Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 03:32 am GMT

PDB ID	:	6GAW
EMDB ID	:	EMD-4368
Title	:	Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the complete 55S ribosome.
Authors	:	Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on	:	2018-04-13
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

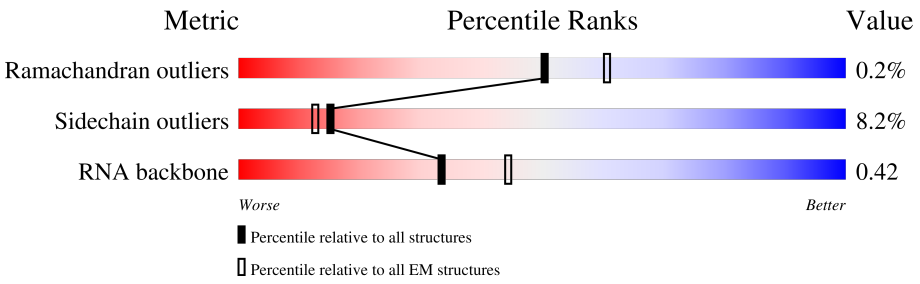
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	BL	198	35% / 35% / 65%
1	CL	198	21% / 21% / 77%
1	DL	198	14% / 13% / 86%
1	EL	198	14% / 13% / 86%
1	FL	198	14% / 13% / 86%
1	GL	198	14% / 13% / 86%
1	HL	198	13% / 12% / 87%
2	B0	148	70% / 26%

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Mol	Chain	Length	Quality of chain
3	B1	256	6% 86% 9% 5%
4	B2	252	65% 6% 29%
5	B3	161	68% 6% 27%
6	B4	126	11% 31% 5% 64%
7	B5	188	53% 5% 41%
8	B6	65	14% 77% 20%
9	B7	95	45% 52%
10	B8	188	44% 6% 49%
11	B9	100	34% 62%
12	BA	1571	68% 29%
13	BB	73	38% 58% 34% 8%
14	BC	650	38% 86% 12%
15	BD	306	72% 7% 22%
16	BE	348	80% 8% 12%
17	BF	294	77% 8% 15%
18	BI	268	6% 34% 63%
19	BJ	262	31% 78% 19%
20	BK	192	66% 89% 8%
21	BN	178	90% 9%
22	BO	145	71% 8% 21%
23	BP	296	87% 10%
24	BQ	251	83% 5% 12%
25	BR	169	83% 8% 9%
26	BS	180	76% 21%
27	BT	292	9% 75% 7% 18%

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Mol	Chain	Length	Quality of chain
28	BU	149	89% 5% 6%
29	BV	209	68% 6% 26%
30	BW	210	74% 5% 21%
31	BX	150	16% 92% 7%
32	BY	216	17% 86% 9% 5%
33	Ba	423	85% 8% 7%
34	Bb	380	85% 8% 7%
35	Bc	334	6% 84% 12%
36	Bd	206	18% 43% 5% 52%
37	Be	135	8% 79% 11% 10%
38	Bf	142	15% 65% 9% 24%
39	Bg	159	81% 13% 7%
40	Bh	332	80% 8% 13%
41	Bi	306	23% 80% 5% 15%
42	Bj	279	49% 73% 5% 22%
43	Bk	212	19% 60% 36%
44	Bl	166	73% 7% 20%
45	Bm	159	28% 65% 31%
46	Bn	128	67% 9% 24%
47	Bo	124	73% 6% 22%
48	Bp	112	22% 83% 13%
49	Bq	138	24% 45% 51%
50	Bt	102	78% 14% 8%
51	Bu	205	20% 67% 6% 26%
52	Bv	222	11% 59% 39%

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Mol	Chain	Length	Quality of chain
53	Bw	433	5% 81% 8% 11%
54	Bx	196	9% 75% 7% 17%
55	Bz	82	96% 100%
56	AA	962	9% 75% 25%
57	AB	289	8% 72% 24%
58	AC	167	30% 69% 10% 21%
59	AE	430	26% 74% 5% 20%
60	AF	124	7% 90% 9%
61	AG	242	55% 80% 6% 14%
62	AI	397	48% 78% 5% 17%
63	AJ	201	48% 62% 7% 30%
64	AK	196	7% 65% 5% 30%
65	AL	139	5% 76% 22%
66	AN	128	25% 68% 11% 21%
67	AO	239	15% 69% 5% 27%
68	AP	135	22% 84% 13%
69	AQ	130	10% 78% 8% 14%
70	AR	143	7% 63% 5% 32%
71	AU	87	87% 11%
72	AV	71	58% 65% 34%
73	AX	201	7% 92%
74	AZ	18	89% 100%
75	Aa	382	41% 70% 7% 24%
76	Ab	190	27% 67% 29%
77	Ac	173	18% 91% 7%

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Mol	Chain	Length	Quality of chain
78	Ad	205	28% 82% 14%
79	Ae	455	82% 79% 6% 15%
80	Af	188	11% 49% 47%
81	Ag	397	77% 84% 5% 11%
82	Ah	387	26% 30% 69%
83	Ai	106	51% 89% 5% 7%
84	Aj	218	70% 93% 5%
85	Ak	325	68% 78% 7% 15%
86	Am	118	38% 88% 10%
87	An	199	32% 64%
88	Ao	692	78% 80% 17%
89	Ap	258	28% 67% 7% 26%

2 Entry composition (i)

There are 98 unique types of molecules in this entry. The entry contains 178372 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	CL	45	317	203	52	62	0	0
1	DL	27	213	137	33	43	0	0
1	EL	28	222	143	35	44	0	0
1	FL	27	213	137	33	43	0	0
1	GL	27	213	137	33	43	0	0
1	HL	26	205	131	32	42	0	0
1	BL	70	537	346	93	98	0	0

- Molecule 2 is a protein called Mitochondrial ribosomal protein L27.

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

- Molecule 3 is a protein called Mitochondrial ribosomal protein L28.

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

- Molecule 4 is a protein called Mitochondrial ribosomal protein L47.

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

- Molecule 5 is a protein called uL30m.

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

- Molecule 6 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B4	45	381	239	77	62	3	0	0

- Molecule 7 is a protein called bL32m.

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

- Molecule 8 is a protein called bL33m.

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

- Molecule 9 is a protein called Mitochondrial ribosomal protein L34.

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

- Molecule 10 is a protein called Mitochondrial ribosomal protein L35.

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

- Molecule 11 is a protein called Ribosomal protein.

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

- Molecule 12 is a RNA chain called 16S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	BA	1549	32950	14798	5993	10610	1549	0	0

- Molecule 13 is a RNA chain called tRNA-Phe, mitochondrial.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	71	C	-	insertion	GB 76262549
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 14 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BC	571	4364	2743	765	839	17	0	0

- Molecule 15 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 16 is a protein called ICT1.

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

- Molecule 17 is a protein called Mitochondrial ribosomal protein L4.

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

- Molecule 18 is a protein called Mitochondrial ribosomal protein L9.

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

- Molecule 19 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 20 is a protein called Mitochondrial ribosomal protein L11.

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

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 22 is a protein called uL14m.

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

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 26 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L19.

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

- Molecule 28 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 29 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 30 is a protein called uL22m.

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

- Molecule 31 is a protein called uL23m.

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

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 33 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 34 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 35 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 36 is a protein called 39S ribosomal protein L40, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Bd	99	832	528	148	155	1	0	0

- Molecule 37 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 38 is a protein called mL42.

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

- Molecule 39 is a protein called mL43.

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

- Molecule 40 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 41 is a protein called mL45.

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

- Molecule 42 is a protein called Mitochondrial ribosomal protein L46.

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

- Molecule 43 is a protein called Mitochondrial ribosomal protein L48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Bk	136	1087	692	185	205	5	0	0

- Molecule 44 is a protein called 39S ribosomal protein L49, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 45 is a protein called mL50.

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

- Molecule 46 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 47 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 48 is a protein called mL53.

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

- Molecule 49 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Bq	68	542	344	102	95	1	0	0

- Molecule 50 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 51 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 52 is a protein called mL64.

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

- Molecule 53 is a protein called mL65.

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

- Molecule 54 is a protein called Mitochondrial ribosomal protein S18A.

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

- Molecule 55 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	Bz	82	410	246	82	82	0	0

- Molecule 56 is a RNA chain called 12S ribosomal RNA, mitochondrial.

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

- Molecule 57 is a protein called Mitochondrial ribosomal protein S2.

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

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

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

- Molecule 59 is a protein called Mitochondrial ribosomal protein S5.

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

- Molecule 60 is a protein called Mitochondrial ribosomal protein S6.

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

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

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

- Molecule 62 is a protein called 28S ribosomal protein S9, mitochondrial.

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

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

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

- Molecule 64 is a protein called 28S ribosomal protein S11, mitochondrial.

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

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

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

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

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

- Molecule 67 is a protein called Uncharacterized protein.

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

- Molecule 68 is a protein called bS16m.

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

- Molecule 69 is a protein called uS17m.

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

- Molecule 70 is a protein called Mitochondrial ribosomal protein S18C.

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

- Molecule 71 is a protein called bS21m.

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

- Molecule 72 is a RNA chain called P-site fMet-tRNAMet, mitochondrial.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1390216722
AV	70	C	-	insertion	GB 1390216722
AV	71	A	-	insertion	GB 1390216722

- Molecule 73 is a RNA chain called MT-CO3 mRNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
73	AX	17	354	161	65	112	16	0	0

- Molecule 74 is a protein called unassigned secondary structure elements.

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

- Molecule 75 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 76 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 77 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 78 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 79 is a protein called mS27.

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

- Molecule 80 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 81 is a protein called Death associated protein 3.

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

- Molecule 82 is a protein called mS31.

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

- Molecule 83 is a protein called mS33.

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

- Molecule 84 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 85 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 86 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 87 is a protein called Aurora kinase A interacting protein 1.

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

- Molecule 88 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 89 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
90	B3	1	1	1	0
90	BA	202	202	202	0
90	BB	1	1	1	0
90	BC	2	2	2	0
90	BD	3	3	3	0

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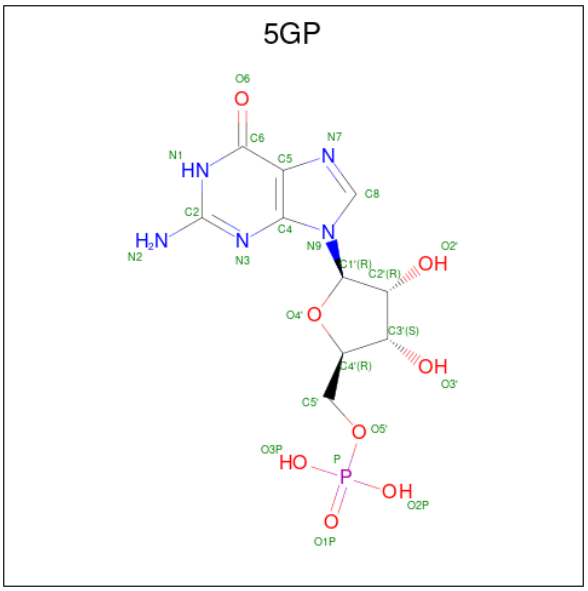
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
90	BE	1	1	1	0
90	BJ	1	1	1	0
90	BP	2	2	2	0
90	Be	1	1	1	0
90	Bl	1	1	1	0
90	Bt	2	2	2	0
90	AA	105	105	105	0
90	AB	1	1	1	0
90	AX	1	1	1	0
90	Ag	1	1	1	0
90	An	1	1	1	0

- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

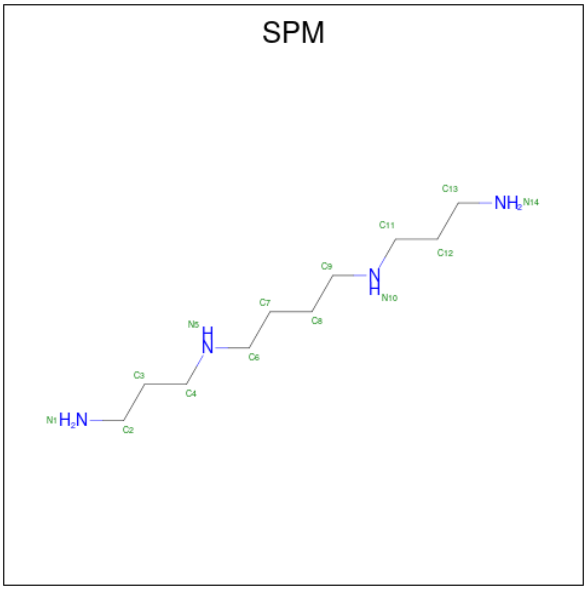
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
91	B5	1	1	1	0
91	B9	1	1	1	0
91	Bx	1	1	1	0
91	AR	1	1	1	0
91	Ac	1	1	1	0
91	Ap	1	1	1	0

- Molecule 92 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	BA	1	48	20	10	16	2	0
			Total	C	N	O	P	
92	BA	1	48	20	10	16	2	0

- Molecule 93 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
93	BA	1	14	10	4	0
			Total	C	N	
93	BR	1	14	10	4	0

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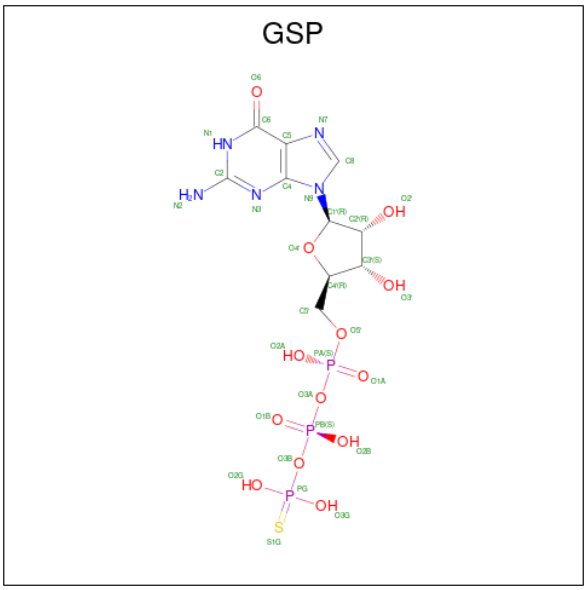
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
93	AA	1	14	10	4	0

- Molecule 94 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

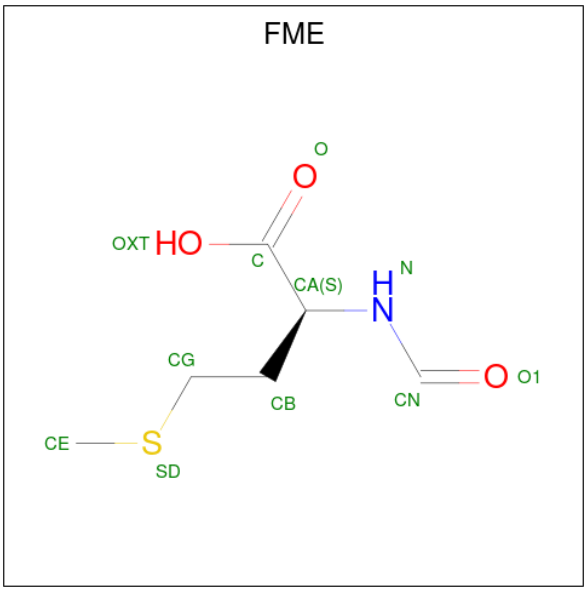


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
94	BC	1	32	10	5	13	3	1	0

- Molecule 95 is SODIUM ION (three-letter code: NA) (formula: Na).

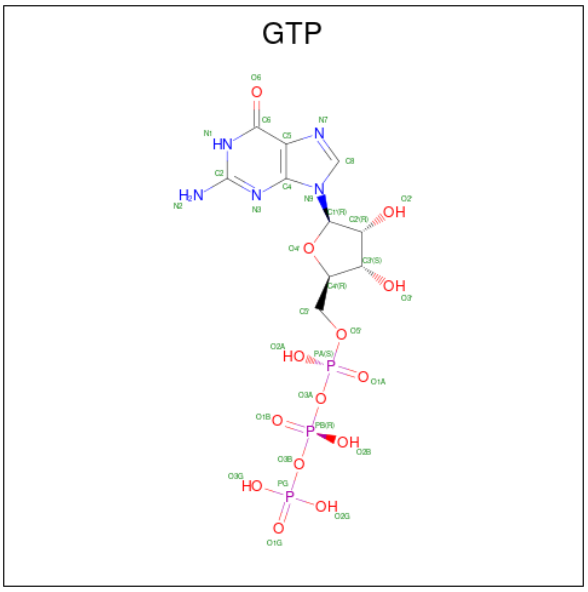
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
95	BC	1	1	1	0

- Molecule 96 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
96	AV	1	10	6	1	2	1	0

- Molecule 97 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
98	BC	2	2	2	0
			Total	O	
98	Ag	3	3	3	0

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 L12

Chain CL: 21% 21% 77%

MET LEU PRO ALA ALA ALA SER SER LEU TRP GLY PRO CYS PHE GLY LEU ARG ALA ALA ALA LEU ARG VAL ALA ARG HIS GLN GLY PRO ARG LEU CYS GLY VAL ARG LEU MET ARG CYS SER SER HIS ARG LYS GLY E10 A11 L12 A13 G14 A15 P16 L17 D18 N19 A20 P21 K22 E23 Y24

P25 P26 K27 I28 Q29 Q30 L31 V32 Q33 D34 I35 A36 S37 L38 T39 L40 L41 E42 I43 S44 D45 L46 N47 E48 L49 L50 K51 K52 T53 L54 LYS ILE GLN ASP VAL GLY PHE MET PRO MET GLY ALA VAL ALA PRO GLY ALA PRO PRO ALA ALA ALA ALA PRO GLU ALA ALA GLU GLU ASP

LEU PRO LYS ARG LYS GLU GLN THR HIS PHE THR VAL ARG LEU THR GLU ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE LYS SER HIS ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL PRO LYS ALA GLU

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

• Molecule 1: Mitochondrial ribosomal protein L12

Chain DL: 14% 13% 86%

MET LEU PRO ALA ALA SER SER LEU TRP GLY PRO CYS PHE GLY LEU ARG ALA ALA ALA LEU ARG VAL ALA ARG HIS GLN GLY PRO ARG LEU CYS GLY VAL ARG LEU MET ARG CYS SER SER HIS ARG LYS GLY GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU TYR

PRO PRO LYS I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 LYS ILE GLN ASP VAL GLY PHE MET PRO MET GLY ALA VAL ALA PRO GLY ALA PRO PRO ALA ALA ALA ALA PRO GLU ALA ALA GLU GLU ASP

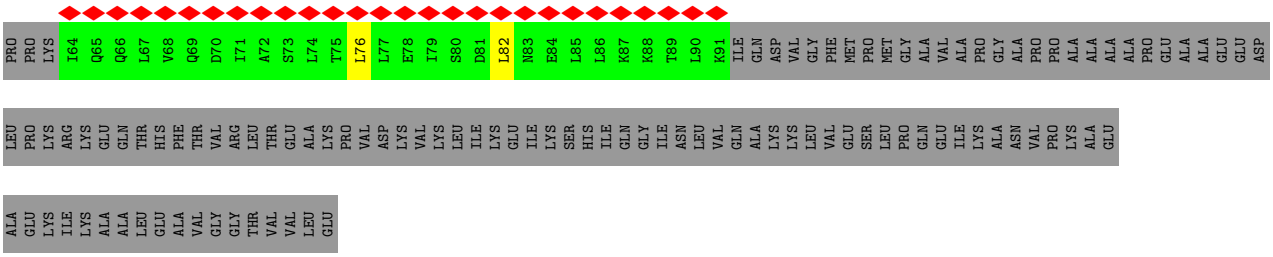
LEU PRO LYS ARG LYS GLU GLN THR HIS PHE THR VAL ARG LEU THR GLU ALA LYS PRO VAL ASP LYS VAL LYS LEU ILE LYS GLU ILE LYS SER HIS ILE GLN GLY ILE ASN LEU VAL GLN ALA LYS LYS LEU VAL GLU SER LEU PRO GLN GLU ILE LYS ALA ASN VAL PRO LYS ALA GLU

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

• Molecule 1: Mitochondrial ribosomal protein L12

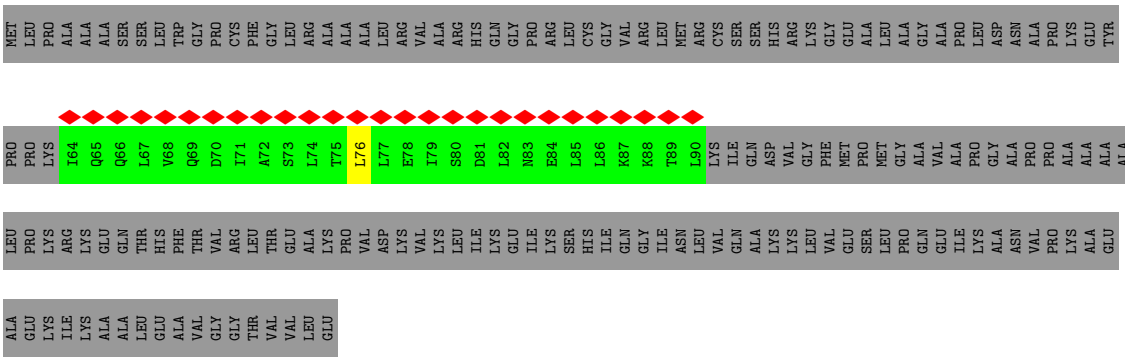
Chain EL: 14% 13% 86%

MET LEU PRO ALA ALA ALA SER SER LEU TRP GLY PRO CYS PHE GLY LEU ARG ALA ALA ALA LEU ARG VAL ALA ARG HIS GLN GLY PRO ARG LEU CYS GLY VAL ARG LEU MET ARG CYS SER SER HIS ARG LYS GLY GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU TYR



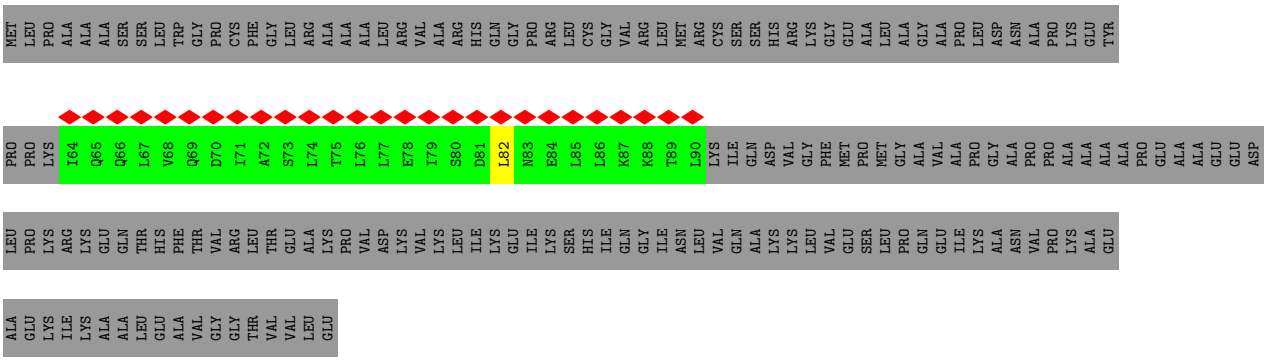
- Molecule 1: Mitochondrial ribosomal protein L12

Chain FL:



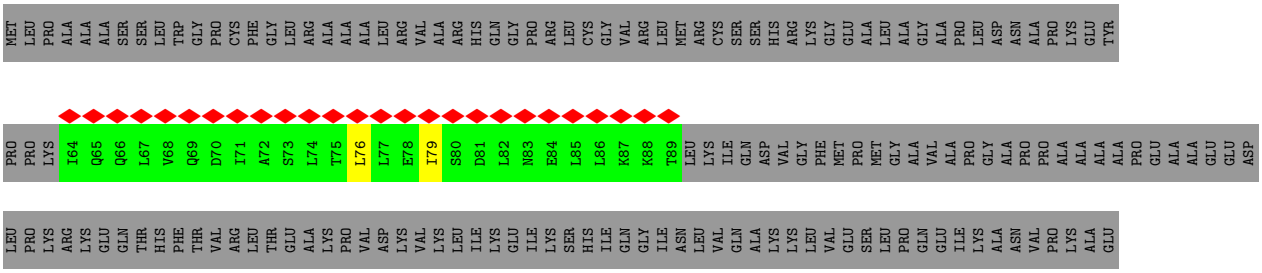
- Molecule 1: Mitochondrial ribosomal protein L12

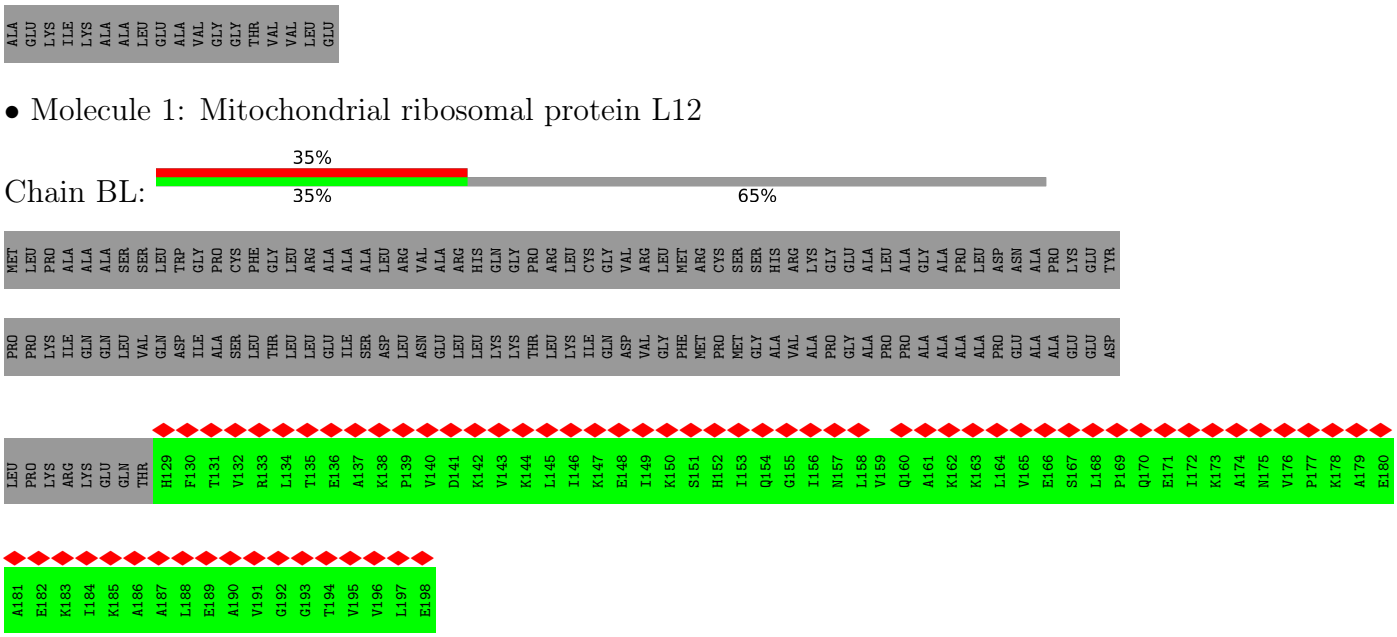
Chain GL:

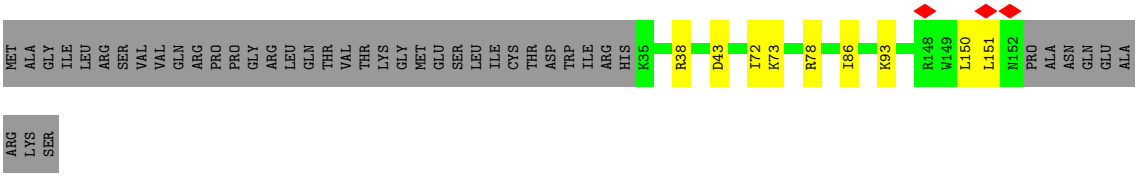


- Molecule 1: Mitochondrial ribosomal protein L12

Chain HL:

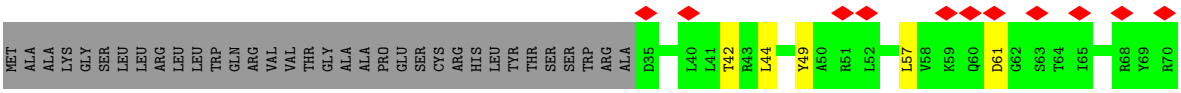


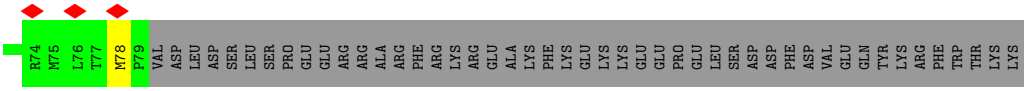

ALA GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU
• Molecule 1: Mitochondrial ribosomal protein L12
Chain BL:
35%
35%
65%
MET LEU PRO ALA ALA ALA SER SER LEU TRP GLY PRO CYS PHE GLY LEU ARG ALA ALA ALA LEU ARG VAL ALA ARG HIS GLN GLY PRO ARG LEU CYS GLY VAL ARG LEU MET ARG CYS SER SER HIS ARG LYS GLY GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU TYR
PRO PRO LYS ILE GLN GLN LEU VAL GLN ASP ILE ALA SER LEU THR LEU LEU GLU ILE SER ASP LEU ASN VAL GLU LEU LEU LYS LYS THR LEU LYS ILE GLN ASP VAL GLY PHE MET PRO MET GLY ALA VAL ALA PRO GLY ALA PRO PRO ALA ALA ALA PRO GLU ALA ALA GLU GLU ASP
LEU PRO LYS ARG LYS GLU GLN THR H129 F130 T131 V132 R133 L134 T135 E136 A137 K138 P139 V140 D141 K142 V143 K144 L145 I146 K147 E148 I149 K150 S151 H152 I153 Q154 G155 I156 N157 L158 V159 Q160 A161 K162 K163 L164 V165 E166 S167 L168 P169 Q170 E171 I172 K173 A174 N175 V176 P177 K178 A179 E180
A181 E182 K183 I184 K185 A186 A187 L188 E189 A190 V191 G192 G193 T194 V195 V196 L197 E198
• Molecule 2: Mitochondrial ribosomal protein L27
Chain B0:
70%
26%
MET ALA LEU ALA VAL LEU ALA LEU ARG THR ARG ALA ALA VAL THR ALA LEU LEU SER PRO PRO GLN ALA ALA ALA LEU ALA VAL ARG TYR ALA SER LYS LYS THR GLY GLY SER S39 K40 K45 R50 I53 C88 L126 T141 L148
• Molecule 3: Mitochondrial ribosomal protein L28
Chain B1:
6%
86%
9%
5%
MET P2 V6 R15 L16 W17 R26 R30 S31 L32 E33 E34 A35 R36 H46 R61 D64 S75 Q76 L77 G78 L79 V104 R112 D120 T126 T148 D152 L161 Q172 H177 P178 D179 D189 R190 D209 R216 D222 P223
I224 Q237 L238 Q241 A242 L243 S244 E245 PRO ALA VAL VAL GLN THR ARG ALA SER ARG LYS
• Molecule 4: Mitochondrial ribosomal protein L47
Chain B2:
65%
6%
29%
MET ALA ALA ALA GLY LEU ALA VAL PHE CYS ARG ARG VAL SER ALA ALA LEU LYS ALA CYS ARG LEU LEU ILE ARG PRO GLN ALA PRO PRO SER THR SER CYS ARG PHE SER PRO SER LEU LEU PRO LYS ASN THR PRO ASN VAL THR SER PHE HIS GLN PHE ARG ILE PHE HIS THR THR
PHE SER ARG ARG G65 L66 E67 E68 D72 L108 E118 L126 L144 D145 D153 L158 R171 I174 N197 Q218 L228 E229 R230 E238 H242 L243 SER GLU THR GLN LYS SER SER HIS VAL
• Molecule 5: uL30m
Chain B3:
68%
6%
27%



• Molecule 6: 39S ribosomal protein L55, mitochondrial

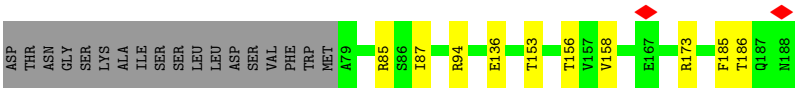
Chain B4:





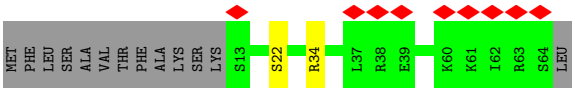
• Molecule 7: bL32m

Chain B5:



• Molecule 8: bL33m

Chain B6:

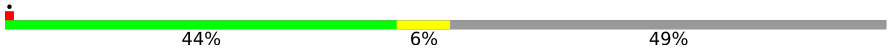


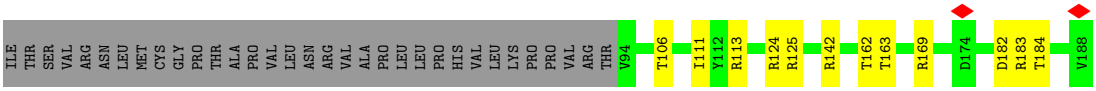
• Molecule 9: Mitochondrial ribosomal protein L34

Chain B7:

• Molecule 10: Mitochondrial ribosomal protein L35

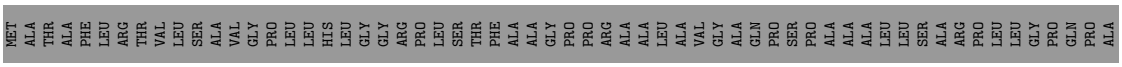
Chain B8:

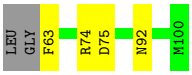




- Molecule 11: Ribosomal protein

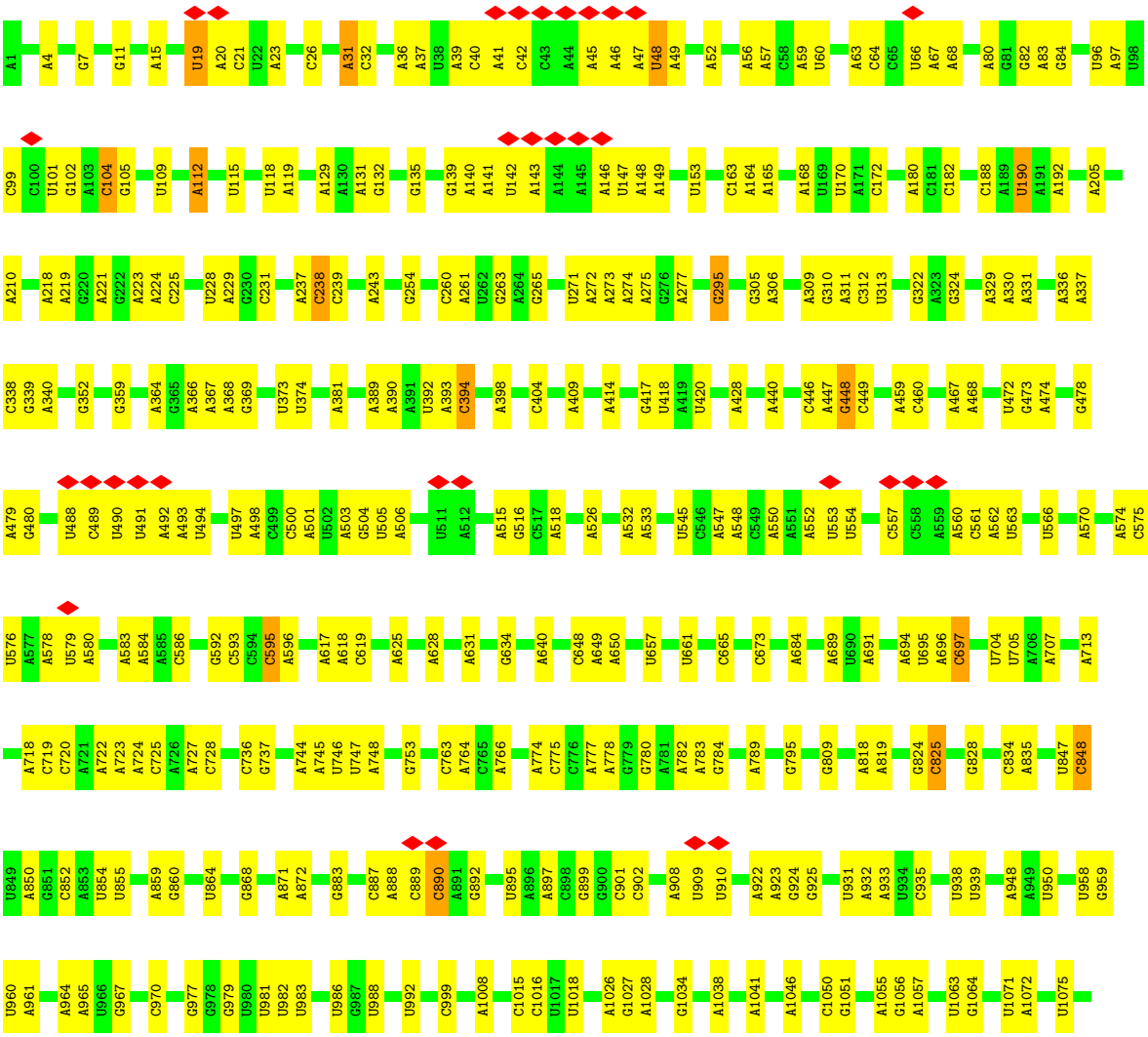
Chain B9:

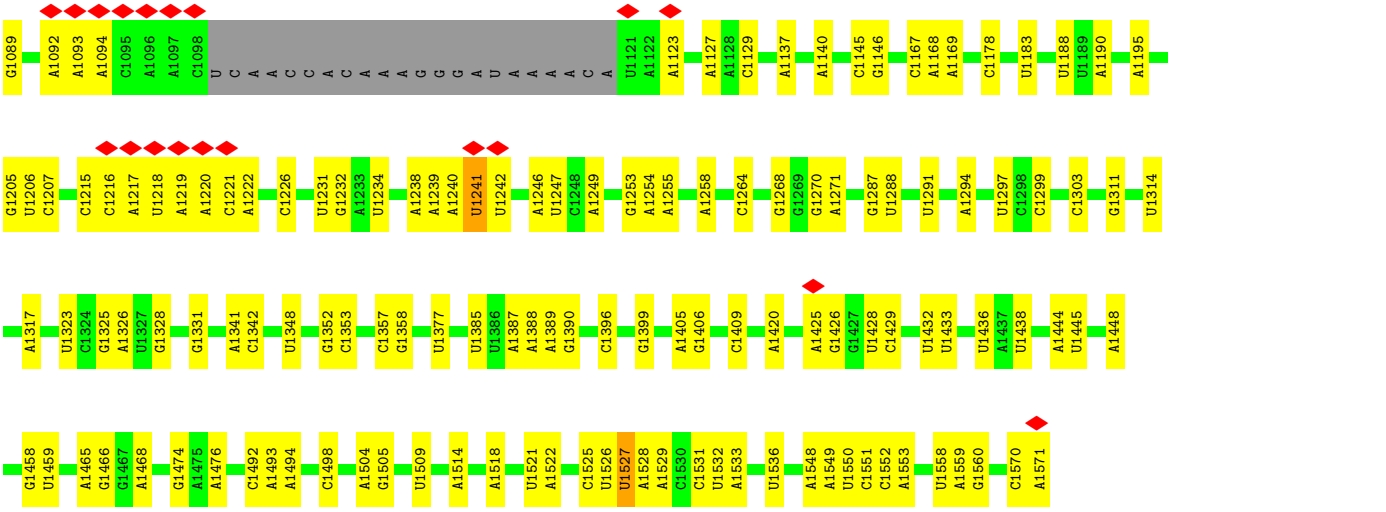




- Molecule 12: 16S ribosomal RNA, mitochondrial

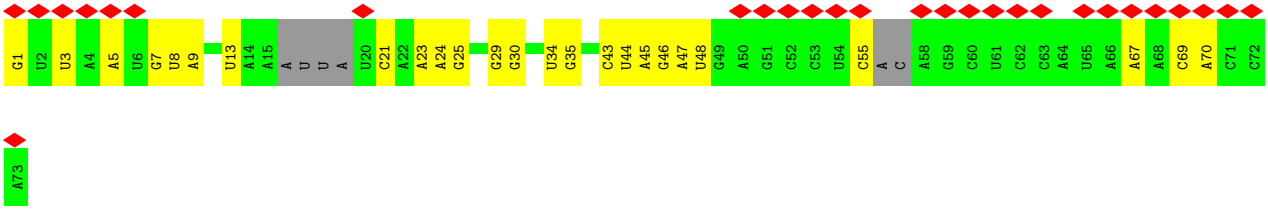
Chain BA:





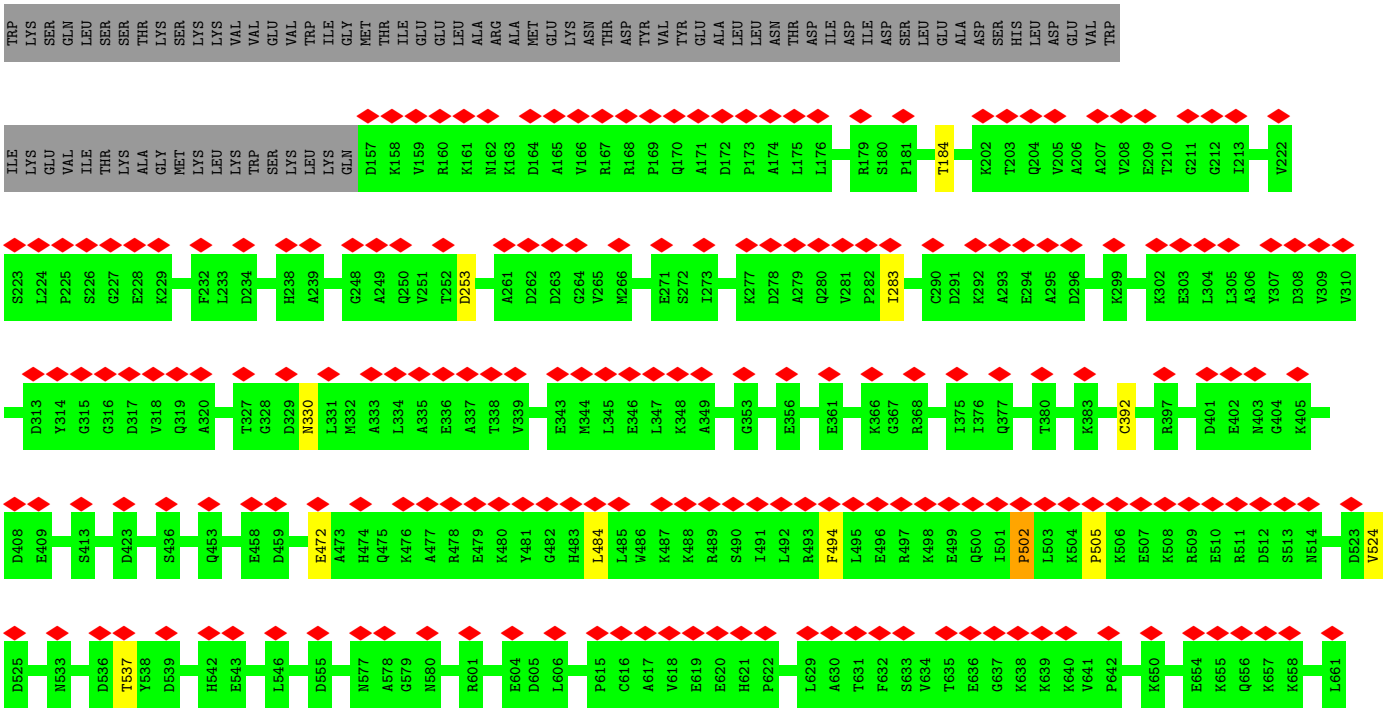
- Molecule 13: tRNA-Phe, mitochondrial

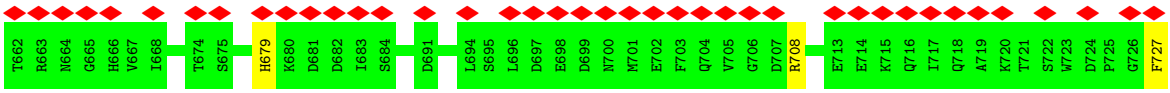
Chain BB:



- Molecule 14: Translation initiation factor IF-2, mitochondrial

Chain BC:



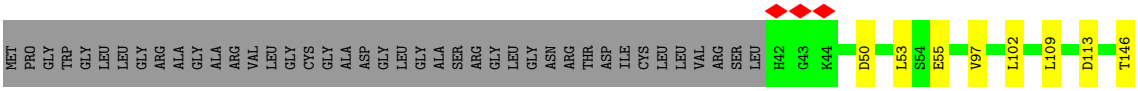


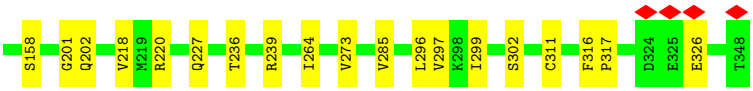
• Molecule 15: 39S ribosomal protein L2, mitochondrial

Chain BD:

• Molecule 16: ICT1

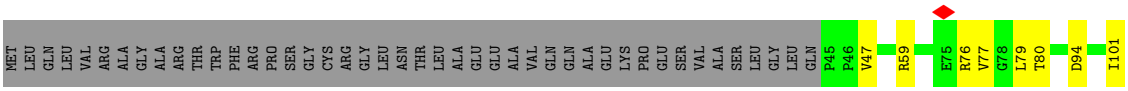
Chain BE:

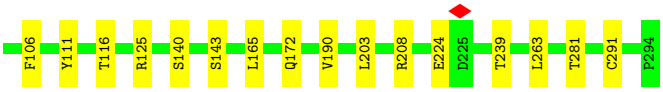




• Molecule 17: Mitochondrial ribosomal protein L4

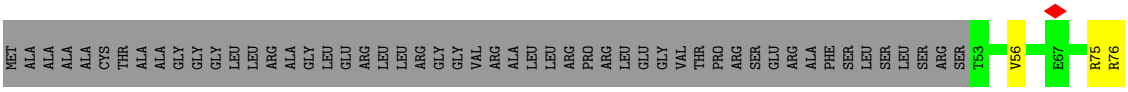
Chain BF:

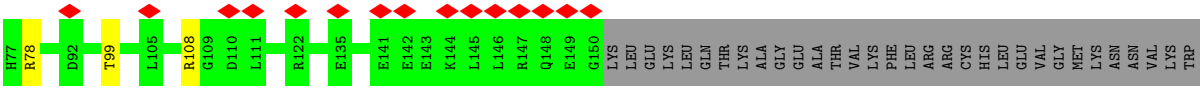


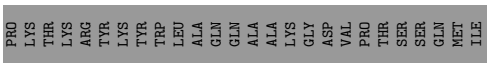


• Molecule 18: Mitochondrial ribosomal protein L9

Chain BI:

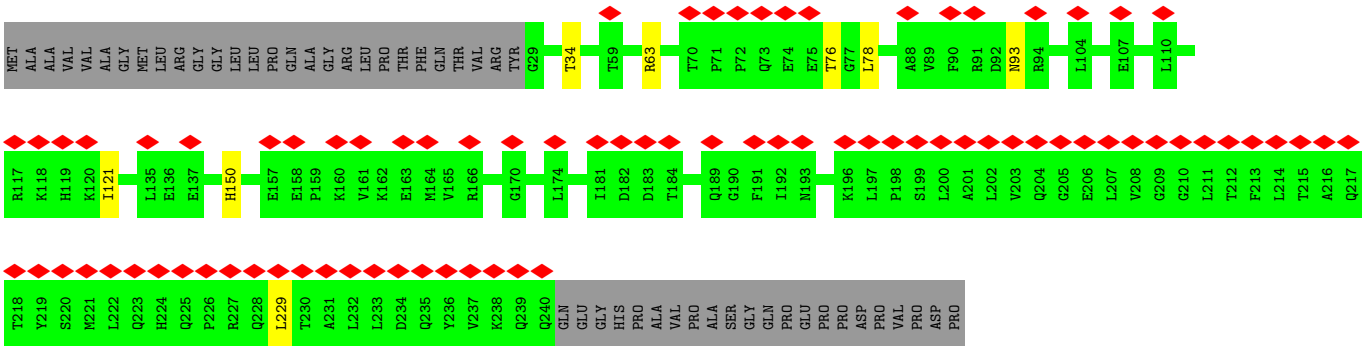






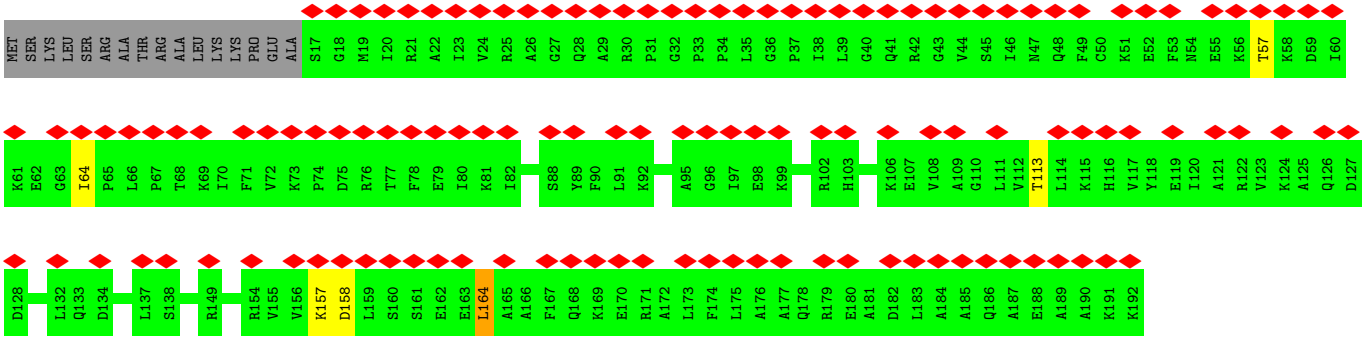
• Molecule 19: Mitochondrial ribosomal protein L10

Chain BJ:



• Molecule 20: Mitochondrial ribosomal protein L11

Chain BK:

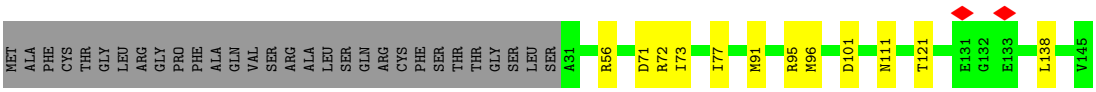


• Molecule 21: 39S ribosomal protein L13, mitochondrial

Chain BN:

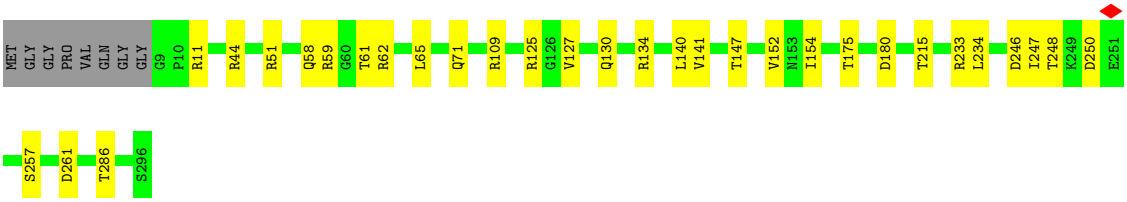
• Molecule 22: uL14m

Chain BO:



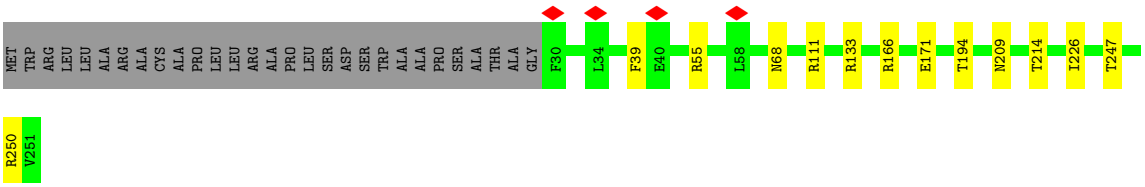
• Molecule 23: 39S ribosomal protein L15, mitochondrial

Chain BP:



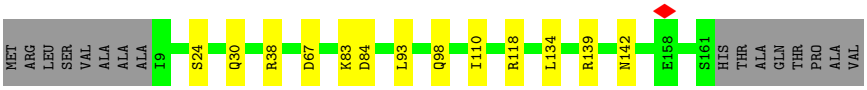
• Molecule 24: 39S ribosomal protein L16, mitochondrial

Chain BQ:



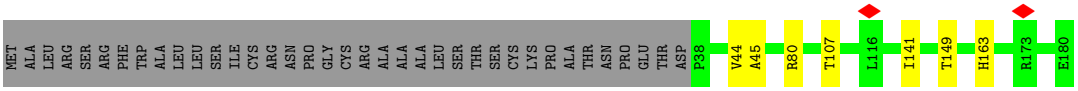
• Molecule 25: 39S ribosomal protein L17, mitochondrial

Chain BR:



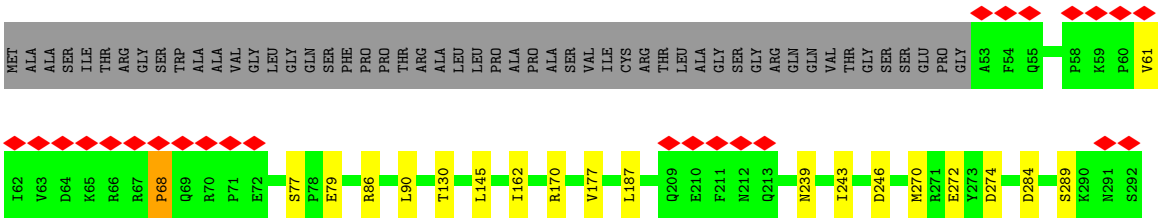
• Molecule 26: Mitochondrial ribosomal protein L18

Chain BS:



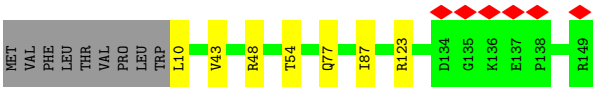
• Molecule 27: Mitochondrial ribosomal protein L19

Chain BT:



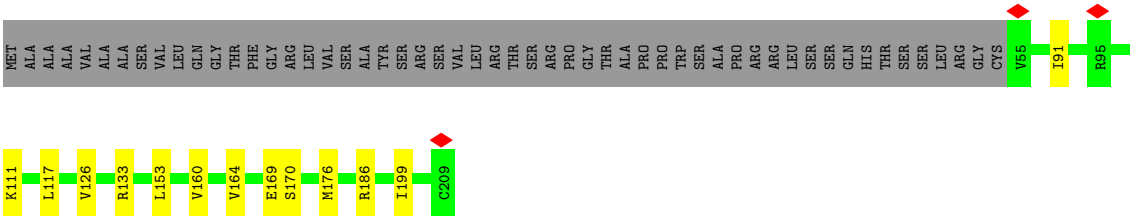
• Molecule 28: Mitochondrial ribosomal protein L20

Chain BU:



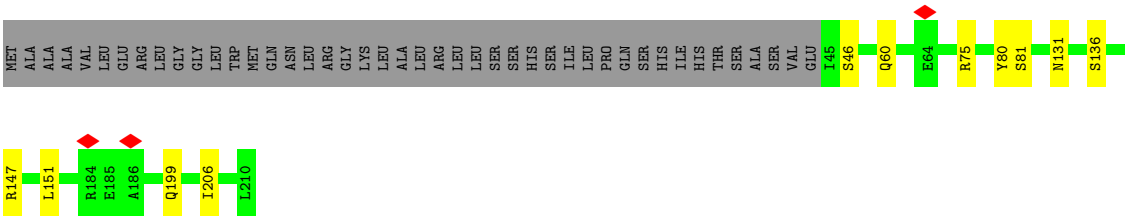
• Molecule 29: Mitochondrial ribosomal protein L21

Chain BV:



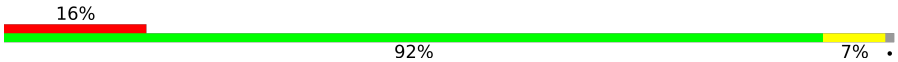
• Molecule 30: uL22m

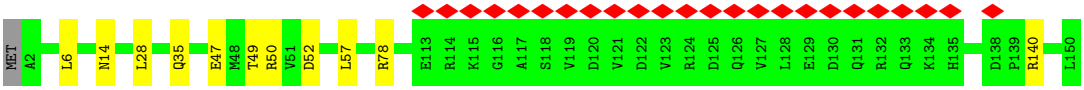
Chain BW:



• Molecule 31: uL23m

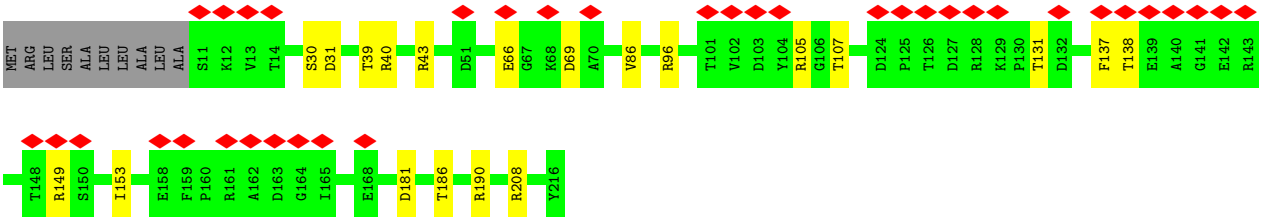
Chain BX:





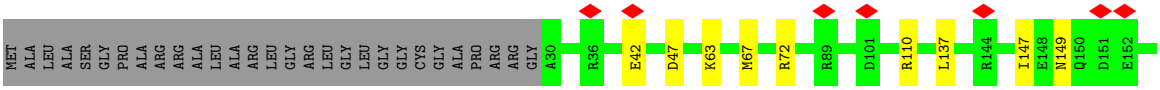
• Molecule 32: 39S ribosomal protein L24, mitochondrial

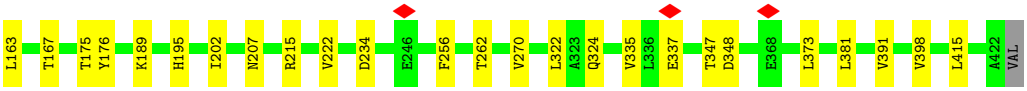
Chain BY:



• Molecule 33: Mitochondrial ribosomal protein L37

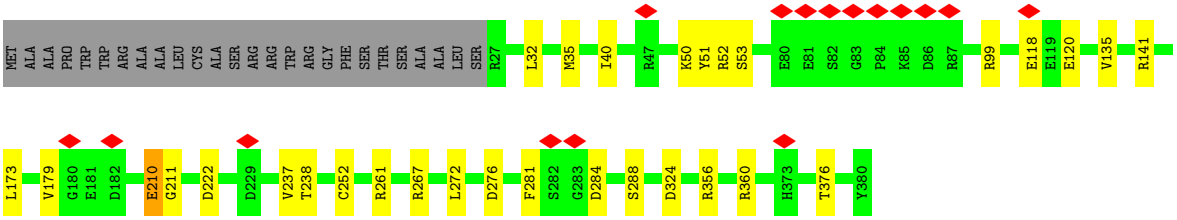
Chain Ba:





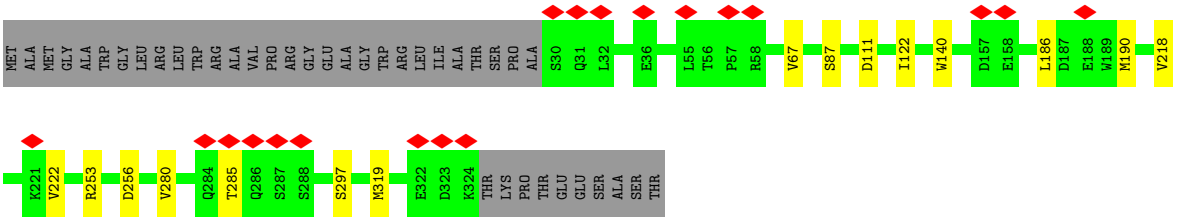
• Molecule 34: Mitochondrial ribosomal protein L38

Chain Bb:



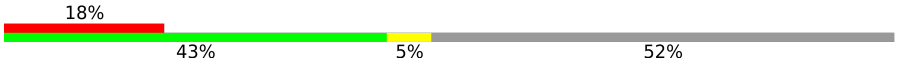
• Molecule 35: Mitochondrial ribosomal protein L39

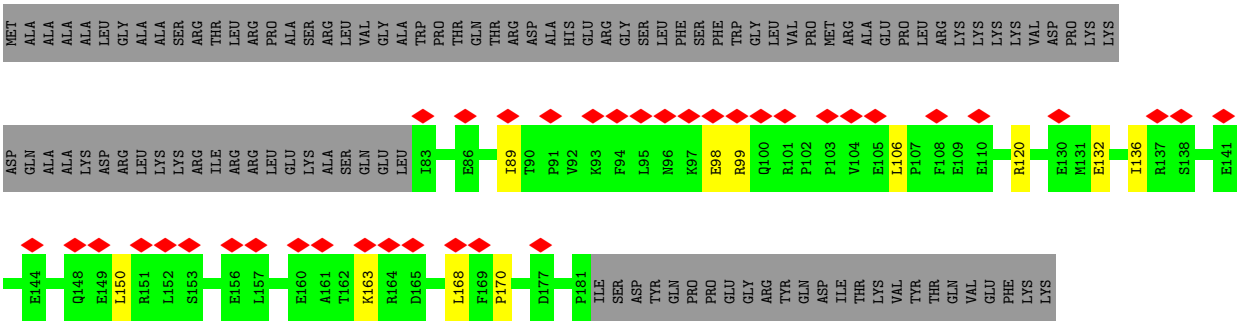
Chain Bc:



• Molecule 36: 39S ribosomal protein L40, mitochondrial isoform 1

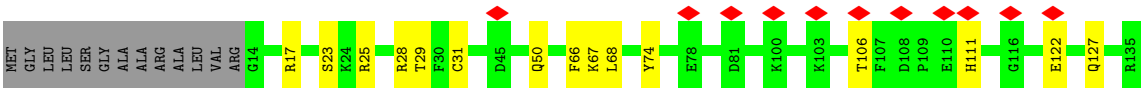
Chain Bd:





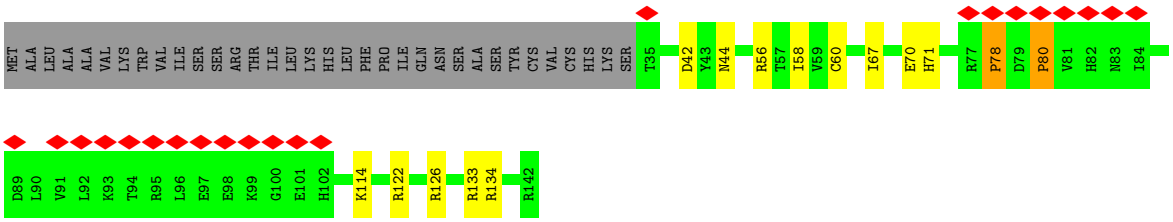
• Molecule 37: Mitochondrial ribosomal protein L41

Chain Be:



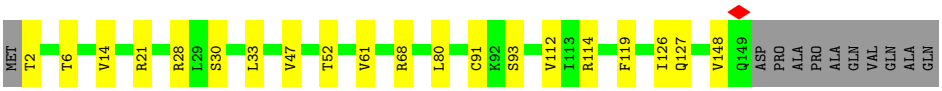
• Molecule 38: mL42

Chain Bf:



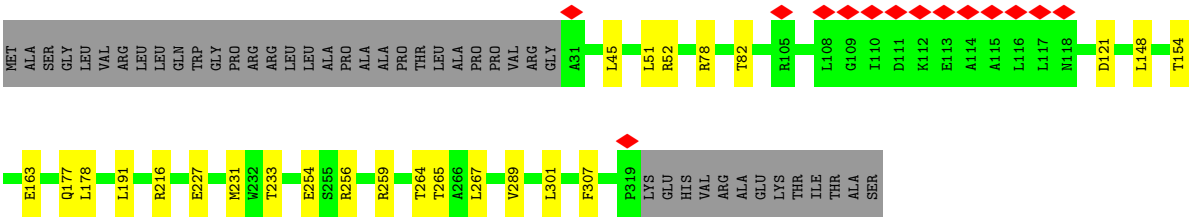
• Molecule 39: mL43

Chain Bg:



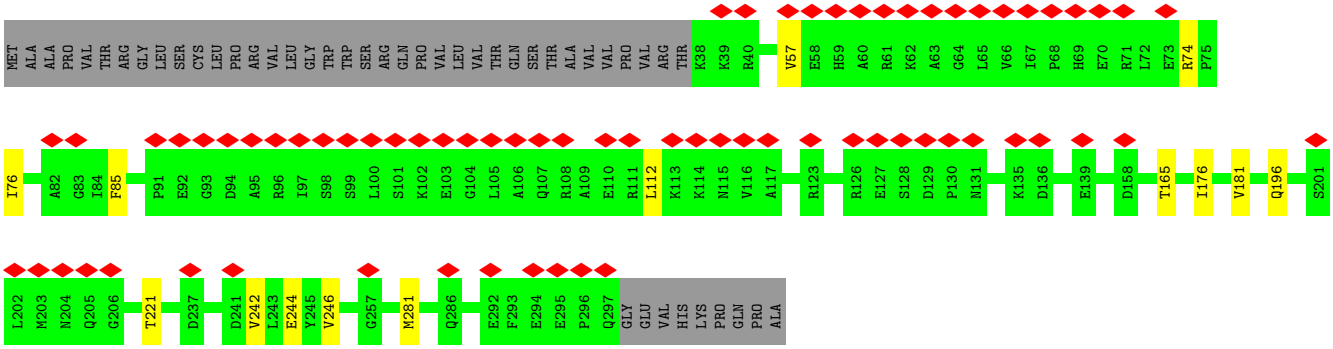
• Molecule 40: 39S ribosomal protein L44, mitochondrial

Chain Bh:



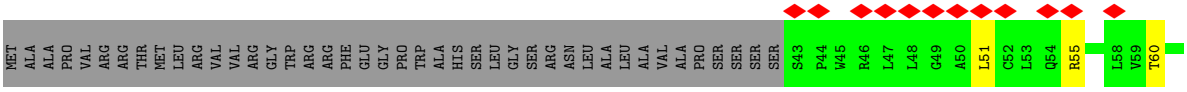
• Molecule 41: mL45

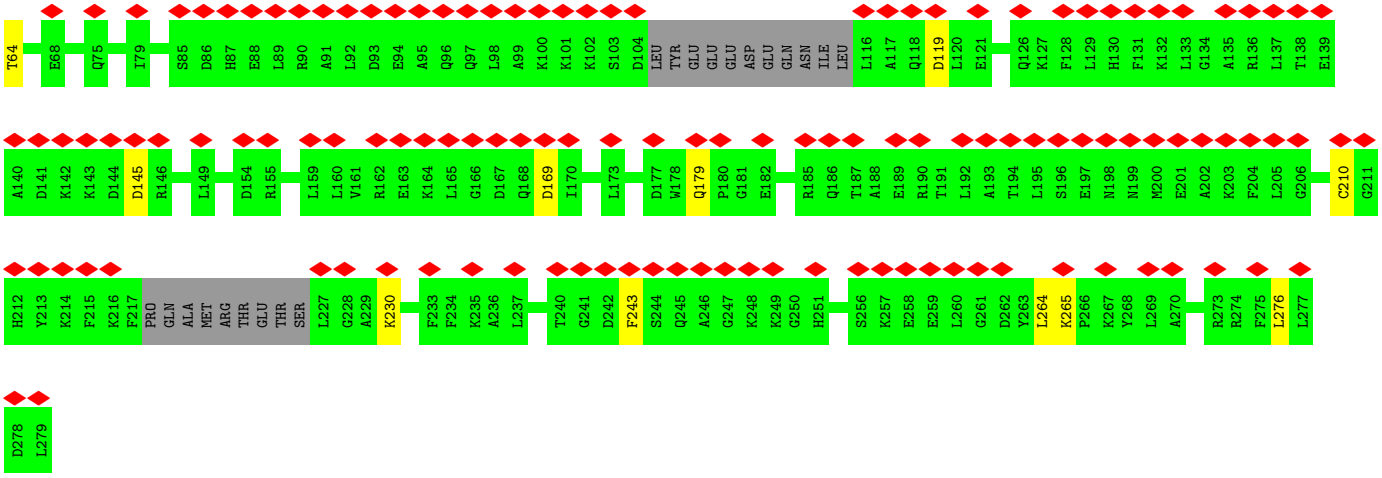
Chain Bi:



• Molecule 42: Mitochondrial ribosomal protein L46

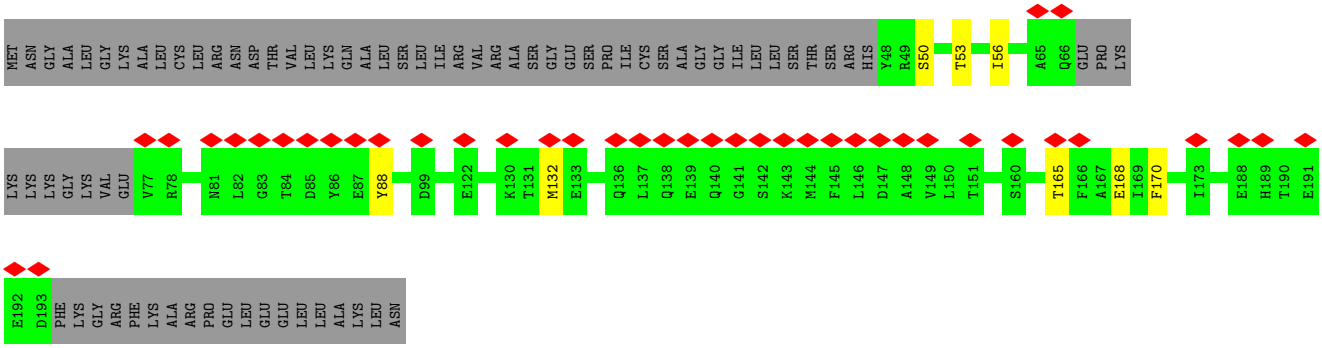
Chain Bj:





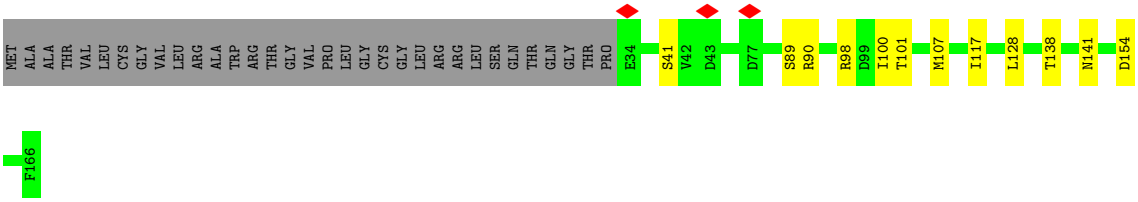
- Molecule 43: Mitochondrial ribosomal protein L48

Chain Bk:



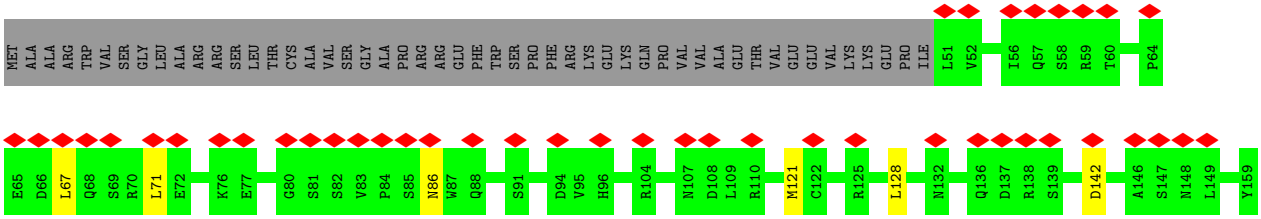
- Molecule 44: 39S ribosomal protein L49, mitochondrial

Chain Bl:



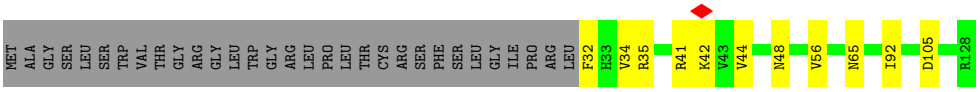
- Molecule 45: mL50

Chain Bm:



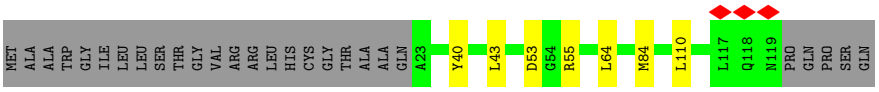
- Molecule 46: Mitochondrial ribosomal protein L51

Chain Bn:



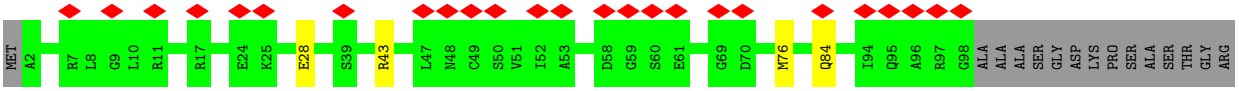
- Molecule 47: 39S ribosomal protein L52, mitochondrial

Chain Bo:



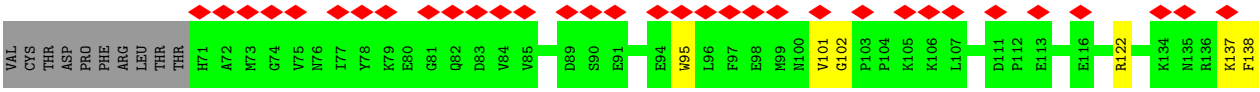
- Molecule 48: mL53

Chain Bp:



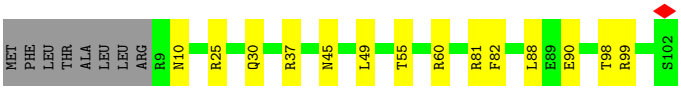
- Molecule 49: mL54

Chain Bq:



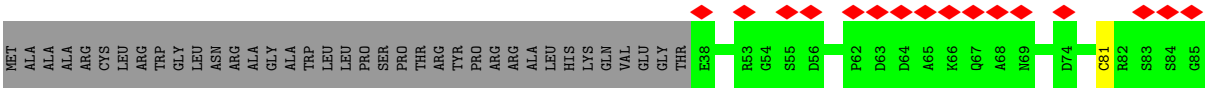
- Molecule 50: Mitochondrial ribosomal protein L57

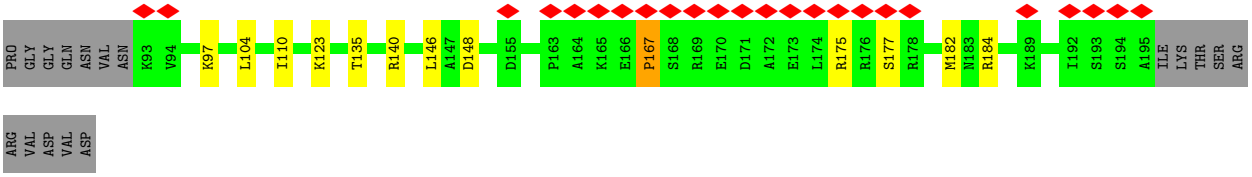
Chain Bt:



- Molecule 51: Peptidyl-tRNA hydrolase ICT1, mitochondrial

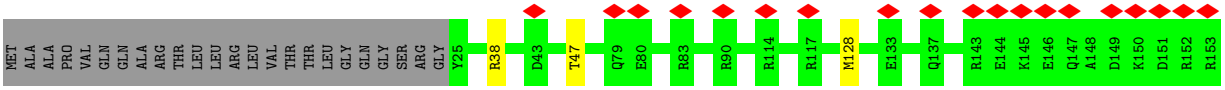
Chain Bu:

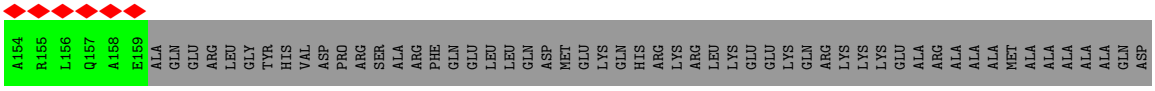




- Molecule 52: mL64

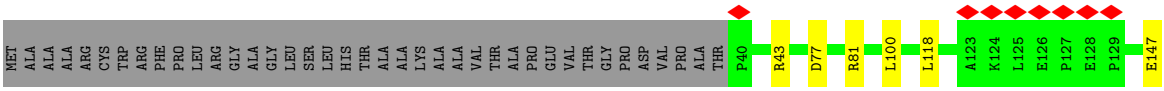
Chain Bv:

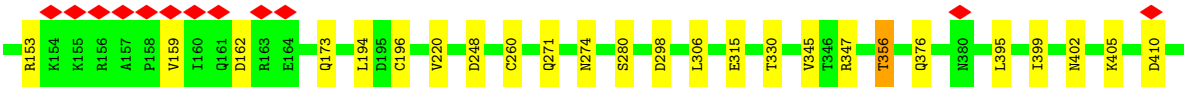


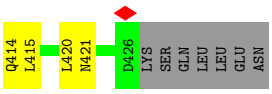


- Molecule 53: mL65

Chain Bw:

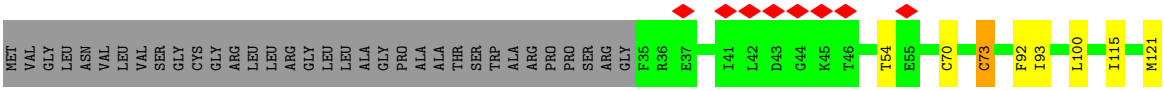


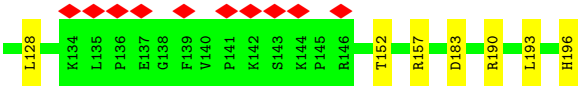




- Molecule 54: Mitochondrial ribosomal protein S18A

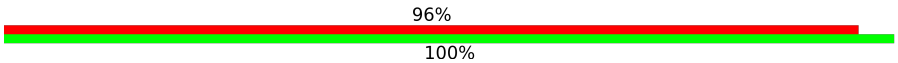
Chain Bx:





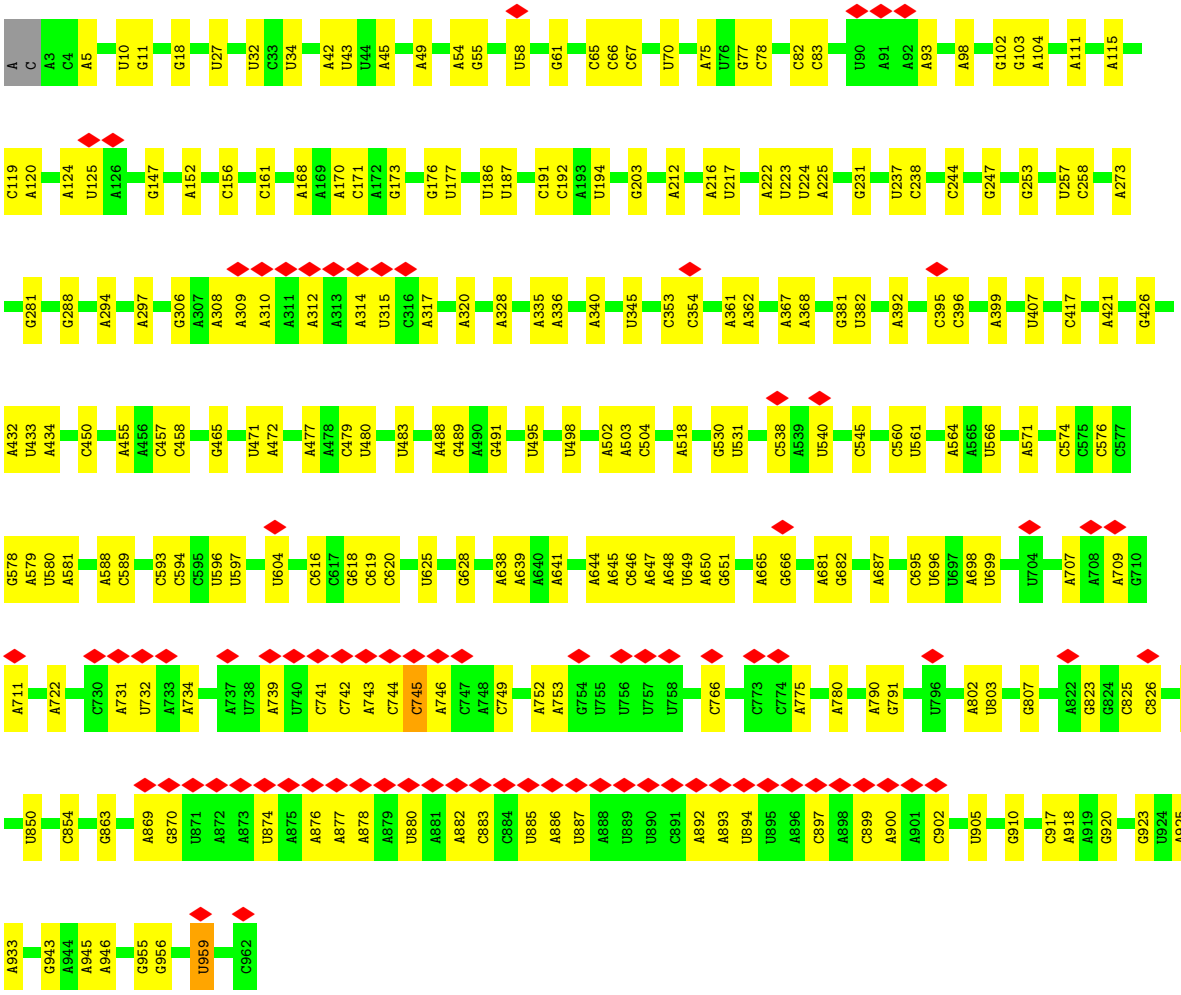
- Molecule 55: unassigned secondary structure elements

Chain Bz:



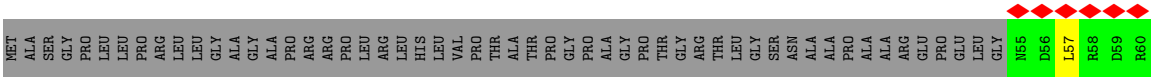
• Molecule 56: 12S ribosomal RNA, mitochondrial

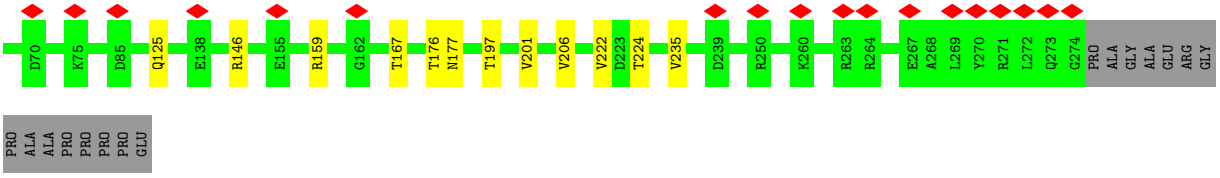
Chain AA:



• Molecule 57: Mitochondrial ribosomal protein S2

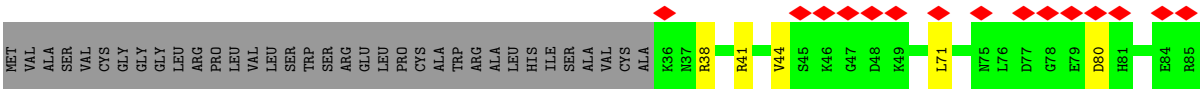
Chain AB:

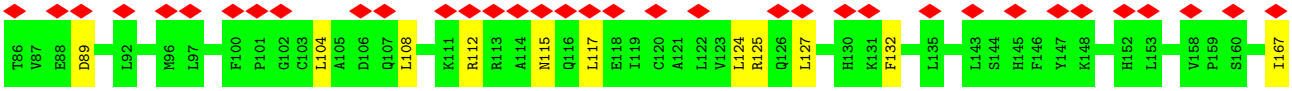




• Molecule 58: Mitochondrial ribosomal protein S24

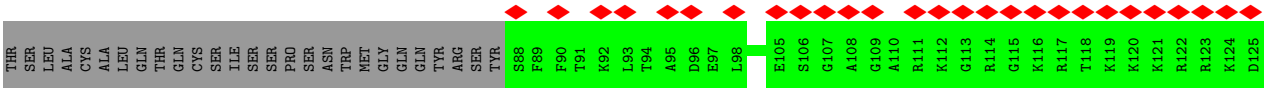
Chain AC:

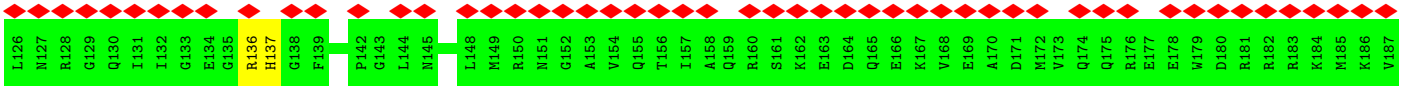


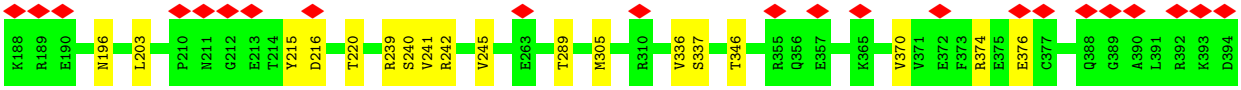


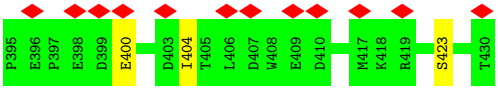
• Molecule 59: Mitochondrial ribosomal protein S5

Chain AE:



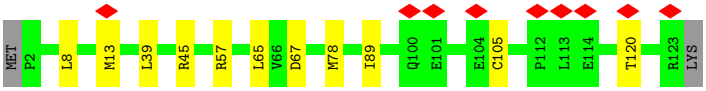






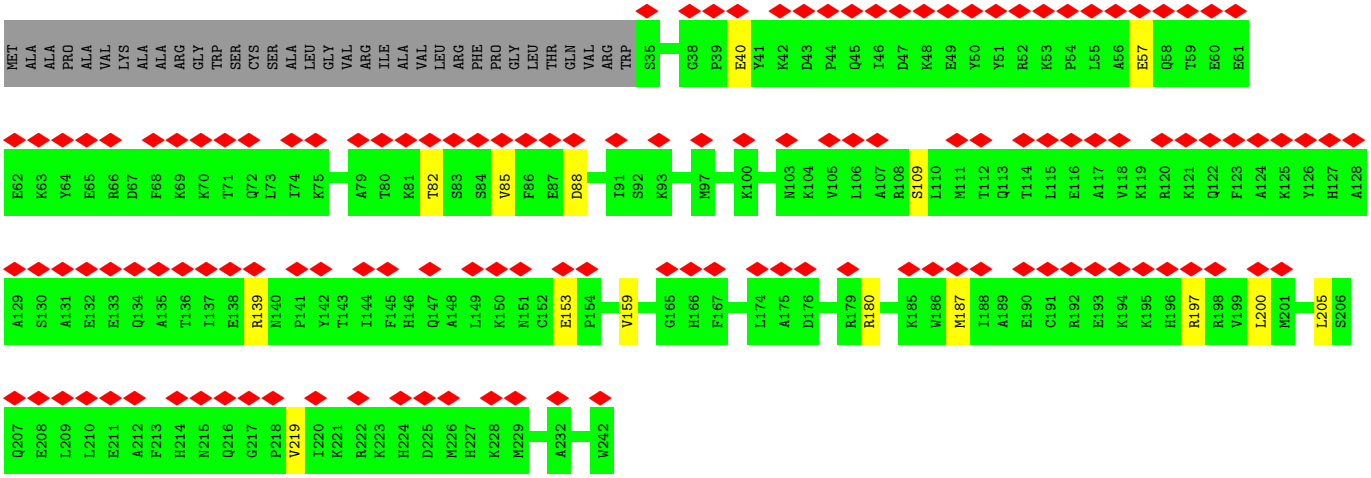
• Molecule 60: Mitochondrial ribosomal protein S6

Chain AF:



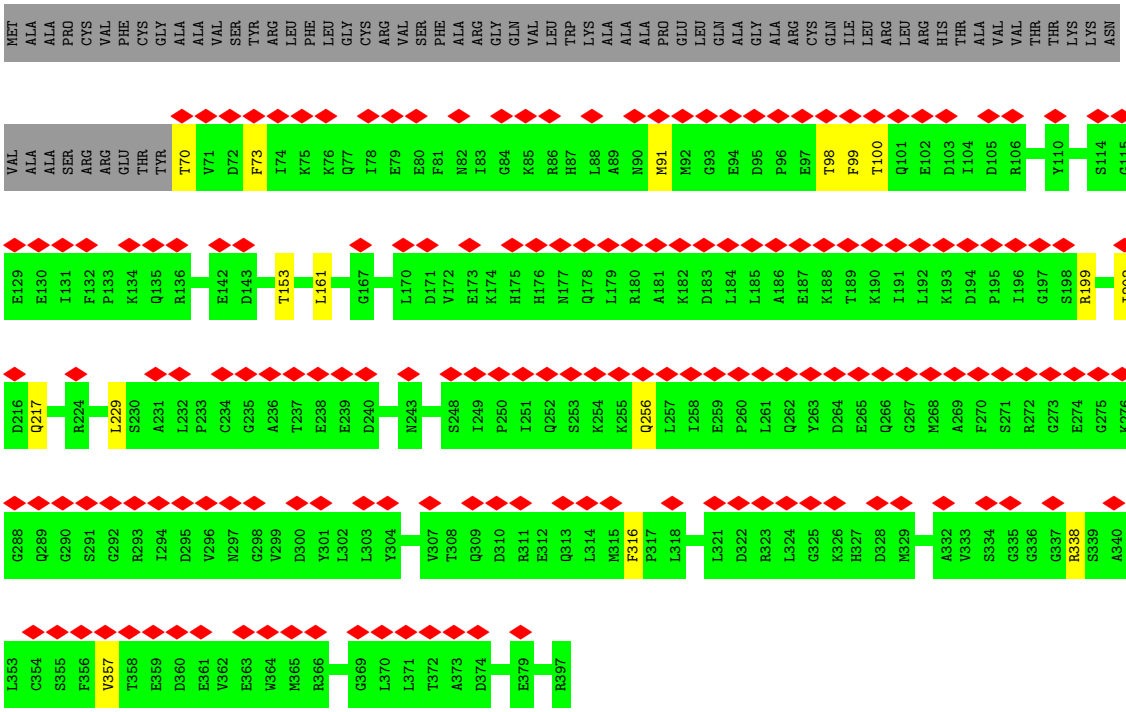
• Molecule 61: Mitochondrial ribosomal protein S7

Chain AG:



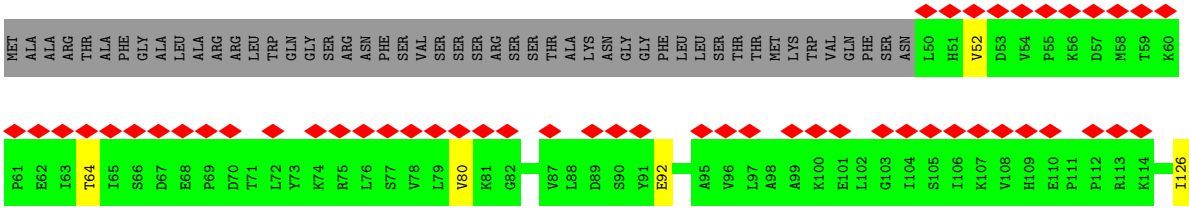
- Molecule 62: 28S ribosomal protein S9, mitochondrial

Chain AI:



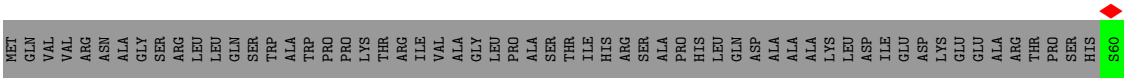
- Molecule 63: Mitochondrial ribosomal protein S10

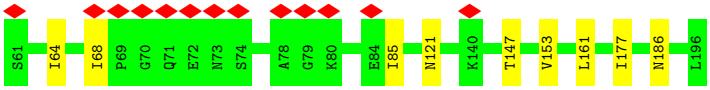
Chain AJ:



• Molecule 64: 28S ribosomal protein S11, mitochondrial

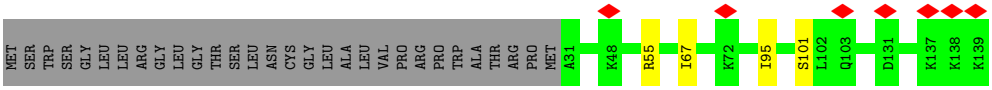
Chain AK:





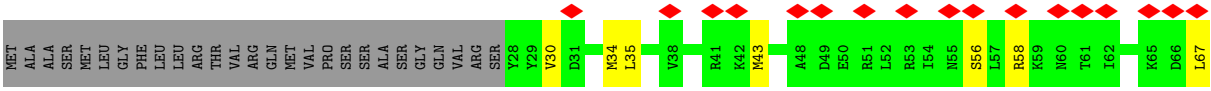
• Molecule 65: Mitochondrial ribosomal protein S12

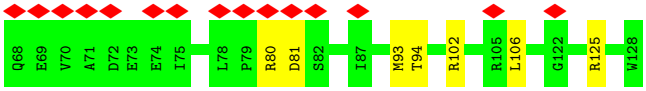
Chain AL:



• Molecule 66: Mitochondrial ribosomal protein S14

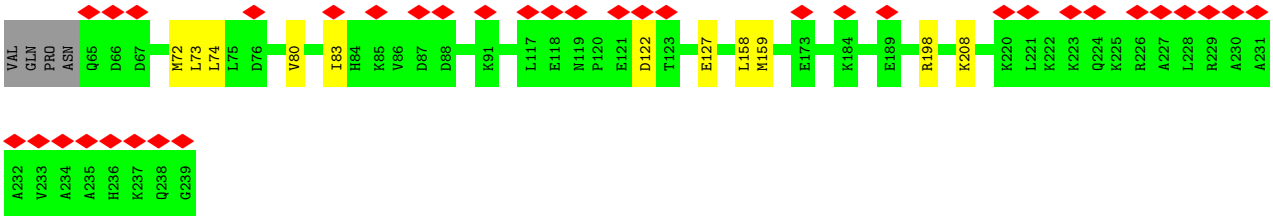
Chain AN:





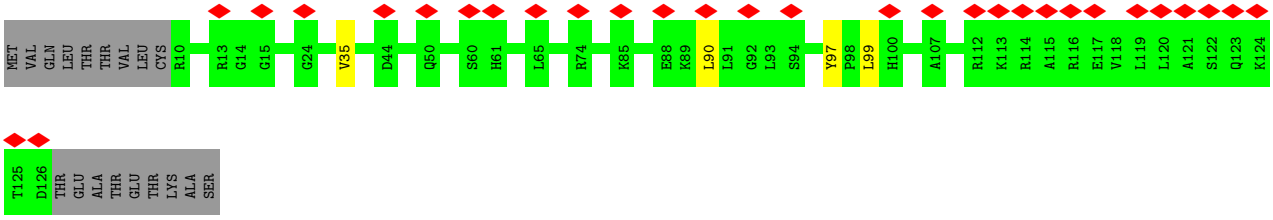
• Molecule 67: Uncharacterized protein

Chain AO:



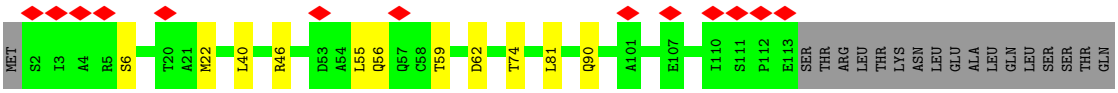
• Molecule 68: bS16m

Chain AP:



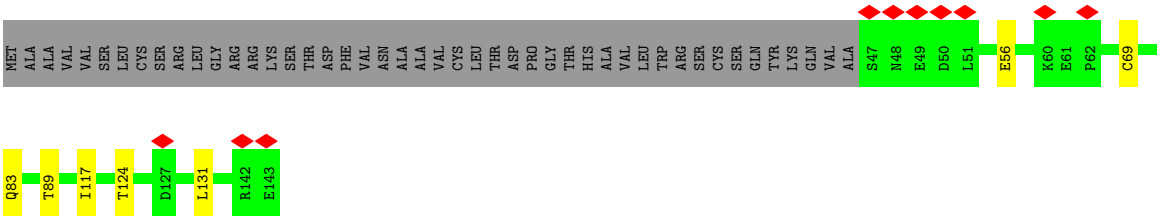
- Molecule 69: uS17m

Chain AQ:



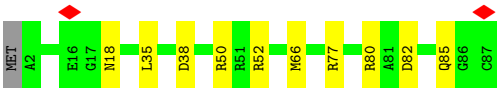
- Molecule 70: Mitochondrial ribosomal protein S18C

Chain AR:



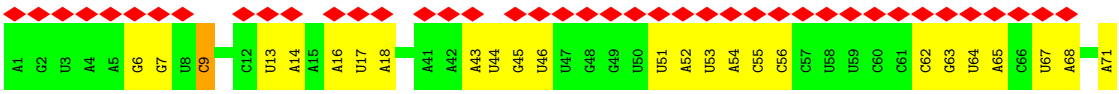
- Molecule 71: bS21m

Chain AU:



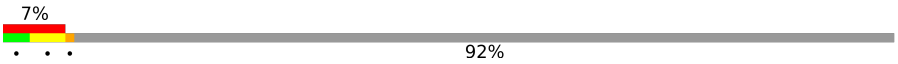
- Molecule 72: P-site fMet-tRNAMet, mitochondrial

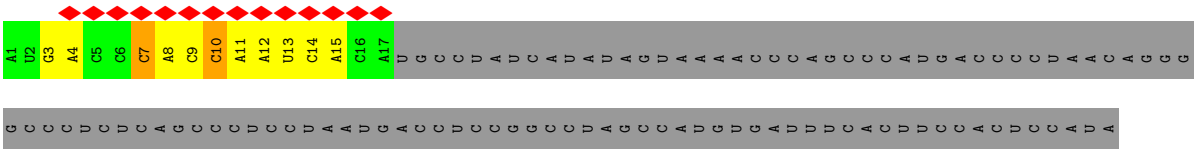
Chain AV:



- Molecule 73: MT-CO3 mRNA, mitochondrial

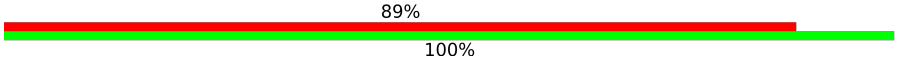
Chain AX:

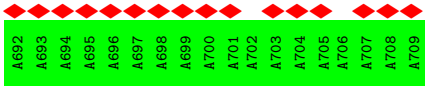




- Molecule 74: unassigned secondary structure elements

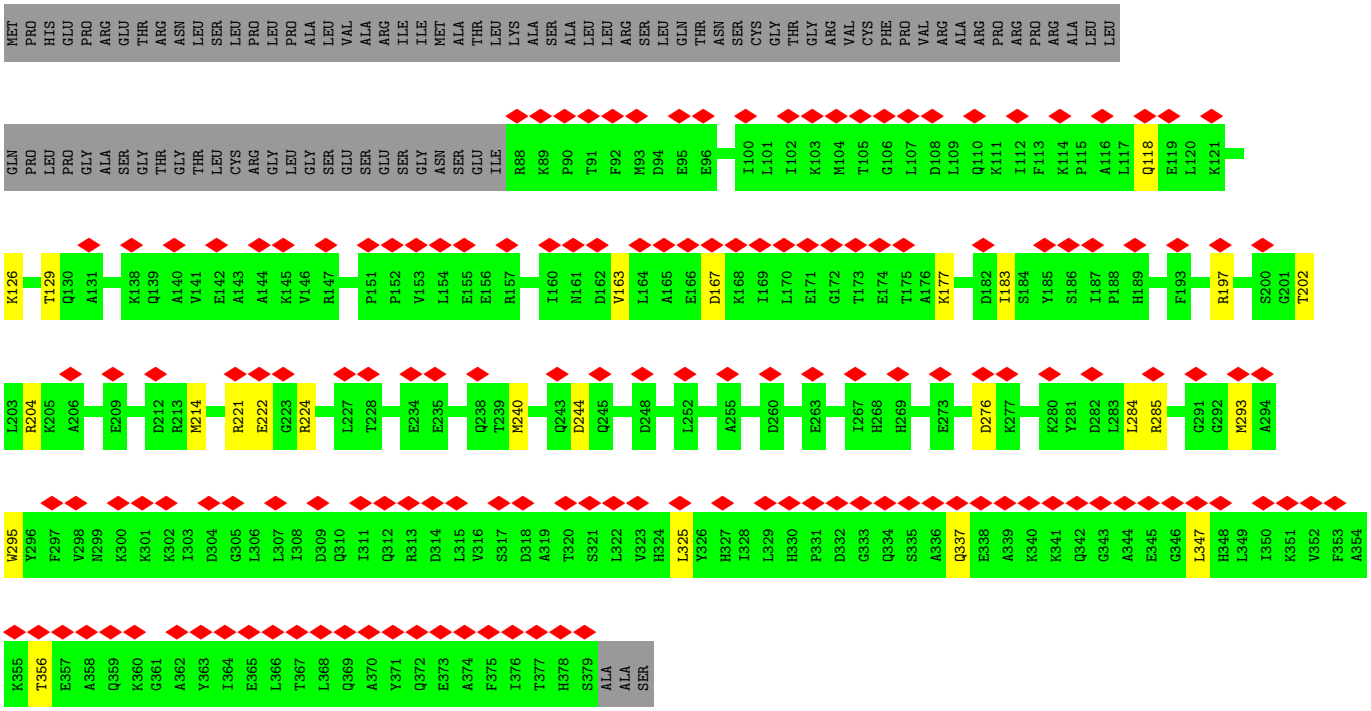
Chain AZ:





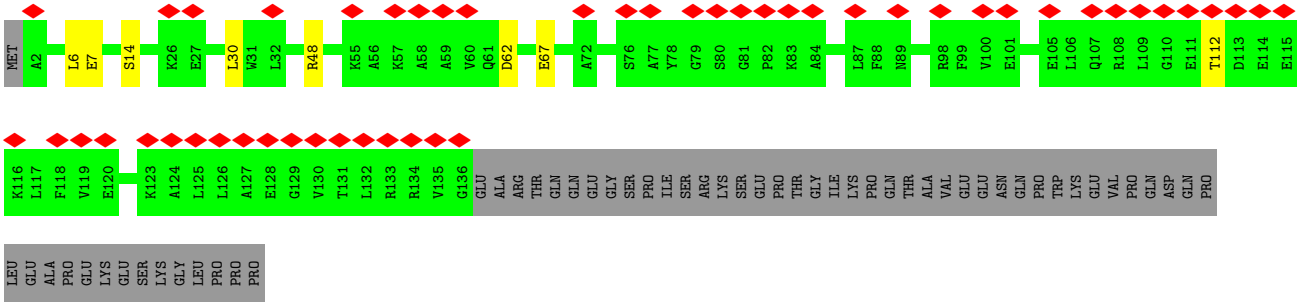
- Molecule 75: Mitochondrial ribosomal protein S22

Chain Aa:



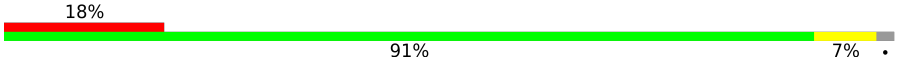
- Molecule 76: 28S ribosomal protein S23, mitochondrial

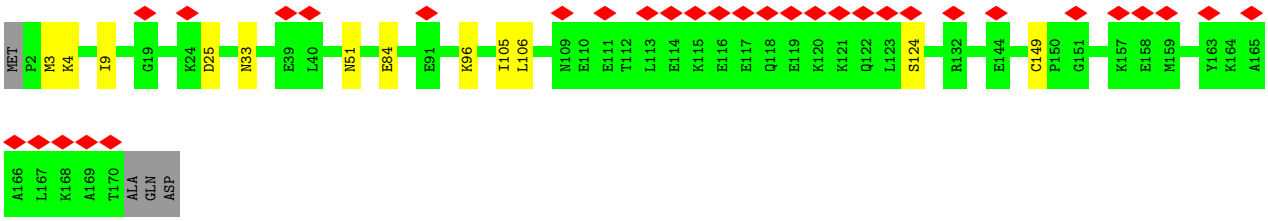
Chain Ab:



- Molecule 77: Mitochondrial ribosomal protein S25

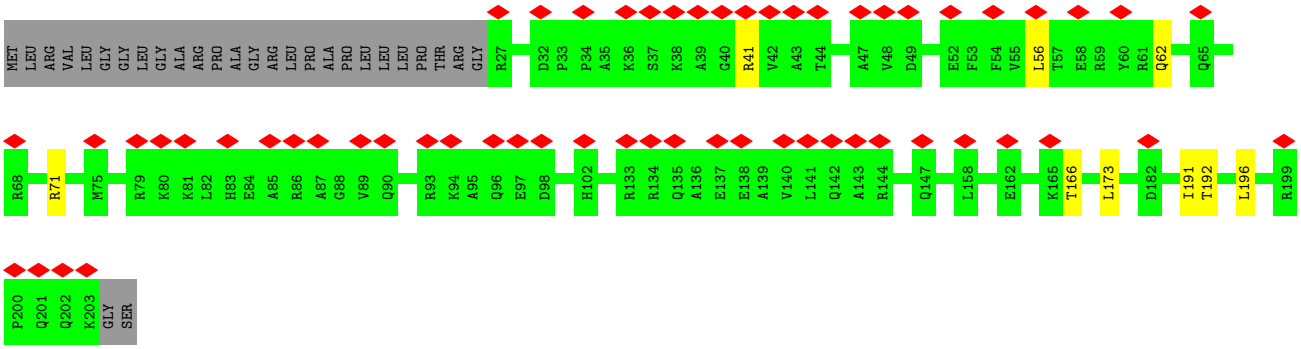
Chain Ac:





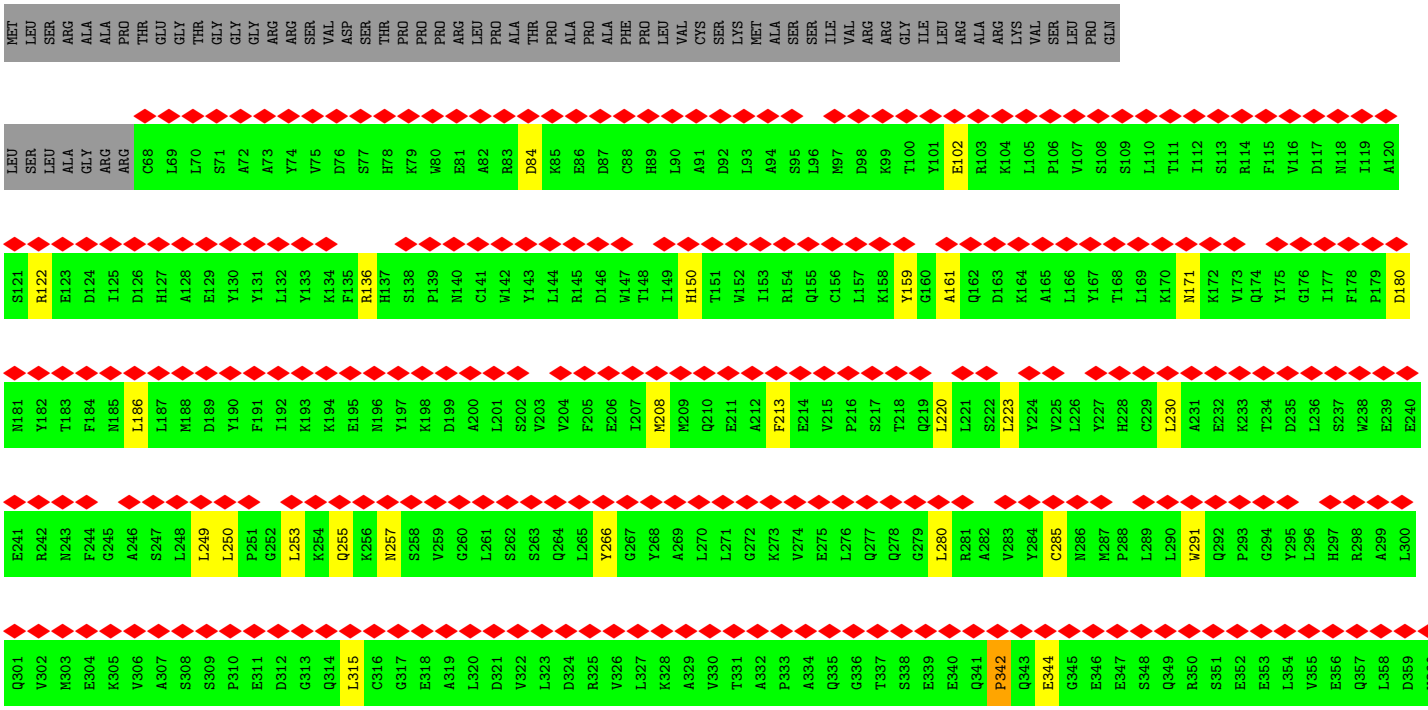
- Molecule 78: Mitochondrial ribosomal protein S26

Chain Ad:



- Molecule 79: mS27

Chain Ae:



E361 E362 T363 E364 Q365 S366 K367 L368 P369 Q370 Y371 L372 E373 R374 F375 E376 A377 L378 R379 S380 K381 L382 Q383 A384 L385 G386 K387 V388 E389 S390 E391 S392 L393 L394 T395 L396 S397 T398 Q399 L400 A401 K402 A403 Q404 L405 P406 T407 C408 E409 A410 E411 D412 I413 A414 V415 Y416 E417 Q418 R419 L420

Q421 Q422 W423 H424 G425 E426 R427 V428 R429 L430 I431 Q432 R433 E434 Q435 E436 Q437 R438 E439 R440 A441 R442 Q443 D444 Y445 E446 A447 R448 R449 A450 A451 K452 A453 S454 A455

- Molecule 80: 28S ribosomal protein S28, mitochondrial

Chain Af: 11% 49% • 47%

MET ALA ALA LEU CYS ARG THR ARG ALA VAL THR ALA LYS SER HIS PHE LEU ARG VAL PHE PHE PHE SER ARG PRO CYS ARG GLY THR GLY THR GLU SER GLY SER GLY SER GLU SER SER GLU SER THR GLU PRO LYS GLN ARG PRO GLY GLY PHE ALA SER ALA LEU GLU ARG HIS SER

GLU LEU GLN GLN LYS ALA GLU PHE GLY ARG MET ARG GLY SER PRO LYS ASN V78 E79 M84 L85 L90 K97 E110 D111 D112 E129 V130 D131 G132 E133 K134 R144 L148 R153 F154 L155 T162 D167 A168 V169 L170 L173 Q174 E175 S176 LYS ASP SER

LYS SER LYS GLU GLU ARG HIS GLU LYS

- Molecule 81: Death associated protein 3

Chain Ag: 77% 84% 5% 11%

MET LEU LYS GLY VAL THR ARG LEU ILE SER ARG VAL HIS LYS LEU ASP PRO GLY HIS VAL LEU TYR MET GLY THR GLN ALA PRO GLN SER LEU ALA ALA HIS LEU ASP ASN GLN VAL PRO VAL LYS SER PRO R45 A46 I47 S48 R49 T50 S51 E52 D53 D54 P55 A56 K57 H58 R59 E60

Q61 H62 E63 G64 Q65 H66 Y67 N68 L71 Q72 E73 L74 K75 T76 V77 F78 P79 H80 G81 L82 P83 P84 R85 F86 A87 M88 Q89 V90 K91 T92 F93 N94 E95 A96 C97 L98 M99 V100 R101 K102 P103 A104 L105 E106 L107 L108 H109 Y110 L111 K112 N113 T114 N115 F116 A117 H118 P119 A120 V121

R122 Y123 V124 L125 Y126 G127 E128 K129 K133 T134 L135 S136 L137 C138 H139 I140 L141 H142 F143 C144 A145 K146 Q147 N148 W149 L150 I151 L152 H153 I154 P155 D156 A157 H158 I159 W160 V161 K162 N163 C164 R165 D166 L167 L168 Q169 S170 N171 Y172 N173 K174 Q175 R176 F177 D178 Q179 P180 L181 E182 A183

S184 T185 W186 L187 K188 N189 F190 K191 T192 A193 N194 E195 H196 F197 L198 S199 Q200 I201 K202 V203 Q204 E205 K206 Y207 V208 W209 N210 K211 R212 E213 S214 T215 E216 K217 G218 R219 P220 L221 G222 E223 V224 V225 E226 Q227 G228 I229 M230 R231 V232 R233 N234 A235 T236 D237 A238 V239 G240 I241 V242 L243

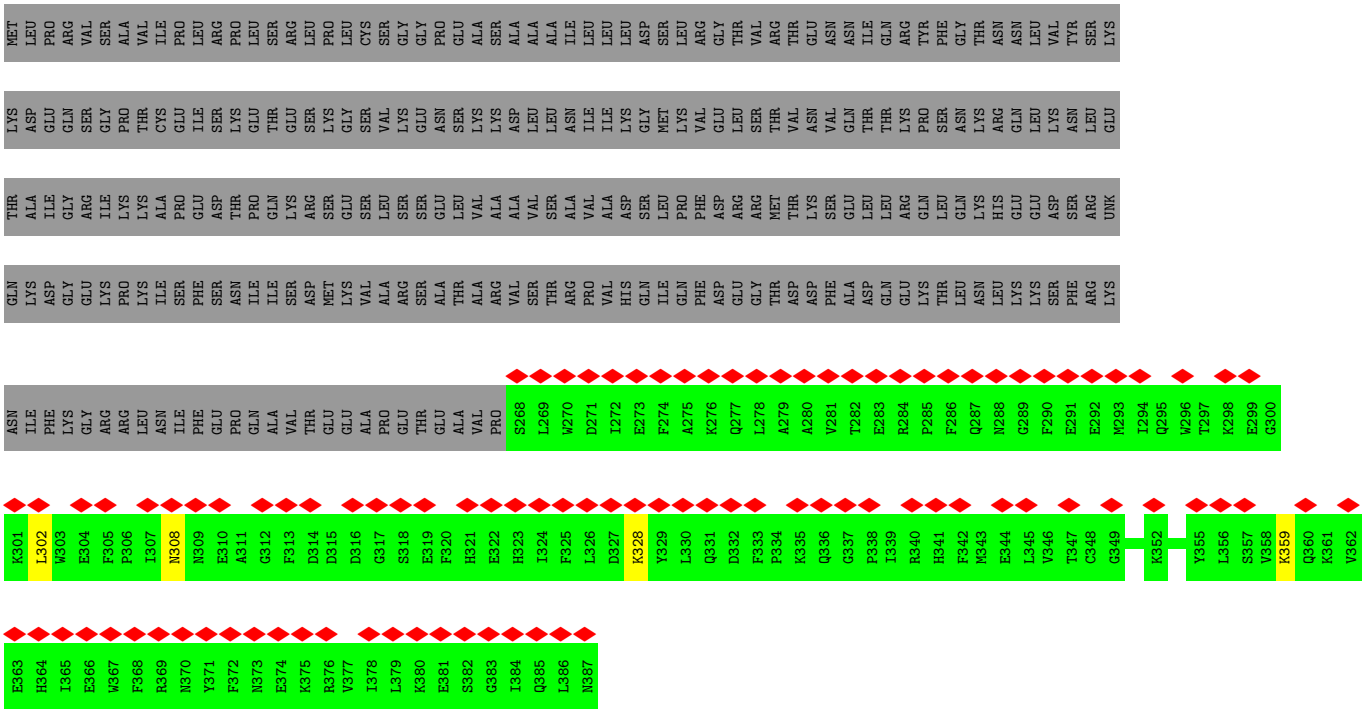
K244 E245 L246 K247 R248 Q249 S250 S251 L252 G253 I254 F255 H256 L257 L258 V259 A260 V261 D262 G263 V264 N265 A266 L267 W268 G269 R270 T271 T272 L273 K274 R275 E276 D277 K278 S279 P280 I281 A282 P283 E284 E285 L286 A287 L288 I289 H290 N291 L292 R293 K294 M295 V296 K297 N298 D299 W300 Q301 G302 G303

A304 I305 V306 L307 T308 V309 S310 Q311 K317 P318 R319 N320 A321 Y322 L323 P324 Q325 E326 L327 L328 G329 K330 E331 G332 F333 D334 A335 L336 D337 P338 F339 I340 P341 I342 L343 V344 S345 N346 P349 K350 E351 F352 E353 S354 C355 I356 Q357 Y358 Y359 L360 E361 N362 N363 W364 L365 Q366 H367 E368

K369 A370 H371 T372 E373 E374 G375 K376 K377 E378 L379 L380 F381 L382 S383 N384 R385 N386 P387 L390 E391 R392 L393 C394 A395 Y396 L397

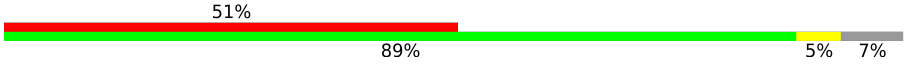
- Molecule 82: mS31

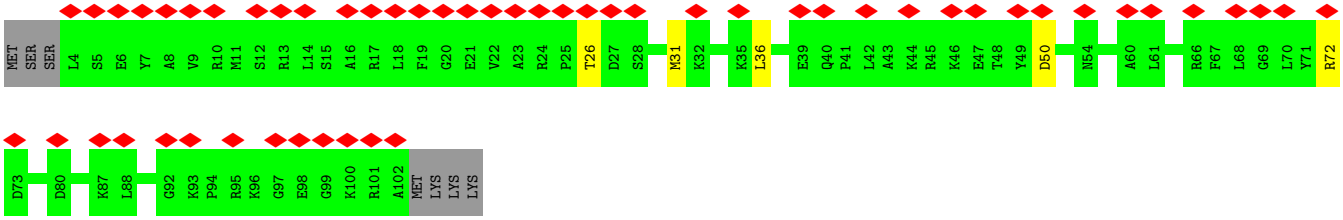
Chain Ah:



- Molecule 83: mS33

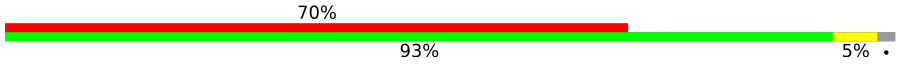
Chain Ai:

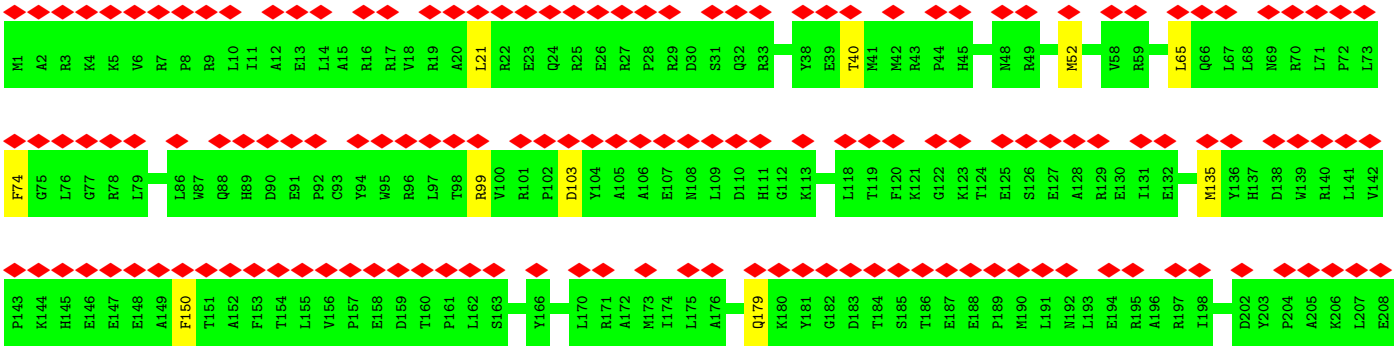


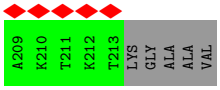


- Molecule 84: 28S ribosomal protein S34, mitochondrial

Chain Aj:

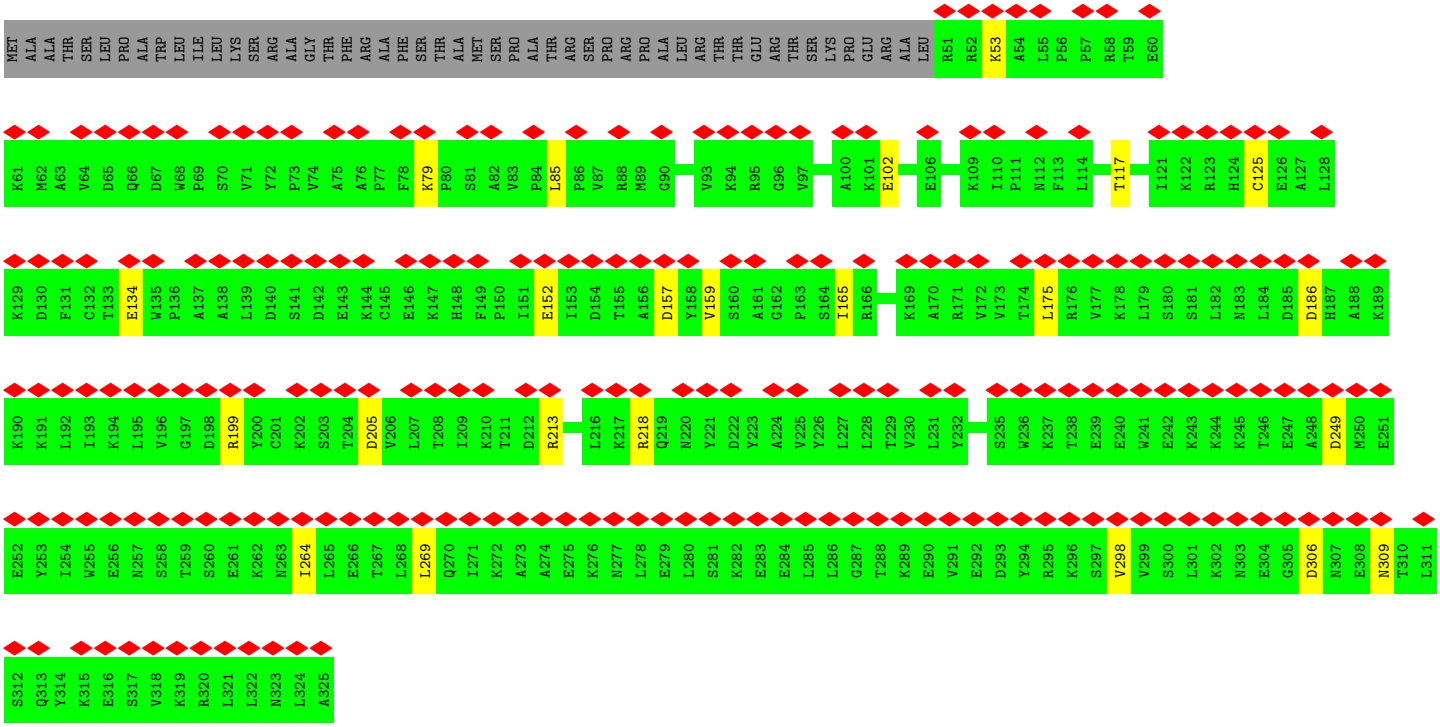






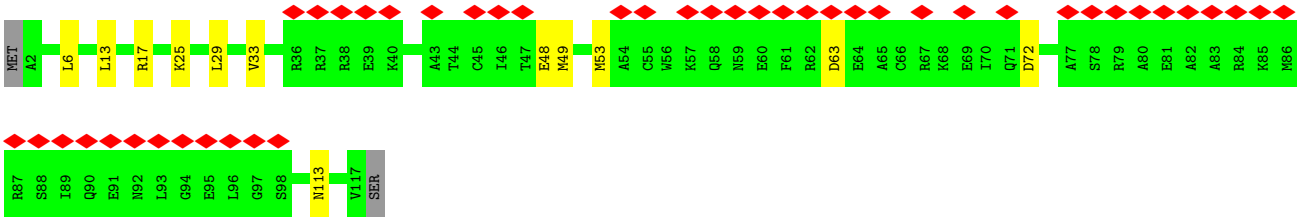
- Molecule 85: 28S ribosomal protein S35, mitochondrial

Chain Ak:



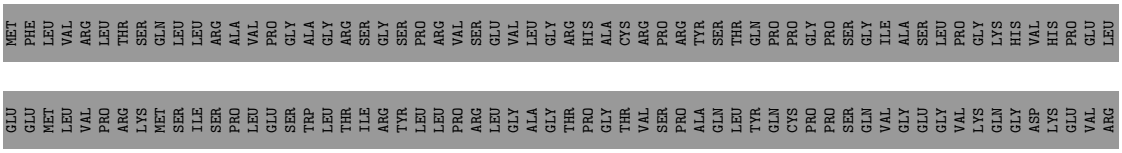
- Molecule 86: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain Am:



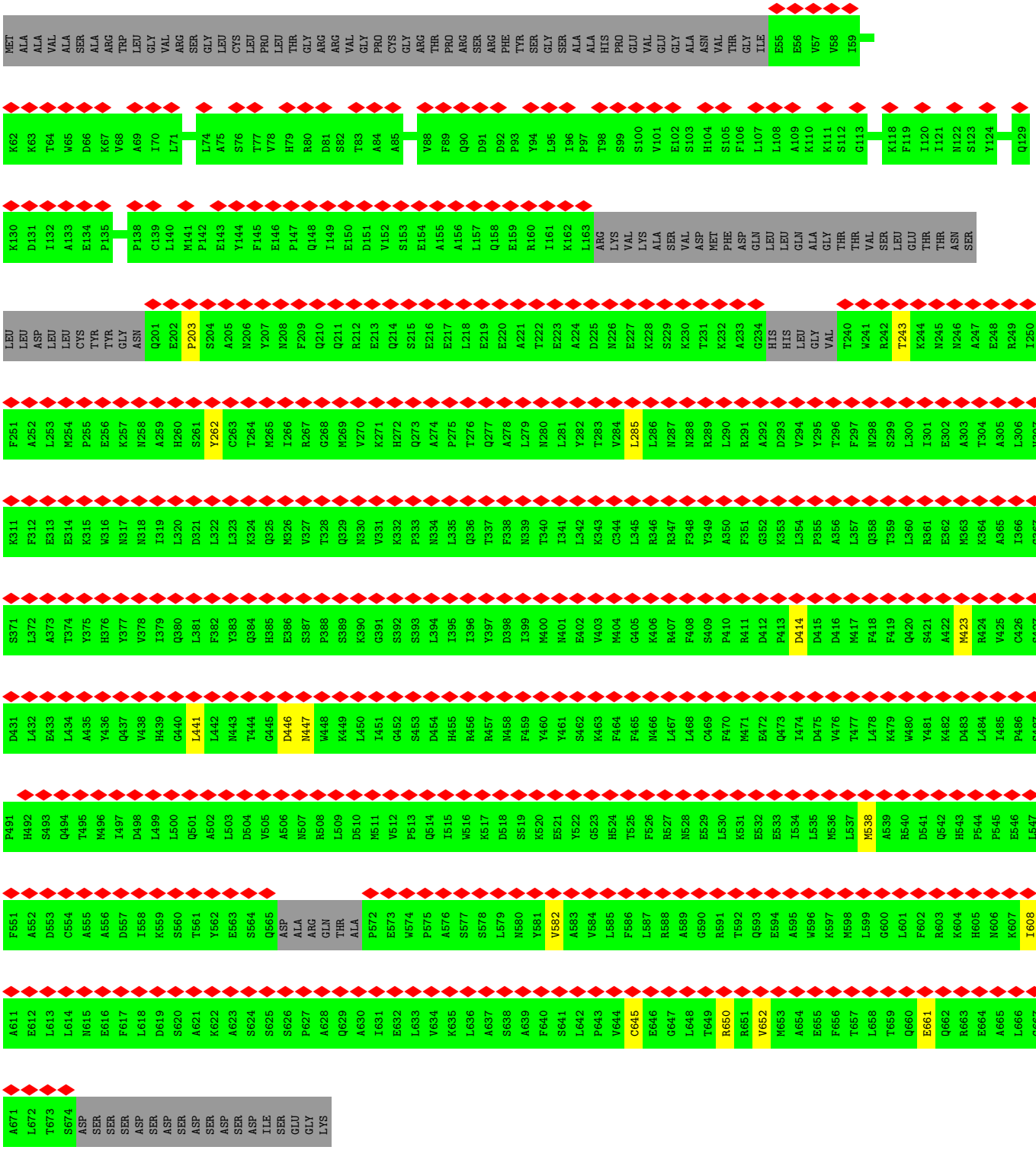
- Molecule 87: Aurora kinase A interacting protein 1

Chain An:



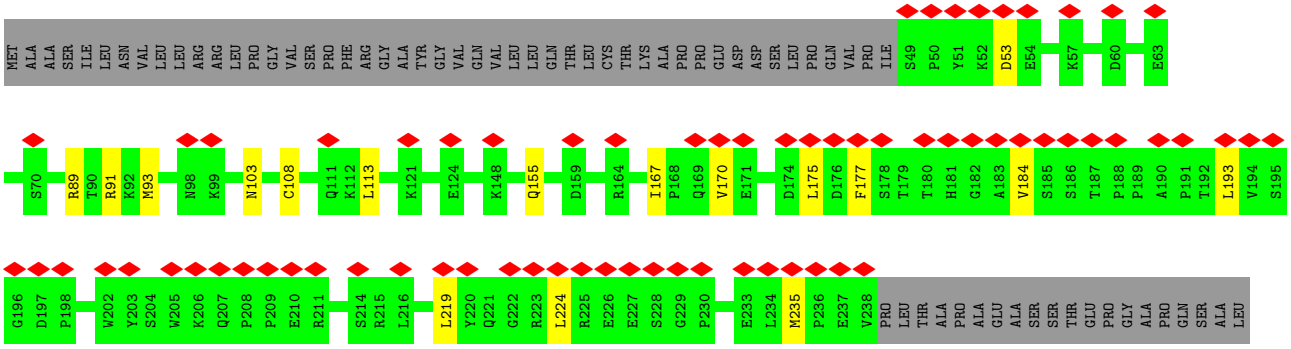
• Molecule 88: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain Ao:



• Molecule 89: 28S ribosomal protein S18b, mitochondrial

Chain Ap:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139206	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	1.453	Depositor
Minimum map value	-0.743	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	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: FME, MG, NA, 5GP, SPM, ZN, GTP, GSP

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	BL	0.34	0/542	0.48	0/729
1	CL	0.36	0/319	0.67	2/435 (0.5%)
1	DL	0.31	0/212	0.43	0/286
1	EL	0.36	0/221	0.48	0/297
1	FL	0.36	0/212	0.49	0/286
1	GL	0.37	0/212	0.44	0/286
1	HL	0.38	0/204	0.49	0/275
2	B0	0.50	0/880	0.53	0/1189
3	B1	0.34	0/2093	0.48	0/2835
4	B2	0.40	0/1586	0.52	0/2123
5	B3	0.43	0/993	0.58	0/1341
6	B4	0.25	0/388	0.50	0/523
7	B5	0.42	0/917	0.53	0/1227
8	B6	0.31	0/430	0.50	0/570
9	B7	0.54	0/395	0.58	0/524
10	B8	0.51	0/853	0.58	0/1136
11	B9	0.45	0/342	0.56	0/450
12	BA	0.81	0/36903	0.97	29/57455 (0.1%)
13	BB	0.44	1/1595 (0.1%)	0.84	0/2475
14	BC	0.30	0/4432	0.49	2/5989 (0.0%)
15	BD	0.42	0/1898	0.57	0/2555
16	BE	0.44	0/2493	0.62	2/3387 (0.1%)
17	BF	0.47	0/2069	0.59	0/2816
18	BI	0.35	0/819	0.52	0/1101
19	BJ	0.31	0/1742	0.47	0/2358
20	BK	0.29	0/1323	0.49	1/1785 (0.1%)
21	BN	0.44	0/1487	0.53	0/2017
22	BO	0.41	0/912	0.57	0/1231
23	BP	0.42	0/2368	0.54	0/3198
24	BQ	0.39	0/1850	0.53	0/2491
25	BR	0.46	0/1262	0.57	0/1700
26	BS	0.38	0/1197	0.54	0/1624

