Full wwPDB EM Validation Report

Nov 10, 2024 – 12:54 am GMT

PDB ID	:	7NQL
EMDB ID	:	EMD-12529
Title	:	55S mammalian mitochondrial ribosome with ICT1 and P site tRNAMet
Authors	:	Kummer, E.; Schubert, K.; Ban, N.
Deposited on	:	2021-03-01
Resolution	:	3.40 Å(reported)

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:

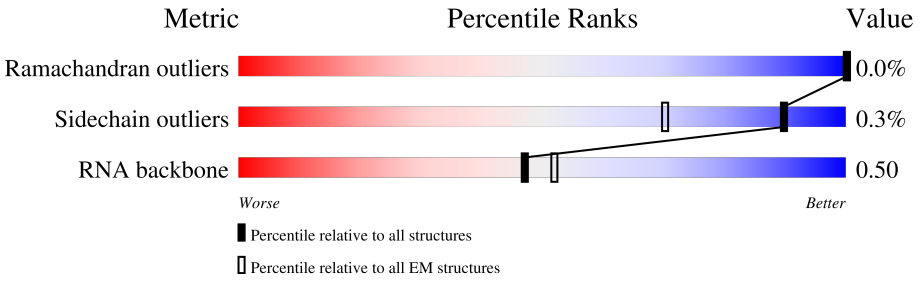
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	B7	95	48% 52%
2	B8	188	50% 49%
3	B9	100	38% 62%
4	BA	1571	5% 72% 26%
5	BB	73	38% 70% 22% 8%
6	BD	306	78% 22%
7	BE	399	77% 23%
8	BF	294	85% 15%

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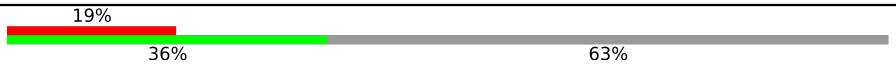
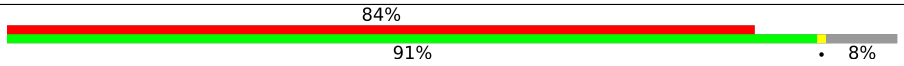
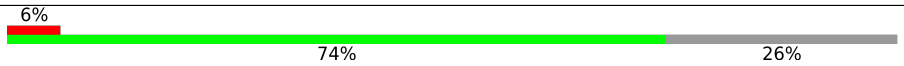
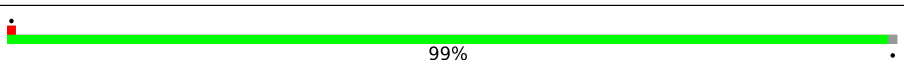
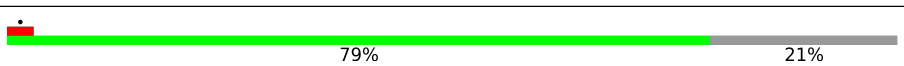
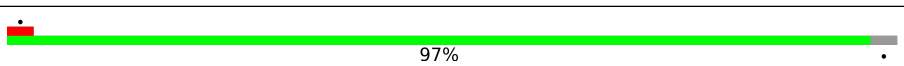
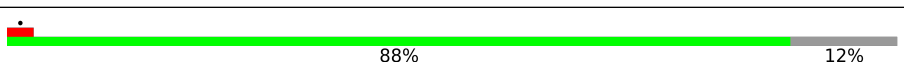
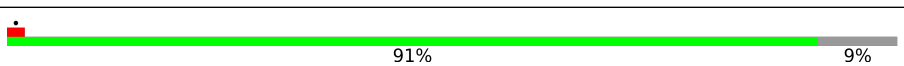
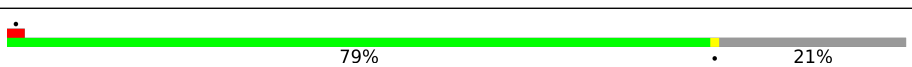
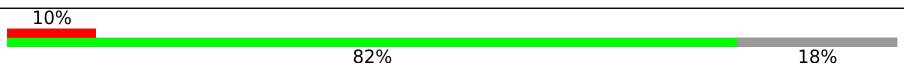
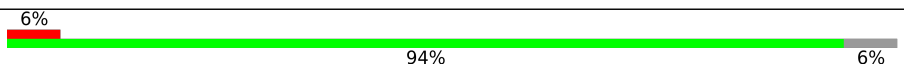
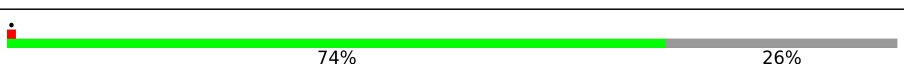
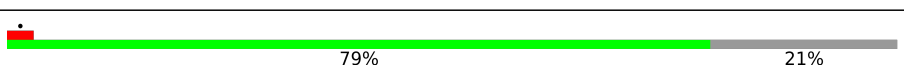
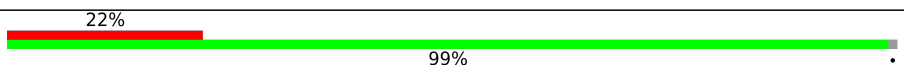
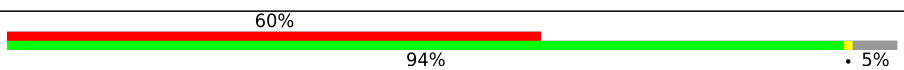
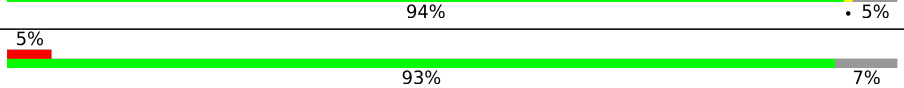
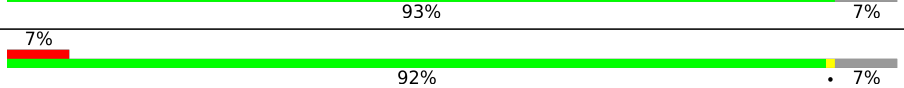
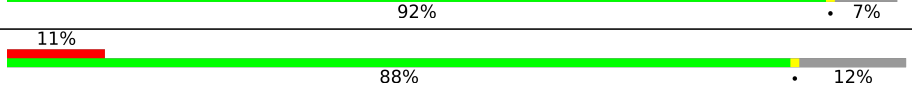
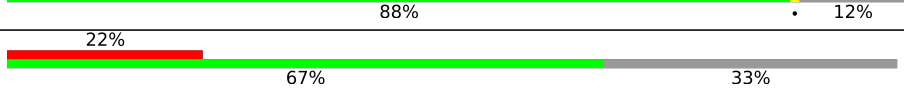
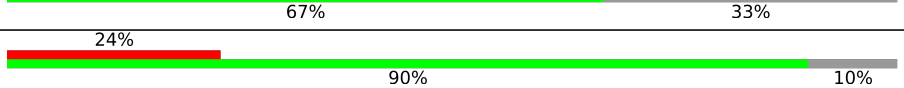
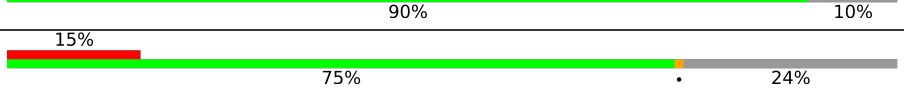
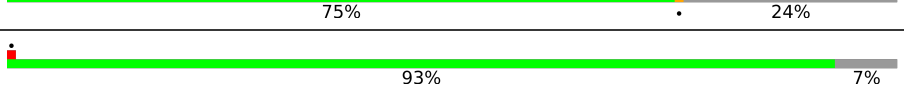
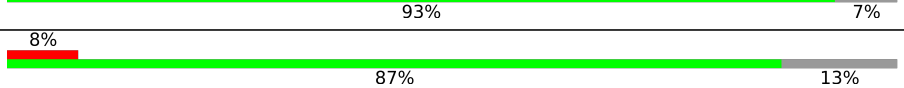
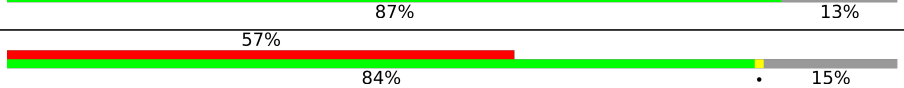
Mol	Chain	Length	Quality of chain
9	BI	268	
10	BJ	262	
11	BK	192	
12	BL	184	
13	BN	178	
14	BO	145	
15	BP	296	
16	BQ	251	
17	BR	169	
18	BS	180	
19	BT	292	
20	BU	149	
21	BV	209	
22	BW	210	
23	BX	150	
24	BY	216	
25	Ba	423	
26	Bb	380	
27	Bc	334	
28	Bd	206	
29	Be	135	
30	Bf	142	
31	Bg	159	
32	Bh	332	
33	Bi	306	

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Mol	Chain	Length	Quality of chain
34	Bj	279	32% 78% 22%
35	Bk	269	15% 58% 42%
36	Bl	166	80% 20%
37	Bm	198	40% 55% 45%
38	Bn	128	75% 24%
39	Bo	124	7% 78% 22%
40	Bp	112	59% 87% 13%
41	Bq	138	25% 39% 61%
42	Bt	102	92% 8%
43	Bu	205	32% 73% 26%
44	Bv	222	27% 61% 39%
45	Bw	433	8% 89% 11%
46	Bx	196	13% 82% 17%
47	AA	962	8% 81% 19%
48	CL	198	23% 23% 77%
48	DL	198	14% 13% 86%
48	EL	198	14% 14% 86%
48	FL	198	14% 14% 86%
48	GL	198	14% 14% 86%
48	HL	198	13% 13% 87%
49	AB	289	8% 76% 24%
50	AC	167	10% 79% 21%
51	AE	430	24% 79% 20%
52	AF	276	44% 56%
53	AG	242	20% 86% 14%

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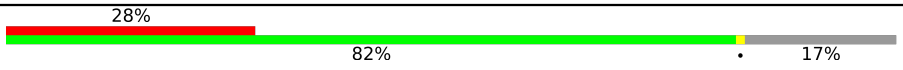
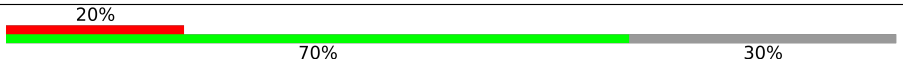
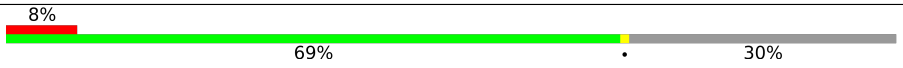
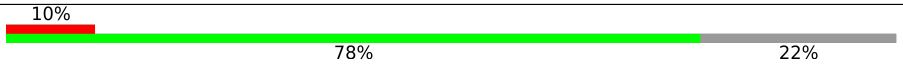
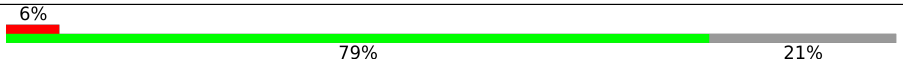
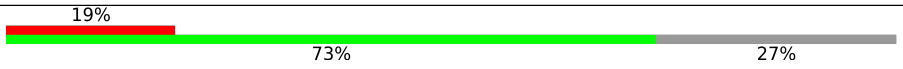
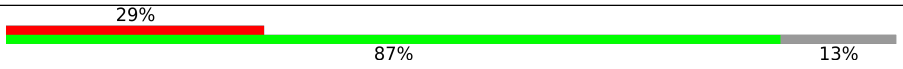
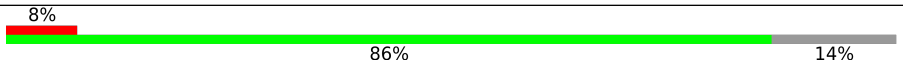
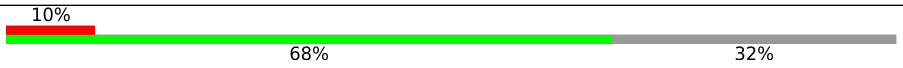
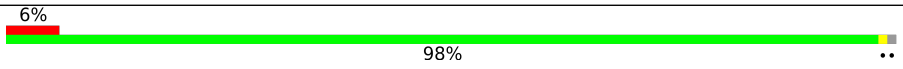
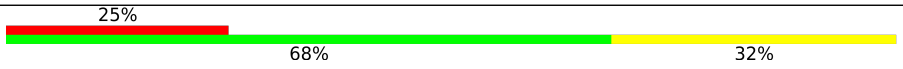
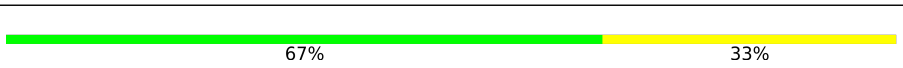
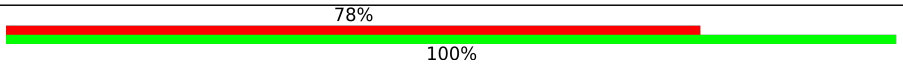
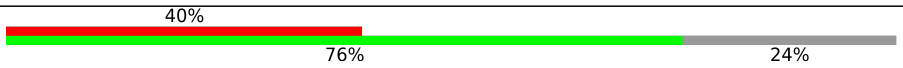
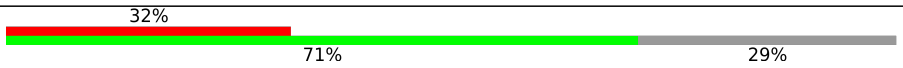
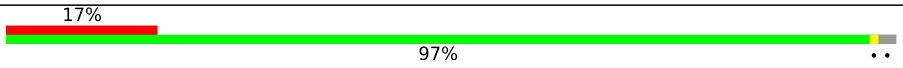
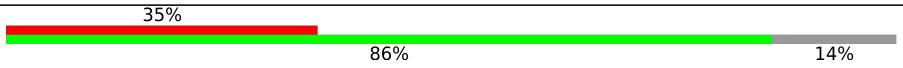
Mol	Chain	Length	Quality of chain
54	AI	397	
55	AJ	200	
56	AK	196	
57	AL	139	
58	AN	128	
59	AO	239	
60	AP	135	
61	AQ	130	
62	AR	143	
63	AU	87	
64	AV	71	
65	AX	6	
66	AZ	18	
67	Aa	382	
68	Ab	190	
69	Ac	173	
70	Ad	205	
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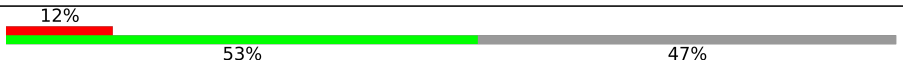
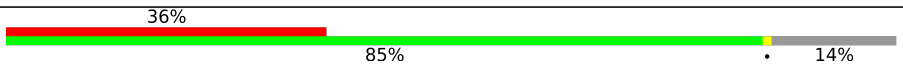
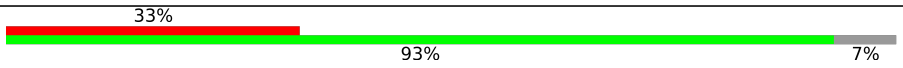
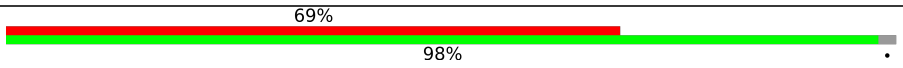
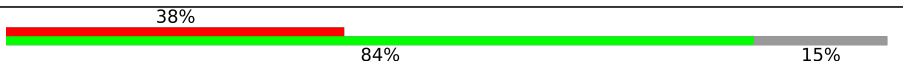
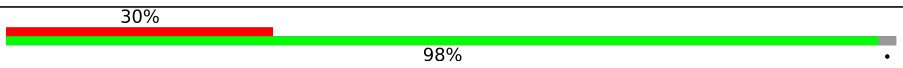
72	Af	188	
73	Ag	410	
74	Ah	387	
75	Ai	106	
76	Aj	218	
77	Ak	325	
78	Am	118	

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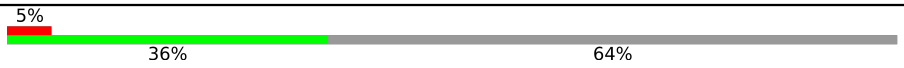
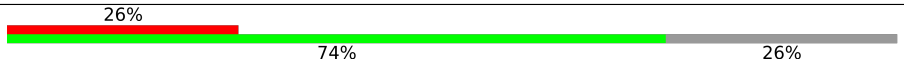
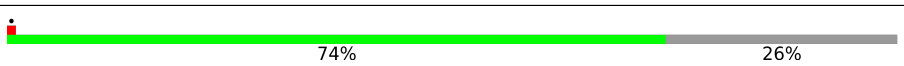
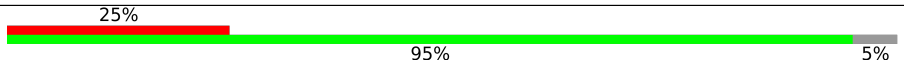
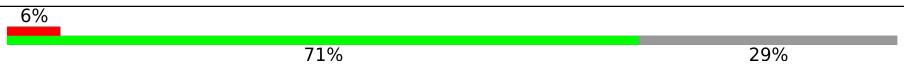
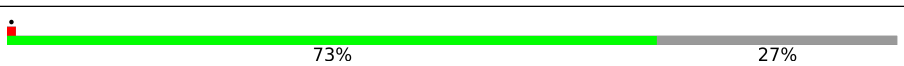
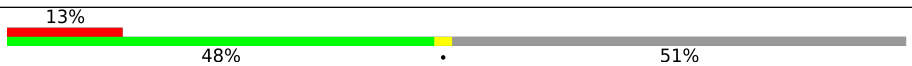
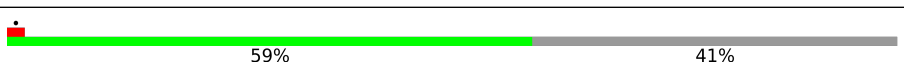
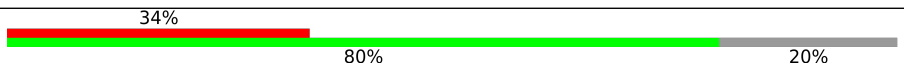
Mol	Chain	Length	Quality of chain
79	An	199	
80	Ao	699	
81	Ap	258	
82	B0	148	
83	B1	256	
84	B2	252	
85	B3	161	
86	B4	126	
87	B5	188	
88	B6	65	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 174319 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B7	46	387	239	89	58	1	0	0

- Molecule 2 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B8	95	833	539	163	129	2	0	0

- Molecule 3 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B9	38	335	214	70	47	4	0	0

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	BA	1544	32844	14750	5972	10578	1544	0	0

- Molecule 5 is a RNA chain called CP tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	BB	67	1427	640	261	459	67	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 6 is a protein called uL2m.

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

- Molecule 7 is a protein called ICT1.

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

- Molecule 8 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	BI	98	Total	C	N	O	0	0
			805	509	155	141		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 11 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BK	176	Total	C	N	O	S	0	0
			1303	830	236	235	2		

- Molecule 12 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BL	137	Total	C	N	O	S	0	0
			1113	683	219	206	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	23	SER	-	expression tag	UNP Q14197
BL	24	GLY	-	expression tag	UNP Q14197
BL	25	GLY	-	expression tag	UNP Q14197
BL	26	SER	-	expression tag	UNP Q14197
BL	27	GLY	-	expression tag	UNP Q14197
BL	28	SER	-	expression tag	UNP Q14197
BL	29	GLY	-	expression tag	UNP Q14197

- Molecule 13 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 14 is a protein called uL14m.

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

- Molecule 15 is a protein called uL15m.

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

- Molecule 16 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BQ	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
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 17 is a protein called bL17m.

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

- Molecule 18 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 19 is a protein called Mitochondrial ribosomal protein L19.

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

- Molecule 20 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 21 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 22 is a protein called uL22m.

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

- Molecule 23 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 24 is a protein called uL24m.

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

- Molecule 25 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 26 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 28 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bd	138	Total	C	N	O	S	0	0
			1158	729	211	217	1		

- Molecule 29 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 30 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 31 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 32 is a protein called mL44.

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

- Molecule 33 is a protein called Mitochondrial ribosomal protein L45.

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

- Molecule 34 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 35 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bk	155	Total	C	N	O	S	0	0
			1246	796	214	231	5		

- Molecule 36 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bl	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
Bl	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 37 is a protein called Mitochondrial ribosomal protein L50.

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

- Molecule 38 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 39 is a protein called mL52.

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

- Molecule 40 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bp	12	ALA	SER	conflict	UNP A0A341D604
Bp	107	SER	GLY	conflict	UNP A0A341D604

- Molecule 41 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bq	54	Total	C	N	O	S	0	0
			474	304	88	81	1		

- Molecule 42 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 43 is a protein called mL62 (ICT1).

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

- Molecule 44 is a protein called mL64.

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

- Molecule 45 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 46 is a protein called Mitochondrial ribosomal protein S18A.

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

- Molecule 47 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 48 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	CL	45	Total	C	N	O	0	0
			317	203	52	62		
48	DL	27	Total	C	N	O	0	0
			213	137	33	43		
48	EL	28	Total	C	N	O	0	0
			222	143	35	44		
48	FL	27	Total	C	N	O	0	0
			213	137	33	43		
48	GL	27	Total	C	N	O	0	0
			213	137	33	43		
48	HL	26	Total	C	N	O	0	0
			205	131	32	42		

- Molecule 49 is a protein called Mitochondrial ribosomal protein S2.

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

- Molecule 50 is a protein called Mitochondrial ribosomal protein S24.

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

- Molecule 51 is a protein called Mitochondrial ribosomal protein S5.

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

- Molecule 52 is a protein called bS6m.

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

- Molecule 53 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 54 is a protein called uS9m.

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

- Molecule 55 is a protein called Mitochondrial ribosomal protein S10.

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

- Molecule 56 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AK	137	Total	C	N	O	S	0	0
			1007	631	193	180	3		

- Molecule 57 is a protein called Mitochondrial ribosomal protein S12.

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

- Molecule 58 is a protein called Mitochondrial ribosomal protein S14.

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

- Molecule 59 is a protein called uS15m.

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

- Molecule 60 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 61 is a protein called uS17m.

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

- Molecule 62 is a protein called Mitochondrial ribosomal protein S18C.

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

- Molecule 63 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 64 is a RNA chain called fMet-tRNAMet (P site).

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 65 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AX	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 66 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 67 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 68 is a protein called mS23.

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

- Molecule 69 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 70 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 71 is a protein called Mitochondrial ribosomal protein S27.

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

- Molecule 72 is a protein called Mitoribosomal protein ms28, mrps28.

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

- Molecule 73 is a protein called Death associated protein 3.

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

- Molecule 74 is a protein called Mitochondrial ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ah	120	Total	C	N	O	S	0	0
			1015	659	168	185	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	180	UNK	-	insertion	UNP F1RME2
Ah	181	GLN	-	insertion	UNP F1RME2
Ah	182	LYS	-	insertion	UNP F1RME2
Ah	184	GLY	-	insertion	UNP F1RME2
Ah	185	GLU	LYS	conflict	UNP F1RME2
Ah	187	PRO	LYS	conflict	UNP F1RME2
Ah	189	ILE	LEU	conflict	UNP F1RME2
Ah	190	SER	ILE	conflict	UNP F1RME2
Ah	237	SER	-	insertion	UNP F1RME2
Ah	238	PHE	-	insertion	UNP F1RME2

- Molecule 75 is a protein called mS33.

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

- Molecule 76 is a protein called mS34.

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

- Molecule 77 is a protein called Mitochondrial ribosomal protein S35.

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

- Molecule 78 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 79 is a protein called Aurora kinase A interacting protein 1.

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

- Molecule 80 is a protein called Pentatricopeptide repeat domain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ao	572	Total	C	N	O	S	0	0
			4526	2898	770	834	24		

- Molecule 81 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 82 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	B0	110	Total	C	N	O	S	0	0
			857	553	156	145	3		

- Molecule 83 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 84 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	B2	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 85 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 86 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	B4	62	Total	C	N	O	S	0	0
			474	296	94	81	3		

- Molecule 87 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 88 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
89	B9	1	Total Zn 1 1	0
89	Bx	1	Total Zn 1 1	0
89	AR	1	Total Zn 1 1	0
89	Ac	1	Total Zn 1 1	0
89	Ap	1	Total Zn 1 1	0
89	B5	1	Total Zn 1 1	0

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

Mol	Chain	Residues	Atoms	AltConf
90	BA	212	Total Mg 212 212	0
90	BB	1	Total Mg 1 1	0
90	BD	3	Total Mg 3 3	0
90	BE	1	Total Mg 1 1	0
90	BP	3	Total Mg 3 3	0
90	BQ	1	Total Mg 1 1	0
90	BR	1	Total Mg 1 1	0
90	Be	2	Total Mg 2 2	0
90	Bl	1	Total Mg 1 1	0
90	Bt	1	Total Mg 1 1	0
90	AA	101	Total Mg 101 101	0
90	AB	1	Total Mg 1 1	0
90	AL	1	Total Mg 1 1	0
90	AV	1	Total Mg 1 1	0

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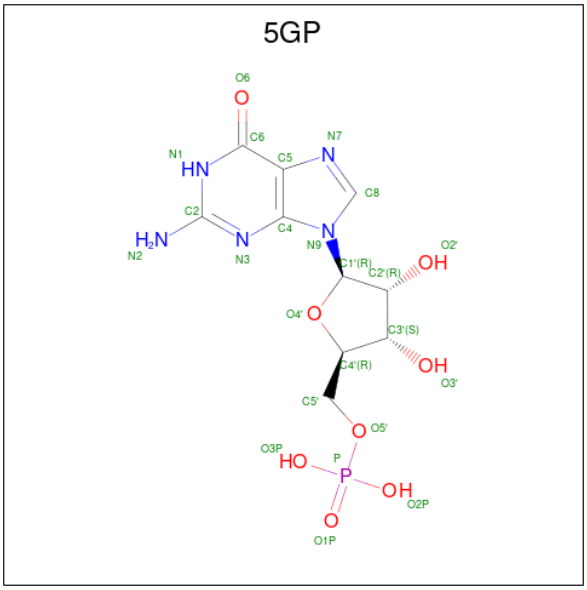
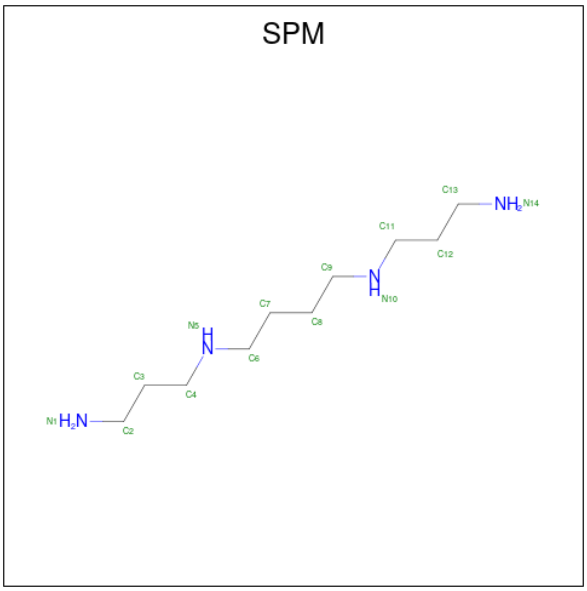
Mol	Chain	Residues	Atoms	AltConf
90	AX	1	Total Mg 1 1	0
90	Ag	1	Total Mg 1 1	0
90	Am	1	Total Mg 1 1	0
90	An	1	Total Mg 1 1	0
90	B3	1	Total Mg 1 1	0

- Molecule 91 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



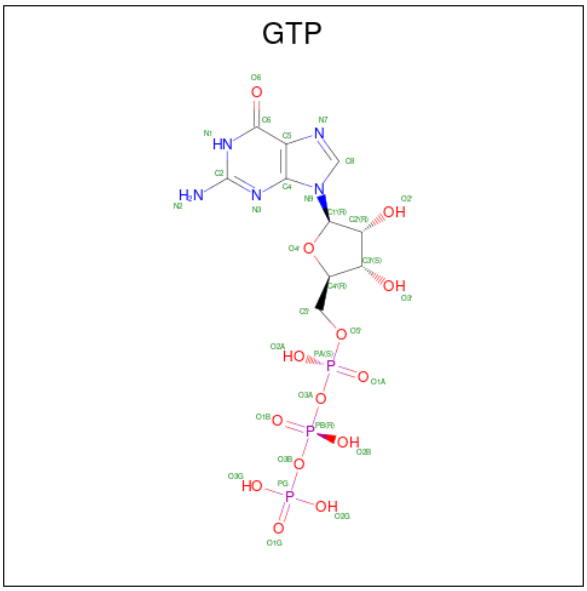
Mol	Chain	Residues	Atoms	AltConf
91	BA	1	Total C N O P 24 10 5 8 1	0
91	BA	1	Total C N O P 24 10 5 8 1	0

- Molecule 92 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
93	Ag	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 94 is water.

