5'
2	B	9	1MA	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AA	936	MA6	2	0
1	A	2815	OMG	1	0
25	AA	937	MA6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	39	PSU	3	0
25	AA	841	5MC	2	0
2	B	10	2MG	1	0
62	AI	184	5F0	2	0
1	A	3040	OMG	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 261 ligands modelled in this entry, 254 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	$\# Z > 2$
96	FES	AE	201	69,58	0,4,4	-	-	-		
98	GDP	AX	503	-	28,30,30	0.37	0	44,47,47	0.43	0
93	VAL	B	101	-	4,6,7	0.58	0	6,7,9	0.66	0
96	FES	r	201	7,55	0,4,4	-	-	-		
94	NAD	AA	1002	92	45,48,48	0.39	0	63,73,73	0.62	1 (1%)
96	FES	AT	201	73,66	0,4,4	-	-	-		
97	ATP	AX	501	92	29,33,33	0.37	0	44,52,52	0.64	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
96	FES	AE	201	69,58	-	-	0/1/1/1
98	GDP	AX	503	-	-	1/16/32/32	0/3/3/3
93	VAL	B	101	-	-	0/5/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	FES	r	201	7,55	-	-	0/1/1/1
94	NAD	AA	1002	92	-	5/30/62/62	0/5/5/5
96	FES	AT	201	73,66	-	-	0/1/1/1
97	ATP	AX	501	92	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	AA	1002	NAD	PN-O3-PA	-2.54	124.12	132.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	AA	1002	NAD	C3D-C4D-C5D-O5D
94	AA	1002	NAD	O4B-C4B-C5B-O5B
94	AA	1002	NAD	O4D-C4D-C5D-O5D
94	AA	1002	NAD	C5B-O5B-PA-O3
98	AX	503	GDP	C5'-O5'-PA-O1A
94	AA	1002	NAD	C3B-C4B-C5B-O5B

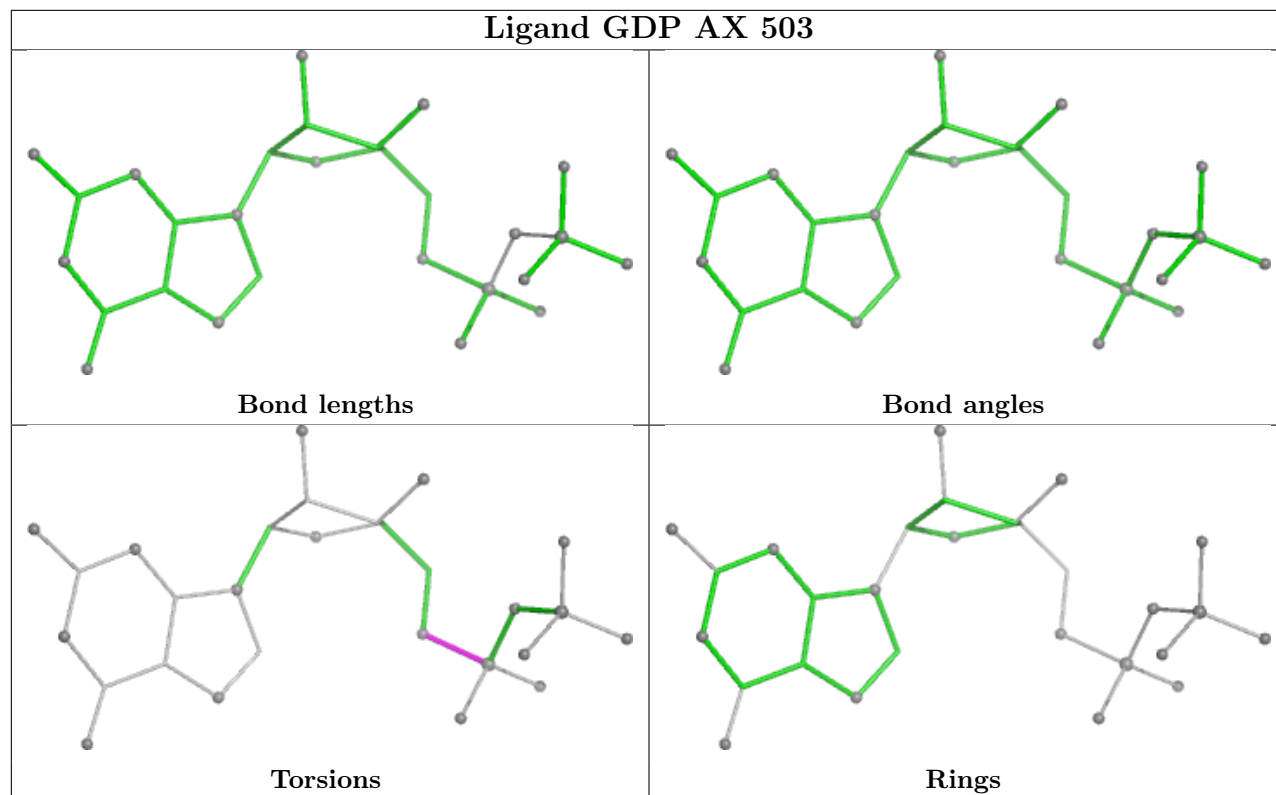
There are no ring outliers.

