wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 06:56 pm BST

PDB ID	:	5AJ4
EMDB ID	:	EMD-2914
Title	:	Structure of the 55S mammalian mitoribosome.
Authors	:	Greber, B.J.; Bieri, P.; Leibundgut, M.; Leitner, A.; Aebersold, R.; Boehringer, D.; Ban, N.
Deposited on	:	2015-02-20
Resolution	:	3.80 Å(reported)

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

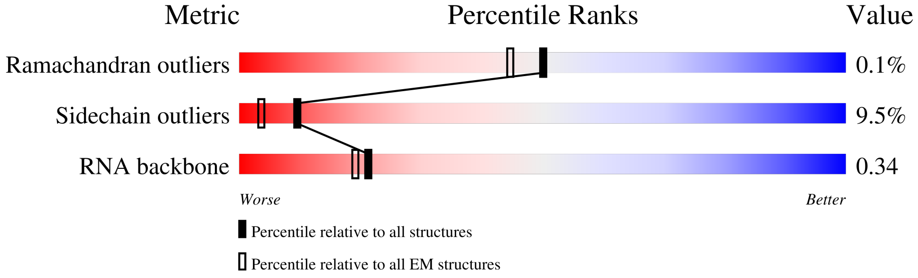
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

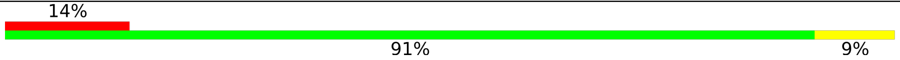
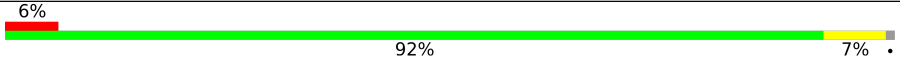
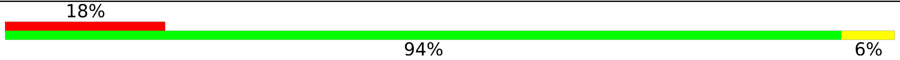
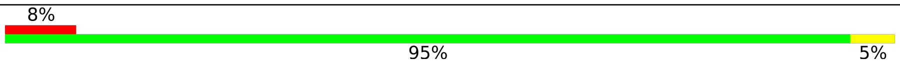
The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	AA	962	
2	AB	220	
3	AC	132	
4	AE	328	
5	AF	124	
6	AG	208	
7	AI	311	
8	AJ	201	

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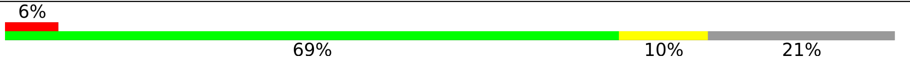
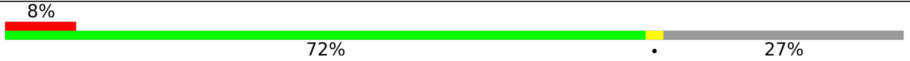
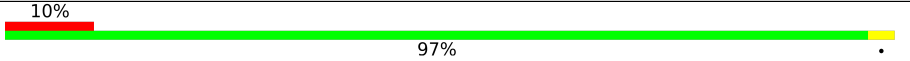
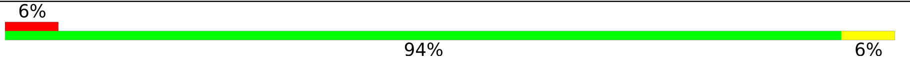
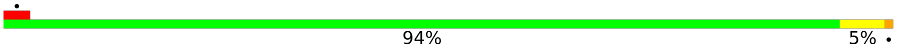
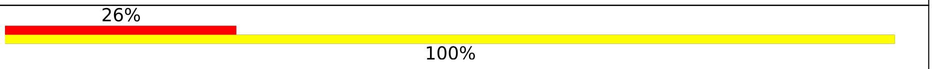
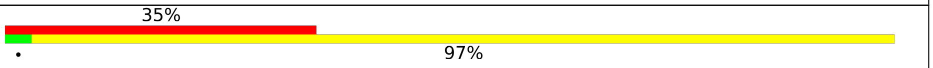
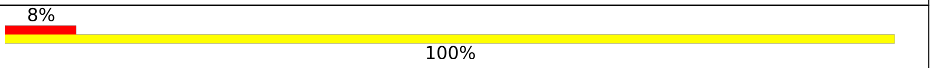
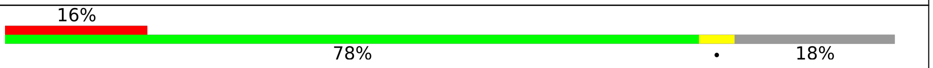
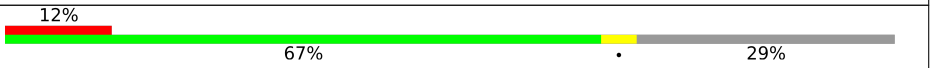
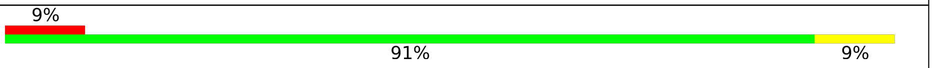
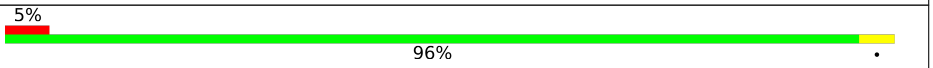
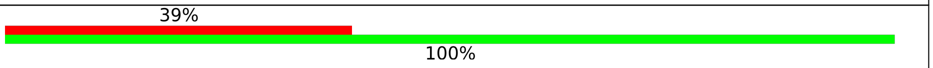
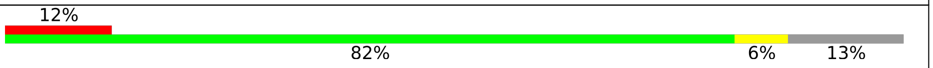
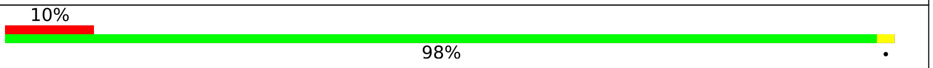
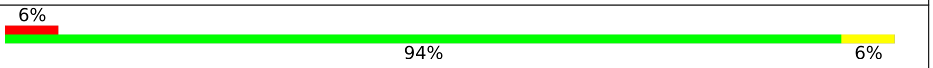
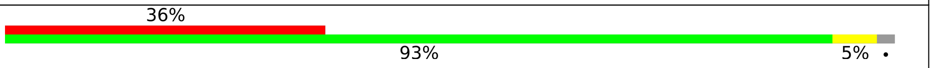
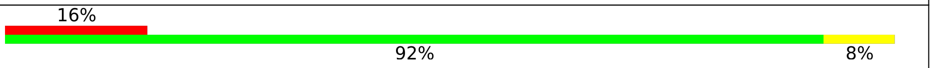
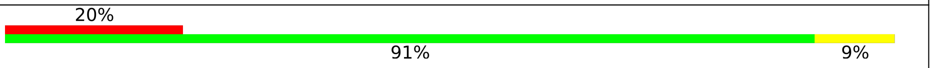
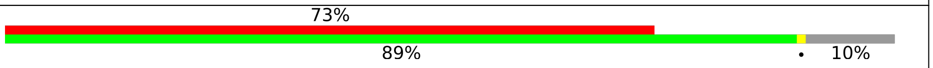
Mol	Chain	Length	Quality of chain
9	AK	136	
10	AL	109	
11	AN	128	
12	AO	239	
13	AP	117	
14	AQ	109	
15	AR	97	
16	AU	86	
17	AV	69	
17	AY	69	
18	AX	13	
19	Aa	356	
20	Ab	190	
21	Ac	169	
22	Ad	177	
23	Ae	336	
24	Af	188	
25	Ag	397	
26	Ah	103	
27	Ai	99	
28	Aj	218	
29	Ak	275	
30	Am	116	
31	An	72	
32	Ao	530	

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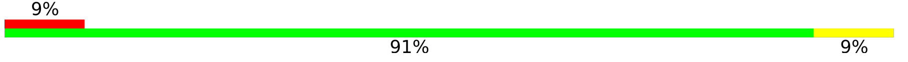
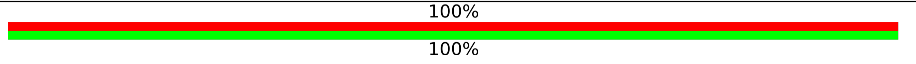
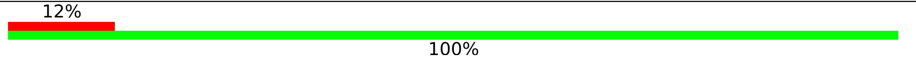
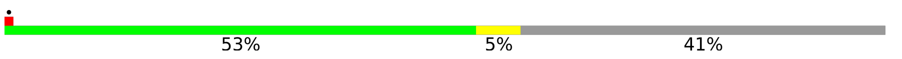
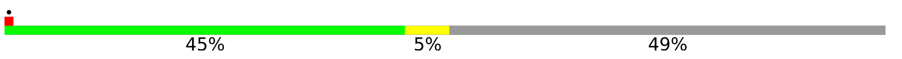
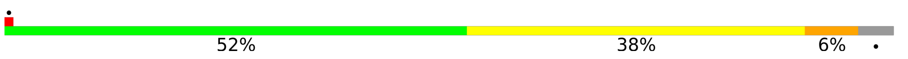
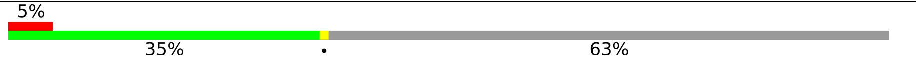
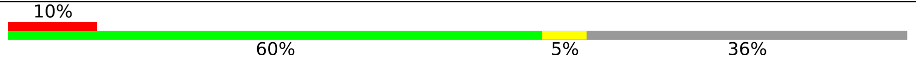
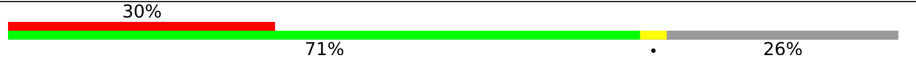
Mol	Chain	Length	Quality of chain
33	Ap	188	
34	As	16	
35	Az	17	
36	B0	148	
37	B1	256	
38	B2	252	
39	B3	161	
40	B4	126	
41	B5	188	
42	B6	65	
43	B7	95	
44	B8	188	
45	B9	100	
46	BA	1570	
47	BB	51	
48	BD	306	
49	BE	348	
50	BF	294	
51	BI	268	
52	BJ	262	
53	BK	192	
54	BN	178	
55	BO	145	
56	BP	296	
57	BQ	251	

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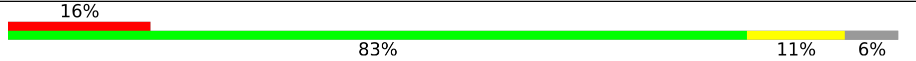
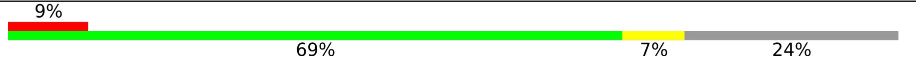
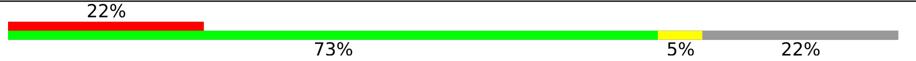
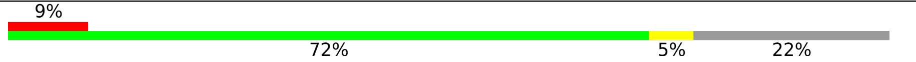
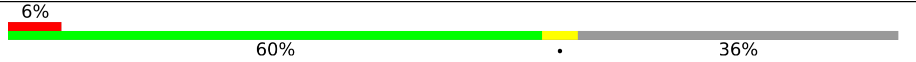
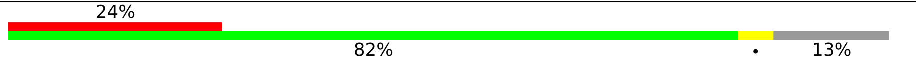
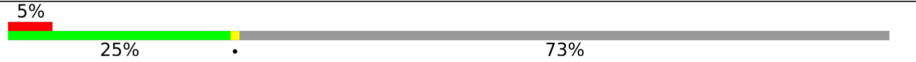
Mol	Chain	Length	Quality of chain
58	BR	169	
59	BS	180	
60	BT	292	
61	BU	149	
62	BV	209	
63	BW	210	
64	BX	150	
65	BY	216	
66	Ba	423	
67	Bb	380	
68	Bc	334	
69	Bd	206	
70	Be	135	
71	Bf	142	
72	Bg	159	
73	Bh	332	
74	Bi	312	
75	Bj	279	
76	Bk	212	
77	Bl	166	
78	Bm	159	
79	Bn	128	
80	Bo	124	
81	Bp	112	
82	Bq	138	

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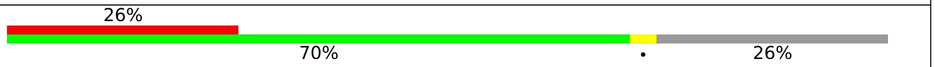
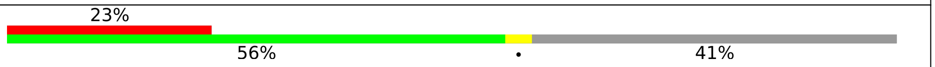
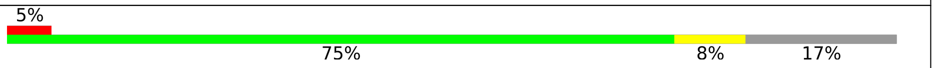
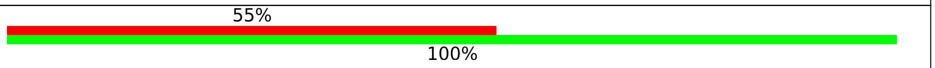
Mol	Chain	Length	Quality of chain
83	Bt	102	
84	Bu	205	
85	Bv	222	
86	Bw	433	
87	Bx	196	
88	Bz	94	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 167915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called MITORIBOSOMAL 12S Ribosomal RNA.

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

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN US2M, MRPS2.

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

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN US3M, MRPS24.

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

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN US5M, MRPS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AE	328	2621	1641	498	471	11	0	0

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BS6M, MRPS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AF	123	990	626	180	178	6	0	0

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN US7M, MRPS7.

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

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN US9M, MRPS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AI	311	2498	1586	450	449	13	0	0

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN US10M, MRPS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AJ	129	1067	690	182	192	3	0	0

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN US11M, MRPS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AK	136	1001	628	192	178	3	0	0

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN US12M, MRPS12.

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

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN US14M, MRPS14.

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

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN US15M, MRPS15.

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

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN BS16M, MRPS16.

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

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN US17M, MRPS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AQ	109	Total 853	C 555	N 150	O 145	S 3	0	0

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN BS18M, MRPS18C.

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

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN BS21M, MRPS21.

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

- Molecule 17 is a RNA chain called P-SITE AND A-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AV	69	Total 1251	C 625	N 146	O 412	P 68	0	0
17	AY	69	Total 1251	C 625	N 146	O 412	P 68	0	0

- Molecule 18 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AX	13	Total 231	C 117	N 26	O 76	P 12	0	0

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN MS22, MRPS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Aa	292	Total 2296	C 1476	N 394	O 417	S 9	0	0

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN MS23, MRPS23.

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

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN MS25, MRPS25.

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

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN MS26, MRPS26.

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

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN MS27, MRPS27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Ae	336	Total 2016	C 1344	N 336	O 336	0	0

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN MS28, MRPS28.

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

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN MS29, MRPS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ag	346	Total 2774	C 1786	N 489	O 489	S 10	0	0

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN MS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ah	103	Total 876	C 569	N 145	O 159	S 3	0	0

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN MS33, MRPS33.

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

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN MS34, MRPS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Aj	213	1777	1123	339	308	7	0	0

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN MS35, MRPS35.

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

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN MS37, MRPS37.

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

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN MS38, MRPS38.