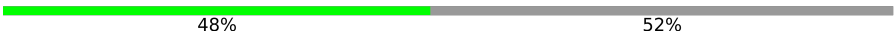
Mol	Chain	Residues	Atoms		AltConf
94	Ag	3	Total	O	0
			3	3	

3 Residue-property plots (i)

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

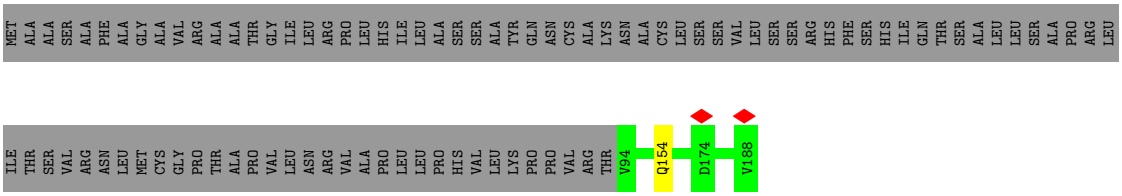
• Molecule 1: Mitochondrial ribosomal protein L34

Chain B7:



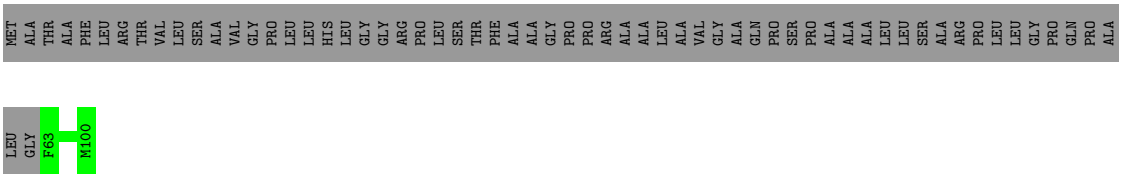
• Molecule 2: Mitochondrial ribosomal protein L35

Chain B8:



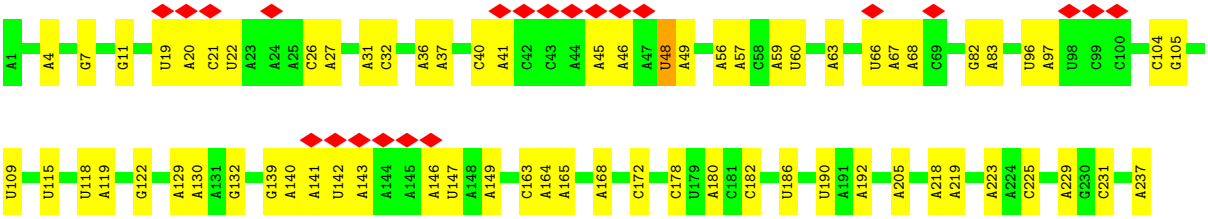
• Molecule 3: Ribosomal protein

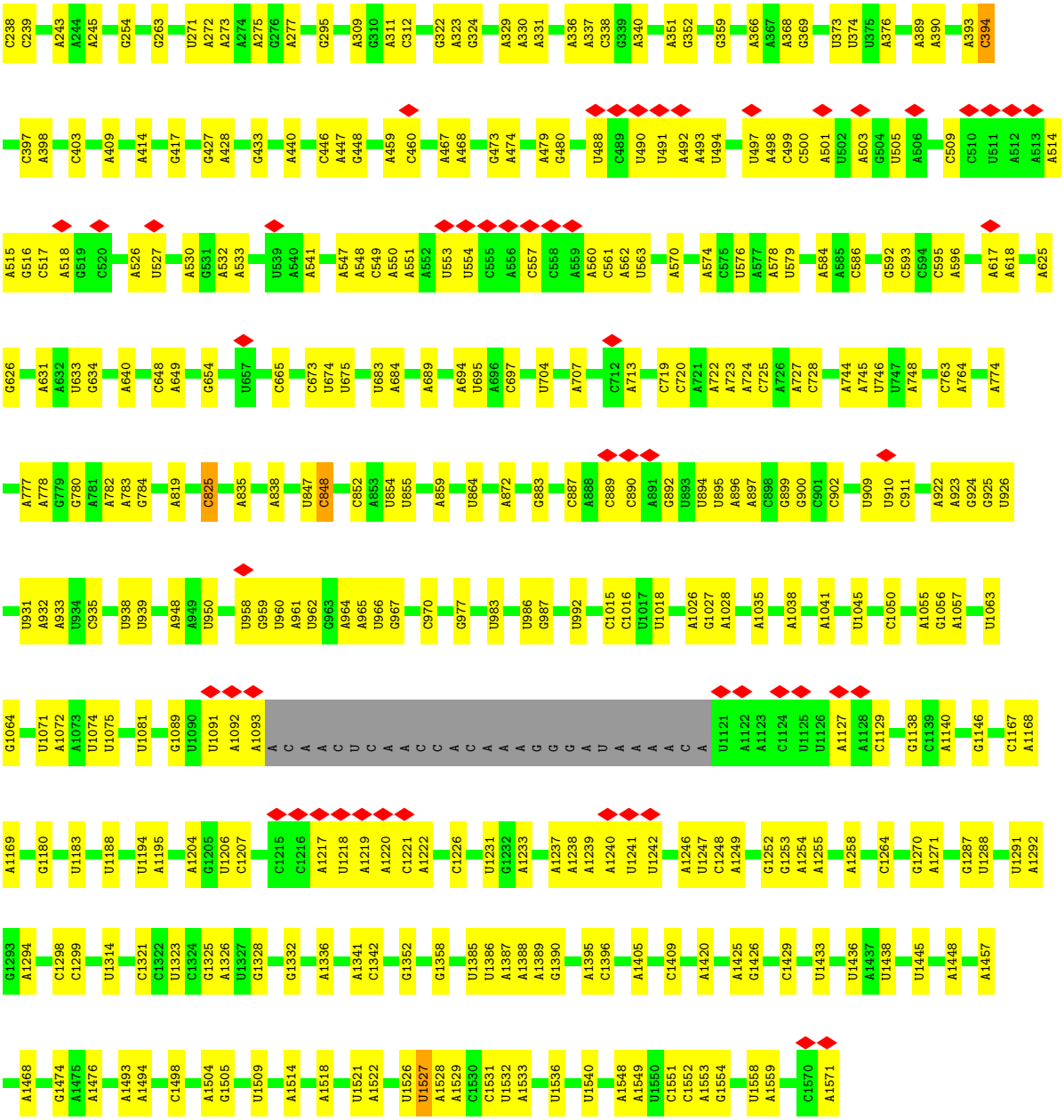
Chain B9:



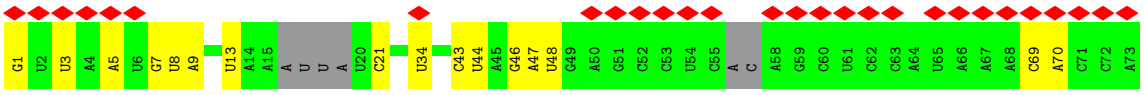
• Molecule 4: 16S rRNA

Chain BA:

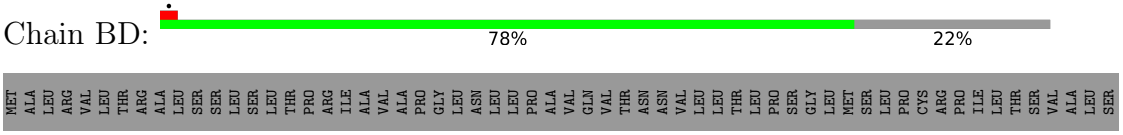


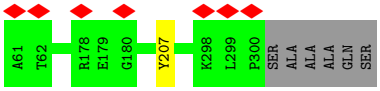


• Molecule 5: CP tRNAPhe



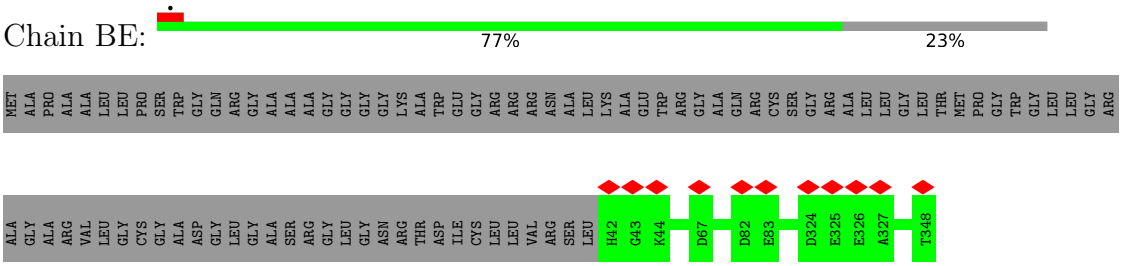
• Molecule 6: uL2m





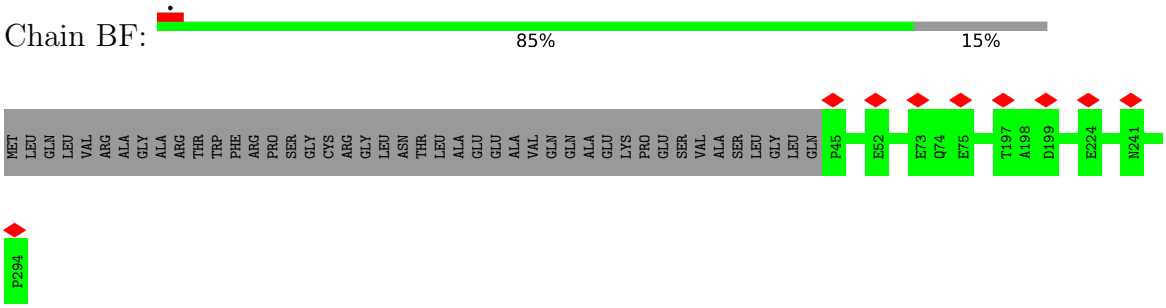
• Molecule 7: ICT1

Chain BE:



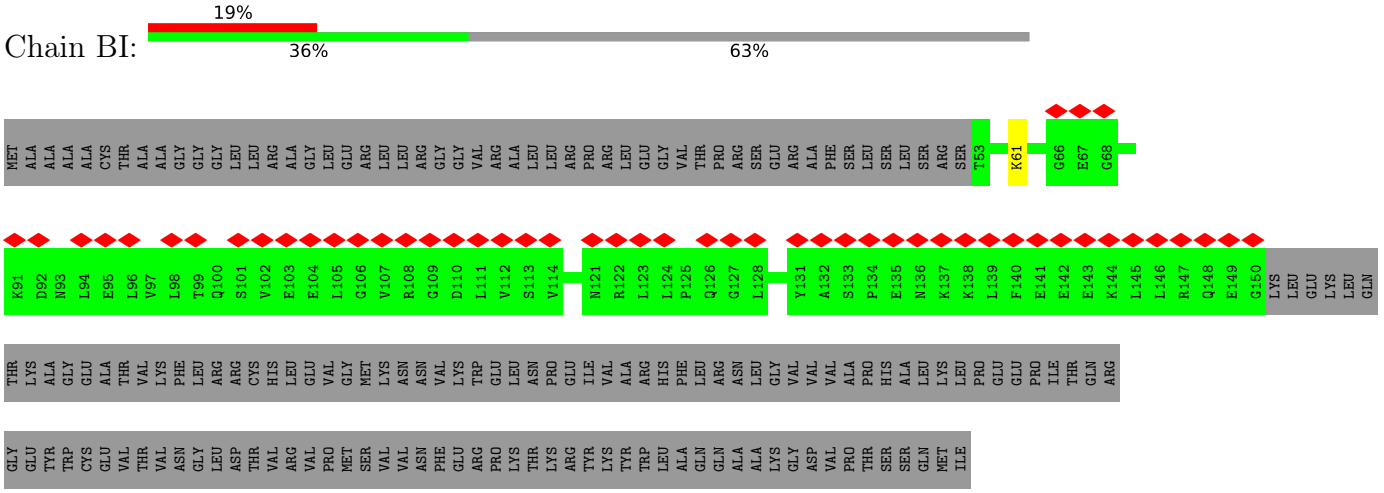
• Molecule 8: Mitochondrial ribosomal protein L4

Chain BF:



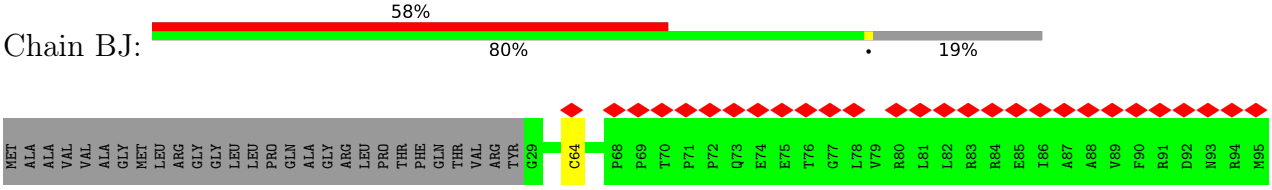
• Molecule 9: Mitochondrial ribosomal protein L9

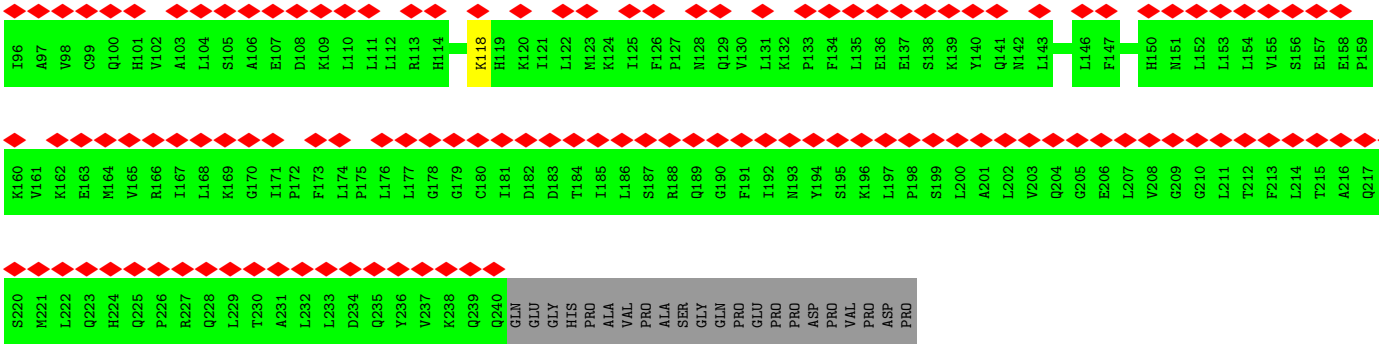
Chain BI:



• Molecule 10: Mitochondrial ribosomal protein L10

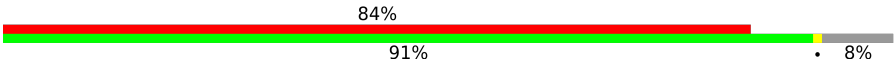
Chain BJ:

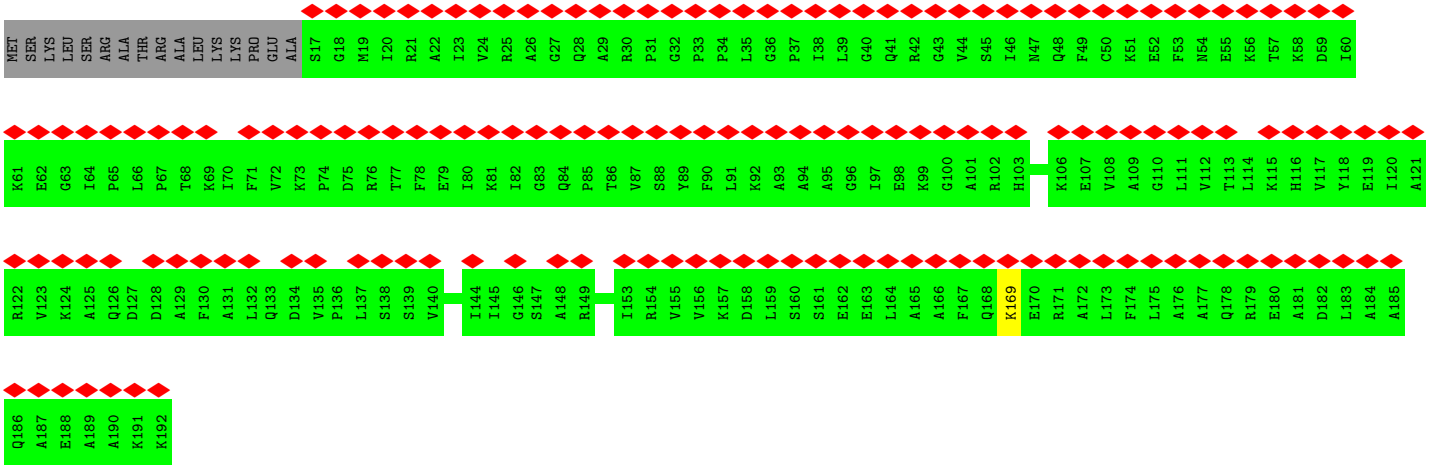




• Molecule 11: Mitochondrial ribosomal protein L11

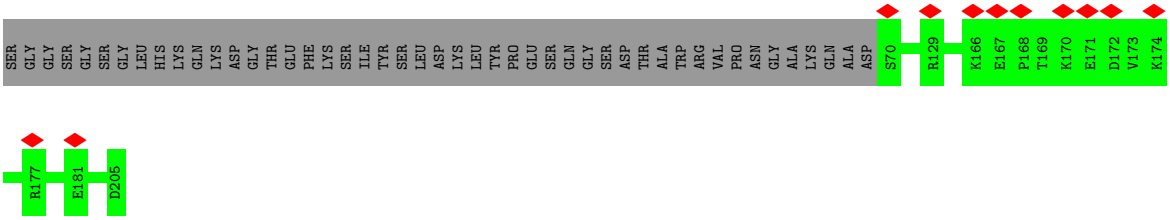
Chain BK:





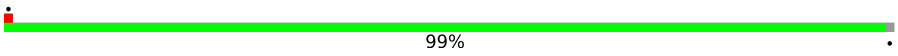
• Molecule 12: Peptidyl-tRNA hydrolase ICT1, mitochondrial

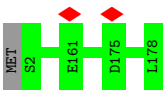
Chain BL:



• Molecule 13: uL13m

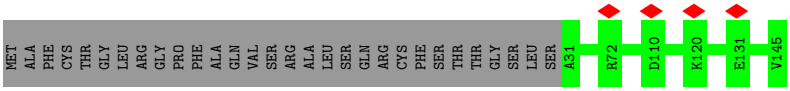
Chain BN:





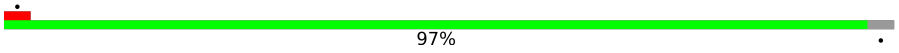
• Molecule 14: uL14m

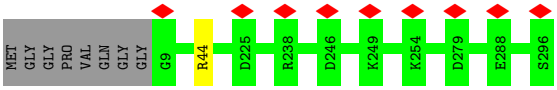
Chain BO:



• Molecule 15: uL15m

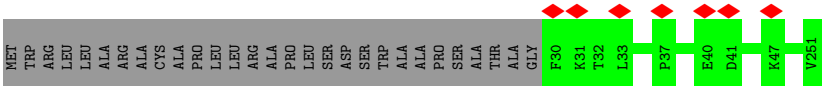
Chain BP:





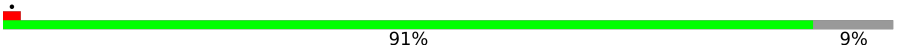
• Molecule 16: uL16m

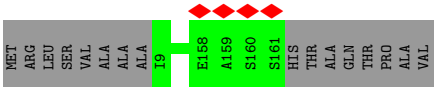
Chain BQ:



• Molecule 17: bL17m

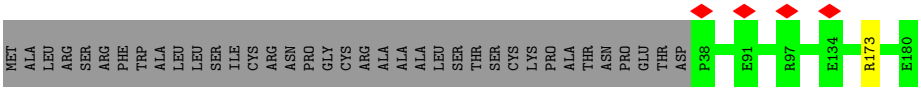
Chain BR:





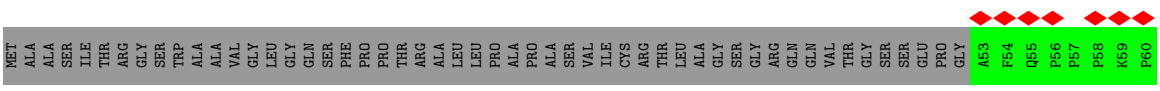
• Molecule 18: Mitochondrial ribosomal protein L18

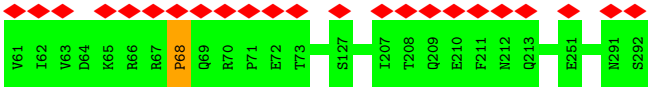
Chain BS:



• Molecule 19: Mitochondrial ribosomal protein L19

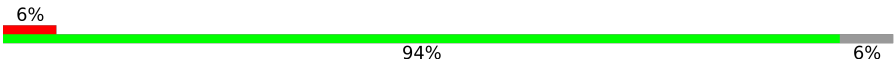
Chain BT:

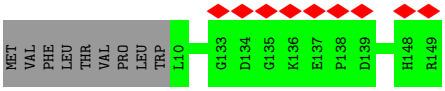




• Molecule 20: Mitochondrial ribosomal protein L20

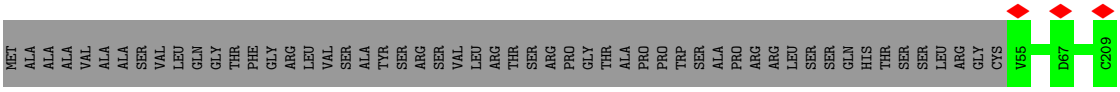
Chain BU:





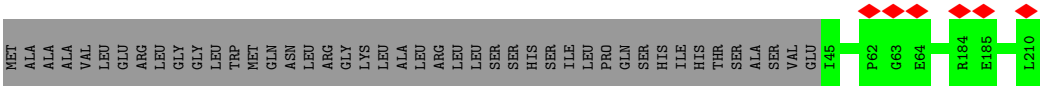
• Molecule 21: Mitochondrial ribosomal protein L21

Chain BV:



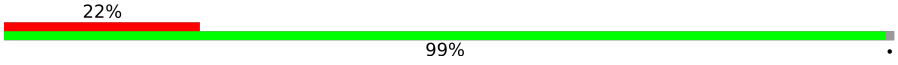
• Molecule 22: uL22m

Chain BW:



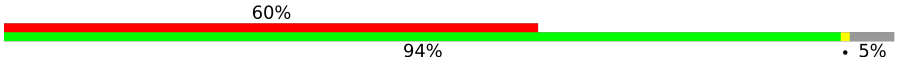
• Molecule 23: uL23m

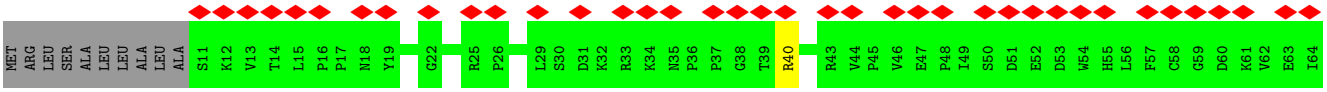
Chain BX:

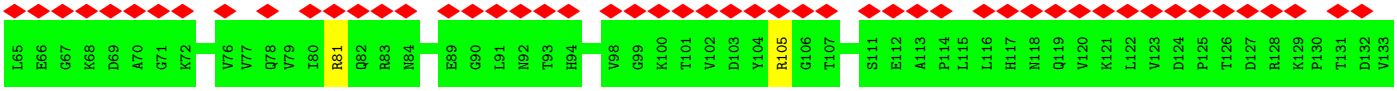


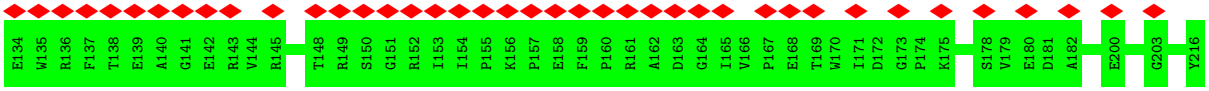
• Molecule 24: uL24m

Chain BY:



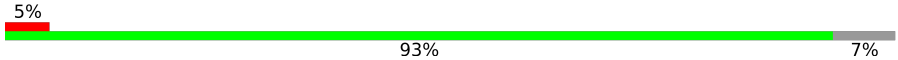


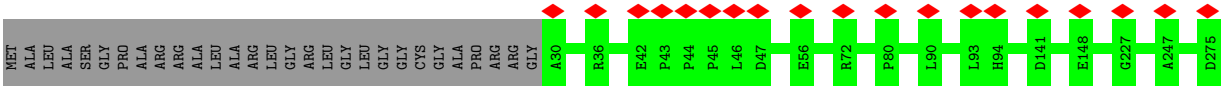


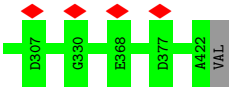


• Molecule 25: Mitochondrial ribosomal protein L37

Chain Ba:

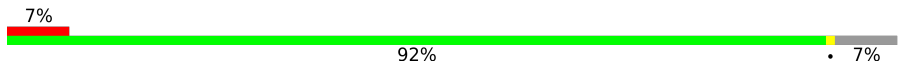


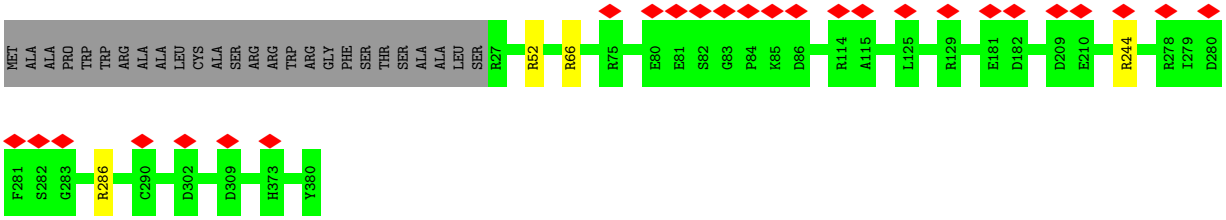




• Molecule 26: Mitochondrial ribosomal protein L38

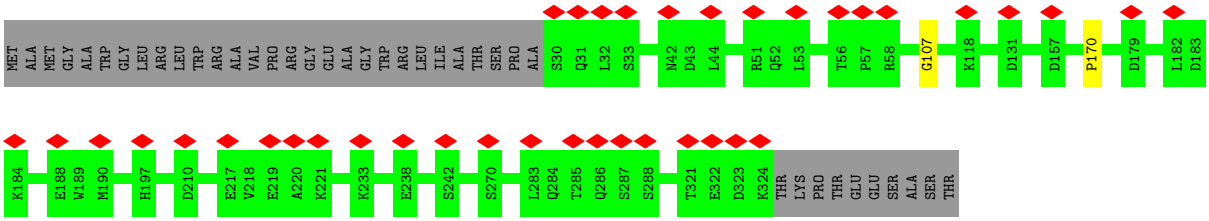
Chain Bb:





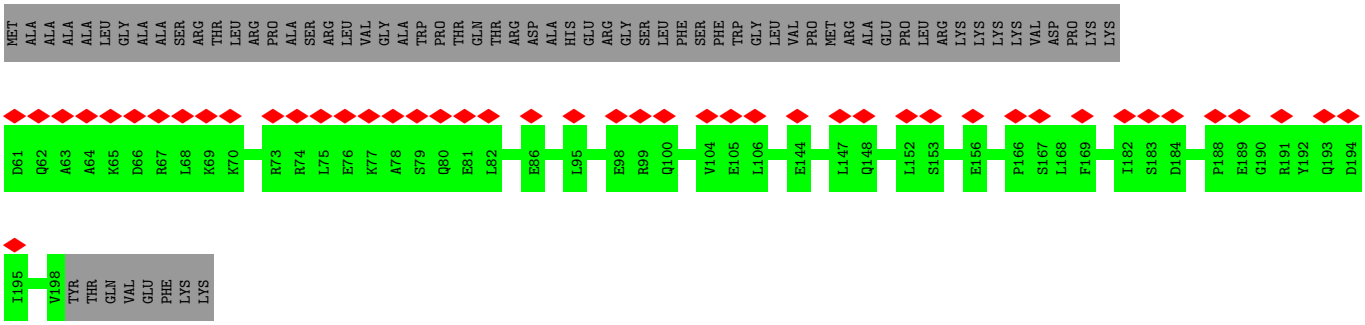
• Molecule 27: Mitochondrial ribosomal protein L39

Chain Bc:



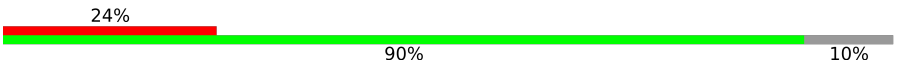
• Molecule 28: Mitochondrial ribosomal protein L40

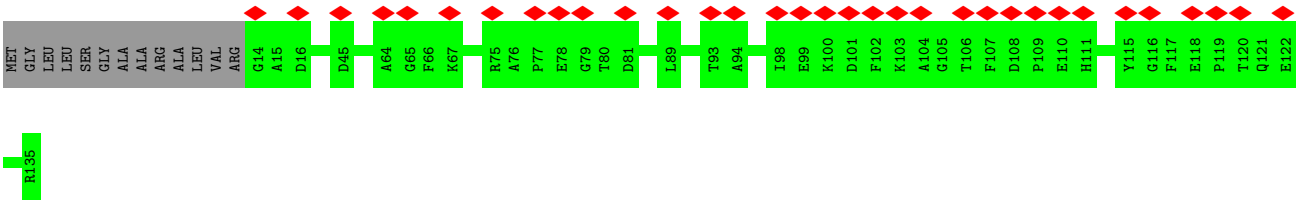
Chain Bd:



• Molecule 29: Mitochondrial ribosomal protein L41

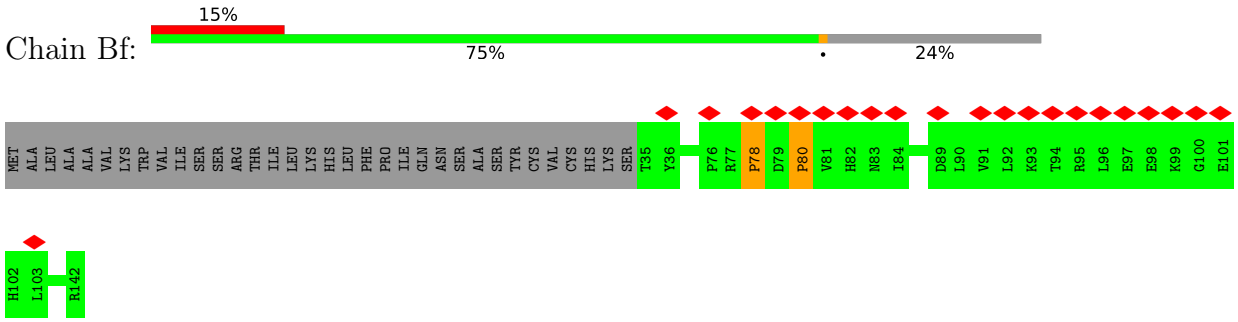
Chain Be:





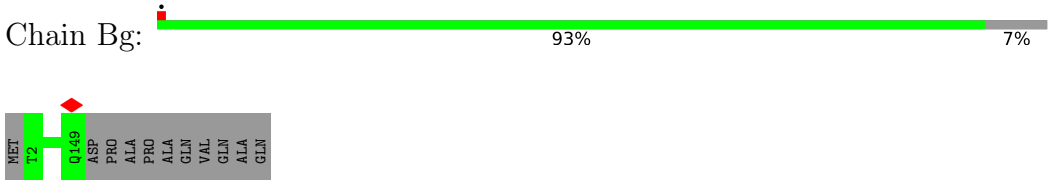
• Molecule 30: mL42

Chain Bf:



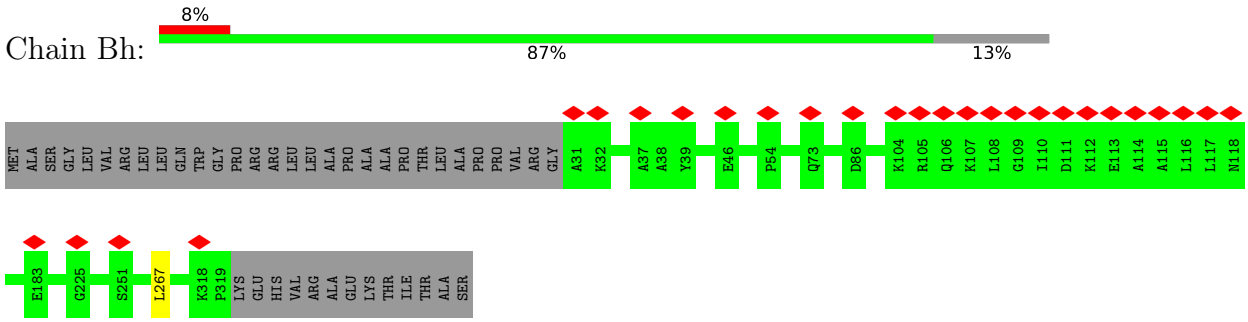
• Molecule 31: Mitochondrial ribosomal protein L43

Chain Bg:



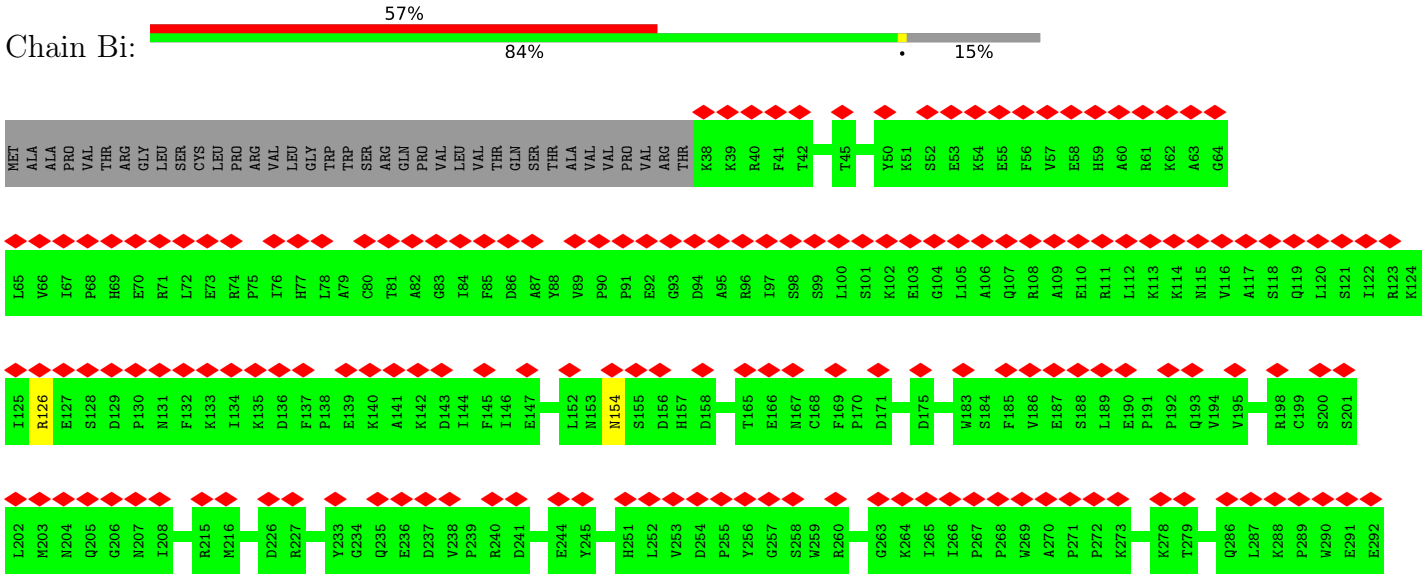
• Molecule 32: mL44

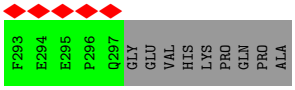
Chain Bh:



• Molecule 33: Mitochondrial ribosomal protein L45

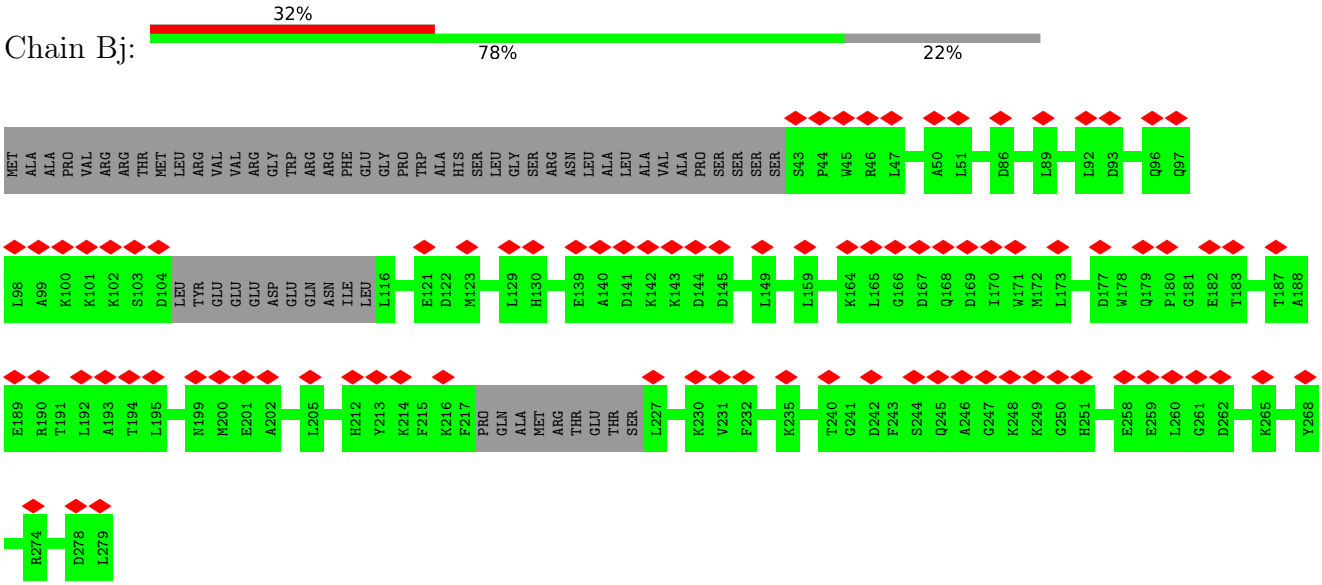
Chain Bi:





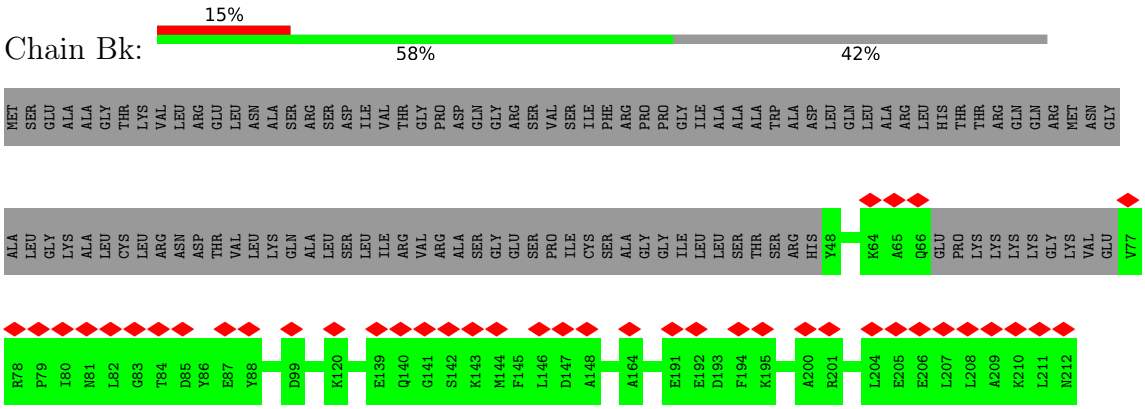
• Molecule 34: Mitochondrial ribosomal protein L46

Chain Bj:



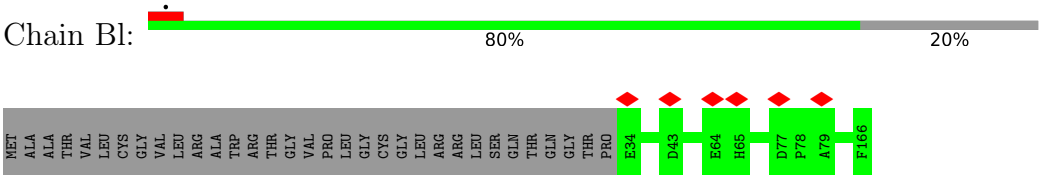
• Molecule 35: 39S ribosomal protein L48, mitochondrial

Chain Bk:



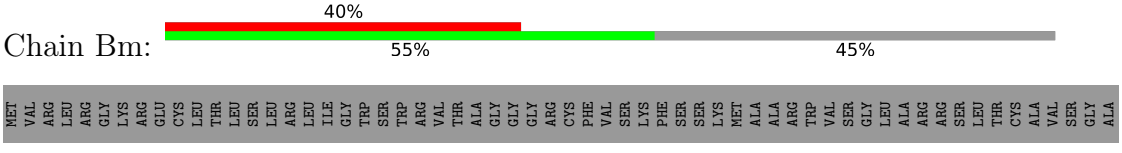
• Molecule 36: Mrpl34

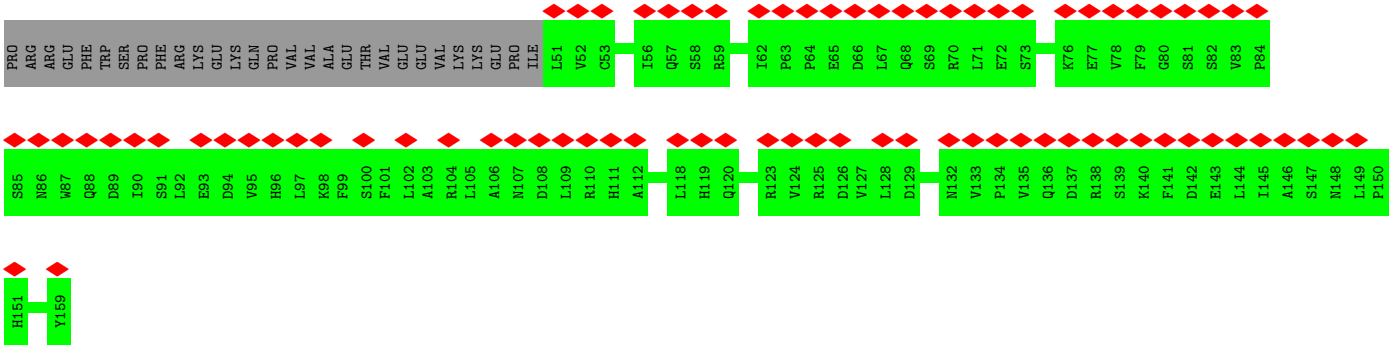
Chain Bl:



• Molecule 37: Mitochondrial ribosomal protein L50

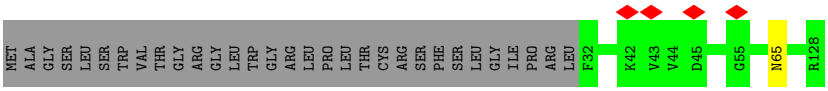
Chain Bm:





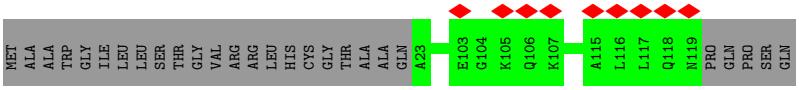
• Molecule 38: Mitochondrial ribosomal protein L51

Chain Bn:



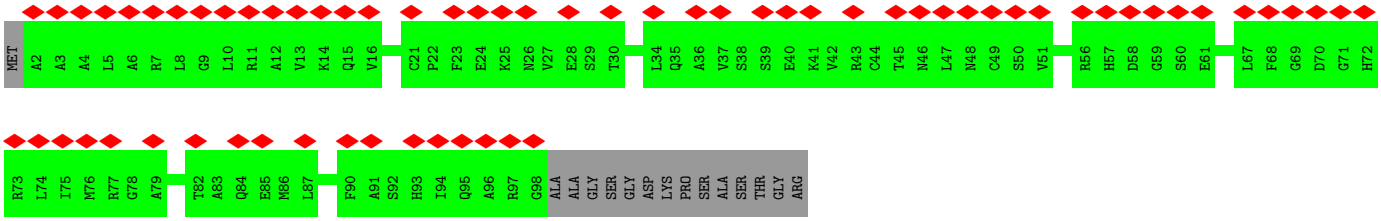
• Molecule 39: mL52

Chain Bo:



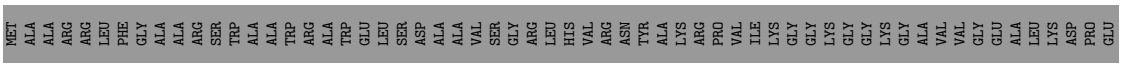
• Molecule 40: mL53

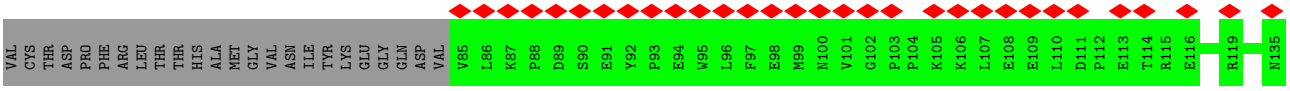
Chain Bp:



• Molecule 41: mL54

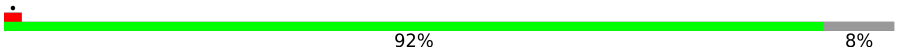
Chain Bq:

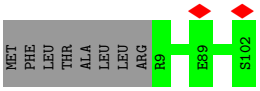




• Molecule 42: Mitochondrial ribosomal protein L57

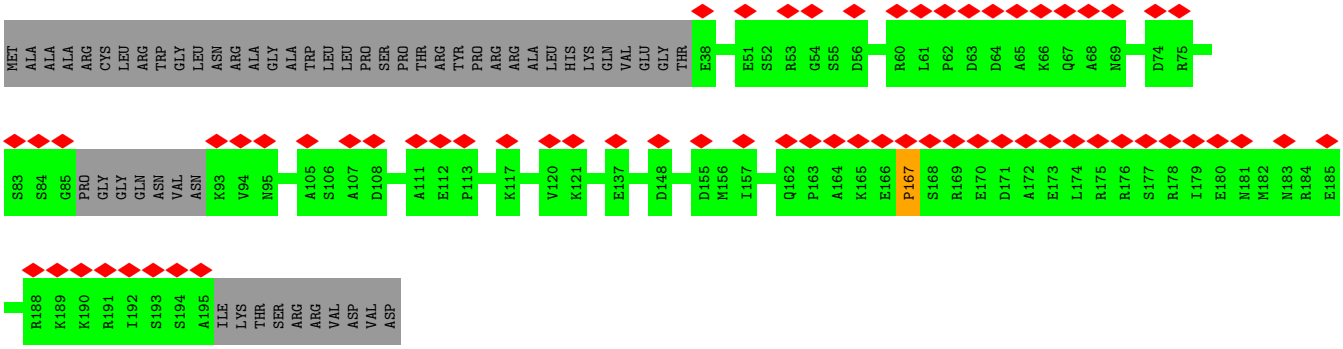
Chain Bt:





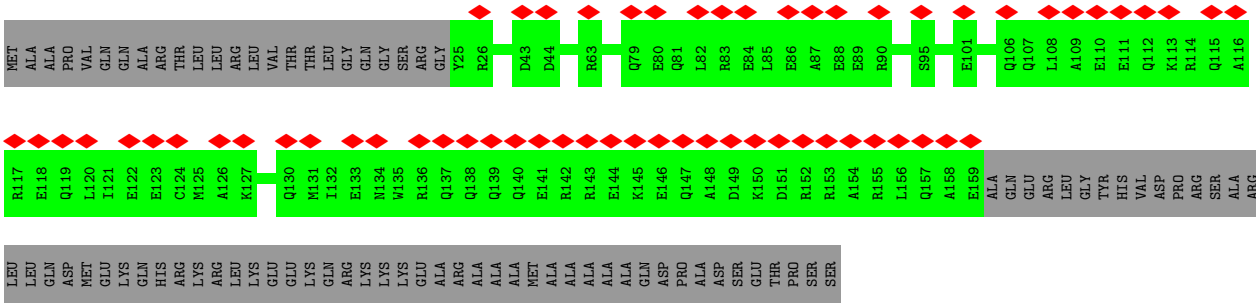
• Molecule 43: mL62 (ICT1)

Chain Bu:



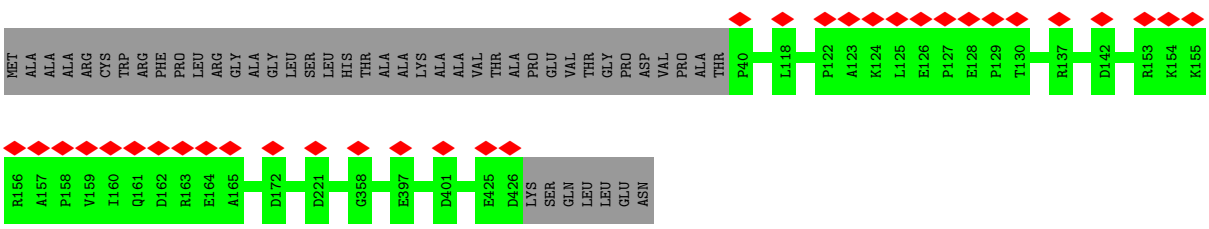
• Molecule 44: mL64

Chain Bv:



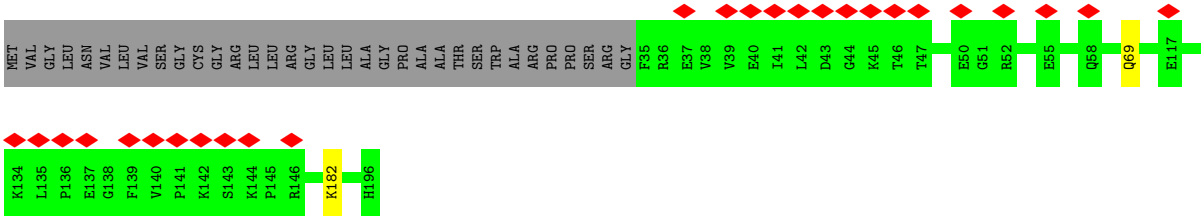
• Molecule 45: 39S ribosomal protein S30, mitochondrial

Chain Bw:



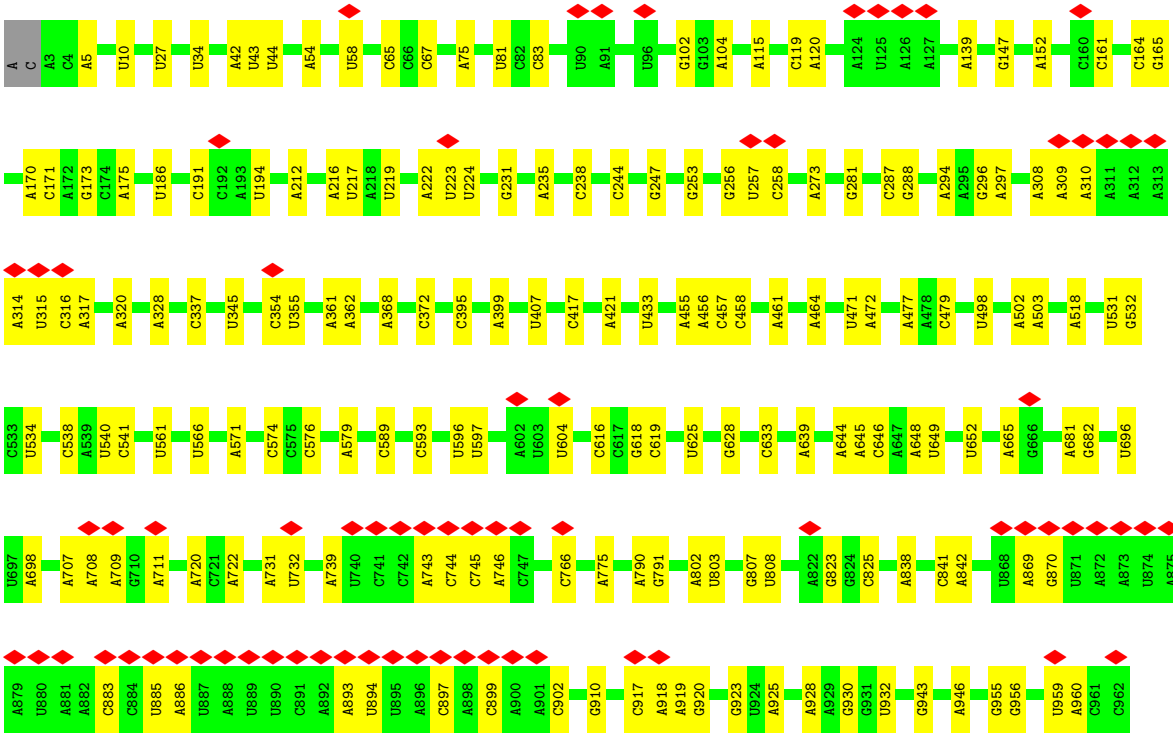
• Molecule 46: Mitochondrial ribosomal protein S18A

Chain Bx:



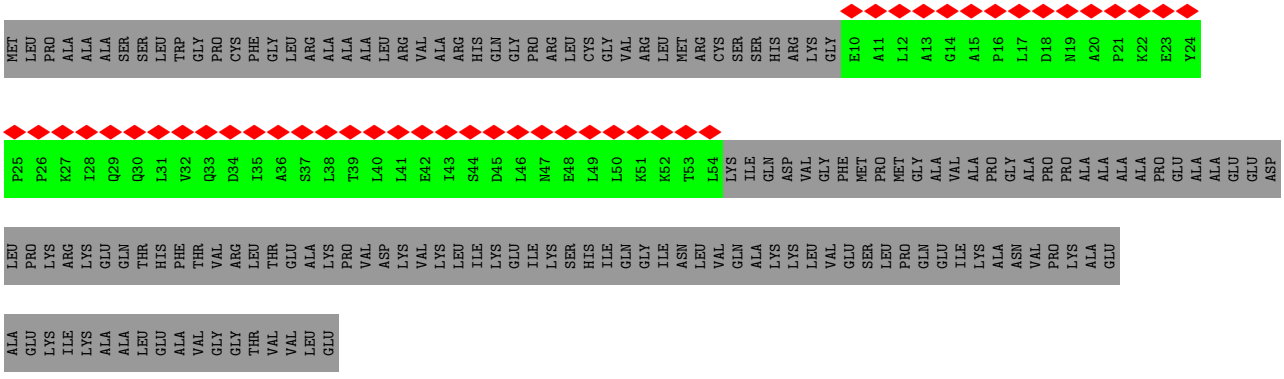
• Molecule 47: 12S rRNA

Chain AA:



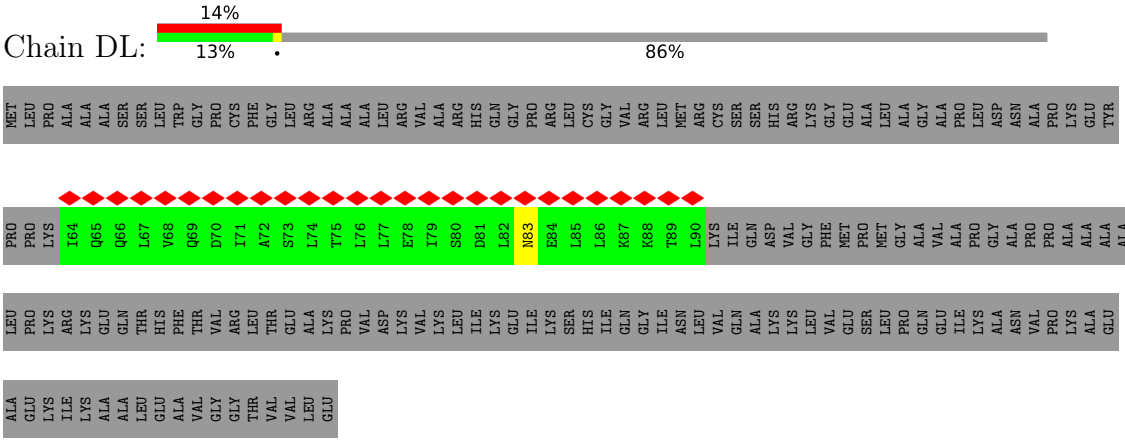
• Molecule 48: Mitochondrial ribosomal protein L12

Chain CL:



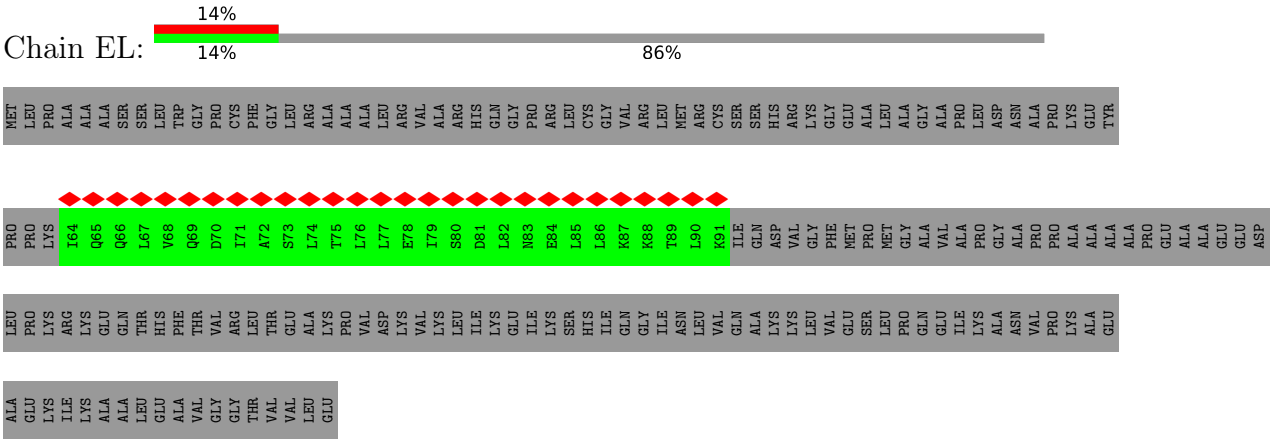
• Molecule 48: Mitochondrial ribosomal protein L12

Chain DL:



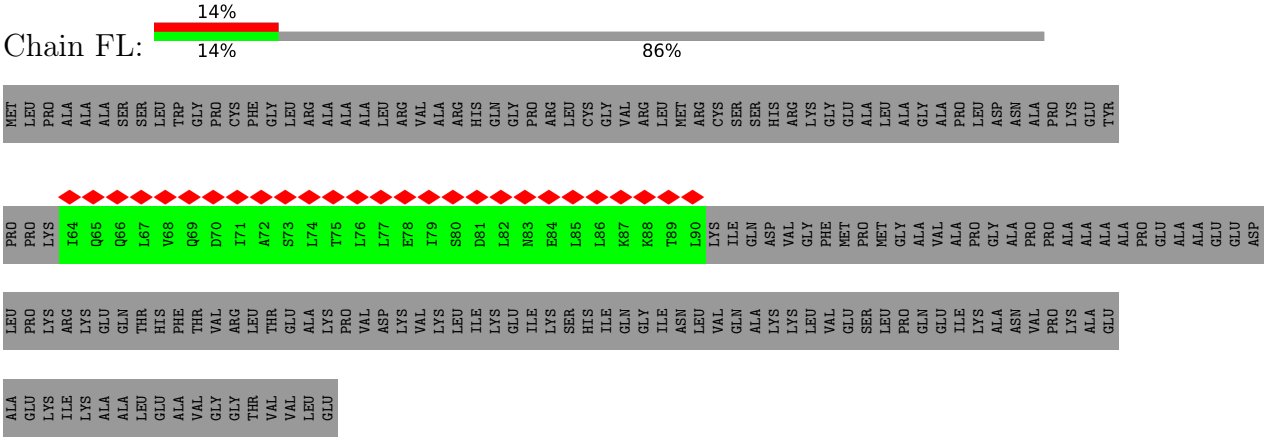
• Molecule 48: Mitochondrial ribosomal protein L12