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	BT	0.41	0/2002	0.57	1/2708 (0.0%)
28	BU	0.52	0/1179	0.58	0/1578
29	BV	0.46	0/1256	0.59	0/1706
30	BW	0.47	0/1407	0.55	0/1891
31	BX	0.42	0/1211	0.55	0/1646
32	BY	0.28	0/1719	0.50	0/2329
33	Ba	0.37	0/3267	0.53	0/4455
34	Bb	0.35	0/3047	0.53	1/4139 (0.0%)
35	Bc	0.34	0/2464	0.49	0/3330
36	Bd	0.28	0/853	0.50	0/1153
37	Be	0.36	0/1000	0.58	0/1345
38	Bf	0.37	0/851	0.55	2/1159 (0.2%)
39	Bg	0.45	0/1191	0.56	0/1614
40	Bh	0.36	0/2372	0.54	0/3211
41	Bi	0.31	0/2199	0.49	0/2980
42	Bj	0.28	0/1811	0.48	0/2436
43	Bk	0.30	0/1108	0.49	0/1499
44	Bl	0.38	0/1135	0.51	0/1549
45	Bm	0.26	0/917	0.44	0/1248
46	Bn	0.51	0/860	0.61	0/1150
47	Bo	0.37	0/787	0.51	0/1056
48	Bp	0.29	0/752	0.50	0/1013
49	Bq	0.32	0/558	0.48	1/756 (0.1%)
50	Bt	0.45	0/798	0.58	0/1073
51	Bu	0.28	0/1214	0.48	1/1630 (0.1%)
52	Bv	0.28	0/1157	0.39	0/1560
53	Bw	0.42	0/3206	0.55	0/4354
54	Bx	0.42	0/1364	0.61	1/1849 (0.1%)
55	Bz	0.29	0/404	0.29	0/556
56	AA	0.53	0/22852	0.93	17/35580 (0.0%)
57	AB	0.45	0/1804	0.54	0/2445
58	AC	0.39	0/1105	0.50	0/1496
59	AE	0.34	0/2785	0.49	0/3735
60	AF	0.35	0/999	0.56	1/1347 (0.1%)
61	AG	0.38	0/1763	0.47	0/2368
62	AI	0.38	0/2707	0.46	0/3636
63	AJ	0.40	0/1181	0.52	0/1597
64	AK	0.35	0/1027	0.58	0/1389
65	AL	0.31	0/858	0.53	0/1152
66	AN	0.46	0/874	0.50	0/1171
67	AO	0.37	0/1473	0.52	0/1970
68	AP	0.50	0/954	0.55	0/1284
69	AQ	0.39	0/894	0.55	0/1213

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
70	AR	0.47	1/802 (0.1%)	0.59	0/1079
71	AU	0.39	0/745	0.55	0/993
72	AV	0.37	0/1673	0.93	5/2602 (0.2%)
73	AX	0.41	0/395	1.08	4/612 (0.7%)
74	AZ	0.35	0/89	0.44	0/123
75	Aa	0.44	0/2428	0.51	0/3279
76	Ab	0.40	0/1126	0.50	0/1514
77	Ac	0.42	0/1399	0.52	0/1881
78	Ad	0.43	0/1490	0.47	0/2005
79	Ae	0.32	0/3171	0.51	1/4292 (0.0%)
80	Af	0.40	0/790	0.57	0/1064
81	Ag	0.34	0/2945	0.47	0/3984
82	Ah	0.40	0/1045	0.45	0/1409
83	Ai	0.38	0/841	0.46	0/1121
84	Aj	0.35	0/1835	0.49	0/2484
85	Ak	0.36	0/2268	0.46	0/3069
86	Am	0.34	0/947	0.49	0/1268
87	An	0.38	0/650	0.54	0/858
88	Ao	0.32	0/4626	0.48	1/6269 (0.0%)
89	Ap	0.38	0/1616	0.49	0/2195
All	All	0.51	2/187395 (0.0%)	0.71	72/266151 (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	B4	0	1
16	BE	0	1
34	Bb	0	1
46	Bn	0	1
53	Bw	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BB	1	G	OP3-P	-10.43	1.48	1.61
70	AR	69	CYS	CB-SG	5.52	1.91	1.82

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BT	68	PRO	N-CA-CB	8.66	113.70	103.30
56	AA	959	U	N1-C2-O2	8.45	128.72	122.80
72	AV	9	C	C2-N1-C1'	8.28	127.90	118.80
56	AA	959	U	C2-N1-C1'	8.21	127.55	117.70
12	BA	448	G	O5'-P-OP2	-8.04	98.47	105.70
72	AV	9	C	N1-C2-O2	7.79	123.58	118.90
56	AA	959	U	N3-C2-O2	-7.03	117.28	122.20
12	BA	595	C	C6-N1-C2	-6.88	117.55	120.30
12	BA	52	A	O4'-C1'-N9	6.83	113.67	108.20
14	BC	502	PRO	N-CA-CB	6.75	111.40	103.30
72	AV	9	C	N3-C2-O2	-6.65	117.25	121.90
73	AX	10	C	N1-C2-O2	6.48	122.79	118.90
73	AX	7	C	C2-N1-C1'	6.45	125.90	118.80
72	AV	9	C	C6-N1-C2	-6.41	117.74	120.30
12	BA	697	C	C6-N1-C2	-6.37	117.75	120.30
1	CL	21	PRO	N-CA-CB	6.35	110.92	103.30
16	BE	201	GLY	N-CA-C	-6.34	97.24	113.10
12	BA	190	U	N3-C2-O2	-6.28	117.81	122.20
1	CL	16	PRO	N-CA-CB	6.23	110.77	103.30
12	BA	848	C	C2-N1-C1'	6.17	125.59	118.80
12	BA	697	C	C5-C6-N1	6.14	124.07	121.00
88	Ao	203	PRO	N-CA-CB	6.13	110.65	103.30
12	BA	64	C	C6-N1-C2	-6.07	117.87	120.30
12	BA	64	C	N3-C2-O2	-5.93	117.75	121.90
12	BA	170	U	N3-C2-O2	-5.79	118.15	122.20
51	Bu	167	PRO	N-CA-CB	5.77	110.23	103.30
38	Bf	80	PRO	N-CA-CB	5.76	110.21	103.30
12	BA	825	C	C2-N1-C1'	5.73	125.10	118.80
12	BA	295	G	O4'-C1'-N9	5.72	112.78	108.20
12	BA	112	A	O4'-C1'-N9	5.71	112.77	108.20
56	AA	119	C	C2-N1-C1'	5.68	125.05	118.80
14	BC	505	PRO	N-CA-CB	5.65	110.08	103.30
79	Ae	342	PRO	N-CA-CB	5.64	110.07	103.30
73	AX	10	C	C2-N1-C1'	5.63	125.00	118.80
56	AA	745	C	C2-N1-C1'	5.62	124.98	118.80
12	BA	48	U	P-O3'-C3'	5.61	126.43	119.70
12	BA	999	C	C6-N1-C2	-5.57	118.07	120.30
56	AA	70	U	C5-C6-N1	-5.56	119.92	122.70
38	Bf	78	PRO	N-CA-CB	5.53	109.94	103.30
12	BA	104	C	C2-N1-C1'	5.51	124.86	118.80
12	BA	19	U	C5-C6-N1	5.49	125.44	122.70
56	AA	119	C	C6-N1-C1'	-5.48	114.22	120.80
12	BA	848	C	N1-C2-O2	5.44	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	BE	102	LEU	CA-CB-CG	5.42	127.77	115.30
72	AV	9	C	C6-N1-C1'	-5.41	114.31	120.80
56	AA	959	U	C6-N1-C1'	-5.41	113.63	121.20
12	BA	697	C	C2-N1-C1'	5.38	124.72	118.80
60	AF	105	CYS	CA-CB-SG	5.37	123.67	114.00
56	AA	745	C	C6-N1-C2	-5.35	118.16	120.30
12	BA	890	C	N1-C2-O2	5.33	122.10	118.90
34	Bb	211	GLY	N-CA-C	-5.32	99.80	113.10
12	BA	238	C	O4'-C1'-N1	5.29	112.43	108.20
12	BA	404	C	N1-C2-O2	5.29	122.07	118.90
56	AA	841	C	N1-C2-O2	5.28	122.07	118.90
56	AA	959	U	C5-C6-N1	5.27	125.34	122.70
49	Bq	102	GLY	N-CA-C	5.23	126.19	113.10
12	BA	595	C	C2-N1-C1'	5.22	124.54	118.80
56	AA	156	C	C6-N1-C2	5.21	122.39	120.30
12	BA	825	C	C6-N1-C2	-5.20	118.22	120.30
54	Bx	73	CYS	CA-CB-SG	-5.20	104.64	114.00
56	AA	382	U	C5-C6-N1	-5.18	120.11	122.70
12	BA	394	C	C6-N1-C2	-5.16	118.23	120.30
12	BA	1241	U	P-O3'-C3'	5.13	125.86	119.70
12	BA	1527	U	N1-C2-O2	5.13	126.39	122.80
12	BA	31	A	C8-N9-C4	5.10	107.84	105.80
73	AX	7	C	C6-N1-C1'	-5.09	114.69	120.80
20	BK	164	LEU	CA-CB-CG	-5.07	103.65	115.30
12	BA	404	C	C2-N1-C1'	5.05	124.35	118.80
56	AA	177	U	C5-C6-N1	-5.03	120.18	122.70
56	AA	841	C	C2-N1-C1'	5.01	124.31	118.80
56	AA	745	C	N1-C2-O2	5.00	121.90	118.90
56	AA	119	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B4	61	ASP	Peptide
16	BE	316	PHE	Peptide
34	Bb	210	GLU	Peptide
46	Bn	65	ASN	Peptide
53	Bw	356	THR	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	BL	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
1	CL	43/198 (22%)	41 (95%)	1 (2%)	1 (2%)	6	34
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	25 (96%)	1 (4%)	0	100	100
1	FL	25/198 (13%)	25 (100%)	0	0	100	100
1	GL	25/198 (13%)	25 (100%)	0	0	100	100
1	HL	24/198 (12%)	24 (100%)	0	0	100	100
2	B0	108/148 (73%)	104 (96%)	4 (4%)	0	100	100
3	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
4	B2	177/252 (70%)	172 (97%)	5 (3%)	0	100	100
5	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
6	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
7	B5	108/188 (57%)	106 (98%)	2 (2%)	0	100	100
8	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
9	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
10	B8	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
11	B9	36/100 (36%)	36 (100%)	0	0	100	100
14	BC	569/650 (88%)	548 (96%)	20 (4%)	1 (0%)	47	79
15	BD	238/306 (78%)	226 (95%)	12 (5%)	0	100	100
16	BE	305/348 (88%)	284 (93%)	18 (6%)	3 (1%)	15	54
17	BF	248/294 (84%)	237 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
19	BJ	210/262 (80%)	202 (96%)	8 (4%)	0	100	100
20	BK	174/192 (91%)	166 (95%)	7 (4%)	1 (1%)	25	64
21	BN	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
22	BO	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
23	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
24	BQ	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
25	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
26	BS	141/180 (78%)	131 (93%)	9 (6%)	1 (1%)	22	61
27	BT	238/292 (82%)	229 (96%)	8 (3%)	1 (0%)	34	69
28	BU	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
29	BV	153/209 (73%)	147 (96%)	6 (4%)	0	100	100
30	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
31	BX	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
32	BY	204/216 (94%)	193 (95%)	11 (5%)	0	100	100
33	Ba	391/423 (92%)	377 (96%)	14 (4%)	0	100	100
34	Bb	352/380 (93%)	329 (94%)	23 (6%)	0	100	100
35	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100
36	Bd	97/206 (47%)	89 (92%)	7 (7%)	1 (1%)	15	54
37	Be	120/135 (89%)	115 (96%)	5 (4%)	0	100	100
38	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	8	39
39	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
40	Bh	287/332 (86%)	276 (96%)	11 (4%)	0	100	100
41	Bi	258/306 (84%)	248 (96%)	10 (4%)	0	100	100
42	Bj	211/279 (76%)	199 (94%)	12 (6%)	0	100	100
43	Bk	132/212 (62%)	126 (96%)	6 (4%)	0	100	100
44	Bl	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
45	Bm	107/159 (67%)	104 (97%)	3 (3%)	0	100	100
46	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
47	Bo	95/124 (77%)	91 (96%)	4 (4%)	0	100	100
48	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Bq	66/138 (48%)	64 (97%)	1 (2%)	1 (2%)	10	44
50	Bt	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
51	Bu	147/205 (72%)	136 (92%)	10 (7%)	1 (1%)	22	61
52	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
53	Bw	385/433 (89%)	365 (95%)	18 (5%)	2 (0%)	29	67
54	Bx	160/196 (82%)	156 (98%)	3 (2%)	1 (1%)	25	64
55	Bz	70/82 (85%)	70 (100%)	0	0	100	100
57	AB	218/289 (75%)	213 (98%)	5 (2%)	0	100	100
58	AC	130/167 (78%)	122 (94%)	8 (6%)	0	100	100
59	AE	341/430 (79%)	327 (96%)	14 (4%)	0	100	100
60	AF	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
61	AG	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
62	AI	326/397 (82%)	313 (96%)	13 (4%)	0	100	100
63	AJ	138/201 (69%)	129 (94%)	7 (5%)	2 (1%)	11	46
64	AK	135/196 (69%)	129 (96%)	5 (4%)	1 (1%)	22	61
65	AL	107/139 (77%)	105 (98%)	2 (2%)	0	100	100
66	AN	99/128 (77%)	99 (100%)	0	0	100	100
67	AO	173/239 (72%)	167 (96%)	6 (4%)	0	100	100
68	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100	100
69	AQ	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
70	AR	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
71	AU	84/87 (97%)	84 (100%)	0	0	100	100
74	AZ	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
75	Aa	290/382 (76%)	284 (98%)	6 (2%)	0	100	100
76	Ab	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
77	Ac	167/173 (96%)	157 (94%)	9 (5%)	1 (1%)	25	64
78	Ad	175/205 (85%)	170 (97%)	5 (3%)	0	100	100
79	Ae	386/455 (85%)	350 (91%)	32 (8%)	4 (1%)	15	54
80	Af	97/188 (52%)	92 (95%)	5 (5%)	0	100	100
81	Ag	351/397 (88%)	338 (96%)	13 (4%)	0	100	100
82	Ah	118/387 (30%)	116 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	Ai	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
84	Aj	211/218 (97%)	207 (98%)	4 (2%)	0	100	100
85	Ak	273/325 (84%)	265 (97%)	8 (3%)	0	100	100
86	Am	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
87	An	70/199 (35%)	68 (97%)	2 (3%)	0	100	100
88	Ao	564/692 (82%)	532 (94%)	32 (6%)	0	100	100
89	Ap	188/258 (73%)	182 (97%)	6 (3%)	0	100	100
All	All	14839/20063 (74%)	14258 (96%)	557 (4%)	24 (0%)	50	79

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CL	21	PRO
14	BC	502	PRO
27	BT	68	PRO
38	Bf	78	PRO
38	Bf	80	PRO
51	Bu	167	PRO
16	BE	202	GLN
53	Bw	159	VAL
54	Bx	93	ILE
63	AJ	179	GLN
63	AJ	185	ARG
16	BE	317	PRO
79	Ae	285	CYS
20	BK	157	LYS
49	Bq	101	VAL
53	Bw	100	LEU
77	Ac	105	ILE
79	Ae	161	ALA
79	Ae	342	PRO
79	Ae	344	GLU
16	BE	264	ILE
64	AK	186	ASN
36	Bd	170	PRO
26	BS	45	ALA

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	BL	59/157 (38%)	59 (100%)	0	100	100
1	CL	30/157 (19%)	29 (97%)	1 (3%)	38	71
1	DL	26/157 (17%)	24 (92%)	2 (8%)	13	44
1	EL	27/157 (17%)	25 (93%)	2 (7%)	13	46
1	FL	26/157 (17%)	25 (96%)	1 (4%)	33	67
1	GL	26/157 (17%)	25 (96%)	1 (4%)	33	67
1	HL	25/157 (16%)	23 (92%)	2 (8%)	12	42
2	B0	90/115 (78%)	84 (93%)	6 (7%)	16	50
3	B1	219/229 (96%)	195 (89%)	24 (11%)	6	26
4	B2	164/228 (72%)	148 (90%)	16 (10%)	8	31
5	B3	110/147 (75%)	101 (92%)	9 (8%)	11	41
6	B4	42/114 (37%)	37 (88%)	5 (12%)	5	22
7	B5	99/163 (61%)	89 (90%)	10 (10%)	7	29
8	B6	49/60 (82%)	47 (96%)	2 (4%)	30	66
9	B7	41/78 (53%)	38 (93%)	3 (7%)	14	46
10	B8	87/162 (54%)	75 (86%)	12 (14%)	3	16
11	B9	36/77 (47%)	32 (89%)	4 (11%)	6	25
14	BC	464/553 (84%)	451 (97%)	13 (3%)	43	74
15	BD	193/248 (78%)	172 (89%)	21 (11%)	6	26
16	BE	263/290 (91%)	242 (92%)	21 (8%)	12	42
17	BF	217/251 (86%)	193 (89%)	24 (11%)	6	25
18	BI	88/228 (39%)	82 (93%)	6 (7%)	16	49
19	BJ	192/230 (84%)	184 (96%)	8 (4%)	30	65
20	BK	129/151 (85%)	124 (96%)	5 (4%)	32	67
21	BN	156/157 (99%)	140 (90%)	16 (10%)	7	29
22	BO	99/123 (80%)	87 (88%)	12 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	BP	245/249 (98%)	214 (87%)	31 (13%)	4	20
24	BQ	190/210 (90%)	177 (93%)	13 (7%)	16	49
25	BR	132/143 (92%)	119 (90%)	13 (10%)	8	31
26	BS	123/153 (80%)	117 (95%)	6 (5%)	25	61
27	BT	212/258 (82%)	193 (91%)	19 (9%)	9	34
28	BU	118/127 (93%)	111 (94%)	7 (6%)	19	54
29	BV	136/178 (76%)	123 (90%)	13 (10%)	8	32
30	BW	144/180 (80%)	133 (92%)	11 (8%)	13	45
31	BX	116/134 (87%)	105 (90%)	11 (10%)	8	32
32	BY	185/192 (96%)	165 (89%)	20 (11%)	6	27
33	Ba	348/365 (95%)	314 (90%)	34 (10%)	8	31
34	Bb	310/328 (94%)	280 (90%)	30 (10%)	8	31
35	Bc	271/299 (91%)	256 (94%)	15 (6%)	21	57
36	Bd	92/181 (51%)	82 (89%)	10 (11%)	6	26
37	Be	100/108 (93%)	85 (85%)	15 (15%)	3	14
38	Bf	80/133 (60%)	67 (84%)	13 (16%)	2	11
39	Bg	128/136 (94%)	108 (84%)	20 (16%)	2	12
40	Bh	251/284 (88%)	226 (90%)	25 (10%)	7	30
41	Bi	236/275 (86%)	222 (94%)	14 (6%)	19	54
42	Bj	190/242 (78%)	176 (93%)	14 (7%)	13	46
43	Bk	119/181 (66%)	111 (93%)	8 (7%)	16	50
44	Bl	122/147 (83%)	110 (90%)	12 (10%)	8	31
45	Bm	103/145 (71%)	97 (94%)	6 (6%)	20	55
46	Bn	88/113 (78%)	78 (89%)	10 (11%)	5	24
47	Bo	77/97 (79%)	70 (91%)	7 (9%)	9	34
48	Bp	79/88 (90%)	75 (95%)	4 (5%)	24	60
49	Bq	50/114 (44%)	46 (92%)	4 (8%)	12	42
50	Bt	75/82 (92%)	61 (81%)	14 (19%)	1	8
51	Bu	126/177 (71%)	113 (90%)	13 (10%)	7	29
52	Bv	115/183 (63%)	112 (97%)	3 (3%)	46	76
53	Bw	340/373 (91%)	307 (90%)	33 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	Bx	149/173 (86%)	135 (91%)	14 (9%)	8	33
57	AB	187/233 (80%)	174 (93%)	13 (7%)	15	48
58	AC	115/142 (81%)	99 (86%)	16 (14%)	3	16
59	AE	282/351 (80%)	259 (92%)	23 (8%)	11	41
60	AF	107/109 (98%)	97 (91%)	10 (9%)	9	33
61	AG	181/205 (88%)	166 (92%)	15 (8%)	11	40
62	AI	273/333 (82%)	255 (93%)	18 (7%)	16	51
63	AJ	130/181 (72%)	117 (90%)	13 (10%)	7	30
64	AK	103/151 (68%)	95 (92%)	8 (8%)	12	43
65	AL	92/116 (79%)	88 (96%)	4 (4%)	29	64
66	AN	92/114 (81%)	78 (85%)	14 (15%)	3	13
67	AO	159/205 (78%)	148 (93%)	11 (7%)	15	49
68	AP	97/113 (86%)	93 (96%)	4 (4%)	30	66
69	AQ	97/114 (85%)	86 (89%)	11 (11%)	6	25
70	AR	89/127 (70%)	83 (93%)	6 (7%)	16	50
71	AU	77/78 (99%)	67 (87%)	10 (13%)	4	19
75	Aa	258/330 (78%)	233 (90%)	25 (10%)	8	31
76	Ab	113/162 (70%)	105 (93%)	8 (7%)	14	47
77	Ac	152/155 (98%)	141 (93%)	11 (7%)	14	47
78	Ad	149/168 (89%)	140 (94%)	9 (6%)	19	54
79	Ae	325/393 (83%)	300 (92%)	25 (8%)	13	44
80	Af	86/160 (54%)	80 (93%)	6 (7%)	15	48
81	Ag	312/350 (89%)	292 (94%)	20 (6%)	17	52
82	Ah	109/346 (32%)	105 (96%)	4 (4%)	34	68
83	Ai	86/93 (92%)	81 (94%)	5 (6%)	20	55
84	Aj	188/190 (99%)	178 (95%)	10 (5%)	22	58
85	Ak	249/289 (86%)	226 (91%)	23 (9%)	9	33
86	Am	100/102 (98%)	88 (88%)	12 (12%)	5	22
87	An	66/174 (38%)	58 (88%)	8 (12%)	5	22
88	Ao	478/604 (79%)	462 (97%)	16 (3%)	38	71
89	Ap	170/225 (76%)	153 (90%)	17 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12929/17064 (76%)	11866 (92%)	1063 (8%)	15 41

All (1063) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CL	40	LEU
1	DL	75	THR
1	DL	86	LEU
1	EL	76	LEU
1	EL	82	LEU
1	FL	76	LEU
1	GL	82	LEU
1	HL	76	LEU
1	HL	79	ILE
2	B0	45	LYS
2	B0	50	ARG
2	B0	53	ILE
2	B0	88	CYS
2	B0	126	LEU
2	B0	141	THR
3	B1	6	VAL
3	B1	31	SER
3	B1	46	HIS
3	B1	61	ARG
3	B1	64	ASP
3	B1	75	SER
3	B1	77	LEU
3	B1	79	LEU
3	B1	104	VAL
3	B1	112	ARG
3	B1	120	ASP
3	B1	126	THR
3	B1	148	THR
3	B1	152	ASP
3	B1	161	LEU
3	B1	172	GLN
3	B1	177	HIS
3	B1	179	ASP
3	B1	190	ARG
3	B1	209	ASP
3	B1	216	ARG
3	B1	222	ASP

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Mol	Chain	Res	Type
3	B1	224	ILE
3	B1	238	LEU
4	B2	67	GLU
4	B2	68	GLU
4	B2	72	ASP
4	B2	108	LEU
4	B2	118	GLU
4	B2	126	LEU
4	B2	144	LEU
4	B2	145	ASP
4	B2	153	ASP
4	B2	158	LEU
4	B2	171	ARG
4	B2	174	ILE
4	B2	197	ASN
4	B2	218	GLN
4	B2	228	LEU
4	B2	230	ARG
5	B3	38	ARG
5	B3	43	ASP
5	B3	72	ILE
5	B3	73	LYS
5	B3	78	ARG
5	B3	86	ILE
5	B3	93	LYS
5	B3	150	LEU
5	B3	151	LEU
6	B4	42	THR
6	B4	44	LEU
6	B4	49	TYR
6	B4	57	LEU
6	B4	78	MET
7	B5	85	ARG
7	B5	87	ILE
7	B5	94	ARG
7	B5	136	GLU
7	B5	153	THR
7	B5	156	THR
7	B5	158	VAL
7	B5	173	ARG
7	B5	185	PHE
7	B5	186	THR

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Mol	Chain	Res	Type
8	B6	22	SER
8	B6	34	ARG
9	B7	65	HIS
9	B7	75	THR
9	B7	92	SER
10	B8	106	THR
10	B8	111	ILE
10	B8	113	ARG
10	B8	124	ARG
10	B8	125	ARG
10	B8	142	ARG
10	B8	162	THR
10	B8	163	THR
10	B8	169	ARG
10	B8	182	ASP
10	B8	183	ARG
10	B8	184	THR
11	B9	63	PHE
11	B9	74	ARG
11	B9	75	ASP
11	B9	92	ASN
14	BC	184	THR
14	BC	253	ASP
14	BC	283	ILE
14	BC	330	ASN
14	BC	392	CYS
14	BC	472	GLU
14	BC	484	LEU
14	BC	494	PHE
14	BC	524	VAL
14	BC	537	THR
14	BC	679	HIS
14	BC	708	ARG
14	BC	727	PHE
15	BD	62	THR
15	BD	64	VAL
15	BD	69	ARG
15	BD	74	VAL
15	BD	75	MET
15	BD	85	ARG
15	BD	90	GLN
15	BD	103	ARG

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Mol	Chain	Res	Type
15	BD	105	ARG
15	BD	111	ARG
15	BD	148	ARG
15	BD	150	ARG
15	BD	155	THR
15	BD	158	MET
15	BD	163	THR
15	BD	172	ARG
15	BD	190	VAL
15	BD	198	GLU
15	BD	224	THR
15	BD	240	THR
15	BD	285	ARG
16	BE	50	ASP
16	BE	53	LEU
16	BE	55	GLU
16	BE	97	VAL
16	BE	109	LEU
16	BE	113	ASP
16	BE	146	THR
16	BE	158	SER
16	BE	218	VAL
16	BE	220	ARG
16	BE	227	GLN
16	BE	236	THR
16	BE	239	ARG
16	BE	273	VAL
16	BE	285	VAL
16	BE	296	LEU
16	BE	297	VAL
16	BE	299	ILE
16	BE	302	SER
16	BE	311	CYS
16	BE	326	GLU
17	BF	47	VAL
17	BF	59	ARG
17	BF	76	ARG
17	BF	77	VAL
17	BF	79	LEU
17	BF	80	THR
17	BF	94	ASP
17	BF	101	ILE

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Mol	Chain	Res	Type
17	BF	106	PHE
17	BF	111	TYR
17	BF	116	THR
17	BF	125	ARG
17	BF	140	SER
17	BF	143	SER
17	BF	165	LEU
17	BF	172	GLN
17	BF	190	VAL
17	BF	203	LEU
17	BF	208	ARG
17	BF	224	GLU
17	BF	239	THR
17	BF	263	LEU
17	BF	281	THR
17	BF	291	CYS
18	BI	56	VAL
18	BI	75	ARG
18	BI	76	ARG
18	BI	78	ARG
18	BI	99	THR
18	BI	108	ARG
19	BJ	34	THR
19	BJ	63	ARG
19	BJ	76	THR
19	BJ	78	LEU
19	BJ	93	ASN
19	BJ	121	ILE
19	BJ	150	HIS
19	BJ	229	LEU
20	BK	57	THR
20	BK	64	ILE
20	BK	113	THR
20	BK	158	ASP
20	BK	164	LEU
21	BN	10	GLN
21	BN	24	LYS
21	BN	31	LEU
21	BN	39	LEU
21	BN	65	ILE
21	BN	67	PHE
21	BN	78	SER

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Mol	Chain	Res	Type
21	BN	91	THR
21	BN	101	VAL
21	BN	104	VAL
21	BN	118	ARG
21	BN	123	GLN
21	BN	131	GLU
21	BN	136	ASP
21	BN	153	ARG
21	BN	177	ARG
22	BO	56	ARG
22	BO	71	ASP
22	BO	72	ARG
22	BO	73	ILE
22	BO	77	ILE
22	BO	91	MET
22	BO	95	ARG
22	BO	96	MET
22	BO	101	ASP
22	BO	111	ASN
22	BO	121	THR
22	BO	138	LEU
23	BP	11	ARG
23	BP	44	ARG
23	BP	51	ARG
23	BP	58	GLN
23	BP	59	ARG
23	BP	61	THR
23	BP	62	ARG
23	BP	65	LEU
23	BP	71	GLN
23	BP	109	ARG
23	BP	125	ARG
23	BP	127	VAL
23	BP	130	GLN
23	BP	134	ARG
23	BP	140	LEU
23	BP	141	VAL
23	BP	147	THR
23	BP	152	VAL
23	BP	154	ILE
23	BP	175	THR
23	BP	180	ASP

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Mol	Chain	Res	Type
23	BP	215	THR
23	BP	233	ARG
23	BP	234	LEU
23	BP	246	ASP
23	BP	247	ILE
23	BP	248	THR
23	BP	250	ASP
23	BP	257	SER
23	BP	261	ASP
23	BP	286	THR
24	BQ	39	PHE
24	BQ	55	ARG
24	BQ	68	ASN
24	BQ	111	ARG
24	BQ	133	ARG
24	BQ	166	ARG
24	BQ	171	GLU
24	BQ	194	THR
24	BQ	209	ASN
24	BQ	214	THR
24	BQ	226	ILE
24	BQ	247	THR
24	BQ	250	ARG
25	BR	24	SER
25	BR	30	GLN
25	BR	38	ARG
25	BR	67	ASP
25	BR	83	LYS
25	BR	84	ASP
25	BR	93	LEU
25	BR	98	GLN
25	BR	110	ILE
25	BR	118	ARG
25	BR	134	LEU
25	BR	139	ARG
25	BR	142	ASN
26	BS	44	VAL
26	BS	80	ARG
26	BS	107	THR
26	BS	141	ILE
26	BS	149	THR
26	BS	163	HIS

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Mol	Chain	Res	Type
27	BT	61	VAL
27	BT	77	SER
27	BT	79	GLU
27	BT	86	ARG
27	BT	90	LEU
27	BT	130	THR
27	BT	145	LEU
27	BT	162	ILE
27	BT	170	ARG
27	BT	177	VAL
27	BT	187	LEU
27	BT	239	ASN
27	BT	243	ILE
27	BT	246	ASP
27	BT	270	MET
27	BT	272	GLU
27	BT	274	ASP
27	BT	284	ASP
27	BT	289	SER
28	BU	10	LEU
28	BU	43	VAL
28	BU	48	ARG
28	BU	54	THR
28	BU	77	GLN
28	BU	87	ILE
28	BU	123	ARG
29	BV	91	ILE
29	BV	111	LYS
29	BV	117	LEU
29	BV	126	VAL
29	BV	133	ARG
29	BV	153	LEU
29	BV	160	VAL
29	BV	164	VAL
29	BV	169	GLU
29	BV	170	SER
29	BV	176	MET
29	BV	186	ARG
29	BV	199	ILE
30	BW	46	SER
30	BW	60	GLN
30	BW	75	ARG

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Mol	Chain	Res	Type
30	BW	80	TYR
30	BW	81	SER
30	BW	131	ASN
30	BW	136	SER
30	BW	147	ARG
30	BW	151	LEU
30	BW	199	GLN
30	BW	206	ILE
31	BX	6	LEU
31	BX	14	ASN
31	BX	28	LEU
31	BX	35	GLN
31	BX	47	GLU
31	BX	49	THR
31	BX	50	ARG
31	BX	52	ASP
31	BX	57	LEU
31	BX	78	ARG
31	BX	140	ARG
32	BY	30	SER
32	BY	31	ASP
32	BY	39	THR
32	BY	40	ARG
32	BY	43	ARG
32	BY	66	GLU
32	BY	69	ASP
32	BY	86	VAL
32	BY	96	ARG
32	BY	105	ARG
32	BY	107	THR
32	BY	131	THR
32	BY	137	PHE
32	BY	138	THR
32	BY	149	ARG
32	BY	153	ILE
32	BY	181	ASP
32	BY	186	THR
32	BY	190	ARG
32	BY	208	ARG
33	Ba	42	GLU
33	Ba	47	ASP
33	Ba	63	LYS

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Mol	Chain	Res	Type
33	Ba	67	MET
33	Ba	72	ARG
33	Ba	110	ARG
33	Ba	137	LEU
33	Ba	147	ILE
33	Ba	149	ASN
33	Ba	163	LEU
33	Ba	167	THR
33	Ba	175	THR
33	Ba	176	TYR
33	Ba	189	LYS
33	Ba	195	HIS
33	Ba	202	ILE
33	Ba	207	ASN
33	Ba	215	ARG
33	Ba	222	VAL
33	Ba	234	ASP
33	Ba	256	PHE
33	Ba	262	THR
33	Ba	270	VAL
33	Ba	322	LEU
33	Ba	324	GLN
33	Ba	335	VAL
33	Ba	337	GLU
33	Ba	347	THR
33	Ba	348	ASP
33	Ba	373	LEU
33	Ba	381	LEU
33	Ba	391	VAL
33	Ba	398	VAL
33	Ba	415	LEU
34	Bb	32	LEU
34	Bb	35	MET
34	Bb	40	ILE
34	Bb	50	LYS
34	Bb	51	TYR
34	Bb	52	ARG
34	Bb	53	SER
34	Bb	99	ARG
34	Bb	118	GLU
34	Bb	120	GLU
34	Bb	135	VAL

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Mol	Chain	Res	Type
34	Bb	141	ARG
34	Bb	173	LEU
34	Bb	179	VAL
34	Bb	210	GLU
34	Bb	222	ASP
34	Bb	237	VAL
34	Bb	238	THR
34	Bb	252	CYS
34	Bb	261	ARG
34	Bb	267	ARG
34	Bb	272	LEU
34	Bb	276	ASP
34	Bb	281	PHE
34	Bb	284	ASP
34	Bb	288	SER
34	Bb	324	ASP
34	Bb	356	ARG
34	Bb	360	ARG
34	Bb	376	THR
35	Bc	67	VAL
35	Bc	87	SER
35	Bc	111	ASP
35	Bc	122	ILE
35	Bc	140	TRP
35	Bc	186	LEU
35	Bc	190	MET
35	Bc	218	VAL
35	Bc	222	VAL
35	Bc	253	ARG
35	Bc	256	ASP
35	Bc	280	VAL
35	Bc	285	THR
35	Bc	297	SER
35	Bc	319	MET
36	Bd	89	ILE
36	Bd	98	GLU
36	Bd	99	ARG
36	Bd	106	LEU
36	Bd	120	ARG
36	Bd	132	GLU
36	Bd	136	ILE
36	Bd	150	LEU

