



Full wwPDB EM Validation Report ⓘ

Jun 19, 2024 – 05:09 pm BST

PDB ID : 8OIN
EMDB ID : EMD-16894
Title : 55S mammalian mitochondrial ribosome with mtRF1 and P-site tRNA
Authors : Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on : 2023-03-23
Resolution : 3.60 Å(reported)
Based on initial models : ., 7NQH, 7QI4

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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

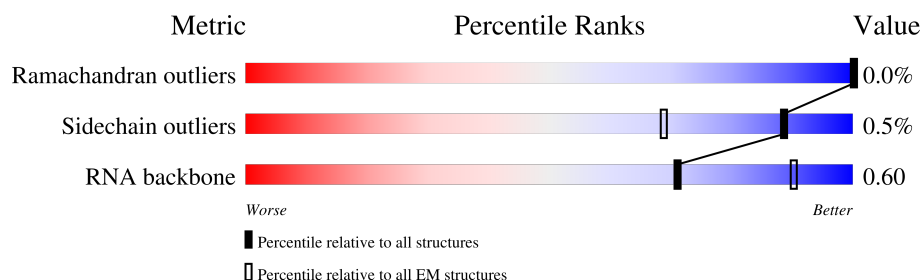
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	B1	198	<div> <div>23%</div> <div>23%</div> <div>77%</div> </div>
1	B2	198	<div> <div>14%</div> <div>14%</div> <div>86%</div> </div>
1	B3	198	<div> <div>14%</div> <div>14%</div> <div>86%</div> </div>
1	B4	198	<div> <div>14%</div> <div>14%</div> <div>86%</div> </div>
1	B5	198	<div> <div>14%</div> <div>14%</div> <div>86%</div> </div>
1	B6	198	<div> <div>13%</div> <div>13%</div> <div>87%</div> </div>
2	B7	3	<div> <div>100%</div> <div>67%</div> <div>33%</div> </div>
3	B8	1571	<div> <div>6%</div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
4	B9	73	
5	BA	210	
6	BB	150	
7	BC	216	
8	BD	148	
9	BE	256	
10	BF	250	
11	BG	161	
12	BH	207	
13	BI	65	
14	BJ	95	
15	BK	188	
16	BL	306	
17	BM	399	
18	BN	294	
19	BO	268	
20	BP	257	
21	BQ	192	
22	BR	197	
23	BS	325	
24	BT	296	
25	BU	251	
26	BV	169	
27	BW	188	
28	BX	303	

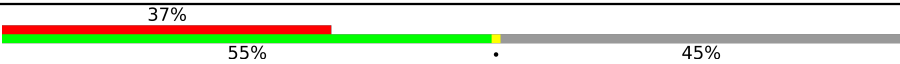


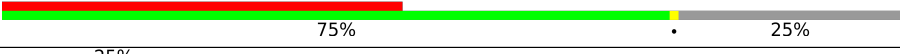
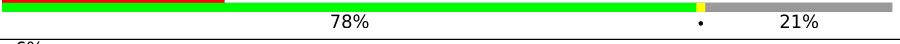

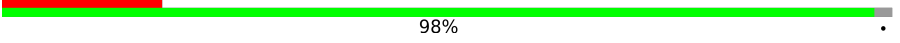









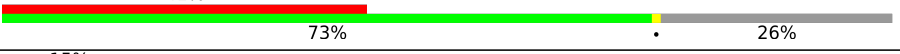

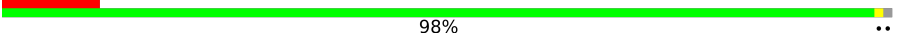


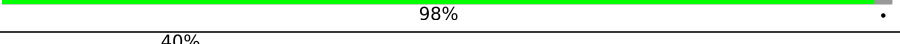

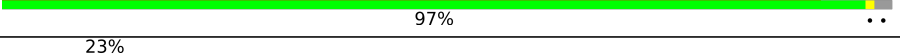

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Mol	Chain	Length	Quality of chain
29	BY	149	
30	BZ	209	
31	Ba	160	
32	Bb	112	
33	Bc	138	
34	Bd	126	
35	Be	102	
36	Bf	205	
37	Bg	222	
38	Bh	196	
39	Bi	433	
40	Bj	304	
41	Bl	100	
42	Bm	423	
43	Bn	380	
44	Bo	334	
45	Bp	162	
46	Bq	135	
47	Br	142	
48	Bs	159	
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	269	
53	Bx	166	

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Mol	Chain	Length	Quality of chain
54	By	198	
55	Bz	128	
56	AA	960	
57	AB	366	
58	AC	167	
59	AD	199	
60	AE	124	
61	AF	242	
62	AG	71	
63	AH	200	
64	AI	9	
65	AJ	139	
66	AK	128	
67	AL	259	
68	AM	135	
69	AN	130	
70	AO	258	
71	AP	143	
72	AQ	87	
73	AR	382	
74	AS	190	
75	AT	173	
76	AU	205	
77	AV	395	
78	AW	188	

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Mol	Chain	Length	Quality of chain
79	AX	410	
80	AY	381	
81	AZ	148	
82	Aa	474	
83	Ab	289	
84	Ac	118	
85	Ad	430	
86	Ae	692	
87	Ag	397	
88	Ai	196	
89	Aj	505	

2 Entry composition [i](#)

There are 100 unique types of molecules in this entry. The entry contains 180624 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 protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B1	45	Total	C	N	O	0	0
			317	203	52	62		
1	B2	27	Total	C	N	O	0	0
			213	137	33	43		
1	B3	28	Total	C	N	O	0	0
			222	143	35	44		
1	B4	27	Total	C	N	O	0	0
			213	137	33	43		
1	B5	27	Total	C	N	O	0	0
			213	137	33	43		
1	B6	26	Total	C	N	O	0	0
			205	131	32	42		

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B7	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B8	1571	Total	C	N	O	P	0	0
			33427	15015	6087	10754	1571		

- Molecule 4 is a RNA chain called CP Phe-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B9	73	Total	C	N	O	P	S	0	0
			1560	703	283	500	73	1		

- Molecule 5 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 6 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	149	Total	C	N	O	S	0	0
			1184	754	227	201	2		

- Molecule 7 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	206	Total	C	N	O	S	0	0
			1678	1056	308	309	5		

- Molecule 8 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	112	Total	C	N	O	S	0	0
			867	558	158	148	3		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BE	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	107	Total	C	N	O	S	0	0
			874	562	159	150	3		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 13 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 14 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 15 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BK	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 16 is a protein called Mitochondrial ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 17 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BM	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 18 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BN	250	Total	C	N	O	S	1	0
			2019	1299	370	344	6		

- Molecule 19 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	202	Total	C	N	O	S	0	0
			1660	1059	311	286	4		

- Molecule 20 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BP	212	Total	C	N	O	S	0	0
			1705	1100	306	290	9		

- Molecule 21 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	176	Total	C	N	O	S	0	0
			1339	851	243	243	2		

- Molecule 22 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	177	Total	C	N	O	S	0	0
			1447	928	258	254	7		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BS	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 24 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BT	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 25 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BU	222	Total	C	N	O	S	0	0
			1803	1156	331	306	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 26 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BV	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 27 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BW	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 28 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BX	240	Total	C	N	O	S	0	0
			1954	1253	338	354	9		

- Molecule 29 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BY	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BZ	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ba	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L53.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bb	97	Total	C	N	O	S	0	0
			745	461	143	135	6		

- Molecule 33 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bc	84	Total	C	N	O	S	0	0
			716	458	128	127	3		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L55.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bd	92	Total	C	N	O	S	0	0
			763	477	148	135	3		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Be	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 36 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bf	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 37 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bg	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 38 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bh	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 39 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 40 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bj	164	Total	C	N	O	S	0	0
			1325	853	217	251	4		

- Molecule 41 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 42 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bn	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 44 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bo	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 45 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	143	Total	C	N	O	S	0	0
			1202	757	217	227	1		

- Molecule 46 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bq	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 47 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	108	Total	C	N	O	S	0	0
			906	570	167	165	4		

- Molecule 48 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	151	Total	C	N	O	S	0	0
			1185	738	227	217	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	2	ACE	-	acetylation	UNP F1S8U4

- Molecule 49 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bt	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 50 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 51 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	238	Total	C	N	O	S	0	0
			1948	1240	338	363	7		

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bw	165	Total	C	N	O	S	0	0
			1295	825	224	241	5		

- Molecule 53 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bx	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bx	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 54 is a protein called Mitochondrial ribosomal protein L50.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	By	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 55 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bz	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 56 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AA	960	Total	C	N	O	P	0	0
			20418	9169	3708	6581	960		

- Molecule 57 is a protein called 28S ribosomal protein S35, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AB	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 58 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 59 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AD	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 60 is a protein called Mitoribosomal protein bs6m, mrps6.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AE	122	Total	C	N	O	S	0	0
			981	620	178	177	6		

- Molecule 61 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AF	208	Total	C	N	O	S	0	0
			1722	1097	314	300	11		

- Molecule 62 is a RNA chain called P-site Met-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AG	71	Total	C	N	O	P	0	0
			1502	673	264	494	71		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	69	C	-	insertion	GB 1208989970
AG	70	C	-	insertion	GB 1208989970
AG	71	A	-	insertion	GB 1208989970

- Molecule 63 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AH	140	Total	C	N	O	S	0	0
			1155	746	197	208	4		

- Molecule 64 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AI	9	Total	C	N	O	P	0	0
			193	88	40	57	8		

- Molecule 65 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AJ	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 66 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AK	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 67 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AL	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 68 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AM	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 69 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AN	112	Total	C	N	O	S	0	0
			875	568	153	151	3		

- Molecule 70 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AO	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 71 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AP	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 72 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AQ	86	Total	C	N	O	S	0	0
			737	455	148	126	8		

- Molecule 73 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AR	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 74 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AS	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 75 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AT	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 76 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AU	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 77 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AV	388	Total	C	N	O	S	0	0
			3109	1971	535	589	14		

- Molecule 78 is a protein called Mitoribosomal protein ms28, mrps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AW	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 79 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AX	353	Total	C	N	O	S	0	0
			2875	1837	515	513	10		

- Molecule 80 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AY	149	Total	C	N	O	S	0	0
			1250	807	211	229	3		

- Molecule 81 is a protein called Mitochondrial ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AZ	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 82 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Aa	381	Total	C	N	O	S	1	0
			3120	1943	572	592	13		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	ASP	-	expression tag	UNP O75570
Aa	454	TYR	-	expression tag	UNP O75570
Aa	455	LYS	-	expression tag	UNP O75570
Aa	456	ASP	-	expression tag	UNP O75570
Aa	457	HIS	-	expression tag	UNP O75570

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	458	ASP	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	ASP	-	expression tag	UNP O75570
Aa	461	TYR	-	expression tag	UNP O75570
Aa	462	LYS	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	HIS	-	expression tag	UNP O75570
Aa	465	ASP	-	expression tag	UNP O75570
Aa	466	ILE	-	expression tag	UNP O75570
Aa	467	ASP	-	expression tag	UNP O75570
Aa	468	TYR	-	expression tag	UNP O75570
Aa	469	LYS	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	ASP	-	expression tag	UNP O75570
Aa	472	ASP	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	LYS	-	expression tag	UNP O75570

- Molecule 83 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ab	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 84 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ac	116	Total	C	N	O	S	0	0
			933	579	185	161	8		

- Molecule 85 is a protein called 28S ribosomal protein S5, mitochondrial isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ad	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 86 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ae	588	Total	C	N	O	S	0	0
			4748	3039	804	879	26		

- Molecule 87 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Ag	328	Total	C	N	O	S	0	0
			2650	1678	478	481	13		

- Molecule 88 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ai	137	Total	C	N	O	S	0	0
			1008	632	192	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ai	186	5F0	ASN	variant	UNP A0A286ZJJ6

- Molecule 89 is a protein called Mitochondrial ribosomal protein S34.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	B8	192	Total	Mg	0
			192	192	
90	B9	1	Total	Mg	0
			1	1	
90	BL	2	Total	Mg	0
			2	2	
90	BM	2	Total	Mg	0
			2	2	
90	BT	1	Total	Mg	0
			1	1	
90	BV	3	Total	Mg	0
			3	3	
90	BY	1	Total	Mg	0
			1	1	
90	Be	1	Total	Mg	0
			1	1	
90	Bq	1	Total	Mg	0
			1	1	

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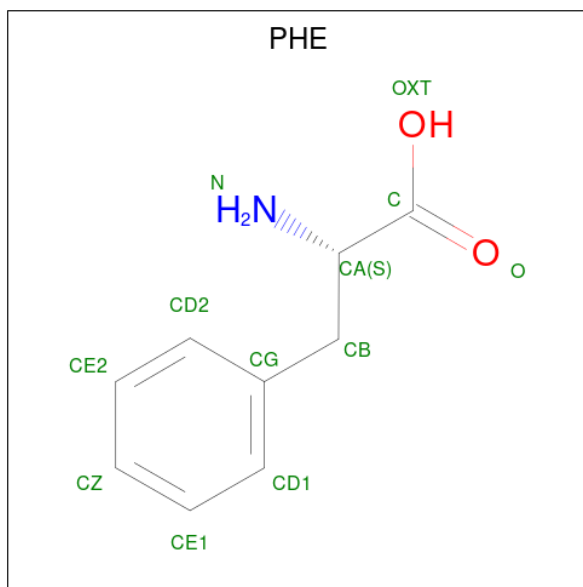
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Mol	Chain	Residues	Atoms		AltConf
90	Bx	1	Total 1	Mg 1	0
90	AA	121	Total 121	Mg 121	0
90	AD	1	Total 1	Mg 1	0
90	AG	1	Total 1	Mg 1	0
90	AI	1	Total 1	Mg 1	0
90	AJ	1	Total 1	Mg 1	0
90	AX	1	Total 1	Mg 1	0
90	Ab	1	Total 1	Mg 1	0

- Molecule 91 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
91	B8	25	Total 25	K 25	0
91	BL	1	Total 1	K 1	0
91	BU	1	Total 1	K 1	0
91	BW	1	Total 1	K 1	0
91	Be	1	Total 1	K 1	0
91	Bz	1	Total 1	K 1	0
91	AA	11	Total 11	K 11	0

- Molecule 92 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).

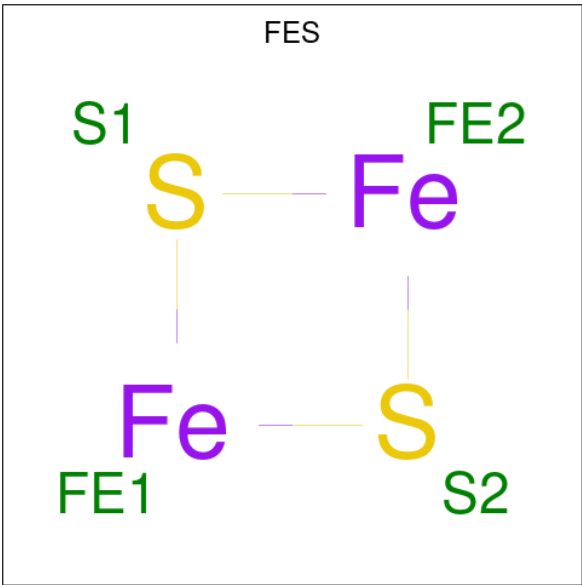


Mol	Chain	Residues	Atoms				AltConf
92	B9	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 93 is ZINC ION (three-letter code: ZN) (formula: Zn).

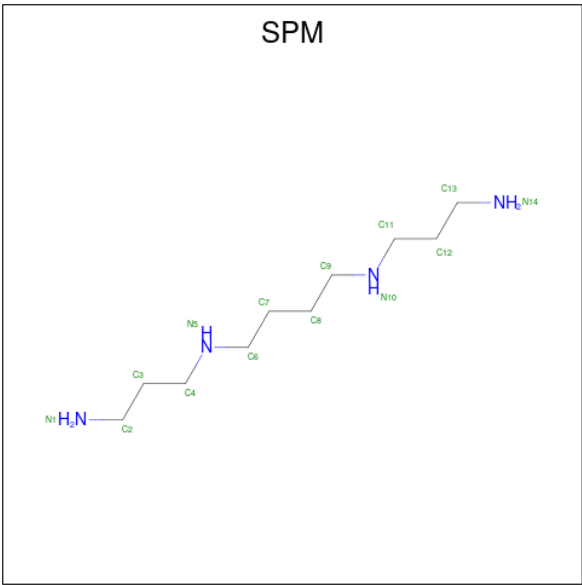
Mol	Chain	Residues	Atoms		AltConf
93	BH	1	Total	Zn	0
			1	1	
93	Bl	1	Total	Zn	0
			1	1	
93	AO	1	Total	Zn	0
			1	1	

- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



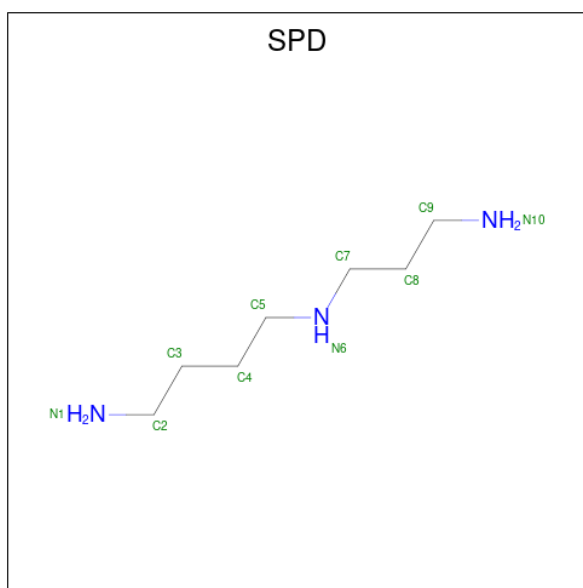
Mol	Chain	Residues	Atoms			AltConf
94	Bh	1	Total	Fe	S	0
			4	2	2	
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 95 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



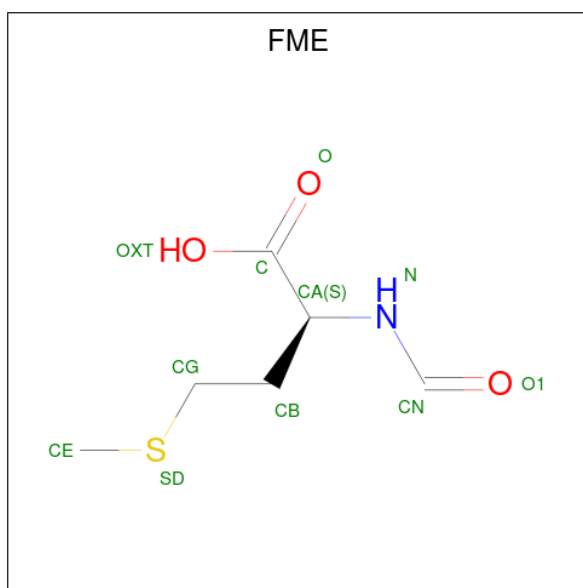
Mol	Chain	Residues	Atoms			AltConf
95	AA	1	Total	C	N	0
			14	10	4	

- Molecule 96 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

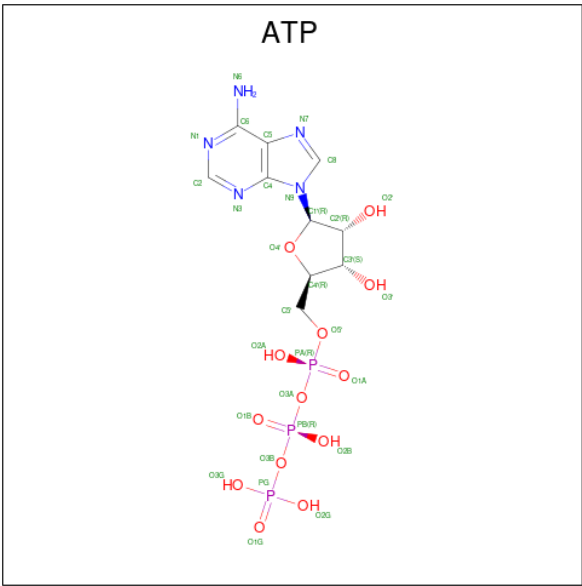
- Molecule 97 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
97	AG	1	Total	C	N	O	S	0
			10	6	1	2	1	

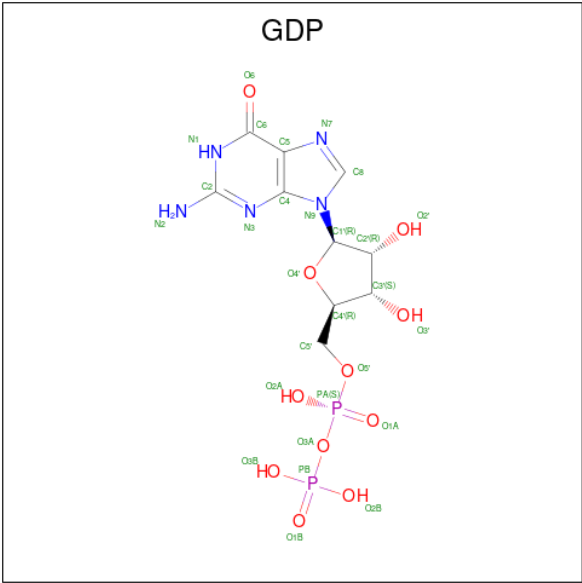
- Molecule 98 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 99 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



- Molecule 100 is water.

Mol	Chain	Residues	Atoms		AltConf
100	AX	3	Total	O	0
			3	3	

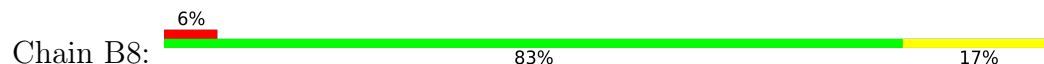
ALA
GLU
LYS
ILE
LYS
ALA
ALA
LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
LEU
GLU

• Molecule 2: E-site tRNA



C74
C75
A76

• Molecule 3: 16S rRNA



A1
A15
U19
A20
C21
U22
A23
A24
A25
C26
A27
A31
C32
A36
C40
A41
C42
C43
A44
A45
A46
A47
A56
A57
C58
A59
U60
U66
A67
A68
C69
G82
A83
C100
C104
G105
U109
A112
U115
A129
G139
A140
U142
A143

A144
A145
A146
C163
A164
A168
C172
U179
A180
A189
U190
A191
A192
A205
A218
A219
C225
U228
A229
C239
G254
G263
A272
A273
A274
A275
A276
A277
A311
G322
A323
G324
A329
A330
A331
A336
A340
G352
G359

G369
U373
U374
U375
A376
U392
A409
G427
A428
G433
U434
A445
C446
A447
G448
A459
C460
C475
A479
G480
U488
C489
U490
U491
A492
A493
U497
A498
A501
U502
A503
A506
U511
A512
A515
A518
A532
A533
A534
C549
G557

C558
A559
A560
A570
A574
C575
U576
A577
U578
A580
A584
A585
C586
G592
C595
A596
A617
A618
A625
A631
A632
U633
G634
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A713
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A721
A722
A723
A724
C725
A726

A727
C728
G737
U746
U747
A748
G753
A777
A783
G809
A817
C825
C852
A853
U854
U855
A859
U864
A872
C889
C890
A891
A897
C902
A922
A923
G924
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G959
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U966
G967
G977

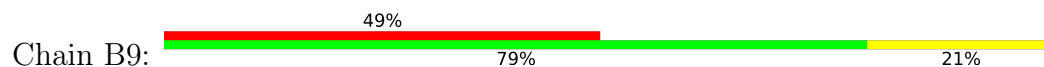
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C1016
U1017
U1018
A1026
G1027
A1028
A1038
C1050
G1051
A1055
G1056
A1057
U1063
G1064
U1091
A1092
A1093
A1094
C1095
A1096
A1097
C1098
U1099
C1100
A1101
A1102
C1103
C1104
A1105
C1106
A1107
A1108
A1109
G1110
G1111
G1112
A1113
U1114
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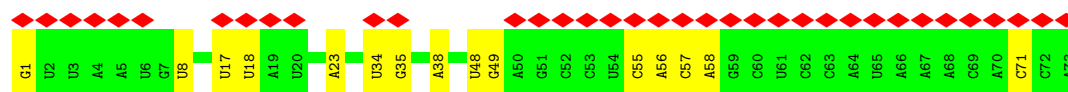
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G1151
C1167
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A1169
G1180
U1183
U1188
A1195
A1204
G1205
U1206
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C1215
A1216
A1217
U1218
A1219
A1220
C1221
A1222
C1226
U1231
G1232
A1233
A1240
U1241
U1242
U1243
A1246
U1247
C1248
A1249
G1253
A1254
C1264
A1271
U1291
U1296
C1299
U1314
G1325

A1326
U1327
G1328
G1332
A1341
C1342
U1375
G1376
A1389
G1390
C1396
U1403
A1425
G1426
U1432
U1433
U1436
U1445
A1448
A1468
A1485
A1493
A1494
C1498
A1504
G1505
U1509
C1525
U1526
U1527
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U1536
C1551
C1552
A1553
U1558
A1561

A1571

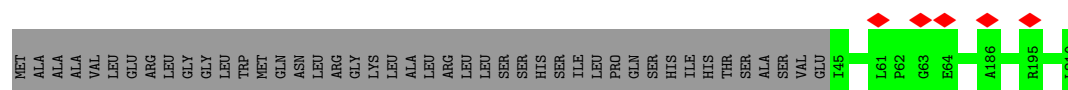
• Molecule 4: CP Phe-tRNA





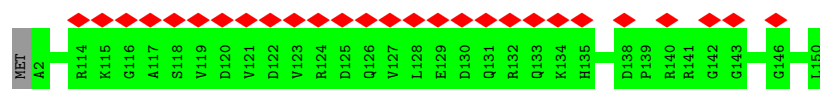
- Molecule 5: Large ribosomal subunit protein uL22m