Chain EL:



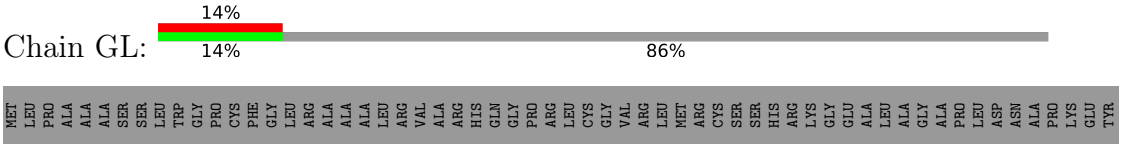
• Molecule 48: Mitochondrial ribosomal protein L12

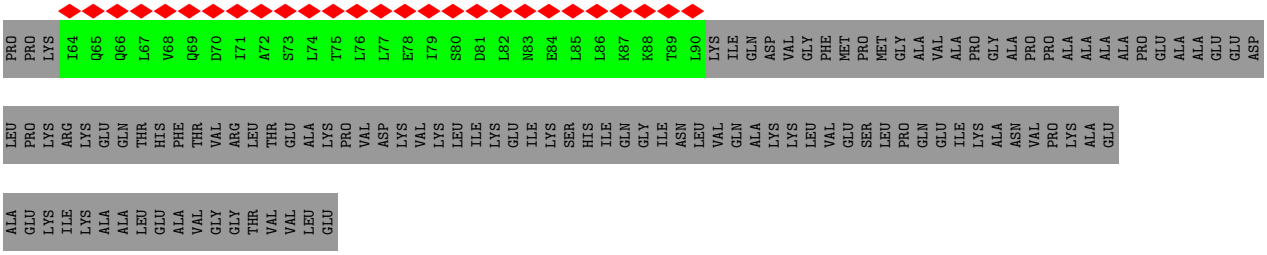
Chain FL:



• Molecule 48: Mitochondrial ribosomal protein L12

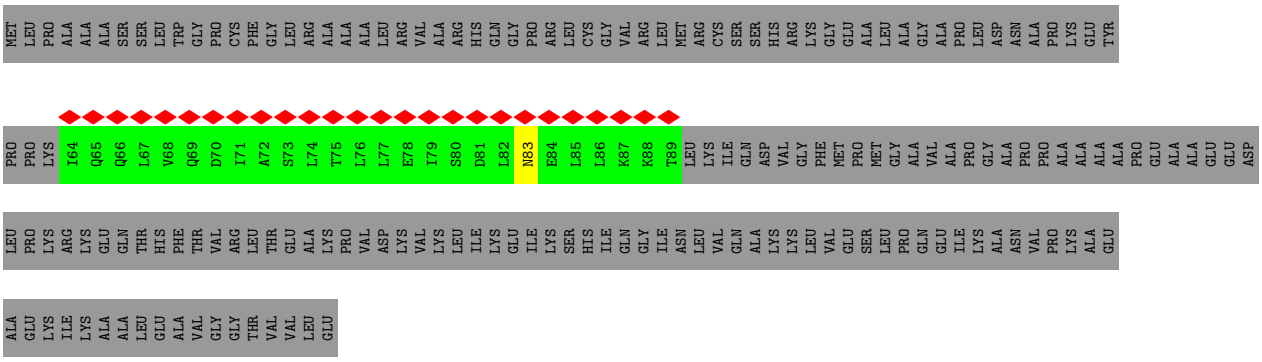
Chain GL:





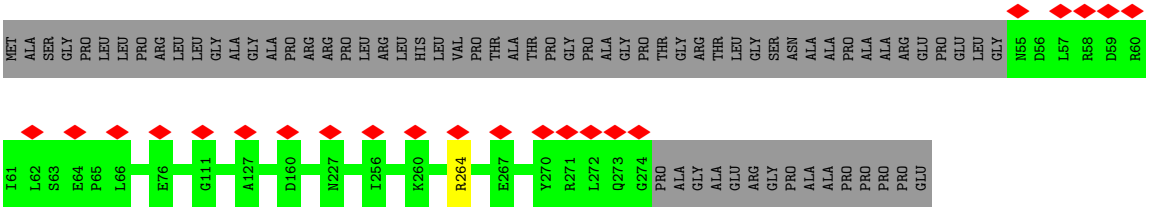
• Molecule 48: Mitochondrial ribosomal protein L12

Chain HL:



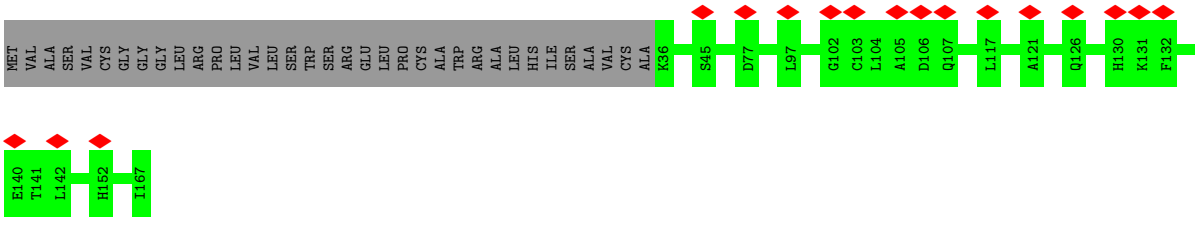
• Molecule 49: Mitochondrial ribosomal protein S2

Chain AB:



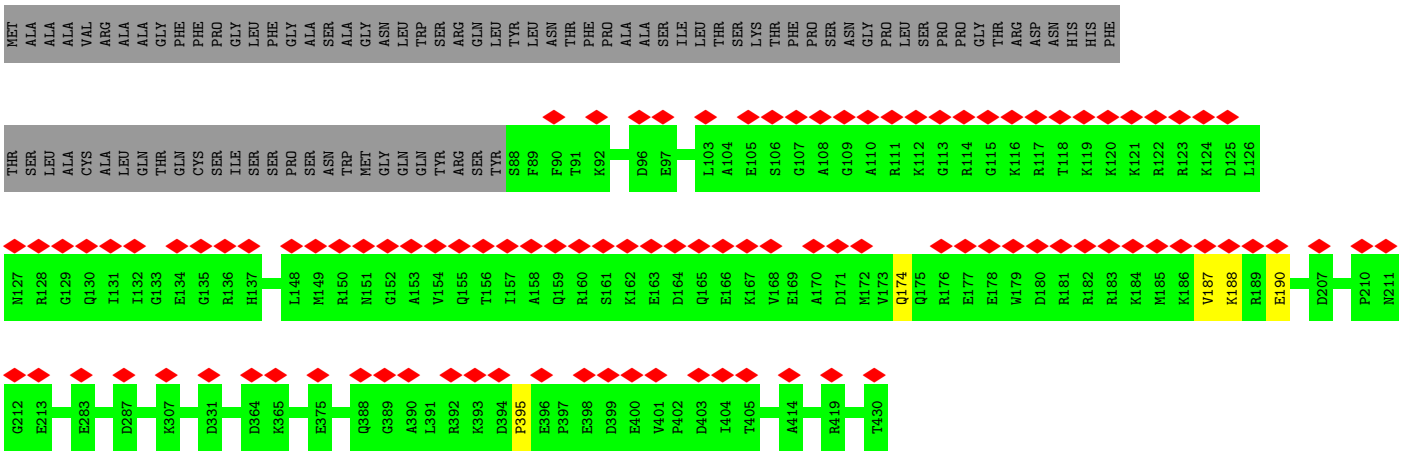
• Molecule 50: Mitochondrial ribosomal protein S24

Chain AC:

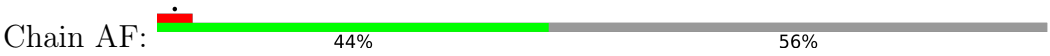


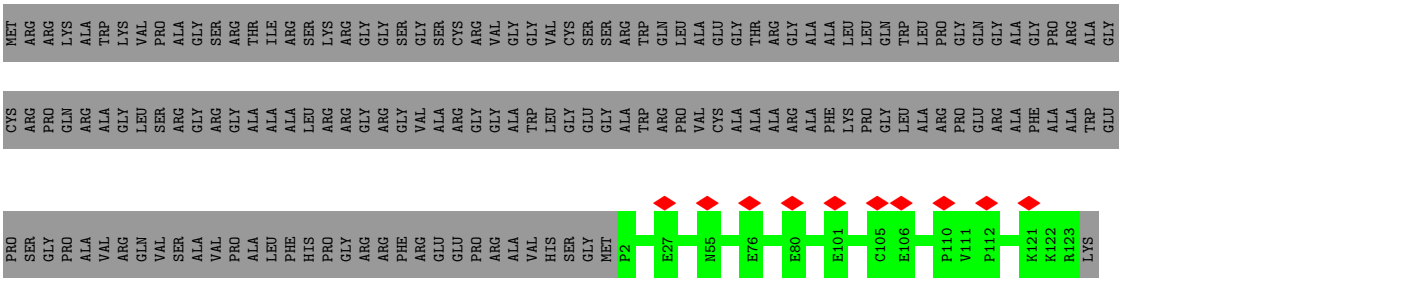
• Molecule 51: Mitochondrial ribosomal protein S5

Chain AE:

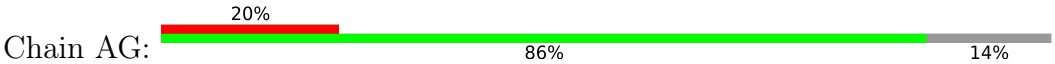


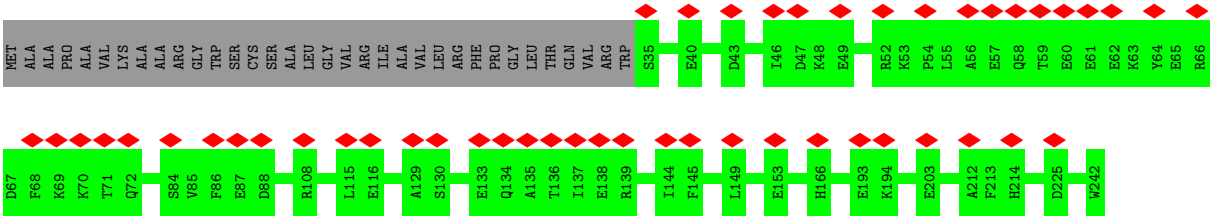
• Molecule 52: bS6m



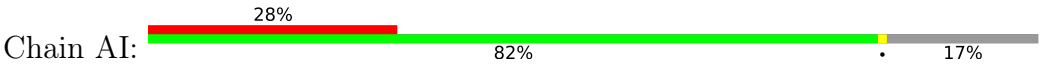


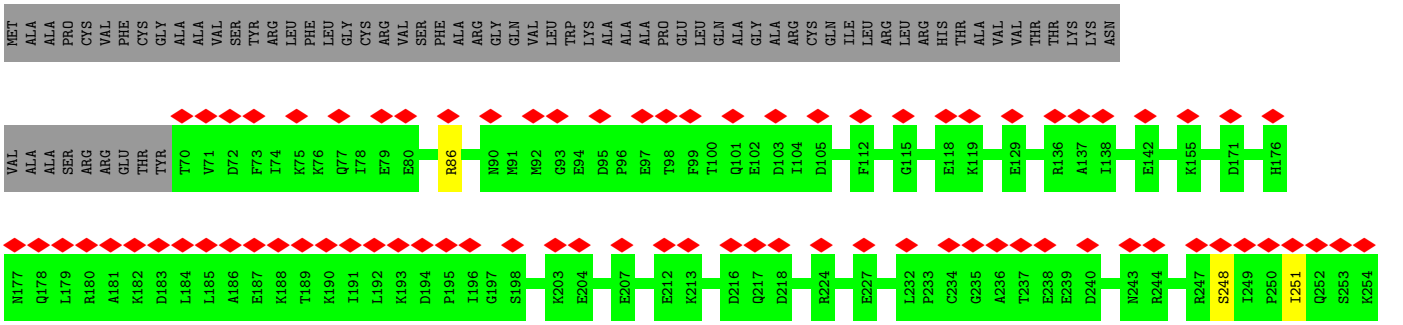
• Molecule 53: Mitochondrial ribosomal protein S7

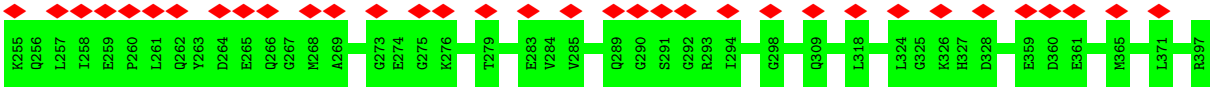




• Molecule 54: uS9m

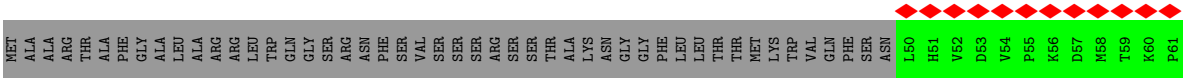


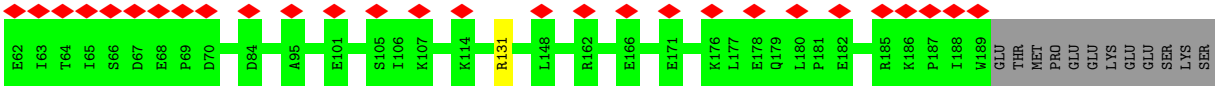




• Molecule 55: Mitochondrial ribosomal protein S10

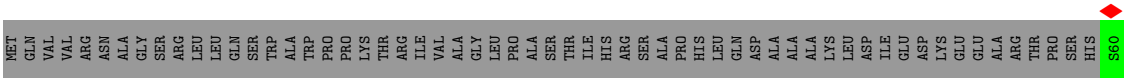
Chain AJ:

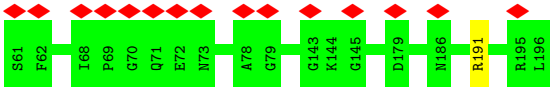




• Molecule 56: uS11m

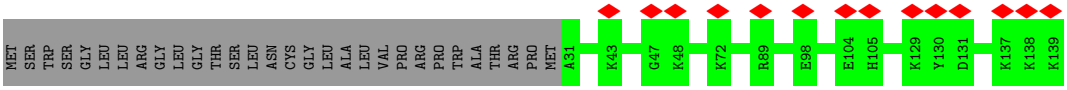
Chain AK:





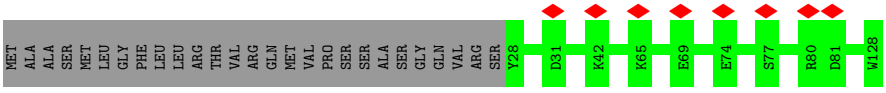
• Molecule 57: Mitochondrial ribosomal protein S12

Chain AL:



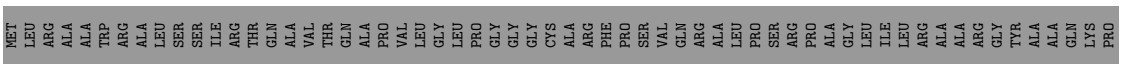
• Molecule 58: Mitochondrial ribosomal protein S14

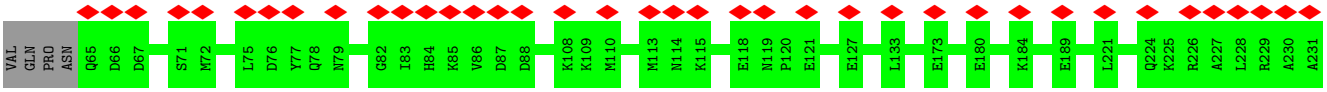
Chain AN:

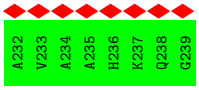


• Molecule 59: uS15m

Chain AO:

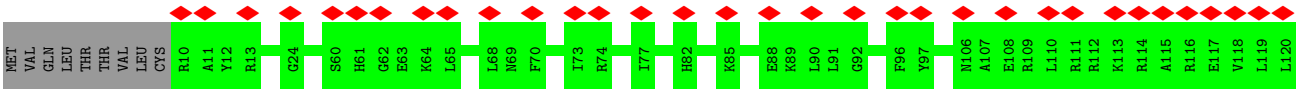


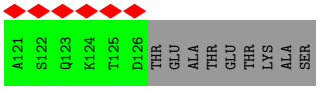




• Molecule 60: 28S ribosomal protein S16, mitochondrial

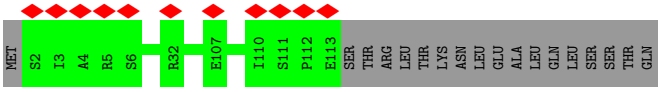
Chain AP:





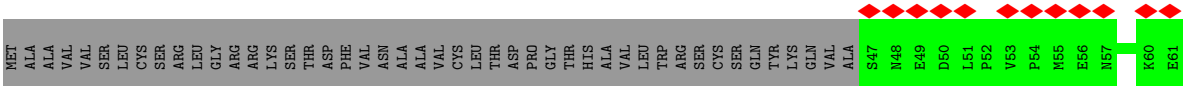
• Molecule 61: uS17m

Chain AQ:



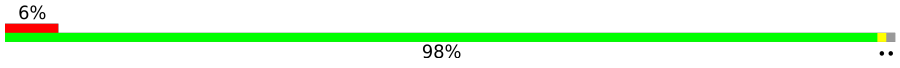
• Molecule 62: Mitochondrial ribosomal protein S18C

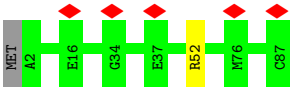
Chain AR:



• Molecule 63: bS21m

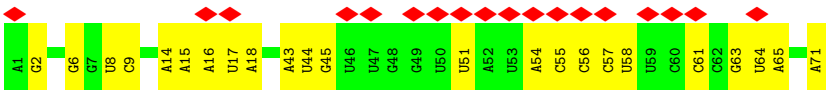
Chain AU:





• Molecule 64: fMet-tRNAMet (P site)

Chain AV:

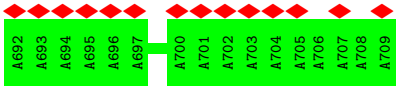


• Molecule 65: mRNA

Chain AX:

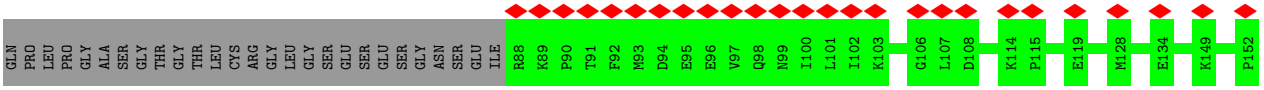
• Molecule 66: unknown

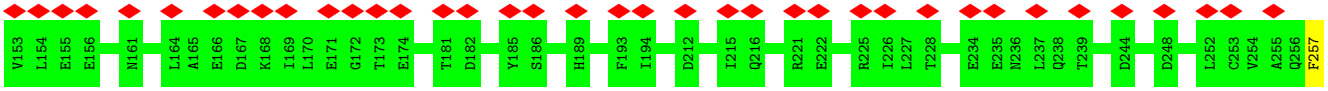
Chain AZ:

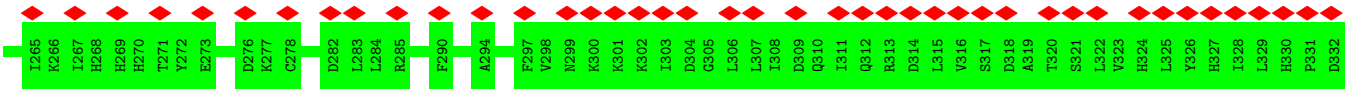


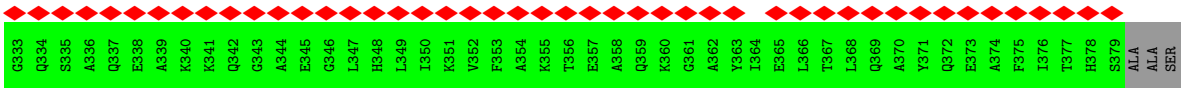
• Molecule 67: Mitochondrial ribosomal protein S22

Chain Aa:



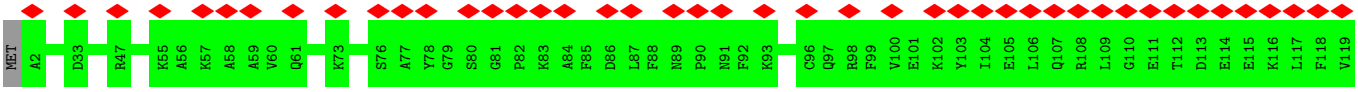


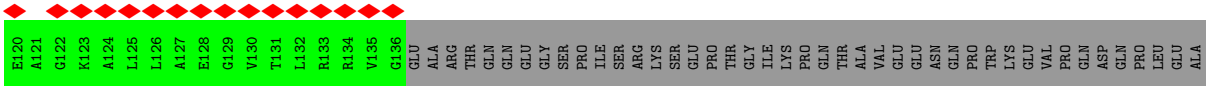


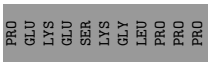


• Molecule 68: mS23

Chain Ab:

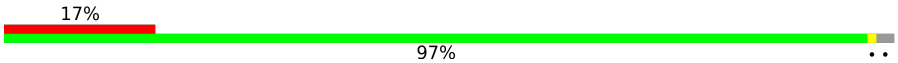


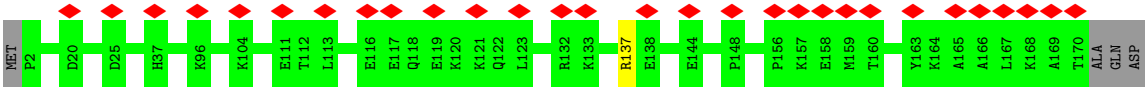




• Molecule 69: Mitochondrial ribosomal protein S25

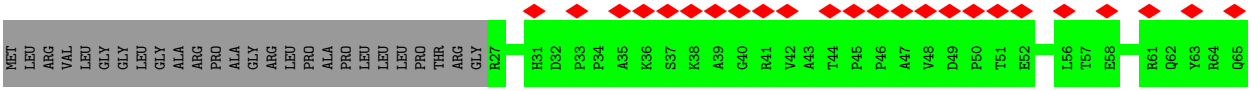
Chain Ac:

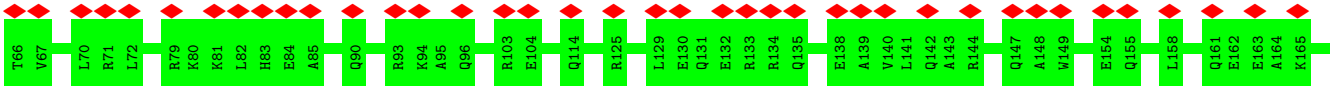


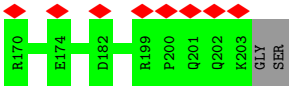


• Molecule 70: Mitochondrial ribosomal protein S26

Chain Ad:

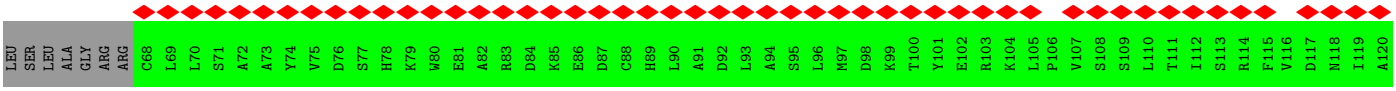


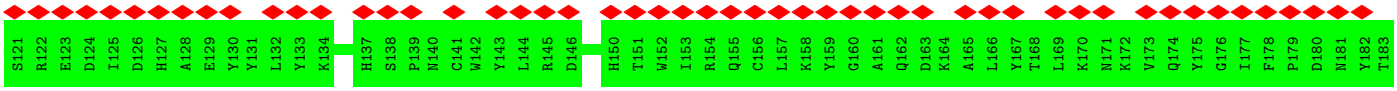


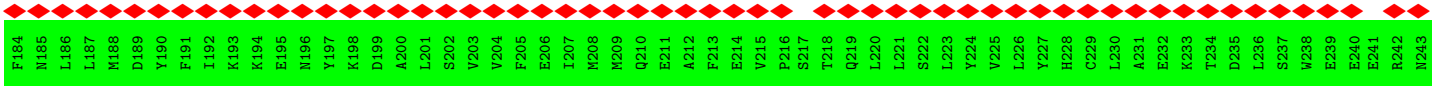


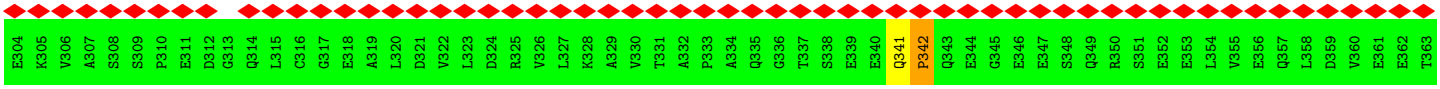
• Molecule 71: Mitochondrial ribosomal protein S27

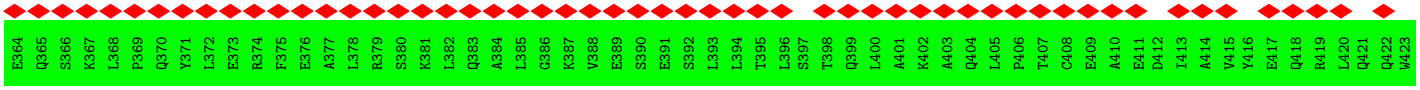
Chain Ae:

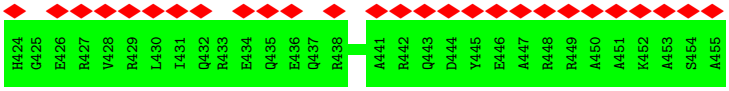






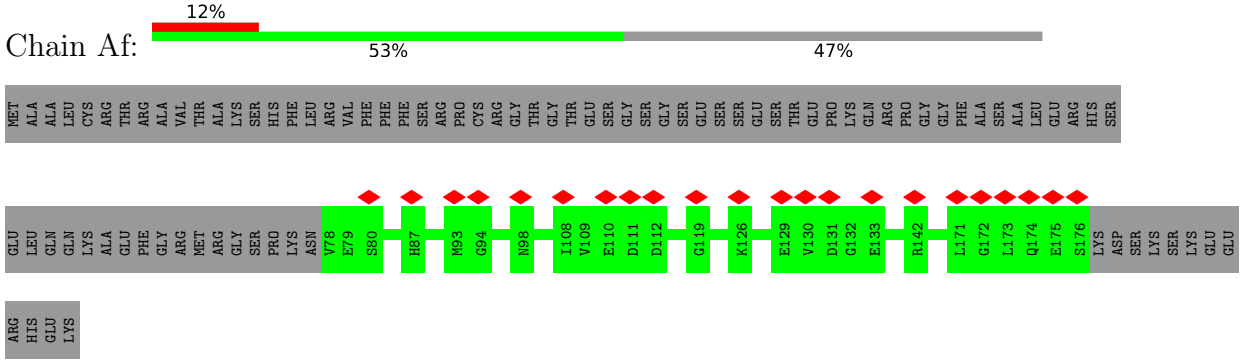






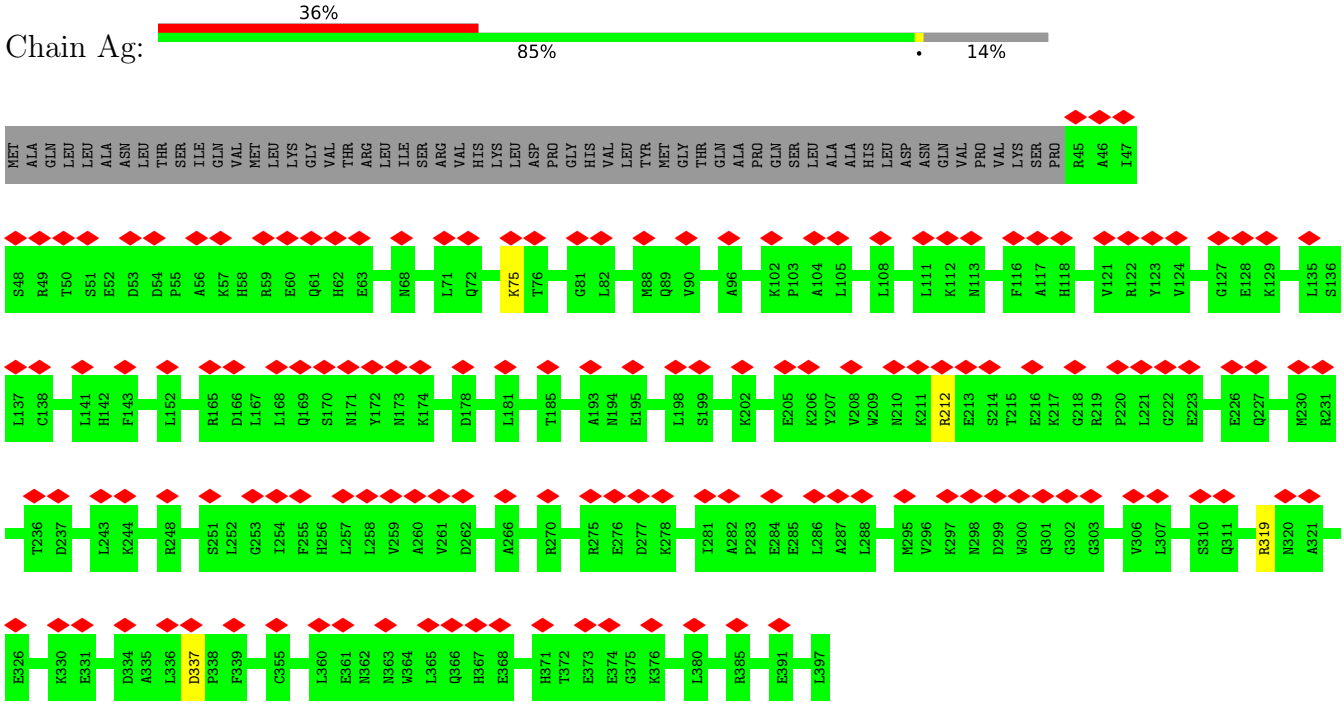
• Molecule 72: Mitoribosomal protein ms28, mrps28