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

- Molecule 32 is a protein called MITORIBOSOMAL PROTEIN MS39, MRPS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Ao	476	3028	2007	500	519	2	0	0

- Molecule 33 is a protein called 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Ap	188	1551	983	290	270	8	0	0

- Molecule 34 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	As	16	96	64	16	16	0	0

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Az	17	102	68	17	17	0	0

- Molecule 36 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B0	114	878	564	160	151	3	0	0

- Molecule 37 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

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

- Molecule 38 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	B2	178	1544	990	289	259	6	0	0

- Molecule 39 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

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

- Molecule 40 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

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

- Molecule 41 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

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

- Molecule 42 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 43 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

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

- Molecule 44 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

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

- Molecule 45 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

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

- Molecule 46 is a RNA chain called MITORIBOSOMAL 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BA	1515	Total	C	N	O	P	0	0
			32233	14473	5860	10385	1515		

- Molecule 47 is a RNA chain called MITORIBOSOMAL CP TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BB	51	Total	C	N	O	P	0	0
			1008	489	162	306	51		

- Molecule 48 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

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

- Molecule 49 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

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

- Molecule 50 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

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

- Molecule 51 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

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

- Molecule 52 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BJ	168	Total 1361	C 879	N 248	O 226	S 8	0	0

- Molecule 53 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	142	Total 1081	C 690	N 197	O 192	S 2	0	0

- Molecule 54 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

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

- Molecule 55 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

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

- Molecule 56 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

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

- Molecule 57 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BQ	221	1792	1147	330	305	10	0	0

- Molecule 58 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

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

- Molecule 59 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

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

- Molecule 60 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	BT	239	1950	1249	339	353	9	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	54	UNK	PHE	conflict	UNP I3LNJ0
BT	55	UNK	GLN	conflict	UNP I3LNJ0
BT	56	UNK	PRO	conflict	UNP I3LNJ0
BT	57	UNK	PRO	conflict	UNP I3LNJ0
BT	58	UNK	PRO	conflict	UNP I3LNJ0
BT	59	UNK	LYS	conflict	UNP I3LNJ0
BT	60	UNK	PRO	conflict	UNP I3LNJ0
BT	61	UNK	VAL	conflict	UNP I3LNJ0
BT	62	UNK	ILE	conflict	UNP I3LNJ0
BT	63	UNK	VAL	conflict	UNP I3LNJ0
BT	64	UNK	ASP	conflict	UNP I3LNJ0
BT	65	UNK	LYS	conflict	UNP I3LNJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
BT	66	UNK	ARG	conflict	UNP I3LNJ0
BT	67	UNK	ARG	conflict	UNP I3LNJ0
BT	68	UNK	PRO	conflict	UNP I3LNJ0

- Molecule 61 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

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

- Molecule 62 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

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

- Molecule 63 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

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

- Molecule 64 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	BX	134	1120	715	217	186	2	0	0

- Molecule 65 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	BY	204	1663	1047	305	306	5	0	0

- Molecule 66 is a protein called MITORIBOSOMAL PROTEIN ML37, MRPL37.

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

- Molecule 67 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

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

- Molecule 68 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

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

- Molecule 69 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

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

- Molecule 70 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Be	121	968	626	167	172	3	0	0

- Molecule 71 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	Bf	108	852	544	154	150	4	0	0

- Molecule 72 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

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

- Molecule 73 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

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

- Molecule 74 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	Bi	242	1979	1266	352	351	10	0	0

- Molecule 75 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

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

- Molecule 76 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

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

- Molecule 77 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

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

- Molecule 78 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

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

- Molecule 79 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

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

- Molecule 80 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Bo	94	747	466	143	136	2	0	0

- Molecule 81 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

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

- Molecule 82 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
82	Bq	37	336	214	69	53	0	0

- Molecule 83 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57.

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

- Molecule 84 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Bu	151	1208	748	233	222	5	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bu	164	UNK	ALA	conflict	UNP W5IDC0
Bu	165	UNK	LYS	conflict	UNP W5IDC0
Bu	166	UNK	GLU	conflict	UNP W5IDC0
Bu	167	UNK	PRO	conflict	UNP W5IDC0
Bu	168	UNK	SER	conflict	UNP W5IDC0
Bu	169	UNK	ARG	conflict	UNP W5IDC0
Bu	170	UNK	GLU	conflict	UNP W5IDC0
Bu	171	UNK	ASP	conflict	UNP W5IDC0
Bu	172	UNK	ALA	conflict	UNP W5IDC0
Bu	173	UNK	GLU	conflict	UNP W5IDC0

- Molecule 85 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Bv	131	1068	662	206	195	5	0	0

- Molecule 86 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

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

- Molecule 87 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

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

- Molecule 88 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	Bz	94	Total 564	C 376	N 94	O 94	0	0

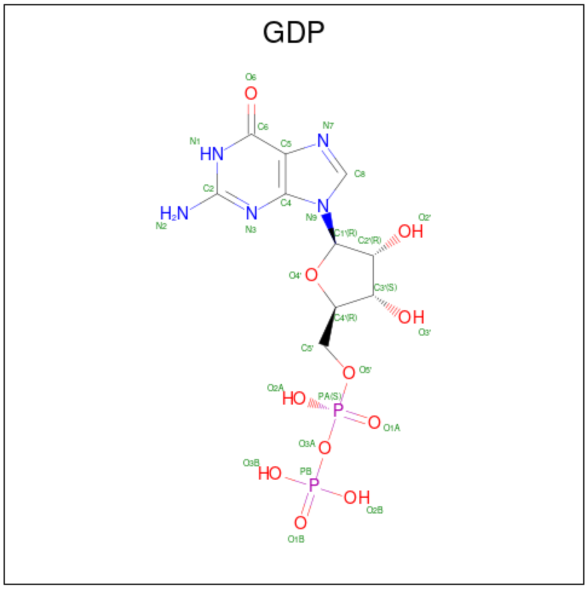
- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	146	Total 146	Mg 146	0
89	Ag	1	Total 1	Mg 1	0
89	B0	1	Total 1	Mg 1	0
89	B2	1	Total 1	Mg 1	0
89	BA	195	Total 195	Mg 195	0
89	BD	2	Total 2	Mg 2	0
89	BE	1	Total 1	Mg 1	0
89	BP	1	Total 1	Mg 1	0
89	BR	2	Total 2	Mg 2	0
89	BX	1	Total 1	Mg 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
92	AA	114	114	114	0
92	Ag	4	4	4	0

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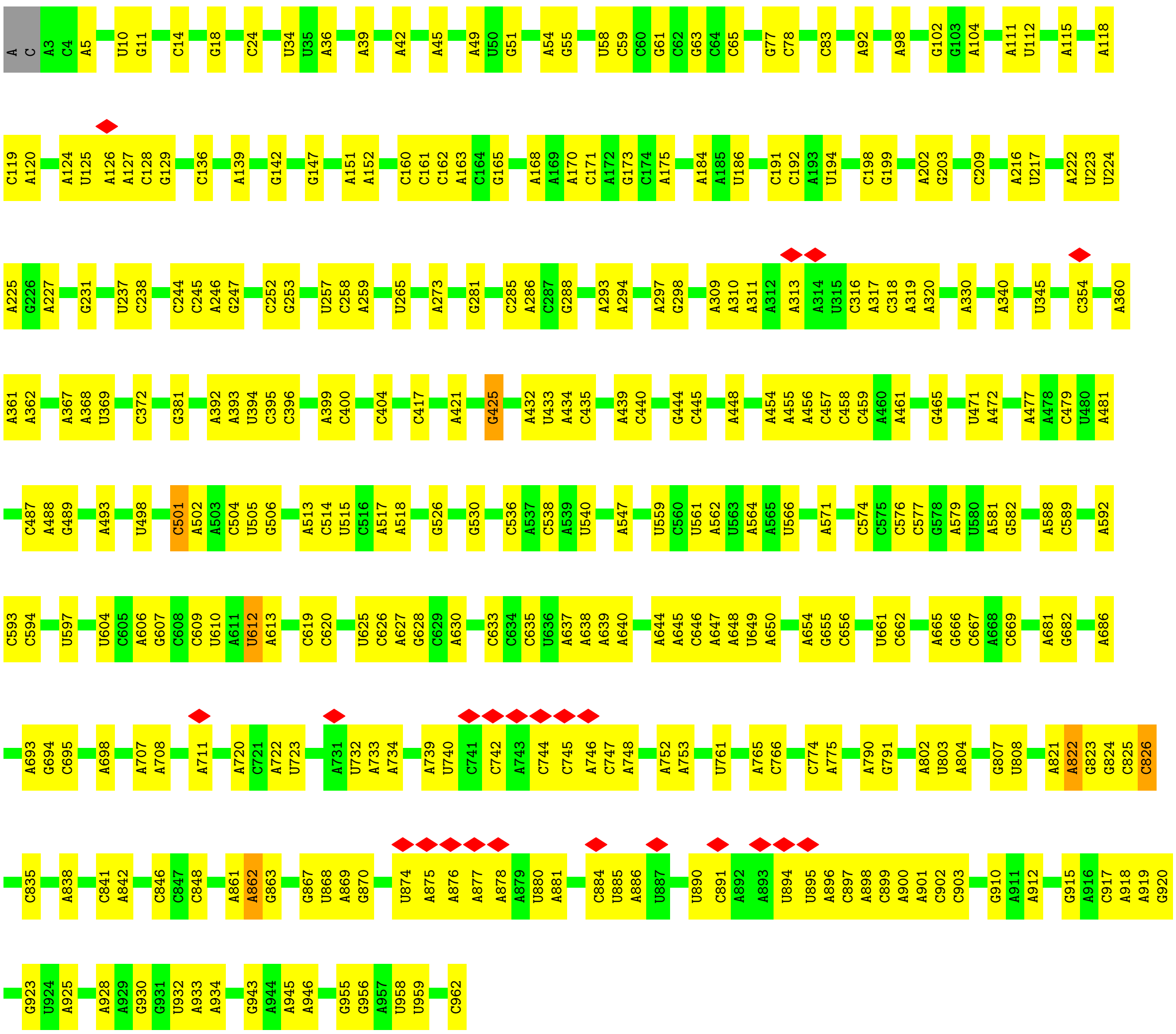
Mol	Chain	Residues	Atoms	AltConf
92	B0	3	Total O 3 3	0
92	B7	2	Total O 2 2	0
92	B8	1	Total O 1 1	0
92	BA	196	Total O 196 196	0
92	BD	3	Total O 3 3	0
92	BF	4	Total O 4 4	0
92	BI	1	Total O 1 1	0
92	BO	2	Total O 2 2	0
92	BP	3	Total O 3 3	0
92	BR	2	Total O 2 2	0
92	BU	1	Total O 1 1	0
92	BW	4	Total O 4 4	0

3 Residue-property plots ⓘ

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

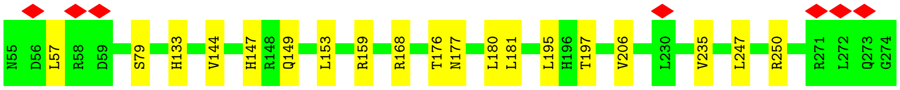
- Molecule 1: MITORIBOSOMAL 12S Ribosomal RNA

Chain AA:



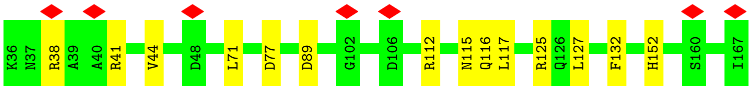
- Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2

Chain AB:



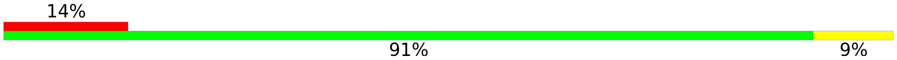
- Molecule 3: MITORIBOSOMAL PROTEIN US3M, MRPS24

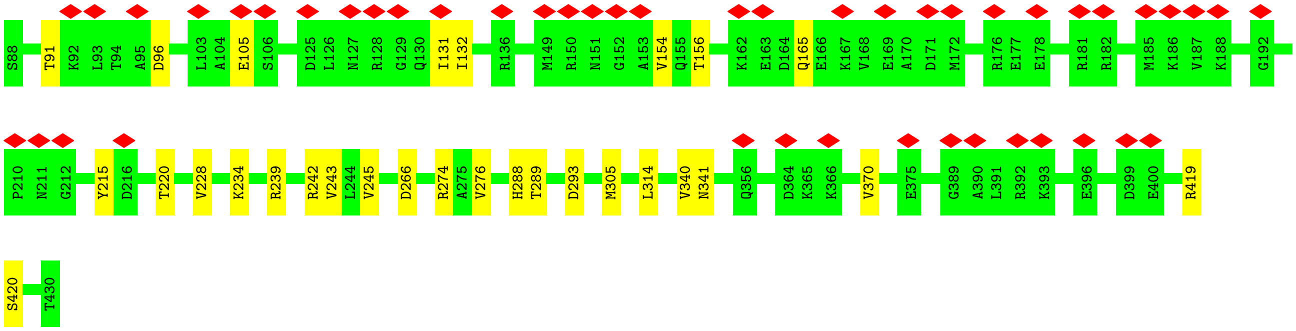
Chain AC:



- Molecule 4: MITORIBOSOMAL PROTEIN US5M, MRPS5

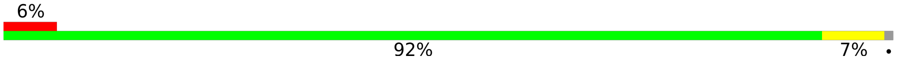
Chain AE:

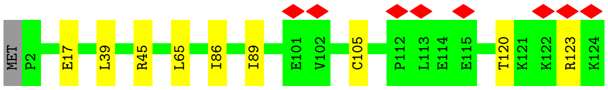




- Molecule 5: MITORIBOSOMAL PROTEIN BS6M, MRPS6

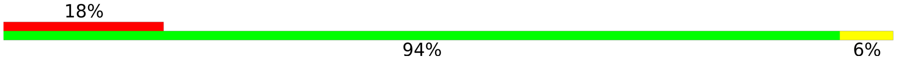
Chain AF:

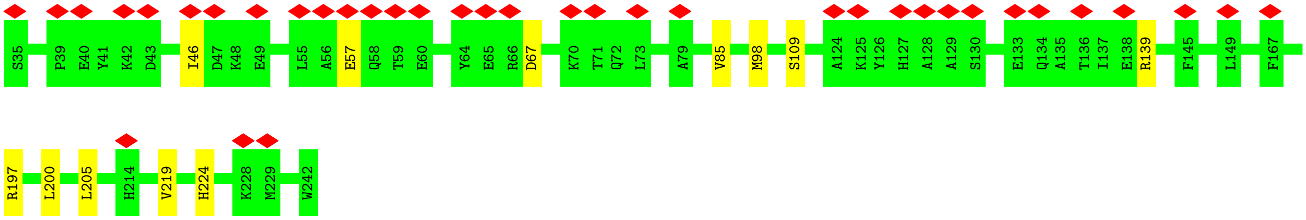




- Molecule 6: MITORIBOSOMAL PROTEIN US7M, MRPS7

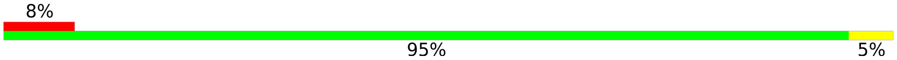
Chain AG:

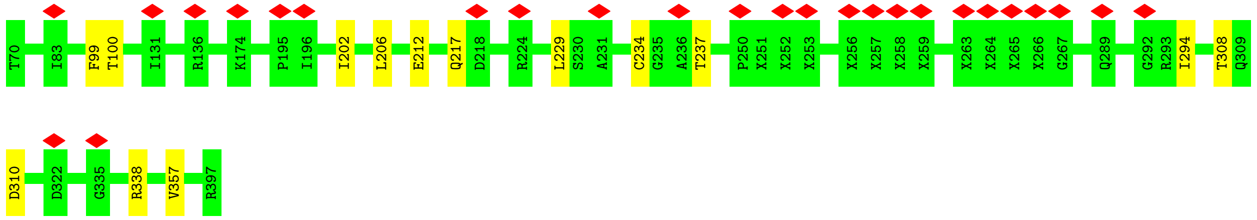




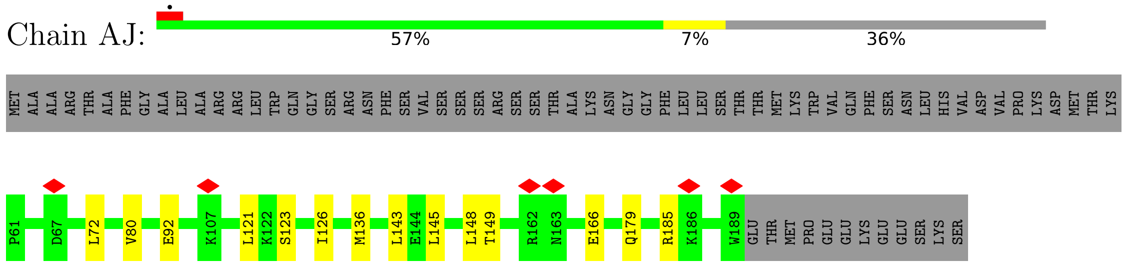
- Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9

Chain AI:

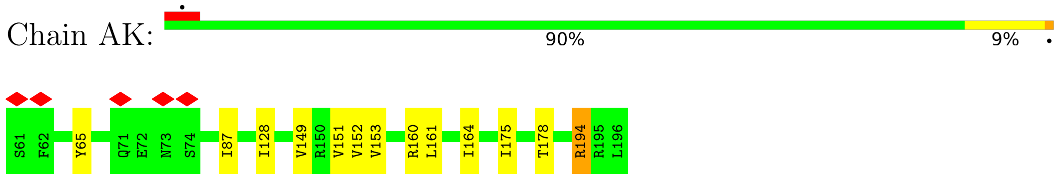




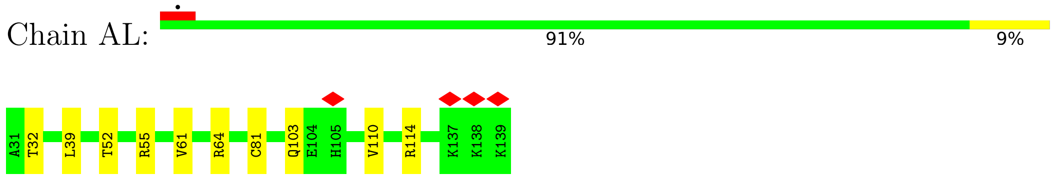
- Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10