Chain BA: 79% 21%



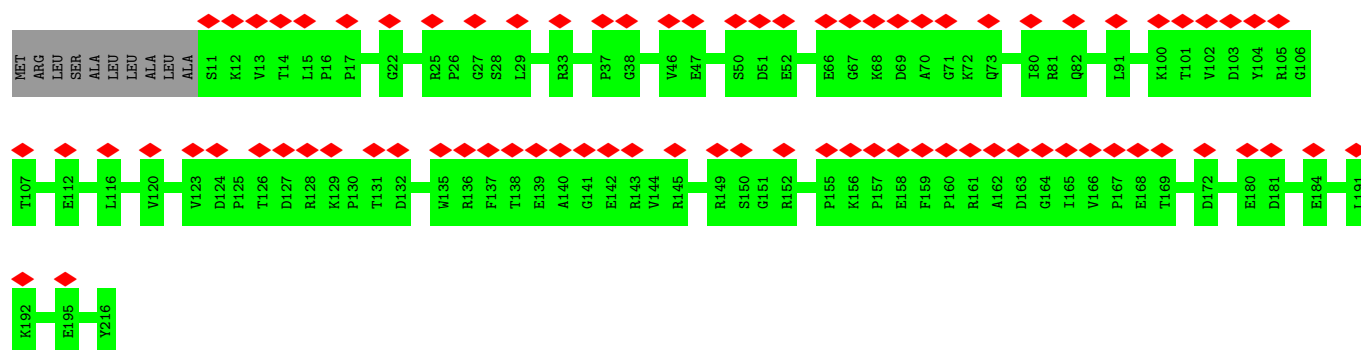
- Molecule 6: 39S ribosomal protein L23, mitochondrial

Chain BB: 18% 99%



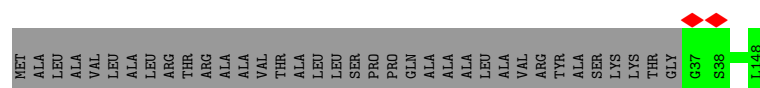
- Molecule 7: uL24m

Chain BC: 38% 95% 5%



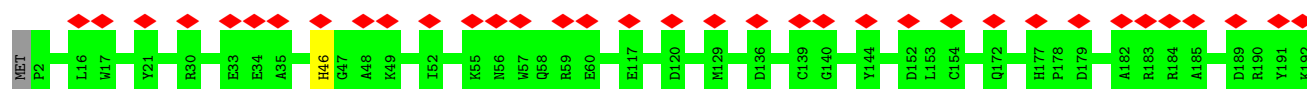
- Molecule 8: 39S ribosomal protein L27, mitochondrial

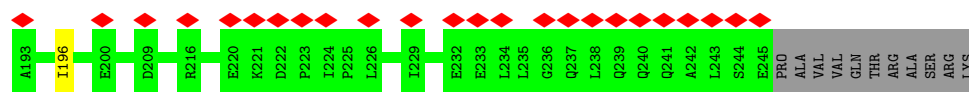
Chain BD: 76% 24%



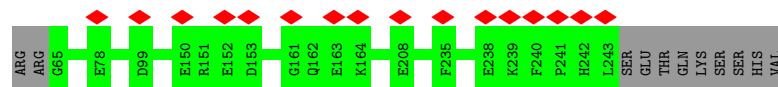
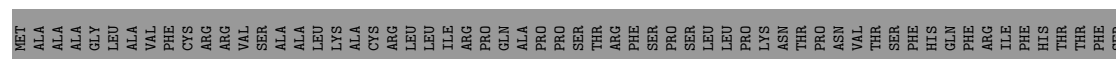
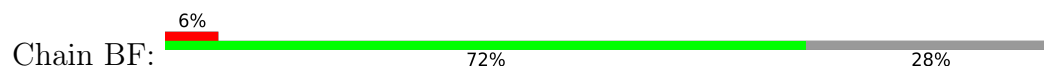
- Molecule 9: Mitochondrial ribosomal protein L28

Chain BE: 23% 95% 5%

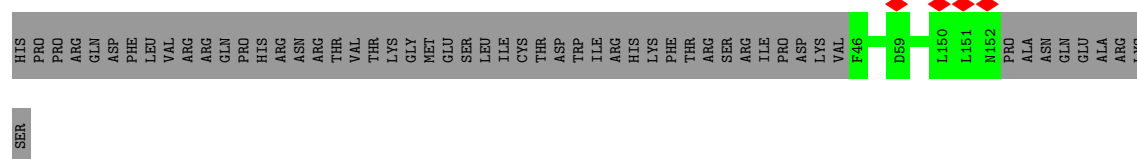




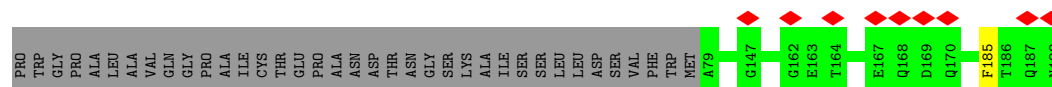
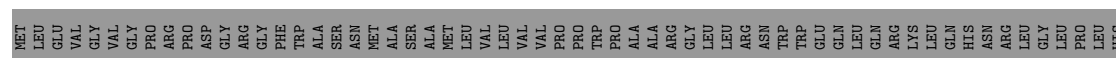
- Molecule 10: Mitochondrial ribosomal protein L47



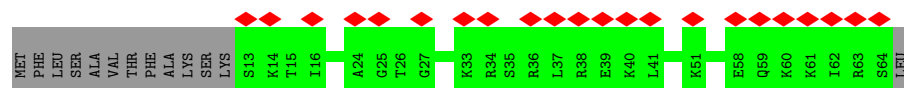
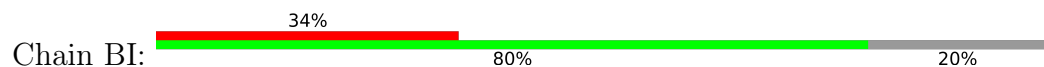
- Molecule 11: Large ribosomal subunit protein uL30m



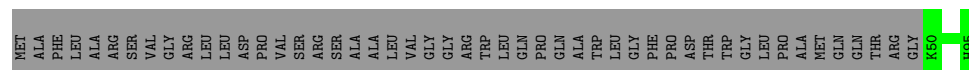
- Molecule 12: Mitochondrial ribosomal protein L32



- Molecule 13: Large ribosomal subunit protein bL33m



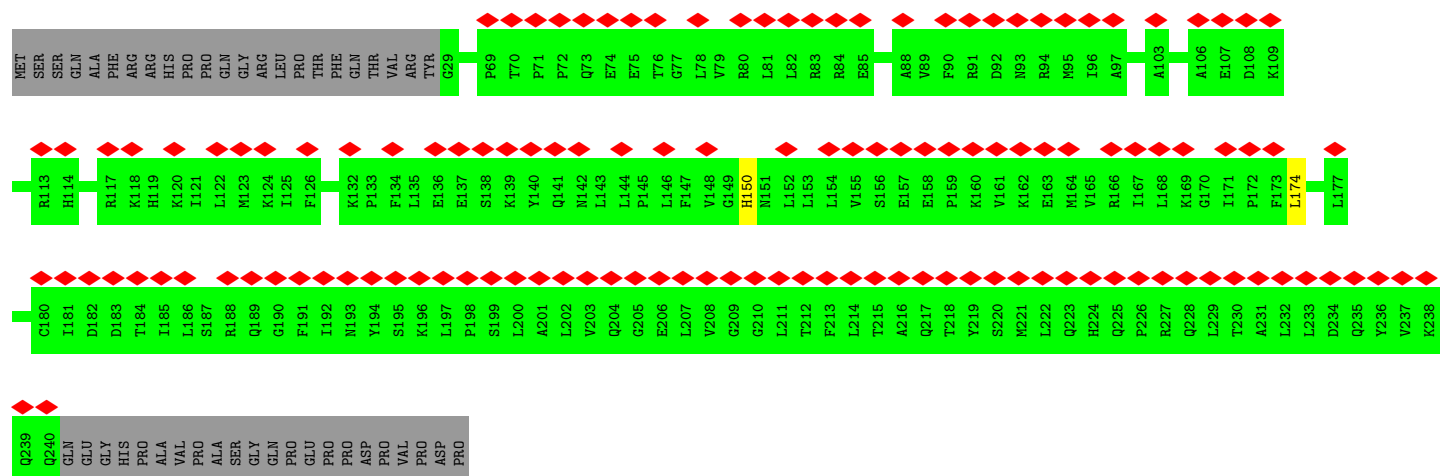
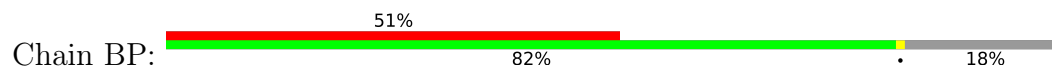
- Molecule 14: Large ribosomal subunit protein bL34m



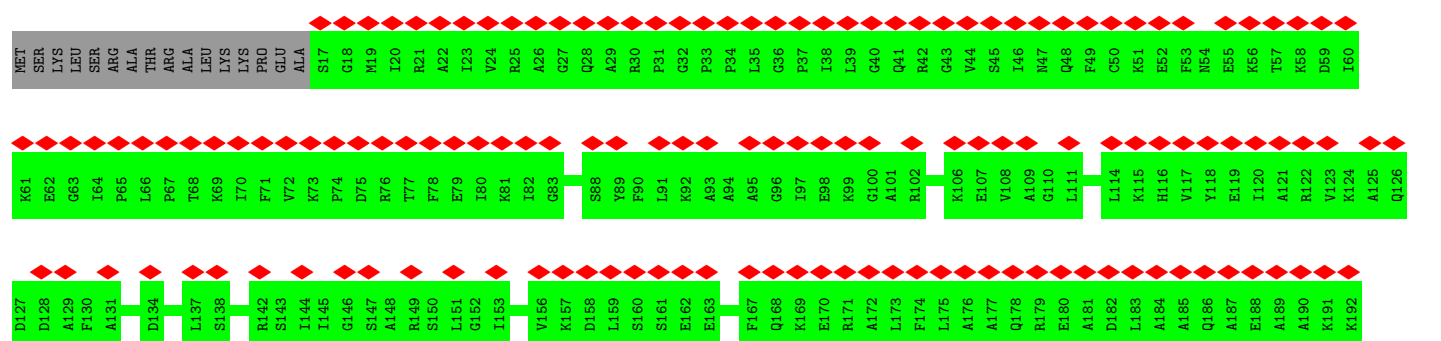
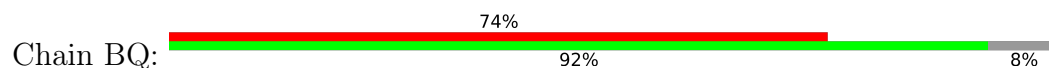
- Molecule 15: 39S ribosomal protein L35, mitochondrial



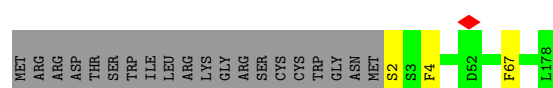
• Molecule 20: Mitochondrial ribosomal protein L10



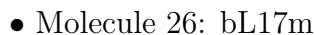
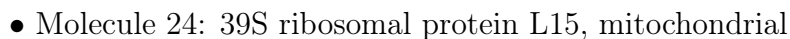
• Molecule 21: Mitochondrial ribosomal protein L11

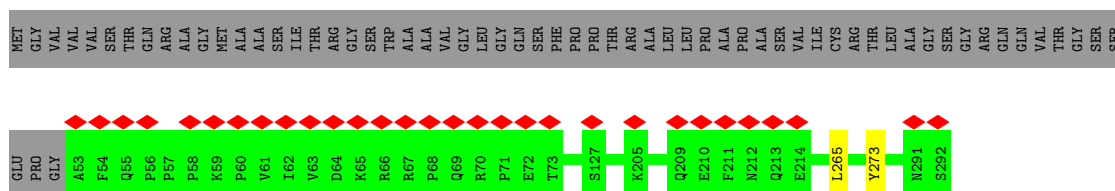


• Molecule 22: 39S ribosomal protein L13, mitochondrial

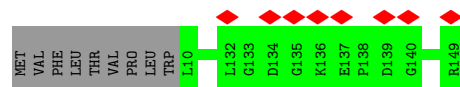


• Molecule 23: Mitochondrial ribosomal protein L14

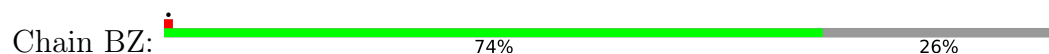




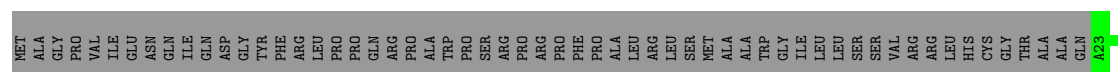
- Molecule 29: Mitochondrial ribosomal protein L20



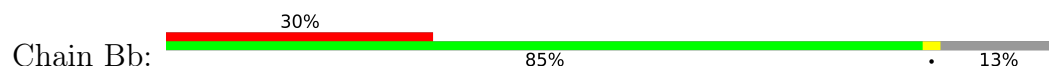
- Molecule 30: Mitochondrial ribosomal protein L21



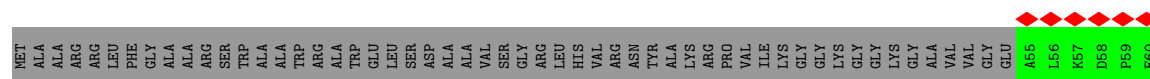
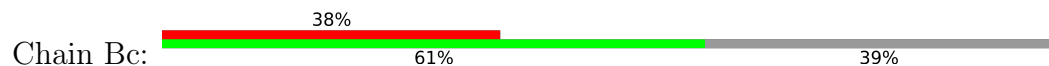
- Molecule 31: 39S ribosomal protein L52, mitochondrial

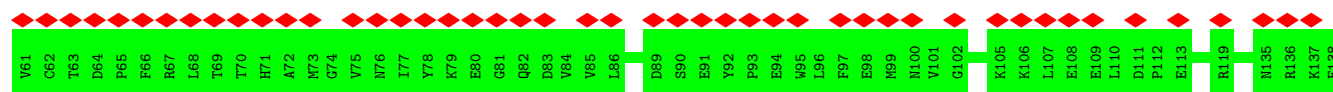


- Molecule 32: Mitochondrial ribosomal protein L53

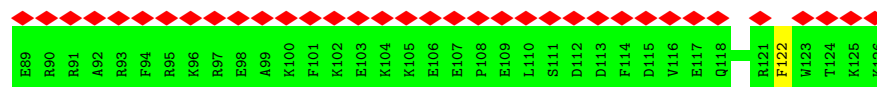
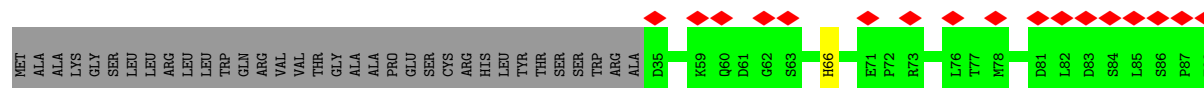
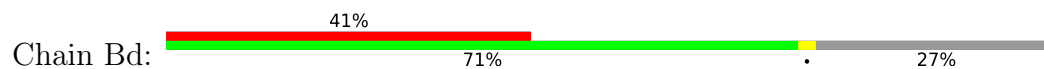


- Molecule 33: mL54

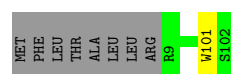




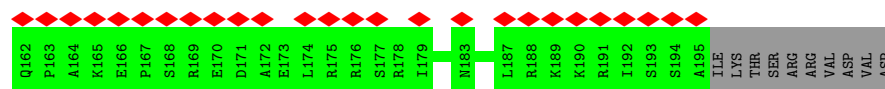
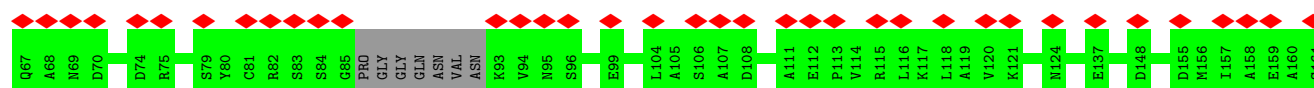
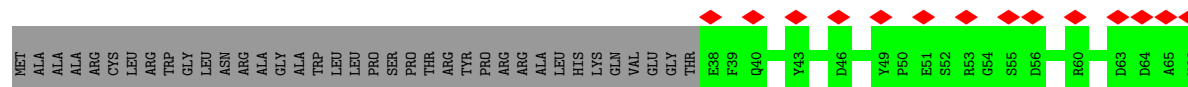
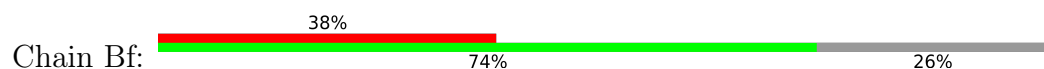
• Molecule 34: Mitochondrial ribosomal protein L55



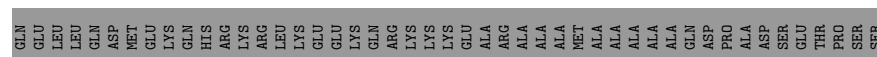
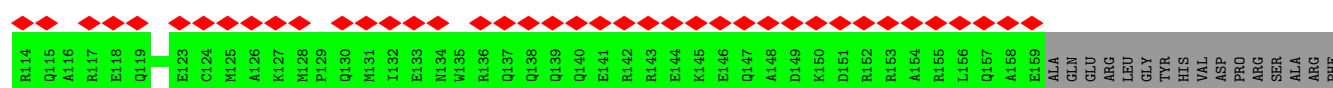
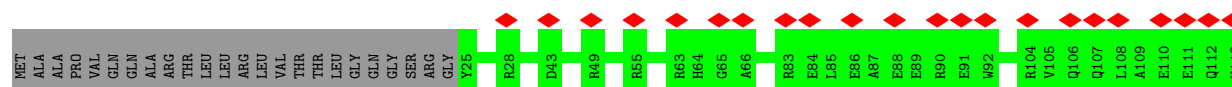
• Molecule 35: Mitochondrial ribosomal protein L57



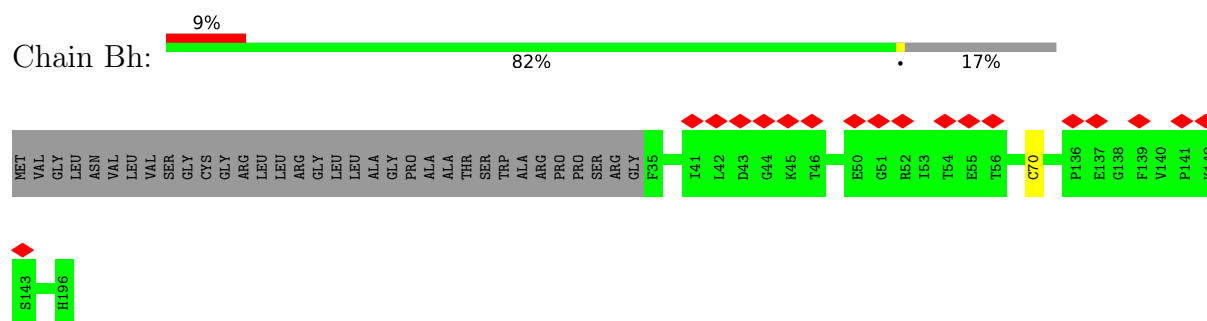
• Molecule 36: mL62 (ICT1)



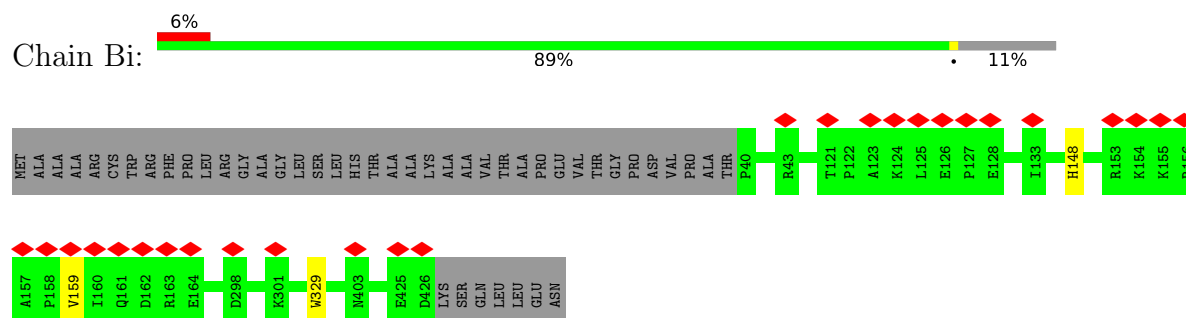
• Molecule 37: mL64



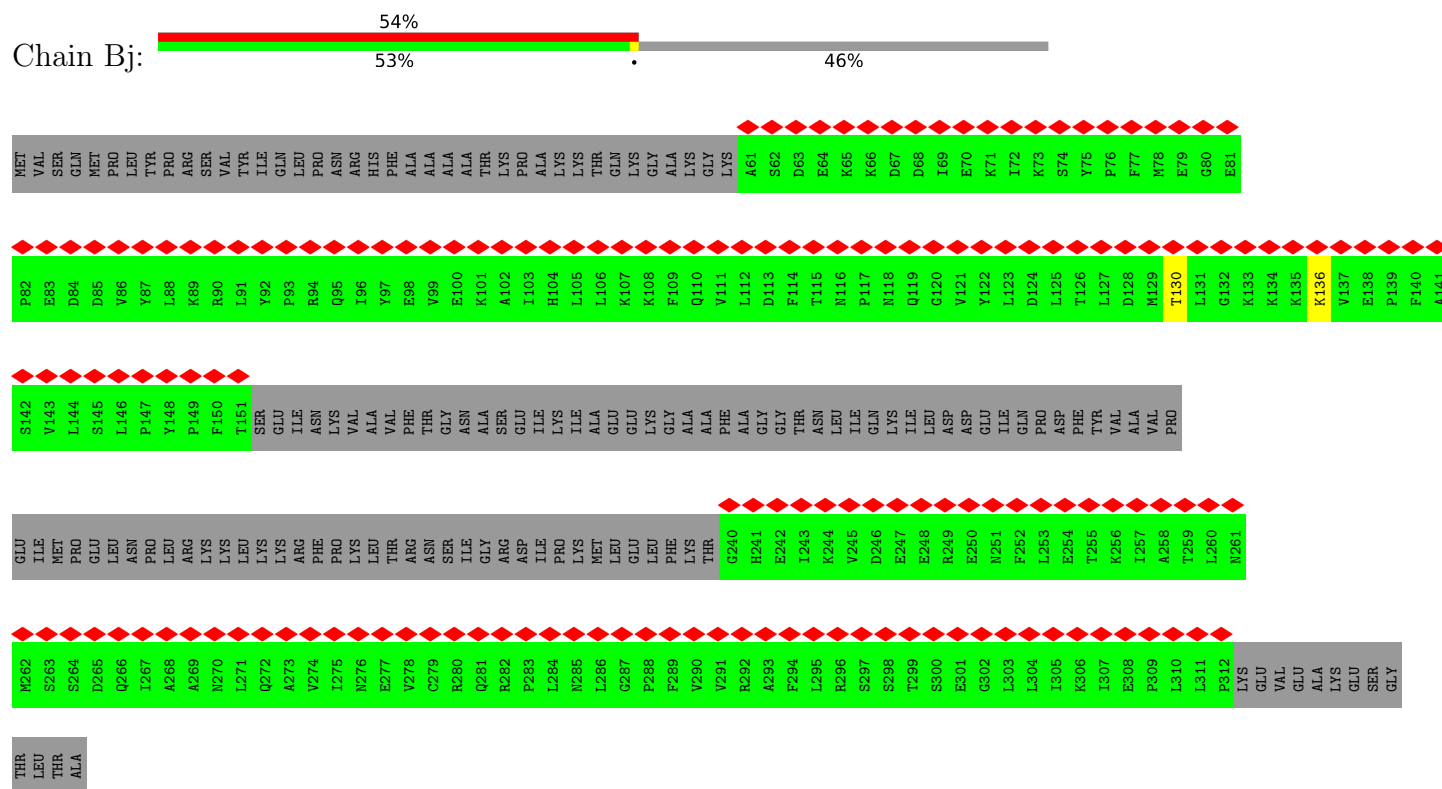
- Molecule 38: Mitochondrial ribosomal protein S18A



- Molecule 39: 39S ribosomal protein S30, mitochondrial

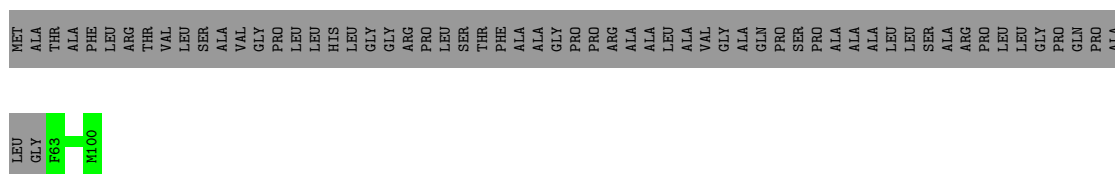


- Molecule 40: 39S ribosomal protein L1, mitochondrial

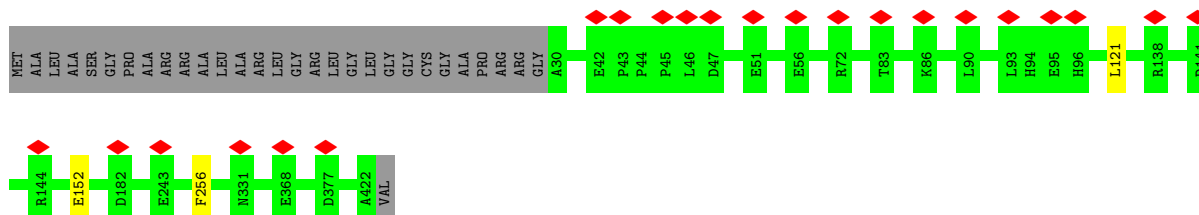


- Molecule 41: Ribosomal protein

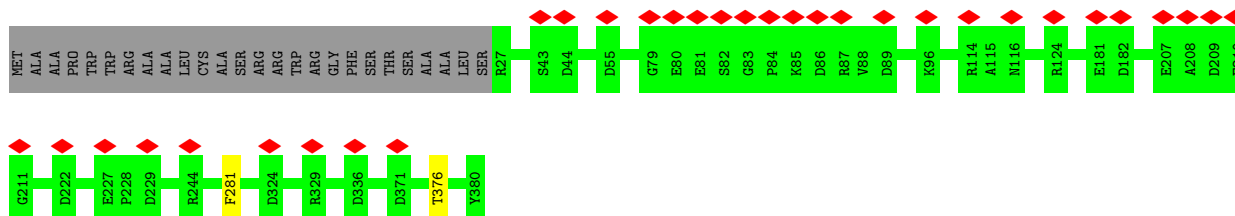




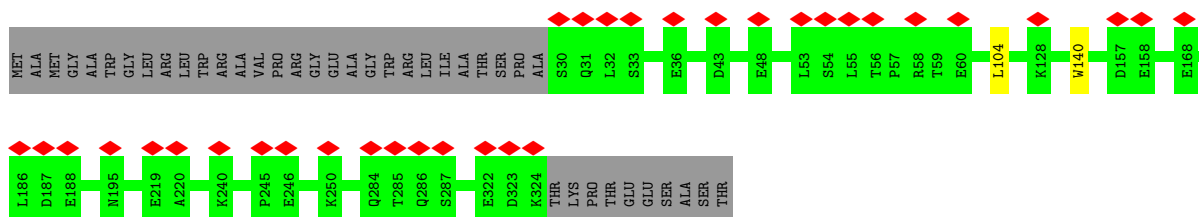
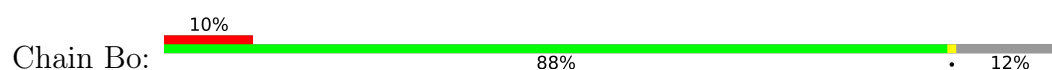
- Molecule 42: Mitochondrial ribosomal protein L37