Chain Af:



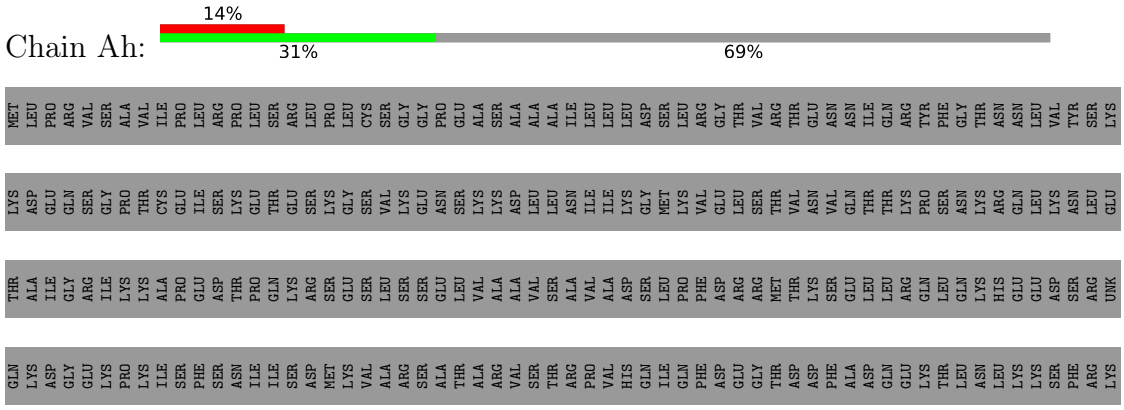
• Molecule 73: Death associated protein 3

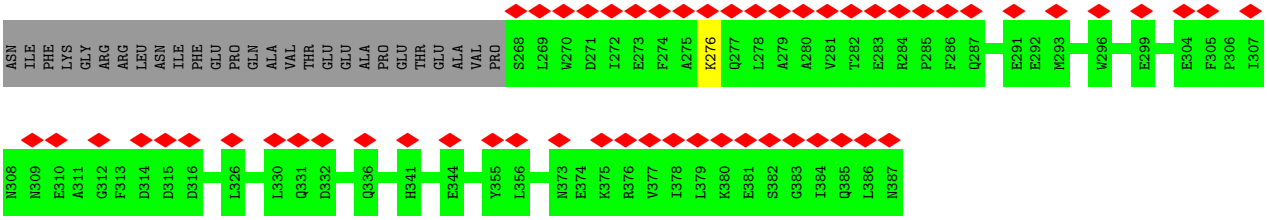
Chain Ag:



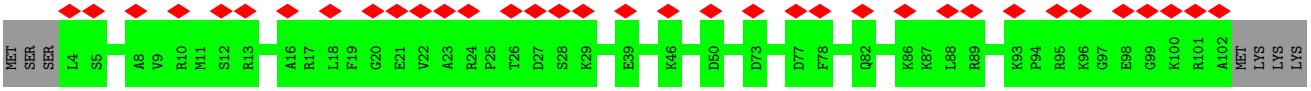
• Molecule 74: Mitochondrial ribosomal protein S31

Chain Ah:

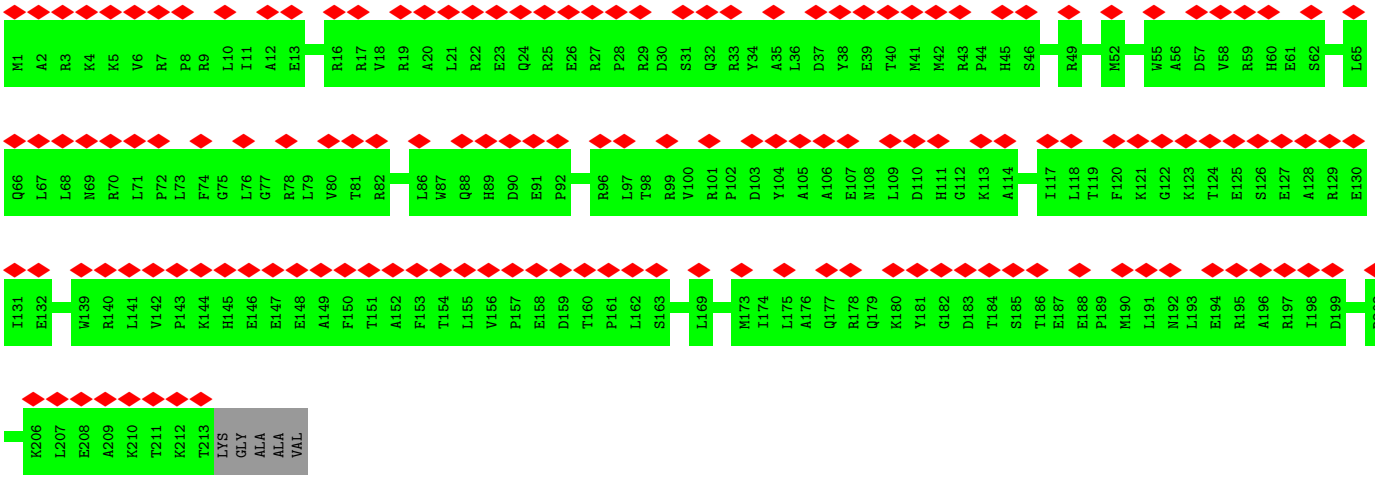




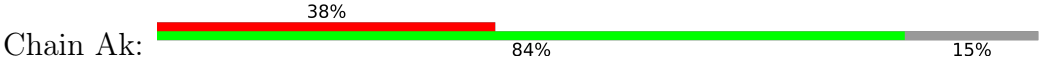
• Molecule 75: mS33

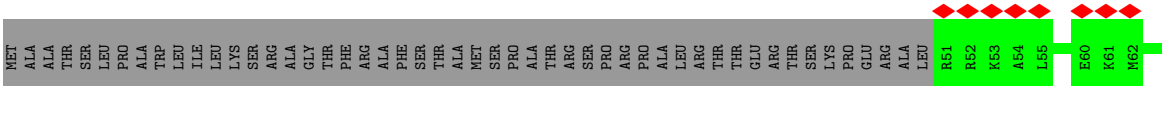


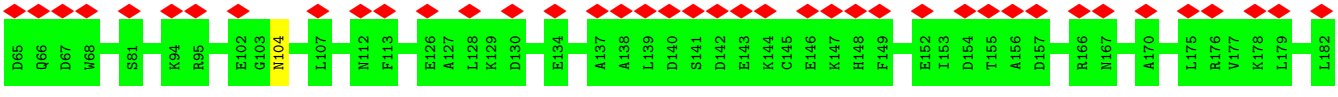
• Molecule 76: mS34

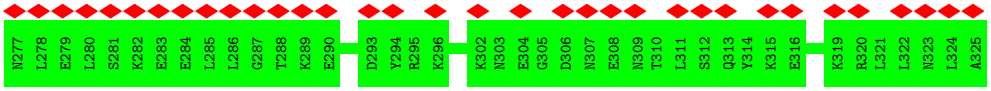


• Molecule 77: Mitochondrial ribosomal protein S35



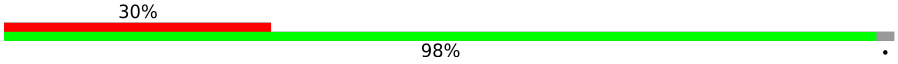


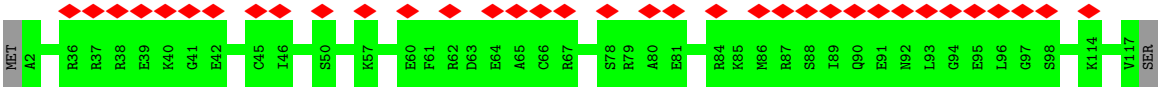




• Molecule 78: mS37

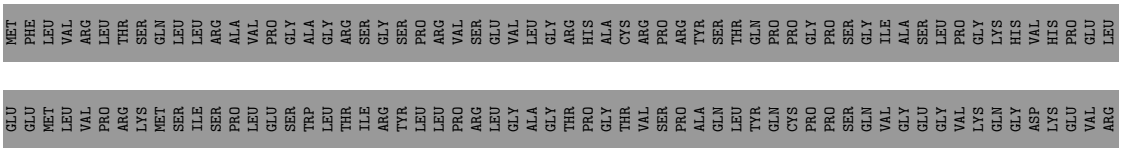
Chain Am:





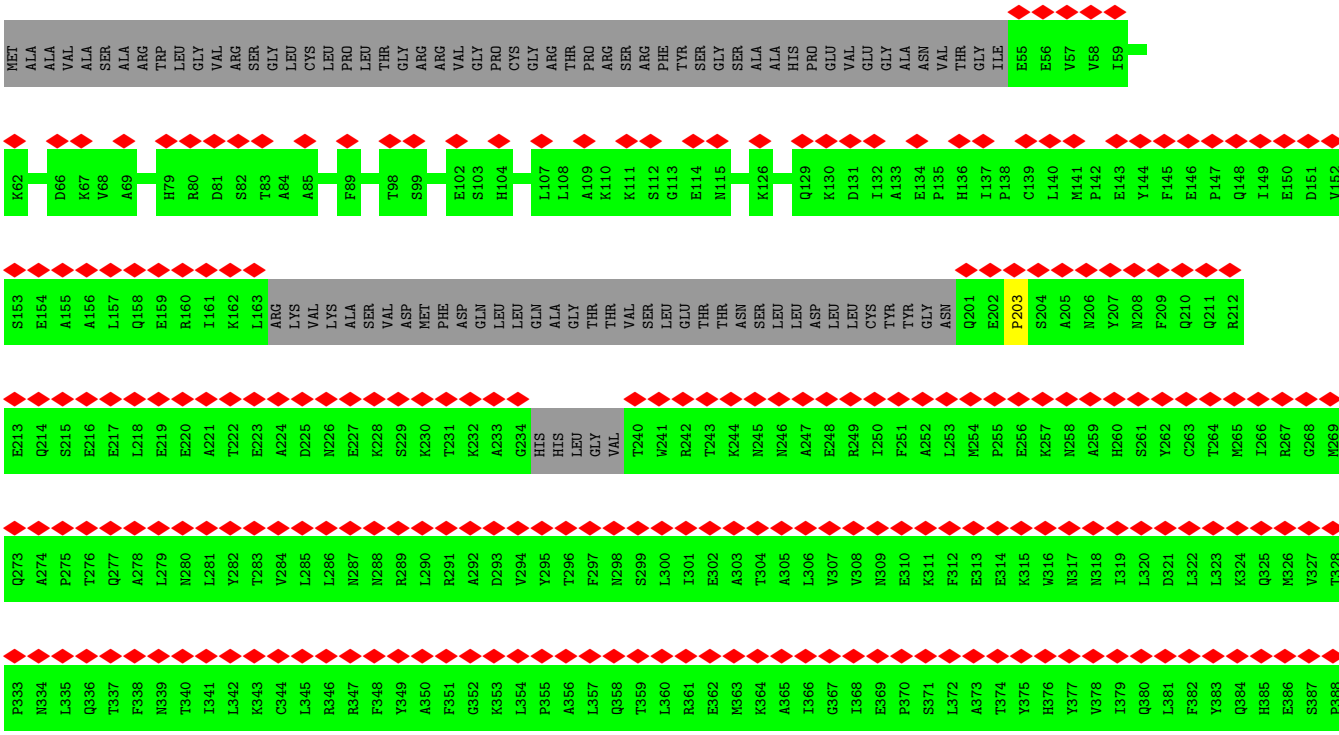
• Molecule 79: Aurora kinase A interacting protein 1

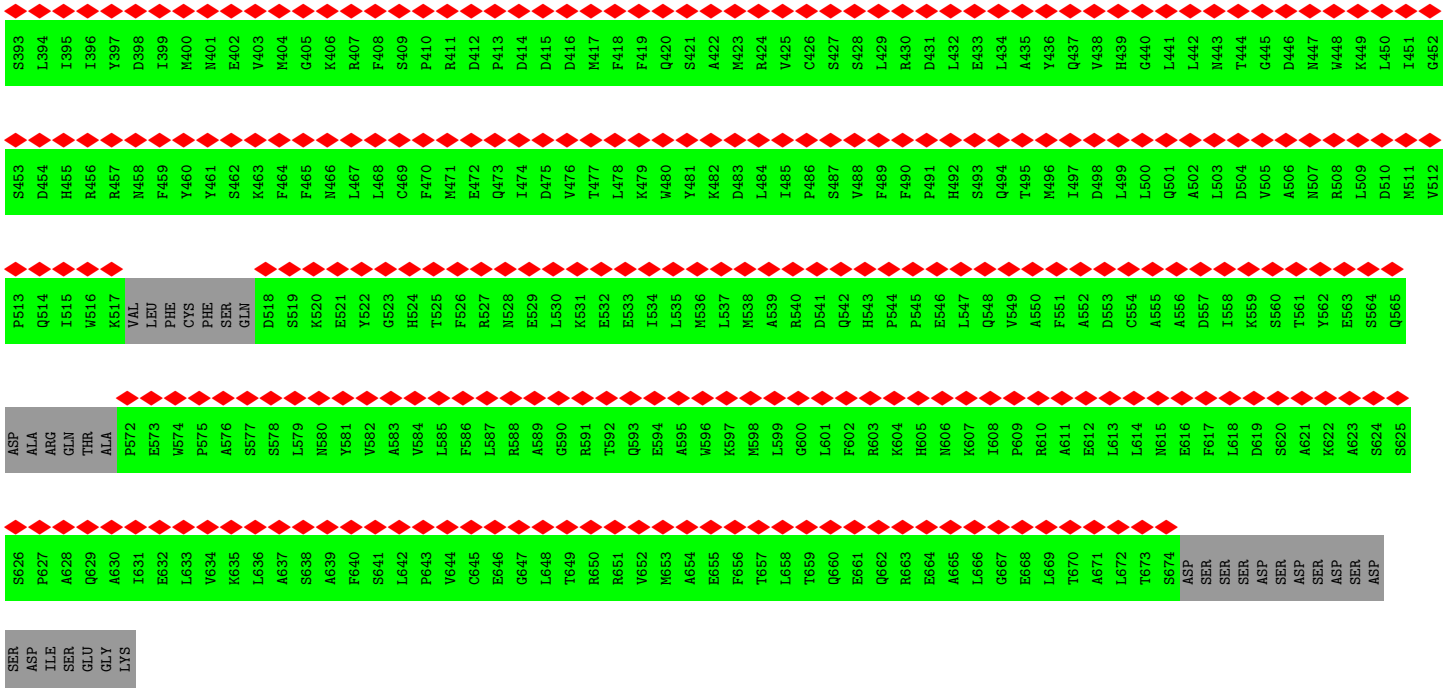
Chain An:



• Molecule 80: Pentatricopeptide repeat domain 3

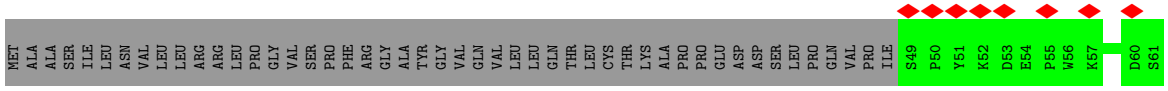
Chain Ao:

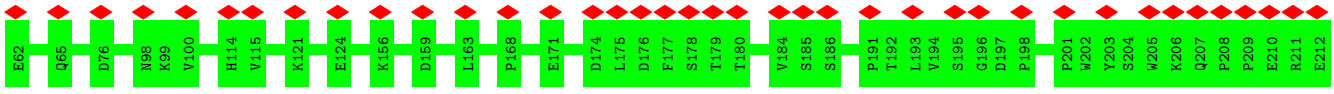


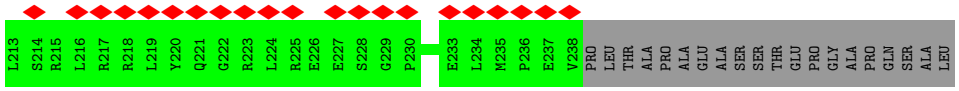


• Molecule 81: 28S ribosomal protein S18b, mitochondrial

Chain Ap:

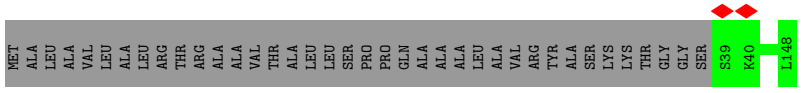






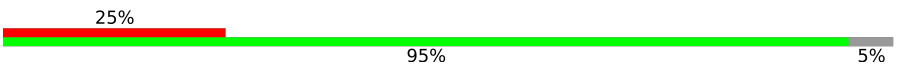
• Molecule 82: Mitochondrial ribosomal protein L27

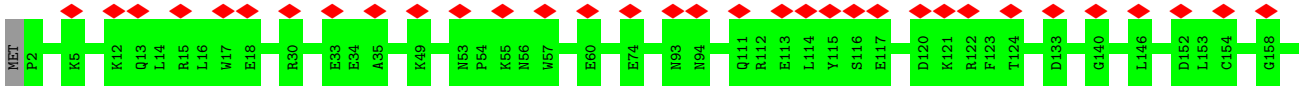
Chain B0:



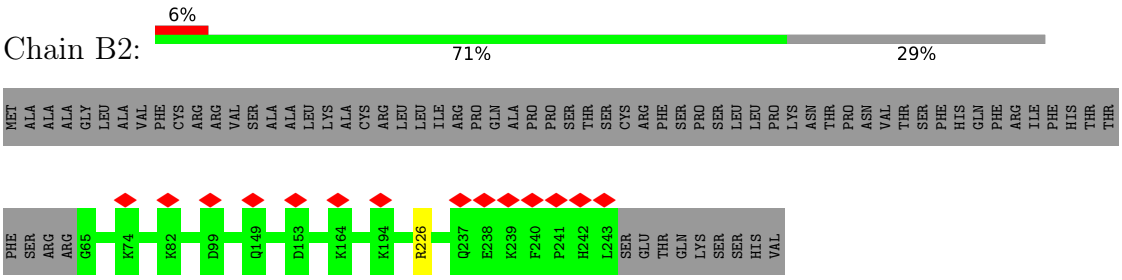
• Molecule 83: Mitochondrial ribosomal protein L28

Chain B1:

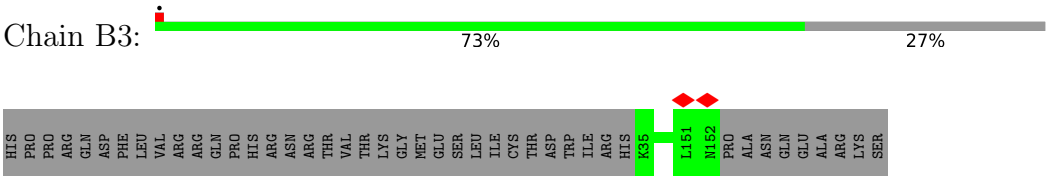




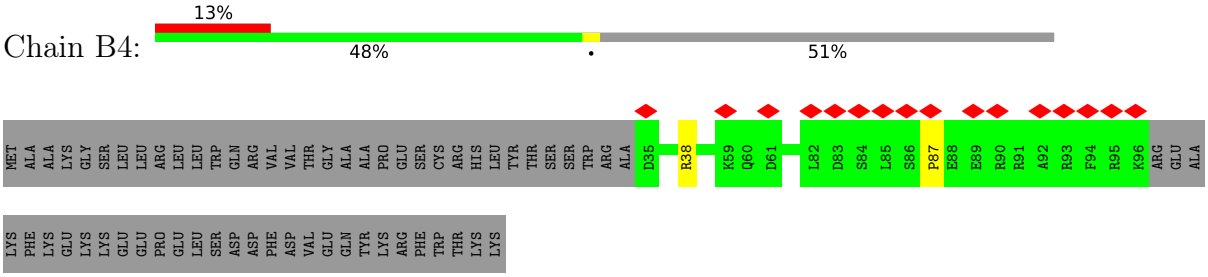
• Molecule 84: Mitochondrial ribosomal protein L47



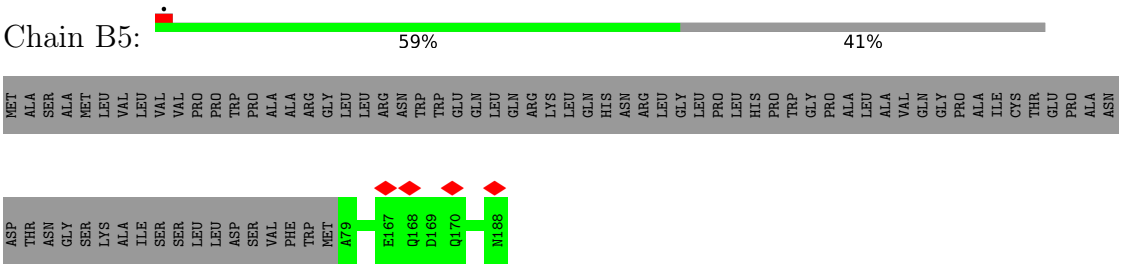
• Molecule 85: uL30m



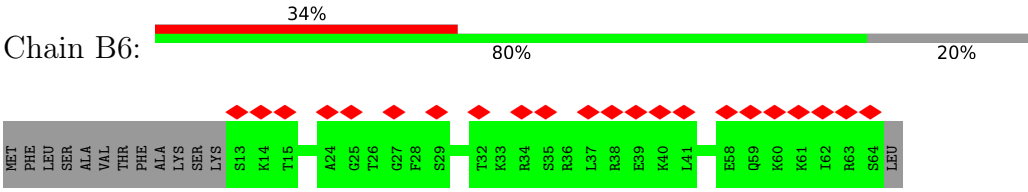
• Molecule 86: bL31m



• Molecule 87: bL32m



• Molecule 88: bL33m



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93623	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.037	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SPM, 5GP, MG, GTP

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	B7	0.23	0/395	0.56	0/524
2	B8	0.23	0/853	0.52	0/1136
3	B9	0.24	0/342	0.55	0/450
4	BA	0.20	0/36784	0.78	14/57270 (0.0%)
5	BB	0.31	1/1595 (0.1%)	0.76	0/2475
6	BD	0.25	0/1898	0.54	0/2555
7	BE	0.26	0/2493	0.46	0/3387
8	BF	0.24	0/2069	0.51	0/2816
9	BI	0.23	0/819	0.55	0/1101
10	BJ	0.25	0/1742	0.51	0/2358
11	BK	0.25	0/1323	0.49	0/1785
12	BL	0.23	0/1127	0.51	0/1512
13	BN	0.24	0/1487	0.46	0/2017
14	BO	0.29	0/912	0.58	0/1231
15	BP	0.25	0/2368	0.53	0/3198
16	BQ	0.25	0/1850	0.51	0/2491
17	BR	0.24	0/1262	0.54	0/1700
18	BS	0.24	0/1197	0.56	0/1624
19	BT	0.27	0/2002	0.50	1/2708 (0.0%)
20	BU	0.25	0/1179	0.55	0/1578
21	BV	0.24	0/1256	0.49	0/1706
22	BW	0.25	0/1407	0.53	0/1891
23	BX	0.26	0/1211	0.52	0/1646
24	BY	0.24	0/1719	0.53	0/2329
25	Ba	0.25	0/3267	0.48	0/4455
26	Bb	0.25	0/3047	0.51	0/4139
27	Bc	0.26	0/2464	0.49	0/3330
28	Bd	0.25	0/1183	0.54	0/1594
29	Be	0.26	0/1000	0.48	0/1345
30	Bf	0.25	0/851	0.58	2/1159 (0.2%)
31	Bg	0.27	0/1191	0.56	0/1614
32	Bh	0.25	0/2372	0.49	1/3211 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	Bi	0.25	0/2199	0.50	0/2980
34	Bj	0.24	0/1811	0.51	0/2436
35	Bk	0.27	0/1270	0.52	0/1714
36	Bl	0.26	0/1135	0.50	0/1549
37	Bm	0.24	0/917	0.48	0/1248
38	Bn	0.24	0/860	0.53	0/1150
39	Bo	0.25	0/787	0.47	0/1056
40	Bp	0.25	0/752	0.55	0/1013
41	Bq	0.25	0/490	0.51	0/662
42	Bt	0.24	0/798	0.55	0/1073
43	Bu	0.24	0/1214	0.54	1/1630 (0.1%)
44	Bv	0.24	0/1157	0.50	0/1560
45	Bw	0.25	0/3206	0.48	0/4354
46	Bx	0.27	0/1364	0.53	0/1849
47	AA	0.17	0/22852	0.75	6/35580 (0.0%)
48	CL	0.23	0/319	0.42	0/435
48	DL	0.22	0/212	0.41	0/286
48	EL	0.22	0/221	0.40	0/297
48	FL	0.22	0/212	0.40	0/286
48	GL	0.22	0/212	0.40	0/286
48	HL	0.22	0/204	0.41	0/275
49	AB	0.26	0/1804	0.53	0/2445
50	AC	0.26	0/1105	0.52	0/1496
51	AE	0.27	0/2785	0.56	2/3735 (0.1%)
52	AF	0.26	0/999	0.57	0/1347
53	AG	0.25	0/1763	0.49	0/2368
54	AI	0.26	0/2707	0.50	0/3636
55	AJ	0.25	0/1181	0.51	0/1597
56	AK	0.25	0/1027	0.52	0/1389
57	AL	0.25	0/858	0.54	0/1152
58	AN	0.23	0/874	0.56	0/1171
59	AO	0.24	0/1473	0.47	0/1970
60	AP	0.25	0/954	0.58	0/1284
61	AQ	0.24	0/894	0.48	0/1213
62	AR	0.25	0/802	0.49	0/1079
63	AU	0.24	0/745	0.54	0/993
64	AV	0.21	0/1673	0.87	1/2602 (0.0%)
65	AX	0.24	0/147	0.80	0/227
66	AZ	0.26	0/89	0.35	0/123
67	Aa	0.25	0/2428	0.50	1/3279 (0.0%)
68	Ab	0.25	0/1126	0.52	0/1514
69	Ac	0.26	0/1399	0.50	0/1881
70	Ad	0.25	0/1490	0.55	0/2005

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
71	Ae	0.25	0/3171	0.50	1/4292 (0.0%)
72	Af	0.24	0/790	0.53	0/1064
73	Ag	0.25	0/2945	0.49	0/3984
74	Ah	0.25	0/1045	0.45	0/1409
75	Ai	0.26	0/841	0.55	0/1121
76	Aj	0.24	0/1835	0.56	0/2484
77	Ak	0.25	0/2268	0.47	0/3069
78	Am	0.24	0/947	0.53	0/1268
79	An	0.23	0/650	0.54	0/858
80	Ao	0.25	0/4626	0.49	1/6269 (0.0%)
81	Ap	0.27	0/1616	0.53	0/2195
82	B0	0.26	0/880	0.48	0/1189
83	B1	0.24	0/2093	0.49	0/2835
84	B2	0.24	0/1586	0.51	0/2123
85	B3	0.24	0/993	0.49	0/1341
86	B4	0.23	0/481	0.63	1/653 (0.2%)
87	B5	0.24	0/917	0.52	0/1227
88	B6	0.25	0/430	0.55	0/570
All	All	0.23	1/183294 (0.0%)	0.62	32/260511 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	BD	0	1
10	BJ	0	1
38	Bn	0	1
73	Ag	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BB	1	G	OP3-P	-10.58	1.48	1.61