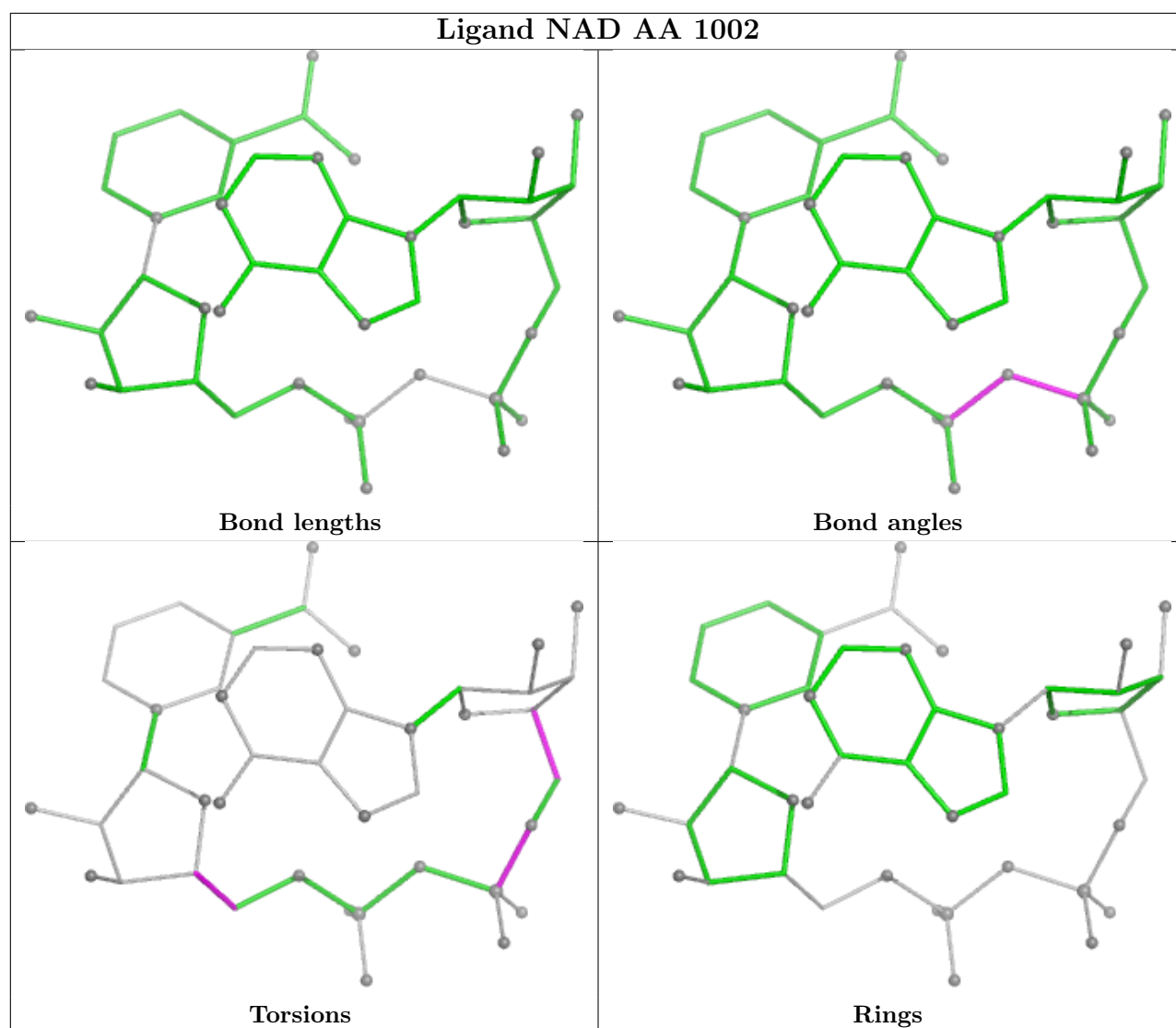
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
96	r	201	FES	5	0
94	AA	1002	NAD	1	0
97	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.





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.

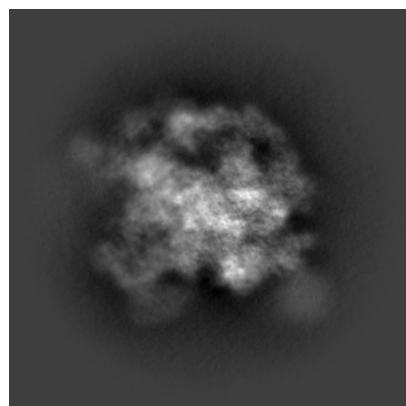
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54640. These allow visual inspection of the internal detail of the map and identification of artifacts.

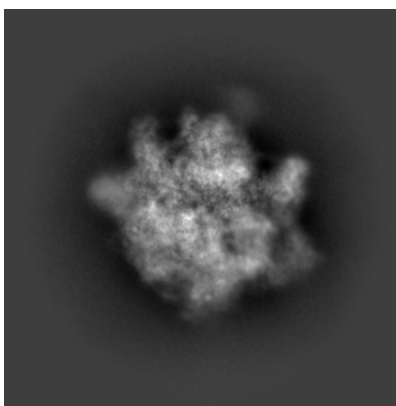
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

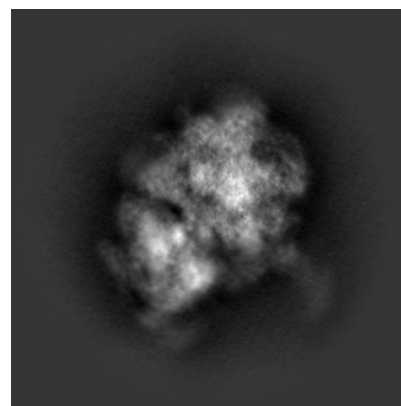
6.1.1 Primary map



X

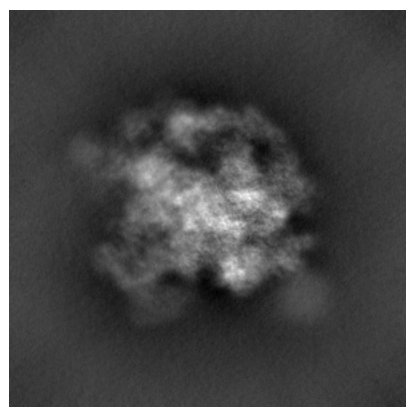


Y

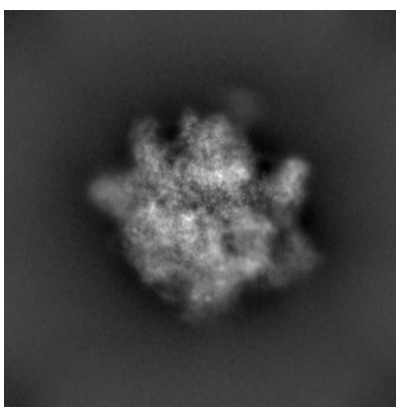


Z

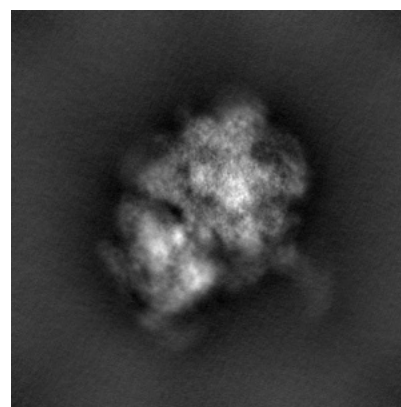
6.1.2 Raw map



X



Y

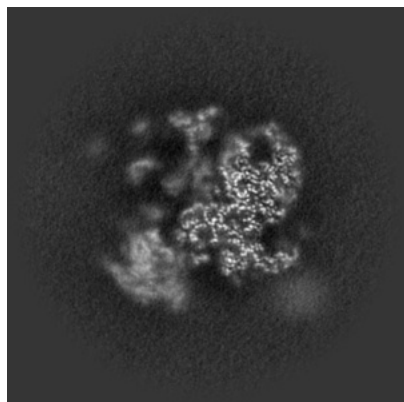


Z

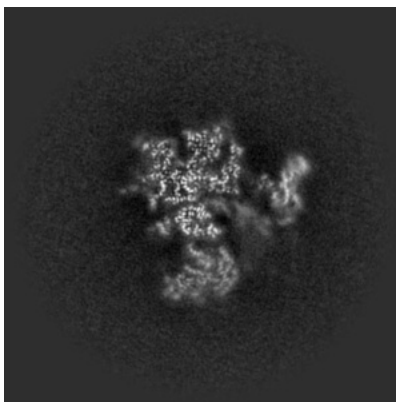
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