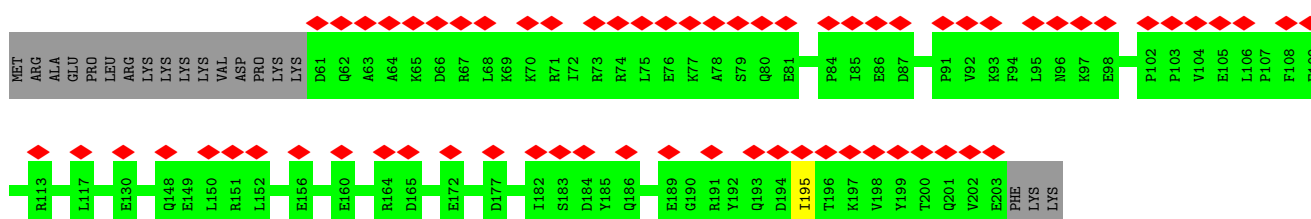
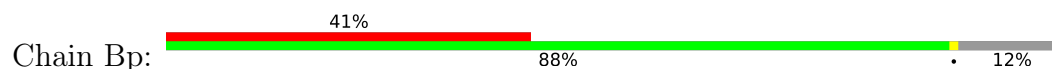
- Molecule 43: Mitochondrial ribosomal protein L38



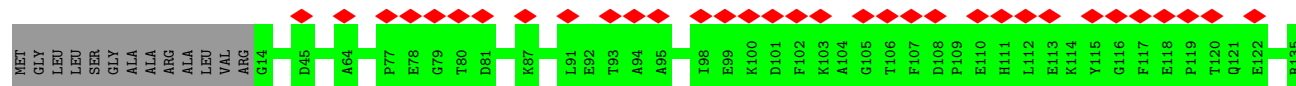
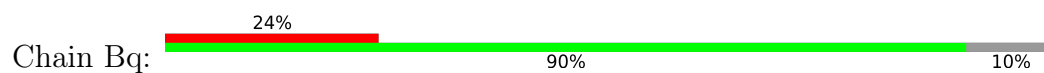
- Molecule 44: Mitochondrial ribosomal protein L39



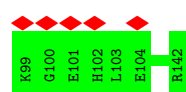
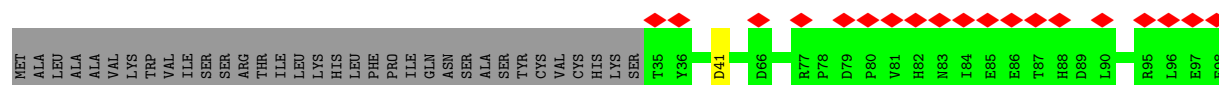
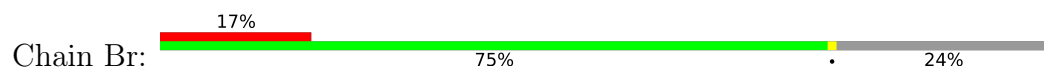
- Molecule 45: Mitochondrial ribosomal protein L40



- Molecule 46: 39S ribosomal protein L41, mitochondrial



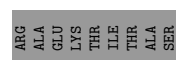
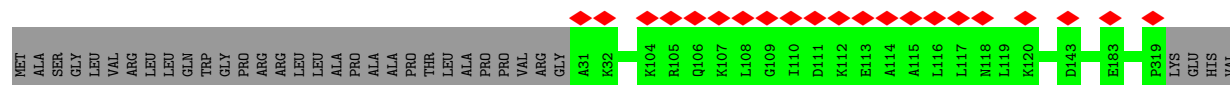
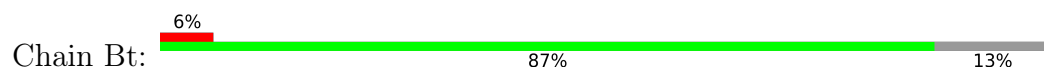
- Molecule 47: mL42



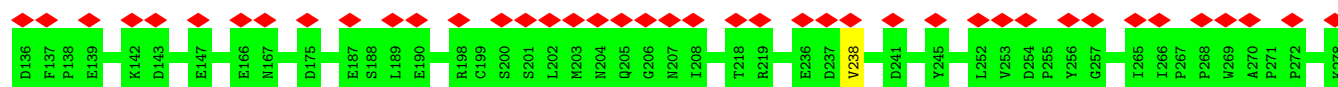
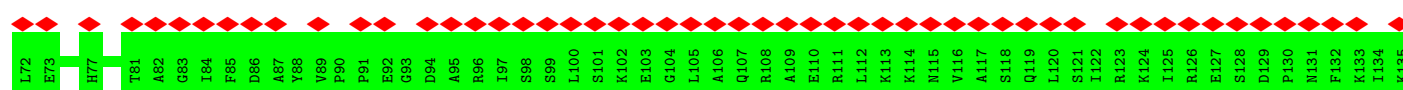
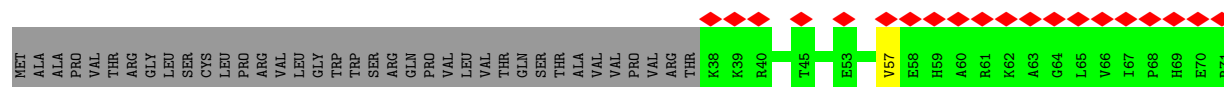
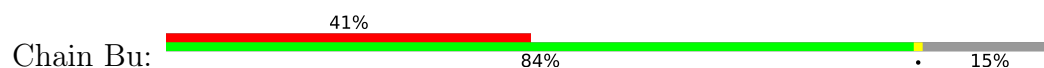
- Molecule 48: Large ribosomal subunit protein mL43

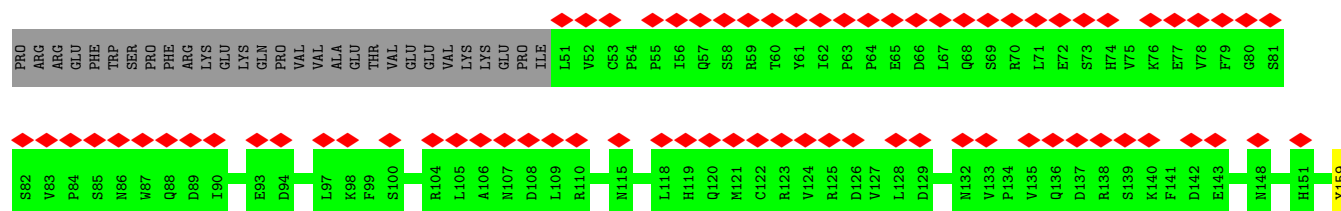


- Molecule 49: mL44

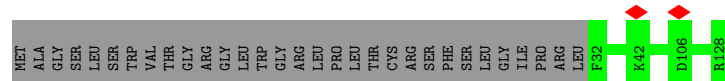
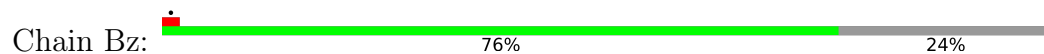


- Molecule 50: Mitochondrial ribosomal protein L45

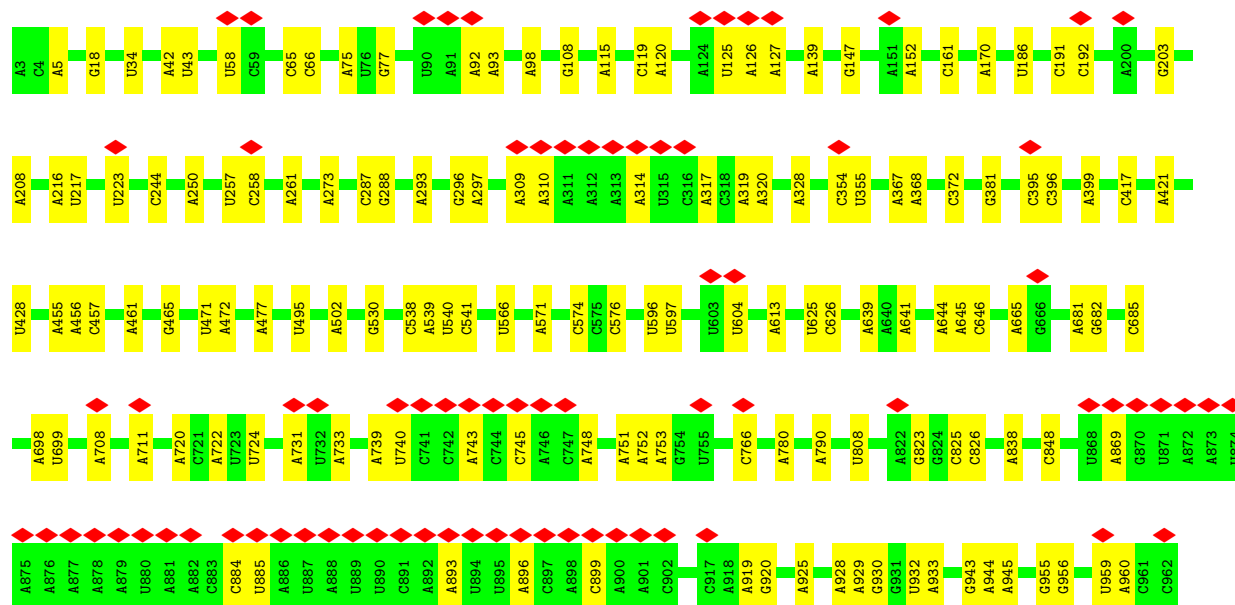
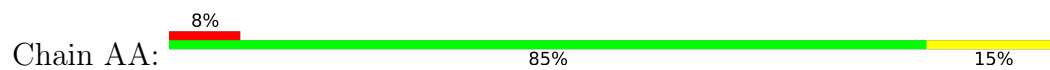




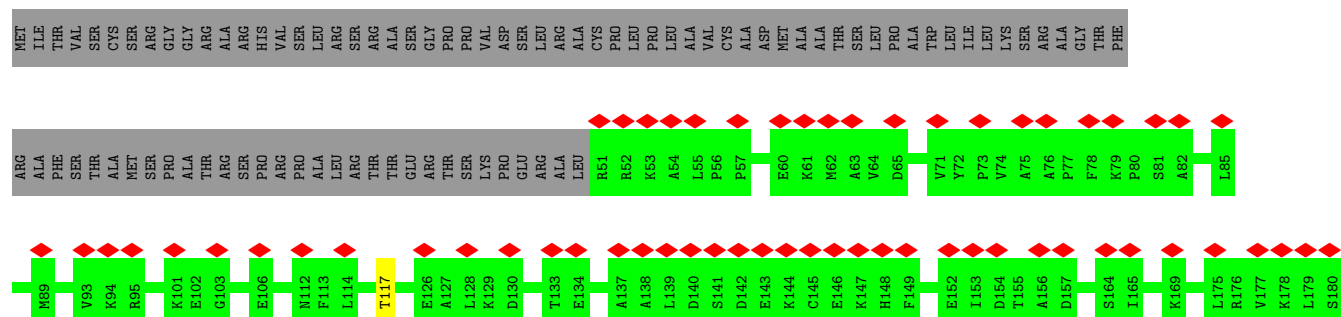
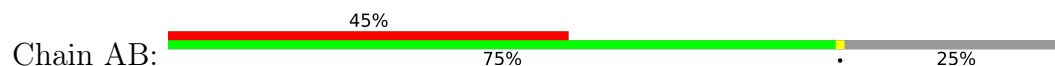
- Molecule 55: Large ribosomal subunit protein mL51

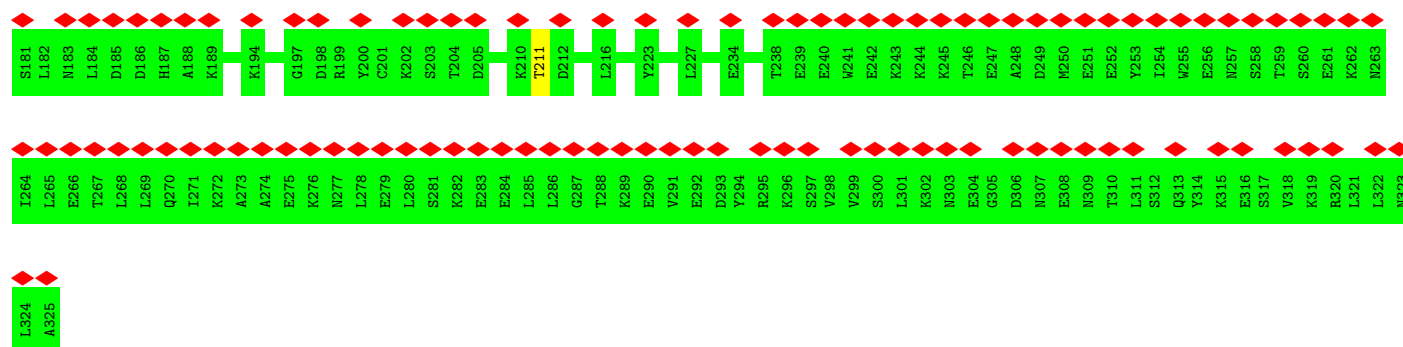


- Molecule 56: 12S rRNA



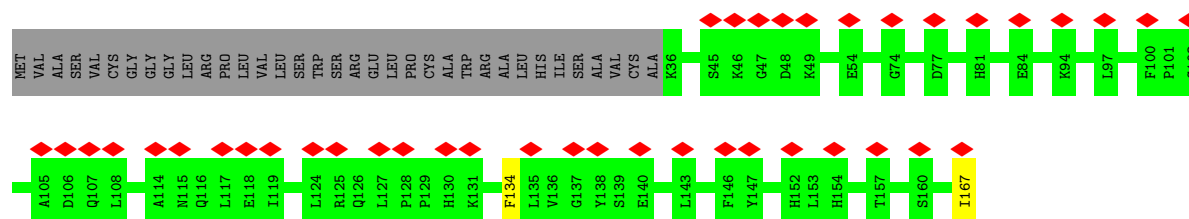
- Molecule 57: 28S ribosomal protein S35, mitochondrial isoform 1





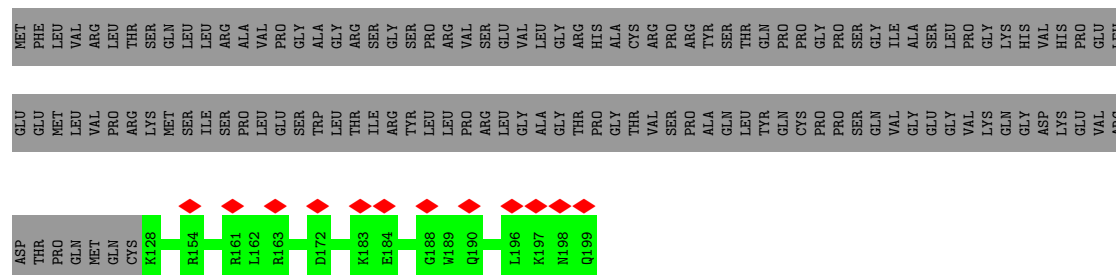
- Molecule 58: Mitochondrial ribosomal protein S24

Chain AC: 25% 78% 21%



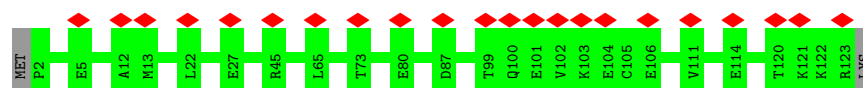
- Molecule 59: Small ribosomal subunit protein mS38

Chain AD: 6% 36% 64%



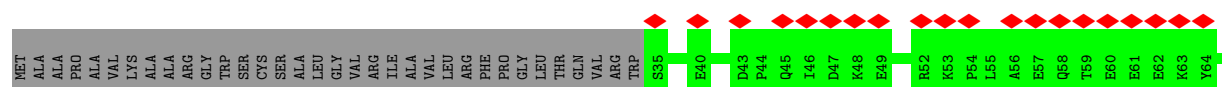
- Molecule 60: Mitochondrial ribosomal protein bs6m, mrps6

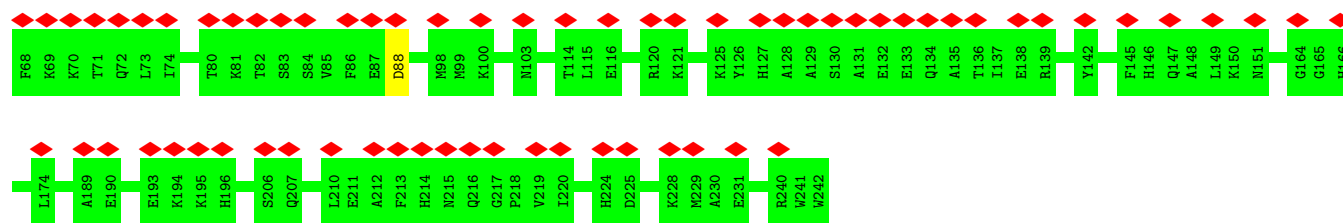
Chain AE: 18% 98%



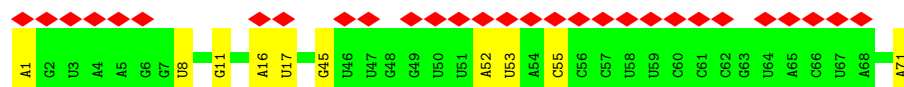
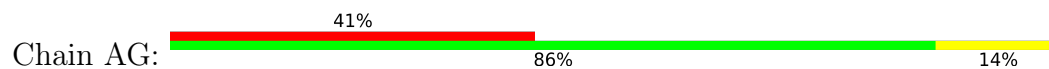
- Molecule 61: Mitochondrial ribosomal protein S7

Chain AF: 36% 86% 14%

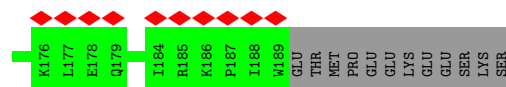
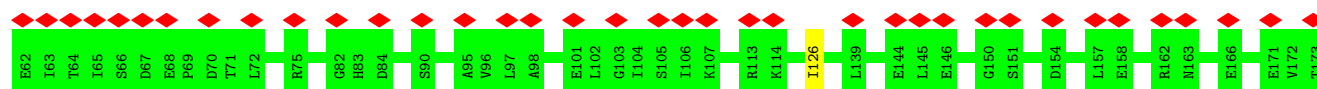
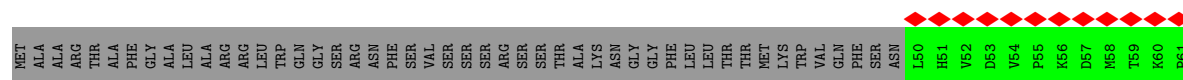
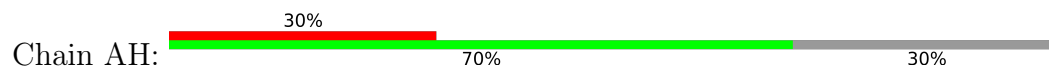




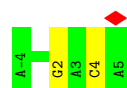
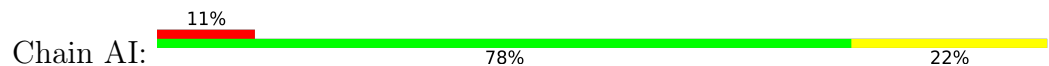
- Molecule 62: P-site Met-tRNA(fMet)



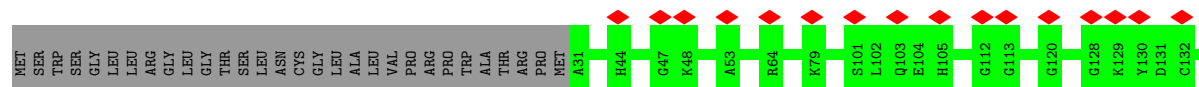
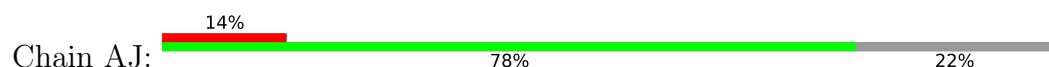
- Molecule 63: Mitochondrial ribosomal protein S10



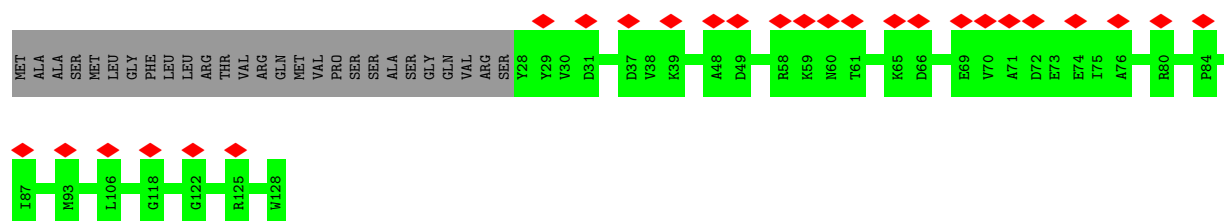
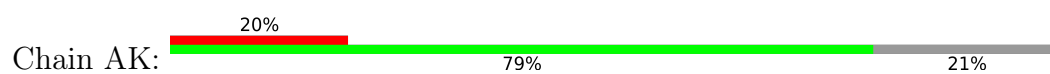
- Molecule 64: mRNA



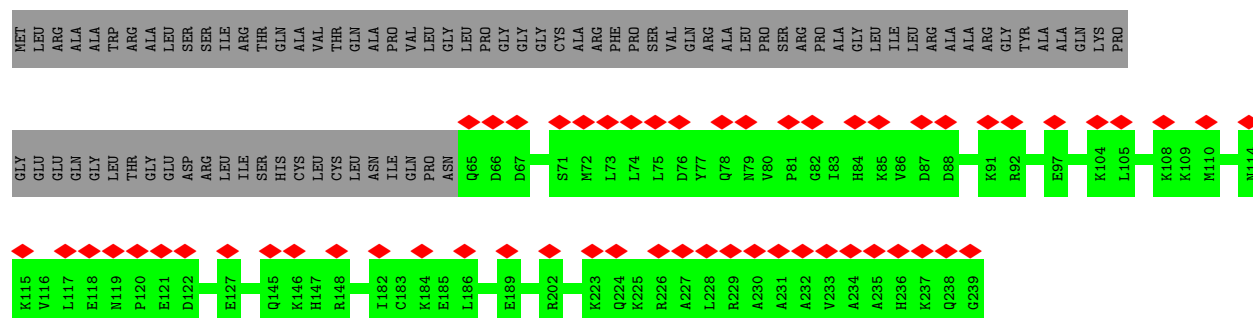
- Molecule 65: Mitochondrial ribosomal protein S12



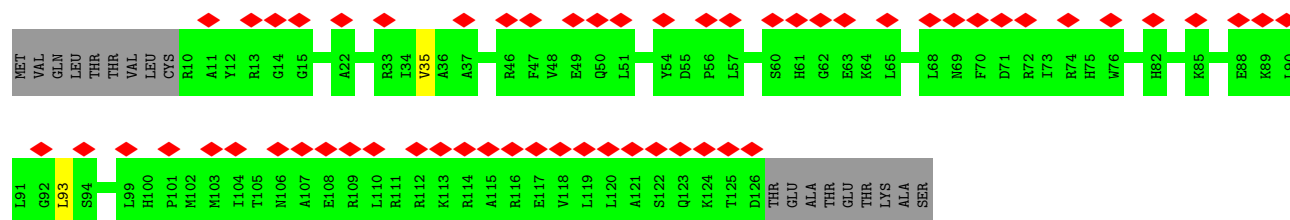
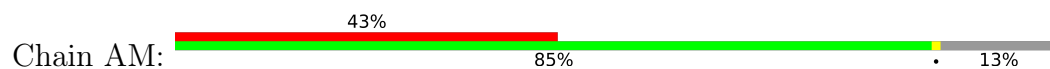
- Molecule 66: Mitochondrial ribosomal protein S14



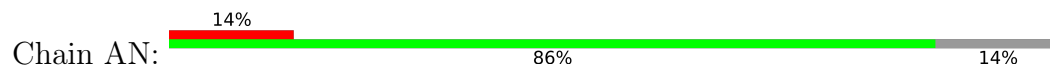
- Molecule 67: 28S ribosomal protein S15, mitochondrial



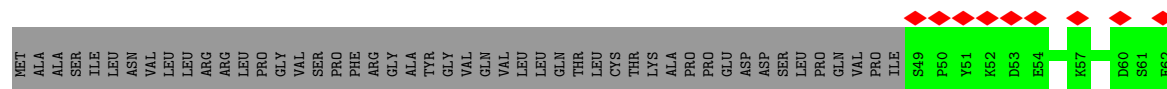
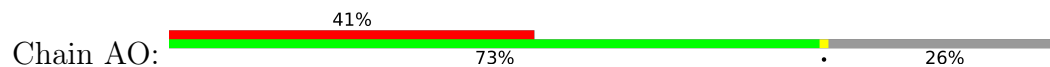
- Molecule 68: 28S ribosomal protein S16, mitochondrial