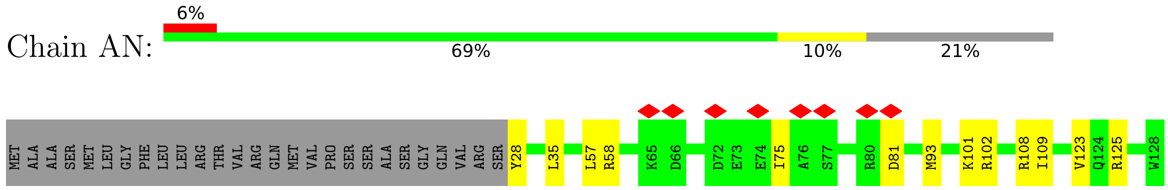
- Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11



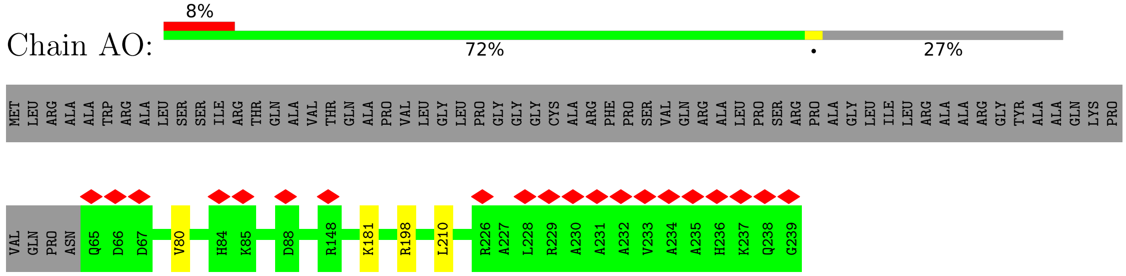
- Molecule 10: MITORIBOSOMAL PROTEIN US12M, MRPS12



- Molecule 11: MITORIBOSOMAL PROTEIN US14M, MRPS14

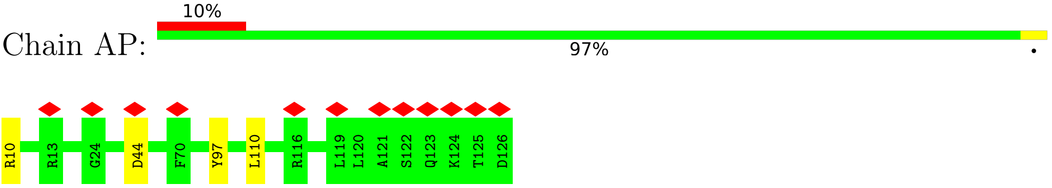


- Molecule 12: MITORIBOSOMAL PROTEIN US15M, MRPS15



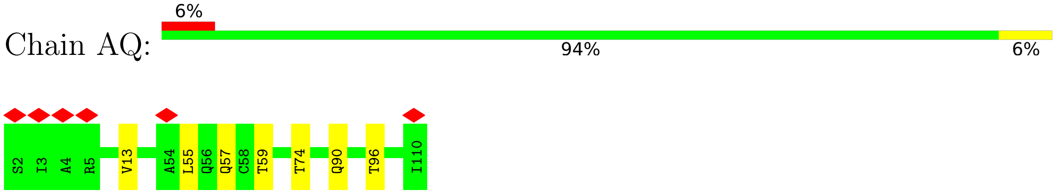
- Molecule 13: MITORIBOSOMAL PROTEIN BS16M, MRPS16

Chain AP:



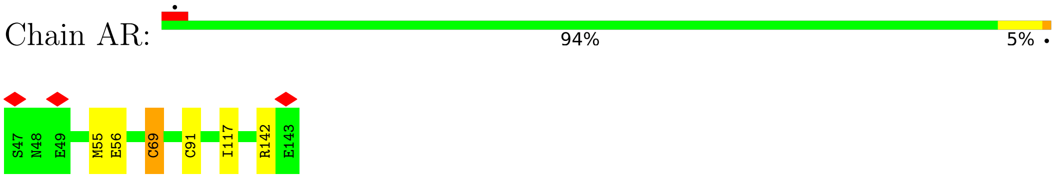
- Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17

Chain AQ:



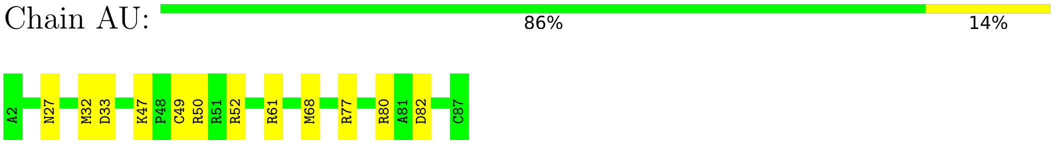
- Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

Chain AR:



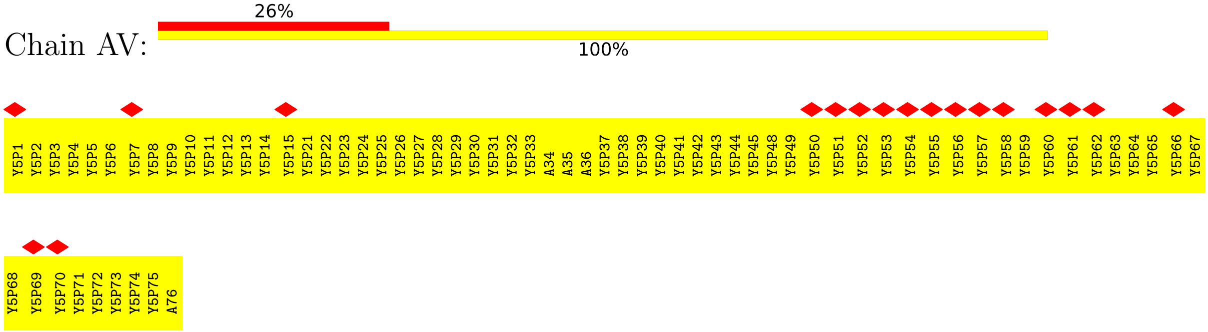
- Molecule 16: MITORIBOSOMAL PROTEIN BS21M, MRPS21

Chain AU:



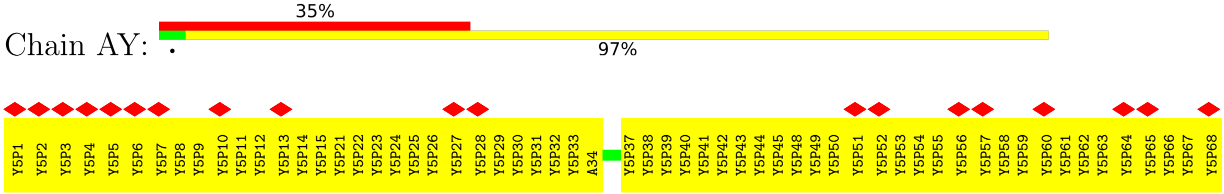
- Molecule 17: P-SITE AND A-SITE TRNA

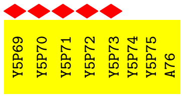
Chain AV:



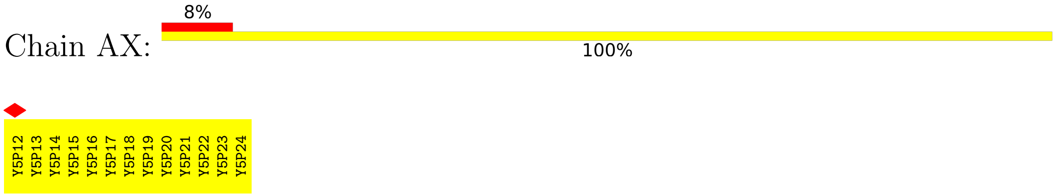
- Molecule 17: P-SITE AND A-SITE TRNA

Chain AY:

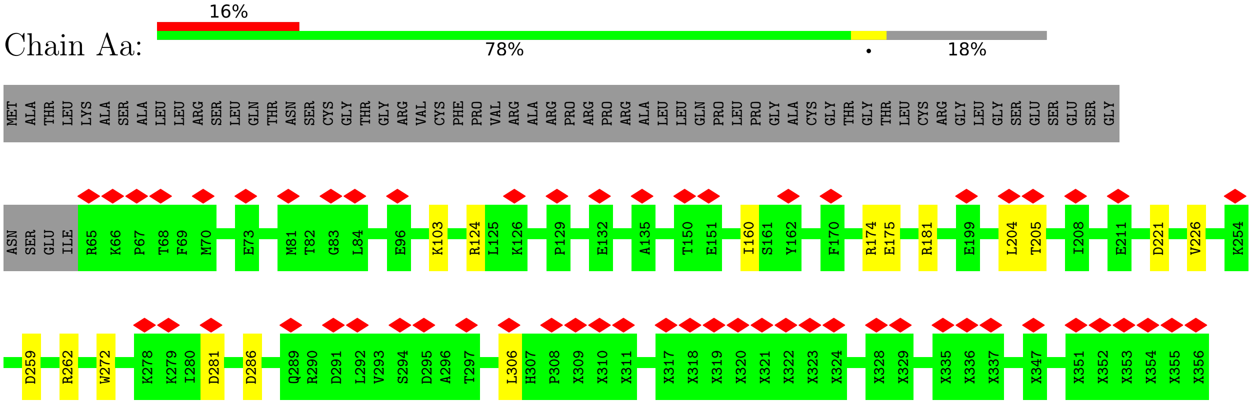




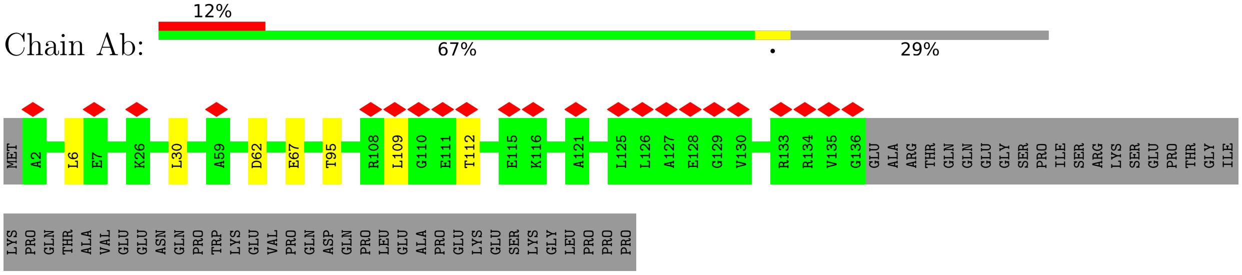
- Molecule 18: MRNA



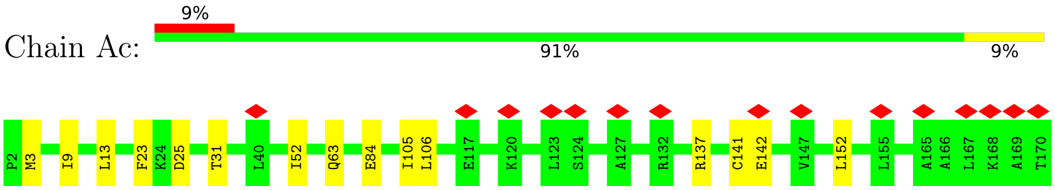
- Molecule 19: MITORIBOSOMAL PROTEIN MS22, MRPS22



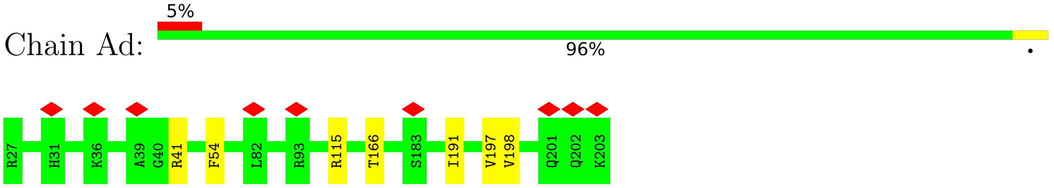
- Molecule 20: MITORIBOSOMAL PROTEIN MS23, MRPS23



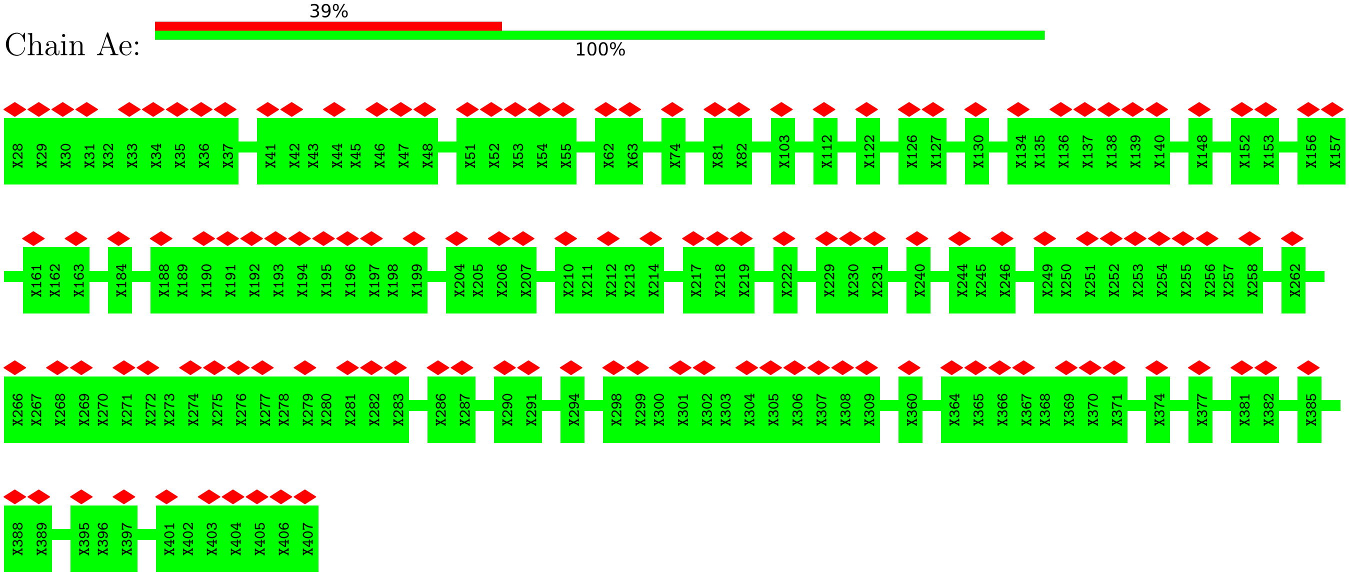
- Molecule 21: MITORIBOSOMAL PROTEIN MS25, MRPS25



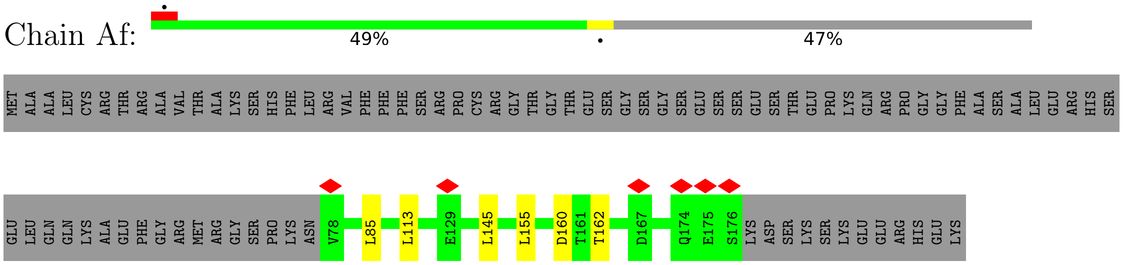
- Molecule 22: MITORIBOSOMAL PROTEIN MS26, MRPS26