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	AE	395	PRO	CA-N-CD	-8.95	98.97	111.50
47	AA	119	C	C2-N1-C1'	8.22	127.84	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	AV	57	C	N3-C2-O2	-7.76	116.47	121.90
4	BA	848	C	C2-N1-C1'	6.95	126.44	118.80
51	AE	395	PRO	N-CD-CG	-6.91	92.83	103.20
4	BA	1527	U	C2-N1-C1'	6.79	125.84	117.70
30	Bf	80	PRO	N-CA-CB	6.55	111.16	103.30
71	Ae	342	PRO	N-CA-CB	6.50	111.11	103.30
30	Bf	78	PRO	N-CA-CB	6.40	110.98	103.30
43	Bu	167	PRO	N-CA-CB	6.38	110.96	103.30
4	BA	825	C	C2-N1-C1'	6.01	125.41	118.80
47	AA	119	C	C6-N1-C1'	-5.94	113.67	120.80
4	BA	1527	U	N1-C2-O2	5.90	126.93	122.80
32	Bh	267	LEU	CA-CB-CG	5.84	128.73	115.30
80	Ao	203	PRO	N-CA-CB	5.68	110.11	103.30
4	BA	825	C	N1-C2-O2	5.65	122.29	118.90
86	B4	87	PRO	N-CA-CB	5.60	110.02	103.30
4	BA	890	C	N1-C2-O2	5.57	122.24	118.90
19	BT	68	PRO	N-CA-CB	5.50	109.91	103.30
4	BA	1527	U	N3-C2-O2	-5.49	118.35	122.20
67	Aa	257	PHE	C-N-CA	5.49	135.43	121.70
4	BA	48	U	OP1-P-O3'	5.46	117.22	105.20
4	BA	890	C	C2-N1-C1'	5.44	124.78	118.80
4	BA	394	C	N1-C2-O2	5.35	122.11	118.90
47	AA	744	C	C2-N1-C1'	5.29	124.61	118.80
4	BA	48	U	P-O3'-C3'	5.27	126.02	119.70
4	BA	397	C	C2-N1-C1'	5.24	124.56	118.80
47	AA	119	C	N1-C2-O2	5.18	122.01	118.90
47	AA	745	C	N1-C2-O2	5.16	121.99	118.90
47	AA	745	C	C2-N1-C1'	5.14	124.46	118.80
4	BA	394	C	C2-N1-C1'	5.09	124.39	118.80
4	BA	397	C	N1-C2-O2	5.08	121.95	118.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
73	Ag	337	ASP	Peptide
6	BD	207	TYR	Peptide
10	BJ	64	CYS	Peptide
38	Bn	65	ASN	Peptide

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	B7	44/95 (46%)	44 (100%)	0	0	100	100
2	B8	93/188 (50%)	93 (100%)	0	0	100	100
3	B9	36/100 (36%)	36 (100%)	0	0	100	100
6	BD	238/306 (78%)	231 (97%)	7 (3%)	0	100	100
7	BE	305/399 (76%)	291 (95%)	14 (5%)	0	100	100
8	BF	248/294 (84%)	242 (98%)	6 (2%)	0	100	100
9	BI	96/268 (36%)	95 (99%)	1 (1%)	0	100	100
10	BJ	210/262 (80%)	199 (95%)	11 (5%)	0	100	100
11	BK	174/192 (91%)	172 (99%)	2 (1%)	0	100	100
12	BL	135/184 (73%)	133 (98%)	2 (2%)	0	100	100
13	BN	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
14	BO	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
15	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
16	BQ	220/251 (88%)	217 (99%)	3 (1%)	0	100	100
17	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
18	BS	141/180 (78%)	131 (93%)	10 (7%)	0	100	100
19	BT	238/292 (82%)	233 (98%)	4 (2%)	1 (0%)	30	60
20	BU	138/149 (93%)	138 (100%)	0	0	100	100
21	BV	153/209 (73%)	149 (97%)	4 (3%)	0	100	100
22	BW	164/210 (78%)	158 (96%)	6 (4%)	0	100	100
23	BX	147/150 (98%)	145 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BY	204/216 (94%)	197 (97%)	7 (3%)	0	100	100
25	Ba	391/423 (92%)	378 (97%)	13 (3%)	0	100	100
26	Bb	352/380 (93%)	333 (95%)	19 (5%)	0	100	100
27	Bc	293/334 (88%)	281 (96%)	11 (4%)	1 (0%)	37	66
28	Bd	136/206 (66%)	129 (95%)	7 (5%)	0	100	100
29	Be	120/135 (89%)	112 (93%)	8 (7%)	0	100	100
30	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	6	26
31	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
32	Bh	287/332 (86%)	274 (96%)	13 (4%)	0	100	100
33	Bi	258/306 (84%)	244 (95%)	14 (5%)	0	100	100
34	Bj	211/279 (76%)	200 (95%)	11 (5%)	0	100	100
35	Bk	151/269 (56%)	144 (95%)	7 (5%)	0	100	100
36	Bl	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
37	Bm	107/198 (54%)	106 (99%)	1 (1%)	0	100	100
38	Bn	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
39	Bo	95/124 (77%)	94 (99%)	1 (1%)	0	100	100
40	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
41	Bq	52/138 (38%)	49 (94%)	3 (6%)	0	100	100
42	Bt	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
43	Bu	147/205 (72%)	139 (95%)	7 (5%)	1 (1%)	19	47
44	Bv	133/222 (60%)	133 (100%)	0	0	100	100
45	Bw	385/433 (89%)	365 (95%)	20 (5%)	0	100	100
46	Bx	160/196 (82%)	152 (95%)	8 (5%)	0	100	100
48	CL	43/198 (22%)	43 (100%)	0	0	100	100
48	DL	25/198 (13%)	25 (100%)	0	0	100	100
48	EL	26/198 (13%)	26 (100%)	0	0	100	100
48	FL	25/198 (13%)	25 (100%)	0	0	100	100
48	GL	25/198 (13%)	25 (100%)	0	0	100	100
48	HL	24/198 (12%)	24 (100%)	0	0	100	100
49	AB	218/289 (75%)	211 (97%)	7 (3%)	0	100	100
50	AC	130/167 (78%)	123 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	AE	341/430 (79%)	329 (96%)	12 (4%)	0	100	100
52	AF	120/276 (44%)	119 (99%)	1 (1%)	0	100	100
53	AG	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
54	AI	326/397 (82%)	320 (98%)	6 (2%)	0	100	100
55	AJ	138/200 (69%)	125 (91%)	13 (9%)	0	100	100
56	AK	135/196 (69%)	130 (96%)	5 (4%)	0	100	100
57	AL	107/139 (77%)	99 (92%)	8 (8%)	0	100	100
58	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
59	AO	173/239 (72%)	169 (98%)	4 (2%)	0	100	100
60	AP	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
61	AQ	110/130 (85%)	108 (98%)	2 (2%)	0	100	100
62	AR	95/143 (66%)	95 (100%)	0	0	100	100
63	AU	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
66	AZ	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
67	Aa	290/382 (76%)	284 (98%)	6 (2%)	0	100	100
68	Ab	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
69	Ac	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
70	Ad	175/205 (85%)	175 (100%)	0	0	100	100
71	Ae	386/455 (85%)	361 (94%)	23 (6%)	2 (0%)	25	54
72	Af	97/188 (52%)	95 (98%)	2 (2%)	0	100	100
73	Ag	351/410 (86%)	337 (96%)	14 (4%)	0	100	100
74	Ah	118/387 (30%)	117 (99%)	1 (1%)	0	100	100
75	Ai	97/106 (92%)	95 (98%)	2 (2%)	0	100	100
76	Aj	211/218 (97%)	205 (97%)	6 (3%)	0	100	100
77	Ak	273/325 (84%)	266 (97%)	7 (3%)	0	100	100
78	Am	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
79	An	70/199 (35%)	69 (99%)	1 (1%)	0	100	100
80	Ao	564/699 (81%)	548 (97%)	16 (3%)	0	100	100
81	Ap	188/258 (73%)	182 (97%)	6 (3%)	0	100	100
82	B0	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
83	B1	242/256 (94%)	241 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	B2	177/252 (70%)	172 (97%)	5 (3%)	0	100	100
85	B3	116/161 (72%)	113 (97%)	3 (3%)	0	100	100
86	B4	60/126 (48%)	55 (92%)	5 (8%)	0	100	100
87	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
88	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
All	All	14328/19635 (73%)	13864 (97%)	457 (3%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	BT	68	PRO
30	Bf	80	PRO
43	Bu	167	PRO
30	Bf	78	PRO
71	Ae	342	PRO
71	Ae	341	GLN
27	Bc	107	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B7	41/78 (53%)	41 (100%)	0	100	100
2	B8	87/162 (54%)	86 (99%)	1 (1%)	70	81
3	B9	36/77 (47%)	36 (100%)	0	100	100
6	BD	193/248 (78%)	193 (100%)	0	100	100
7	BE	263/320 (82%)	263 (100%)	0	100	100
8	BF	217/251 (86%)	217 (100%)	0	100	100
9	BI	88/228 (39%)	87 (99%)	1 (1%)	70	81
10	BJ	192/230 (84%)	191 (100%)	1 (0%)	86	91
11	BK	129/151 (85%)	128 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	BL	125/162 (77%)	125 (100%)	0	100	100
13	BN	156/157 (99%)	156 (100%)	0	100	100
14	BO	99/123 (80%)	99 (100%)	0	100	100
15	BP	245/249 (98%)	244 (100%)	1 (0%)	89	93
16	BQ	190/210 (90%)	190 (100%)	0	100	100
17	BR	132/143 (92%)	132 (100%)	0	100	100
18	BS	123/153 (80%)	122 (99%)	1 (1%)	79	87
19	BT	212/258 (82%)	212 (100%)	0	100	100
20	BU	118/127 (93%)	118 (100%)	0	100	100
21	BV	136/178 (76%)	136 (100%)	0	100	100
22	BW	144/180 (80%)	144 (100%)	0	100	100
23	BX	116/134 (87%)	116 (100%)	0	100	100
24	BY	185/192 (96%)	182 (98%)	3 (2%)	58	75
25	Ba	348/365 (95%)	348 (100%)	0	100	100
26	Bb	310/328 (94%)	306 (99%)	4 (1%)	65	78
27	Bc	271/299 (91%)	270 (100%)	1 (0%)	89	93
28	Bd	127/181 (70%)	127 (100%)	0	100	100
29	Be	100/108 (93%)	100 (100%)	0	100	100
30	Bf	80/133 (60%)	80 (100%)	0	100	100
31	Bg	128/136 (94%)	128 (100%)	0	100	100
32	Bh	251/284 (88%)	251 (100%)	0	100	100
33	Bi	236/275 (86%)	234 (99%)	2 (1%)	79	87
34	Bj	190/242 (78%)	190 (100%)	0	100	100
35	Bk	135/226 (60%)	135 (100%)	0	100	100
36	Bl	122/147 (83%)	122 (100%)	0	100	100
37	Bm	103/178 (58%)	103 (100%)	0	100	100
38	Bn	88/113 (78%)	88 (100%)	0	100	100
39	Bo	77/97 (79%)	77 (100%)	0	100	100
40	Bp	79/88 (90%)	79 (100%)	0	100	100
41	Bq	50/114 (44%)	50 (100%)	0	100	100
42	Bt	75/82 (92%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Bu	126/177 (71%)	126 (100%)	0	100	100
44	Bv	115/183 (63%)	115 (100%)	0	100	100
45	Bw	340/373 (91%)	340 (100%)	0	100	100
46	Bx	149/173 (86%)	147 (99%)	2 (1%)	65	78
48	CL	30/157 (19%)	30 (100%)	0	100	100
48	DL	26/157 (17%)	25 (96%)	1 (4%)	28	54
48	EL	27/157 (17%)	27 (100%)	0	100	100
48	FL	26/157 (17%)	26 (100%)	0	100	100
48	GL	26/157 (17%)	26 (100%)	0	100	100
48	HL	25/157 (16%)	24 (96%)	1 (4%)	27	52
49	AB	187/233 (80%)	186 (100%)	1 (0%)	86	91
50	AC	115/142 (81%)	115 (100%)	0	100	100
51	AE	282/351 (80%)	278 (99%)	4 (1%)	62	77
52	AF	107/210 (51%)	107 (100%)	0	100	100
53	AG	181/205 (88%)	181 (100%)	0	100	100
54	AI	273/333 (82%)	270 (99%)	3 (1%)	70	81
55	AJ	130/180 (72%)	129 (99%)	1 (1%)	79	87
56	AK	103/151 (68%)	102 (99%)	1 (1%)	73	83
57	AL	92/116 (79%)	92 (100%)	0	100	100
58	AN	92/114 (81%)	92 (100%)	0	100	100
59	AO	159/205 (78%)	159 (100%)	0	100	100
60	AP	97/113 (86%)	97 (100%)	0	100	100
61	AQ	97/114 (85%)	97 (100%)	0	100	100
62	AR	89/127 (70%)	89 (100%)	0	100	100
63	AU	77/78 (99%)	76 (99%)	1 (1%)	65	78
67	Aa	258/330 (78%)	258 (100%)	0	100	100
68	Ab	113/162 (70%)	113 (100%)	0	100	100
69	Ac	152/155 (98%)	151 (99%)	1 (1%)	81	88
70	Ad	149/168 (89%)	149 (100%)	0	100	100
71	Ae	325/393 (83%)	325 (100%)	0	100	100
72	Af	86/160 (54%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
73	Ag	312/361 (86%)	309 (99%)	3 (1%)	73 83
74	Ah	109/346 (32%)	108 (99%)	1 (1%)	75 86
75	Ai	86/93 (92%)	86 (100%)	0	100 100
76	Aj	188/190 (99%)	188 (100%)	0	100 100
77	Ak	249/289 (86%)	248 (100%)	1 (0%)	89 93
78	Am	100/102 (98%)	100 (100%)	0	100 100
79	An	66/174 (38%)	66 (100%)	0	100 100
80	Ao	478/611 (78%)	477 (100%)	1 (0%)	92 96
81	Ap	170/225 (76%)	170 (100%)	0	100 100
82	B0	90/115 (78%)	90 (100%)	0	100 100
83	B1	219/229 (96%)	219 (100%)	0	100 100
84	B2	164/228 (72%)	163 (99%)	1 (1%)	84 90
85	B3	110/150 (73%)	110 (100%)	0	100 100
86	B4	45/114 (40%)	44 (98%)	1 (2%)	47 68
87	B5	99/163 (61%)	99 (100%)	0	100 100
88	B6	49/60 (82%)	49 (100%)	0	100 100
All	All	12585/16745 (75%)	12545 (100%)	40 (0%)	90 95

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B8	154	GLN
9	BI	61	LYS
10	BJ	118	LYS
11	BK	169	LYS
15	BP	44	ARG
18	BS	173	ARG
24	BY	40	ARG
24	BY	81	ARG
24	BY	105	ARG
26	Bb	52	ARG
26	Bb	66	ARG
26	Bb	244	ARG
26	Bb	286	ARG
27	Bc	170	PRO
33	Bi	126	ARG

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Mol	Chain	Res	Type
33	Bi	154	ASN
46	Bx	69	GLN
46	Bx	182	LYS
48	DL	83	ASN
49	AB	264	ARG
51	AE	174	GLN
51	AE	187	VAL
51	AE	188	LYS
51	AE	190	GLU
54	AI	86	ARG
54	AI	248	SER
54	AI	251	ILE
55	AJ	131	ARG
56	AK	191	ARG
63	AU	52	ARG
69	Ac	137	ARG
73	Ag	75	LYS
73	Ag	212	ARG
73	Ag	319	ARG
74	Ah	276	LYS
77	Ak	104	ASN
80	Ao	329	GLN
48	HL	83	ASN
84	B2	226	ARG
86	B4	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
6	BD	206	GLN
7	BE	154	HIS
8	BF	74	GLN
8	BF	83	HIS
10	BJ	101	HIS
12	BL	182	ASN
14	BO	142	GLN
15	BP	53	HIS
16	BQ	222	ASN
19	BT	158	GLN
25	Ba	324	GLN
26	Bb	354	GLN
29	Be	50	GLN

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Mol	Chain	Res	Type
30	Bf	62	HIS
31	Bg	127	GLN
33	Bi	251	HIS
34	Bj	198	ASN
34	Bj	212	HIS
35	Bk	138	GLN
35	Bk	153	HIS
35	Bk	158	GLN
35	Bk	189	HIS
38	Bn	69	HIS
43	Bu	145	ASN
44	Bv	79	GLN
45	Bw	146	GLN
45	Bw	352	GLN
50	AC	154	HIS
50	AC	156	GLN
54	AI	148	HIS
54	AI	163	HIS
60	AP	106	ASN
62	AR	83	GLN
69	Ac	51	ASN
70	Ad	65	GLN
71	Ae	155	GLN
71	Ae	196	ASN
73	Ag	62	HIS
77	Ak	104	ASN
78	Am	24	ASN
78	Am	105	ASN
80	Ao	420	GLN
85	B3	102	ASN
86	B4	60	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	BA	1542/1571 (98%)	410 (26%)	2 (0%)
47	AA	959/962 (99%)	178 (18%)	0
5	BB	64/73 (87%)	15 (23%)	0
64	AV	70/71 (98%)	22 (31%)	0
65	AX	5/6 (83%)	1 (20%)	1 (20%)
All	All	2640/2683 (98%)	626 (23%)	3 (0%)

All (626) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	BA	4	A
4	BA	7	G
4	BA	11	G
4	BA	19	U
4	BA	20	A
4	BA	21	C
4	BA	22	U
4	BA	26	C
4	BA	27	A
4	BA	31	A
4	BA	32	C
4	BA	36	A
4	BA	37	A
4	BA	40	C
4	BA	41	A
4	BA	45	A
4	BA	46	A
4	BA	49	A
4	BA	56	A
4	BA	57	A
4	BA	59	A
4	BA	60	U
4	BA	63	A
4	BA	66	U
4	BA	67	A
4	BA	68	A
4	BA	82	G
4	BA	83	A
4	BA	96	U
4	BA	97	A
4	BA	104	C
4	BA	105	G
4	BA	109	U
4	BA	115	U
4	BA	118	U
4	BA	119	A
4	BA	122	G
4	BA	129	A
4	BA	130	A
4	BA	132	G
4	BA	139	G
4	BA	140	A

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Mol	Chain	Res	Type
4	BA	141	A
4	BA	142	U
4	BA	143	A
4	BA	146	A
4	BA	147	U
4	BA	149	A
4	BA	163	C
4	BA	164	A
4	BA	165	A
4	BA	168	A
4	BA	172	C
4	BA	178	C
4	BA	180	A
4	BA	182	C
4	BA	186	U
4	BA	190	U
4	BA	192	A
4	BA	205	A
4	BA	218	A
4	BA	219	A
4	BA	223	A
4	BA	225	C
4	BA	229	A
4	BA	231	C
4	BA	237	A
4	BA	238	C
4	BA	239	C
4	BA	243	A
4	BA	245	A
4	BA	254	G
4	BA	263	G
4	BA	271	U
4	BA	272	A
4	BA	273	A
4	BA	275	A
4	BA	277	A
4	BA	295	G
4	BA	309	A
4	BA	311	A
4	BA	312	C
4	BA	322	G
4	BA	323	A

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Mol	Chain	Res	Type
4	BA	324	G
4	BA	329	A
4	BA	330	A
4	BA	331	A
4	BA	336	A
4	BA	337	A
4	BA	338	C
4	BA	340	A
4	BA	351	A
4	BA	352	G
4	BA	359	G
4	BA	366	A
4	BA	368	A
4	BA	369	G
4	BA	373	U
4	BA	374	U
4	BA	376	A
4	BA	389	A
4	BA	390	A
4	BA	393	A
4	BA	394	C
4	BA	398	A
4	BA	403	C
4	BA	409	A
4	BA	414	A
4	BA	417	G
4	BA	427	G
4	BA	428	A
4	BA	433	G
4	BA	440	A
4	BA	446	C
4	BA	447	A
4	BA	448	G
4	BA	459	A
4	BA	460	C
4	BA	467	A
4	BA	468	A
4	BA	473	G
4	BA	474	A
4	BA	479	A
4	BA	480	G
4	BA	488	U

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Mol	Chain	Res	Type
4	BA	490	U
4	BA	491	U
4	BA	492	A
4	BA	493	A
4	BA	494	U
4	BA	497	U
4	BA	498	A
4	BA	499	C
4	BA	500	C
4	BA	501	A
4	BA	503	A
4	BA	505	U
4	BA	509	C
4	BA	514	A
4	BA	515	A
4	BA	516	G
4	BA	517	C
4	BA	518	A
4	BA	526	A
4	BA	527	U
4	BA	530	A
4	BA	532	A
4	BA	533	A
4	BA	541	A
4	BA	547	A
4	BA	548	A
4	BA	549	C
4	BA	550	A
4	BA	551	A
4	BA	553	U
4	BA	554	U
4	BA	557	C
4	BA	560	A
4	BA	561	C
4	BA	562	A
4	BA	563	U
4	BA	570	A
4	BA	574	A
4	BA	576	U
4	BA	578	A
4	BA	579	U
4	BA	584	A

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Mol	Chain	Res	Type
4	BA	586	C
4	BA	592	G
4	BA	593	C
4	BA	595	C
4	BA	596	A
4	BA	617	A
4	BA	618	A
4	BA	625	A
4	BA	626	G
4	BA	631	A
4	BA	633	U
4	BA	634	G
4	BA	640	A
4	BA	648	C
4	BA	649	A
4	BA	654	G
4	BA	665	C
4	BA	673	C
4	BA	674	U
4	BA	675	U
4	BA	683	U
4	BA	684	A
4	BA	689	A
4	BA	694	A
4	BA	695	U
4	BA	697	C
4	BA	704	U
4	BA	707	A
4	BA	713	A
4	BA	719	C
4	BA	720	C
4	BA	722	A
4	BA	723	A
4	BA	724	A
4	BA	725	C
4	BA	727	A
4	BA	728	C
4	BA	744	A
4	BA	745	A
4	BA	746	U
4	BA	748	A
4	BA	763	C

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Mol	Chain	Res	Type
4	BA	764	A
4	BA	774	A
4	BA	777	A
4	BA	778	A
4	BA	780	G
4	BA	782	A
4	BA	783	A
4	BA	784	G
4	BA	819	A
4	BA	825	C
4	BA	835	A
4	BA	838	A
4	BA	847	U
4	BA	848	C
4	BA	852	C
4	BA	854	U
4	BA	855	U
4	BA	859	A
4	BA	864	U
4	BA	872	A
4	BA	883	G
4	BA	887	C
4	BA	889	C
4	BA	892	G
4	BA	894	U
4	BA	895	U
4	BA	896	A
4	BA	897	A
4	BA	899	G
4	BA	900	G
4	BA	902	C
4	BA	909	U
4	BA	910	U
4	BA	911	C
4	BA	922	A
4	BA	923	A
4	BA	924	G
4	BA	925	G
4	BA	926	U
4	BA	931	U
4	BA	932	A
4	BA	933	A

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Mol	Chain	Res	Type
4	BA	935	C
4	BA	938	U
4	BA	939	U
4	BA	948	A
4	BA	950	U
4	BA	958	U
4	BA	959	G
4	BA	960	U
4	BA	961	A
4	BA	962	U
4	BA	964	A
4	BA	965	A
4	BA	966	U
4	BA	967	G
4	BA	970	C
4	BA	977	G
4	BA	983	U
4	BA	986	U
4	BA	987	G
4	BA	992	U
4	BA	1015	C
4	BA	1016	C
4	BA	1018	U
4	BA	1026	A
4	BA	1027	G
4	BA	1028	A
4	BA	1035	A
4	BA	1038	A
4	BA	1041	A
4	BA	1045	U
4	BA	1050	C
4	BA	1055	A
4	BA	1056	G
4	BA	1057	A
4	BA	1063	U
4	BA	1064	G
4	BA	1071	U
4	BA	1072	A
4	BA	1074	U
4	BA	1075	U
4	BA	1081	U
4	BA	1089	G

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Mol	Chain	Res	Type
4	BA	1091	U
4	BA	1092	A
4	BA	1093	A
4	BA	1127	A
4	BA	1129	C
4	BA	1138	G
4	BA	1140	A
4	BA	1146	G
4	BA	1167	C
4	BA	1168	A
4	BA	1169	A
4	BA	1180	G
4	BA	1183	U
4	BA	1188	U
4	BA	1194	U
4	BA	1195	A
4	BA	1204	A
4	BA	1206	U
4	BA	1207	C
4	BA	1217	A
4	BA	1218	U
4	BA	1219	A
4	BA	1220	A
4	BA	1221	C
4	BA	1222	A
4	BA	1226	C
4	BA	1231	U
4	BA	1233	A
4	BA	1237	A
4	BA	1238	A
4	BA	1239	A
4	BA	1240	A
4	BA	1241	U
4	BA	1242	U
4	BA	1246	A
4	BA	1247	U
4	BA	1248	C
4	BA	1249	A
4	BA	1252	G
4	BA	1253	G
4	BA	1254	A
4	BA	1255	A

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Mol	Chain	Res	Type
4	BA	1258	A
4	BA	1264	C
4	BA	1270	G
4	BA	1271	A
4	BA	1287	G
4	BA	1288	U
4	BA	1291	U
4	BA	1292	A
4	BA	1294	A
4	BA	1298	C
4	BA	1299	C
4	BA	1314	U
4	BA	1321	C
4	BA	1323	U
4	BA	1325	G
4	BA	1326	A
4	BA	1328	G
4	BA	1332	G
4	BA	1336	A
4	BA	1341	A
4	BA	1342	C
4	BA	1352	G
4	BA	1358	G
4	BA	1385	U
4	BA	1386	U
4	BA	1387	A
4	BA	1388	A
4	BA	1389	A
4	BA	1390	G
4	BA	1395	A
4	BA	1396	C
4	BA	1405	A
4	BA	1409	C
4	BA	1420	A
4	BA	1425	A
4	BA	1426	G
4	BA	1429	C
4	BA	1433	U
4	BA	1436	U
4	BA	1438	U
4	BA	1445	U
4	BA	1448	A

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Mol	Chain	Res	Type
4	BA	1457	A
4	BA	1468	A
4	BA	1474	G
4	BA	1476	A
4	BA	1493	A
4	BA	1494	A
4	BA	1498	C
4	BA	1504	A
4	BA	1505	G
4	BA	1509	U
4	BA	1514	A
4	BA	1518	A
4	BA	1521	U
4	BA	1522	A
4	BA	1526	U
4	BA	1527	U
4	BA	1528	A
4	BA	1529	A
4	BA	1531	C
4	BA	1532	U
4	BA	1533	A
4	BA	1536	U
4	BA	1540	U
4	BA	1548	A
4	BA	1549	A
4	BA	1551	C
4	BA	1552	C
4	BA	1553	A
4	BA	1554	G
4	BA	1558	U
4	BA	1559	A
4	BA	1571	A
5	BB	3	U
5	BB	5	A
5	BB	7	G
5	BB	8	U
5	BB	9	A
5	BB	13	U
5	BB	21	C
5	BB	34	U
5	BB	43	C
5	BB	44	U

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Mol	Chain	Res	Type
5	BB	46	G
5	BB	47	A
5	BB	48	U
5	BB	69	C
5	BB	70	A
47	AA	5	A
47	AA	10	U
47	AA	27	U
47	AA	34	U
47	AA	42	A
47	AA	43	U
47	AA	44	U
47	AA	54	A
47	AA	58	U
47	AA	65	C
47	AA	67	C
47	AA	75	A
47	AA	81	U
47	AA	83	C
47	AA	102	G
47	AA	104	A
47	AA	115	A
47	AA	120	A
47	AA	139	A
47	AA	147	G
47	AA	152	A
47	AA	161	C
47	AA	164	C
47	AA	165	G
47	AA	170	A
47	AA	171	C
47	AA	173	G
47	AA	175	A
47	AA	186	U
47	AA	191	C
47	AA	194	U
47	AA	212	A
47	AA	216	A
47	AA	217	U
47	AA	219	U
47	AA	222	A
47	AA	223	U

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Mol	Chain	Res	Type
47	AA	224	U
47	AA	231	G
47	AA	235	A
47	AA	238	C
47	AA	244	C
47	AA	247	G
47	AA	253	G
47	AA	256	G
47	AA	257	U
47	AA	258	C
47	AA	273	A
47	AA	281	G
47	AA	287	C
47	AA	288	G
47	AA	294	A
47	AA	296	G
47	AA	297	A
47	AA	308	A
47	AA	309	A
47	AA	310	A
47	AA	314	A
47	AA	315	U
47	AA	316	C
47	AA	317	A
47	AA	320	A
47	AA	328	A
47	AA	337	C
47	AA	345	U
47	AA	354	C
47	AA	355	U
47	AA	361	A
47	AA	362	A
47	AA	368	A
47	AA	372	C
47	AA	395	C
47	AA	399	A
47	AA	407	U
47	AA	417	C
47	AA	421	A
47	AA	433	U
47	AA	455	A
47	AA	456	A

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Mol	Chain	Res	Type
47	AA	457	C
47	AA	458	C
47	AA	461	A
47	AA	464	A
47	AA	471	U
47	AA	472	A
47	AA	477	A
47	AA	479	C
47	AA	498	U
47	AA	502	A
47	AA	503	A
47	AA	518	A
47	AA	531	U
47	AA	532	G
47	AA	534	U
47	AA	538	C
47	AA	540	U
47	AA	541	C
47	AA	561	U
47	AA	566	U
47	AA	571	A
47	AA	574	C
47	AA	576	C
47	AA	579	A
47	AA	589	C
47	AA	593	C
47	AA	596	U
47	AA	597	U
47	AA	604	U
47	AA	616	C
47	AA	618	G
47	AA	619	C
47	AA	625	U
47	AA	628	G
47	AA	633	C
47	AA	639	A
47	AA	644	A
47	AA	645	A
47	AA	646	C
47	AA	648	A
47	AA	649	U
47	AA	652	U

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Mol	Chain	Res	Type
47	AA	665	A
47	AA	681	A
47	AA	682	G
47	AA	696	U
47	AA	698	A
47	AA	707	A
47	AA	708	A
47	AA	709	A
47	AA	711	A
47	AA	720	A
47	AA	722	A
47	AA	731	A
47	AA	732	U
47	AA	739	A
47	AA	743	A
47	AA	746	A
47	AA	766	C
47	AA	775	A
47	AA	790	A
47	AA	791	G
47	AA	802	A
47	AA	803	U
47	AA	807	G
47	AA	808	U
47	AA	823	G
47	AA	825	C
47	AA	838	A
47	AA	841	C
47	AA	842	A
47	AA	869	A
47	AA	870	G
47	AA	876	A
47	AA	877	A
47	AA	883	C
47	AA	885	U
47	AA	886	A
47	AA	893	A
47	AA	894	U
47	AA	897	C
47	AA	899	C
47	AA	902	C
47	AA	910	G

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Mol	Chain	Res	Type
47	AA	917	C
47	AA	918	A
47	AA	919	A
47	AA	920	G
47	AA	923	G
47	AA	925	A
47	AA	928	A
47	AA	930	G
47	AA	932	U
47	AA	943	G
47	AA	946	A
47	AA	955	G
47	AA	956	G
47	AA	959	U
47	AA	960	A
64	AV	2	G
64	AV	6	G
64	AV	8	U
64	AV	9	C
64	AV	14	A
64	AV	15	A
64	AV	16	A
64	AV	17	U
64	AV	18	A
64	AV	43	A
64	AV	44	U
64	AV	45	G
64	AV	51	U
64	AV	54	A
64	AV	55	C
64	AV	56	C
64	AV	58	U
64	AV	61	C
64	AV	63	G
64	AV	64	U
64	AV	65	A
64	AV	71	A
65	AX	3	A

All (3) RNA pucker outliers are listed below:

Continued on next page...