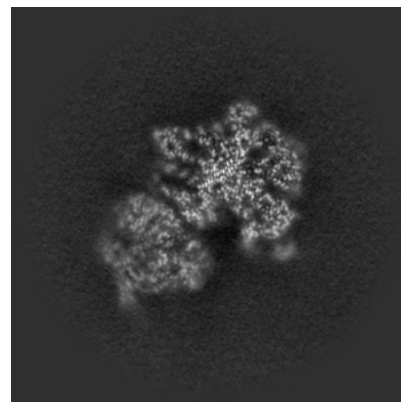
6.2.1 Primary map



X Index: 200

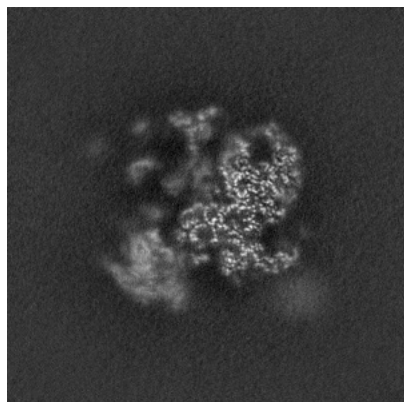


Y Index: 200

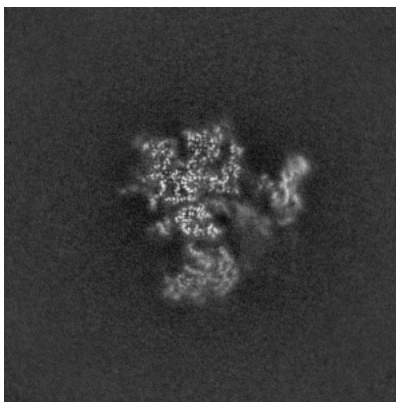


Z Index: 200

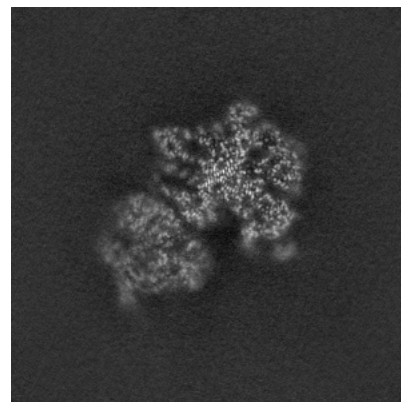
6.2.2 Raw map



X Index: 200



Y Index: 200

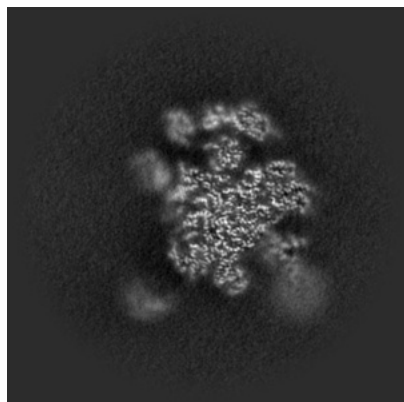


Z Index: 200

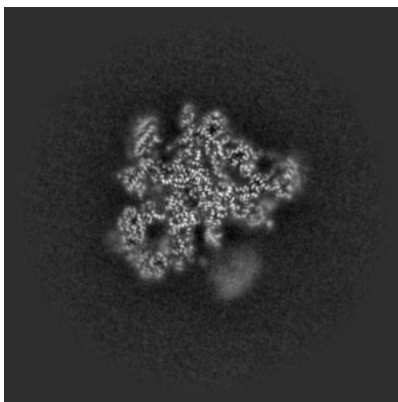
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

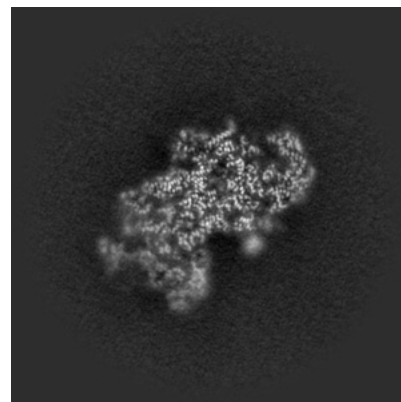
6.3.1 Primary map



X Index: 230

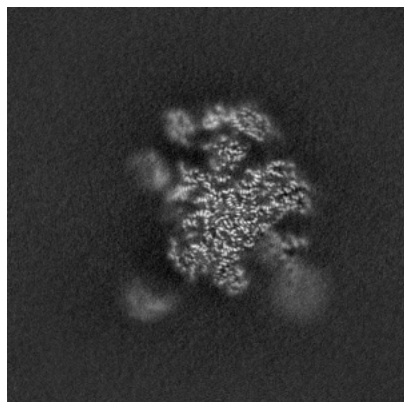


Y Index: 230

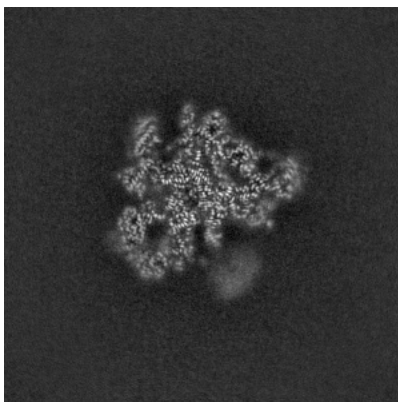


Z Index: 185

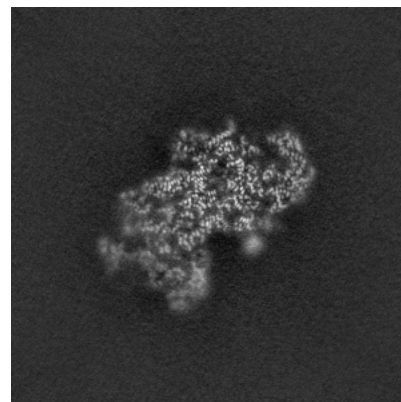
6.3.2 Raw map



X Index: 229



Y Index: 230

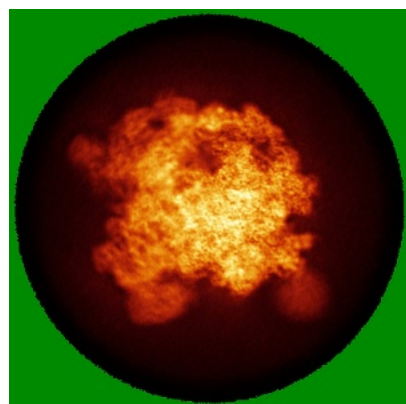


Z Index: 185

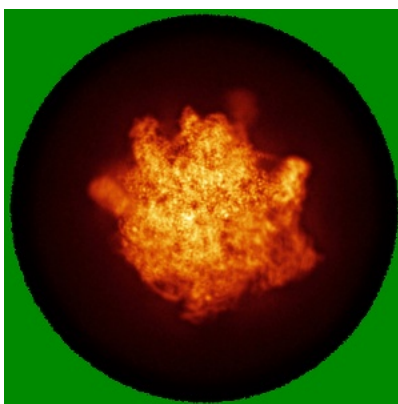
The images above show the largest variance slices of the map in three orthogonal directions.