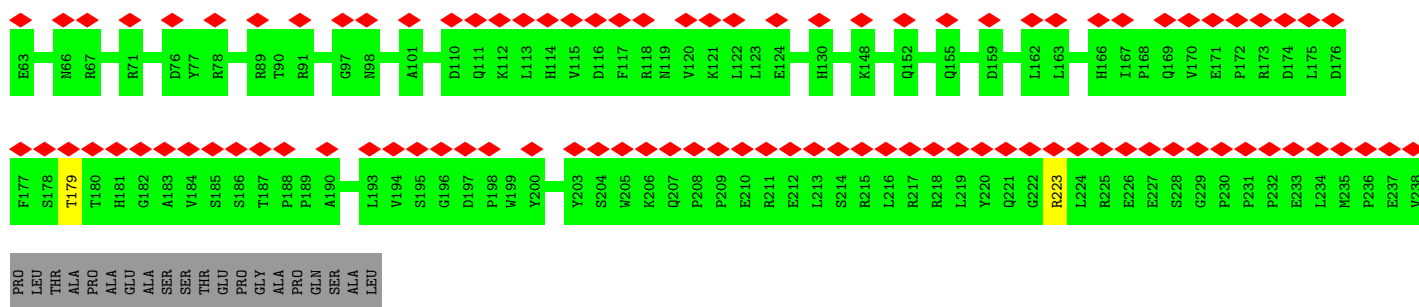


- Molecule 69: 28S ribosomal protein S17, mitochondrial

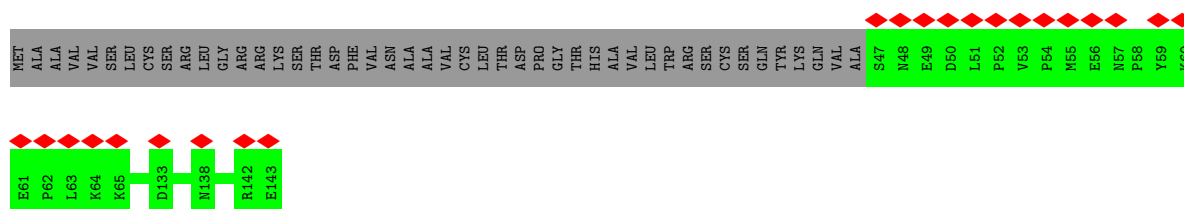


- Molecule 70: 28S ribosomal protein S18b, mitochondrial

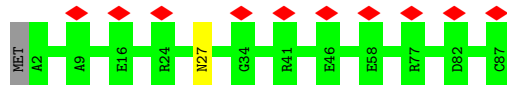




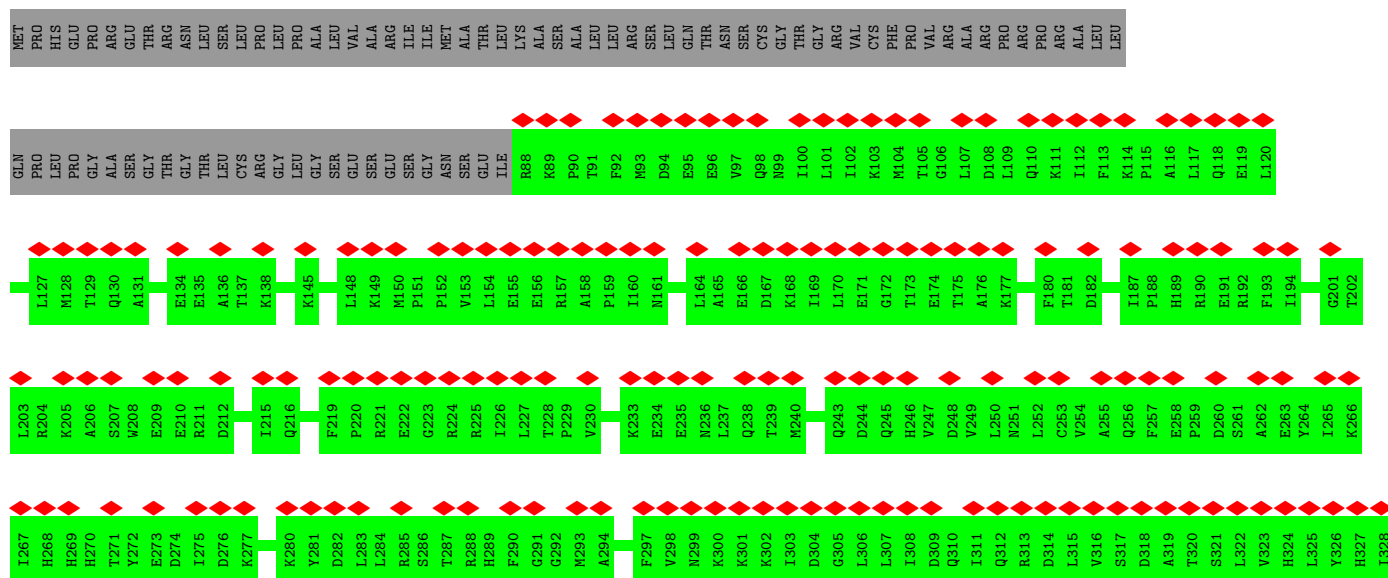
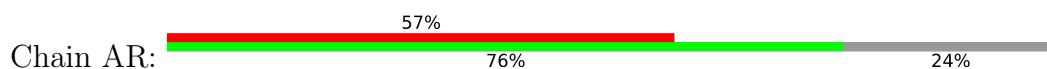
• Molecule 71: Mitochondrial ribosomal protein S18C

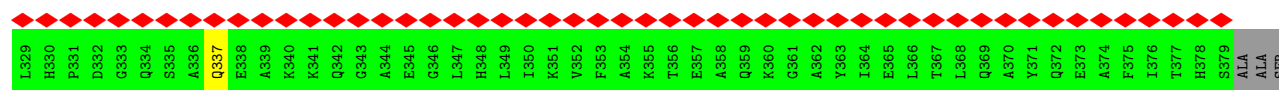


• Molecule 72: 28S ribosomal protein S21, mitochondrial

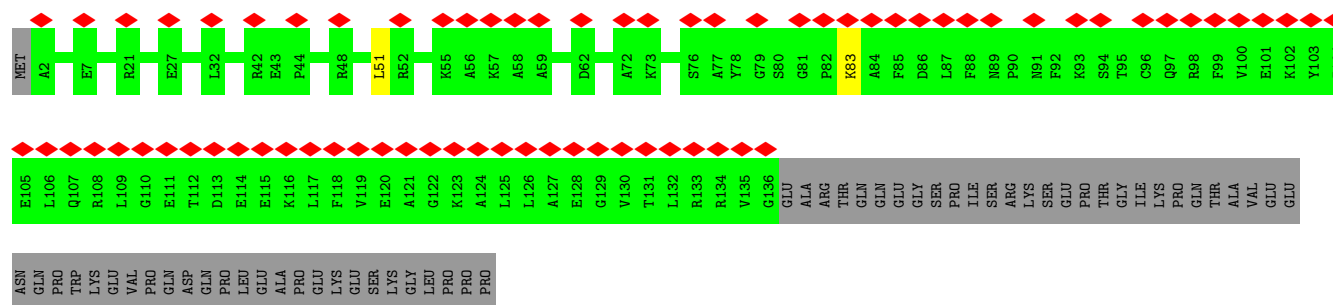
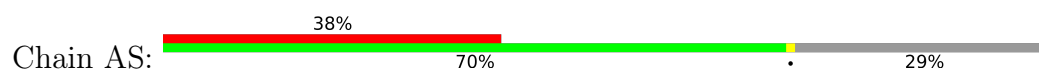


• Molecule 73: Mitochondrial ribosomal protein S22

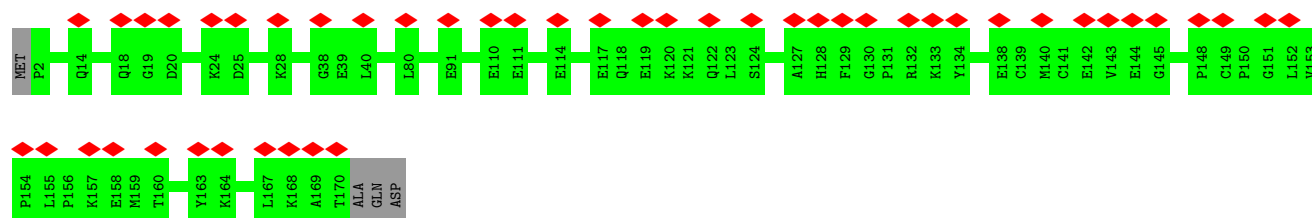




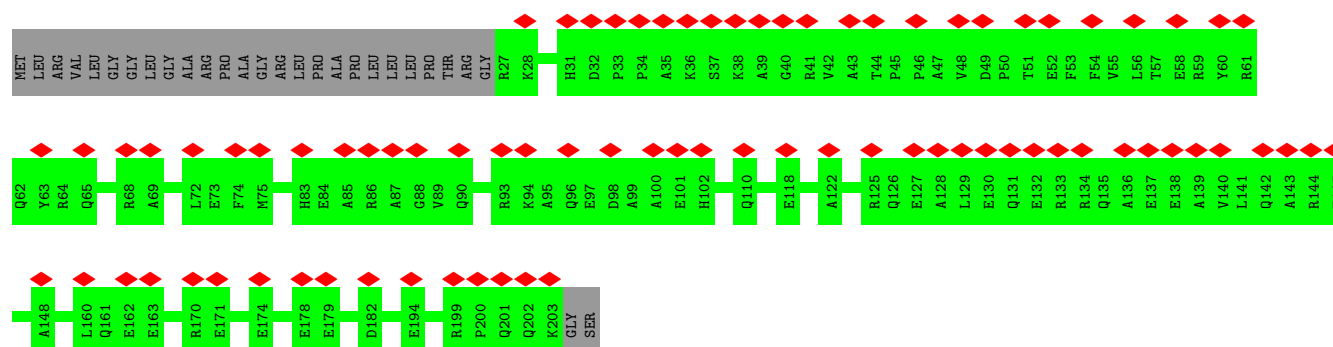
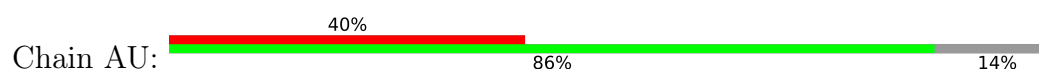
• Molecule 74: mS23



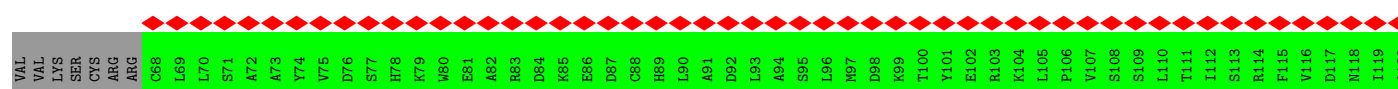
• Molecule 75: Mitochondrial ribosomal protein S25

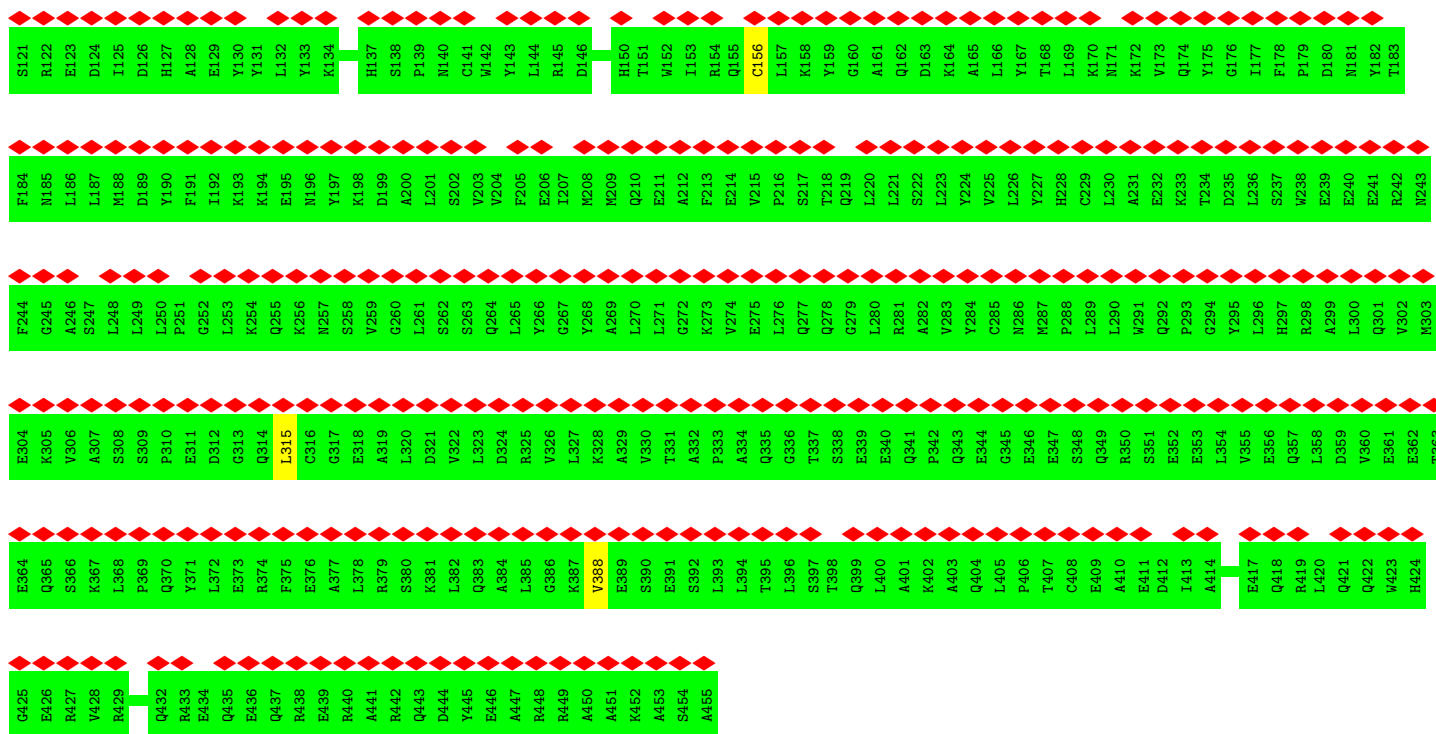


• Molecule 76: Mitochondrial ribosomal protein S26

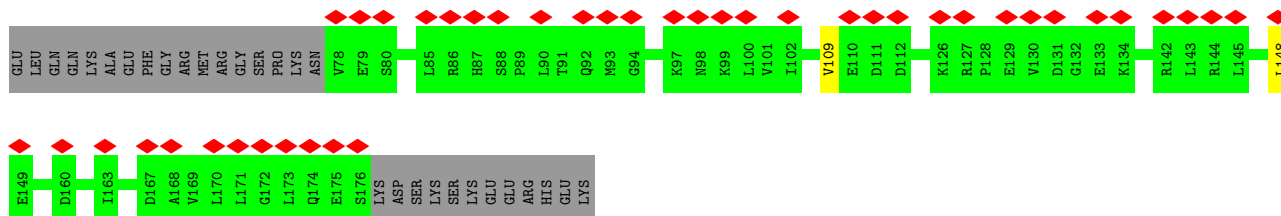
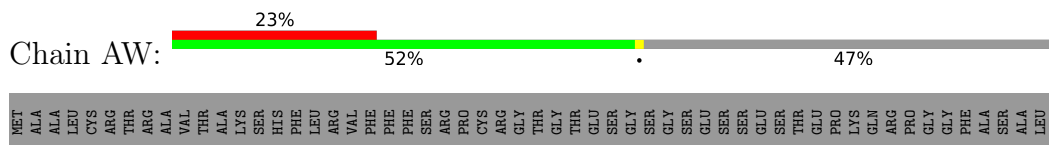


• Molecule 77: Mitochondrial ribosomal protein S27

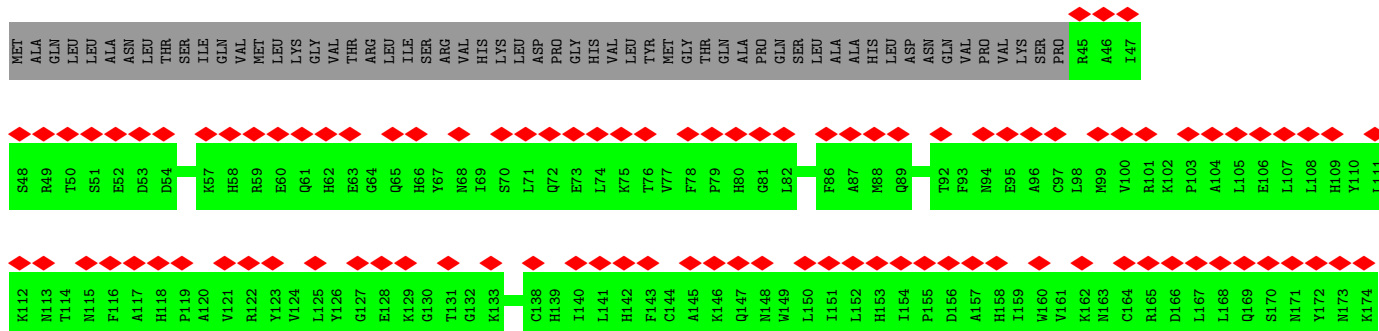
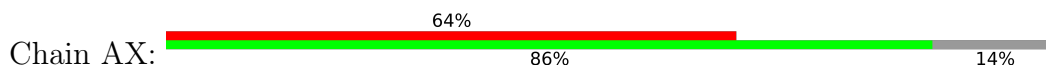


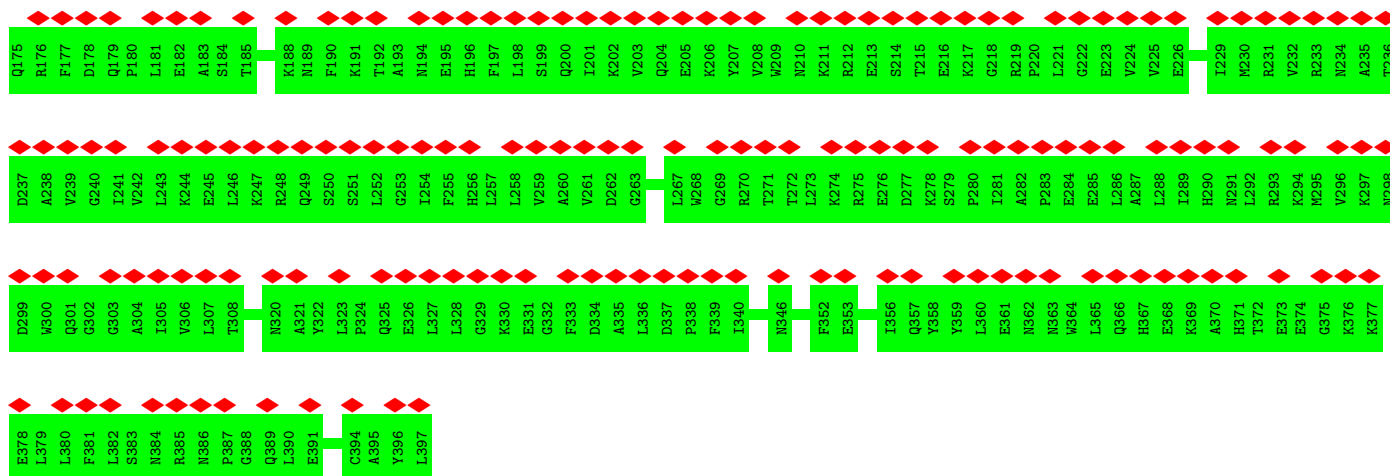


- Molecule 78: Mitoribosomal protein ms28, mrps28

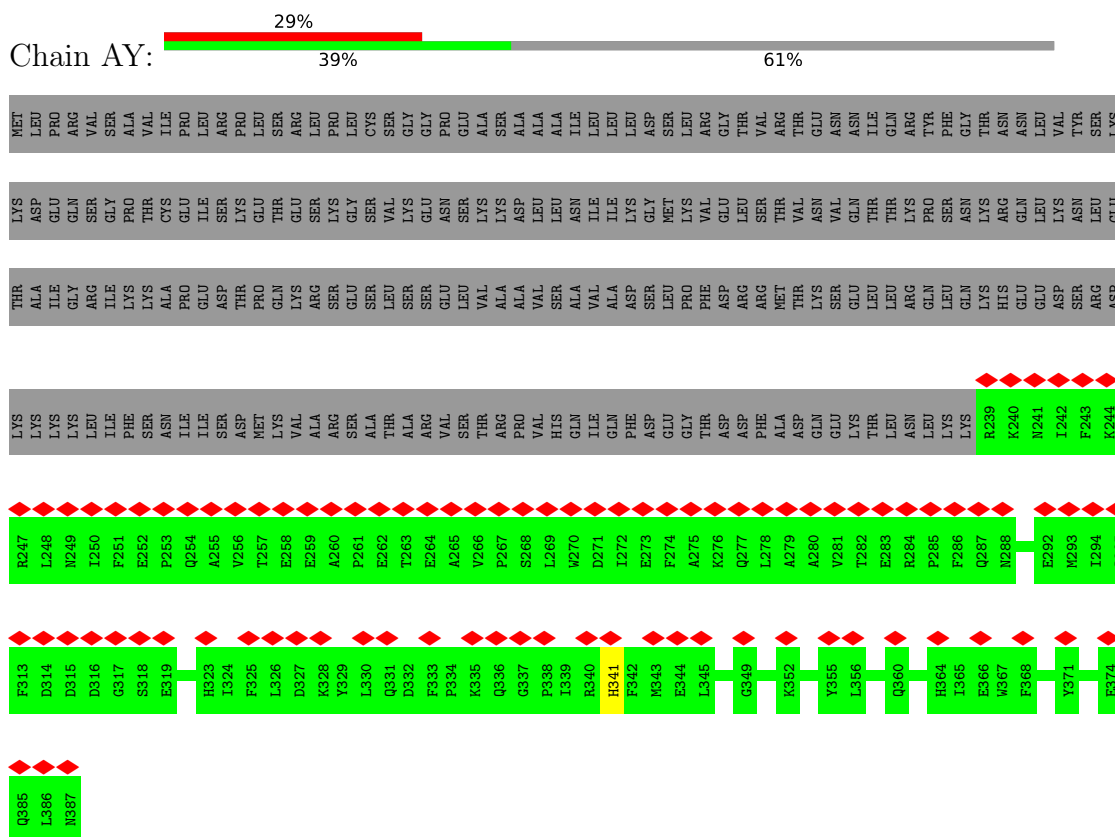


- Molecule 79: Small ribosomal subunit protein mS29

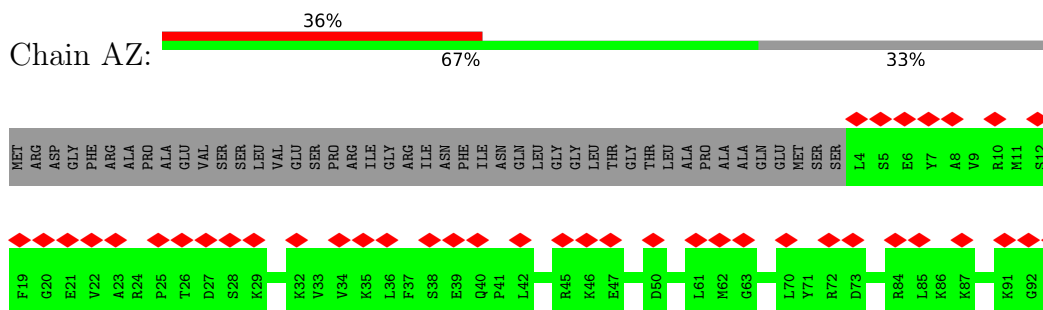




- Molecule 80: 28S ribosomal protein S31, mitochondrial

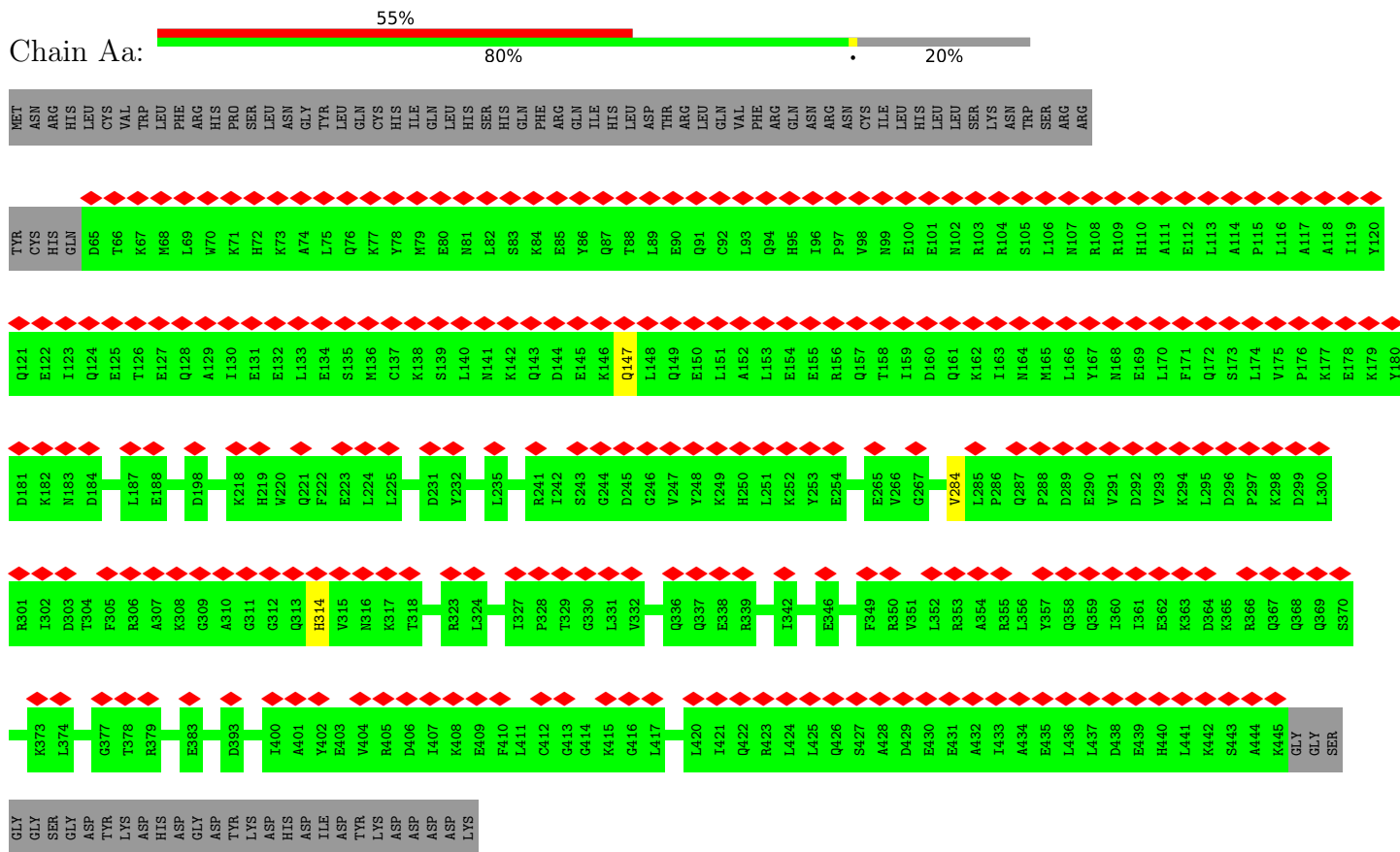


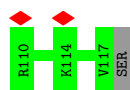
- Molecule 81: Mitochondrial ribosomal protein S33