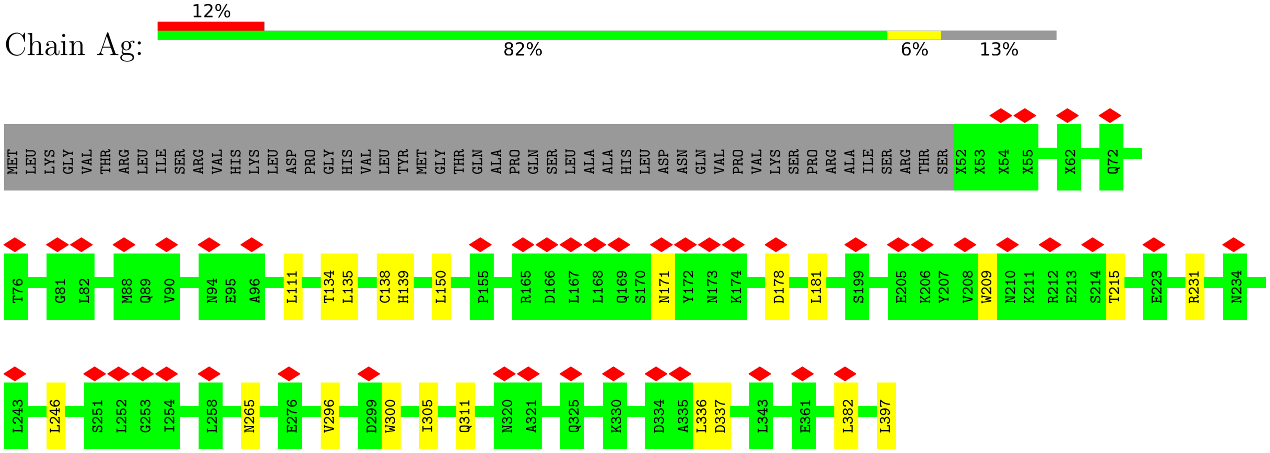
• Molecule 23: MITORIBOSOMAL PROTEIN MS27, MRPS27



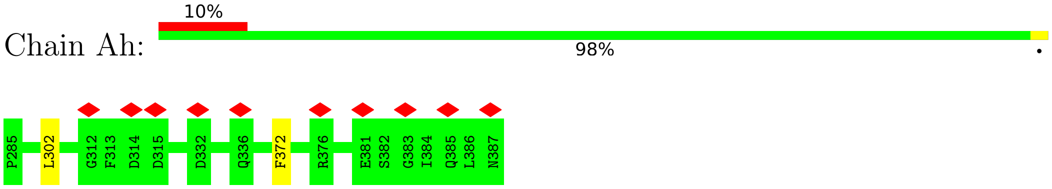
• Molecule 24: MITORIBOSOMAL PROTEIN MS28, MRPS28



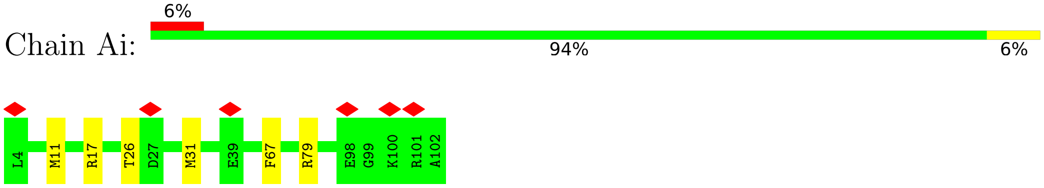
• Molecule 25: MITORIBOSOMAL PROTEIN MS29, MRPS29



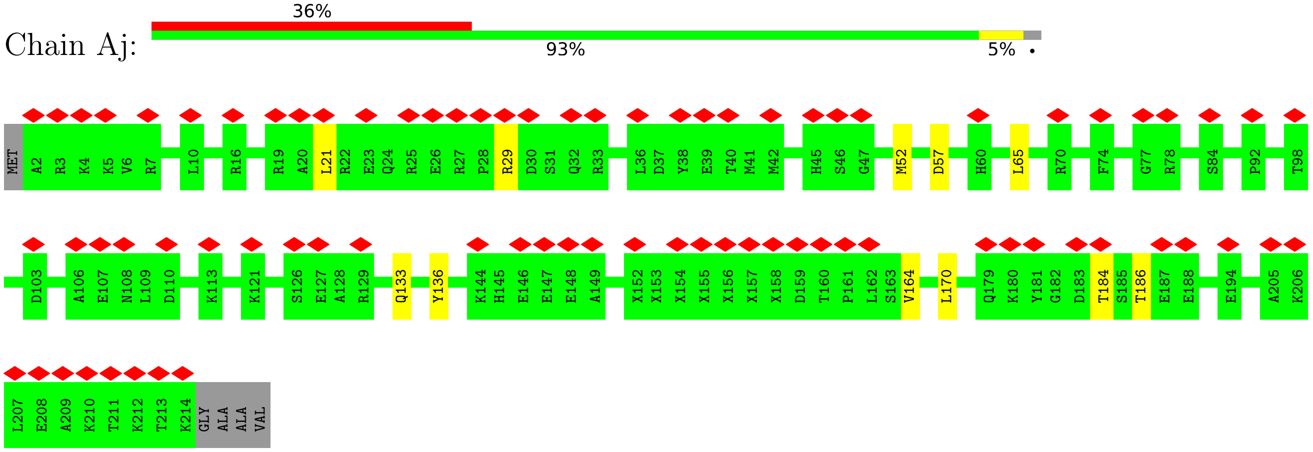
• Molecule 26: MITORIBOSOMAL PROTEIN MS31, MRPS31



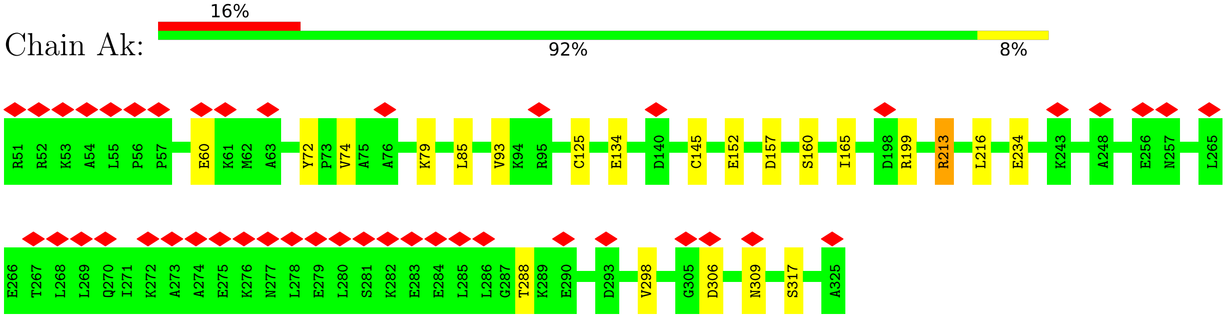
- Molecule 27: MITORIBOSOMAL PROTEIN MS33, MRPS33



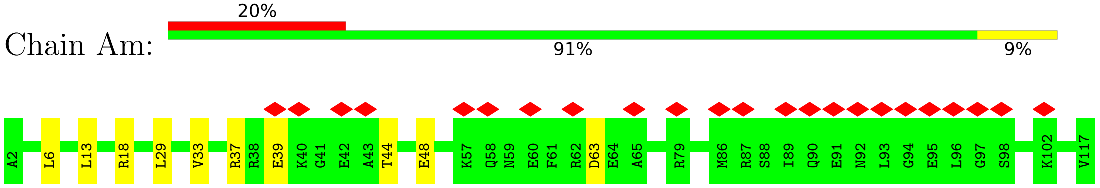
- Molecule 28: MITORIBOSOMAL PROTEIN MS34, MRPS34



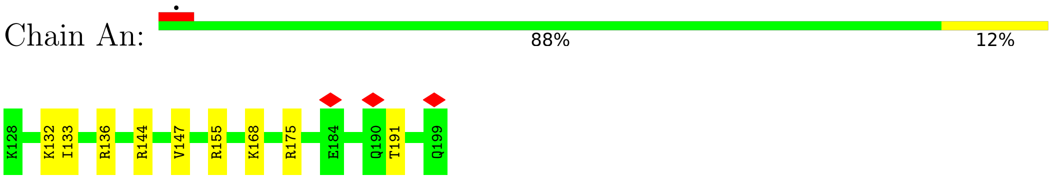
- Molecule 29: MITORIBOSOMAL PROTEIN MS35, MRPS35



- Molecule 30: MITORIBOSOMAL PROTEIN MS37, MRPS37

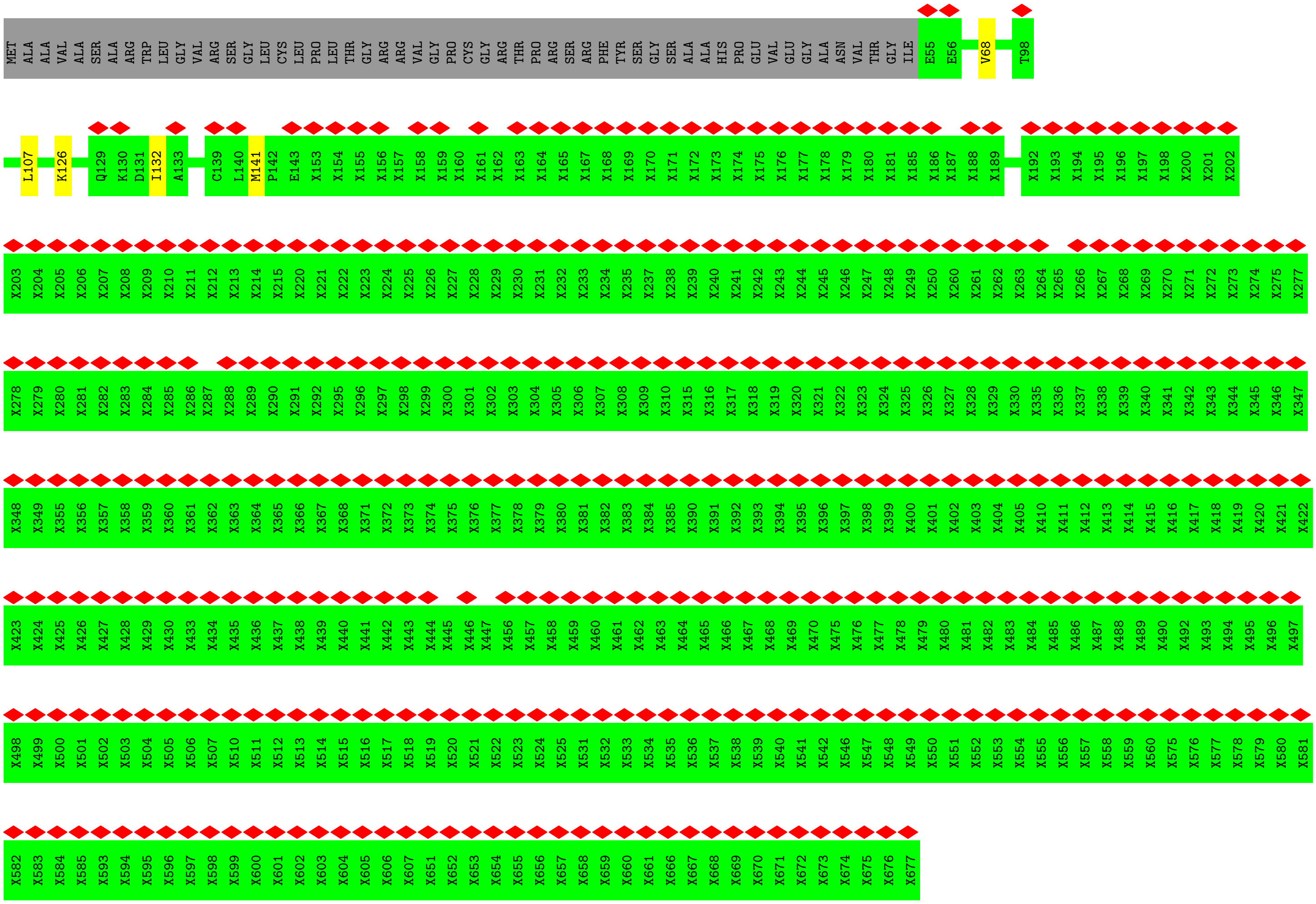


- Molecule 31: MITORIBOSOMAL PROTEIN MS38, MRPS38



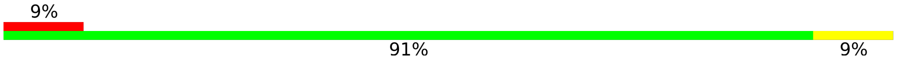
- Molecule 32: MITORIBOSOMAL PROTEIN MS39, MRPS39

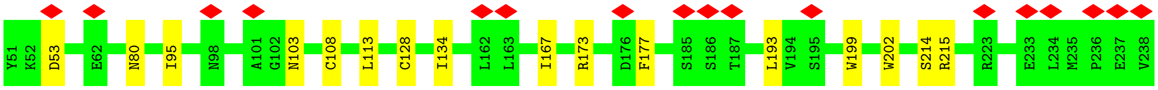
Chain Ao:



- Molecule 33: 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL

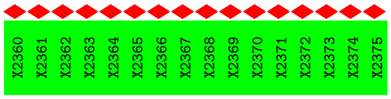
Chain Ap:





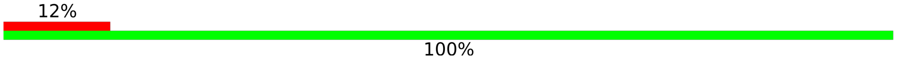
- Molecule 34: UNASSIGNED HELICES

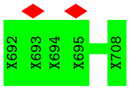
Chain As:



- Molecule 35: UNASSIGNED HELICES

Chain Az:



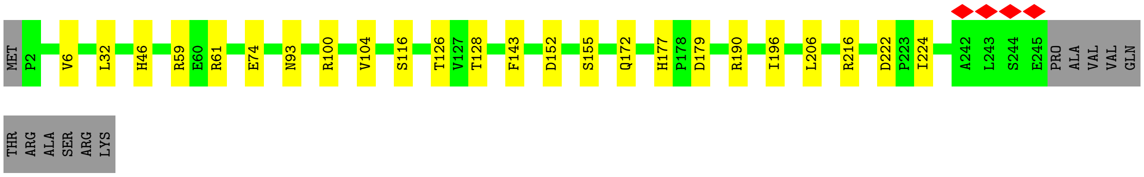


- Molecule 36: MITORIBOSOMAL PROTEIN BL27M, MRPL27

Chain B0:

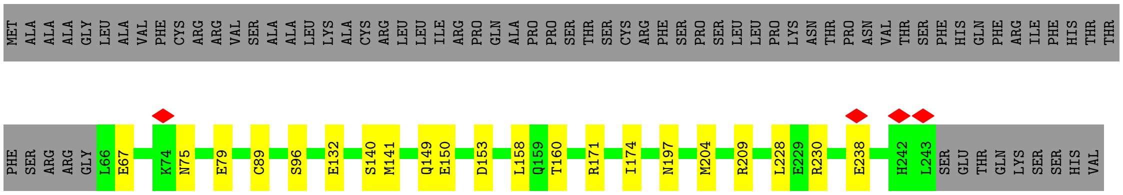
- Molecule 37: MITORIBOSOMAL PROTEIN BL28M, MRPL28

Chain B1:



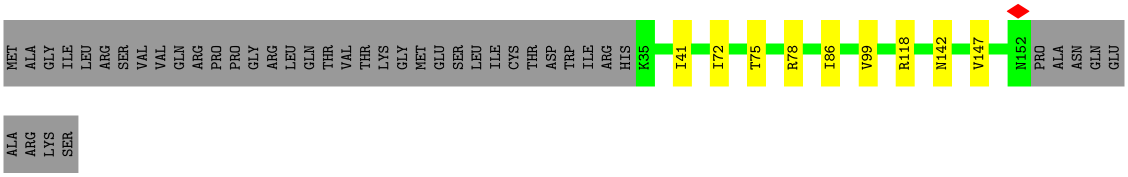
- Molecule 38: MITORIBOSOMAL PROTEIN UL29M, MRPL47

Chain B2:



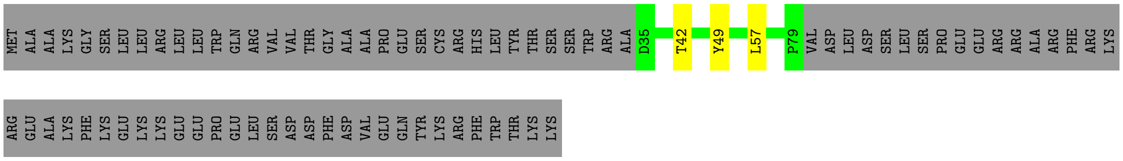
- Molecule 39: MITORIBOSOMAL PROTEIN UL30M, MRPL30

Chain B3:

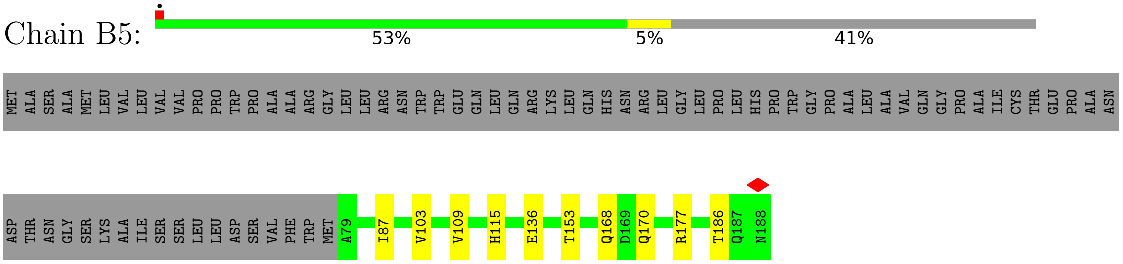


- Molecule 40: MITORIBOSOMAL PROTEIN BL31M, MRPL55

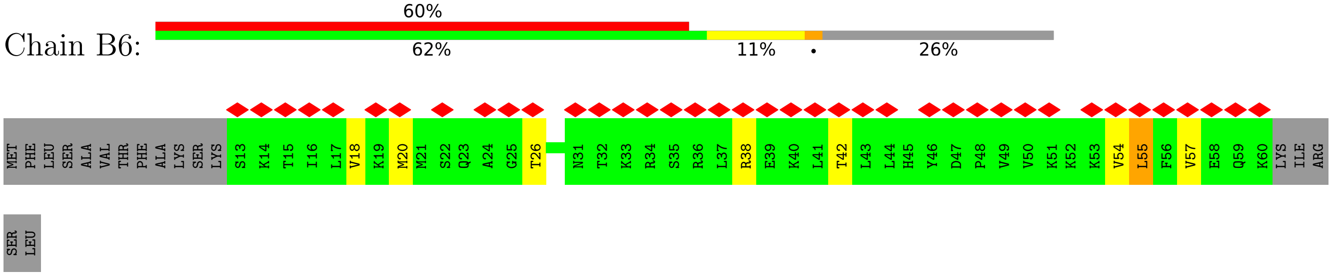
Chain B4:



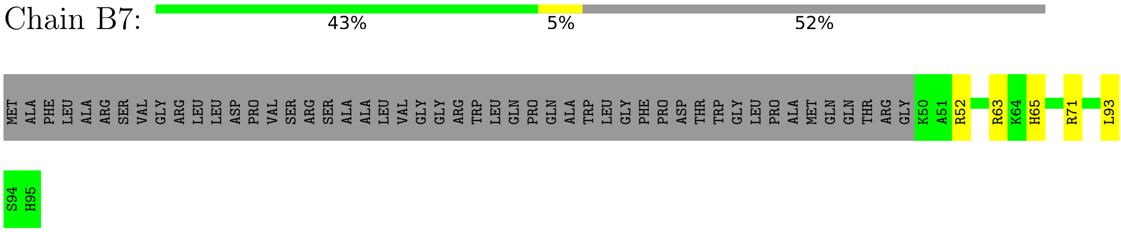
- Molecule 41: MITORIBOSOMAL PROTEIN BL32M, MRPL32



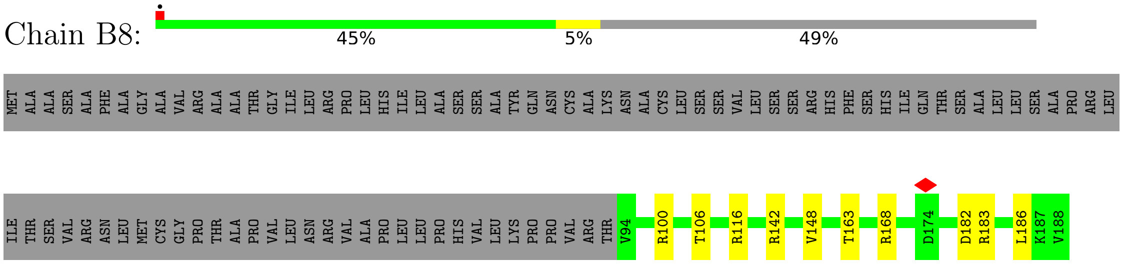
- Molecule 42: MITORIBOSOMAL PROTEIN BL33M, MRPL33



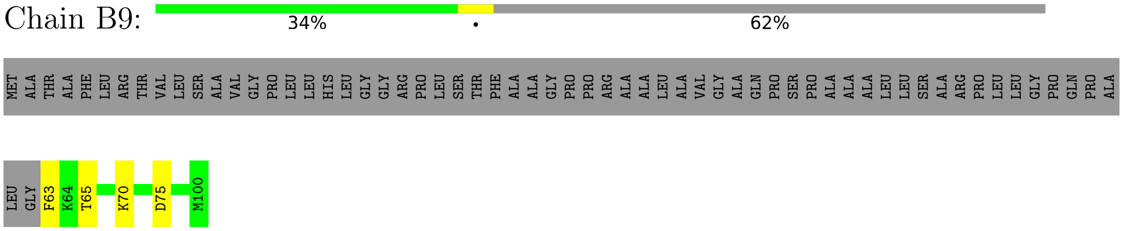
- Molecule 43: MITORIBOSOMAL PROTEIN BL34M, MRPL34



- Molecule 44: MITORIBOSOMAL PROTEIN BL35M, MRPL35

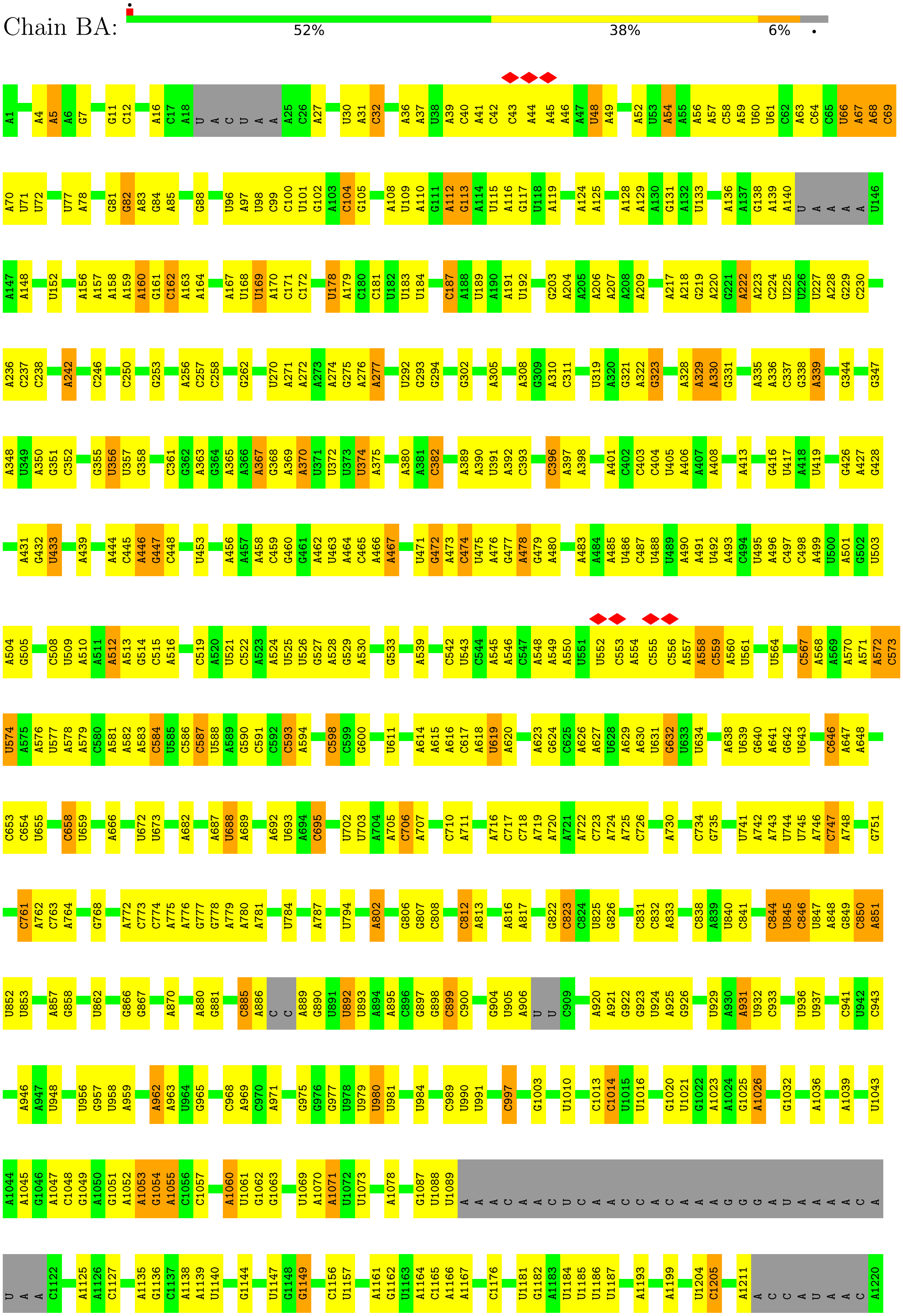


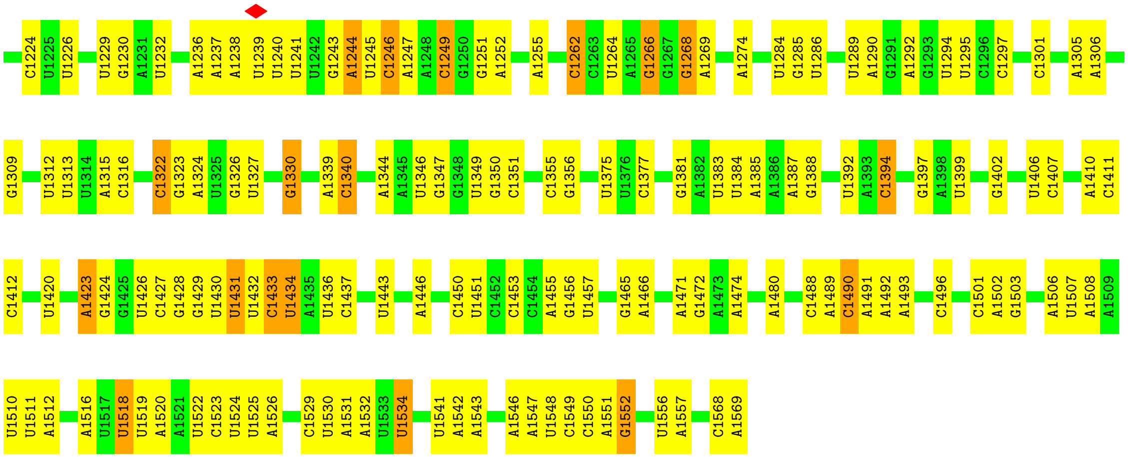
- Molecule 45: MITORIBOSOMAL PROTEIN BL36M, MRPL36



- Molecule 46: MITORIBOSOMAL 16S Ribosomal RNA

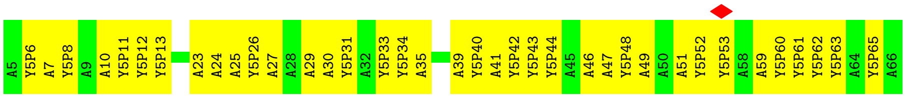
Chain BA:


52%
38%
6%
A1 A4 A5 A6 G7 G11 C12 A16 C17 A18 U A C U A A A25 C26 A27 U30 A31 C32 A36 A37 U38 A39 C40 A41 C42 C43 A44 A45 A46 A47 U48 A49 A52 U53 A54 A55 A56 A57 C58 A59 U60 U61 C62 A63 C64 C65 U66 A67 A68 C69
A70 U71 U72 U77 A78 G81 G82 A83 G84 A85 G88 U96 A97 U98 C99 C100 U101 G102 A103 C104 G105 A108 U109 A110 G111 A112 G113 A114 U115 U116 G117 U118 A119 A124 A125 A128 A129 A130 G131 A132 U133 A136 A137 G138 A139 A140 U A A A A U146
A147 A148 U152 A156 A157 A158 A159 A160 G161 C162 A163 A164 A167 U168 U169 A170 C171 C172 U178 A179 C180 C181 U182 U183 U184 C187 A188 U189 A190 A191 U192 G203 A204 A205 A206 A207 A208 A209 A217 A218 G219 A220 G221 A222 A223 C224 U225 U226 U227 A228 G229 C230
A236 C237 C238 A242 C246 C250 G253 A256 C257 C258 G262 U270 A271 A272 A273 A274 G275 A276 A277 U292 G293 G294 G302 A305 A308 G309 A310 C311 U319 A320 G321 A322 G323 A328 A329 A330 G331 A335 A336 C337 G338 A339 G344 G347
A348 U349 A350 G351 C352 G355 U356 U357 G358 C361 G362 A363 G364 A365 A366 A367 G368 A369 A370 U371 U372 U373 U374 A375 A380 A381 C382 A389 A390 U391 A392 C393 C396 A397 A398 A401 C402 C403 C404 U405 A406 A407 A408 A413 G416 U417 A418 U419 G426 A427 G428
A431 G432 U433 A439 A444 C445 A446 G447 C448 U453 A456 A457 A458 C459 G460 G461 A462 U463 A464 C465 A466 A467 U471 G472 A473 C474 U475 A476 G477 A478 G479 A480 A483 A484 A485 U486 C487 U488 U489 A490 A491 U492 A493 C494 U495 A496 C497 C498 A499 U500 A501 G502 U503
A504 G505 C508 U509 A510 A511 A512 A513 G514 C515 A516 C519 A520 U521 C522 A523 A524 U525 U526 C527 A528 G529 A530 G533 A539 C542 U543 C544 A545 A546 C547 A548 A549 A550 U551 U552 C553 A554 C555 C556 A557 A558 C559 A560 U561 U564 C567 A568 A569 A570 A571 A572 C573
U574 A575 A576 U577 A578 A579 C580 A581 A582 A583 C584 U585 C586 C587 U588 A589 G590 C591 C592 C593 A594 C598 C599 G600 U611 A614 A615 A616 C617 A618 U619 A620 A623 G624 C625 A626 A627 U628 A629 A630 U631 G632 U633 U634 A638 U639 G640 A641 G642 U643 C646 A647 A648
C653 C654 U655 C658 U659 A666 U672 U673 A682 A687 U688 A689 A692 U693 A694 C695 U702 U703 A704 A705 C706 A707 C710 A711 A716 C717 C718 A719 A720 A721 A722 C723 A724 A725 C726 A730 C734 G735 U741 A742 A743 U744 U745 A746 C747 A748 G751
C761 A762 C763 A764 G768 A772 C773 C774 A775 A776 G777 G778 A779 A780 A781 U784 A787 U794 A802 G806 G807 C808 C812 A813 A816 A817 G822 C823 C824 U825 G826 C831 C832 A833 C838 A839 U840 C841 C844 U845 C846 U847 A848 G849 C850 A851
U852 U853 A857 G858 U862 G866 G867 A870 A880 G881 C885 A886 C C A889 G890 U891 U892 U893 A894 A895 C896 G897 G898 C899 C900 G904 U905 A906 U U C909 A920 A921 G922 G923 U924 A925 G926 U929 A930 A931 U932 C933 U936 U937 C941 U942 C943
A946 A947 U948 U956 G957 U958 A959 A962 A963 U964 G965 C968 A969 C970 A971 G975 G976 G977 U978 U979 U980 U981 U984 C989 U990 U991 C997 G1003 U1010 C1013 C1014 U1015 U1016 G1020 U1021 G1022 A1023 A1024 G1025 A1026 G1032 A1036 A1039 U1043
A1044 A1045 G1046 A1047 C1048 G1049 A1050 G1051 A1052 A1053 G1054 A1055 C1056 C1057 A1060 U1061 G1062 G1063 U1069 A1070 A1071 U1072 U1073 A1078 G1087 U1088 U1089 A A A C A A C U C A A C C A C A A A G G A U A A A A C A
U A A C1122 A1125 A1126 C1127 A1135 G1136 C1137 A1138 A1139 U1140 G1144 U1147 G1148 G1149 C1156 U1157 A1161 G1162 U1163 A1164 C1165 A1166 A1167 C1176 U1181 G1182 A1183 U1184 U1185 U1186 U1187 A1193 A1199 U1204 C1205 A1211 A C C A U A A C A1220



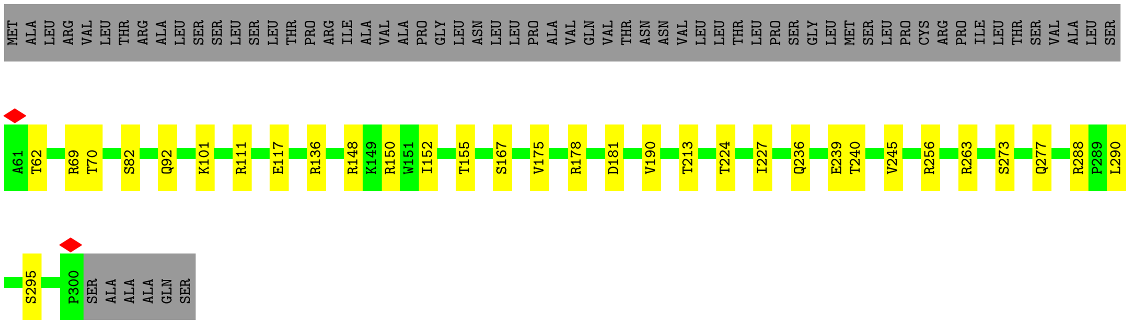
- Molecule 47: MITORIBOSOMAL CP TRNA

Chain BB:



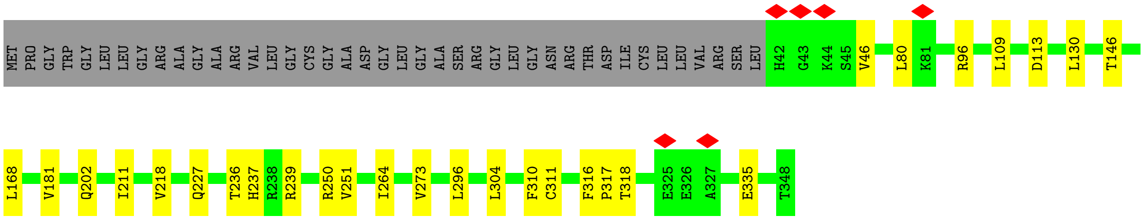
- Molecule 48: MITORIBOSOMAL PROTEIN UL2M, MRPL2

Chain BD:



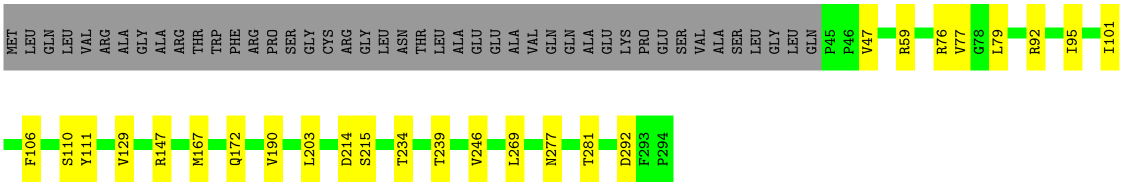
- Molecule 49: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain BE:



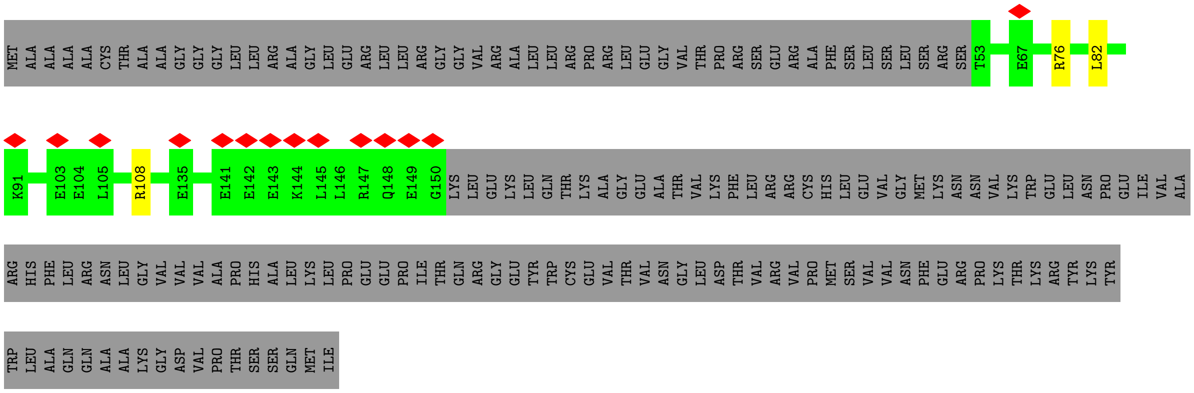
- Molecule 50: MITORIBOSOMAL PROTEIN UL4M, MRPL4

Chain BF:



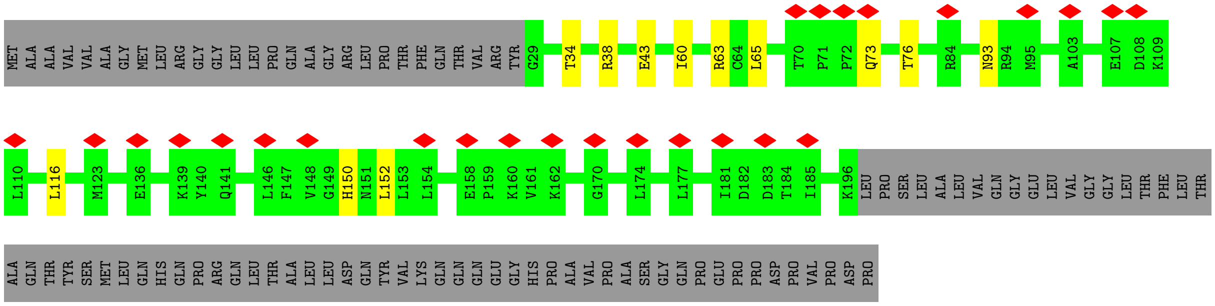
- Molecule 51: MITORIBOSOMAL PROTEIN BL9M, MRPL9

Chain BI:



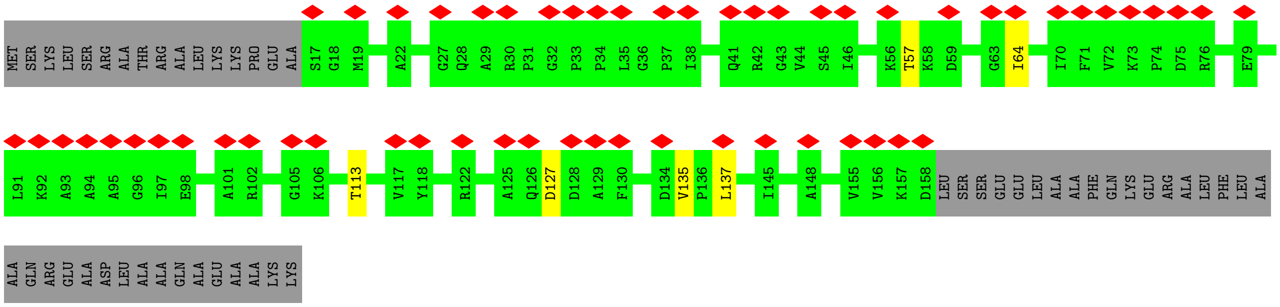
- Molecule 52: MITORIBOSOMAL PROTEIN UL10M, MRPL10

Chain BJ:

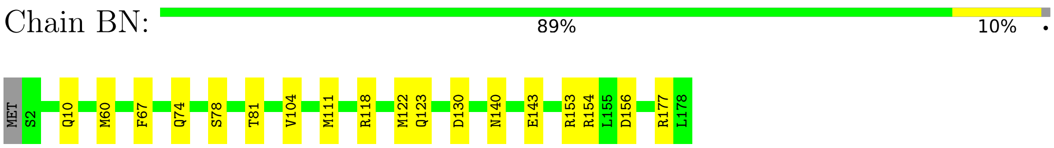


- Molecule 53: MITORIBOSOMAL PROTEIN UL11M, MRPL11

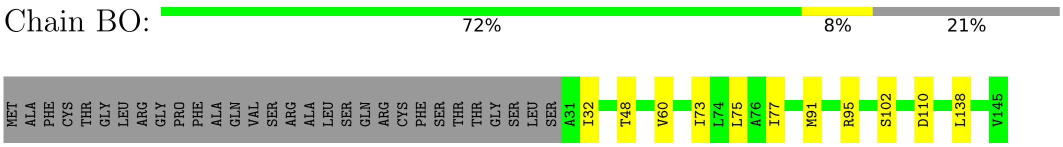
Chain BK:



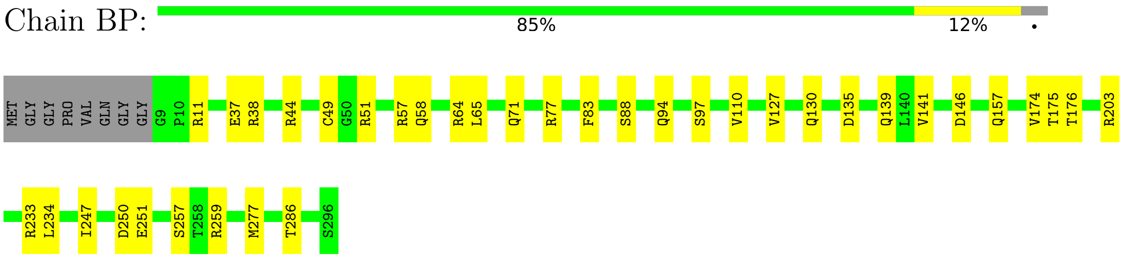
- Molecule 54: MITORIBOSOMAL PROTEIN UL13M, MRPL13



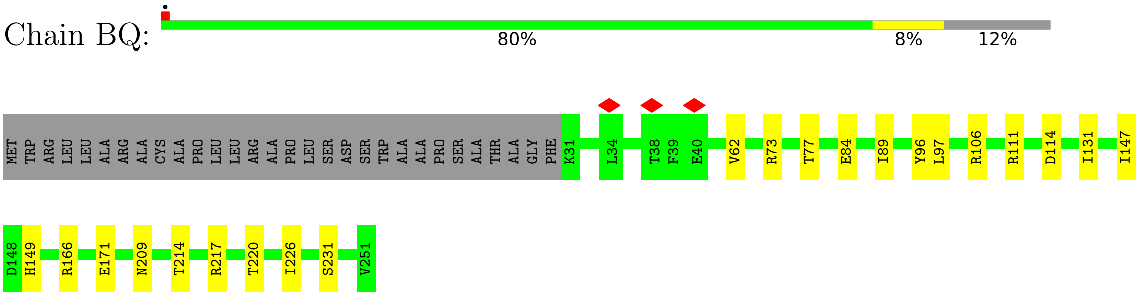
- Molecule 55: MITORIBOSOMAL PROTEIN UL14M, MRPL14



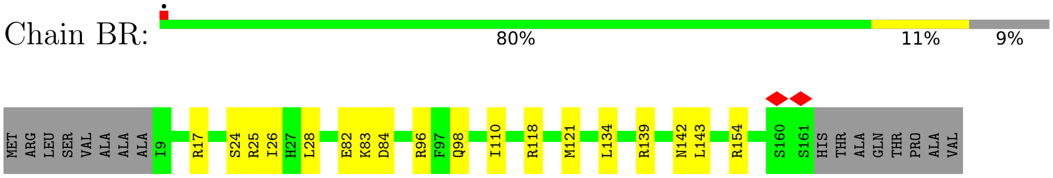
- Molecule 56: MITORIBOSOMAL PROTEIN UL15M, MRPL15



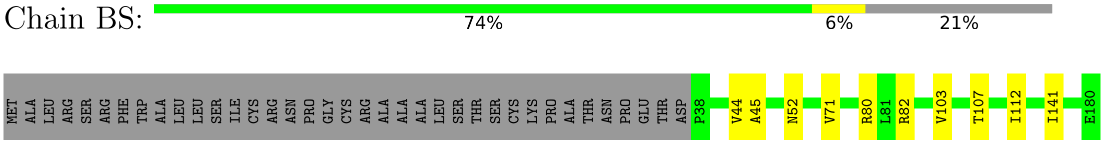
- Molecule 57: MITORIBOSOMAL PROTEIN UL16M, MRPL16



- Molecule 58: MITORIBOSOMAL PROTEIN BL17M, MRPL17

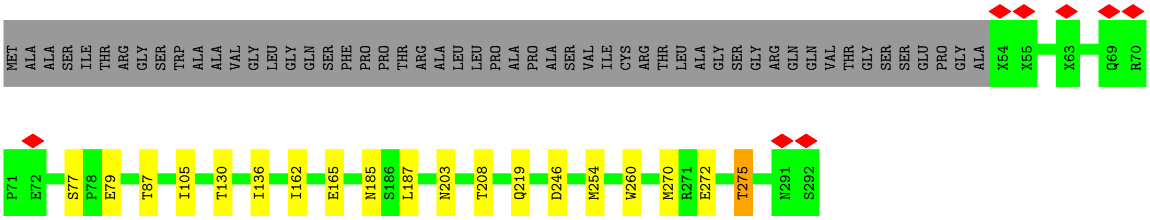


- Molecule 59: MITORIBOSOMAL PROTEIN UL18M, MRPL18



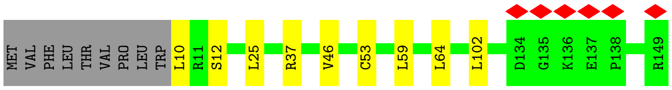
- Molecule 60: MITORIBOSOMAL PROTEIN BL19M, MRPL19

Chain BT:



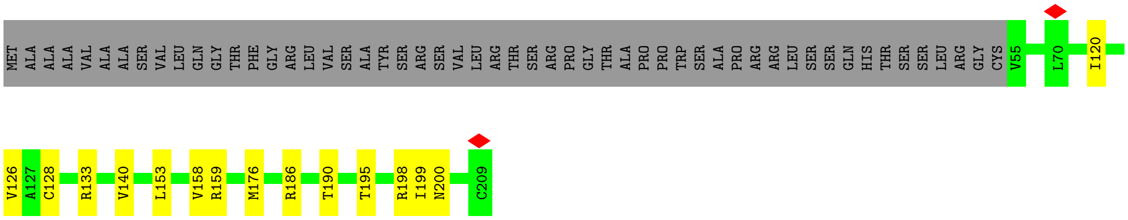
- Molecule 61: MITORIBOSOMAL PROTEIN BL20M, MRPL20

Chain BU:



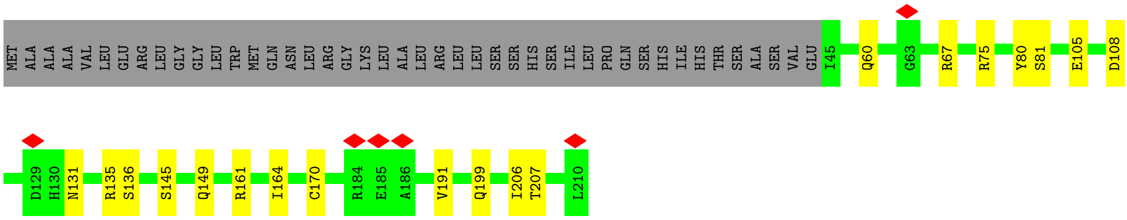
- Molecule 62: MITORIBOSOMAL PROTEIN BL21M, MRPL21

Chain BV:



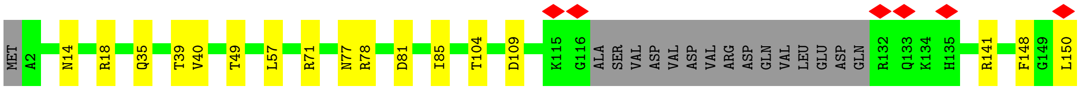
- Molecule 63: MITORIBOSOMAL PROTEIN UL22M, MRPL22

Chain BW:



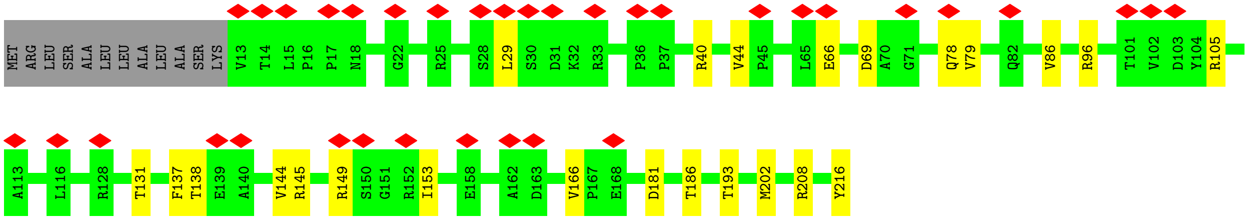
- Molecule 64: MITORIBOSOMAL PROTEIN UL23M, MRPL23

Chain BX:

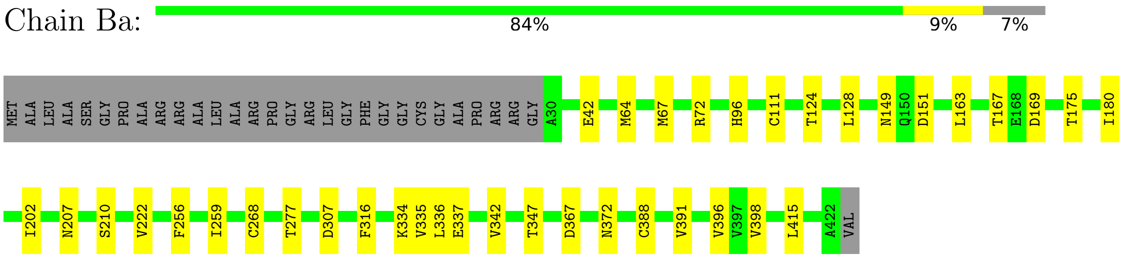


- Molecule 65: MITORIBOSOMAL PROTEIN UL24M, MRPL24

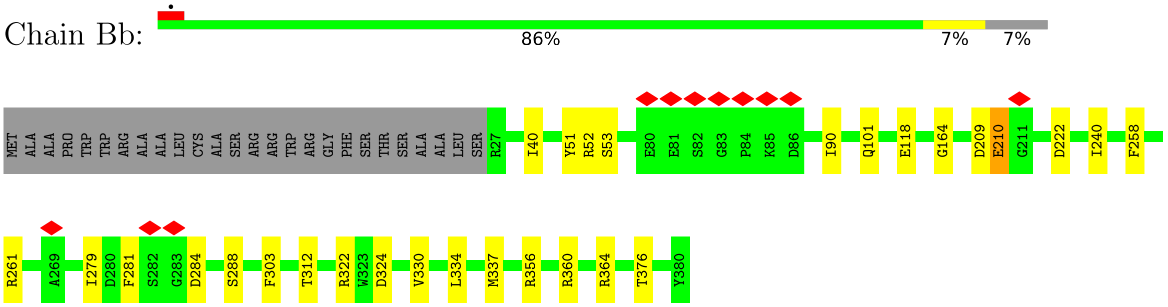
Chain BY:



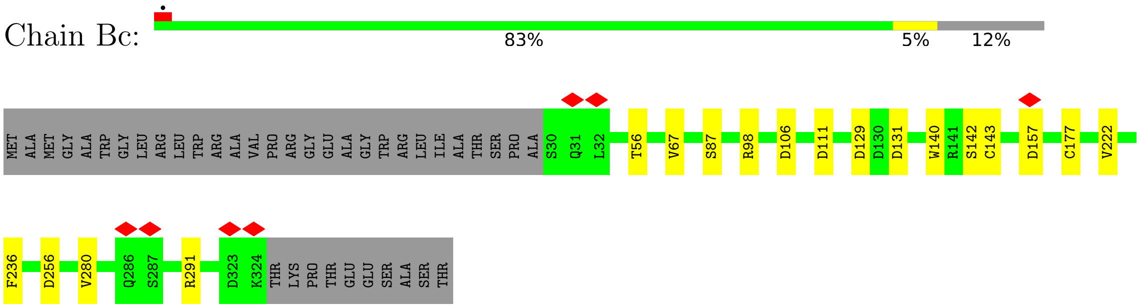
- Molecule 66: MITORIBOSOMAL PROTEIN ML37, MRPL37



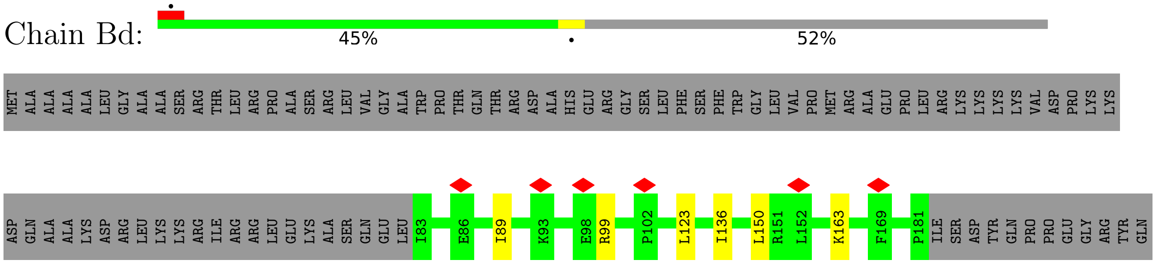
- Molecule 67: MITORIBOSOMAL PROTEIN ML38, MRPL38



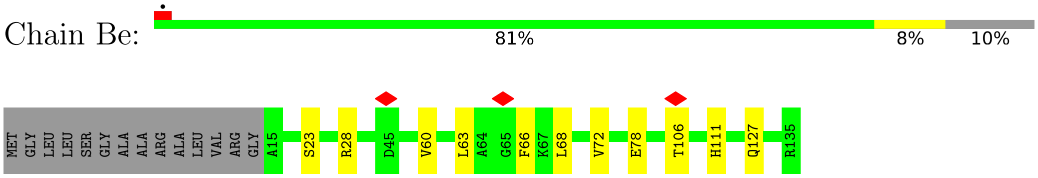
- Molecule 68: MITORIBOSOMAL PROTEIN ML39, MRPL39



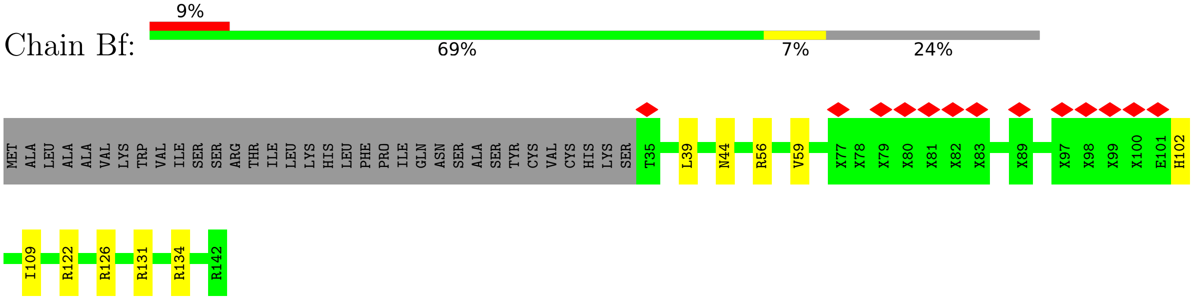
- Molecule 69: MITORIBOSOMAL PROTEIN ML40, MRPL40



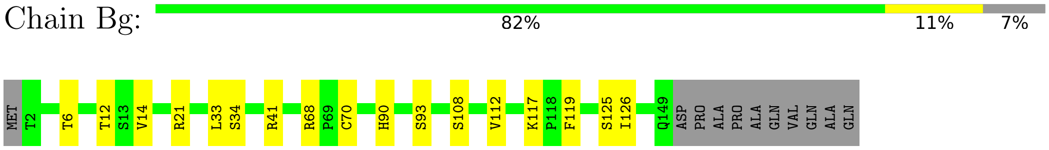
• Molecule 70: MITORIBOSOMAL PROTEIN ML41, MRPL41



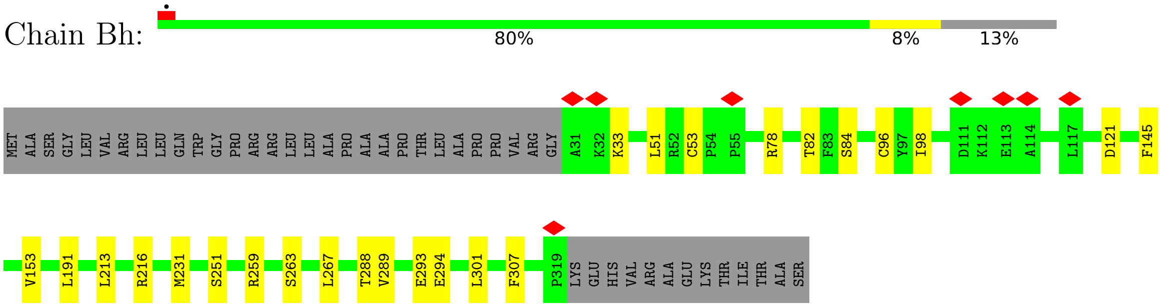
• Molecule 71: MITORIBOSOMAL PROTEIN ML42, MRPL42



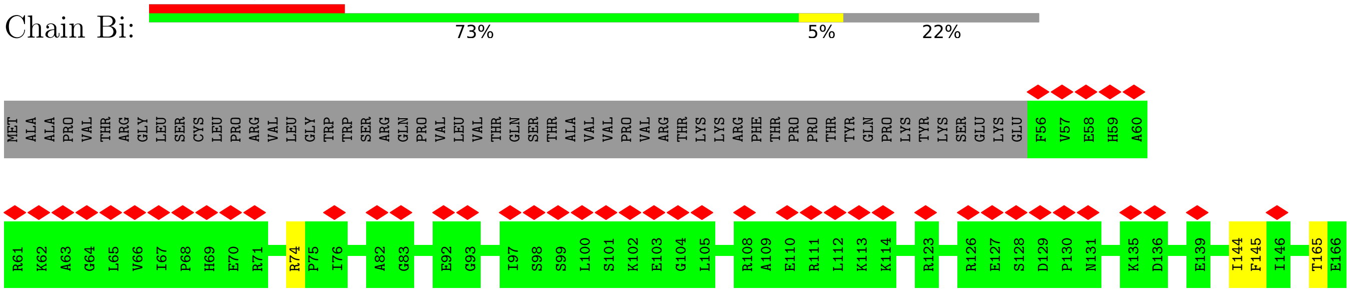
• Molecule 72: MITORIBOSOMAL PROTEIN ML43, MRPL43

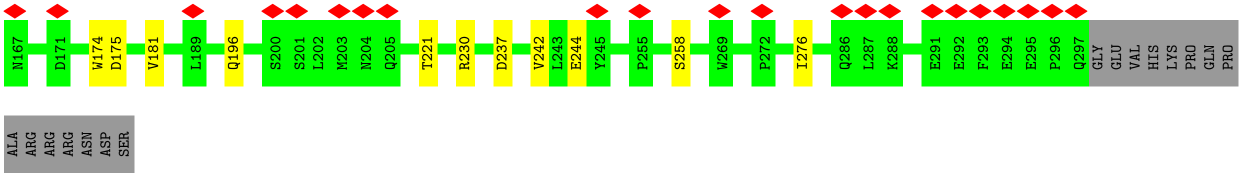


• Molecule 73: MITORIBOSOMAL PROTEIN ML44, MRPL44



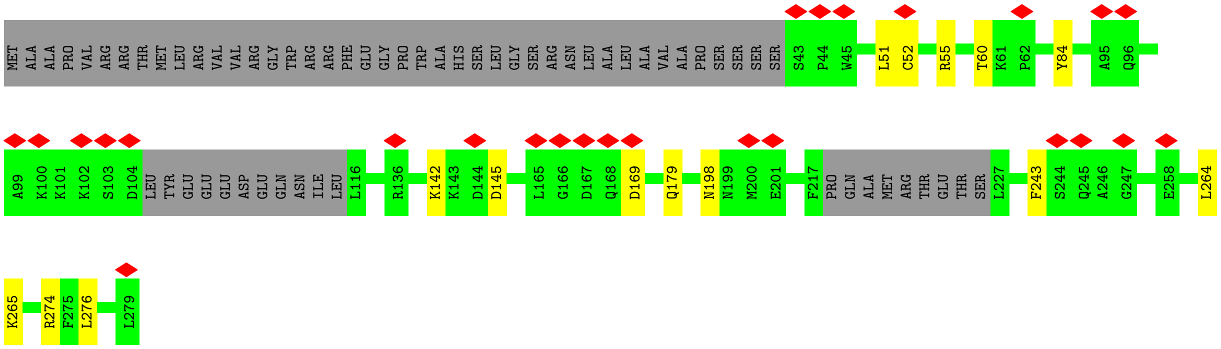
• Molecule 74: MITORIBOSOMAL PROTEIN ML45, MRPL45





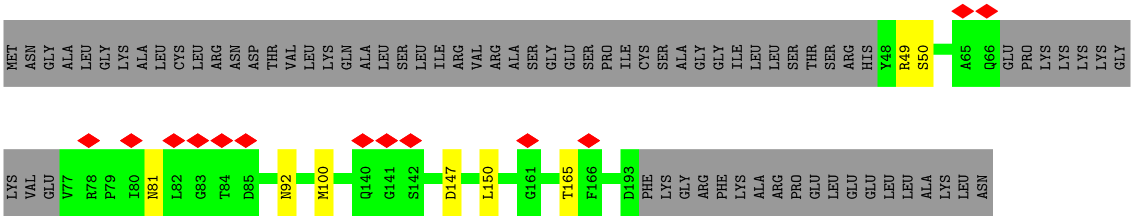
- Molecule 75: MITORIBOSOMAL PROTEIN ML46, MRPL46

Chain Bj:



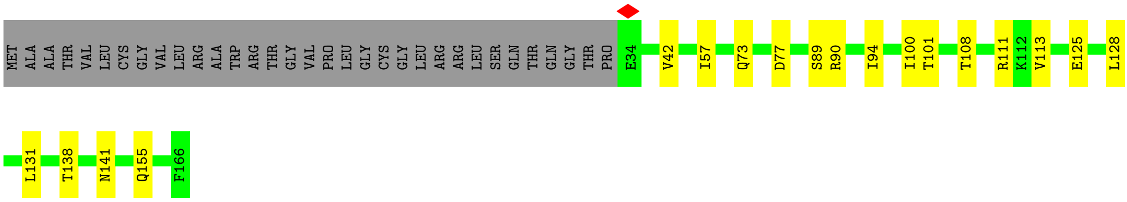
- Molecule 76: MITORIBOSOMAL PROTEIN ML48, MRPL48

Chain Bk:



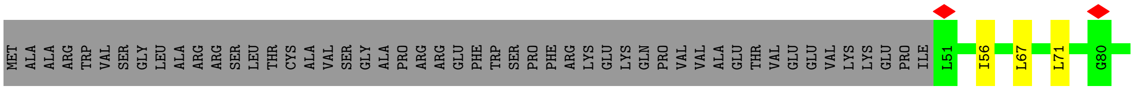
- Molecule 77: MITORIBOSOMAL PROTEIN ML49, MRPL49

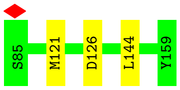
Chain Bl:



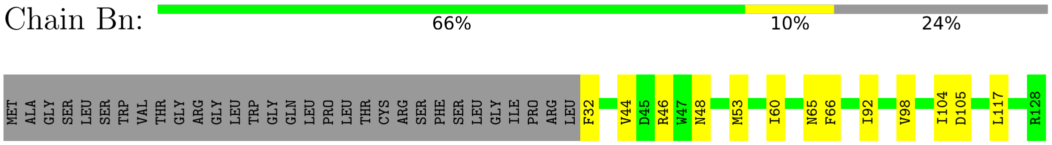
- Molecule 78: MITORIBOSOMAL PROTEIN ML50, MRPL50

Chain Bm:

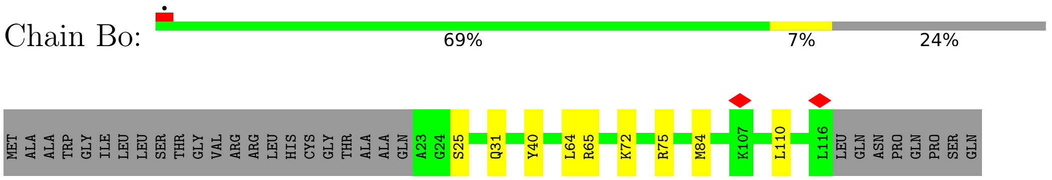




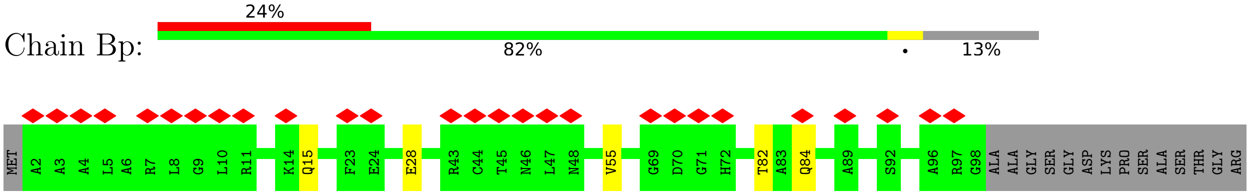
- Molecule 79: MITORIBOSOMAL PROTEIN ML51, MRPL51



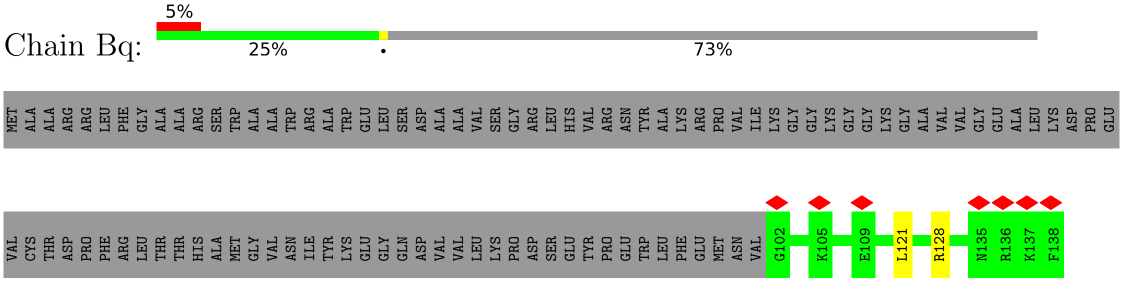
- Molecule 80: MITORIBOSOMAL PROTEIN ML52, MRPL52



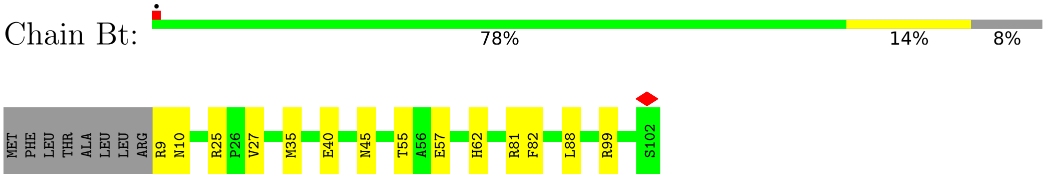
- Molecule 81: MITORIBOSOMAL PROTEIN ML53, MRPL53