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

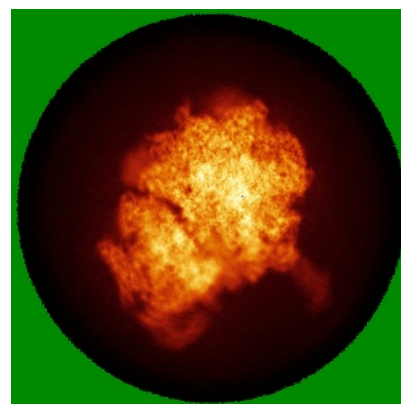
6.4.1 Primary map



X

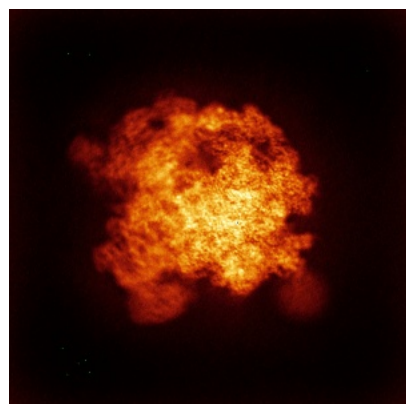


Y

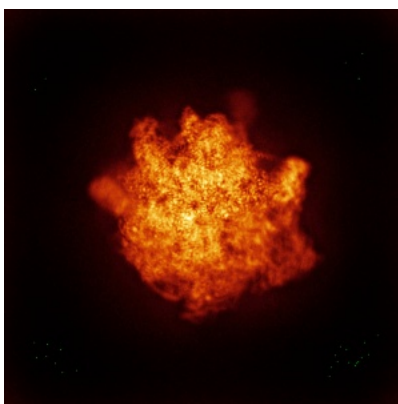


Z

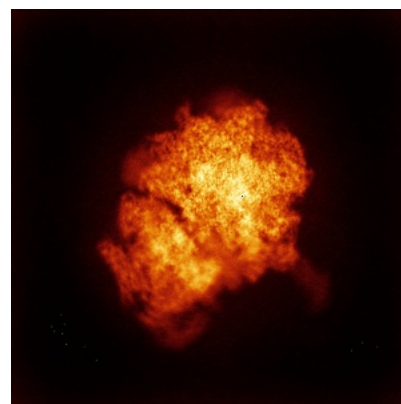
6.4.2 Raw map



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 0.7. 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.

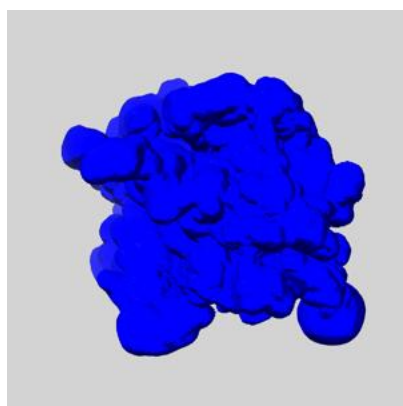
6.6 Mask visualisation [i](#)

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

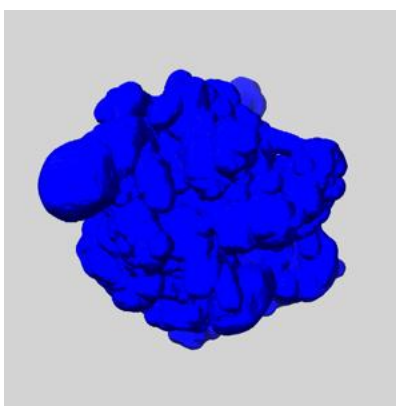
A mask typically either:

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

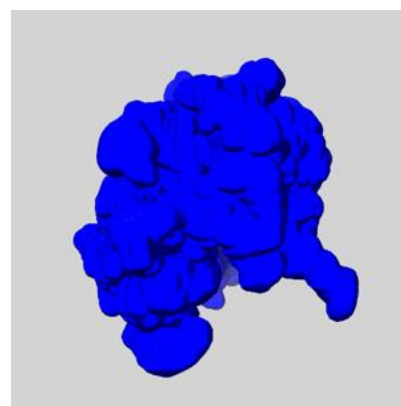
6.6.1 emd_54640_msk_1.map [i](#)