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Mol	Chain	Res	Type
36	Bd	163	LYS
36	Bd	168	LEU
37	Be	17	ARG
37	Be	23	SER
37	Be	25	ARG
37	Be	28	ARG
37	Be	29	THR
37	Be	31	CYS
37	Be	50	GLN
37	Be	66	PHE
37	Be	67	LYS
37	Be	68	LEU
37	Be	74	TYR
37	Be	106	THR
37	Be	111	HIS
37	Be	122	GLU
37	Be	127	GLN
38	Bf	42	ASP
38	Bf	44	ASN
38	Bf	56	ARG
38	Bf	58	ILE
38	Bf	60	CYS
38	Bf	67	ILE
38	Bf	70	GLU
38	Bf	71	HIS
38	Bf	114	LYS
38	Bf	122	ARG
38	Bf	126	ARG
38	Bf	133	ARG
38	Bf	134	ARG
39	Bg	2	THR
39	Bg	6	THR
39	Bg	14	VAL
39	Bg	21	ARG
39	Bg	28	ARG
39	Bg	30	SER
39	Bg	33	LEU
39	Bg	47	VAL
39	Bg	52	THR
39	Bg	61	VAL
39	Bg	68	ARG
39	Bg	80	LEU

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Mol	Chain	Res	Type
39	Bg	91	CYS
39	Bg	93	SER
39	Bg	112	VAL
39	Bg	114	ARG
39	Bg	119	PHE
39	Bg	126	ILE
39	Bg	127	GLN
39	Bg	148	VAL
40	Bh	45	LEU
40	Bh	51	LEU
40	Bh	52	ARG
40	Bh	78	ARG
40	Bh	82	THR
40	Bh	121	ASP
40	Bh	148	LEU
40	Bh	154	THR
40	Bh	163	GLU
40	Bh	177	GLN
40	Bh	178	LEU
40	Bh	191	LEU
40	Bh	216	ARG
40	Bh	227	GLU
40	Bh	231	MET
40	Bh	233	THR
40	Bh	254	GLU
40	Bh	256	ARG
40	Bh	259	ARG
40	Bh	264	THR
40	Bh	265	THR
40	Bh	267	LEU
40	Bh	289	VAL
40	Bh	301	LEU
40	Bh	307	PHE
41	Bi	57	VAL
41	Bi	74	ARG
41	Bi	76	ILE
41	Bi	85	PHE
41	Bi	112	LEU
41	Bi	165	THR
41	Bi	176	ILE
41	Bi	181	VAL
41	Bi	196	GLN

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Mol	Chain	Res	Type
41	Bi	221	THR
41	Bi	242	VAL
41	Bi	244	GLU
41	Bi	246	VAL
41	Bi	281	MET
42	Bj	51	LEU
42	Bj	55	ARG
42	Bj	60	THR
42	Bj	64	THR
42	Bj	119	ASP
42	Bj	145	ASP
42	Bj	169	ASP
42	Bj	179	GLN
42	Bj	210	CYS
42	Bj	230	LYS
42	Bj	243	PHE
42	Bj	264	LEU
42	Bj	265	LYS
42	Bj	276	LEU
43	Bk	50	SER
43	Bk	53	THR
43	Bk	56	ILE
43	Bk	88	TYR
43	Bk	132	MET
43	Bk	165	THR
43	Bk	168	GLU
43	Bk	170	PHE
44	Bl	41	SER
44	Bl	89	SER
44	Bl	90	ARG
44	Bl	98	ARG
44	Bl	100	ILE
44	Bl	101	THR
44	Bl	107	MET
44	Bl	117	ILE
44	Bl	128	LEU
44	Bl	138	THR
44	Bl	141	ASN
44	Bl	154	ASP
45	Bm	67	LEU
45	Bm	71	LEU
45	Bm	86	ASN

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Mol	Chain	Res	Type
45	Bm	121	MET
45	Bm	128	LEU
45	Bm	142	ASP
46	Bn	32	PHE
46	Bn	34	VAL
46	Bn	35	ARG
46	Bn	41	ARG
46	Bn	42	LYS
46	Bn	44	VAL
46	Bn	48	ASN
46	Bn	56	VAL
46	Bn	92	ILE
46	Bn	105	ASP
47	Bo	40	TYR
47	Bo	43	LEU
47	Bo	53	ASP
47	Bo	55	ARG
47	Bo	64	LEU
47	Bo	84	MET
47	Bo	110	LEU
48	Bp	28	GLU
48	Bp	43	ARG
48	Bp	76	MET
48	Bp	84	GLN
49	Bq	95	TRP
49	Bq	122	ARG
49	Bq	137	LYS
49	Bq	138	PHE
50	Bt	10	ASN
50	Bt	25	ARG
50	Bt	30	GLN
50	Bt	37	ARG
50	Bt	45	ASN
50	Bt	49	LEU
50	Bt	55	THR
50	Bt	60	ARG
50	Bt	81	ARG
50	Bt	82	PHE
50	Bt	88	LEU
50	Bt	90	GLU
50	Bt	98	THR
50	Bt	99	ARG

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Mol	Chain	Res	Type
51	Bu	81	CYS
51	Bu	97	LYS
51	Bu	104	LEU
51	Bu	110	ILE
51	Bu	123	LYS
51	Bu	135	THR
51	Bu	140	ARG
51	Bu	146	LEU
51	Bu	148	ASP
51	Bu	175	ARG
51	Bu	177	SER
51	Bu	182	MET
51	Bu	184	ARG
52	Bv	38	ARG
52	Bv	47	THR
52	Bv	128	MET
53	Bw	43	ARG
53	Bw	77	ASP
53	Bw	81	ARG
53	Bw	118	LEU
53	Bw	147	GLU
53	Bw	153	ARG
53	Bw	162	ASP
53	Bw	173	GLN
53	Bw	194	LEU
53	Bw	196	CYS
53	Bw	220	VAL
53	Bw	248	ASP
53	Bw	260	CYS
53	Bw	271	GLN
53	Bw	274	ASN
53	Bw	280	SER
53	Bw	298	ASP
53	Bw	306	LEU
53	Bw	315	GLU
53	Bw	330	THR
53	Bw	345	VAL
53	Bw	347	ARG
53	Bw	356	THR
53	Bw	376	GLN
53	Bw	395	LEU
53	Bw	399	ILE

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Mol	Chain	Res	Type
53	Bw	402	ASN
53	Bw	405	LYS
53	Bw	410	ASP
53	Bw	414	GLN
53	Bw	415	LEU
53	Bw	420	LEU
53	Bw	421	ASN
54	Bx	54	THR
54	Bx	70	CYS
54	Bx	73	CYS
54	Bx	92	PHE
54	Bx	100	LEU
54	Bx	115	ILE
54	Bx	121	MET
54	Bx	128	LEU
54	Bx	152	THR
54	Bx	157	ARG
54	Bx	183	ASP
54	Bx	190	ARG
54	Bx	193	LEU
54	Bx	196	HIS
57	AB	57	LEU
57	AB	125	GLN
57	AB	146	ARG
57	AB	159	ARG
57	AB	167	THR
57	AB	176	THR
57	AB	177	ASN
57	AB	197	THR
57	AB	201	VAL
57	AB	206	VAL
57	AB	222	VAL
57	AB	224	THR
57	AB	235	VAL
58	AC	38	ARG
58	AC	41	ARG
58	AC	44	VAL
58	AC	71	LEU
58	AC	80	ASP
58	AC	89	ASP
58	AC	104	LEU
58	AC	108	LEU

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Mol	Chain	Res	Type
58	AC	112	ARG
58	AC	115	ASN
58	AC	117	LEU
58	AC	124	LEU
58	AC	125	ARG
58	AC	127	LEU
58	AC	132	PHE
58	AC	167	ILE
59	AE	136	ARG
59	AE	137	HIS
59	AE	196	ASN
59	AE	203	LEU
59	AE	215	TYR
59	AE	216	ASP
59	AE	220	THR
59	AE	239	ARG
59	AE	240	SER
59	AE	241	VAL
59	AE	242	ARG
59	AE	245	VAL
59	AE	289	THR
59	AE	305	MET
59	AE	336	VAL
59	AE	337	SER
59	AE	346	THR
59	AE	370	VAL
59	AE	374	ARG
59	AE	376	GLU
59	AE	400	GLU
59	AE	404	ILE
59	AE	423	SER
60	AF	8	LEU
60	AF	13	MET
60	AF	39	LEU
60	AF	45	ARG
60	AF	57	ARG
60	AF	65	LEU
60	AF	67	ASP
60	AF	78	MET
60	AF	89	ILE
60	AF	120	THR
61	AG	40	GLU

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Mol	Chain	Res	Type
61	AG	57	GLU
61	AG	82	THR
61	AG	85	VAL
61	AG	88	ASP
61	AG	109	SER
61	AG	139	ARG
61	AG	153	GLU
61	AG	159	VAL
61	AG	180	ARG
61	AG	187	MET
61	AG	197	ARG
61	AG	200	LEU
61	AG	205	LEU
61	AG	219	VAL
62	AI	70	THR
62	AI	73	PHE
62	AI	91	MET
62	AI	98	THR
62	AI	99	PHE
62	AI	100	THR
62	AI	153	THR
62	AI	161	LEU
62	AI	199	ARG
62	AI	202	ILE
62	AI	206	LEU
62	AI	217	GLN
62	AI	229	LEU
62	AI	256	GLN
62	AI	277	ARG
62	AI	316	PHE
62	AI	338	ARG
62	AI	357	VAL
63	AJ	52	VAL
63	AJ	64	THR
63	AJ	80	VAL
63	AJ	92	GLU
63	AJ	126	ILE
63	AJ	133	GLN
63	AJ	136	MET
63	AJ	145	LEU
63	AJ	148	LEU
63	AJ	158	GLU

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Mol	Chain	Res	Type
63	AJ	166	GLU
63	AJ	168	VAL
63	AJ	175	THR
64	AK	64	ILE
64	AK	68	ILE
64	AK	85	ILE
64	AK	121	ASN
64	AK	147	THR
64	AK	153	VAL
64	AK	161	LEU
64	AK	177	ILE
65	AL	55	ARG
65	AL	67	ILE
65	AL	95	ILE
65	AL	101	SER
66	AN	30	VAL
66	AN	34	MET
66	AN	35	LEU
66	AN	43	MET
66	AN	56	SER
66	AN	58	ARG
66	AN	67	LEU
66	AN	80	ARG
66	AN	81	ASP
66	AN	93	MET
66	AN	94	THR
66	AN	102	ARG
66	AN	106	LEU
66	AN	125	ARG
67	AO	72	MET
67	AO	73	LEU
67	AO	74	LEU
67	AO	80	VAL
67	AO	83	ILE
67	AO	122	ASP
67	AO	127	GLU
67	AO	158	LEU
67	AO	159	MET
67	AO	198	ARG
67	AO	208	LYS
68	AP	35	VAL
68	AP	90	LEU

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Mol	Chain	Res	Type
68	AP	97	TYR
68	AP	99	LEU
69	AQ	6	SER
69	AQ	22	MET
69	AQ	40	LEU
69	AQ	46	ARG
69	AQ	55	LEU
69	AQ	56	GLN
69	AQ	59	THR
69	AQ	62	ASP
69	AQ	74	THR
69	AQ	81	LEU
69	AQ	90	GLN
70	AR	56	GLU
70	AR	83	GLN
70	AR	89	THR
70	AR	117	ILE
70	AR	124	THR
70	AR	131	LEU
71	AU	18	ASN
71	AU	35	LEU
71	AU	38	ASP
71	AU	50	ARG
71	AU	52	ARG
71	AU	66	MET
71	AU	77	ARG
71	AU	80	ARG
71	AU	82	ASP
71	AU	85	GLN
75	Aa	118	GLN
75	Aa	126	LYS
75	Aa	129	THR
75	Aa	163	VAL
75	Aa	167	ASP
75	Aa	177	LYS
75	Aa	183	ILE
75	Aa	197	ARG
75	Aa	202	THR
75	Aa	204	ARG
75	Aa	214	MET
75	Aa	221	ARG
75	Aa	222	GLU

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Mol	Chain	Res	Type
75	Aa	224	ARG
75	Aa	240	MET
75	Aa	244	ASP
75	Aa	276	ASP
75	Aa	284	LEU
75	Aa	285	ARG
75	Aa	293	MET
75	Aa	295	TRP
75	Aa	325	LEU
75	Aa	337	GLN
75	Aa	347	LEU
75	Aa	356	THR
76	Ab	6	LEU
76	Ab	7	GLU
76	Ab	14	SER
76	Ab	30	LEU
76	Ab	48	ARG
76	Ab	62	ASP
76	Ab	67	GLU
76	Ab	112	THR
77	Ac	3	MET
77	Ac	4	LYS
77	Ac	9	ILE
77	Ac	25	ASP
77	Ac	33	ASN
77	Ac	51	ASN
77	Ac	84	GLU
77	Ac	96	LYS
77	Ac	106	LEU
77	Ac	124	SER
77	Ac	149	CYS
78	Ad	41	ARG
78	Ad	56	LEU
78	Ad	62	GLN
78	Ad	71	ARG
78	Ad	166	THR
78	Ad	173	LEU
78	Ad	191	ILE
78	Ad	192	THR
78	Ad	196	LEU
79	Ae	84	ASP
79	Ae	102	GLU

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Mol	Chain	Res	Type
79	Ae	122	ARG
79	Ae	136	ARG
79	Ae	150	HIS
79	Ae	159	TYR
79	Ae	171	ASN
79	Ae	180	ASP
79	Ae	186	LEU
79	Ae	208	MET
79	Ae	213	PHE
79	Ae	220	LEU
79	Ae	223	LEU
79	Ae	230	LEU
79	Ae	249	LEU
79	Ae	250	LEU
79	Ae	253	LEU
79	Ae	255	GLN
79	Ae	257	ASN
79	Ae	266	TYR
79	Ae	280	LEU
79	Ae	291	TRP
79	Ae	315	LEU
79	Ae	388	VAL
79	Ae	421	GLN
80	Af	84	MET
80	Af	85	LEU
80	Af	148	LEU
80	Af	153	ARG
80	Af	155	LEU
80	Af	162	THR
81	Ag	50	THR
81	Ag	78	PHE
81	Ag	98	LEU
81	Ag	135	LEU
81	Ag	138	CYS
81	Ag	142	HIS
81	Ag	172	TYR
81	Ag	178	ASP
81	Ag	181	LEU
81	Ag	194	ASN
81	Ag	255	PHE
81	Ag	264	VAL
81	Ag	265	ASN

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Mol	Chain	Res	Type
81	Ag	270	ARG
81	Ag	296	VAL
81	Ag	305	ILE
81	Ag	334	ASP
81	Ag	336	LEU
81	Ag	337	ASP
81	Ag	372	THR
82	Ah	302	LEU
82	Ah	308	ASN
82	Ah	328	LYS
82	Ah	359	LYS
83	Ai	26	THR
83	Ai	31	MET
83	Ai	36	LEU
83	Ai	50	ASP
83	Ai	72	ARG
84	Aj	21	LEU
84	Aj	40	THR
84	Aj	52	MET
84	Aj	65	LEU
84	Aj	74	PHE
84	Aj	99	ARG
84	Aj	103	ASP
84	Aj	135	MET
84	Aj	150	PHE
84	Aj	179	GLN
85	Ak	53	LYS
85	Ak	79	LYS
85	Ak	85	LEU
85	Ak	102	GLU
85	Ak	117	THR
85	Ak	125	CYS
85	Ak	134	GLU
85	Ak	152	GLU
85	Ak	157	ASP
85	Ak	159	VAL
85	Ak	165	ILE
85	Ak	175	LEU
85	Ak	186	ASP
85	Ak	199	ARG
85	Ak	205	ASP
85	Ak	213	ARG

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Mol	Chain	Res	Type
85	Ak	218	ARG
85	Ak	249	ASP
85	Ak	264	ILE
85	Ak	269	LEU
85	Ak	298	VAL
85	Ak	306	ASP
85	Ak	309	ASN
86	Am	6	LEU
86	Am	13	LEU
86	Am	17	ARG
86	Am	25	LYS
86	Am	29	LEU
86	Am	33	VAL
86	Am	48	GLU
86	Am	49	MET
86	Am	53	MET
86	Am	63	ASP
86	Am	72	ASP
86	Am	113	ASN
87	An	130	ILE
87	An	144	ARG
87	An	155	ARG
87	An	158	ARG
87	An	163	ARG
87	An	164	GLN
87	An	175	ARG
87	An	199	GLN
88	Ao	243	THR
88	Ao	262	TYR
88	Ao	285	LEU
88	Ao	414	ASP
88	Ao	423	MET
88	Ao	441	LEU
88	Ao	446	ASP
88	Ao	447	ASN
88	Ao	488	VAL
88	Ao	538	MET
88	Ao	582	VAL
88	Ao	608	ILE
88	Ao	645	CYS
88	Ao	650	ARG
88	Ao	652	VAL

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Mol	Chain	Res	Type
88	Ao	661	GLU
89	Ap	53	ASP
89	Ap	89	ARG
89	Ap	91	ARG
89	Ap	93	MET
89	Ap	103	ASN
89	Ap	108	CYS
89	Ap	113	LEU
89	Ap	155	GLN
89	Ap	167	ILE
89	Ap	170	VAL
89	Ap	175	LEU
89	Ap	177	PHE
89	Ap	184	VAL
89	Ap	193	LEU
89	Ap	219	LEU
89	Ap	224	LEU
89	Ap	235	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
2	B0	41	ASN
2	B0	59	HIS
2	B0	76	HIS
3	B1	42	HIS
3	B1	172	GLN
4	B2	75	ASN
4	B2	90	GLN
5	B3	67	HIS
6	B4	37	ASN
6	B4	47	GLN
7	B5	118	GLN
7	B5	170	GLN
8	B6	59	GLN
9	B7	65	HIS
10	B8	118	HIS
10	B8	170	ASN
14	BC	188	HIS
14	BC	215	GLN
14	BC	319	GLN
14	BC	330	ASN

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Mol	Chain	Res	Type
15	BD	183	HIS
16	BE	57	ASN
16	BE	128	HIS
16	BE	154	HIS
16	BE	197	HIS
16	BE	281	ASN
16	BE	292	HIS
17	BF	74	GLN
17	BF	83	HIS
17	BF	97	HIS
17	BF	103	GLN
17	BF	105	ASN
17	BF	172	GLN
17	BF	249	ASN
18	BI	88	HIS
18	BI	93	ASN
18	BI	136	ASN
19	BJ	41	HIS
19	BJ	73	GLN
19	BJ	93	ASN
19	BJ	119	HIS
19	BJ	217	GLN
20	BK	54	ASN
20	BK	84	GLN
20	BK	103	HIS
1	BL	152	HIS
21	BN	40	GLN
21	BN	48	HIS
21	BN	74	GLN
21	BN	80	HIS
21	BN	94	GLN
21	BN	140	ASN
22	BO	80	GLN
22	BO	89	HIS
22	BO	103	ASN
22	BO	143	ASN
23	BP	84	ASN
23	BP	87	HIS
23	BP	170	ASN
24	BQ	98	HIS
24	BQ	110	ASN
24	BQ	209	ASN

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Mol	Chain	Res	Type
25	BR	27	HIS
25	BR	112	ASN
25	BR	116	GLN
25	BR	147	ASN
26	BS	52	ASN
26	BS	79	HIS
26	BS	115	HIS
26	BS	147	HIS
28	BU	77	GLN
28	BU	79	HIS
28	BU	94	GLN
29	BV	88	ASN
29	BV	104	HIS
29	BV	109	GLN
29	BV	122	ASN
29	BV	144	ASN
30	BW	131	ASN
30	BW	157	HIS
30	BW	171	HIS
30	BW	199	GLN
30	BW	203	ASN
30	BW	208	HIS
31	BX	4	ASN
31	BX	14	ASN
31	BX	77	ASN
32	BY	35	ASN
32	BY	78	GLN
32	BY	84	ASN
32	BY	210	HIS
33	Ba	65	HIS
33	Ba	108	HIS
33	Ba	119	GLN
33	Ba	156	ASN
33	Ba	195	HIS
33	Ba	207	ASN
33	Ba	223	HIS
33	Ba	266	GLN
33	Ba	289	HIS
33	Ba	343	GLN
33	Ba	358	GLN
33	Ba	360	ASN
34	Bb	220	ASN

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Mol	Chain	Res	Type
34	Bb	224	HIS
34	Bb	307	HIS
34	Bb	308	GLN
34	Bb	354	GLN
35	Bc	252	HIS
35	Bc	274	GLN
35	Bc	294	GLN
36	Bd	143	GLN
38	Bf	44	ASN
38	Bf	62	HIS
38	Bf	71	HIS
38	Bf	121	HIS
38	Bf	130	HIS
39	Bg	17	ASN
39	Bg	127	GLN
39	Bg	131	HIS
39	Bg	135	ASN
40	Bh	94	ASN
40	Bh	118	ASN
40	Bh	128	GLN
40	Bh	177	GLN
41	Bi	115	ASN
41	Bi	196	GLN
42	Bj	87	HIS
42	Bj	150	HIS
43	Bk	61	HIS
43	Bk	111	HIS
43	Bk	177	ASN
44	Bl	141	ASN
45	Bm	115	ASN
46	Bn	33	HIS
46	Bn	69	HIS
46	Bn	108	HIS
46	Bn	122	ASN
47	Bo	63	GLN
48	Bp	15	GLN
48	Bp	84	GLN
48	Bp	93	HIS
49	Bq	129	HIS
50	Bt	30	GLN
50	Bt	34	ASN
50	Bt	45	ASN

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Mol	Chain	Res	Type
50	Bt	85	HIS
51	Bu	103	HIS
51	Bu	145	ASN
52	Bv	107	GLN
53	Bw	96	GLN
53	Bw	104	ASN
53	Bw	201	HIS
53	Bw	234	GLN
53	Bw	271	GLN
53	Bw	381	ASN
53	Bw	385	ASN
54	Bx	112	HIS
54	Bx	131	HIS
54	Bx	164	ASN
54	Bx	184	ASN
54	Bx	196	HIS
57	AB	68	HIS
57	AB	152	HIS
58	AC	72	HIS
58	AC	75	ASN
58	AC	115	ASN
58	AC	145	HIS
59	AE	145	ASN
59	AE	155	GLN
59	AE	196	ASN
59	AE	292	HIS
59	AE	317	HIS
59	AE	356	GLN
59	AE	369	HIS
59	AE	415	GLN
60	AF	41	ASN
61	AG	146	HIS
61	AG	196	HIS
61	AG	227	HIS
61	AG	233	ASN
61	AG	238	HIS
62	AI	87	HIS
62	AI	101	GLN
62	AI	127	HIS
62	AI	156	GLN
62	AI	176	HIS
62	AI	327	HIS

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Mol	Chain	Res	Type
63	AJ	109	HIS
63	AJ	133	GLN
64	AK	89	HIS
65	AL	35	GLN
65	AL	37	HIS
65	AL	77	ASN
65	AL	100	HIS
65	AL	105	HIS
66	AN	60	ASN
66	AN	117	HIS
67	AO	84	HIS
67	AO	147	HIS
67	AO	153	HIS
67	AO	170	ASN
68	AP	28	ASN
69	AQ	23	GLN
69	AQ	44	ASN
69	AQ	56	GLN
69	AQ	76	HIS
70	AR	77	ASN
70	AR	116	GLN
71	AU	3	ASN
75	Aa	99	ASN
75	Aa	245	GLN
75	Aa	246	HIS
75	Aa	299	ASN
77	Ac	51	ASN
77	Ac	56	GLN
77	Ac	59	ASN
77	Ac	63	GLN
77	Ac	69	ASN
77	Ac	95	ASN
77	Ac	125	HIS
77	Ac	146	GLN
78	Ad	62	GLN
78	Ad	102	HIS
79	Ae	140	ASN
79	Ae	185	ASN
79	Ae	257	ASN
79	Ae	314	GLN
79	Ae	404	GLN
79	Ae	421	GLN

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Mol	Chain	Res	Type
79	Ae	424	HIS
80	Af	87	HIS
80	Af	98	ASN
81	Ag	58	HIS
81	Ag	142	HIS
81	Ag	153	HIS
81	Ag	227	GLN
81	Ag	301	GLN
81	Ag	325	GLN
81	Ag	386	ASN
82	Ah	288	ASN
82	Ah	309	ASN
82	Ah	321	HIS
82	Ah	323	HIS
82	Ah	364	HIS
83	Ai	75	HIS
84	Aj	32	GLN
84	Aj	111	HIS
84	Aj	145	HIS
85	Ak	263	ASN
85	Ak	270	GLN
86	Am	24	ASN
86	Am	32	HIS
86	Am	113	ASN
87	An	164	GLN
88	Ao	129	GLN
88	Ao	258	ASN
88	Ao	272	HIS
88	Ao	318	ASN
88	Ao	329	GLN
88	Ao	385	HIS
88	Ao	543	HIS
89	Ap	130	HIS
89	Ap	136	HIS
89	Ap	147	HIS
89	Ap	169	GLN
89	Ap	181	HIS

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	BA	1547/1571 (98%)	471 (30%)	7 (0%)
13	BB	64/73 (87%)	24 (37%)	0
56	AA	959/962 (99%)	237 (24%)	3 (0%)
72	AV	70/71 (98%)	25 (35%)	0
73	AX	16/201 (7%)	10 (62%)	1 (6%)
All	All	2656/2878 (92%)	767 (28%)	11 (0%)

All (767) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	BA	4	A
12	BA	7	G
12	BA	11	G
12	BA	15	A
12	BA	19	U
12	BA	20	A
12	BA	21	C
12	BA	23	A
12	BA	26	C
12	BA	31	A
12	BA	32	C
12	BA	36	A
12	BA	37	A
12	BA	39	A
12	BA	40	C
12	BA	41	A
12	BA	42	C
12	BA	45	A
12	BA	46	A
12	BA	47	A
12	BA	48	U
12	BA	49	A
12	BA	56	A
12	BA	57	A
12	BA	59	A
12	BA	60	U
12	BA	63	A
12	BA	66	U
12	BA	67	A
12	BA	68	A
12	BA	80	A

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Mol	Chain	Res	Type
12	BA	82	G
12	BA	83	A
12	BA	84	G
12	BA	96	U
12	BA	97	A
12	BA	99	C
12	BA	101	U
12	BA	102	G
12	BA	104	C
12	BA	105	G
12	BA	109	U
12	BA	112	A
12	BA	115	U
12	BA	118	U
12	BA	119	A
12	BA	129	A
12	BA	131	A
12	BA	132	G
12	BA	135	G
12	BA	139	G
12	BA	140	A
12	BA	141	A
12	BA	142	U
12	BA	143	A
12	BA	146	A
12	BA	147	U
12	BA	148	A
12	BA	149	A
12	BA	153	U
12	BA	163	C
12	BA	164	A
12	BA	165	A
12	BA	168	A
12	BA	172	C
12	BA	180	A
12	BA	182	C
12	BA	188	C
12	BA	190	U
12	BA	192	A
12	BA	205	A
12	BA	210	A
12	BA	218	A

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Mol	Chain	Res	Type
12	BA	219	A
12	BA	221	A
12	BA	223	A
12	BA	224	A
12	BA	225	C
12	BA	228	U
12	BA	229	A
12	BA	231	C
12	BA	237	A
12	BA	238	C
12	BA	239	C
12	BA	243	A
12	BA	254	G
12	BA	260	C
12	BA	261	A
12	BA	263	G
12	BA	265	G
12	BA	271	U
12	BA	272	A
12	BA	273	A
12	BA	274	A
12	BA	275	A
12	BA	277	A
12	BA	295	G
12	BA	305	G
12	BA	306	A
12	BA	309	A
12	BA	310	G
12	BA	311	A
12	BA	312	C
12	BA	313	U
12	BA	322	G
12	BA	324	G
12	BA	329	A
12	BA	330	A
12	BA	331	A
12	BA	336	A
12	BA	337	A
12	BA	338	C
12	BA	339	G
12	BA	340	A
12	BA	352	G

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Mol	Chain	Res	Type
12	BA	359	G
12	BA	364	A
12	BA	366	A
12	BA	367	A
12	BA	368	A
12	BA	369	G
12	BA	373	U
12	BA	374	U
12	BA	381	A
12	BA	389	A
12	BA	390	A
12	BA	392	U
12	BA	393	A
12	BA	394	C
12	BA	398	A
12	BA	409	A
12	BA	414	A
12	BA	417	G
12	BA	418	U
12	BA	420	U
12	BA	428	A
12	BA	440	A
12	BA	446	C
12	BA	447	A
12	BA	448	G
12	BA	449	C
12	BA	459	A
12	BA	460	C
12	BA	467	A
12	BA	468	A
12	BA	472	U
12	BA	473	G
12	BA	474	A
12	BA	478	G
12	BA	479	A
12	BA	480	G
12	BA	488	U
12	BA	489	C
12	BA	490	U
12	BA	491	U
12	BA	492	A
12	BA	493	A

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Mol	Chain	Res	Type
12	BA	494	U
12	BA	497	U
12	BA	498	A
12	BA	500	C
12	BA	501	A
12	BA	503	A
12	BA	504	G
12	BA	505	U
12	BA	506	A
12	BA	515	A
12	BA	516	G
12	BA	518	A
12	BA	526	A
12	BA	532	A
12	BA	533	A
12	BA	545	U
12	BA	547	A
12	BA	548	A
12	BA	550	A
12	BA	552	A
12	BA	553	U
12	BA	554	U
12	BA	557	C
12	BA	560	A
12	BA	561	C
12	BA	562	A
12	BA	563	U
12	BA	566	U
12	BA	570	A
12	BA	574	A
12	BA	575	C
12	BA	576	U
12	BA	578	A
12	BA	579	U
12	BA	580	A
12	BA	583	A
12	BA	584	A
12	BA	586	C
12	BA	592	G
12	BA	593	C
12	BA	595	C
12	BA	596	A

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Mol	Chain	Res	Type
12	BA	617	A
12	BA	618	A
12	BA	619	C
12	BA	625	A
12	BA	628	A
12	BA	631	A
12	BA	634	G
12	BA	640	A
12	BA	648	C
12	BA	649	A
12	BA	650	A
12	BA	657	U
12	BA	661	U
12	BA	665	C
12	BA	673	C
12	BA	684	A
12	BA	689	A
12	BA	691	A
12	BA	694	A
12	BA	695	U
12	BA	696	A
12	BA	697	C
12	BA	704	U
12	BA	705	U
12	BA	707	A
12	BA	713	A
12	BA	718	A
12	BA	719	C
12	BA	720	C
12	BA	722	A
12	BA	723	A
12	BA	724	A
12	BA	725	C
12	BA	727	A
12	BA	728	C
12	BA	736	C
12	BA	737	G
12	BA	744	A
12	BA	745	A
12	BA	746	U
12	BA	747	U
12	BA	748	A

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Mol	Chain	Res	Type
12	BA	753	G
12	BA	763	C
12	BA	764	A
12	BA	766	A
12	BA	774	A
12	BA	775	C
12	BA	777	A
12	BA	778	A
12	BA	780	G
12	BA	782	A
12	BA	783	A
12	BA	784	G
12	BA	789	A
12	BA	795	G
12	BA	809	G
12	BA	818	A
12	BA	819	A
12	BA	824	G
12	BA	825	C
12	BA	828	G
12	BA	834	C
12	BA	835	A
12	BA	847	U
12	BA	848	C
12	BA	850	A
12	BA	852	C
12	BA	854	U
12	BA	855	U
12	BA	859	A
12	BA	860	G
12	BA	864	U
12	BA	868	G
12	BA	871	A
12	BA	872	A
12	BA	883	G
12	BA	887	C
12	BA	888	A
12	BA	889	C
12	BA	890	C
12	BA	892	G
12	BA	895	U
12	BA	897	A

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Mol	Chain	Res	Type
12	BA	899	G
12	BA	901	C
12	BA	902	C
12	BA	908	A
12	BA	909	U
12	BA	910	U
12	BA	922	A
12	BA	923	A
12	BA	924	G
12	BA	925	G
12	BA	931	U
12	BA	932	A
12	BA	933	A
12	BA	935	C
12	BA	938	U
12	BA	939	U
12	BA	948	A
12	BA	950	U
12	BA	958	U
12	BA	959	G
12	BA	960	U
12	BA	961	A
12	BA	964	A
12	BA	965	A
12	BA	967	G
12	BA	970	C
12	BA	977	G
12	BA	979	G
12	BA	981	U
12	BA	982	U
12	BA	983	U
12	BA	986	U
12	BA	988	U
12	BA	992	U
12	BA	1008	A
12	BA	1015	C
12	BA	1016	C
12	BA	1018	U
12	BA	1026	A
12	BA	1027	G
12	BA	1028	A
12	BA	1034	G

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Mol	Chain	Res	Type
12	BA	1038	A
12	BA	1041	A
12	BA	1046	A
12	BA	1050	C
12	BA	1051	G
12	BA	1055	A
12	BA	1056	G
12	BA	1057	A
12	BA	1063	U
12	BA	1064	G
12	BA	1071	U
12	BA	1072	A
12	BA	1075	U
12	BA	1089	G
12	BA	1092	A
12	BA	1093	A
12	BA	1094	A
12	BA	1123	A
12	BA	1127	A
12	BA	1129	C
12	BA	1137	A
12	BA	1140	A
12	BA	1145	C
12	BA	1146	G
12	BA	1167	C
12	BA	1168	A
12	BA	1169	A
12	BA	1178	C
12	BA	1183	U
12	BA	1188	U
12	BA	1190	A
12	BA	1195	A
12	BA	1205	G
12	BA	1206	U
12	BA	1207	C
12	BA	1215	C
12	BA	1216	C
12	BA	1217	A
12	BA	1218	U
12	BA	1219	A
12	BA	1220	A
12	BA	1221	C