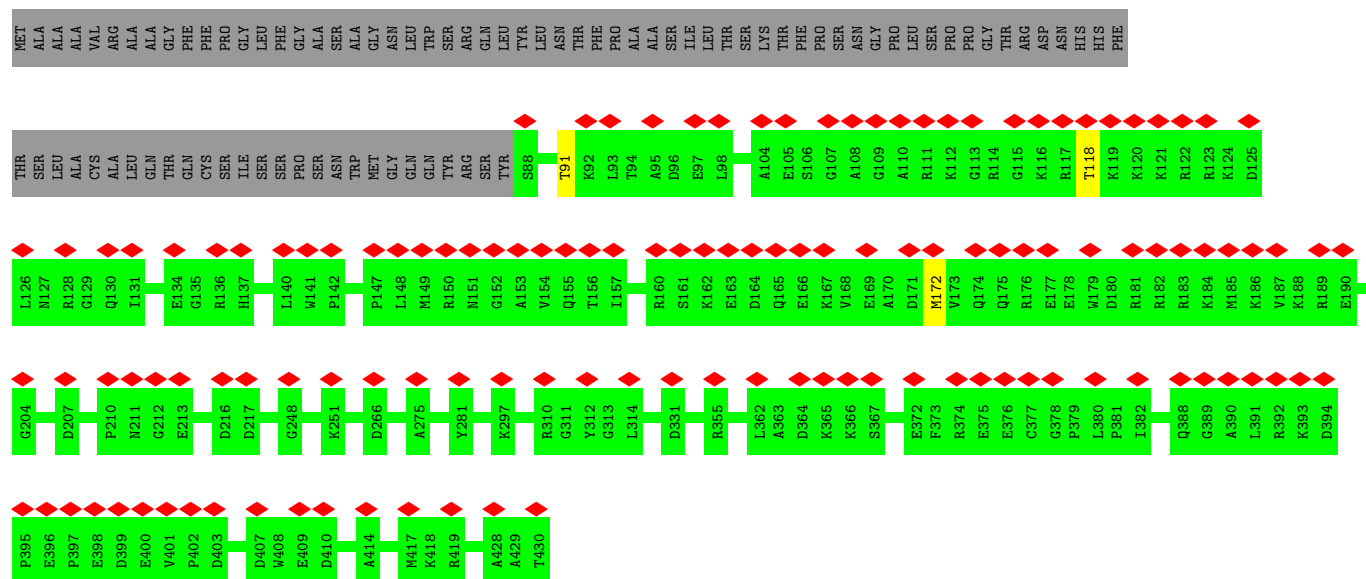
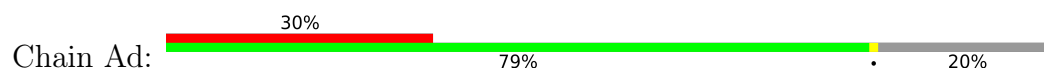
● Molecule 82: Peptide chain release factor 1, mitochondrial

Chain Aa:

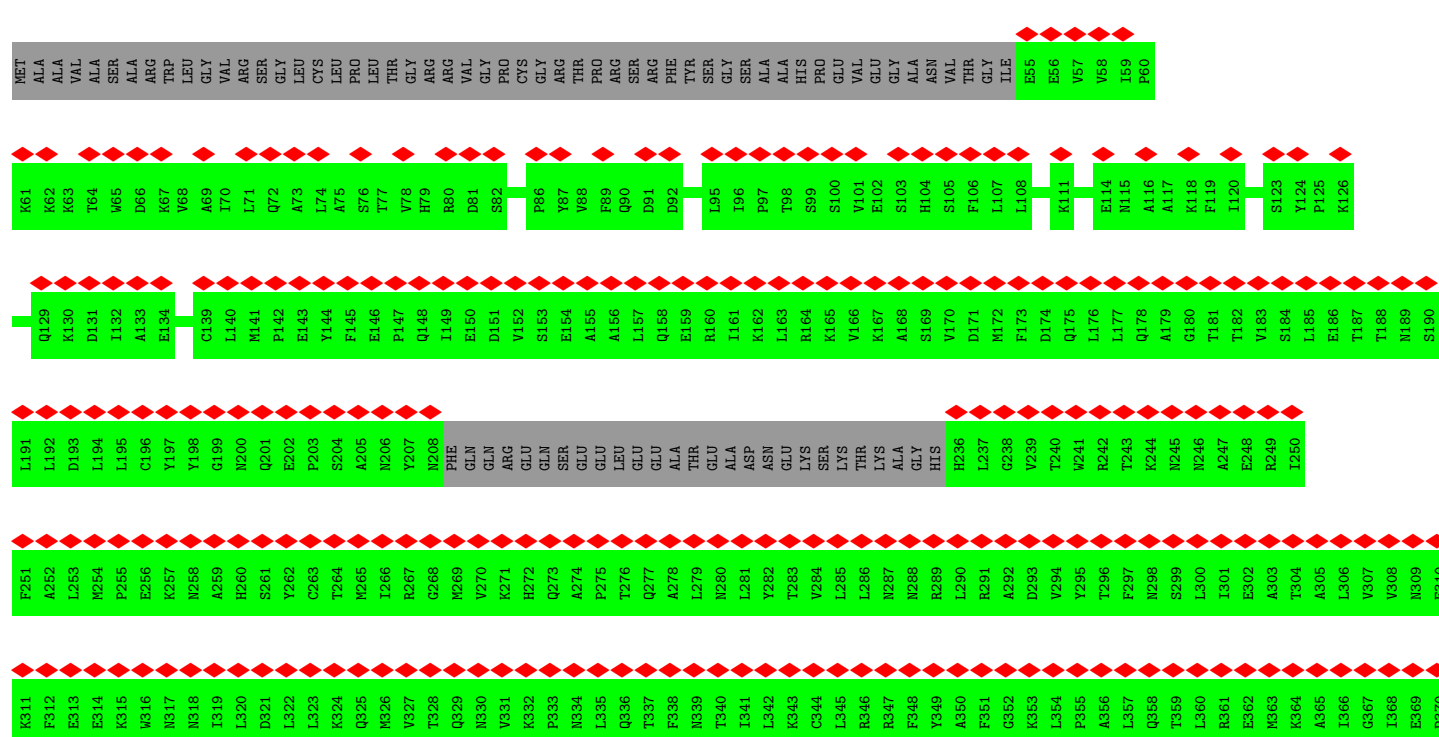
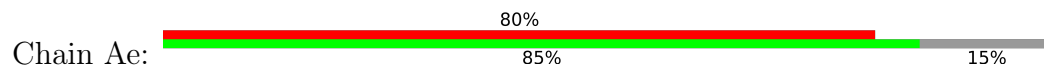




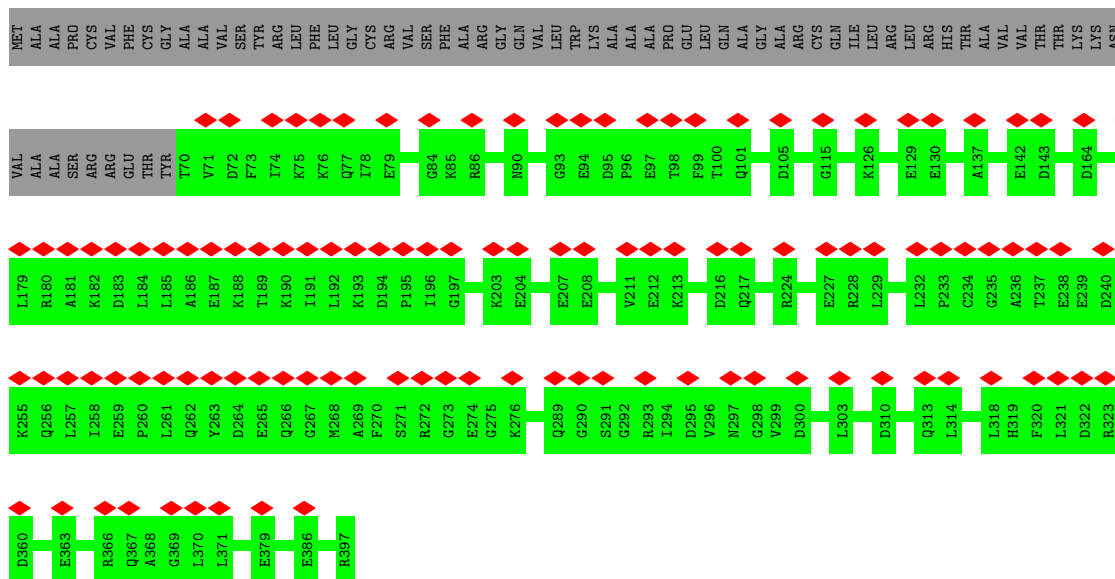
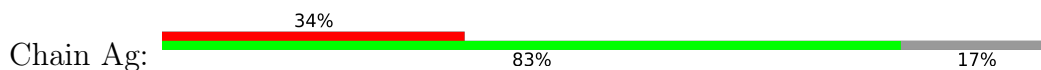
- Molecule 85: 28S ribosomal protein S5, mitochondrial isoform X2



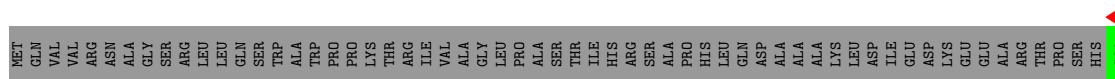
- Molecule 86: mS39

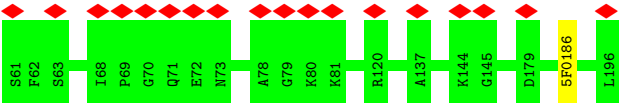


- Molecule 87: uS9m

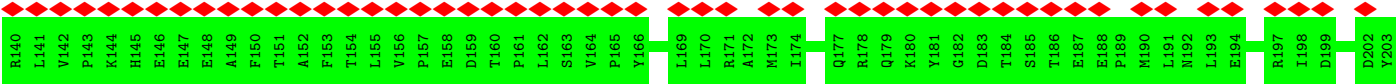
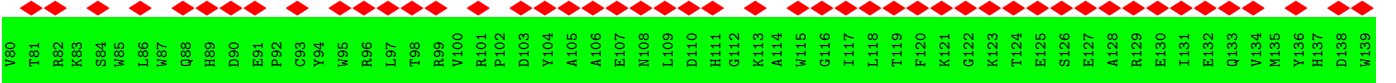
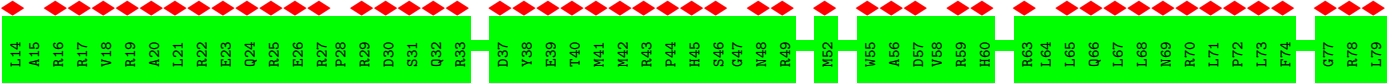
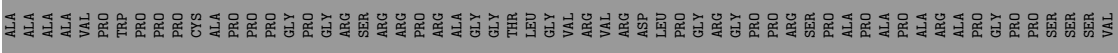
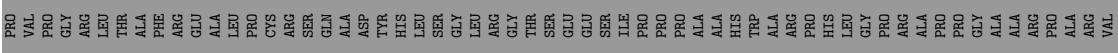
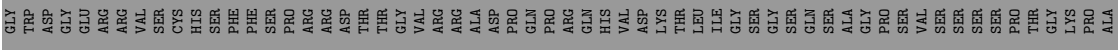
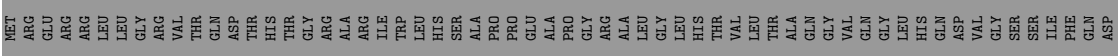


- Molecule 88: Mitochondrial ribosomal protein S11





● Molecule 89: Mitochondrial ribosomal protein S34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50622	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.040	Depositor
Minimum map value	-1.903	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	532.5, 532.5, 532.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	B1	0.23	0/319	0.37	0/435
1	B2	0.21	0/212	0.35	0/286
1	B3	0.22	0/221	0.35	0/297
1	B4	0.22	0/212	0.33	0/286
1	B5	0.22	0/212	0.32	0/286
1	B6	0.22	0/204	0.36	0/275
2	B7	0.12	0/68	0.66	0/103
3	B8	0.20	0/37315	0.69	6/58099 (0.0%)
4	B9	0.30	1/1712 (0.1%)	0.69	0/2659
5	BA	0.25	0/1407	0.48	0/1891
6	BB	0.25	0/1206	0.52	0/1639
7	BC	0.23	0/1719	0.50	0/2329
8	BD	0.25	0/890	0.45	0/1202
9	BE	0.23	0/2093	0.46	0/2835
10	BF	0.23	0/1586	0.47	0/2123
11	BG	0.23	0/897	0.45	0/1213
12	BH	0.24	0/917	0.51	0/1227
13	BI	0.24	0/430	0.48	0/570
14	BJ	0.22	0/395	0.54	0/524
15	BK	0.24	0/853	0.51	0/1136
16	BL	0.25	0/1898	0.52	0/2555
17	BM	0.24	0/2493	0.44	0/3387
18	BN	0.24	0/2080	0.49	0/2830
19	BO	0.23	0/1695	0.49	0/2288
20	BP	0.24	0/1742	0.46	0/2358
21	BQ	0.24	0/1359	0.46	0/1828
22	BR	0.28	1/1481 (0.1%)	0.44	0/2009
23	BS	0.24	0/912	0.53	0/1231
24	BT	0.25	0/2368	0.51	0/3198
25	BU	0.25	0/1850	0.50	0/2491
26	BV	0.23	0/1262	0.50	0/1700

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BW	0.23	0/1197	0.51	0/1624
28	BX	0.25	0/2002	0.47	0/2708
29	BY	0.24	0/1179	0.53	0/1578
30	BZ	0.24	0/1256	0.49	0/1706
31	Ba	0.24	0/787	0.46	0/1056
32	Bb	0.24	0/747	0.51	0/1006
33	Bc	0.23	0/737	0.46	0/997
34	Bd	0.23	0/778	0.54	0/1048
35	Be	0.23	0/798	0.54	0/1073
36	Bf	0.23	0/1214	0.51	0/1630
37	Bg	0.23	0/1157	0.48	0/1560
38	Bh	0.24	0/1364	0.49	0/1849
39	Bi	0.25	0/3206	0.46	0/4354
40	Bj	0.24	0/1350	0.44	0/1823
41	Bl	0.24	0/342	0.53	0/450
42	Bm	0.25	0/3267	0.47	0/4455
43	Bn	0.25	0/3047	0.49	0/4139
44	Bo	0.24	0/2464	0.43	0/3330
45	Bp	0.24	0/1228	0.48	0/1656
46	Bq	0.26	0/1000	0.46	0/1345
47	Br	0.25	0/934	0.50	0/1267
48	Bs	0.25	0/1208	0.53	0/1639
49	Bt	0.24	0/2372	0.45	0/3211
50	Bu	0.24	0/2199	0.47	0/2980
51	Bv	0.23	0/1988	0.44	0/2678
52	Bw	0.24	0/1320	0.47	1/1785 (0.1%)
53	Bx	0.25	0/1135	0.47	0/1549
54	By	0.24	0/917	0.45	0/1248
55	Bz	0.24	0/860	0.48	0/1150
56	AA	0.16	0/22734	0.67	2/35392 (0.0%)
57	AB	0.23	0/2268	0.44	0/3069
58	AC	0.24	0/1105	0.47	0/1496
59	AD	0.23	0/650	0.53	0/858
60	AE	0.25	0/999	0.51	0/1347
61	AF	0.24	0/1764	0.45	0/2368
62	AG	0.30	1/1677 (0.1%)	0.69	0/2606
63	AH	0.24	0/1181	0.47	0/1597
64	AI	0.17	0/217	0.66	0/337
65	AJ	0.25	0/858	0.53	0/1152
66	AK	0.22	0/874	0.53	0/1171
67	AL	0.23	0/1473	0.44	0/1970
68	AM	0.24	0/954	0.51	0/1284
69	AN	0.24	0/894	0.47	0/1213

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AO	0.24	0/1616	0.47	0/2195
71	AP	0.24	0/802	0.42	0/1079
72	AQ	0.24	0/740	0.53	0/986
73	AR	0.23	0/2428	0.43	0/3279
74	AS	0.25	0/1126	0.49	0/1514
75	AT	0.25	0/1399	0.45	0/1881
76	AU	0.23	0/1490	0.49	0/2005
77	AV	0.23	0/3171	0.44	0/4292
78	AW	0.25	0/790	0.49	0/1064
79	AX	0.24	0/2945	0.44	0/3984
80	AY	0.24	0/1285	0.41	0/1734
81	AZ	0.24	0/841	0.48	0/1121
82	Aa	0.23	0/3171	0.45	0/4263
83	Ab	0.24	0/1804	0.48	0/2445
84	Ac	0.23	0/942	0.50	0/1261
85	Ad	0.24	0/2785	0.50	0/3735
86	Ae	0.24	0/4856	0.40	0/6579
87	Ag	0.24	0/2707	0.47	0/3636
88	Ai	0.24	0/1018	0.49	0/1375
89	Aj	0.23	0/1835	0.51	0/2484
All	All	0.23	3/189460 (0.0%)	0.56	9/268956 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	AG	1	A	OP3-P	-10.59	1.48	1.61
4	B9	1	G	OP3-P	-10.53	1.48	1.61
22	BR	4	PHE	C-N	-5.11	1.22	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1527	U	C2-N1-C1'	7.20	126.34	117.70
52	Bw	68	PRO	N-CA-CB	6.15	110.68	103.30
3	B8	1527	U	N1-C2-O2	6.10	127.07	122.80
3	B8	1119	C	N1-C2-O2	5.92	122.45	118.90
56	AA	119	C	C2-N1-C1'	5.74	125.11	118.80
3	B8	1527	U	N3-C2-O2	-5.56	118.31	122.20
56	AA	119	C	N1-C2-O2	5.23	122.04	118.90
3	B8	1119	C	N3-C2-O2	-5.10	118.33	121.90
3	B8	1119	C	C2-N1-C1'	5.00	124.31	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	B1	43/198 (22%)	41 (95%)	2 (5%)	0	100	100
1	B2	25/198 (13%)	25 (100%)	0	0	100	100
1	B3	26/198 (13%)	26 (100%)	0	0	100	100
1	B4	25/198 (13%)	25 (100%)	0	0	100	100
1	B5	25/198 (13%)	25 (100%)	0	0	100	100
1	B6	24/198 (12%)	24 (100%)	0	0	100	100
5	BA	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
6	BB	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
7	BC	204/216 (94%)	199 (98%)	5 (2%)	0	100	100
8	BD	110/148 (74%)	109 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	238 (98%)	4 (2%)	0	100	100
10	BF	177/250 (71%)	175 (99%)	2 (1%)	0	100	100
11	BG	105/161 (65%)	105 (100%)	0	0	100	100
12	BH	108/207 (52%)	108 (100%)	0	0	100	100
13	BI	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
14	BJ	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	238/306 (78%)	229 (96%)	8 (3%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	BM	305/399 (76%)	296 (97%)	9 (3%)	0	100	100
18	BN	249/294 (85%)	247 (99%)	2 (1%)	0	100	100
19	BO	200/268 (75%)	188 (94%)	12 (6%)	0	100	100
20	BP	210/257 (82%)	207 (99%)	3 (1%)	0	100	100
21	BQ	174/192 (91%)	171 (98%)	3 (2%)	0	100	100
22	BR	175/197 (89%)	171 (98%)	4 (2%)	0	100	100
23	BS	113/325 (35%)	112 (99%)	1 (1%)	0	100	100
24	BT	286/296 (97%)	274 (96%)	12 (4%)	0	100	100
25	BU	220/251 (88%)	215 (98%)	5 (2%)	0	100	100
26	BV	151/169 (89%)	147 (97%)	4 (3%)	0	100	100
27	BW	141/188 (75%)	135 (96%)	6 (4%)	0	100	100
28	BX	238/303 (78%)	234 (98%)	4 (2%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	153/209 (73%)	151 (99%)	2 (1%)	0	100	100
31	Ba	95/160 (59%)	94 (99%)	1 (1%)	0	100	100
32	Bb	95/112 (85%)	91 (96%)	4 (4%)	0	100	100
33	Bc	82/138 (59%)	82 (100%)	0	0	100	100
34	Bd	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
35	Be	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
36	Bf	147/205 (72%)	144 (98%)	3 (2%)	0	100	100
37	Bg	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	152 (95%)	8 (5%)	0	100	100
39	Bi	385/433 (89%)	371 (96%)	13 (3%)	1 (0%)	41	75
40	Bj	160/304 (53%)	156 (98%)	4 (2%)	0	100	100
41	Bl	36/100 (36%)	36 (100%)	0	0	100	100
42	Bm	391/423 (92%)	384 (98%)	7 (2%)	0	100	100
43	Bn	352/380 (93%)	334 (95%)	18 (5%)	0	100	100
44	Bo	293/334 (88%)	284 (97%)	9 (3%)	0	100	100
45	Bp	141/162 (87%)	135 (96%)	6 (4%)	0	100	100
46	Bq	120/135 (89%)	115 (96%)	5 (4%)	0	100	100
47	Br	106/142 (75%)	102 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Bs	149/159 (94%)	146 (98%)	3 (2%)	0	100	100
49	Bt	287/332 (86%)	283 (99%)	4 (1%)	0	100	100
50	Bu	258/306 (84%)	253 (98%)	5 (2%)	0	100	100
51	Bv	236/279 (85%)	229 (97%)	7 (3%)	0	100	100
52	Bw	163/269 (61%)	156 (96%)	7 (4%)	0	100	100
53	Bx	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
54	By	107/198 (54%)	104 (97%)	3 (3%)	0	100	100
55	Bz	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
57	AB	273/366 (75%)	270 (99%)	3 (1%)	0	100	100
58	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
59	AD	70/199 (35%)	70 (100%)	0	0	100	100
60	AE	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
61	AF	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
63	AH	138/200 (69%)	134 (97%)	3 (2%)	1 (1%)	22	61
65	AJ	107/139 (77%)	106 (99%)	1 (1%)	0	100	100
66	AK	99/128 (77%)	99 (100%)	0	0	100	100
67	AL	173/259 (67%)	170 (98%)	3 (2%)	0	100	100
68	AM	115/135 (85%)	111 (96%)	4 (4%)	0	100	100
69	AN	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
70	AO	188/258 (73%)	187 (100%)	1 (0%)	0	100	100
71	AP	95/143 (66%)	95 (100%)	0	0	100	100
72	AQ	84/87 (97%)	84 (100%)	0	0	100	100
73	AR	290/382 (76%)	287 (99%)	3 (1%)	0	100	100
74	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
75	AT	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
76	AU	175/205 (85%)	175 (100%)	0	0	100	100
77	AV	386/395 (98%)	373 (97%)	13 (3%)	0	100	100
78	AW	97/188 (52%)	96 (99%)	1 (1%)	0	100	100
79	AX	351/410 (86%)	344 (98%)	7 (2%)	0	100	100
80	AY	147/381 (39%)	145 (99%)	2 (1%)	0	100	100
81	AZ	97/148 (66%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	Aa	380/474 (80%)	373 (98%)	7 (2%)	0	100	100
83	Ab	218/289 (75%)	211 (97%)	7 (3%)	0	100	100
84	Ac	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
85	Ad	341/430 (79%)	332 (97%)	9 (3%)	0	100	100
86	Ae	584/692 (84%)	576 (99%)	8 (1%)	0	100	100
87	Ag	326/397 (82%)	322 (99%)	4 (1%)	0	100	100
88	Ai	134/196 (68%)	131 (98%)	3 (2%)	0	100	100
89	Aj	211/505 (42%)	209 (99%)	2 (1%)	0	100	100
All	All	14966/20598 (73%)	14638 (98%)	325 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
63	AH	126	ILE
39	Bi	159	VAL
16	BL	208	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	30/157 (19%)	30 (100%)	0	100	100
1	B2	26/157 (17%)	26 (100%)	0	100	100
1	B3	27/157 (17%)	27 (100%)	0	100	100
1	B4	26/157 (17%)	26 (100%)	0	100	100
1	B5	26/157 (17%)	26 (100%)	0	100	100
1	B6	25/157 (16%)	25 (100%)	0	100	100
5	BA	144/180 (80%)	144 (100%)	0	100	100
6	BB	116/134 (87%)	116 (100%)	0	100	100
7	BC	185/192 (96%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BD	91/115 (79%)	91 (100%)	0	100	100
9	BE	219/229 (96%)	217 (99%)	2 (1%)	78	90
10	BF	164/226 (73%)	164 (100%)	0	100	100
11	BG	99/150 (66%)	99 (100%)	0	100	100
12	BH	99/177 (56%)	98 (99%)	1 (1%)	76	88
13	BI	49/60 (82%)	49 (100%)	0	100	100
14	BJ	41/78 (53%)	41 (100%)	0	100	100
15	BK	87/162 (54%)	87 (100%)	0	100	100
16	BL	193/248 (78%)	192 (100%)	1 (0%)	88	95
17	BM	263/320 (82%)	263 (100%)	0	100	100
18	BN	218/251 (87%)	217 (100%)	1 (0%)	88	95
19	BO	181/228 (79%)	181 (100%)	0	100	100
20	BP	192/231 (83%)	190 (99%)	2 (1%)	76	88
21	BQ	138/151 (91%)	138 (100%)	0	100	100
22	BR	155/173 (90%)	154 (99%)	1 (1%)	86	94
23	BS	99/243 (41%)	98 (99%)	1 (1%)	76	88
24	BT	245/249 (98%)	244 (100%)	1 (0%)	91	97
25	BU	190/210 (90%)	190 (100%)	0	100	100
26	BV	132/143 (92%)	132 (100%)	0	100	100
27	BW	123/161 (76%)	122 (99%)	1 (1%)	81	91
28	BX	212/266 (80%)	210 (99%)	2 (1%)	78	90
29	BY	118/127 (93%)	118 (100%)	0	100	100
30	BZ	136/178 (76%)	136 (100%)	0	100	100
31	Ba	77/129 (60%)	77 (100%)	0	100	100
32	Bb	79/88 (90%)	77 (98%)	2 (2%)	47	75
33	Bc	79/114 (69%)	79 (100%)	0	100	100
34	Bd	79/114 (69%)	77 (98%)	2 (2%)	47	75
35	Be	75/82 (92%)	74 (99%)	1 (1%)	69	86
36	Bf	126/177 (71%)	126 (100%)	0	100	100
37	Bg	115/183 (63%)	115 (100%)	0	100	100
38	Bh	149/173 (86%)	148 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Bi	340/373 (91%)	338 (99%)	2 (1%)	86	94
40	Bj	150/267 (56%)	148 (99%)	2 (1%)	69	86
41	Bl	36/77 (47%)	36 (100%)	0	100	100
42	Bm	348/365 (95%)	345 (99%)	3 (1%)	78	90
43	Bn	310/328 (94%)	308 (99%)	2 (1%)	86	94
44	Bo	271/299 (91%)	269 (99%)	2 (1%)	84	93
45	Bp	132/150 (88%)	131 (99%)	1 (1%)	81	91
46	Bq	100/108 (93%)	100 (100%)	0	100	100
47	Br	103/133 (77%)	102 (99%)	1 (1%)	76	88
48	Bs	130/135 (96%)	128 (98%)	2 (2%)	65	84
49	Bt	251/284 (88%)	251 (100%)	0	100	100
50	Bu	236/275 (86%)	234 (99%)	2 (1%)	81	91
51	Bv	210/242 (87%)	210 (100%)	0	100	100
52	Bw	135/226 (60%)	133 (98%)	2 (2%)	65	84
53	Bx	122/147 (83%)	122 (100%)	0	100	100
54	By	103/178 (58%)	102 (99%)	1 (1%)	76	88
55	Bz	88/113 (78%)	88 (100%)	0	100	100
57	AB	249/322 (77%)	247 (99%)	2 (1%)	81	91
58	AC	115/142 (81%)	113 (98%)	2 (2%)	60	82
59	AD	66/174 (38%)	66 (100%)	0	100	100
60	AE	107/109 (98%)	107 (100%)	0	100	100
61	AF	181/205 (88%)	180 (99%)	1 (1%)	86	94
63	AH	130/180 (72%)	130 (100%)	0	100	100
65	AJ	92/116 (79%)	92 (100%)	0	100	100
66	AK	92/114 (81%)	92 (100%)	0	100	100
67	AL	159/222 (72%)	159 (100%)	0	100	100
68	AM	97/113 (86%)	95 (98%)	2 (2%)	53	78
69	AN	97/114 (85%)	97 (100%)	0	100	100
70	AO	170/225 (76%)	168 (99%)	2 (1%)	71	87
71	AP	89/127 (70%)	89 (100%)	0	100	100
72	AQ	77/78 (99%)	76 (99%)	1 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	AR	258/330 (78%)	257 (100%)	1 (0%)	91	97
74	AS	113/162 (70%)	111 (98%)	2 (2%)	59	81
75	AT	152/155 (98%)	152 (100%)	0	100	100
76	AU	149/168 (89%)	149 (100%)	0	100	100
77	AV	325/347 (94%)	322 (99%)	3 (1%)	78	90
78	AW	86/160 (54%)	84 (98%)	2 (2%)	50	76
79	AX	312/361 (86%)	312 (100%)	0	100	100
80	AY	134/342 (39%)	133 (99%)	1 (1%)	84	93
81	AZ	86/125 (69%)	86 (100%)	0	100	100
82	Aa	339/424 (80%)	336 (99%)	3 (1%)	78	90
83	Ab	187/233 (80%)	187 (100%)	0	100	100
84	Ac	100/102 (98%)	100 (100%)	0	100	100
85	Ad	282/351 (80%)	279 (99%)	3 (1%)	73	88
86	Ae	521/604 (86%)	521 (100%)	0	100	100
87	Ag	273/333 (82%)	273 (100%)	0	100	100
88	Ai	102/150 (68%)	102 (100%)	0	100	100
89	Aj	188/404 (46%)	187 (100%)	1 (0%)	88	95
All	All	13221/17576 (75%)	13156 (100%)	65 (0%)	89	95