X



Y

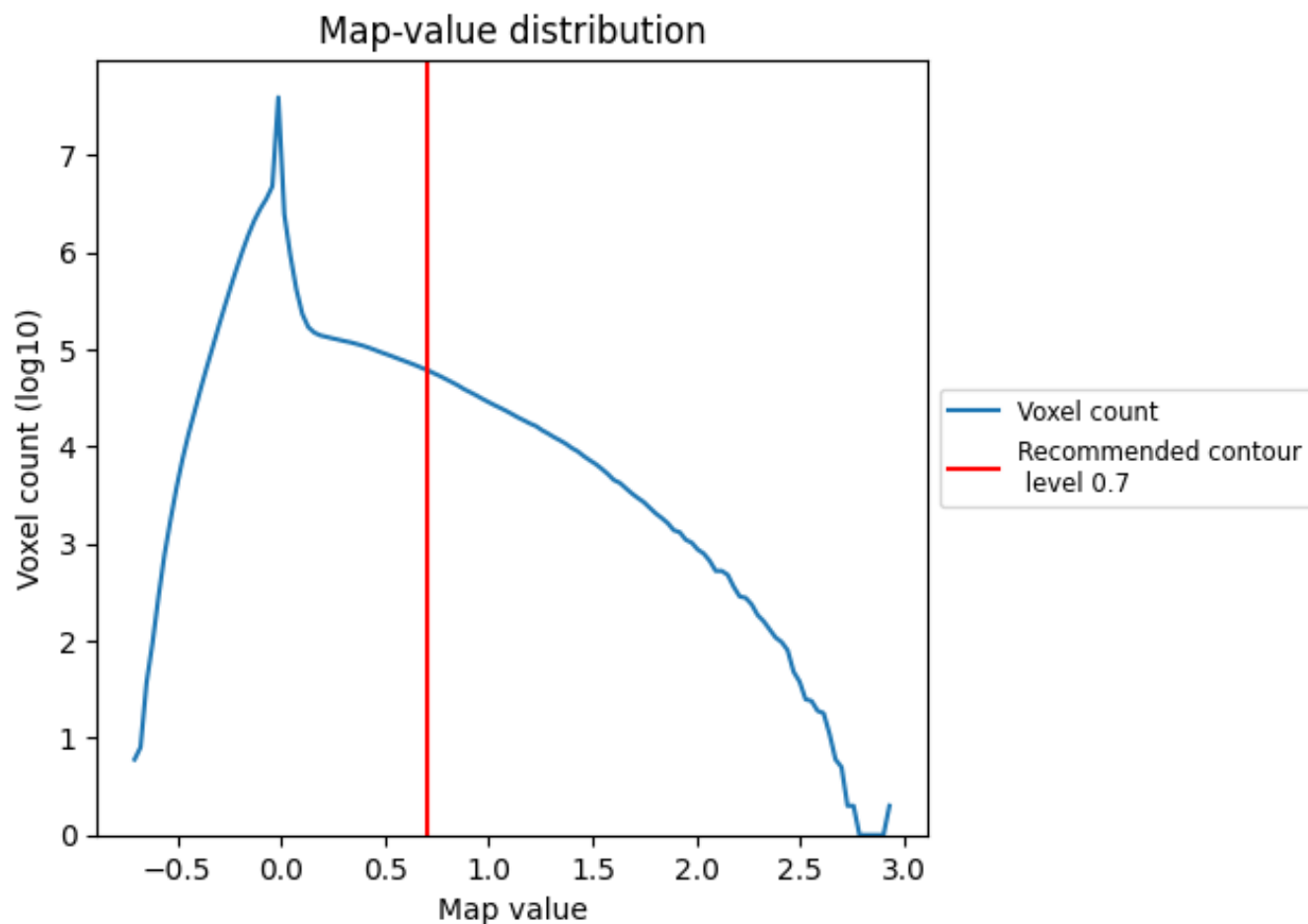


Z

7 Map analysis [i](#)

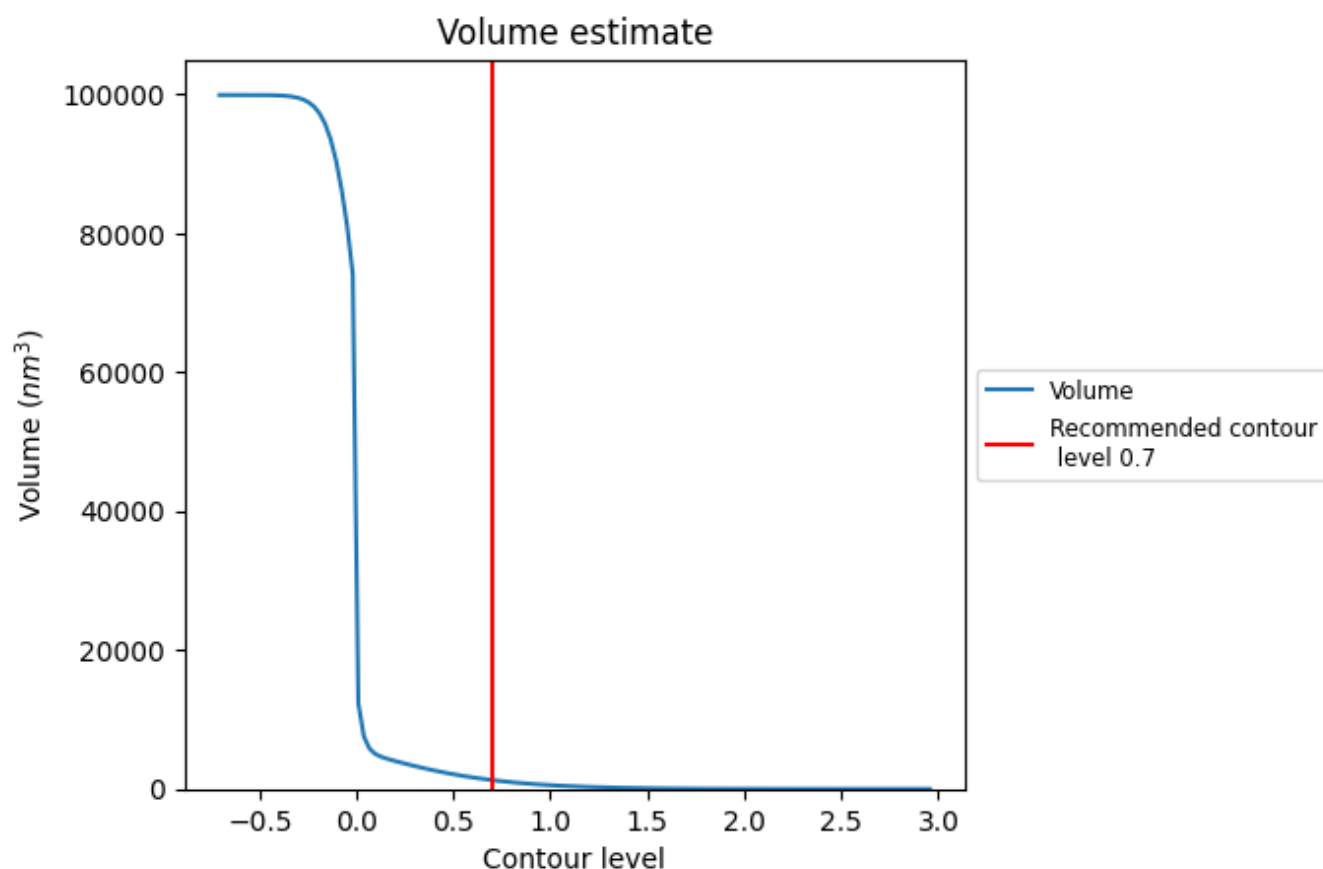
This section contains the results of statistical analysis of the map.

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.