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Mol	Chain	Res	Type
4	BA	48	U
4	BA	1241	U
65	AX	2	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 347 ligands modelled in this entry, 341 are monoatomic - leaving 6 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	SPM	AA	3001	-	13,13,13	0.34	0	12,12,12	0.79	0
91	5GP	BA	3211	-	22,26,26	1.23	2 (9%)	26,40,40	1.26	4 (15%)
92	SPM	BA	3213	-	13,13,13	0.33	0	12,12,12	0.79	0
91	5GP	BA	3212	90	22,26,26	1.24	2 (9%)	26,40,40	1.25	4 (15%)
92	SPM	BA	3214	-	13,13,13	0.35	0	12,12,12	0.77	0
93	GTP	Ag	500	90	26,34,34	1.12	2 (7%)	32,54,54	1.59	7 (21%)

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	SPM	AA	3001	-	-	2/11/11/11	-
91	5GP	BA	3211	-	-	1/6/26/26	0/3/3/3
92	SPM	BA	3213	-	-	3/11/11/11	-
91	5GP	BA	3212	90	-	1/6/26/26	0/3/3/3
92	SPM	BA	3214	-	-	3/11/11/11	-
93	GTP	Ag	500	90	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	BA	3212	5GP	C5-C6	-4.09	1.39	1.47
91	BA	3211	5GP	C5-C6	-4.03	1.39	1.47
93	Ag	500	GTP	C5-C6	-3.95	1.39	1.47
91	BA	3211	5GP	C6-N1	-2.53	1.34	1.37
91	BA	3212	5GP	C6-N1	-2.47	1.34	1.37
93	Ag	500	GTP	C2-N3	2.22	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
93	Ag	500	GTP	PA-O3A-PB	-3.98	119.16	132.83
93	Ag	500	GTP	C5-C6-N1	3.25	119.69	113.95
93	Ag	500	GTP	C3'-C2'-C1'	3.21	105.81	100.98
91	BA	3211	5GP	C5-C6-N1	3.14	119.50	113.95
91	BA	3212	5GP	C5-C6-N1	3.13	119.47	113.95
93	Ag	500	GTP	PB-O3B-PG	-3.10	122.20	132.83
93	Ag	500	GTP	C8-N7-C5	2.99	108.69	102.99
93	Ag	500	GTP	C2-N1-C6	-2.93	119.71	125.10
91	BA	3211	5GP	C8-N7-C5	2.40	107.55	102.99
91	BA	3212	5GP	C8-N7-C5	2.39	107.54	102.99
91	BA	3211	5GP	C2-N1-C6	-2.33	120.81	125.10
91	BA	3212	5GP	C2-N1-C6	-2.29	120.88	125.10
93	Ag	500	GTP	O6-C6-C5	-2.17	120.13	124.37
91	BA	3211	5GP	O6-C6-C5	-2.08	120.31	124.37
91	BA	3212	5GP	O6-C6-C5	-2.07	120.33	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	BA	3213	SPM	C7-C8-C9-N10

Continued on next page...

Continued from previous page...

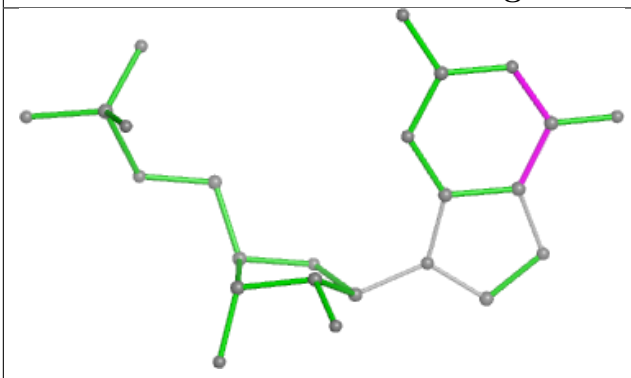
Mol	Chain	Res	Type	Atoms
92	BA	3214	SPM	N5-C6-C7-C8
93	Ag	500	GTP	O4'-C4'-C5'-O5'
93	Ag	500	GTP	C3'-C4'-C5'-O5'
92	AA	3001	SPM	C6-C7-C8-C9
92	BA	3214	SPM	C7-C8-C9-N10
92	BA	3214	SPM	C8-C9-N10-C11
92	AA	3001	SPM	C8-C9-N10-C11
91	BA	3212	5GP	C5'-O5'-P-O3P
92	BA	3213	SPM	C7-C6-N5-C4
91	BA	3211	5GP	O4'-C4'-C5'-O5'
92	BA	3213	SPM	C6-C7-C8-C9

There are no ring outliers.

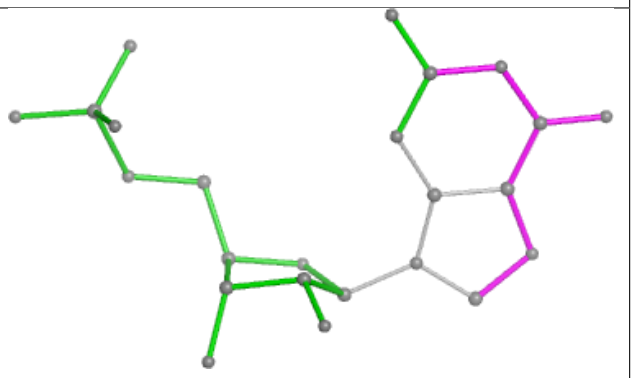
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

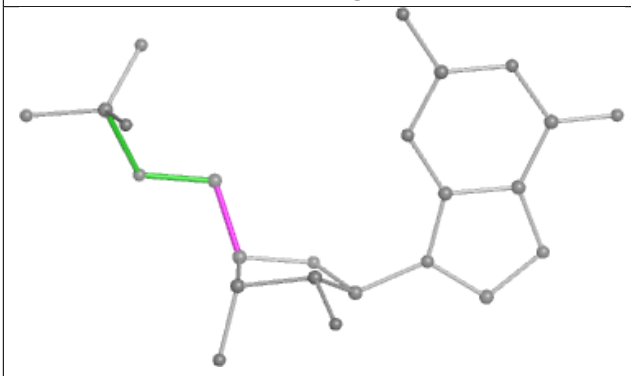
Ligand 5GP BA 3211



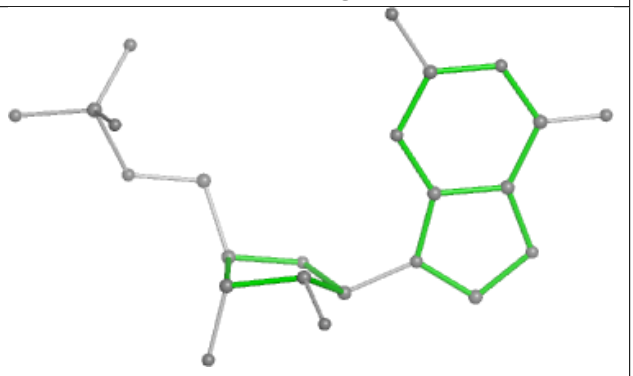
Bond lengths



Bond angles

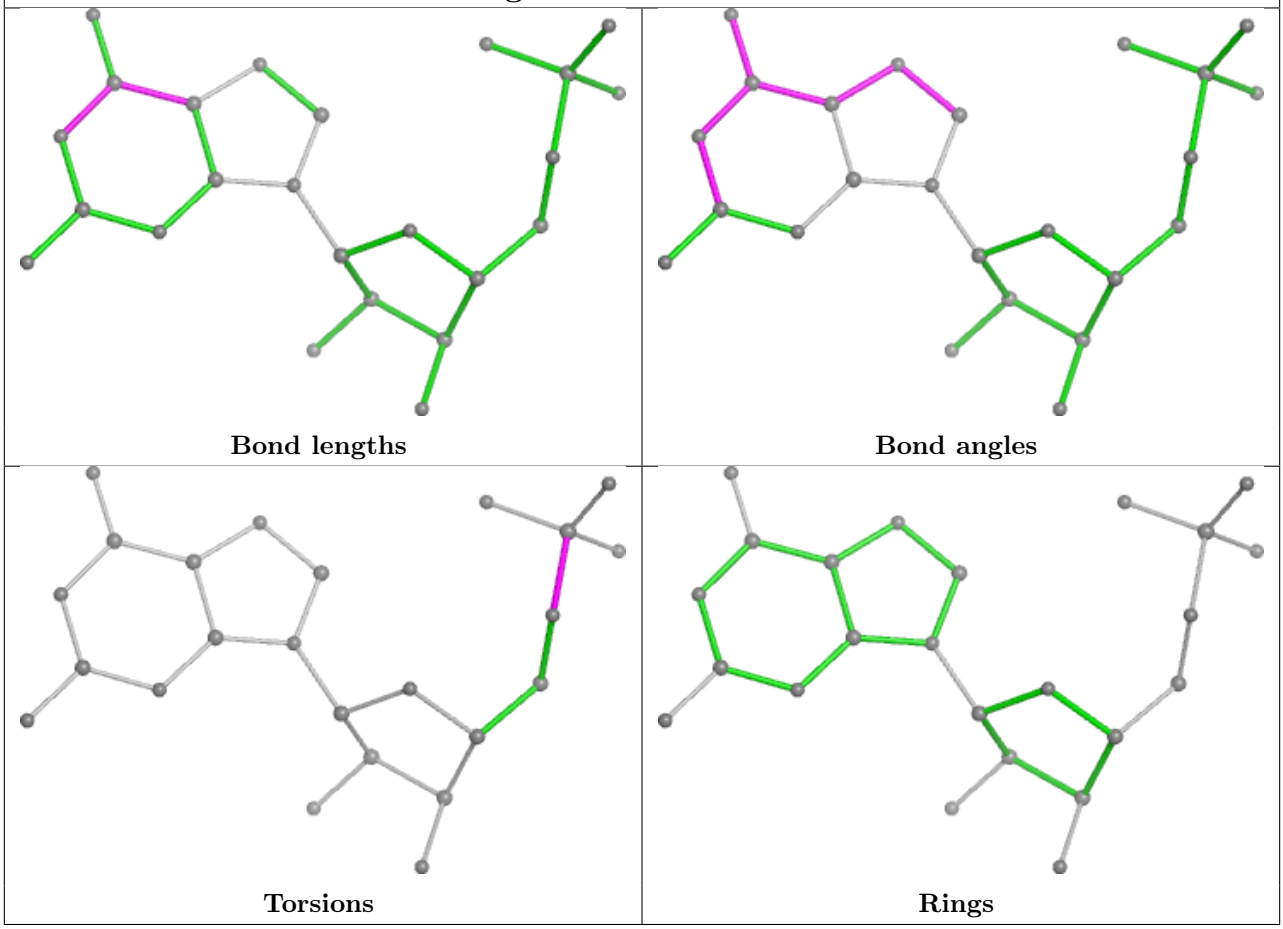


Torsions

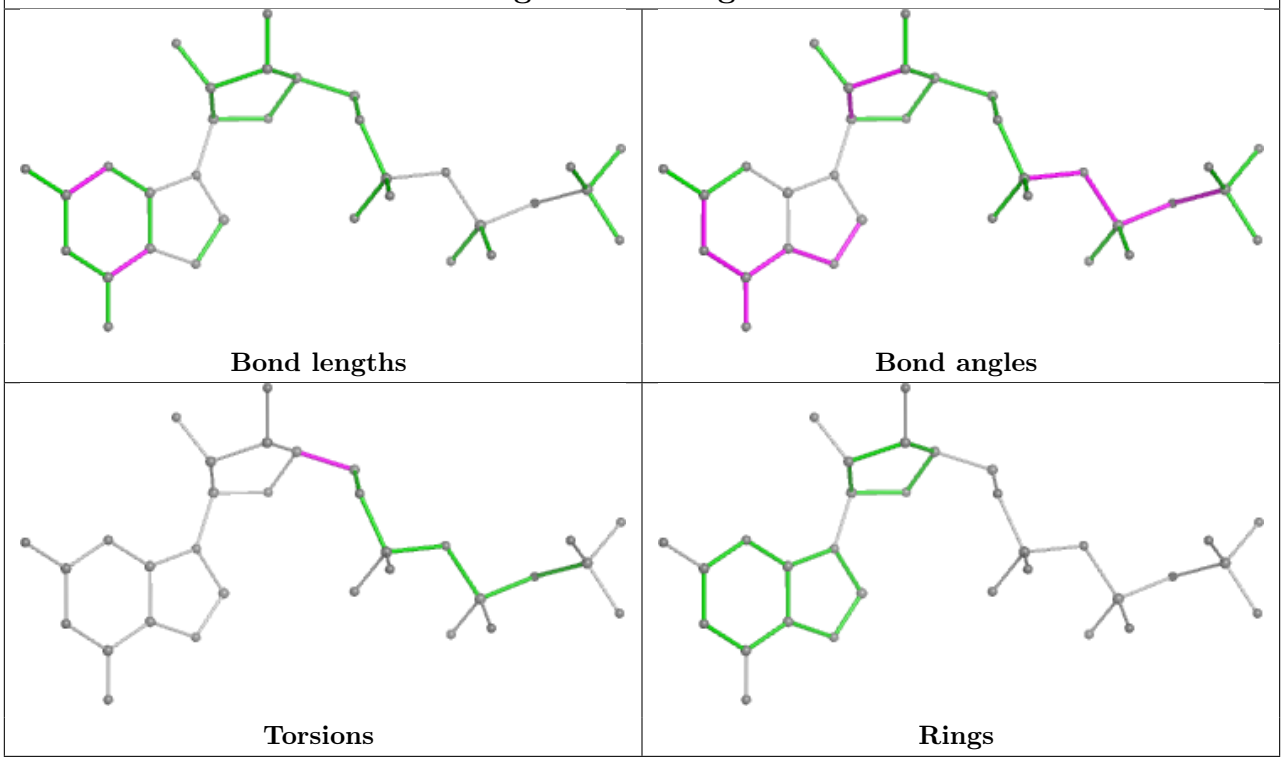


Rings

Ligand 5GP BA 3212



Ligand GTP Ag 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

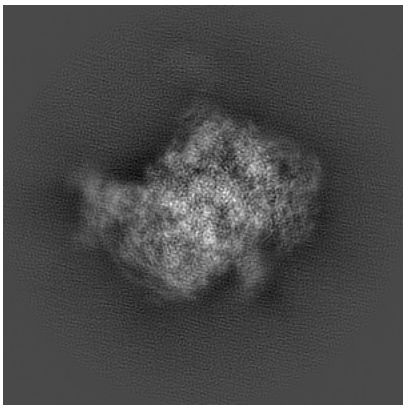
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12529. These allow visual inspection of the internal detail of the map and identification of artifacts.

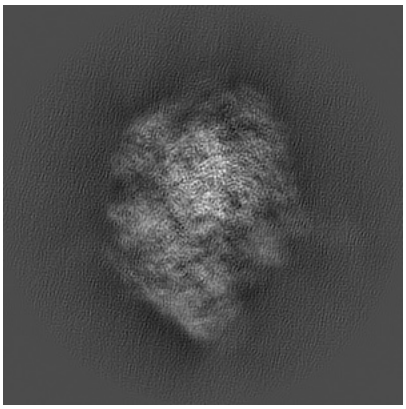
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

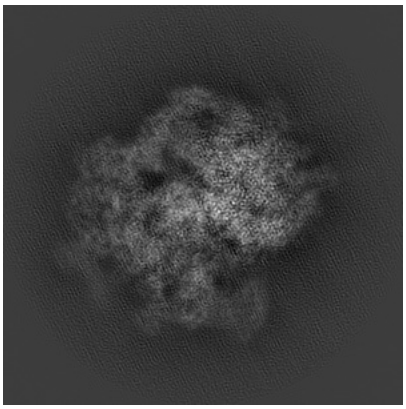
6.1.1 Primary map



X

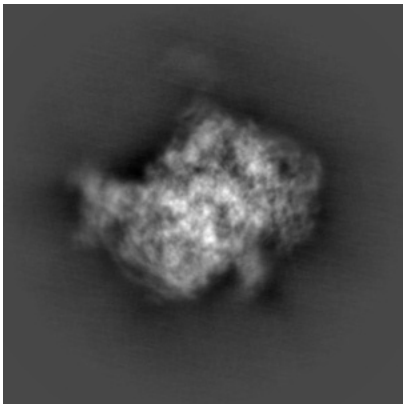


Y

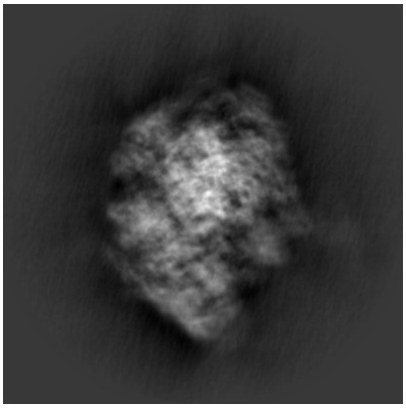


Z

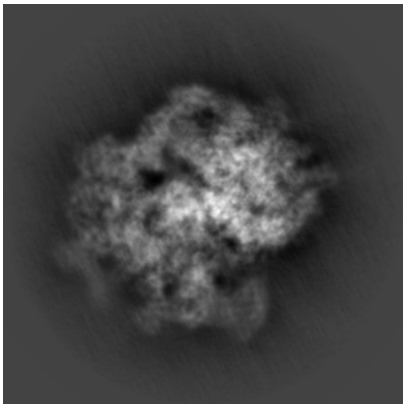
6.1.2 Raw map



X



Y

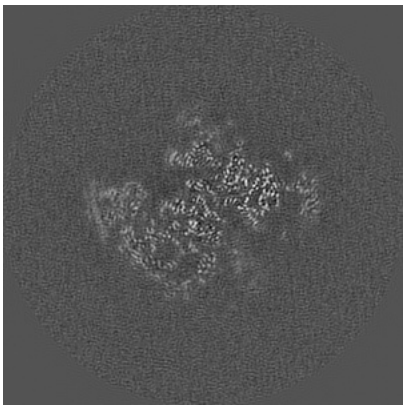


Z

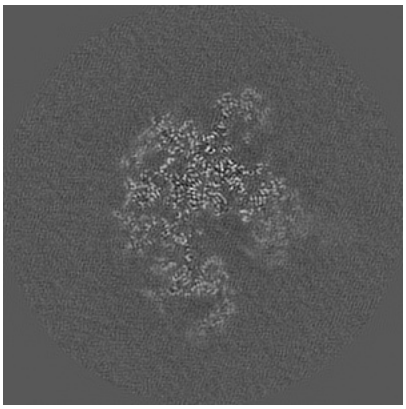
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

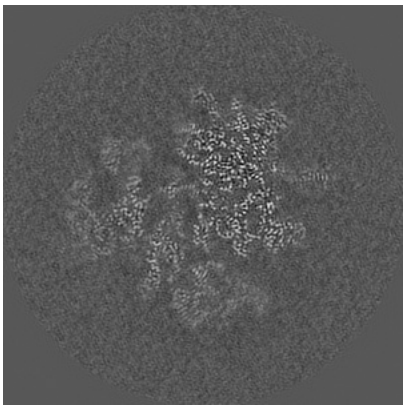
6.2.1 Primary map



X Index: 160

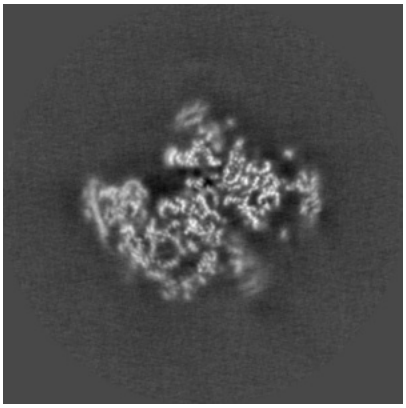


Y Index: 160

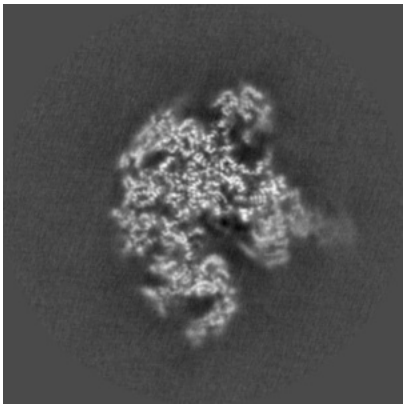


Z Index: 160

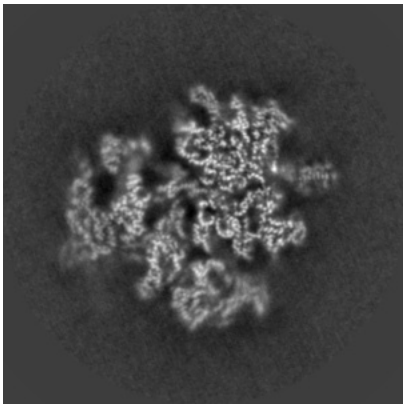
6.2.2 Raw map



X Index: 160



Y Index: 160

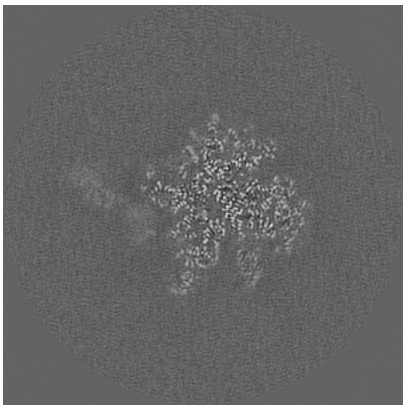


Z Index: 160

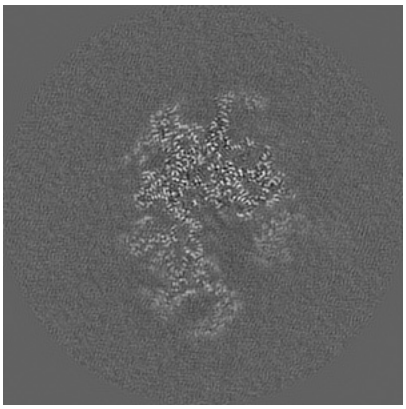
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

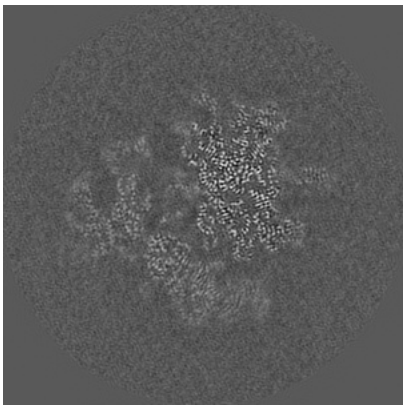
6.3.1 Primary map



X Index: 184

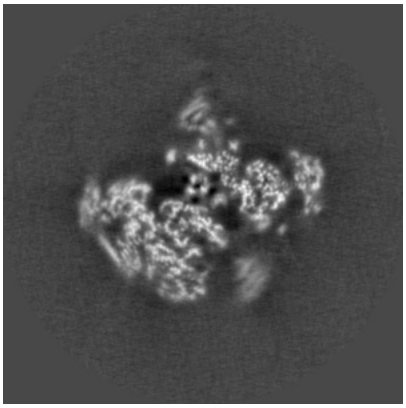


Y Index: 164

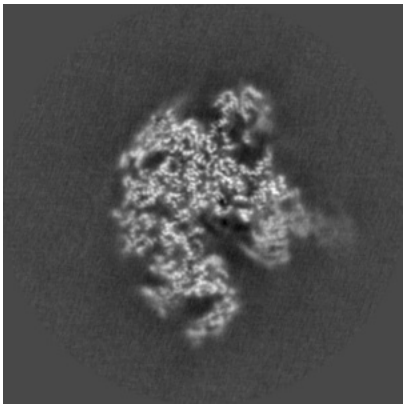


Z Index: 163

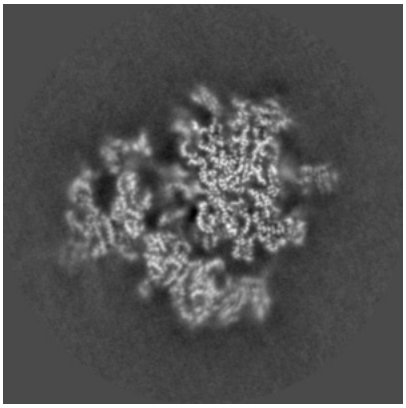
6.3.2 Raw map



X Index: 154



Y Index: 161

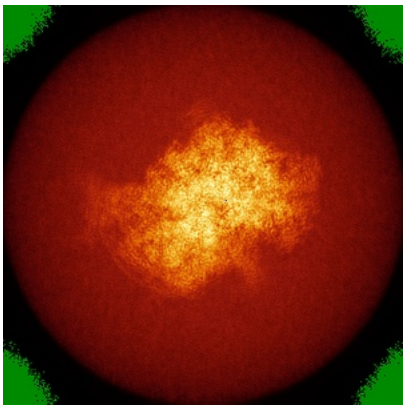


Z Index: 163

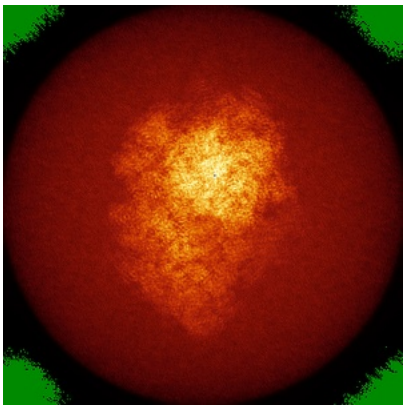
The images above show the largest variance slices of the map in three orthogonal directions.

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

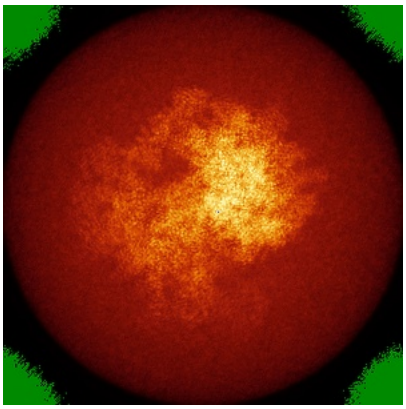
6.4.1 Primary map



X

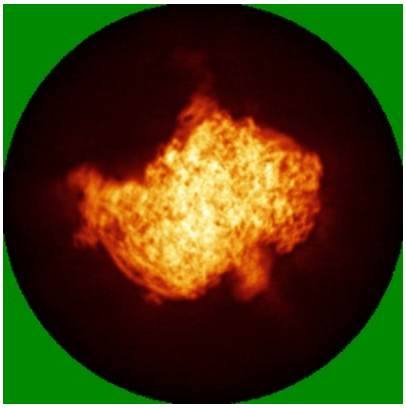


Y

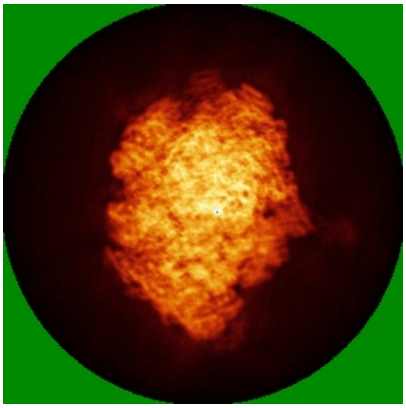


Z

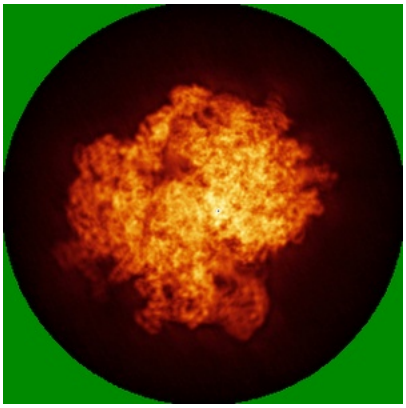
6.4.2 Raw map



X



Y

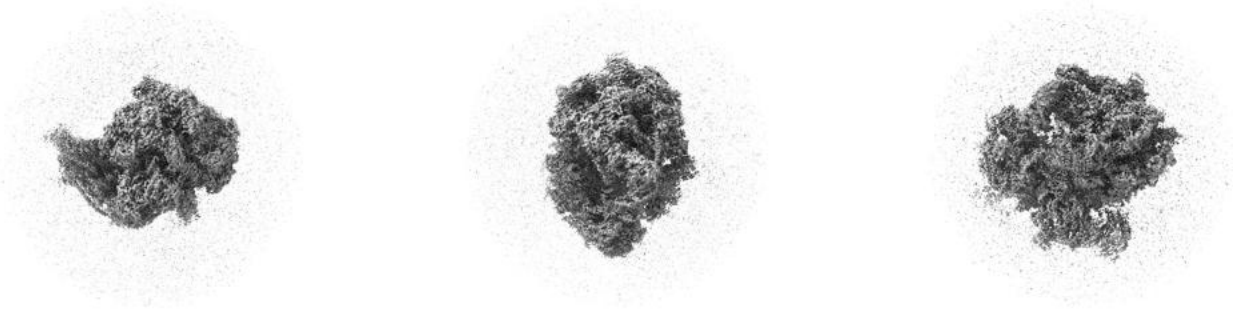


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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

X Y Z

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.