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	BE	46	HIS
9	BE	196	ILE
12	BH	185	PHE
16	BL	173	MET
18	BN	106	PHE
20	BP	150	HIS
20	BP	174	LEU
22	BR	67	PHE
23	BS	89	HIS
24	BT	134	ARG
27	BW	149	THR
28	BX	265	LEU
28	BX	273	TYR
32	Bb	10	LEU

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Mol	Chain	Res	Type
32	Bb	47	LEU
34	Bd	66	HIS
34	Bd	122	PHE
35	Be	101	TRP
38	Bh	70	CYS
39	Bi	148	HIS
39	Bi	329	TRP
40	Bj	130	THR
40	Bj	136	LYS
42	Bm	121	LEU
42	Bm	152	GLU
42	Bm	256	PHE
43	Bn	281	PHE
43	Bn	376	THR
44	Bo	104	LEU
44	Bo	140	TRP
45	Bp	195	ILE
47	Br	41	ASP
48	Bs	84	VAL
48	Bs	127	GLN
50	Bu	57	VAL
50	Bu	238	VAL
52	Bw	84	THR
52	Bw	146	LEU
54	By	159	TYR
57	AB	117	THR
57	AB	211	THR
58	AC	134	PHE
58	AC	167	ILE
61	AF	88	ASP
68	AM	35	VAL
68	AM	93	LEU
70	AO	179	THR
70	AO	223	ARG
72	AQ	27	ASN
73	AR	337	GLN
74	AS	51	LEU
74	AS	83	LYS
77	AV	156	CYS
77	AV	315	LEU
77	AV	388	VAL
78	AW	109	VAL

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Mol	Chain	Res	Type
78	AW	148	LEU
80	AY	341	HIS
82	Aa	147	GLN
82	Aa	284	VAL
82	Aa	314	HIS
85	Ad	91	THR
85	Ad	118	THR
85	Ad	172	MET
89	Aj	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
5	BA	60	GLN
5	BA	99	GLN
5	BA	113	GLN
5	BA	171	HIS
5	BA	199	GLN
8	BD	107	ASN
10	BF	112	ASN
12	BH	96	ASN
12	BH	144	GLN
14	BJ	57	GLN
15	BK	118	HIS
15	BK	154	GLN
16	BL	228	GLN
17	BM	117	HIS
18	BN	97	HIS
18	BN	241	ASN
18	BN	277	ASN
19	BO	88	HIS
19	BO	178	ASN
19	BO	239	ASN
20	BP	61	ASN
20	BP	73	GLN
20	BP	224	HIS
21	BQ	84	GLN
21	BQ	133	GLN
22	BR	160	GLN
23	BS	33	GLN
23	BS	59	HIS
23	BS	142	GLN

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Mol	Chain	Res	Type
24	BT	87	HIS
24	BT	94	GLN
25	BU	138	GLN
25	BU	202	GLN
26	BV	98	GLN
26	BV	116	GLN
27	BW	79	HIS
27	BW	96	HIS
28	BX	253	GLN
29	BY	94	GLN
29	BY	147	GLN
30	BZ	183	ASN
32	Bb	84	GLN
33	Bc	82	GLN
33	Bc	124	HIS
34	Bd	60	GLN
35	Be	30	GLN
35	Be	58	GLN
36	Bf	103	HIS
37	Bg	106	GLN
37	Bg	119	GLN
37	Bg	130	GLN
39	Bi	148	HIS
39	Bi	173	GLN
39	Bi	228	ASN
39	Bi	379	GLN
39	Bi	414	GLN
40	Bj	266	GLN
42	Bm	119	GLN
42	Bm	186	GLN
42	Bm	266	GLN
42	Bm	280	GLN
42	Bm	358	GLN
43	Bn	320	GLN
44	Bo	197	HIS
44	Bo	305	HIS
45	Bp	186	GLN
47	Br	71	HIS
48	Bs	24	GLN
48	Bs	58	ASN
48	Bs	129	GLN
49	Bt	42	GLN

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Mol	Chain	Res	Type
49	Bt	69	HIS
49	Bt	193	GLN
50	Bu	69	HIS
50	Bu	167	ASN
50	Bu	196	GLN
50	Bu	217	HIS
51	Bv	113	ASN
51	Bv	251	HIS
52	Bw	54	HIS
52	Bw	66	GLN
52	Bw	136	GLN
53	Bx	93	ASN
53	Bx	155	GLN
54	By	86	ASN
54	By	88	GLN
55	Bz	69	HIS
58	AC	81	HIS
58	AC	156	GLN
60	AE	38	ASN
60	AE	92	ASN
61	AF	227	HIS
61	AF	238	HIS
65	AJ	57	GLN
66	AK	68	GLN
67	AL	78	GLN
67	AL	139	ASN
67	AL	147	HIS
67	AL	153	HIS
68	AM	100	HIS
69	AN	76	HIS
71	AP	83	GLN
73	AR	132	GLN
73	AR	337	GLN
75	AT	95	ASN
75	AT	146	GLN
76	AU	135	GLN
76	AU	155	GLN
76	AU	161	GLN
77	AV	137	HIS
77	AV	162	GLN
77	AV	185	ASN
77	AV	196	ASN

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Mol	Chain	Res	Type
77	AV	228	HIS
77	AV	301	GLN
77	AV	399	GLN
78	AW	104	GLN
79	AX	169	GLN
79	AX	175	GLN
79	AX	301	GLN
82	Aa	107	ASN
82	Aa	124	GLN
82	Aa	341	GLN
82	Aa	381	GLN
82	Aa	392	GLN
83	Ab	166	HIS
83	Ab	177	ASN
83	Ab	253	GLN
83	Ab	265	GLN
85	Ad	130	GLN
85	Ad	155	GLN
85	Ad	196	ASN
85	Ad	308	GLN
85	Ad	341	ASN
85	Ad	360	GLN
85	Ad	415	GLN
86	Ae	136	HIS
86	Ae	380	GLN
86	Ae	494	GLN
86	Ae	543	HIS
87	Ag	127	HIS
87	Ag	163	HIS
87	Ag	256	GLN
88	Ai	107	GLN
89	Aj	32	GLN
89	Aj	88	GLN
89	Aj	111	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1570/1571 (99%)	259 (16%)	0
4	B9	71/73 (97%)	13 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	AA	956/960 (99%)	139 (14%)	0
62	AG	70/71 (98%)	9 (12%)	0
64	AI	8/9 (88%)	2 (25%)	0
All	All	2677/2687 (99%)	423 (15%)	0

All (423) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	15	A
3	B8	19	U
3	B8	20	A
3	B8	21	C
3	B8	27	A
3	B8	31	A
3	B8	32	C
3	B8	36	A
3	B8	40	C
3	B8	42	C
3	B8	45	A
3	B8	46	A
3	B8	56	A
3	B8	57	A
3	B8	59	A
3	B8	60	U
3	B8	68	A
3	B8	69	C
3	B8	82	G
3	B8	83	A
3	B8	104	C
3	B8	105	G
3	B8	109	U
3	B8	112	A
3	B8	115	U
3	B8	129	A
3	B8	139	G
3	B8	140	A
3	B8	141	A
3	B8	142	U
3	B8	143	A
3	B8	163	C
3	B8	164	A

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Mol	Chain	Res	Type
3	B8	168	A
3	B8	172	C
3	B8	179	U
3	B8	180	A
3	B8	189	A
3	B8	190	U
3	B8	192	A
3	B8	205	A
3	B8	218	A
3	B8	219	A
3	B8	225	C
3	B8	228	U
3	B8	229	A
3	B8	239	C
3	B8	254	G
3	B8	263	G
3	B8	272	A
3	B8	273	A
3	B8	275	A
3	B8	277	A
3	B8	311	A
3	B8	322	G
3	B8	324	G
3	B8	329	A
3	B8	330	A
3	B8	331	A
3	B8	336	A
3	B8	340	A
3	B8	352	G
3	B8	359	G
3	B8	369	G
3	B8	373	U
3	B8	374	U
3	B8	376	A
3	B8	392	U
3	B8	409	A
3	B8	427	G
3	B8	428	A
3	B8	433	G
3	B8	434	U
3	B8	445	A
3	B8	446	C

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Mol	Chain	Res	Type
3	B8	448	G
3	B8	459	A
3	B8	460	C
3	B8	475	C
3	B8	479	A
3	B8	480	G
3	B8	488	U
3	B8	490	U
3	B8	491	U
3	B8	492	A
3	B8	497	U
3	B8	498	A
3	B8	501	A
3	B8	502	U
3	B8	503	A
3	B8	506	A
3	B8	515	A
3	B8	518	A
3	B8	532	A
3	B8	534	A
3	B8	549	C
3	B8	560	A
3	B8	570	A
3	B8	574	A
3	B8	575	C
3	B8	576	U
3	B8	578	A
3	B8	579	U
3	B8	580	A
3	B8	584	A
3	B8	586	C
3	B8	592	G
3	B8	595	C
3	B8	596	A
3	B8	617	A
3	B8	618	A
3	B8	625	A
3	B8	631	A
3	B8	633	U
3	B8	634	G
3	B8	640	A
3	B8	684	A

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Mol	Chain	Res	Type
3	B8	689	A
3	B8	693	U
3	B8	695	U
3	B8	704	U
3	B8	707	A
3	B8	713	A
3	B8	720	C
3	B8	722	A
3	B8	724	A
3	B8	725	C
3	B8	727	A
3	B8	728	C
3	B8	737	G
3	B8	746	U
3	B8	747	U
3	B8	748	A
3	B8	753	G
3	B8	777	A
3	B8	783	A
3	B8	809	G
3	B8	817	A
3	B8	825	C
3	B8	852	C
3	B8	854	U
3	B8	855	U
3	B8	859	A
3	B8	864	U
3	B8	872	A
3	B8	889	C
3	B8	890	C
3	B8	897	A
3	B8	902	C
3	B8	922	A
3	B8	923	A
3	B8	924	G
3	B8	925	G
3	B8	933	A
3	B8	950	U
3	B8	958	U
3	B8	959	G
3	B8	960	U
3	B8	964	A

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Mol	Chain	Res	Type
3	B8	965	A
3	B8	967	G
3	B8	977	G
3	B8	1015	C
3	B8	1016	C
3	B8	1018	U
3	B8	1026	A
3	B8	1027	G
3	B8	1028	A
3	B8	1038	A
3	B8	1050	C
3	B8	1051	G
3	B8	1055	A
3	B8	1056	G
3	B8	1057	A
3	B8	1063	U
3	B8	1064	G
3	B8	1093	A
3	B8	1094	A
3	B8	1095	C
3	B8	1096	A
3	B8	1097	A
3	B8	1099	U
3	B8	1100	C
3	B8	1105	A
3	B8	1107	A
3	B8	1113	A
3	B8	1114	U
3	B8	1115	A
3	B8	1119	C
3	B8	1120	A
3	B8	1121	U
3	B8	1146	G
3	B8	1167	C
3	B8	1168	A
3	B8	1169	A
3	B8	1180	G
3	B8	1183	U
3	B8	1188	U
3	B8	1195	A
3	B8	1204	A
3	B8	1206	U

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Mol	Chain	Res	Type
3	B8	1207	C
3	B8	1215	C
3	B8	1217	A
3	B8	1218	U
3	B8	1220	A
3	B8	1221	C
3	B8	1222	A
3	B8	1226	C
3	B8	1231	U
3	B8	1233	A
3	B8	1240	A
3	B8	1241	U
3	B8	1243	U
3	B8	1246	A
3	B8	1247	U
3	B8	1249	A
3	B8	1253	G
3	B8	1254	A
3	B8	1264	C
3	B8	1271	A
3	B8	1291	U
3	B8	1299	C
3	B8	1314	U
3	B8	1325	G
3	B8	1326	A
3	B8	1327	U
3	B8	1328	G
3	B8	1332	G
3	B8	1341	A
3	B8	1342	C
3	B8	1389	A
3	B8	1390	G
3	B8	1396	C
3	B8	1425	A
3	B8	1426	G
3	B8	1432	U
3	B8	1433	U
3	B8	1436	U
3	B8	1445	U
3	B8	1448	A
3	B8	1468	A
3	B8	1485	A

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Mol	Chain	Res	Type
3	B8	1493	A
3	B8	1494	A
3	B8	1498	C
3	B8	1504	A
3	B8	1505	G
3	B8	1509	U
3	B8	1525	C
3	B8	1526	U
3	B8	1527	U
3	B8	1528	A
3	B8	1536	U
3	B8	1551	C
3	B8	1553	A
3	B8	1558	U
3	B8	1561	A
3	B8	1571	A
4	B9	8	U
4	B9	17	U
4	B9	18	U
4	B9	23	A
4	B9	34	U
4	B9	35	G
4	B9	48	U
4	B9	49	G
4	B9	55	C
4	B9	56	A
4	B9	57	C
4	B9	58	A
4	B9	71	C
56	AA	5	A
56	AA	18	G
56	AA	34	U
56	AA	42	A
56	AA	43	U
56	AA	58	U
56	AA	65	C
56	AA	66	C
56	AA	75	A
56	AA	77	G
56	AA	92	A
56	AA	93	A
56	AA	98	A

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Mol	Chain	Res	Type
56	AA	108	G
56	AA	115	A
56	AA	120	A
56	AA	125	U
56	AA	126	A
56	AA	127	A
56	AA	139	A
56	AA	147	G
56	AA	152	A
56	AA	161	C
56	AA	170	A
56	AA	186	U
56	AA	191	C
56	AA	192	C
56	AA	203	G
56	AA	208	A
56	AA	216	A
56	AA	217	U
56	AA	223	U
56	AA	244	C
56	AA	250	A
56	AA	257	U
56	AA	258	C
56	AA	261	A
56	AA	273	A
56	AA	287	C
56	AA	288	G
56	AA	293	A
56	AA	296	G
56	AA	297	A
56	AA	309	A
56	AA	310	A
56	AA	314	A
56	AA	317	A
56	AA	319	A
56	AA	320	A
56	AA	328	A
56	AA	354	C
56	AA	355	U
56	AA	367	A
56	AA	368	A
56	AA	372	C

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Mol	Chain	Res	Type
56	AA	381	G
56	AA	395	C
56	AA	396	C
56	AA	399	A
56	AA	417	C
56	AA	421	A
56	AA	455	A
56	AA	456	A
56	AA	457	C
56	AA	461	A
56	AA	465	G
56	AA	471	U
56	AA	472	A
56	AA	477	A
56	AA	495	U
56	AA	502	A
56	AA	530	G
56	AA	538	C
56	AA	539	A
56	AA	540	U
56	AA	541	C
56	AA	566	U
56	AA	571	A
56	AA	574	C
56	AA	576	C
56	AA	596	U
56	AA	597	U
56	AA	604	U
56	AA	613	A
56	AA	625	U
56	AA	626	C
56	AA	639	A
56	AA	641	A
56	AA	644	A
56	AA	645	A
56	AA	646	C
56	AA	665	A
56	AA	681	A
56	AA	682	G
56	AA	685	C
56	AA	698	A
56	AA	699	U

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Mol	Chain	Res	Type
56	AA	708	A
56	AA	711	A
56	AA	720	A
56	AA	722	A
56	AA	724	U
56	AA	731	A
56	AA	733	A
56	AA	739	A
56	AA	740	U
56	AA	743	A
56	AA	745	C
56	AA	748	A
56	AA	751	A
56	AA	752	A
56	AA	753	A
56	AA	766	C
56	AA	780	A
56	AA	790	A
56	AA	808	U
56	AA	823	G
56	AA	825	C
56	AA	826	C
56	AA	838	A
56	AA	869	A
56	AA	884	C
56	AA	885	U
56	AA	893	A
56	AA	896	A
56	AA	899	C
56	AA	919	A
56	AA	920	G
56	AA	925	A
56	AA	928	A
56	AA	929	A
56	AA	930	G
56	AA	932	U
56	AA	933	A
56	AA	943	G
56	AA	955	G
56	AA	956	G
56	AA	959	U
56	AA	960	A

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Mol	Chain	Res	Type
62	AG	8	U
62	AG	11	G
62	AG	16	A
62	AG	17	U
62	AG	45	G
62	AG	52	A
62	AG	53	U
62	AG	55	C
62	AG	71	A
64	AI	2	G
64	AI	4	C

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	B8	1403	3	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
4	MIA	B9	38	4	24,31,32	0.85	1 (4%)	26,44,47	4.75	2 (7%)
56	MA6	AA	945	56	18,26,27	1.10	2 (11%)	19,38,41	1.91	3 (15%)
3	1MA	B8	949	3	16,25,26	0.89	2 (12%)	18,37,40	1.06	2 (11%)
56	5MU	AA	428	56	19,22,23	1.39	5 (26%)	28,32,35	2.05	6 (21%)
56	5MC	AA	848	56	18,22,23	0.94	2 (11%)	26,32,35	1.08	2 (7%)
56	MA6	AA	944	56	18,26,27	1.11	2 (11%)	19,38,41	2.02	3 (15%)
6	AYA	BB	2	6	6,7,8	0.77	0	5,8,10	0.18	0
3	OMG	B8	1151	62,3,91	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
22	SAC	BR	2	22	7,8,9	0.53	0	8,9,11	0.94	1 (12%)
88	5F0	Ai	186	88	8,8,9	1.46	2 (25%)	7,9,11	1.70	1 (14%)
3	OMU	B8	1375	3,91	19,22,23	1.18	2 (10%)	26,31,34	1.68	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	B8	1376	3	18,26,27	0.93	1 (5%)	19,38,41	1.04	2 (10%)
84	AYA	Ac	2	84	6,7,8	0.78	0	5,8,10	0.28	0
32	AYA	Bb	2	32	6,7,8	0.73	0	5,8,10	0.38	0
72	AYA	AQ	2	72	6,7,8	0.76	0	5,8,10	0.28	0
56	B8T	AA	846	56	19,22,23	0.42	0	26,31,34	0.37	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
3	PSU	B8	1403	3	-	0/7/25/26	0/2/2/2
4	MIA	B9	38	4	-	0/11/33/34	0/3/3/3
56	MA6	AA	945	56	-	4/7/29/30	0/3/3/3
3	1MA	B8	949	3	-	0/3/25/26	0/3/3/3
56	5MU	AA	428	56	-	0/7/25/26	0/2/2/2
56	5MC	AA	848	56	-	0/7/25/26	0/2/2/2
56	MA6	AA	944	56	-	0/7/29/30	0/3/3/3
6	AYA	BB	2	6	-	1/4/6/8	-
3	OMG	B8	1151	62,3,91	-	0/5/27/28	0/3/3/3
22	SAC	BR	2	22	-	4/7/8/10	-
88	5F0	Ai	186	88	-	3/9/9/10	-
3	OMU	B8	1375	3,91	-	0/9/27/28	0/2/2/2
3	OMG	B8	1376	3	-	0/5/27/28	0/3/3/3
84	AYA	Ac	2	84	-	3/4/6/8	-
32	AYA	Bb	2	32	-	3/4/6/8	-
72	AYA	AQ	2	72	-	2/4/6/8	-
56	B8T	AA	846	56	-	0/7/27/28	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AA	944	MA6	C5-N7	3.37	1.51	1.39
56	AA	945	MA6	C5-N7	3.32	1.51	1.39
3	B8	1403	PSU	C6-C5	3.03	1.38	1.35
88	Ai	186	5F0	OD1-C1	2.92	1.40	1.33
3	B8	1403	PSU	C4-N3	-2.76	1.33	1.38
56	AA	848	5MC	C6-C5	2.70	1.39	1.34
56	AA	428	5MU	C6-C5	2.69	1.39	1.34
56	AA	428	5MU	C4-N3	-2.62	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B8	1376	OMG	C6-N1	-2.60	1.34	1.37
3	B8	1151	OMG	C6-N1	-2.54	1.34	1.37
3	B8	1375	OMU	C4-N3	-2.44	1.34	1.38
3	B8	949	1MA	C8-N7	-2.35	1.31	1.35
56	AA	428	5MU	C6-N1	-2.29	1.34	1.38
56	AA	428	5MU	C4-C5	2.24	1.48	1.44
56	AA	848	5MC	C6-N1	-2.23	1.34	1.38
4	B9	38	MIA	C2-S10	2.22	1.77	1.75
56	AA	944	MA6	C4-N3	-2.14	1.32	1.35
3	B8	949	1MA	C5-C4	-2.12	1.37	1.43
3	B8	1375	OMU	C2-N3	-2.11	1.34	1.38
56	AA	945	MA6	C4-N3	-2.11	1.32	1.35
88	Ai	186	5F0	OD1-CXT	-2.10	1.40	1.45
56	AA	428	5MU	C2-N3	-2.06	1.34	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B9	38	MIA	C11-S10-C2	23.84	120.07	102.27
3	B8	1403	PSU	N1-C2-N3	5.88	121.79	115.13
56	AA	944	MA6	C4-C5-N7	-5.83	103.32	109.40
56	AA	945	MA6	C4-C5-N7	-5.13	104.06	109.40
56	AA	428	5MU	C4-N3-C2	-5.10	120.75	127.35
56	AA	428	5MU	N3-C2-N1	4.76	121.20	114.89
56	AA	944	MA6	C1'-N9-C4	-4.68	118.42	126.64
56	AA	428	5MU	C5-C4-N3	4.50	119.15	115.31
3	B8	1375	OMU	C4-N3-C2	-4.49	120.66	126.58
56	AA	945	MA6	C1'-N9-C4	-4.36	118.99	126.64
56	AA	944	MA6	N3-C2-N1	-4.20	122.11	128.68
56	AA	945	MA6	N3-C2-N1	-4.13	122.23	128.68
3	B8	1375	OMU	N3-C2-N1	4.08	120.30	114.89
56	AA	428	5MU	O4-C4-C5	-4.03	120.23	124.90
3	B8	1403	PSU	C4-N3-C2	-3.79	120.88	126.34
56	AA	428	5MU	C5-C6-N1	-3.76	119.47	123.34
3	B8	1375	OMU	C5-C4-N3	3.52	120.11	114.84
56	AA	848	5MC	C5-C6-N1	-3.44	119.80	123.34
88	Ai	186	5F0	OD1-C1-CA	3.35	120.09	111.52
3	B8	1403	PSU	O2-C2-N1	-3.27	119.19	122.79
4	B9	38	MIA	C5-C6-N1	-3.16	118.19	120.81
3	B8	1375	OMU	O4-C4-C5	-3.01	119.87	125.16
22	BR	2	SAC	O-C-CA	-2.54	118.13	124.78
56	AA	428	5MU	O2-C2-N1	-2.52	119.44	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AA	848	5MC	C5-C4-N3	-2.40	119.08	121.67
3	B8	1375	OMU	O2-C2-N1	-2.35	119.67	122.79
3	B8	1376	OMG	C5-C6-N1	2.30	118.02	113.95
3	B8	1151	OMG	C5-C6-N1	2.25	117.92	113.95
3	B8	1376	OMG	C8-N7-C5	2.21	107.20	102.99
3	B8	1151	OMG	C8-N7-C5	2.17	107.13	102.99
3	B8	949	1MA	C5-C6-N1	-2.17	110.66	113.90
3	B8	949	1MA	N1-C6-N6	2.12	125.16	119.77