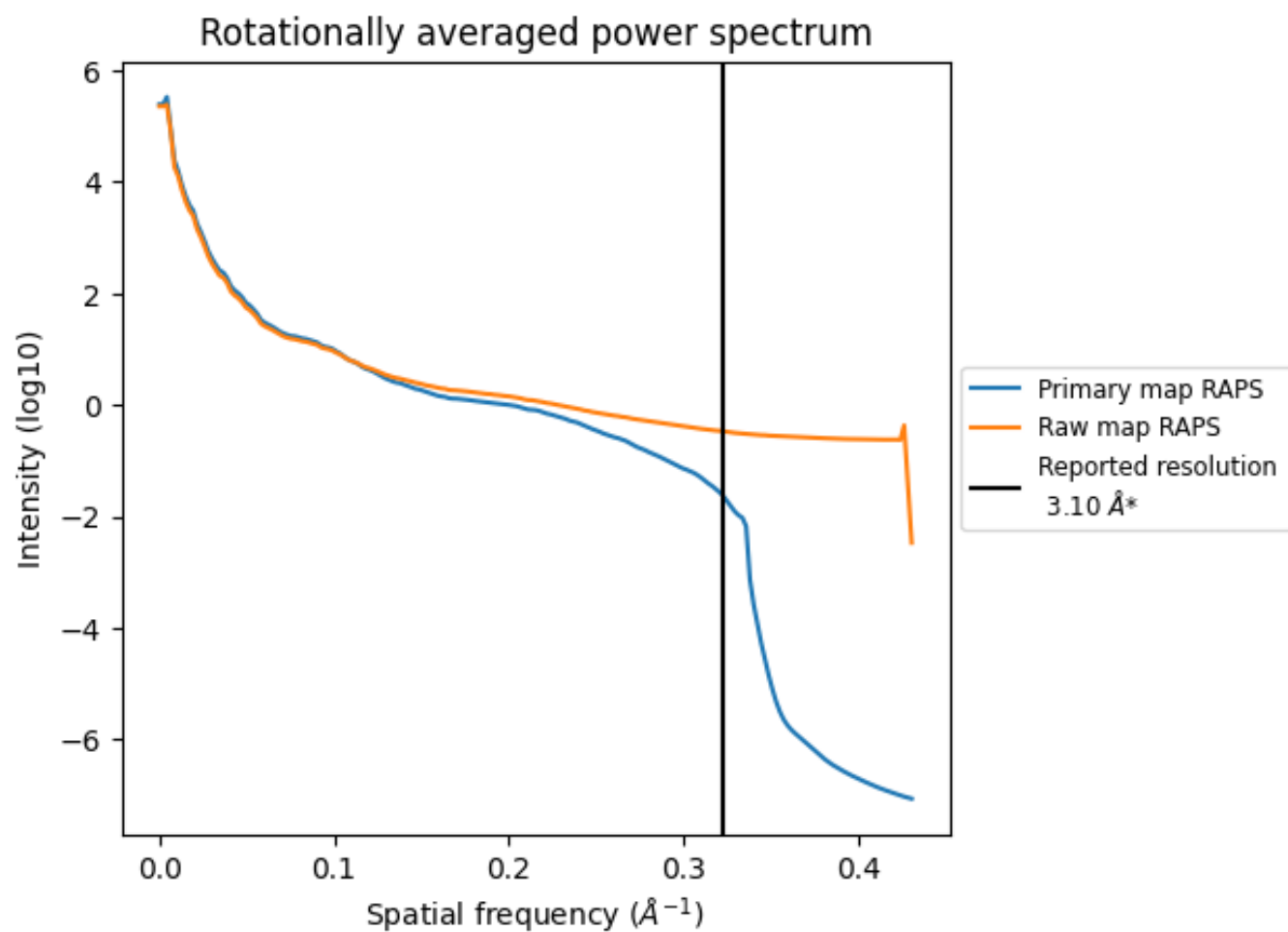
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1276 nm^3 ; this corresponds to an approximate mass of 1152 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 ⓘ