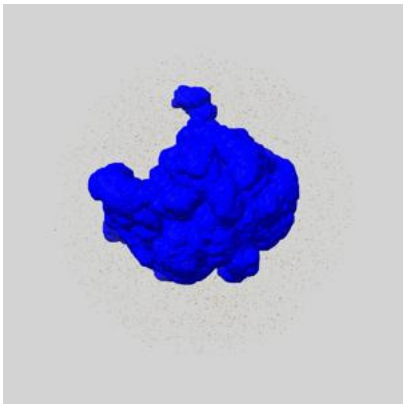
6.6 Mask visualisation

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

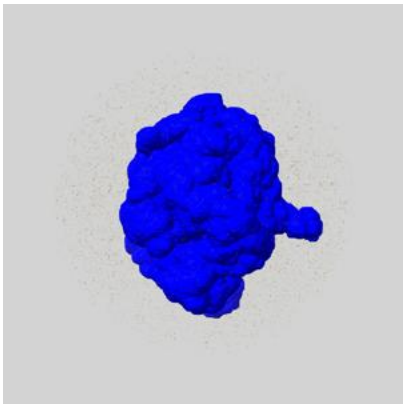
A mask typically either:

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

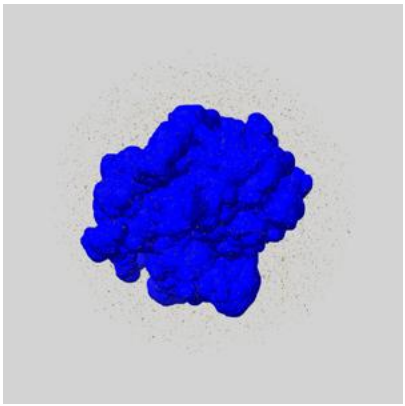
6.6.1 emd_12529_msk_1.map



X



Y

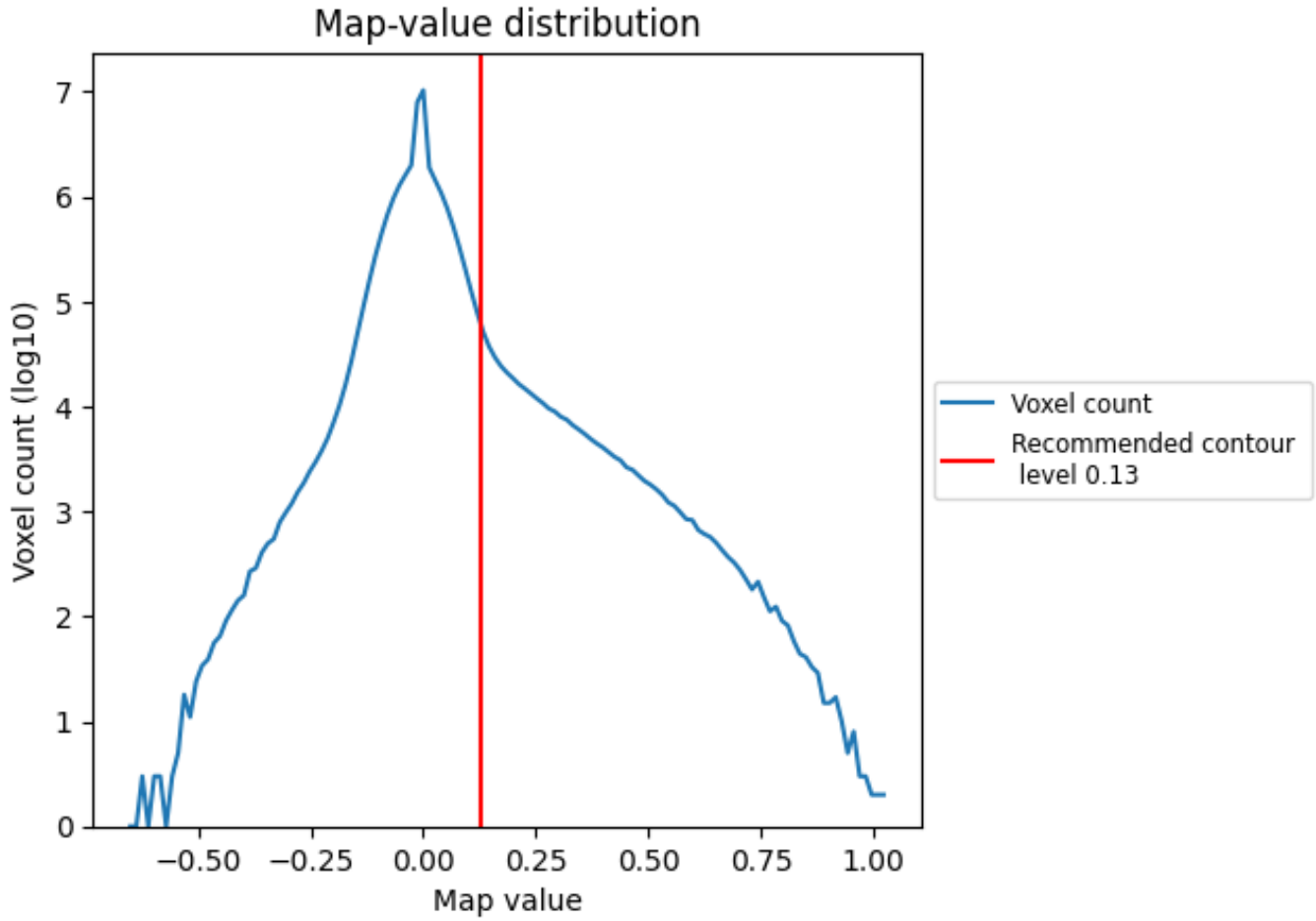


Z

7 Map analysis

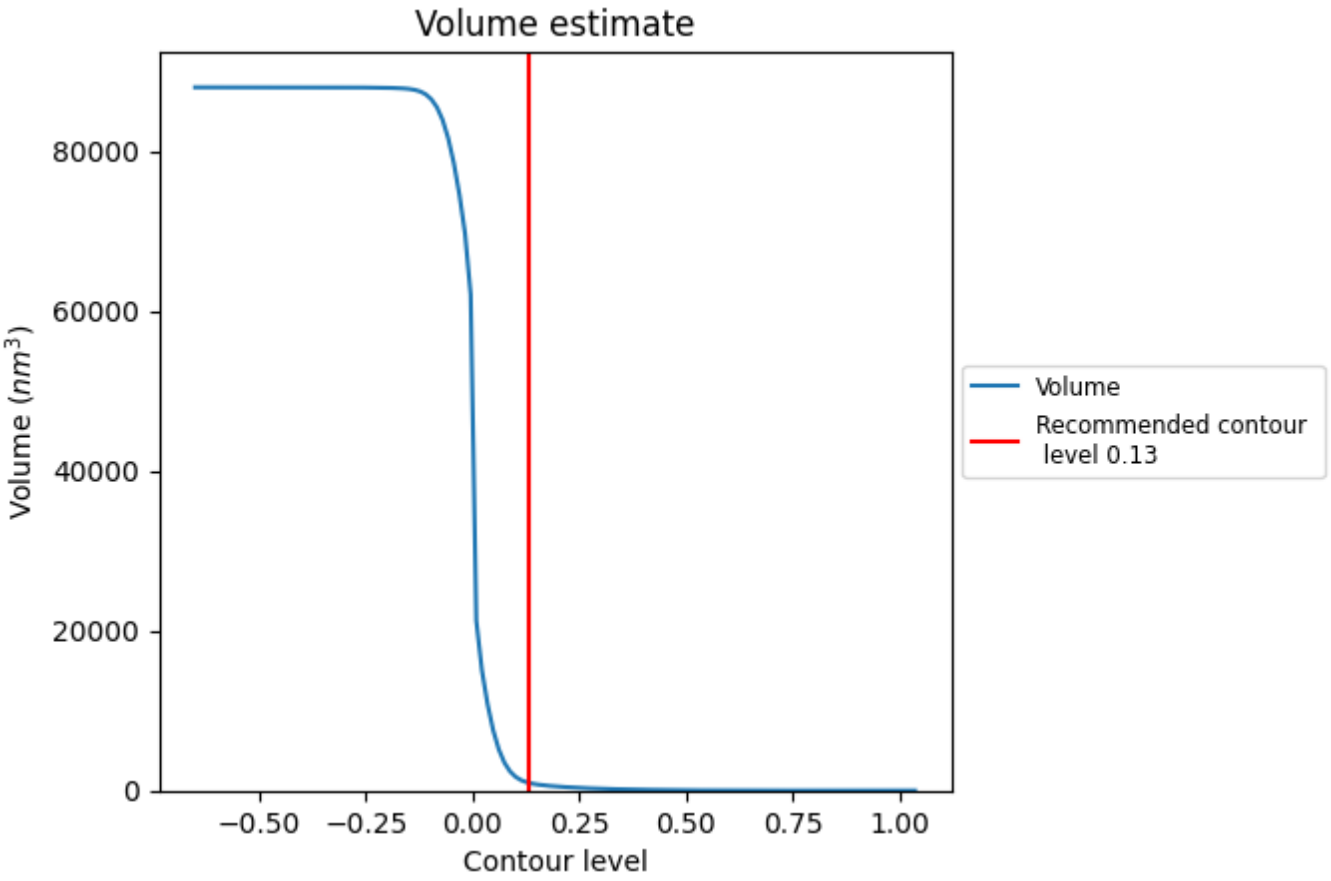
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

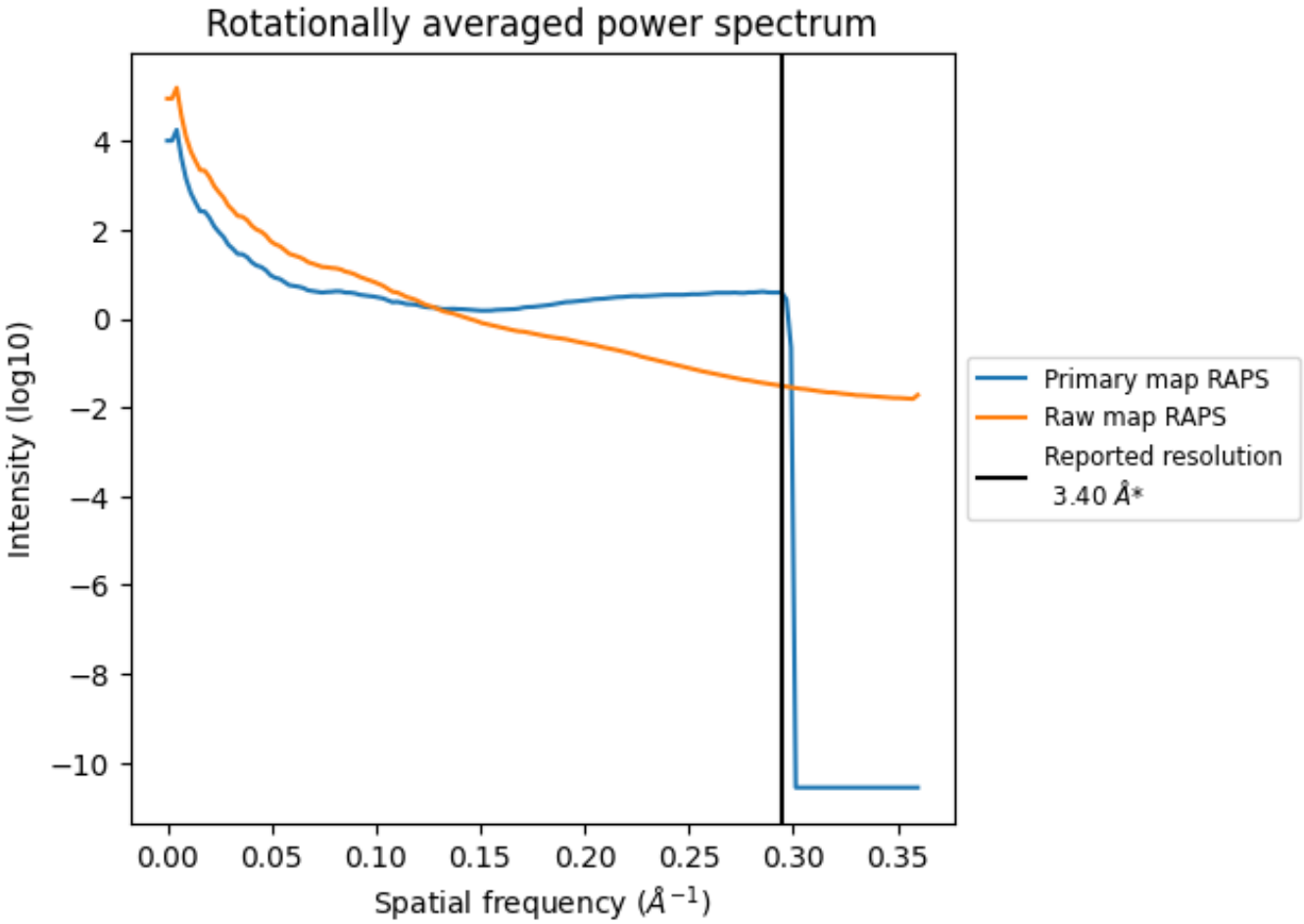
7.2 Volume estimate



The volume at the recommended contour level is 992 nm^3; this corresponds to an approximate mass of 897 kDa.

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

7.3 Rotationally averaged power spectrum (i)

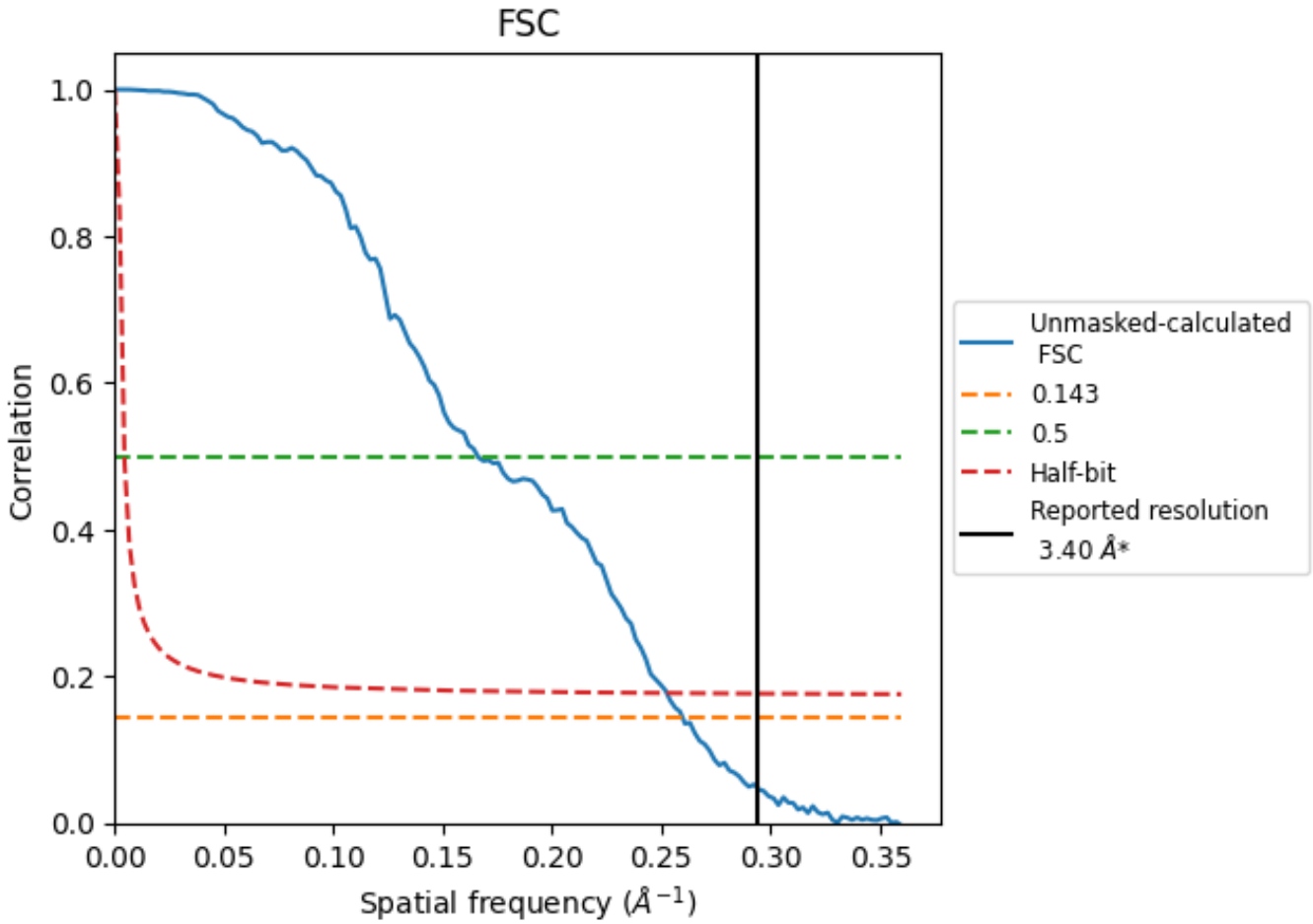


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

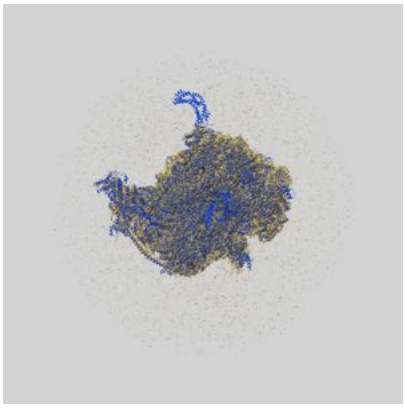
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	6.02	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.4 by more than 10 %

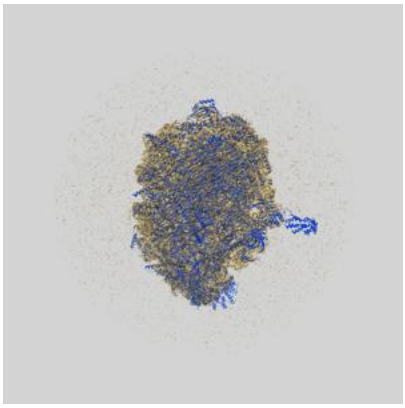
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12529 and PDB model 7NQL. Per-residue inclusion information can be found in section 3 on page 25.

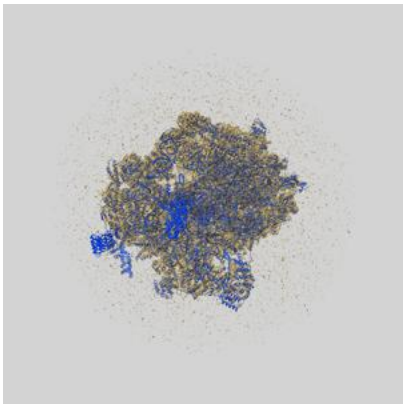
9.1 Map-model overlay



X



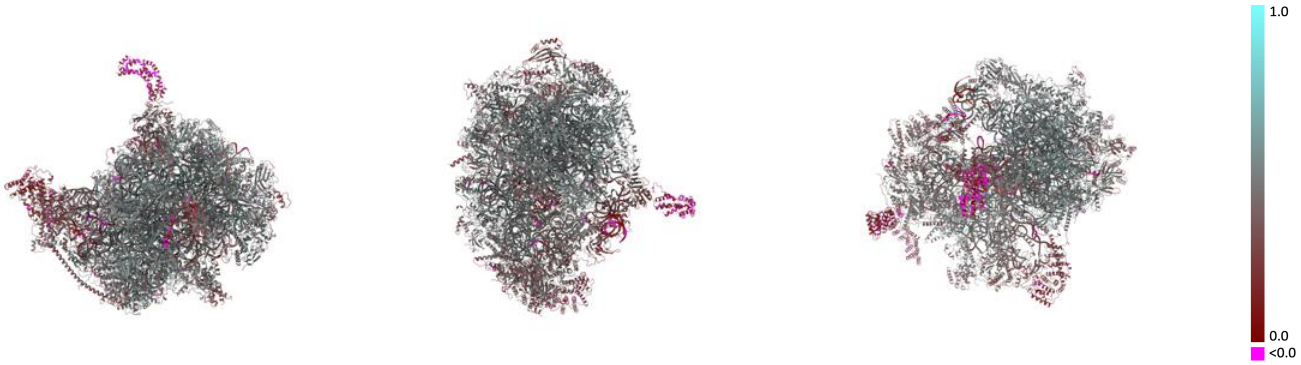
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

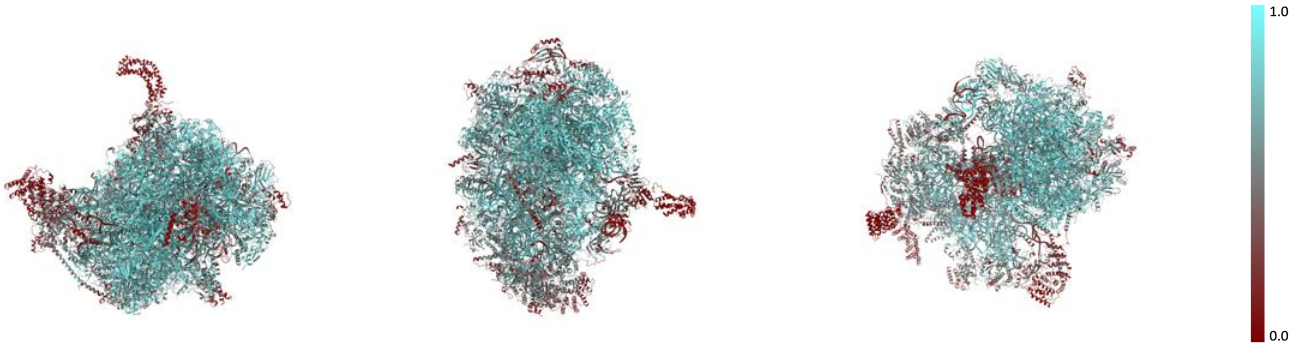
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

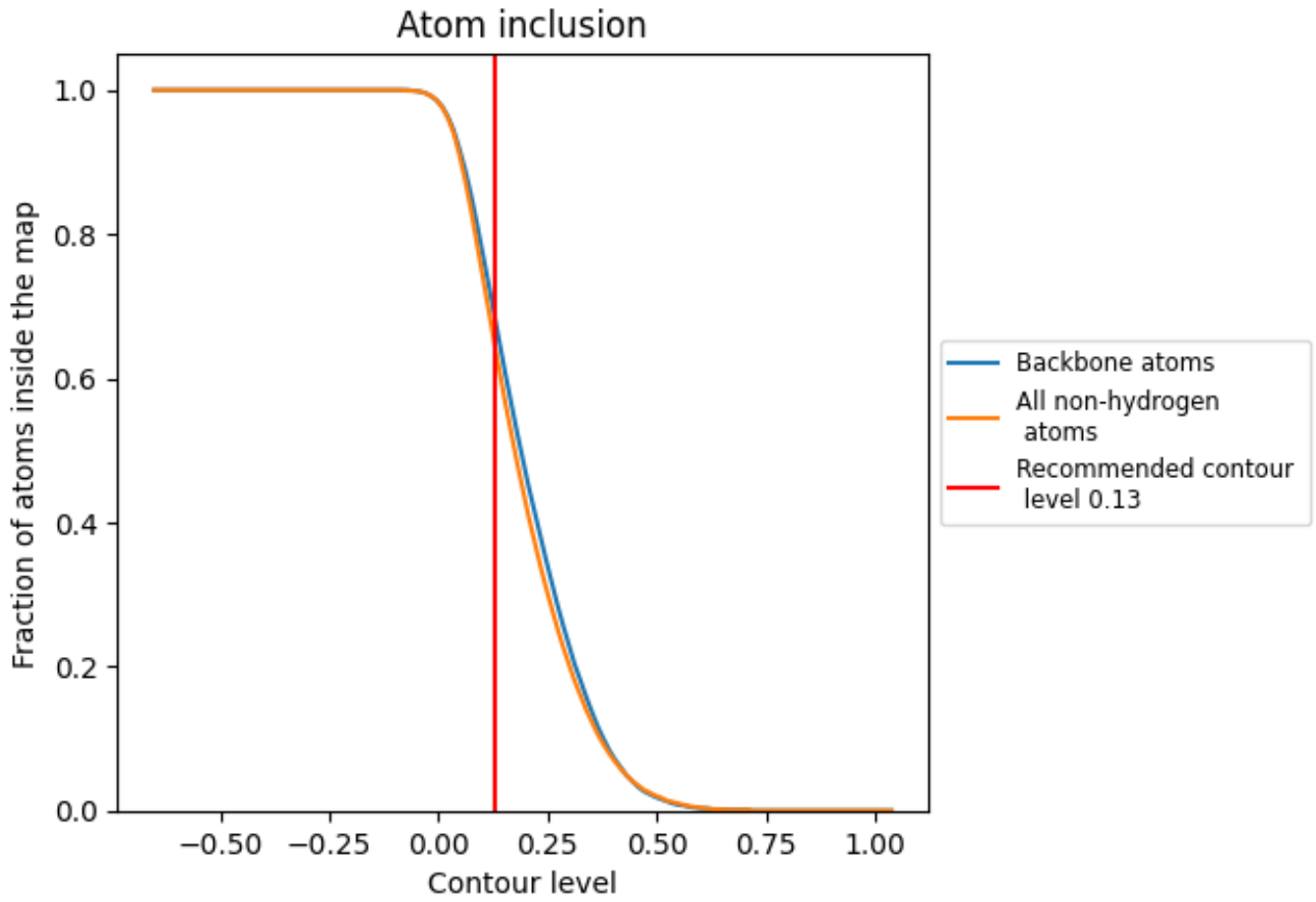
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6420	0.4370
AA	0.7650	0.4380
AB	0.6840	0.4670
AC	0.6190	0.4730
AE	0.5570	0.4510
AF	0.6700	0.4750
AG	0.5490	0.4250
AI	0.5230	0.4100
AJ	0.5500	0.4190
AK	0.6700	0.4770
AL	0.6400	0.4840
AN	0.6800	0.4640
AO	0.5520	0.4330
AP	0.5010	0.3880
AQ	0.6410	0.4620
AR	0.6560	0.4760
AU	0.7080	0.4840
AV	0.6020	0.3620
AX	0.7580	0.4820
AZ	0.3330	0.2130
Aa	0.3800	0.3680
Ab	0.4600	0.4010
Ac	0.6090	0.4400
Ad	0.4730	0.3740
Ae	0.1410	0.2260
Af	0.5650	0.4550
Ag	0.4680	0.3730
Ah	0.4130	0.3570
Ai	0.4960	0.4080
Aj	0.3000	0.3350
Ak	0.4400	0.3790
Am	0.5490	0.4370
An	0.6750	0.5050
Ao	0.0780	0.2060
Ap	0.5070	0.3980

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Chain	Atom inclusion	Q-score
B0	0.8310	0.5370
B1	0.5990	0.4580
B2	0.7020	0.4790
B3	0.8130	0.5250
B4	0.6220	0.4240
B5	0.7420	0.5020
B6	0.4350	0.4340
B7	0.8540	0.5460
B8	0.8430	0.5460
B9	0.8720	0.5440
BA	0.8320	0.4810
BB	0.5350	0.2780
BD	0.7830	0.5180
BE	0.7900	0.5160
BF	0.7670	0.5020
BI	0.4470	0.4260
BJ	0.2770	0.3110
BK	0.1230	0.2410
BL	0.7030	0.4940
BN	0.8280	0.5350
BO	0.7450	0.5080
BP	0.7560	0.4990
BQ	0.7740	0.5150
BR	0.7770	0.5200
BS	0.7680	0.5040
BT	0.6900	0.4910
BU	0.8020	0.5210
BV	0.7890	0.5190
BW	0.7590	0.5210
BX	0.6480	0.4650
BY	0.3520	0.3860
Ba	0.7320	0.4820
Bb	0.7320	0.4660
Bc	0.6420	0.4460
Bd	0.5270	0.3800
Be	0.5600	0.4430
Bf	0.6880	0.4540
Bg	0.7870	0.5140
Bh	0.6970	0.4720
Bi	0.2860	0.3600
Bj	0.4720	0.3200
Bk	0.5550	0.4230

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Chain	Atom inclusion	Q-score
Bl	0.7750	0.5020
Bm	0.2760	0.3810
Bn	0.7940	0.5190
Bo	0.7340	0.4900
Bp	0.3290	0.3560
Bq	0.3680	0.3810
Bt	0.7990	0.5180
Bu	0.4600	0.3940
Bv	0.4510	0.4080
Bw	0.7320	0.4860
Bx	0.7240	0.4710
CL	0.0090	0.1130
DL	0.0050	0.1040
EL	0.0000	0.0740
FL	0.0000	0.0320
GL	0.0000	0.0010
HL	0.0000	0.0060