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	BR	2	SAC	C2A-C1A-N-CA
22	BR	2	SAC	OAC-C1A-N-CA
22	BR	2	SAC	C-CA-CB-OG
72	AQ	2	AYA	OT-CT-N-CA
56	AA	945	MA6	C5-C6-N6-C9
56	AA	945	MA6	C5-C6-N6-C10
88	Ai	186	5F0	OD1-C1-CA-CB
72	AQ	2	AYA	CM-CT-N-CA
84	Ac	2	AYA	CM-CT-N-CA
32	Bb	2	AYA	CM-CT-N-CA
84	Ac	2	AYA	OT-CT-N-CA
56	AA	945	MA6	N1-C6-N6-C9
32	Bb	2	AYA	OT-CT-N-CA
22	BR	2	SAC	N-CA-CB-OG
88	Ai	186	5F0	O1-C1-CA-CB
6	BB	2	AYA	C-CA-N-CT
32	Bb	2	AYA	C-CA-N-CT
56	AA	945	MA6	C4'-C5'-O5'-P
88	Ai	186	5F0	O1-C1-OD1-CXT
84	Ac	2	AYA	C-CA-N-CT

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 385 ligands modelled in this entry, 376 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	PHE	B9	101	4	10,11,12	0.38	0	10,13,15	0.29	0
94	FES	AP	201	71,60	0,4,4	-	-	-		
94	FES	AT	201	75,68	0,4,4	-	-	-		
98	ATP	AX	501	90	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
97	FME	AG	101	62	8,9,10	0.54	0	7,9,11	0.97	1 (14%)
94	FES	Bh	201	20,38	0,4,4	-	-	-		
99	GDP	AX	503	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
96	SPD	AA	1121	-	9,9,9	0.33	0	8,8,8	0.87	0
95	SPM	AA	1120	-	13,13,13	0.35	0	12,12,12	0.94	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
92	PHE	B9	101	4	-	1/5/6/8	0/1/1/1
94	FES	AP	201	71,60	-	-	0/1/1/1
94	FES	AT	201	75,68	-	-	0/1/1/1
98	ATP	AX	501	90	-	3/18/38/38	0/3/3/3
97	FME	AG	101	62	-	2/7/9/11	-
94	FES	Bh	201	20,38	-	-	0/1/1/1
99	GDP	AX	503	-	-	3/12/32/32	0/3/3/3
96	SPD	AA	1121	-	-	0/7/7/7	-
95	SPM	AA	1120	-	-	2/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
99	AX	503	GDP	C6-N1	-2.31	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
99	AX	503	GDP	PA-O3A-PB	-3.64	120.32	132.83
99	AX	503	GDP	C3'-C2'-C1'	3.09	105.63	100.98
97	AG	101	FME	O-C-CA	-2.53	118.14	124.78
99	AX	503	GDP	C8-N7-C5	2.32	107.40	102.99
98	AX	501	ATP	C5-C6-N6	2.30	123.84	120.35
99	AX	503	GDP	C5-C6-N1	2.28	117.98	113.95
98	AX	501	ATP	PB-O3B-PG	2.00	139.71	132.83

There are no chirality outliers.

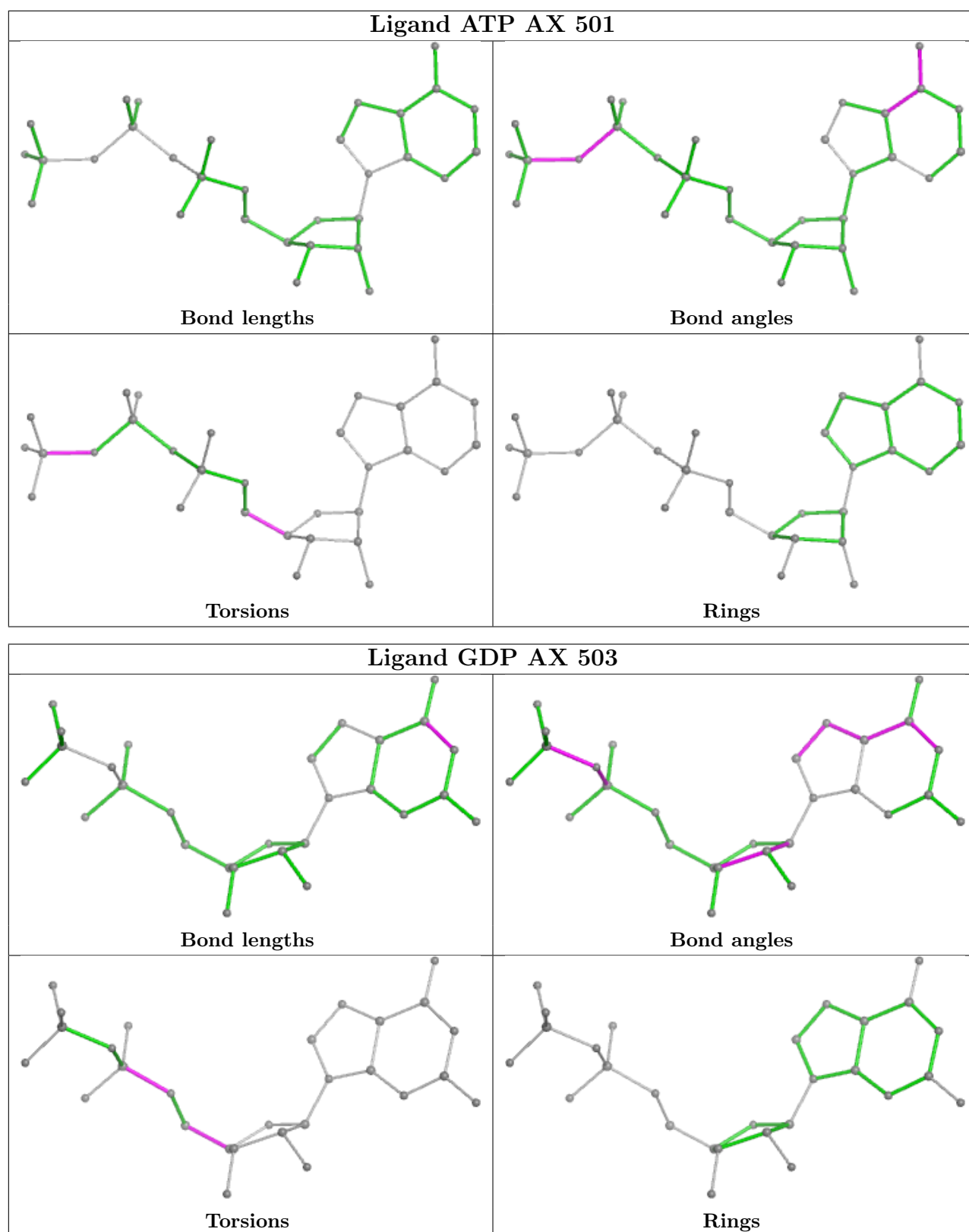
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	B9	101	PHE	O-C-CA-CB
97	AG	101	FME	O1-CN-N-CA
97	AG	101	FME	CB-CA-N-CN
98	AX	501	ATP	O4'-C4'-C5'-O5'
99	AX	503	GDP	O4'-C4'-C5'-O5'
98	AX	501	ATP	C3'-C4'-C5'-O5'
99	AX	503	GDP	C3'-C4'-C5'-O5'
95	AA	1120	SPM	N5-C6-C7-C8
95	AA	1120	SPM	C6-C7-C8-C9
98	AX	501	ATP	PB-O3B-PG-O3G
99	AX	503	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no chain breaks in this entry.

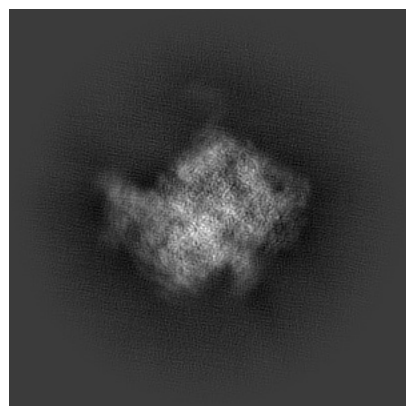
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16894. These allow visual inspection of the internal detail of the map and identification of artifacts.

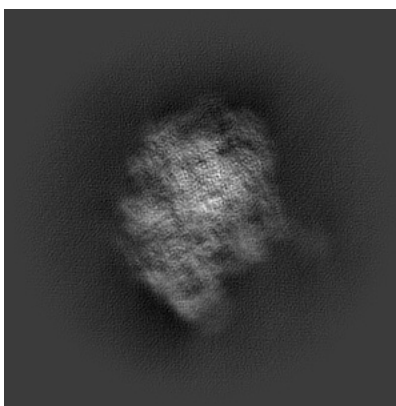
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

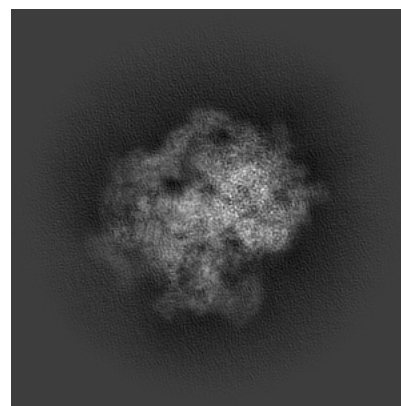
6.1.1 Primary map



X

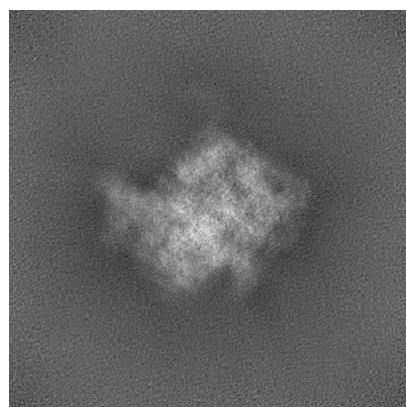


Y

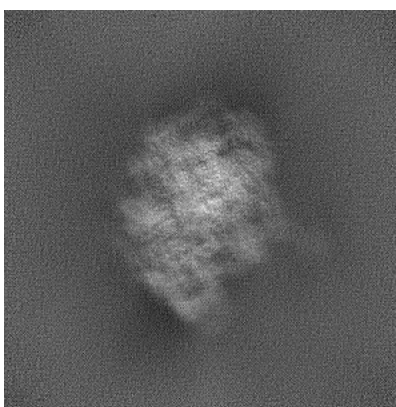


Z

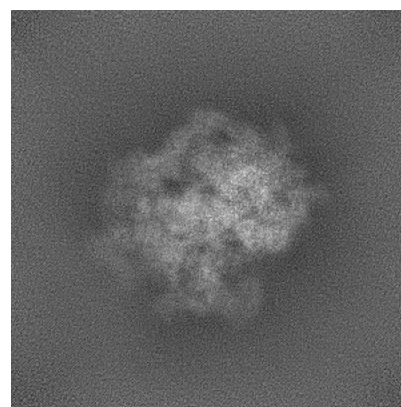
6.1.2 Raw map



X



Y

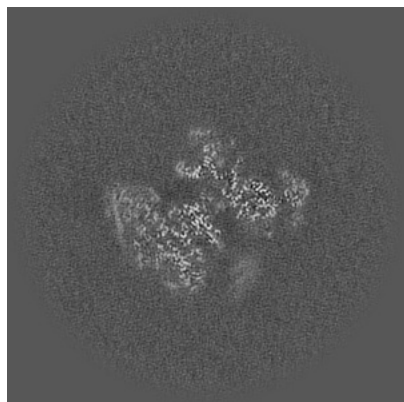


Z

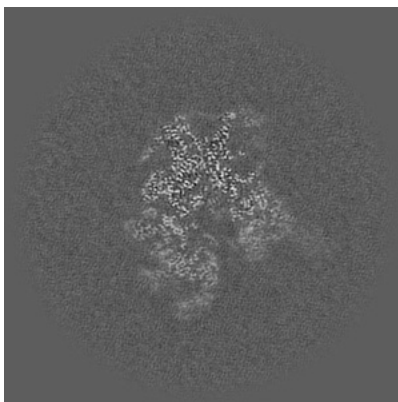
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

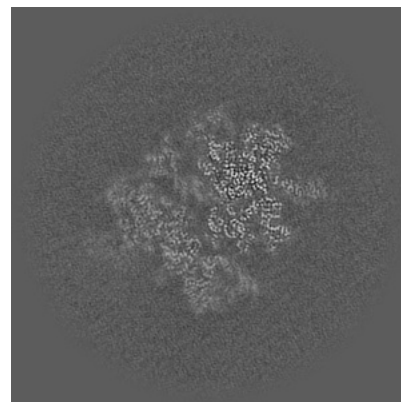
6.2.1 Primary map



X Index: 250

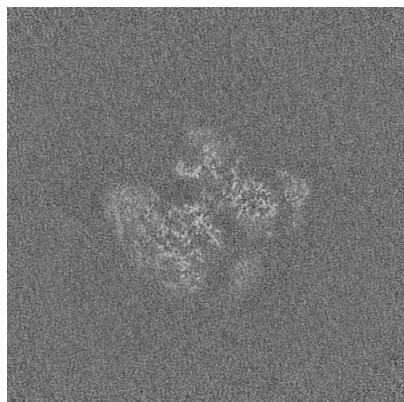


Y Index: 250

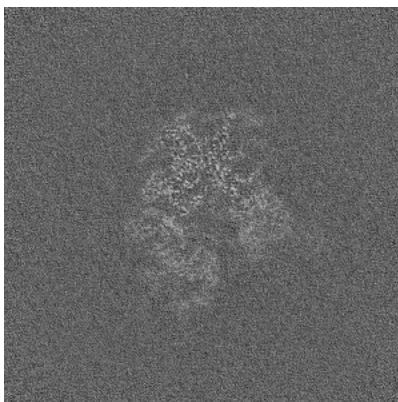


Z Index: 250

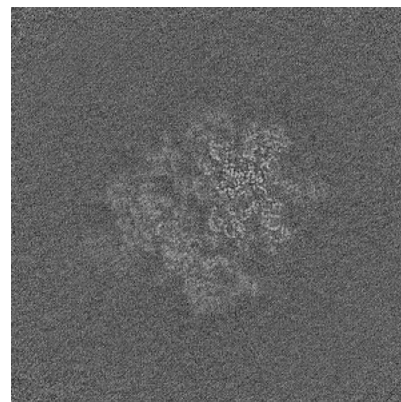
6.2.2 Raw map



X Index: 250



Y Index: 250

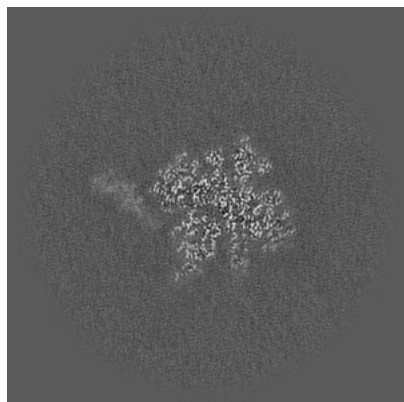


Z Index: 250

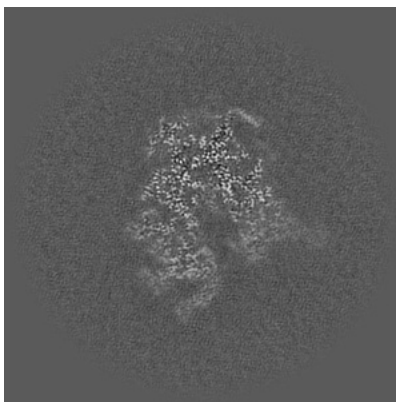
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

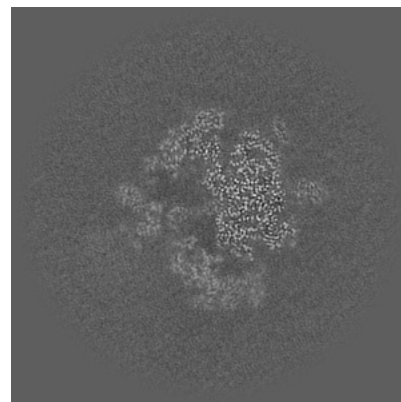
6.3.1 Primary map



X Index: 291

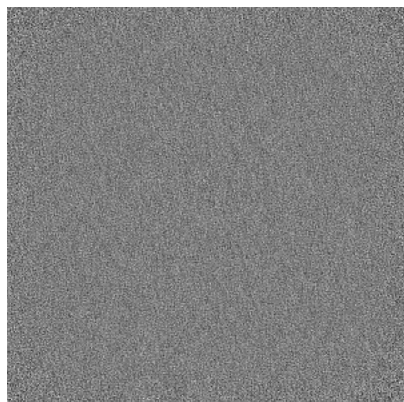


Y Index: 253

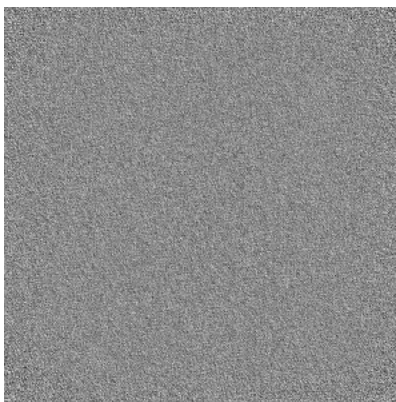


Z Index: 263

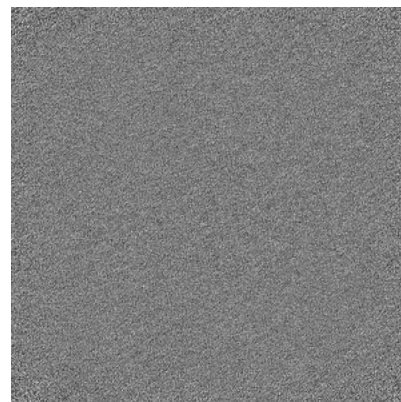
6.3.2 Raw map



X Index: 0



Y Index: 0

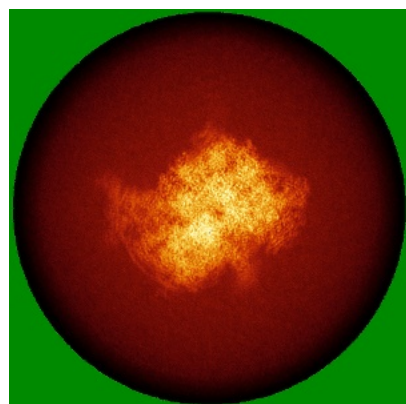


Z Index: 0

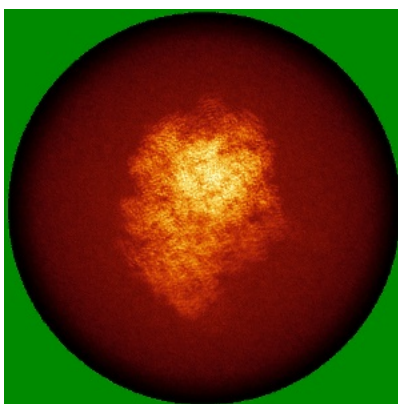
The images above show the largest variance slices of the map in three orthogonal directions.

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

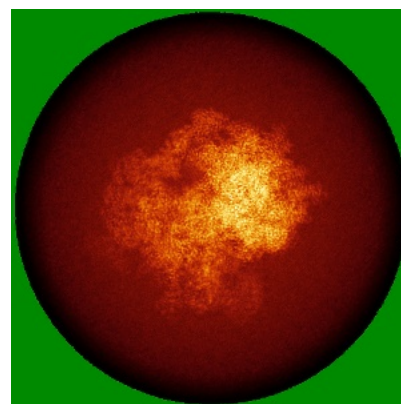
6.4.1 Primary map



X

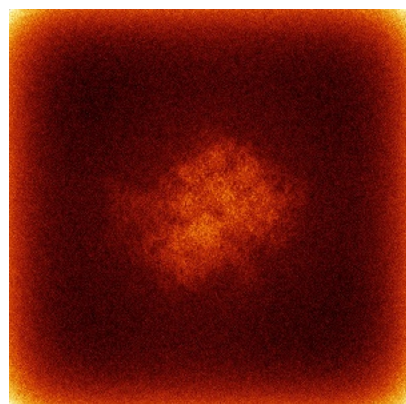


Y

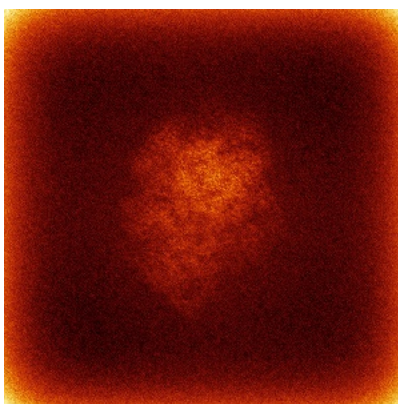


Z

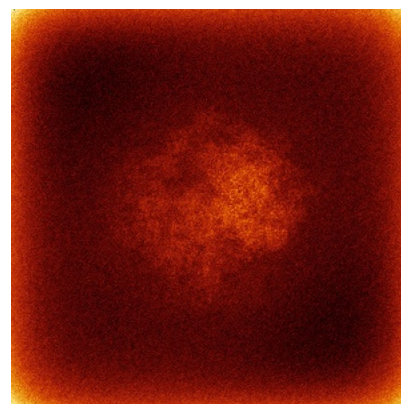
6.4.2 Raw map



X



Y

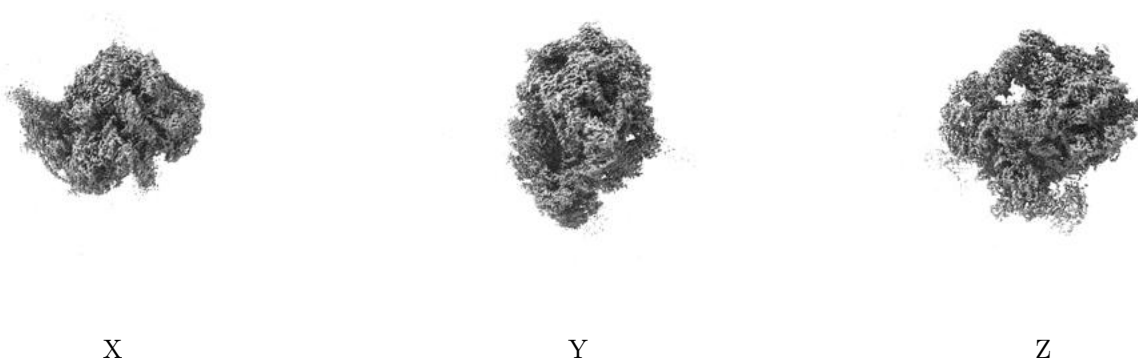


Z

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

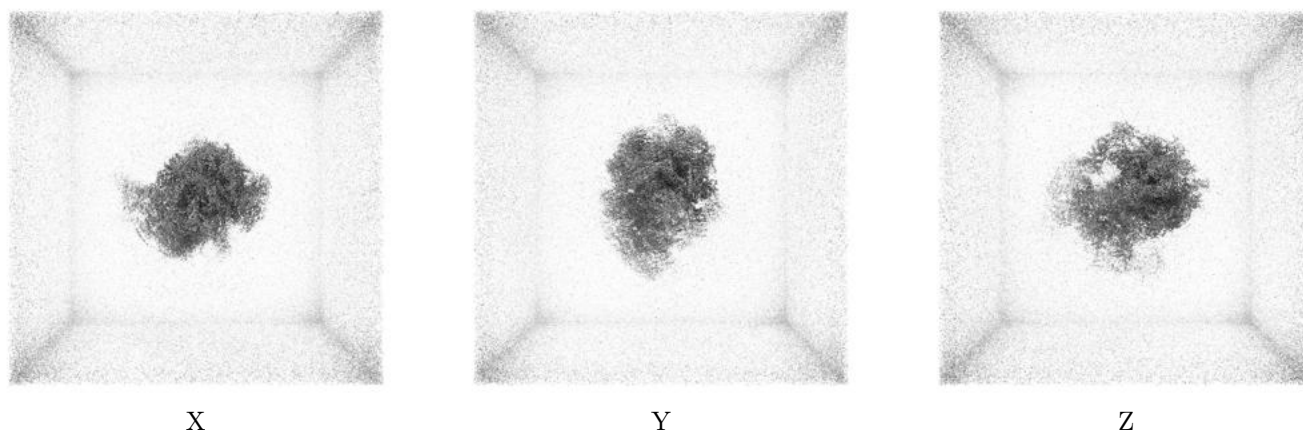
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