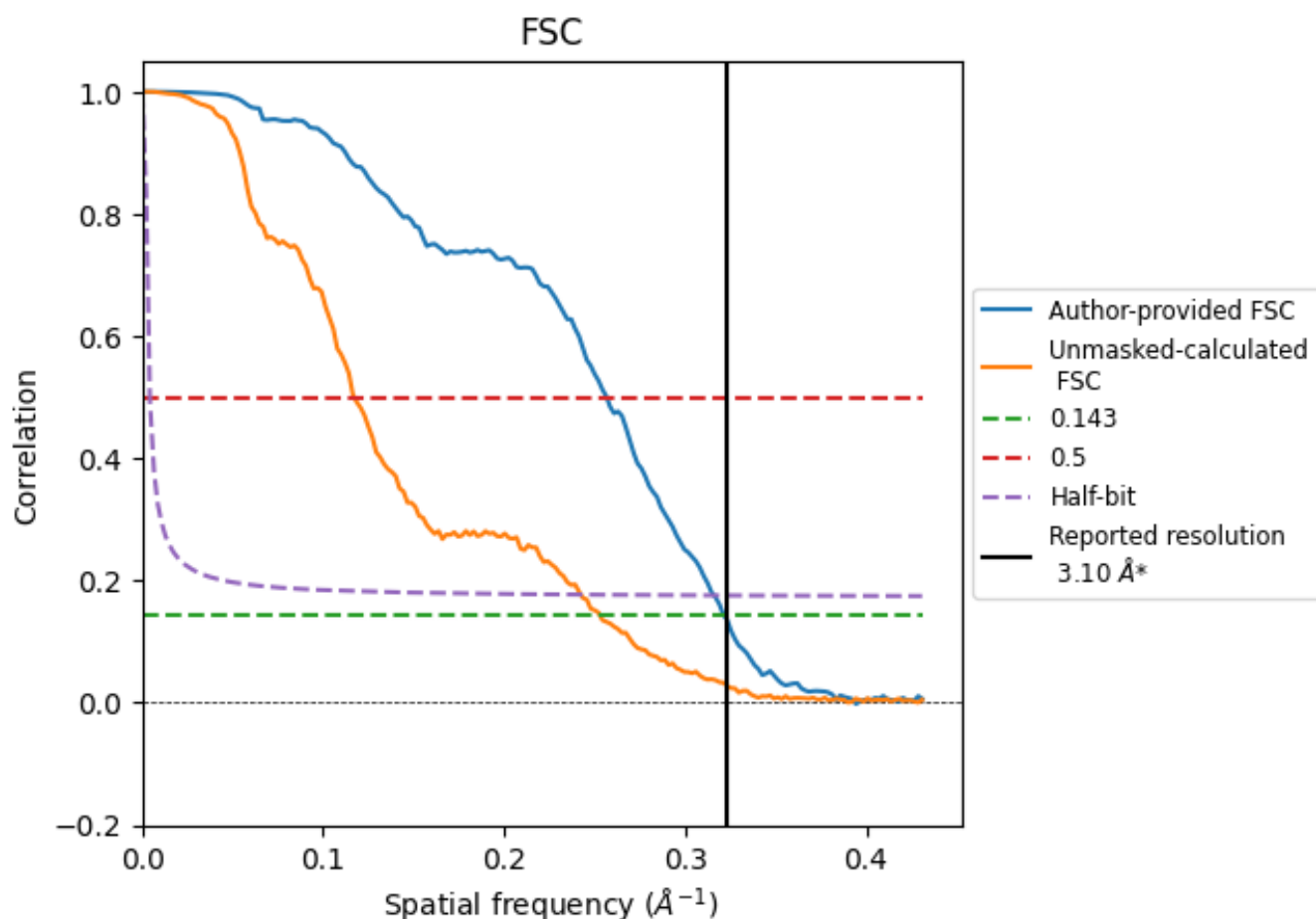


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

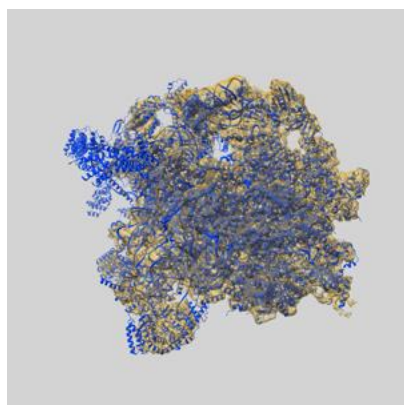
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.90	3.16
Unmasked-calculated*	3.95	8.54	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.1 by more than 10 %

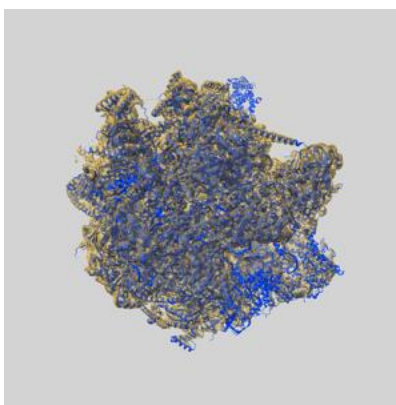
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54640 and PDB model 9S7E. Per-residue inclusion information can be found in section [3](#) on page [26](#).

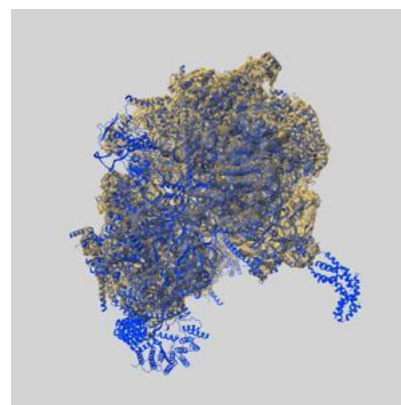
9.1 Map-model overlay [i](#)



X



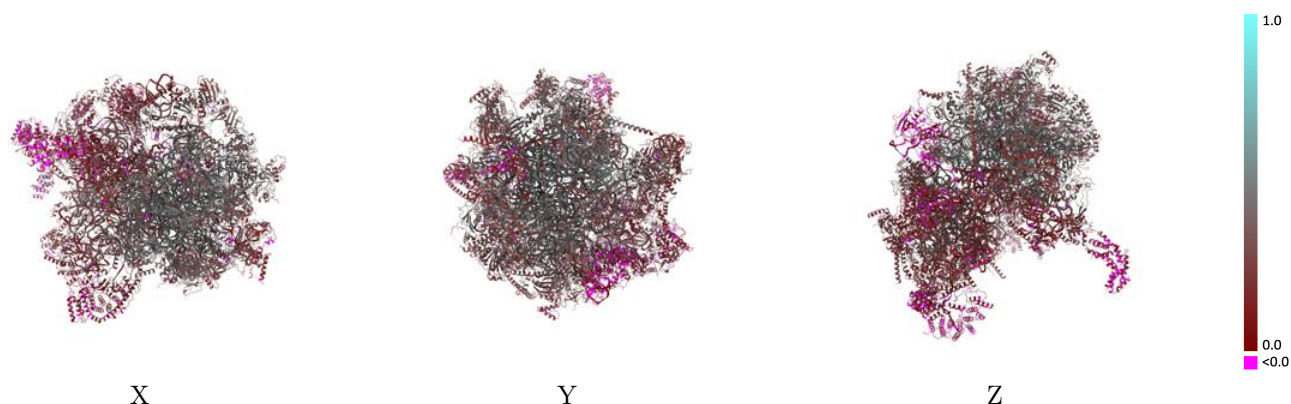
Y



Z

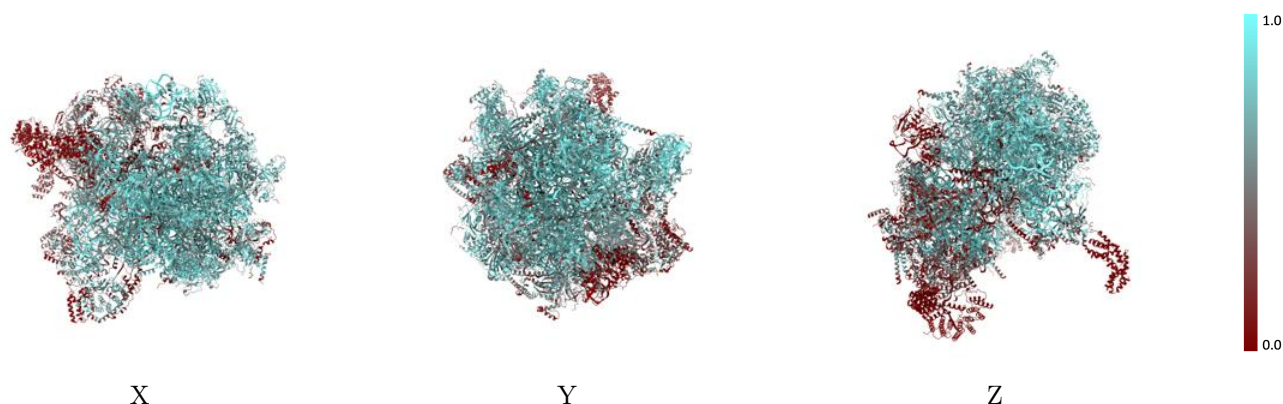
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