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Mol	Chain	Res	Type
12	BA	1222	A
12	BA	1226	C
12	BA	1231	U
12	BA	1232	G
12	BA	1234	U
12	BA	1238	A
12	BA	1239	A
12	BA	1240	A
12	BA	1241	U
12	BA	1242	U
12	BA	1246	A
12	BA	1247	U
12	BA	1249	A
12	BA	1253	G
12	BA	1254	A
12	BA	1255	A
12	BA	1258	A
12	BA	1264	C
12	BA	1268	G
12	BA	1270	G
12	BA	1271	A
12	BA	1287	G
12	BA	1288	U
12	BA	1291	U
12	BA	1294	A
12	BA	1297	U
12	BA	1299	C
12	BA	1303	C
12	BA	1311	G
12	BA	1314	U
12	BA	1317	A
12	BA	1323	U
12	BA	1325	G
12	BA	1326	A
12	BA	1328	G
12	BA	1331	G
12	BA	1341	A
12	BA	1342	C
12	BA	1348	U
12	BA	1352	G
12	BA	1353	C
12	BA	1357	C

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Mol	Chain	Res	Type
12	BA	1358	G
12	BA	1377	U
12	BA	1385	U
12	BA	1387	A
12	BA	1388	A
12	BA	1389	A
12	BA	1390	G
12	BA	1396	C
12	BA	1399	G
12	BA	1405	A
12	BA	1406	G
12	BA	1409	C
12	BA	1420	A
12	BA	1425	A
12	BA	1426	G
12	BA	1428	U
12	BA	1429	C
12	BA	1432	U
12	BA	1433	U
12	BA	1436	U
12	BA	1438	U
12	BA	1444	A
12	BA	1445	U
12	BA	1448	A
12	BA	1458	G
12	BA	1459	U
12	BA	1465	A
12	BA	1466	G
12	BA	1468	A
12	BA	1474	G
12	BA	1476	A
12	BA	1492	C
12	BA	1493	A
12	BA	1494	A
12	BA	1498	C
12	BA	1504	A
12	BA	1505	G
12	BA	1509	U
12	BA	1514	A
12	BA	1518	A
12	BA	1521	U
12	BA	1522	A

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Mol	Chain	Res	Type
12	BA	1525	C
12	BA	1526	U
12	BA	1527	U
12	BA	1528	A
12	BA	1529	A
12	BA	1531	C
12	BA	1532	U
12	BA	1533	A
12	BA	1536	U
12	BA	1548	A
12	BA	1549	A
12	BA	1550	U
12	BA	1551	C
12	BA	1552	C
12	BA	1553	A
12	BA	1558	U
12	BA	1559	A
12	BA	1560	G
12	BA	1570	C
12	BA	1571	A
13	BB	3	U
13	BB	5	A
13	BB	7	G
13	BB	8	U
13	BB	9	A
13	BB	13	U
13	BB	21	C
13	BB	23	A
13	BB	24	A
13	BB	25	G
13	BB	29	G
13	BB	30	G
13	BB	34	U
13	BB	35	G
13	BB	43	C
13	BB	44	U
13	BB	45	A
13	BB	46	G
13	BB	47	A
13	BB	48	U
13	BB	55	C
13	BB	67	A

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Mol	Chain	Res	Type
13	BB	69	C
13	BB	70	A
56	AA	5	A
56	AA	10	U
56	AA	11	G
56	AA	18	G
56	AA	27	U
56	AA	32	U
56	AA	34	U
56	AA	42	A
56	AA	43	U
56	AA	45	A
56	AA	49	A
56	AA	54	A
56	AA	55	G
56	AA	58	U
56	AA	61	G
56	AA	65	C
56	AA	66	C
56	AA	67	C
56	AA	75	A
56	AA	77	G
56	AA	78	C
56	AA	82	C
56	AA	83	C
56	AA	93	A
56	AA	98	A
56	AA	102	G
56	AA	103	G
56	AA	104	A
56	AA	111	A
56	AA	115	A
56	AA	120	A
56	AA	124	A
56	AA	125	U
56	AA	147	G
56	AA	152	A
56	AA	161	C
56	AA	168	A
56	AA	170	A
56	AA	171	C
56	AA	173	G

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Mol	Chain	Res	Type
56	AA	176	G
56	AA	186	U
56	AA	187	U
56	AA	191	C
56	AA	192	C
56	AA	194	U
56	AA	203	G
56	AA	212	A
56	AA	216	A
56	AA	217	U
56	AA	222	A
56	AA	223	U
56	AA	224	U
56	AA	225	A
56	AA	231	G
56	AA	237	U
56	AA	238	C
56	AA	244	C
56	AA	247	G
56	AA	253	G
56	AA	257	U
56	AA	258	C
56	AA	273	A
56	AA	281	G
56	AA	288	G
56	AA	294	A
56	AA	297	A
56	AA	306	G
56	AA	308	A
56	AA	309	A
56	AA	310	A
56	AA	312	A
56	AA	314	A
56	AA	315	U
56	AA	317	A
56	AA	320	A
56	AA	328	A
56	AA	335	A
56	AA	336	A
56	AA	340	A
56	AA	345	U
56	AA	353	C

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Mol	Chain	Res	Type
56	AA	354	C
56	AA	361	A
56	AA	362	A
56	AA	367	A
56	AA	368	A
56	AA	381	G
56	AA	392	A
56	AA	395	C
56	AA	396	C
56	AA	399	A
56	AA	407	U
56	AA	417	C
56	AA	421	A
56	AA	426	G
56	AA	432	A
56	AA	433	U
56	AA	434	A
56	AA	450	C
56	AA	455	A
56	AA	457	C
56	AA	458	C
56	AA	465	G
56	AA	471	U
56	AA	472	A
56	AA	477	A
56	AA	479	C
56	AA	480	U
56	AA	483	U
56	AA	488	A
56	AA	489	G
56	AA	491	G
56	AA	495	U
56	AA	498	U
56	AA	502	A
56	AA	503	A
56	AA	504	C
56	AA	518	A
56	AA	530	G
56	AA	531	U
56	AA	538	C
56	AA	540	U
56	AA	545	C

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Mol	Chain	Res	Type
56	AA	560	C
56	AA	561	U
56	AA	564	A
56	AA	566	U
56	AA	571	A
56	AA	574	C
56	AA	576	C
56	AA	578	G
56	AA	579	A
56	AA	580	U
56	AA	581	A
56	AA	588	A
56	AA	589	C
56	AA	593	C
56	AA	594	C
56	AA	596	U
56	AA	597	U
56	AA	604	U
56	AA	616	C
56	AA	618	G
56	AA	619	C
56	AA	620	C
56	AA	625	U
56	AA	628	G
56	AA	638	A
56	AA	639	A
56	AA	641	A
56	AA	644	A
56	AA	645	A
56	AA	646	C
56	AA	647	A
56	AA	648	A
56	AA	649	U
56	AA	650	A
56	AA	651	G
56	AA	665	A
56	AA	666	G
56	AA	681	A
56	AA	682	G
56	AA	687	A
56	AA	695	C
56	AA	696	U

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Mol	Chain	Res	Type
56	AA	698	A
56	AA	699	U
56	AA	707	A
56	AA	709	A
56	AA	711	A
56	AA	722	A
56	AA	731	A
56	AA	732	U
56	AA	734	A
56	AA	739	A
56	AA	741	C
56	AA	742	C
56	AA	743	A
56	AA	744	C
56	AA	745	C
56	AA	746	A
56	AA	749	C
56	AA	752	A
56	AA	753	A
56	AA	766	C
56	AA	775	A
56	AA	780	A
56	AA	790	A
56	AA	791	G
56	AA	802	A
56	AA	803	U
56	AA	807	G
56	AA	823	G
56	AA	825	C
56	AA	826	C
56	AA	838	A
56	AA	841	C
56	AA	842	A
56	AA	850	U
56	AA	854	C
56	AA	863	G
56	AA	869	A
56	AA	870	G
56	AA	874	U
56	AA	876	A
56	AA	877	A
56	AA	878	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	AA	880	U
56	AA	883	C
56	AA	885	U
56	AA	886	A
56	AA	887	U
56	AA	892	A
56	AA	893	A
56	AA	894	U
56	AA	897	C
56	AA	899	C
56	AA	900	A
56	AA	902	C
56	AA	905	U
56	AA	910	G
56	AA	917	C
56	AA	918	A
56	AA	920	G
56	AA	923	G
56	AA	925	A
56	AA	928	A
56	AA	930	G
56	AA	932	U
56	AA	933	A
56	AA	943	G
56	AA	945	A
56	AA	946	A
56	AA	955	G
56	AA	956	G
56	AA	959	U
72	AV	6	G
72	AV	7	G
72	AV	9	C
72	AV	13	U
72	AV	14	A
72	AV	16	A
72	AV	17	U
72	AV	18	A
72	AV	43	A
72	AV	44	U
72	AV	45	G
72	AV	46	U
72	AV	51	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	AV	52	A
72	AV	53	U
72	AV	54	A
72	AV	55	C
72	AV	56	C
72	AV	62	C
72	AV	63	G
72	AV	64	U
72	AV	65	A
72	AV	67	U
72	AV	68	A
72	AV	71	A
73	AX	3	G
73	AX	4	A
73	AX	7	C
73	AX	8	A
73	AX	9	C
73	AX	10	C
73	AX	11	A
73	AX	13	U
73	AX	14	C
73	AX	15	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	BA	48	U
12	BA	101	U
12	BA	1145	C
12	BA	1219	A
12	BA	1220	A
12	BA	1240	A
12	BA	1241	U
56	AA	395	C
56	AA	743	A
56	AA	882	A
73	AX	12	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 341 ligands modelled in this entry, 333 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
94	GSP	BC	901	90	26,34,34	2.13	3 (11%)	27,54,54	1.49	6 (22%)
96	FME	AV	101	72	8,9,10	0.97	0	7,9,11	0.80	0
93	SPM	AA	3001	-	13,13,13	0.43	0	12,12,12	0.77	0
93	SPM	BA	3205	-	13,13,13	0.23	0	12,12,12	1.02	0
92	5GP	BA	3203	-	22,26,26	1.12	2 (9%)	26,40,40	1.50	4 (15%)
92	5GP	BA	3204	-	22,26,26	1.13	2 (9%)	26,40,40	1.36	5 (19%)
97	GTP	Ag	500	90	26,34,34	1.02	2 (7%)	32,54,54	1.46	9 (28%)
93	SPM	BR	201	-	13,13,13	0.39	0	12,12,12	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	GSP	BC	901	90	-	0/17/38/38	0/3/3/3
96	FME	AV	101	72	-	4/7/9/11	-
93	SPM	AA	3001	-	-	7/11/11/11	-
93	SPM	BA	3205	-	-	4/11/11/11	-
92	5GP	BA	3203	-	-	5/6/26/26	0/3/3/3
92	5GP	BA	3204	-	-	5/6/26/26	0/3/3/3
97	GTP	Ag	500	90	-	6/18/38/38	0/3/3/3
93	SPM	BR	201	-	-	8/11/11/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	BC	901	GSP	PG-S1G	-9.31	1.70	1.90
94	BC	901	GSP	C5-C6	-3.79	1.39	1.47
97	Ag	500	GTP	C5-C6	-3.59	1.40	1.47
92	BA	3204	5GP	C5-C6	-3.52	1.40	1.47
92	BA	3203	5GP	C5-C6	-2.75	1.41	1.47
92	BA	3203	5GP	C6-N1	-2.72	1.33	1.37
94	BC	901	GSP	C2-N3	2.37	1.38	1.33
92	BA	3204	5GP	C6-N1	-2.28	1.34	1.37
97	Ag	500	GTP	C2-N3	2.23	1.38	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	BA	3203	5GP	C5-C6-N1	3.95	120.92	113.95
92	BA	3204	5GP	C5-C6-N1	3.29	119.77	113.95
97	Ag	500	GTP	C5-C6-N1	3.23	119.66	113.95
92	BA	3203	5GP	C8-N7-C5	3.18	109.04	102.99
94	BC	901	GSP	C5-C6-N1	3.15	119.51	113.95
92	BA	3203	5GP	C2-N1-C6	-3.11	119.37	125.10
94	BC	901	GSP	C8-N7-C5	3.10	108.89	102.99
92	BA	3203	5GP	O6-C6-N1	-2.88	117.24	120.65
97	Ag	500	GTP	C8-N7-C5	2.80	108.31	102.99
92	BA	3204	5GP	C2-N1-C6	-2.80	119.95	125.10
94	BC	901	GSP	PA-O3A-PB	-2.75	123.40	132.83
94	BC	901	GSP	C2-N1-C6	-2.74	120.06	125.10
94	BC	901	GSP	C3'-C2'-C1'	2.63	104.93	100.98
97	Ag	500	GTP	C3'-C2'-C1'	2.57	104.84	100.98
92	BA	3204	5GP	C8-N7-C5	2.57	107.88	102.99
97	Ag	500	GTP	C2-N1-C6	-2.42	120.64	125.10
97	Ag	500	GTP	PA-O3A-PB	-2.26	125.08	132.83
97	Ag	500	GTP	O2G-PG-O3B	2.24	112.13	104.64
97	Ag	500	GTP	N1-C2-N3	-2.24	119.14	123.32
92	BA	3204	5GP	O6-C6-C5	-2.10	120.26	124.37
97	Ag	500	GTP	O6-C6-C5	-2.10	120.28	124.37
92	BA	3204	5GP	O2P-P-O5'	-2.06	101.24	106.73
97	Ag	500	GTP	N2-C2-N1	2.06	121.10	116.71
94	BC	901	GSP	O6-C6-C5	-2.05	120.37	124.37

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	BA	3203	5GP	C5'-O5'-P-O2P
92	BA	3203	5GP	C5'-O5'-P-O3P
92	BA	3204	5GP	C5'-O5'-P-O1P
92	BA	3204	5GP	C5'-O5'-P-O3P
96	AV	101	FME	C-CA-CB-CG
96	AV	101	FME	CA-CB-CG-SD
97	Ag	500	GTP	C5'-O5'-PA-O3A
97	Ag	500	GTP	C5'-O5'-PA-O1A
92	BA	3204	5GP	O4'-C4'-C5'-O5'
92	BA	3204	5GP	C3'-C4'-C5'-O5'
97	Ag	500	GTP	O4'-C4'-C5'-O5'
93	BR	201	SPM	C2-C3-C4-N5
93	BR	201	SPM	N5-C6-C7-C8
93	AA	3001	SPM	C7-C8-C9-N10
93	BA	3205	SPM	C7-C8-C9-N10
93	AA	3001	SPM	C8-C9-N10-C11
93	AA	3001	SPM	C12-C11-N10-C9
93	BA	3205	SPM	C7-C6-N5-C4
93	BR	201	SPM	C8-C9-N10-C11
93	AA	3001	SPM	C2-C3-C4-N5
96	AV	101	FME	N-CA-CB-CG
96	AV	101	FME	CB-CG-SD-CE
93	BR	201	SPM	N1-C2-C3-C4
93	BA	3205	SPM	C2-C3-C4-N5
93	BA	3205	SPM	C6-C7-C8-C9
92	BA	3203	5GP	C5'-O5'-P-O1P
93	BR	201	SPM	C6-C7-C8-C9
97	Ag	500	GTP	C3'-C4'-C5'-O5'
92	BA	3203	5GP	C4'-C5'-O5'-P
97	Ag	500	GTP	PA-O3A-PB-O2B
93	BR	201	SPM	N10-C11-C12-C13
93	AA	3001	SPM	N1-C2-C3-C4
93	AA	3001	SPM	C6-C7-C8-C9
92	BA	3204	5GP	C5'-O5'-P-O2P
93	BR	201	SPM	C12-C11-N10-C9
97	Ag	500	GTP	PA-O3A-PB-O1B
93	AA	3001	SPM	C3-C4-N5-C6
93	BR	201	SPM	C7-C8-C9-N10
92	BA	3203	5GP	O4'-C4'-C5'-O5'

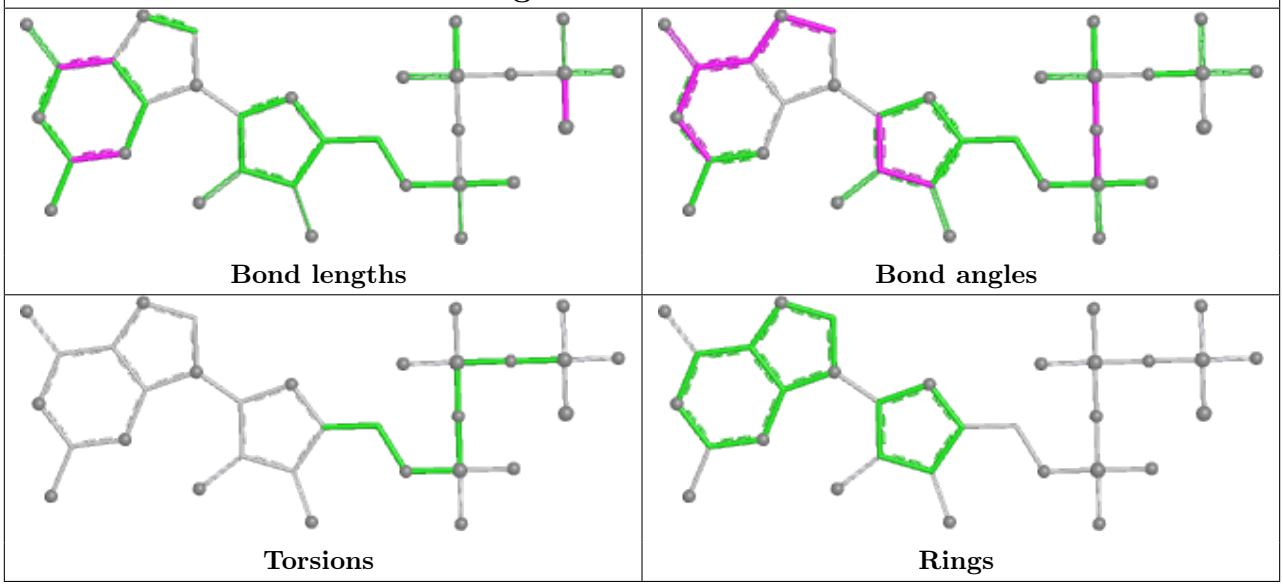
There are no ring outliers.

No monomer is involved in short contacts.

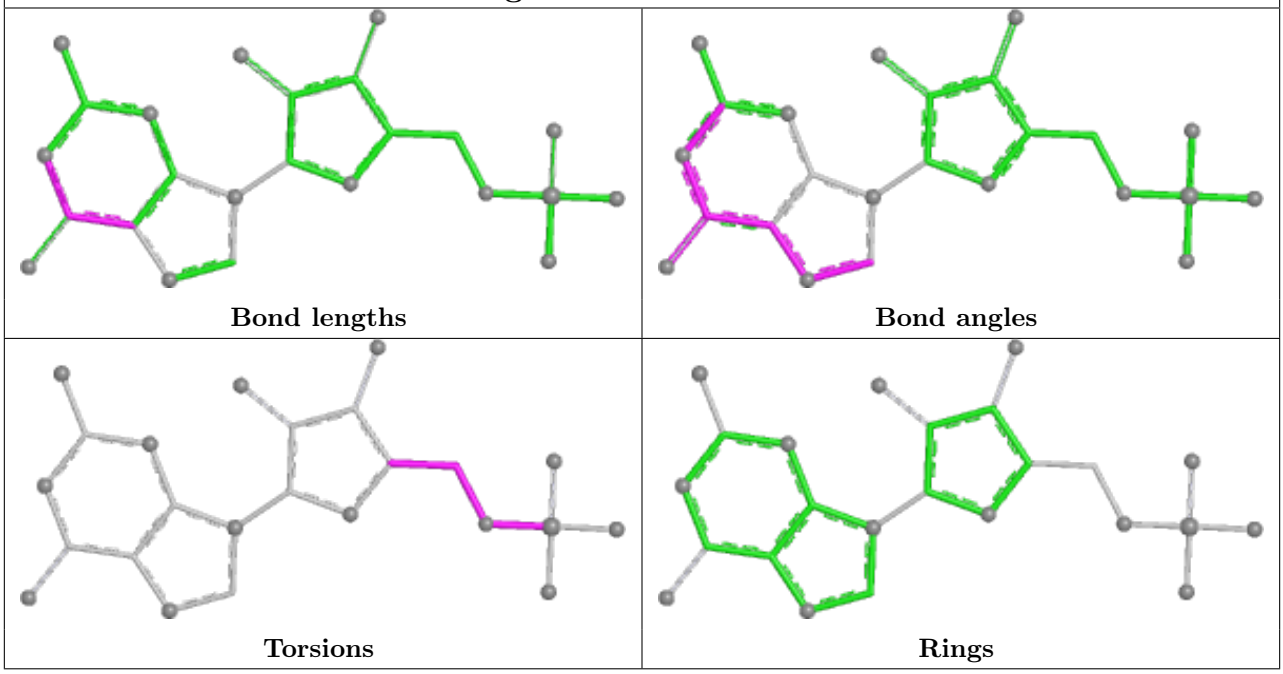
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

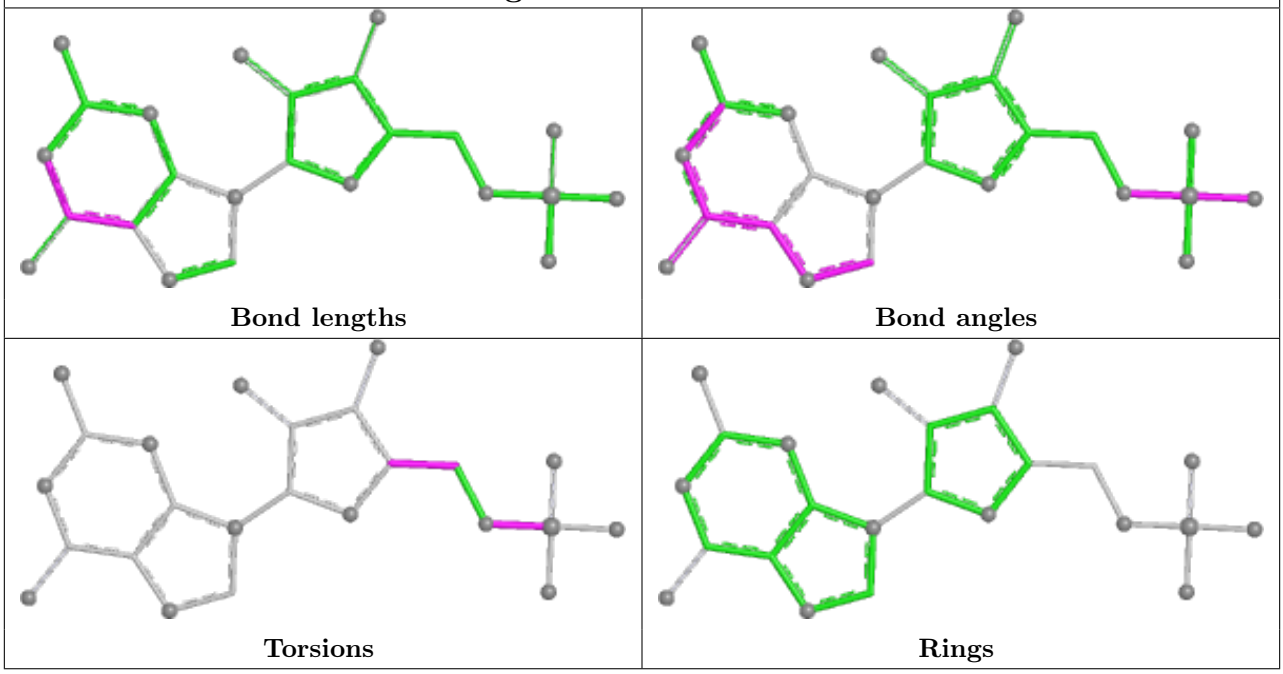
Ligand GSP BC 901



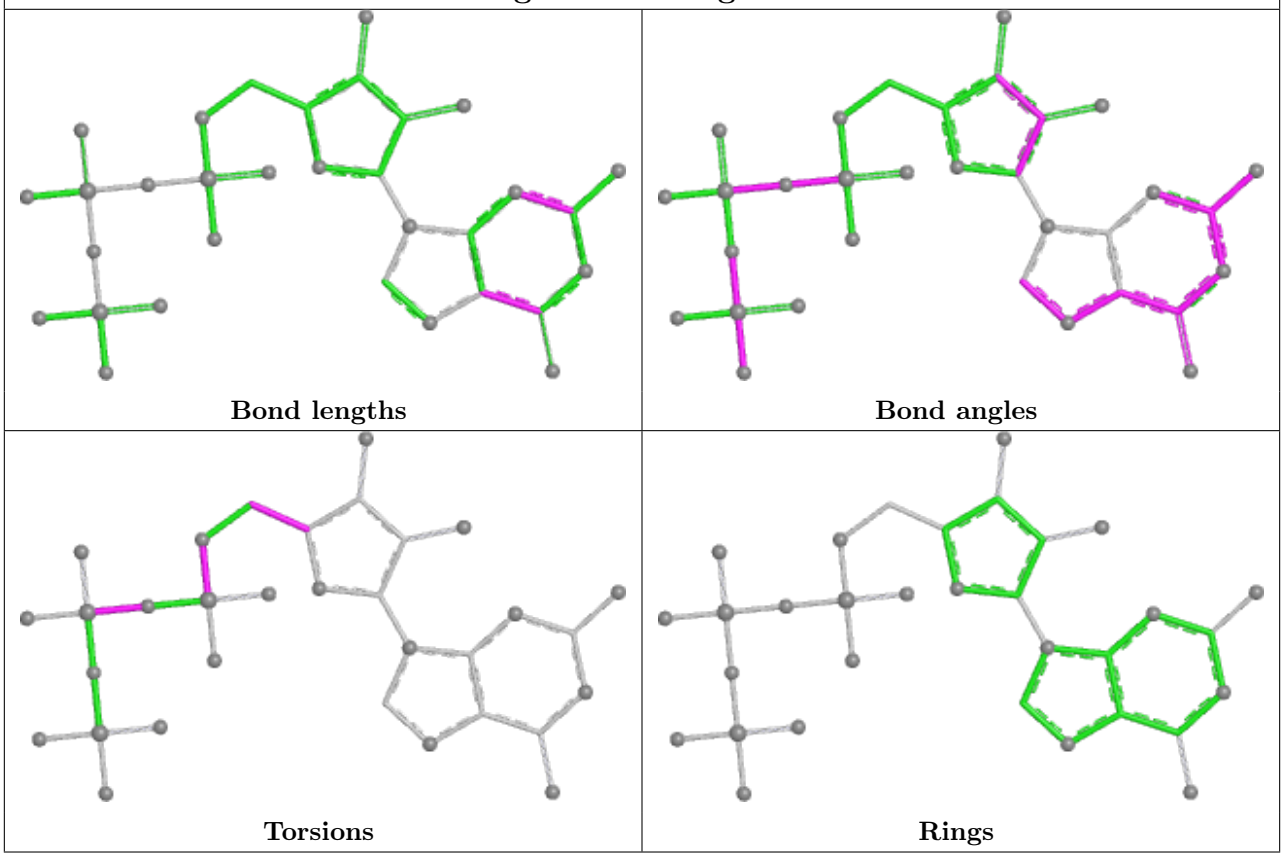
Ligand 5GP BA 3203



Ligand 5GP BA 3204



Ligand GTP Ag 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Bz	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	710:ALA	C	1001:ALA	N	59.86
1	Bz	415:ALA	C	601:ALA	N	51.54
1	Bz	106:ALA	C	301:ALA	N	30.13
1	Bz	615:ALA	C	700:ALA	N	17.90
1	Bz	315:ALA	C	399:ALA	N	16.24

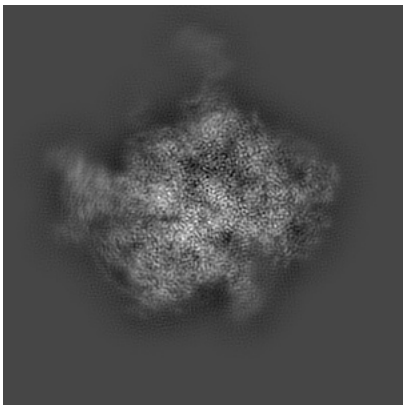
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4368. These allow visual inspection of the internal detail of the map and identification of artifacts.

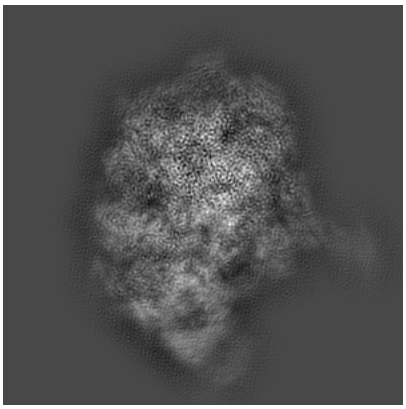
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

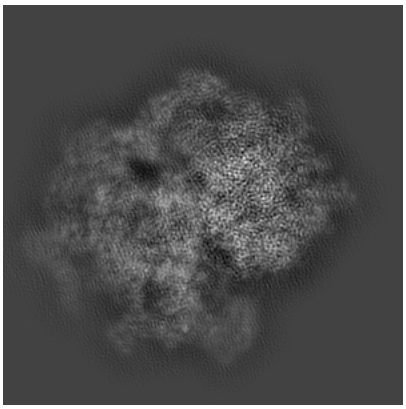
6.1.1 Primary map



X

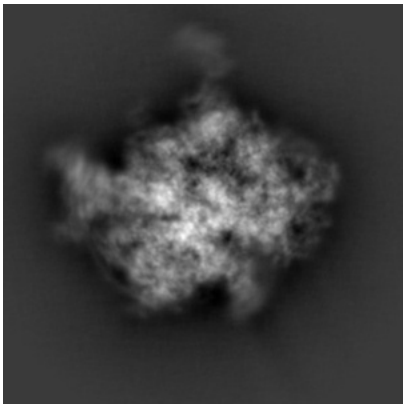


Y

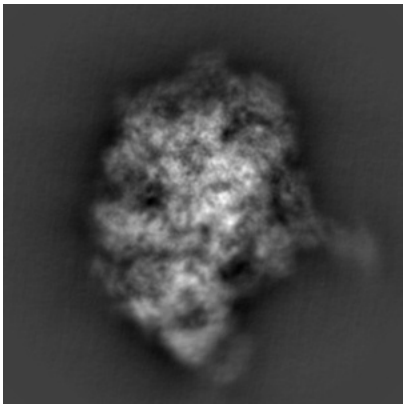


Z

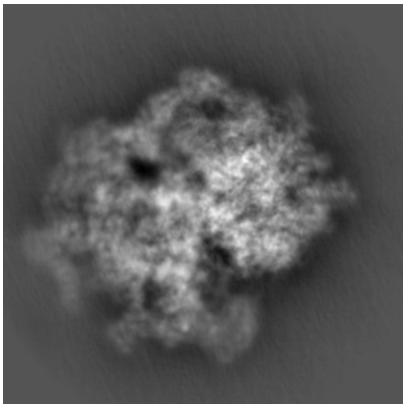
6.1.2 Raw map



X



Y

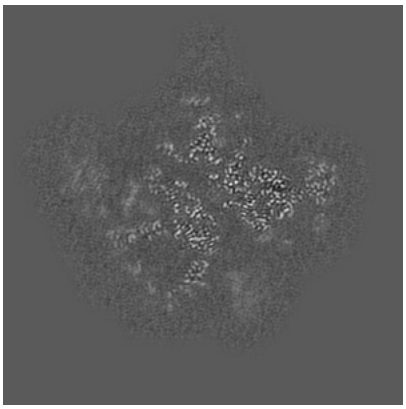


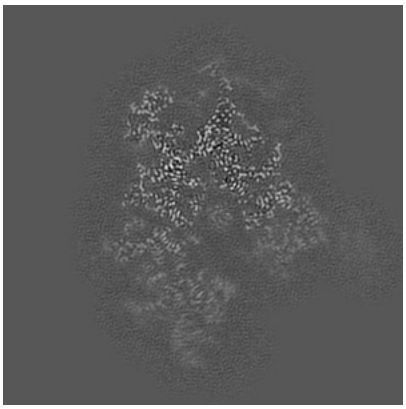
Z

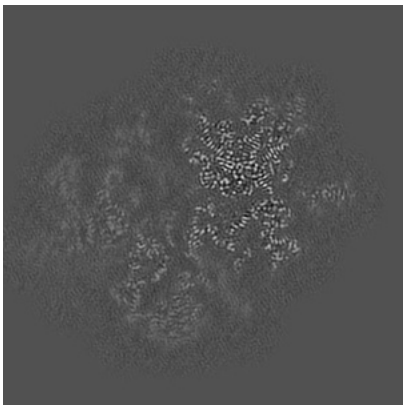
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

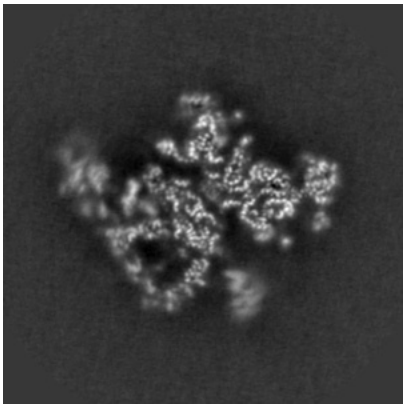
6.2.1 Primary map

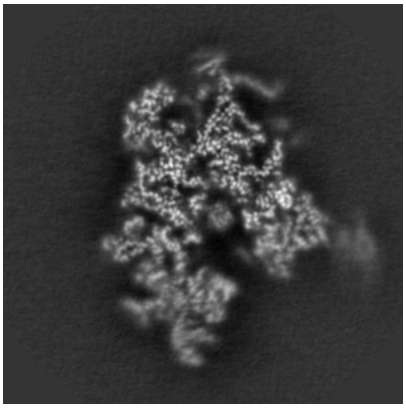

X Index: 140

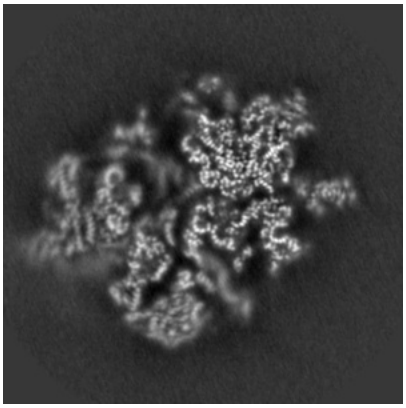

Y Index: 140


Z Index: 140

6.2.2 Raw map


X Index: 140

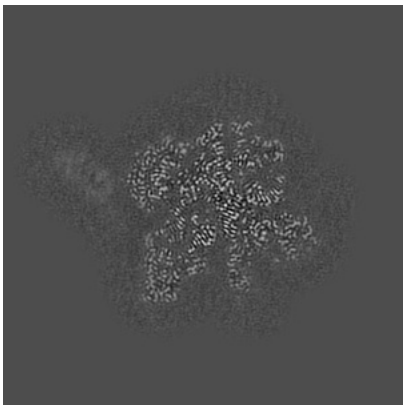

Y Index: 140


Z Index: 140

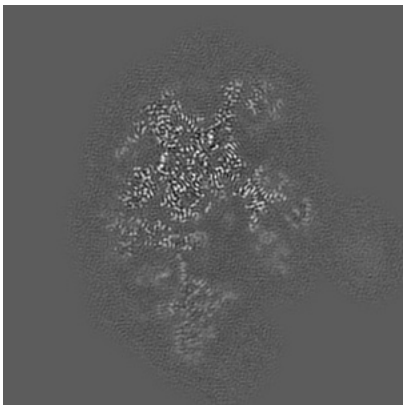
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

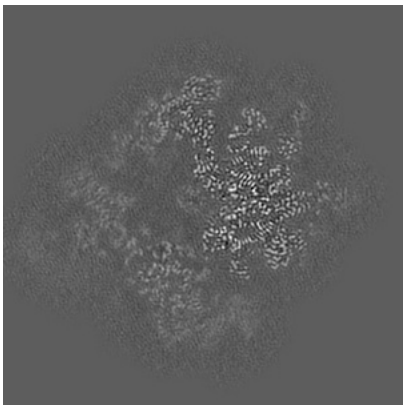
6.3.1 Primary map



X Index: 166

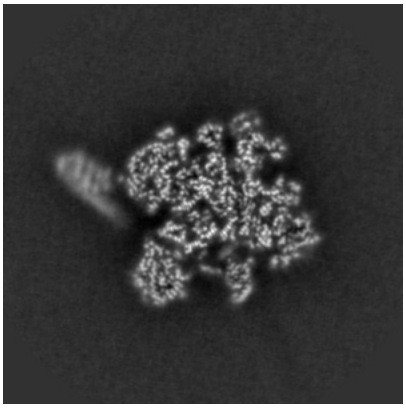


Y Index: 133

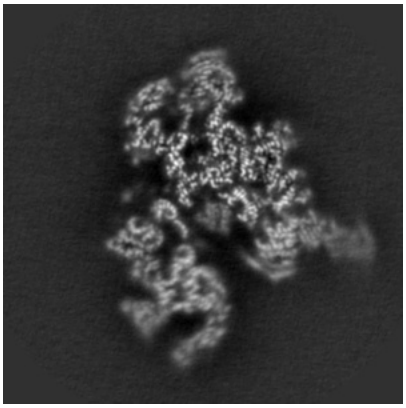


Z Index: 151

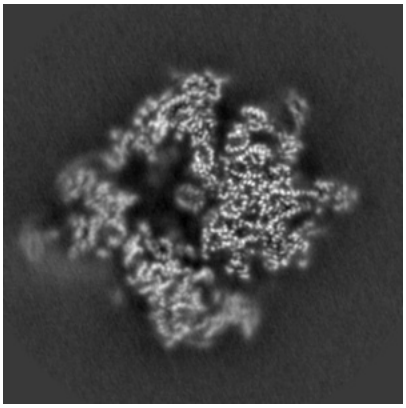
6.3.2 Raw map



X Index: 169



Y Index: 147



Z Index: 150

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

6.4 Orthogonal surface views (i)

6.4.1 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.