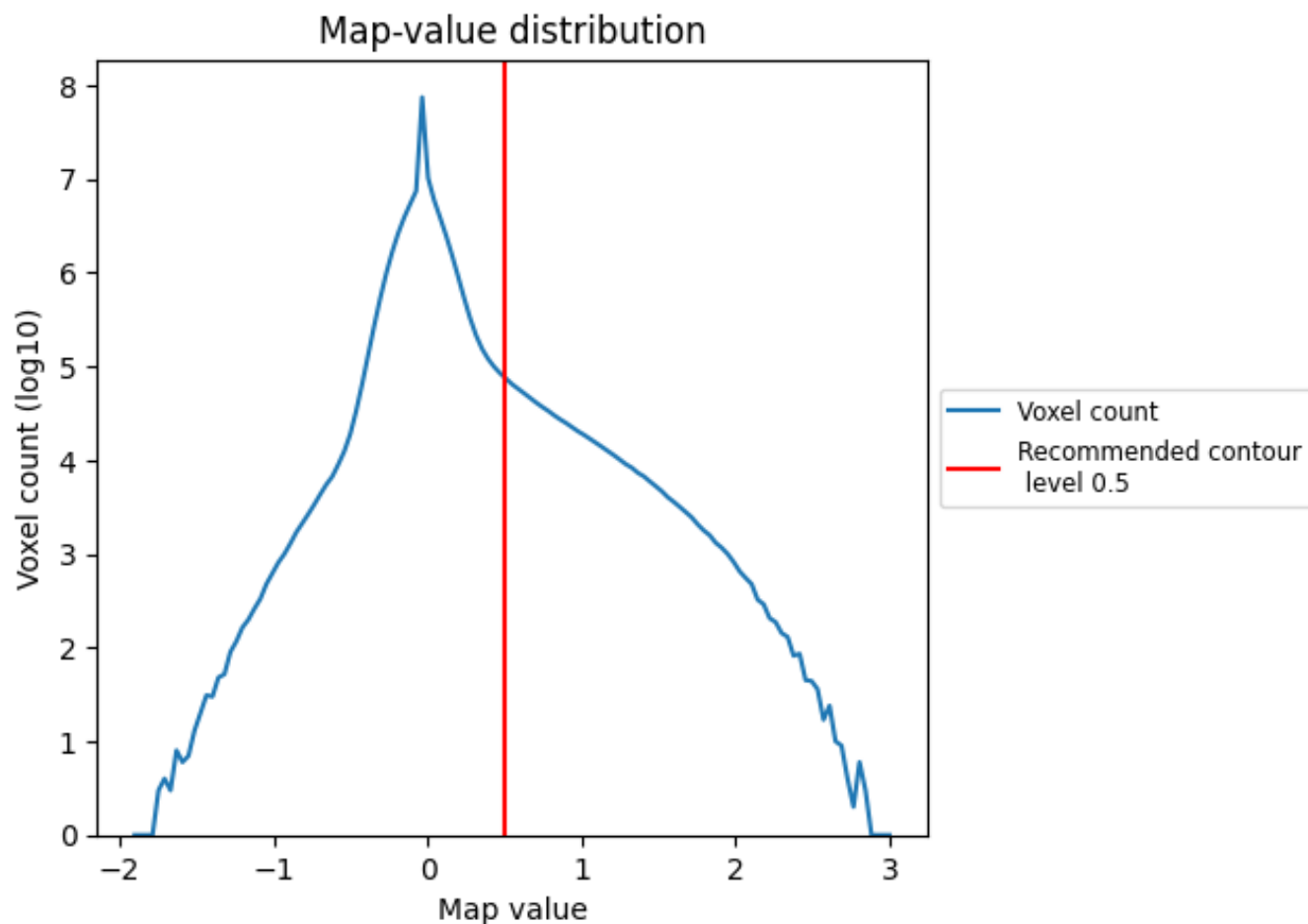
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

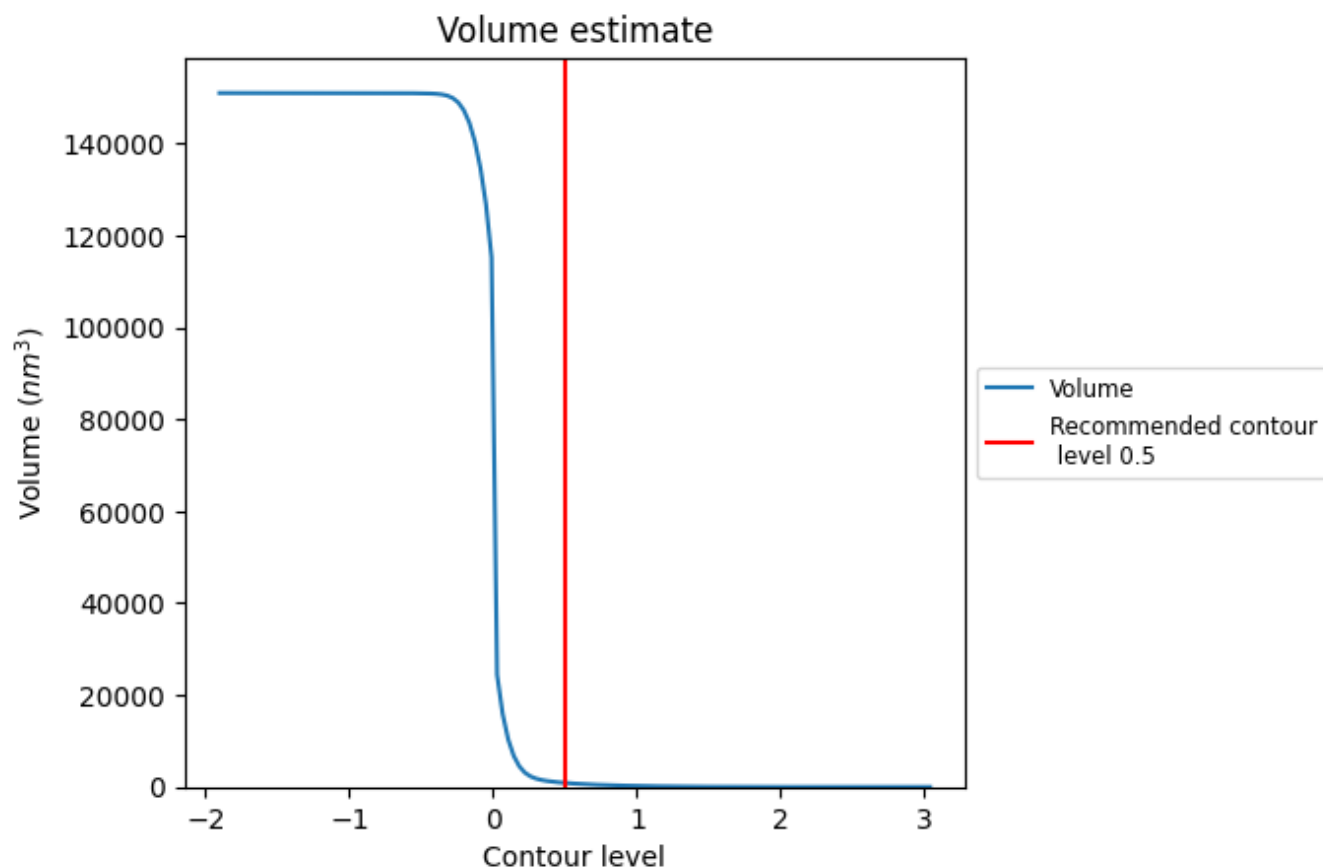
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

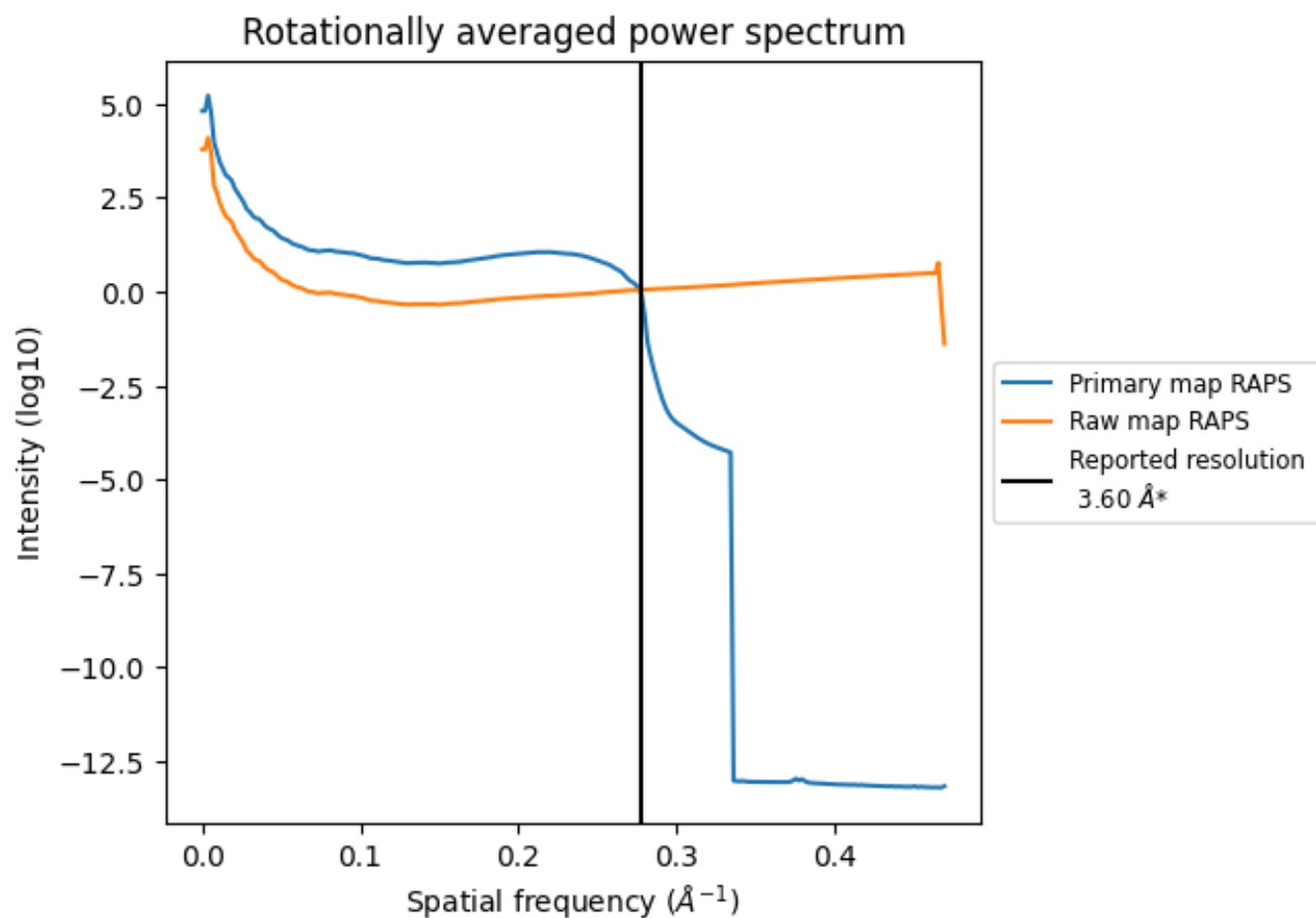
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880 nm³; this corresponds to an approximate mass of 795 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 ⓘ

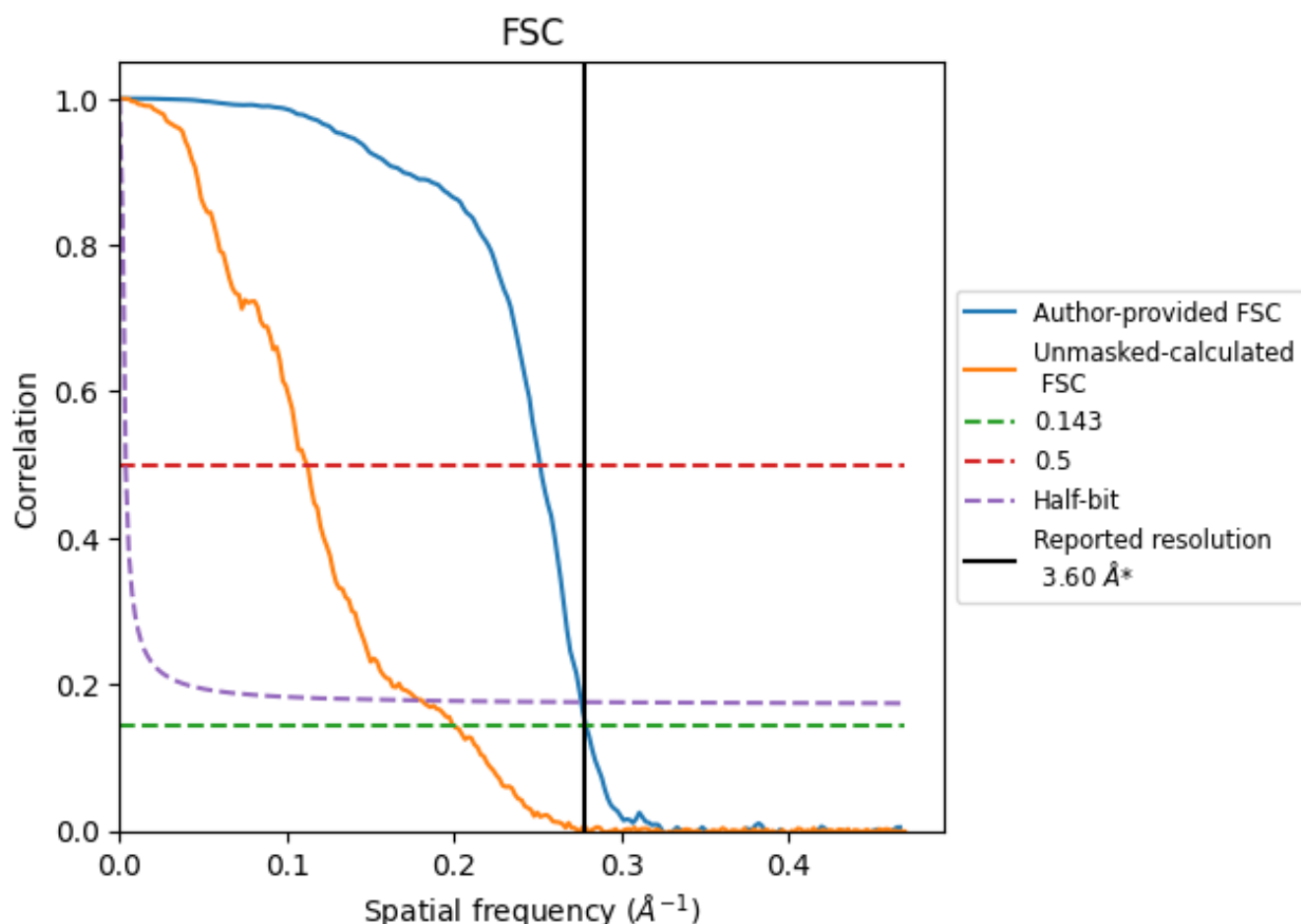


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

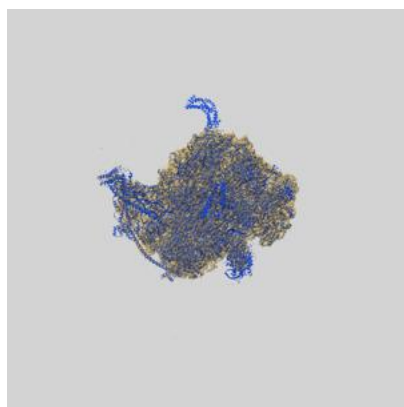
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.98	3.62
Unmasked-calculated*	5.00	8.92	5.53

*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 5.00 differs from the reported value 3.6 by more than 10 %

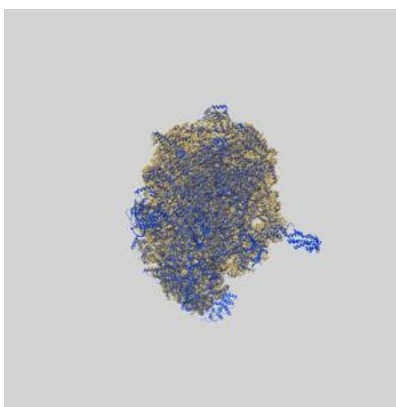
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16894 and PDB model 8OIN. Per-residue inclusion information can be found in section [3](#) on page [28](#).

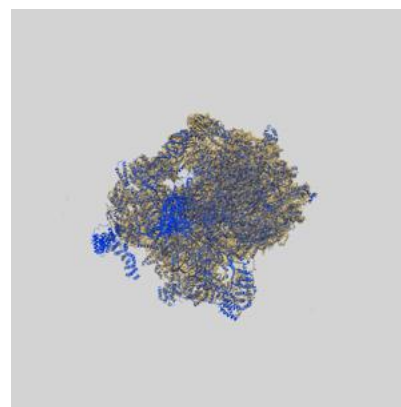
9.1 Map-model overlay [i](#)



X



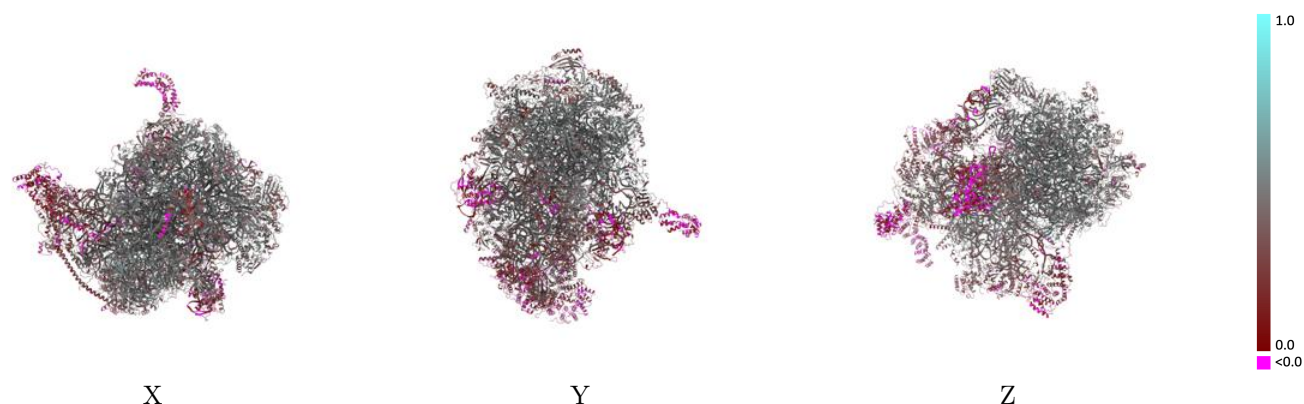
Y



Z

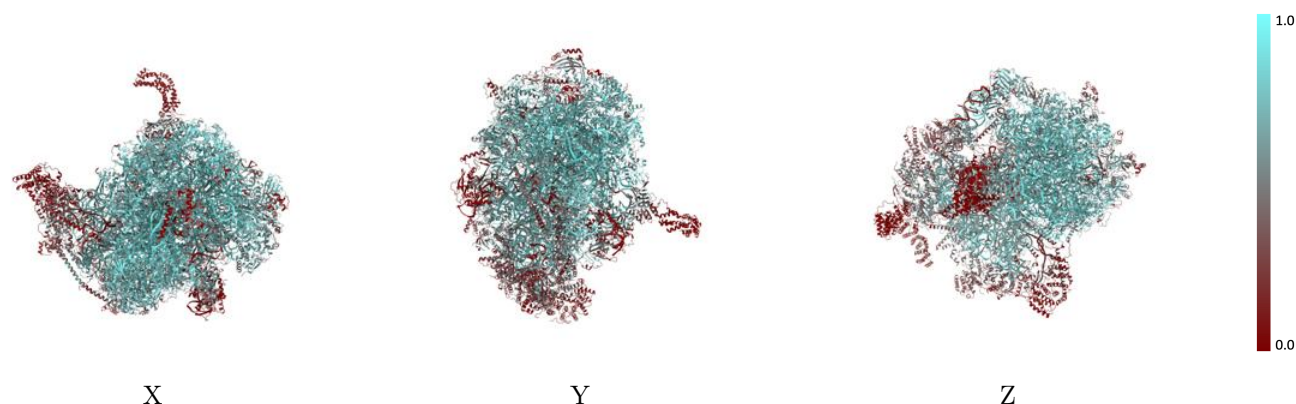
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



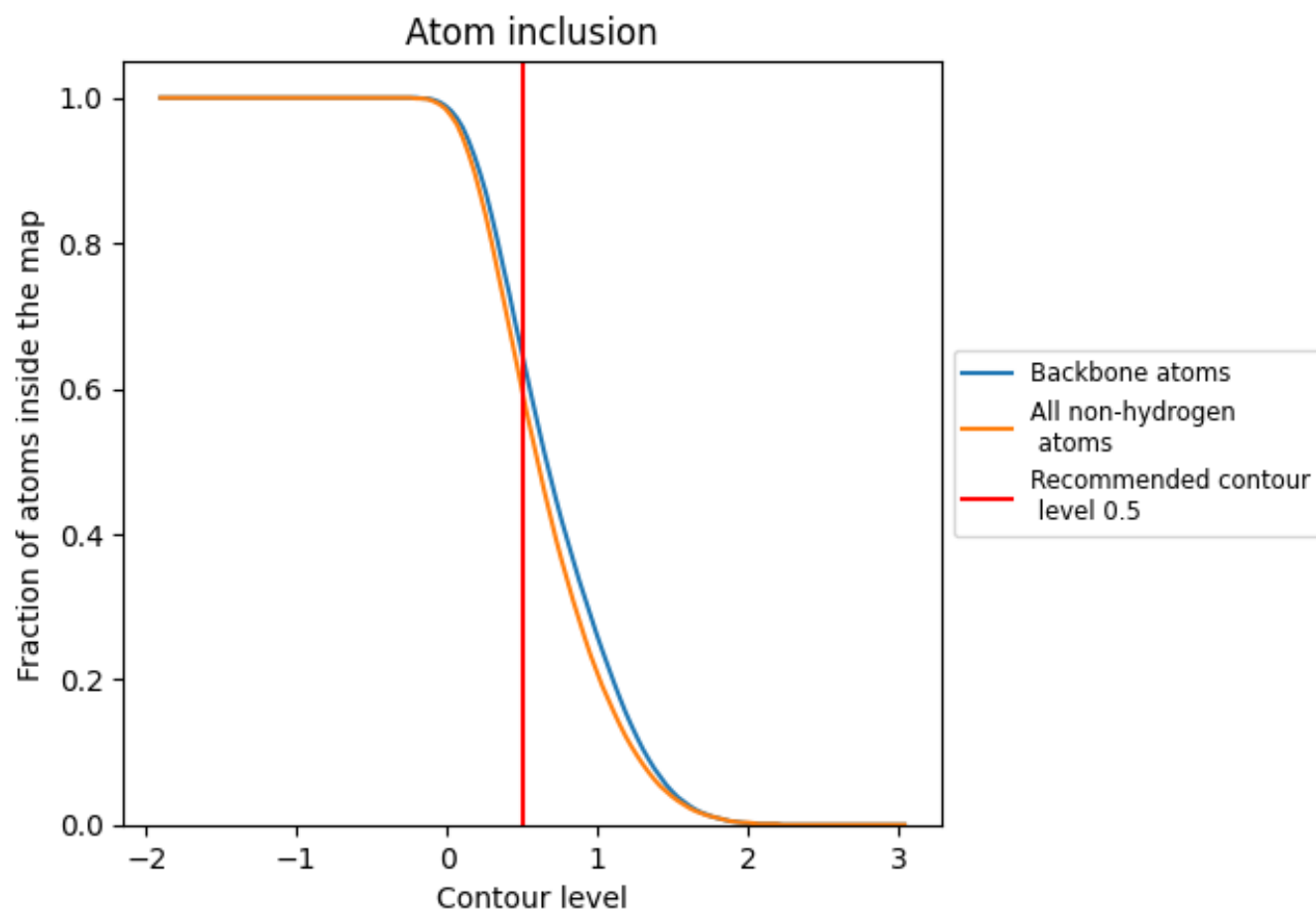
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5970	 0.3840
AA	 0.7520	 0.4070
AB	 0.3430	 0.2840
AC	 0.5180	 0.4150
AD	 0.6490	 0.4510
AE	 0.6030	 0.4180
AF	 0.4550	 0.3200
AG	 0.4840	 0.3230
AH	 0.4450	 0.3420
AI	 0.7470	 0.4470
AJ	 0.5680	 0.4440
AK	 0.5500	 0.4110
AL	 0.5390	 0.3830
AM	 0.4060	 0.3320
AN	 0.5920	 0.4030
AO	 0.3760	 0.3220
AP	 0.5740	 0.4030
AQ	 0.6480	 0.4300
AR	 0.2430	 0.2670
AS	 0.3750	 0.2950
AT	 0.5360	 0.3740
AU	 0.4150	 0.2690
AV	 0.1150	 0.1370
AW	 0.4350	 0.3570
AX	 0.2690	 0.2030
AY	 0.2530	 0.2350
AZ	 0.3890	 0.3370
Aa	 0.2460	 0.2700
Ab	 0.5880	 0.3910
Ac	 0.4780	 0.3630
Ad	 0.4920	 0.3900
Ae	 0.0600	 0.1060
Ag	 0.4520	 0.3230
Ai	 0.6200	 0.4200
Aj	 0.2400	 0.2550







































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Chain	Atom inclusion	Q-score
B1	0.0190	0.0620
B2	0.0000	0.0960
B3	0.0000	0.0660
B4	0.0050	0.0570
B5	0.0000	0.0690
B6	0.0000	0.0150
B7	0.0320	0.1360
B8	0.8300	0.4530
B9	0.4850	0.2420
BA	0.7320	0.4940
BB	0.6760	0.4460
BC	0.4610	0.3960
BD	0.7840	0.5030
BE	0.5830	0.4210
BF	0.7220	0.4600
BG	0.7950	0.4910
BH	0.7190	0.4780
BI	0.4520	0.3930
BJ	0.8210	0.5180
BK	0.8020	0.5130
BL	0.7650	0.4890
BM	0.7590	0.4750
BN	0.7470	0.4830
BO	0.2260	0.2160
BP	0.3440	0.2660
BQ	0.2190	0.2150
BR	0.7910	0.4950
BS	0.7030	0.4750
BT	0.7190	0.4690
BU	0.7610	0.4780
BV	0.7480	0.4920
BW	0.6930	0.4530
BX	0.6500	0.4540
BY	0.7710	0.4940
BZ	0.7550	0.4880
Ba	0.7000	0.4560
Bb	0.4840	0.3510
Bc	0.3490	0.2680
Bd	0.3510	0.2650
Be	0.8110	0.5000
Bf	0.3990	0.3500
Bg	0.4530	0.3670

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Chain	Atom inclusion	Q-score
Bh	 0.7200	 0.4550
Bi	 0.7340	 0.4590
Bj	 0.0300	 0.0700
Bl	 0.8010	 0.4990
Bm	 0.7200	 0.4490
Bn	 0.6980	 0.4250
Bo	 0.6460	 0.4280
Bp	 0.4420	 0.3250
Bq	 0.5770	 0.4220
Br	 0.6210	 0.4300
Bs	 0.7700	 0.4910
Bt	 0.7120	 0.4540
Bu	 0.4000	 0.3590
Bv	 0.3970	 0.2620
Bw	 0.4900	 0.3630
Bx	 0.7250	 0.4680
By	 0.2870	 0.3620
Bz	 0.7870	 0.4960