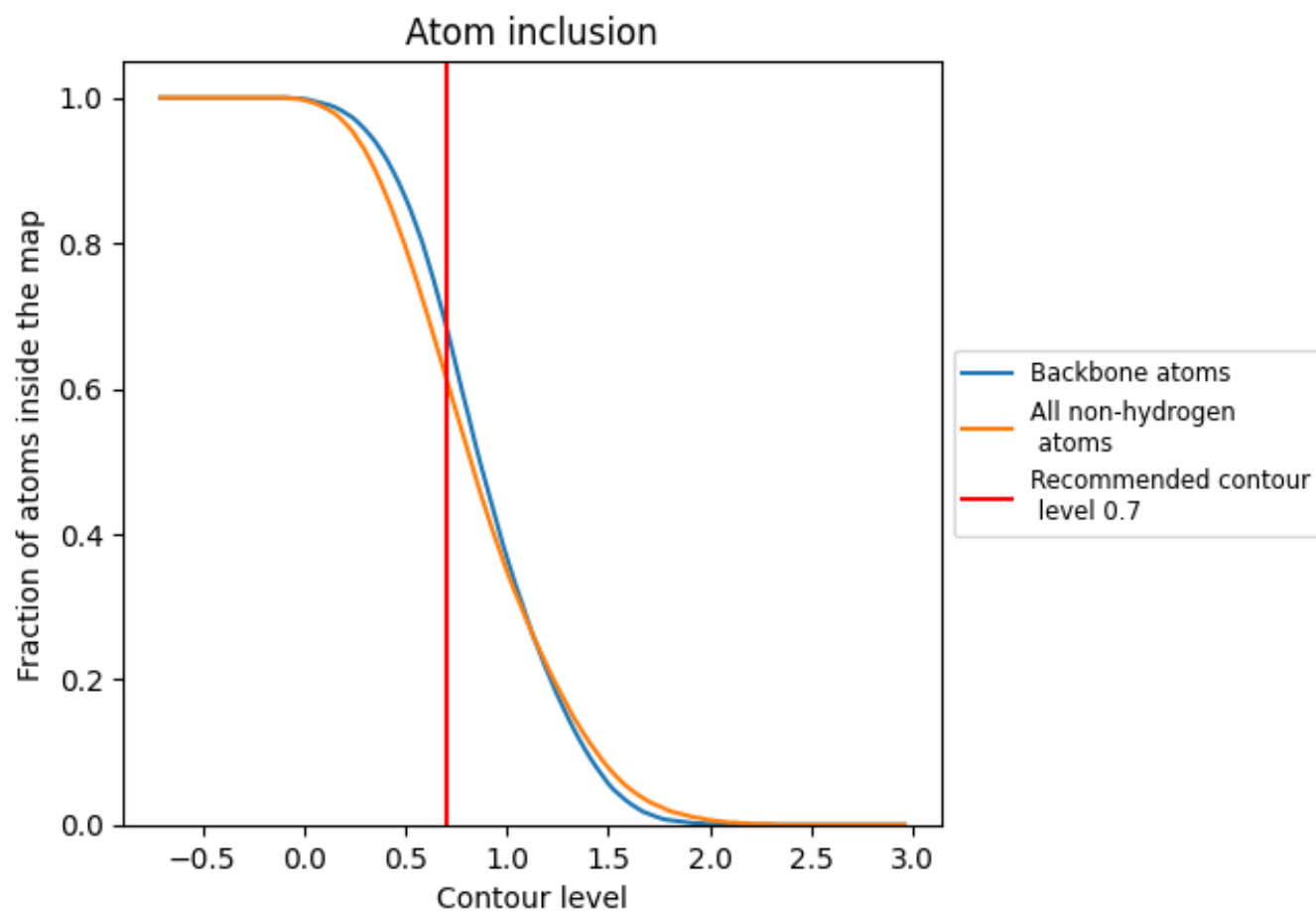
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6150	 0.3140
0	 0.7230	 0.4010
1	 0.6360	 0.3350
2	 0.7920	 0.4820
3	 0.7590	 0.4700
4	 0.8040	 0.3860
5	 0.6680	 0.3500
6	 0.7700	 0.3340
7	 0.7320	 0.3510
8	 0.4310	 0.2570
9	 0.7140	 0.3830
A	 0.8820	 0.4240
A0	 0.4580	 0.1560
A1	 0.2620	 0.2050
A2	 0.2580	 0.2630
A3	 0.4950	 0.3460
A4	 0.0380	 0.1010
AA	 0.8360	 0.3150
AB	 0.5560	 0.2890
AC	 0.3480	 0.2650
AD	 0.3070	 0.2770
AE	 0.4780	 0.3100
AF	 0.3820	 0.2050
AG	 0.3220	 0.2140
AH	 0.3020	 0.2160
AI	 0.6020	 0.3190
AJ	 0.2660	 0.2620
AK	 0.6010	 0.2500
AL	 0.4600	 0.2610
AM	 0.5220	 0.2040
AN	 0.5480	 0.2810
AO	 0.3710	 0.1990
AP	 0.5850	 0.3100
AQ	 0.5280	 0.3200
AR	 0.3130	 0.1850



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AS	 0.3940	 0.2410
AT	 0.4360	 0.2590
AU	 0.5240	 0.2000
AV	 0.3990	 0.1240
AW	 0.3840	 0.2880
AX	 0.3100	 0.1280
AY	 0.2190	 0.1540
AZ	 0.4210	 0.1940
Au	 0.1180	 0.1340
Av	 0.1390	 0.2920
Aw	 0.0330	 0.2110
Ax	 0.4020	 0.2270
Az	 0.1510	 0.1530
B	 0.9080	 0.2540
D	 0.7460	 0.4380
E	 0.7850	 0.4360
F	 0.7510	 0.4300
H	 0.3740	 0.2010
I	 0.4520	 0.2060
J	 0.3640	 0.1390
K	 0.7820	 0.4380
L	 0.6640	 0.4320
M	 0.7680	 0.4230
N	 0.6950	 0.4020
O	 0.7540	 0.4280
P	 0.7970	 0.3710
Q	 0.6130	 0.3890
R	 0.6830	 0.4020
S	 0.7270	 0.4120
T	 0.7070	 0.4310
U	 0.7220	 0.4030
V	 0.4580	 0.2090
W	 0.7590	 0.4490
X	 0.7000	 0.3940
Y	 0.7130	 0.3810
Z	 0.6330	 0.4080
a	 0.5410	 0.3340
b	 0.7210	 0.4130
c	 0.7110	 0.3610
d	 0.5050	 0.2100
e	 0.5950	 0.2030
f	 0.4660	 0.2840

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.7460	 0.4000
h	 0.6440	 0.3240
i	 0.7460	 0.4600
j	 0.6940	 0.3770
k	 0.5640	 0.2320
l	 0.3720	 0.1430
m	 0.4170	 0.1930
o	 0.7870	 0.4380
p	 0.6290	 0.3220
q	 0.5000	 0.2670
r	 0.7740	 0.3900
s	 0.7220	 0.3910
t	 0.0370	 0.1140
u	 0.0000	 0.0860
v	 0.0000	 0.0920
w	 0.0000	 0.0290
x	 0.0000	 0.0210
y	 0.0000	 0.0060
z	 0.0270	 0.0310