6.4.2 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.

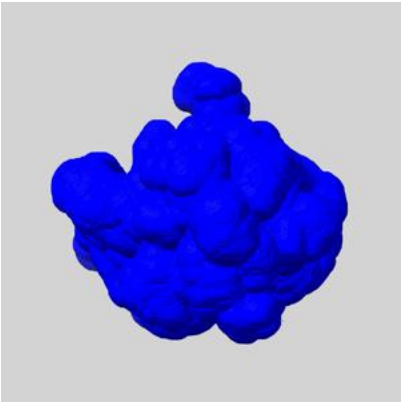
6.5 Mask visualisation (i)

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

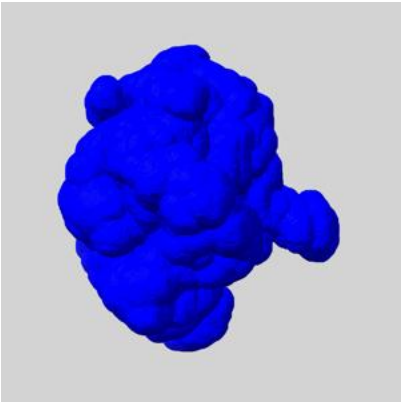
A mask typically either:

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

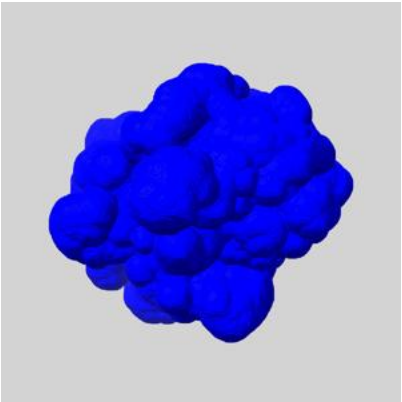
6.5.1 emd_4368_msk_1.map (i)



X



Y

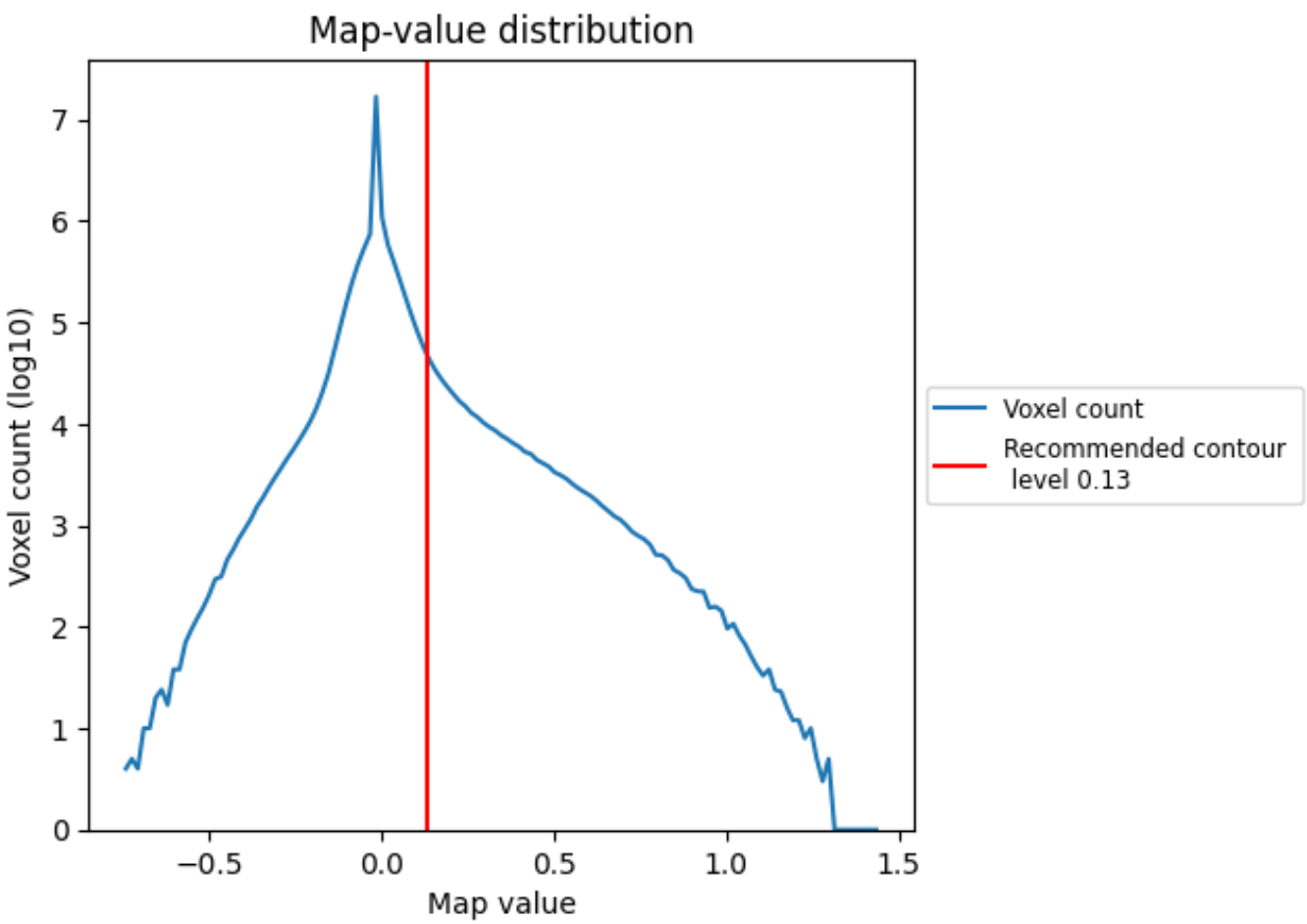


Z

7 Map analysis (i)

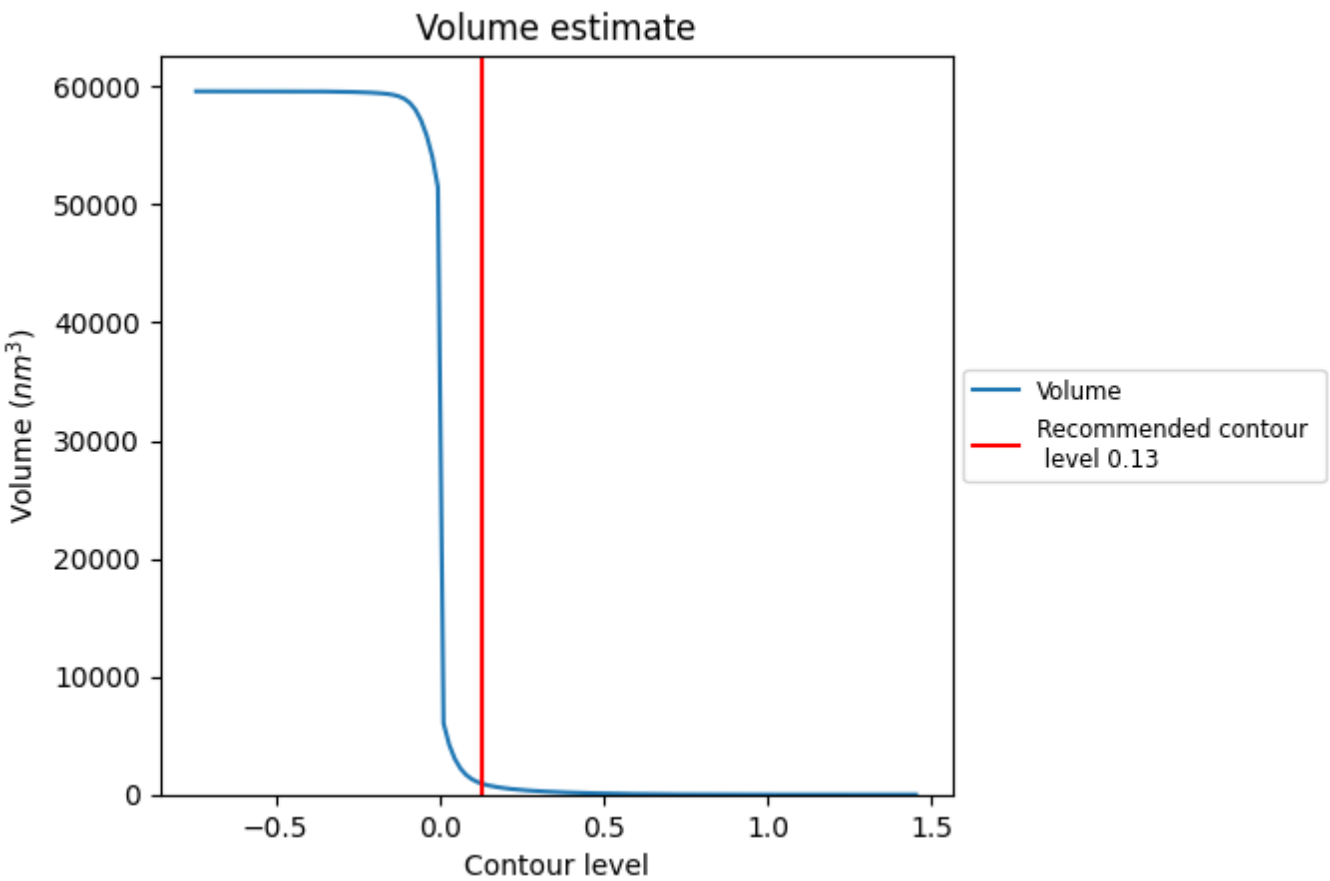
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

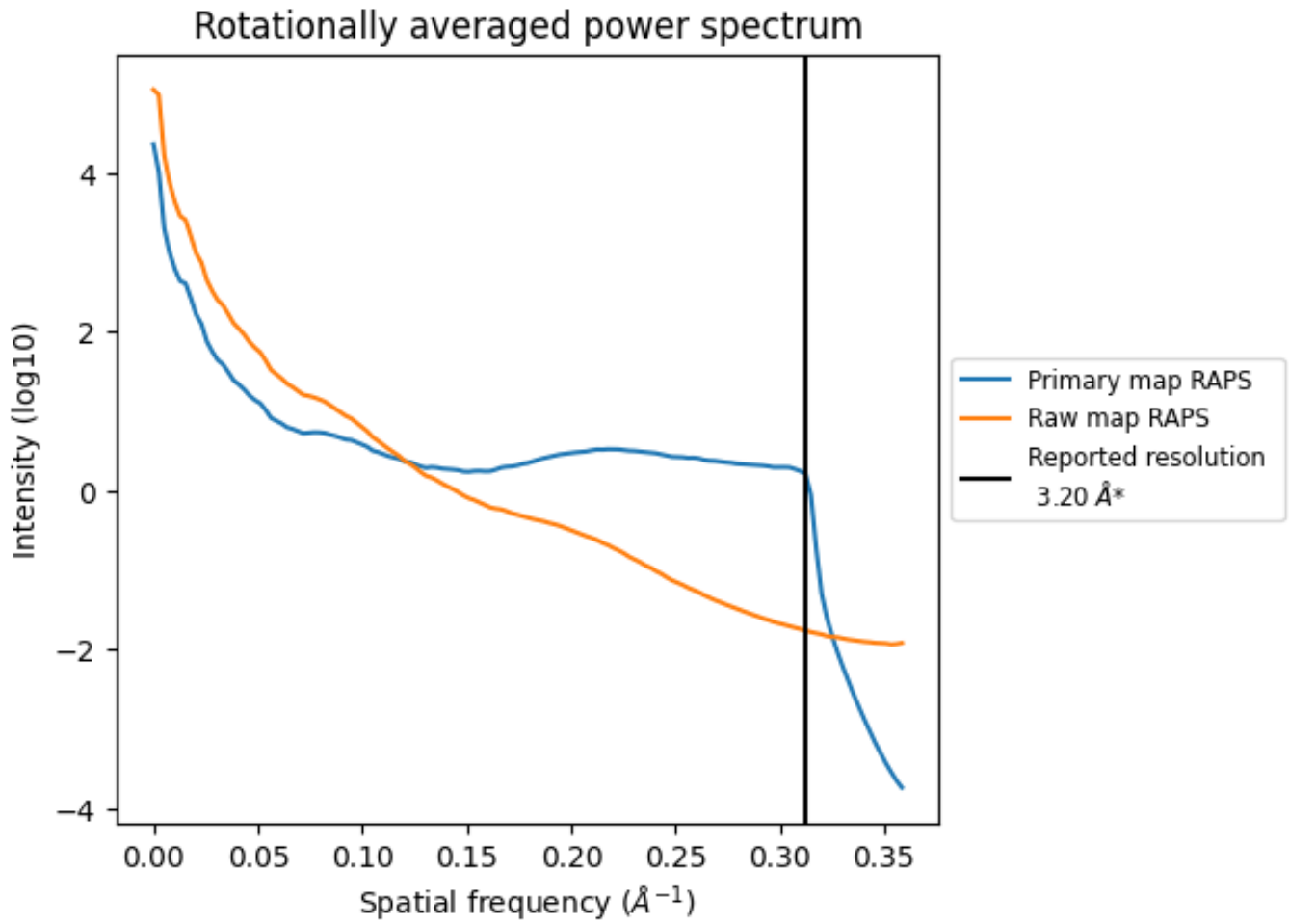
7.2 Volume estimate (i)



The volume at the recommended contour level is 920 nm^3; this corresponds to an approximate mass of 831 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)

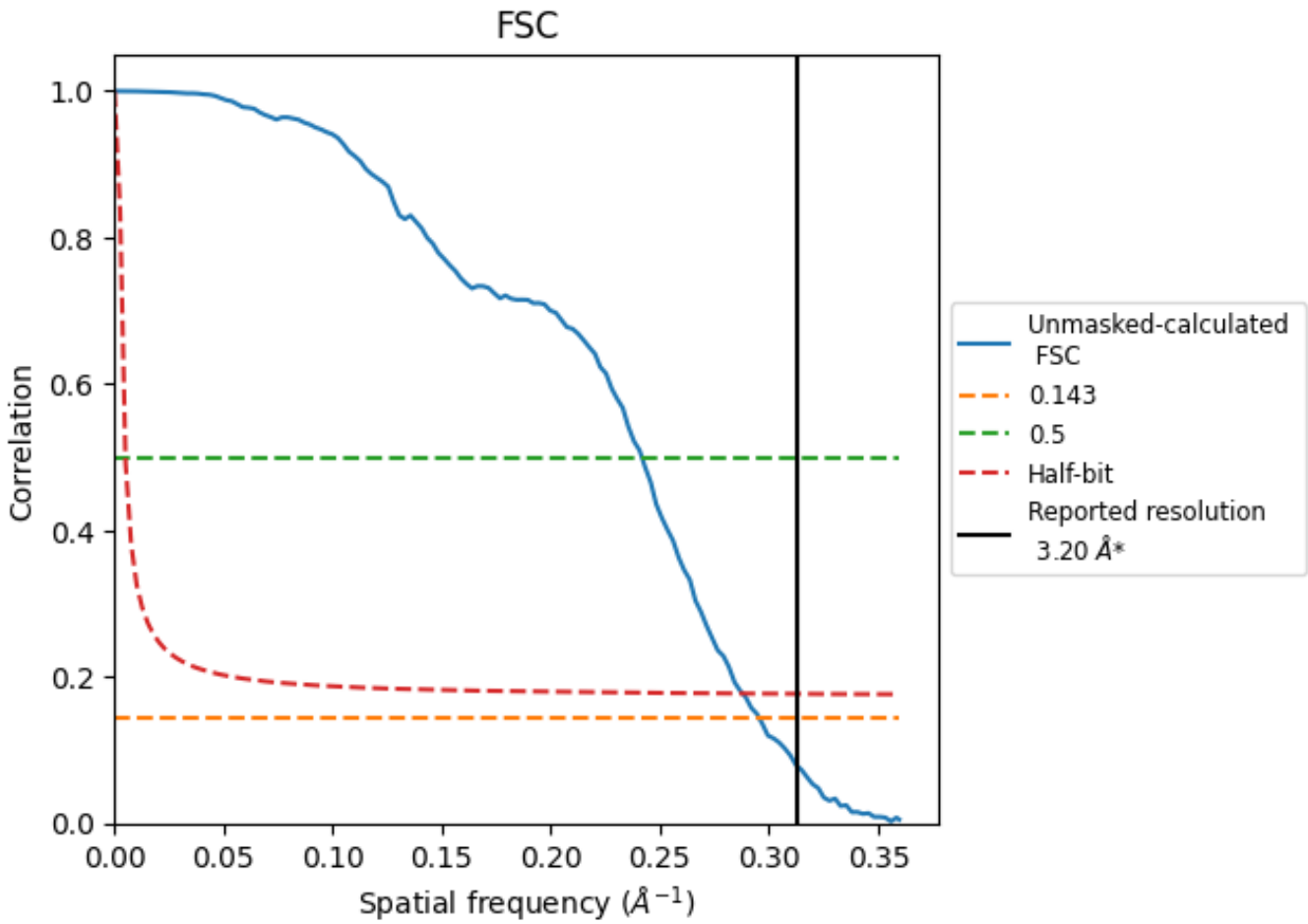


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

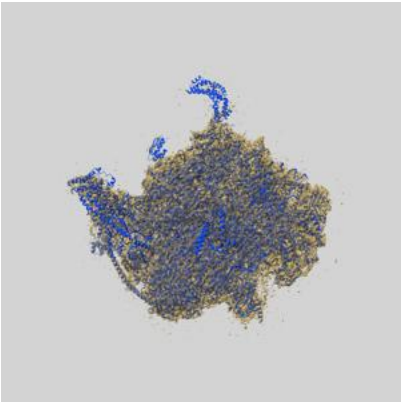
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	4.14	3.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

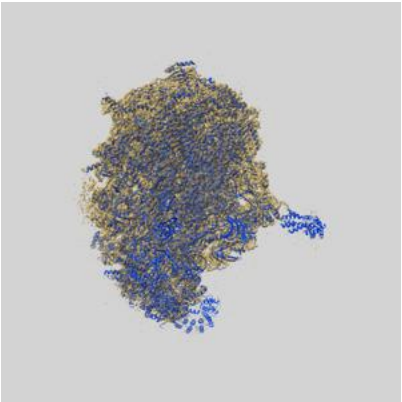
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4368 and PDB model 6GAW. Per-residue inclusion information can be found in section 3 on page 26.

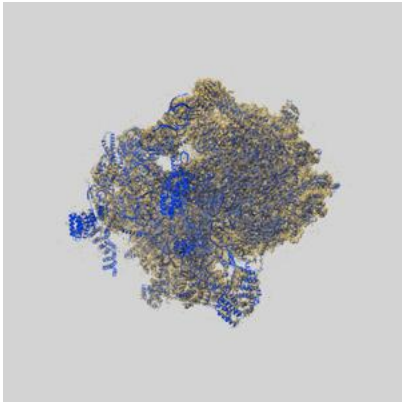
9.1 Map-model overlay (i)



X



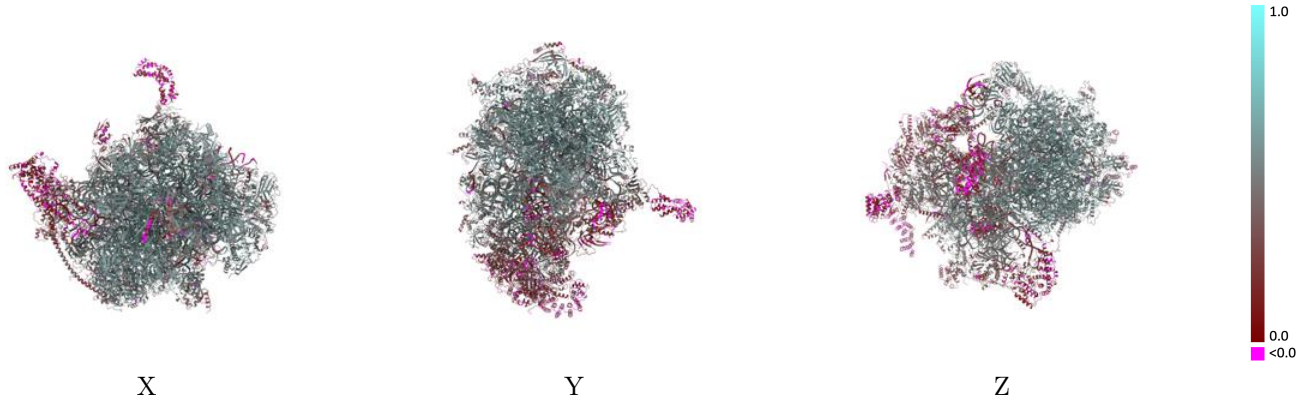
Y



Z

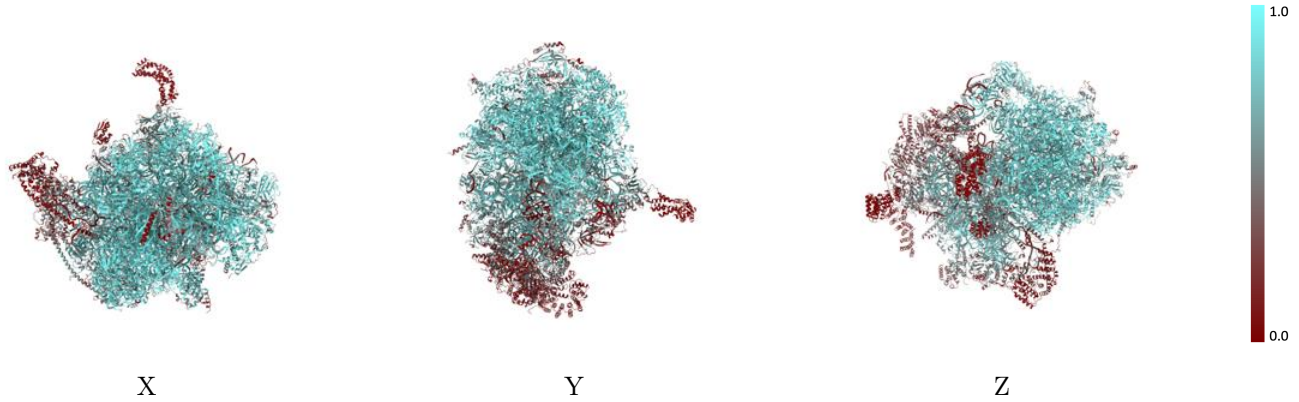
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



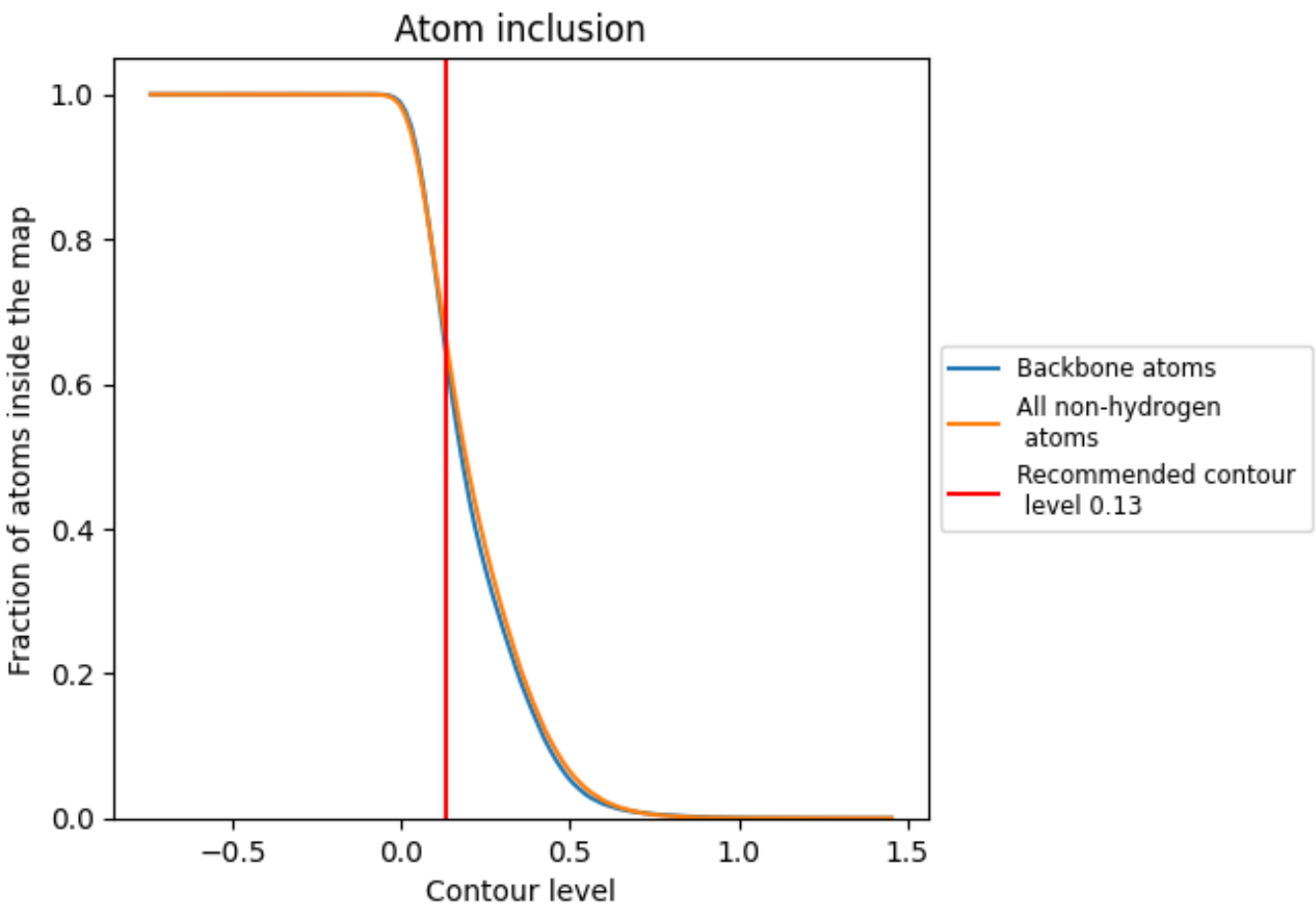
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.6668	0.4490
AA	0.7868	0.4730
AB	0.6540	0.4630
AC	0.4766	0.4340
AE	0.5566	0.4420
AF	0.7107	0.5020
AG	0.3315	0.3290
AI	0.3988	0.3330
AJ	0.3236	0.3080
AK	0.6589	0.4780
AL	0.7302	0.5200
AN	0.5276	0.4060
AO	0.6031	0.4290
AP	0.5495	0.3920
AQ	0.6395	0.4540
AR	0.7050	0.4800
AU	0.7464	0.5060
AV	0.4012	0.3030
AX	0.1803	0.1870
AZ	0.2444	0.2290
Aa	0.3800	0.3060
Ab	0.5329	0.4040
Ac	0.6082	0.4360
Ad	0.5074	0.3310
Ae	0.1274	0.1240
Af	0.5812	0.4450
Ag	0.2044	0.2230
Ah	0.2320	0.2310
Ai	0.3804	0.3240
Aj	0.2889	0.2510
Ak	0.2461	0.2530
Am	0.4917	0.3980
An	0.6951	0.5050
Ao	0.0668	0.1060
Ap	0.5178	0.3850

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Chain	Atom inclusion	Q-score
B0	0.8906	0.5710
B1	0.7649	0.4980
B2	0.8303	0.5390
B3	0.8495	0.5500
B4	0.5552	0.3310
B5	0.8404	0.5470
B6	0.6394	0.4760
B7	0.9268	0.6030
B8	0.9034	0.5850
B9	0.8941	0.5710
BA	0.9147	0.5630
BB	0.5427	0.2790
BC	0.4338	0.3750
BD	0.8541	0.5590
BE	0.8524	0.5520
BF	0.8699	0.5600
BI	0.6739	0.4570
BJ	0.4644	0.3340
BK	0.2674	0.2110
BL	0.0243	0.1230
BN	0.8937	0.5730
BO	0.8230	0.5420
BP	0.8566	0.5520
BQ	0.8269	0.5420
BR	0.8690	0.5640
BS	0.8162	0.5240
BT	0.7611	0.5120
BU	0.8771	0.5630
BV	0.8391	0.5520
BW	0.8638	0.5650
BX	0.7951	0.5120
BY	0.6426	0.4670
Ba	0.8289	0.5310
Bb	0.7842	0.4880
Bc	0.7523	0.4910
Bd	0.4746	0.2810
Be	0.7600	0.4980
Bf	0.7463	0.4730
Bg	0.8778	0.5640
Bh	0.7962	0.5070
Bi	0.5647	0.4090
Bj	0.3397	0.2220

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Chain	Atom inclusion	Q-score
Bk	0.5229	0.3700
Bl	0.8447	0.5460
Bm	0.4908	0.4160
Bn	0.8983	0.5730
Bo	0.7870	0.5200
Bp	0.5691	0.3840
Bq	0.4933	0.3500
Bt	0.8727	0.5670
Bu	0.6081	0.4020
Bv	0.6452	0.4400
Bw	0.8212	0.5270
Bx	0.7887	0.5160
Bz	0.0780	0.0740
CL	0.0949	0.1430
DL	0.0376	0.0930
EL	0.0000	0.0630
FL	0.0047	-0.0030
GL	0.0000	0.0290
HL	0.0000	0.0450