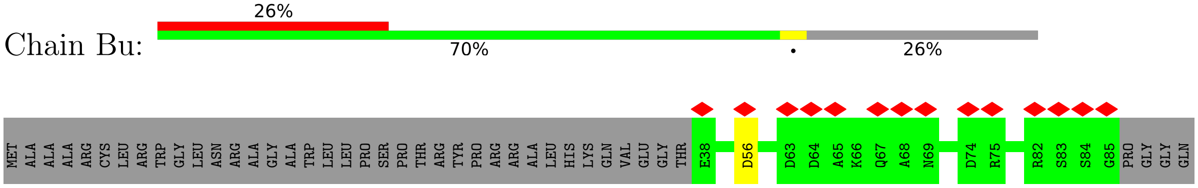
- Molecule 82: MITORIBOSOMAL PROTEIN ML54, MRPL54

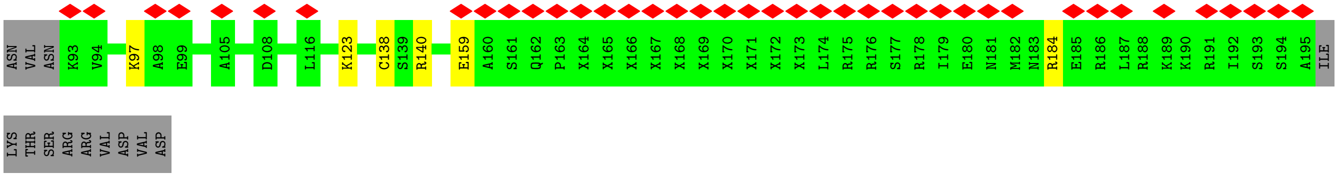


- Molecule 83: MITORIBOSOMAL PROTEIN ML63, MRPL57

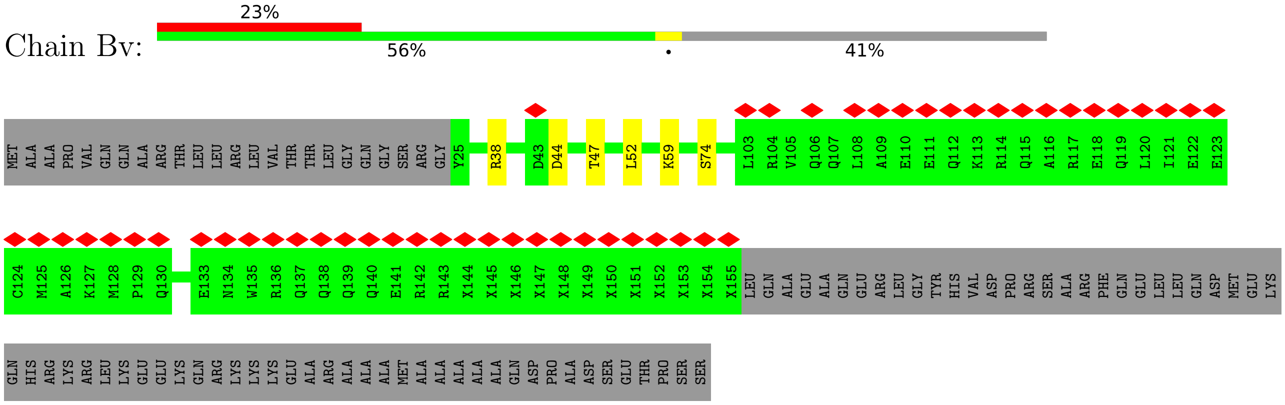


- Molecule 84: MITORIBOSOMAL PROTEIN ML62, MRPL58

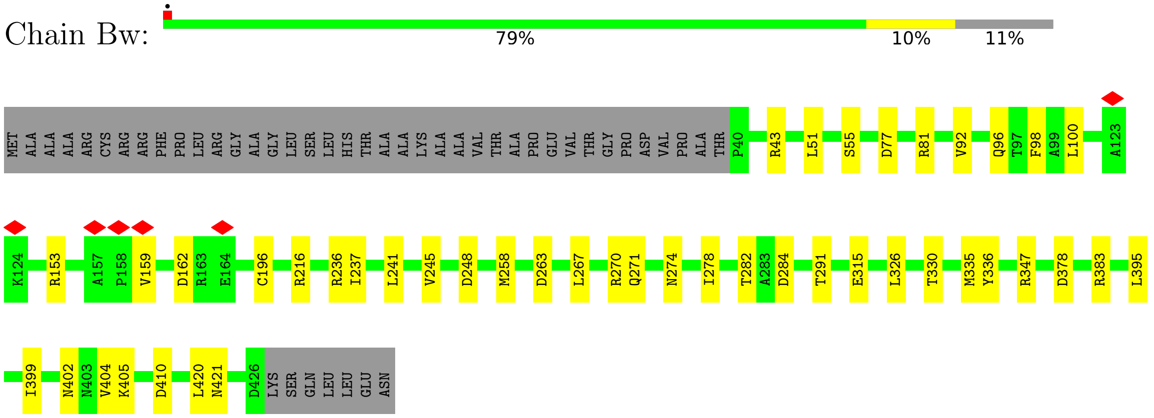




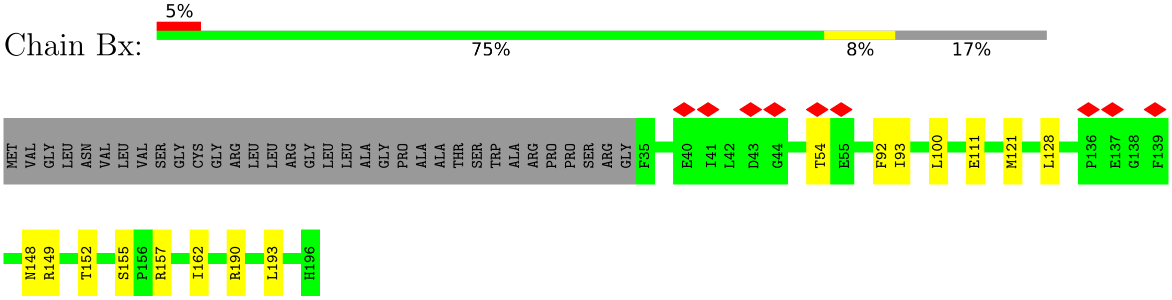
- Molecule 85: MITORIBOSOMAL PROTEIN ML64, MRPL59



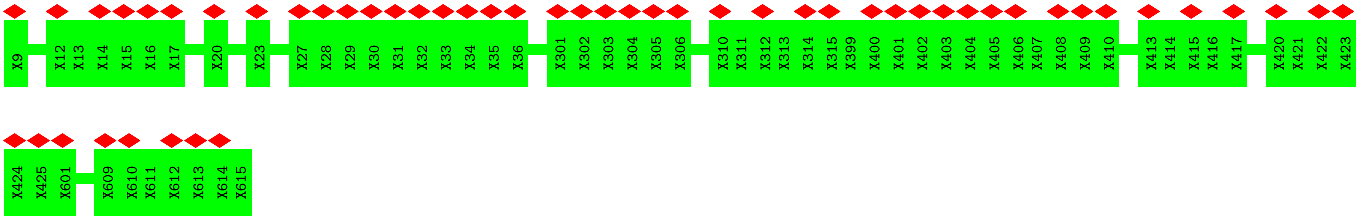
- Molecule 86: MITORIBOSOMAL PROTEIN ML65, MRPS30



- Molecule 87: MITORIBOSOMAL PROTEIN ML66, MRPS18A



- Molecule 88: UNASSIGNED SECONDARY STRUCTURE ELEMENTS


X9
X12
X13
X14
X15
X16
X17
X20
X23
X27
X28
X29
X30
X31
X32
X33
X34
X35
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X420
X421
X422
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X425
X601
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X611
X612
X613
X614
X615

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60872	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	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: P5P, MG, ZN, Y5P, GDP

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	AA	0.47	2/22852 (0.0%)	1.00	23/35580 (0.1%)
2	AB	0.35	0/1804	0.52	0/2445
3	AC	0.32	0/1105	0.53	0/1496
4	AE	0.34	0/2673	0.52	0/3591
5	AF	0.36	0/1008	0.59	0/1358
6	AG	0.34	0/1763	0.49	0/2368
7	AI	0.32	0/2455	0.45	0/3291
8	AJ	0.36	0/1091	0.56	0/1474
9	AK	0.35	0/1021	0.60	0/1381
10	AL	0.31	0/858	0.53	0/1152
11	AN	0.30	0/874	0.46	0/1171
12	AO	0.37	0/1473	0.51	0/1970
13	AP	0.33	0/954	0.49	0/1284
14	AQ	0.34	0/871	0.57	0/1181
15	AR	0.41	1/802 (0.1%)	0.58	0/1079
16	AU	0.37	0/745	0.52	0/993
19	Aa	0.32	0/2052	0.48	0/2774
20	Ab	0.33	0/1126	0.48	0/1514
21	Ac	0.33	0/1399	0.53	0/1881
22	Ad	0.35	0/1490	0.46	0/2005
24	Af	0.33	0/790	0.54	0/1064
25	Ag	0.33	0/2731	0.50	0/3696
26	Ah	0.30	0/903	0.46	0/1215
27	Ai	0.30	0/841	0.48	0/1121
28	Aj	0.30	0/1779	0.53	0/2404
29	Ak	0.31	0/2268	0.49	0/3069
30	Am	0.35	0/947	0.54	0/1268
31	An	0.46	0/650	0.58	0/858
32	Ao	0.31	0/726	0.51	0/988
33	Ap	0.30	0/1602	0.52	0/2175
36	B0	0.54	0/901	0.67	1/1217 (0.1%)
37	B1	0.40	0/2093	0.53	0/2835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	B2	0.42	0/1582	0.56	0/2118
39	B3	0.49	0/993	0.66	0/1341
40	B4	0.29	0/388	0.61	0/523
41	B5	0.45	0/917	0.57	0/1227
42	B6	0.36	0/396	0.62	1/526 (0.2%)
43	B7	0.57	0/395	0.70	0/524
44	B8	0.55	0/853	0.67	0/1136
45	B9	0.59	0/342	0.58	0/450
46	BA	0.81	19/36094 (0.1%)	1.28	247/56186 (0.4%)
48	BD	0.50	0/1898	0.65	0/2555
49	BE	0.46	0/2493	0.66	0/3387
50	BF	0.52	0/2069	0.65	0/2816
51	BI	0.40	0/819	0.58	0/1101
52	BJ	0.36	0/1392	0.56	0/1881
53	BK	0.34	0/1099	0.51	0/1480
54	BN	0.48	0/1487	0.62	0/2017
55	BO	0.49	0/912	0.66	0/1231
56	BP	0.46	0/2368	0.62	0/3198
57	BQ	0.48	0/1838	0.64	1/2475 (0.0%)
58	BR	0.47	0/1262	0.59	0/1700
59	BS	0.42	0/1197	0.59	0/1624
60	BT	0.44	0/1903	0.62	0/2567
61	BU	0.54	0/1179	0.65	0/1578
62	BV	0.51	0/1256	0.65	0/1706
63	BW	0.52	0/1407	0.64	0/1891
64	BX	0.43	0/1149	0.60	0/1554
65	BY	0.34	0/1704	0.56	0/2310
66	Ba	0.39	0/3267	0.58	0/4455
67	Bb	0.39	0/3047	0.59	0/4139
68	Bc	0.36	0/2464	0.54	0/3330
69	Bd	0.32	0/853	0.53	0/1153
70	Be	0.42	0/996	0.60	0/1340
71	Bf	0.42	0/731	0.60	0/990
72	Bg	0.47	0/1191	0.64	0/1614
73	Bh	0.42	0/2372	0.58	0/3211
74	Bi	0.35	0/2034	0.53	0/2759
75	Bj	0.31	0/1811	0.52	0/2436
76	Bk	0.39	0/1108	0.58	0/1499
77	Bl	0.43	0/1135	0.60	0/1549
78	Bm	0.33	0/917	0.52	0/1248
79	Bn	0.57	0/860	0.72	1/1150 (0.1%)
80	Bo	0.45	0/762	0.59	0/1022
81	Bp	0.32	0/752	0.54	0/1013

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\lvert Z\rvert$ >5	RMSZ	#$\lvert Z\rvert$ >5
82	Bq	0.32	0/346	0.44	0/463
83	Bt	0.49	0/798	0.67	0/1073
84	Bu	0.32	0/1163	0.50	0/1557
85	Bv	0.37	0/1022	0.45	0/1382
86	Bw	0.44	0/3206	0.61	0/4354
87	Bx	0.43	0/1364	0.63	0/1849
All	All	0.53	22/166238 (0.0%)	0.86	274/236586 (0.1%)

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
9	AK	0	1
49	BE	0	1
57	BQ	0	1
60	BT	0	1
67	Bb	0	2
79	Bn	0	1
83	Bt	0	1
All	All	0	8

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BA	1255	A	N9-C4	-8.31	1.32	1.37
46	BA	1410	A	N9-C4	-7.55	1.33	1.37
46	BA	52	A	N9-C4	-7.33	1.33	1.37
46	BA	85	A	N9-C4	-6.79	1.33	1.37
46	BA	1047	A	N9-C4	-6.50	1.33	1.37

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	BA	374	U	N3-C2-O2	-11.16	114.39	122.20
1	AA	846	C	C6-N1-C2	-9.81	116.38	120.30
46	BA	374	U	N1-C2-O2	9.67	129.57	122.80
46	BA	12	C	C6-N1-C2	-9.04	116.68	120.30
46	BA	81	G	N3-C4-C5	-9.01	124.09	128.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AK	194	ARG	Peptide
49	BE	316	PHE	Peptide
57	BQ	149	HIS	Peptide
60	BT	275	THR	Peptide
67	Bb	164	GLY	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	AB	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
3	AC	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
4	AE	324/328 (99%)	305 (94%)	18 (6%)	1 (0%)	37	69
5	AF	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
6	AG	206/208 (99%)	203 (98%)	3 (2%)	0	100	100
7	AI	291/311 (94%)	283 (97%)	8 (3%)	0	100	100
8	AJ	127/201 (63%)	119 (94%)	6 (5%)	2 (2%)	8	36
9	AK	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
10	AL	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
11	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
13	AP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
14	AQ	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
15	AR	95/97 (98%)	91 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AU	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
19	Aa	243/356 (68%)	238 (98%)	4 (2%)	1 (0%)	30	63
20	Ab	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	Ac	167/169 (99%)	157 (94%)	9 (5%)	1 (1%)	22	55
22	Ad	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
24	Af	97/188 (52%)	90 (93%)	7 (7%)	0	100	100
25	Ag	327/397 (82%)	317 (97%)	10 (3%)	0	100	100
26	Ah	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
27	Ai	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
28	Aj	204/218 (94%)	194 (95%)	10 (5%)	0	100	100
29	Ak	273/275 (99%)	265 (97%)	7 (3%)	1 (0%)	30	63
30	Am	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
31	An	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
32	Ao	87/530 (16%)	83 (95%)	4 (5%)	0	100	100
33	Ap	186/188 (99%)	175 (94%)	11 (6%)	0	100	100
36	B0	112/148 (76%)	109 (97%)	3 (3%)	0	100	100
37	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
38	B2	176/252 (70%)	167 (95%)	9 (5%)	0	100	100
39	B3	116/161 (72%)	112 (97%)	4 (3%)	0	100	100
40	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
41	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
42	B6	46/65 (71%)	45 (98%)	1 (2%)	0	100	100
43	B7	44/95 (46%)	44 (100%)	0	0	100	100
44	B8	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
45	B9	36/100 (36%)	36 (100%)	0	0	100	100
48	BD	238/306 (78%)	228 (96%)	10 (4%)	0	100	100
49	BE	305/348 (88%)	278 (91%)	24 (8%)	3 (1%)	13	44
50	BF	248/294 (84%)	232 (94%)	16 (6%)	0	100	100
51	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
52	BJ	166/262 (63%)	158 (95%)	8 (5%)	0	100	100
53	BK	140/192 (73%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BN	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
55	BO	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
56	BP	286/296 (97%)	273 (96%)	13 (4%)	0	100	100
57	BQ	219/251 (87%)	218 (100%)	1 (0%)	0	100	100
58	BR	151/169 (89%)	145 (96%)	6 (4%)	0	100	100
59	BS	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	19	52
60	BT	223/292 (76%)	216 (97%)	7 (3%)	0	100	100
61	BU	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
62	BV	153/209 (73%)	146 (95%)	7 (5%)	0	100	100
63	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
64	BX	130/150 (87%)	126 (97%)	4 (3%)	0	100	100
65	BY	202/216 (94%)	190 (94%)	12 (6%)	0	100	100
66	Ba	391/423 (92%)	374 (96%)	17 (4%)	0	100	100
67	Bb	352/380 (93%)	330 (94%)	21 (6%)	1 (0%)	37	69
68	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100
69	Bd	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
70	Be	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
71	Bf	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
72	Bg	146/159 (92%)	138 (94%)	8 (6%)	0	100	100
73	Bh	287/332 (86%)	269 (94%)	18 (6%)	0	100	100
74	Bi	240/312 (77%)	227 (95%)	12 (5%)	1 (0%)	30	63
75	Bj	211/279 (76%)	198 (94%)	12 (6%)	1 (0%)	25	58
76	Bk	132/212 (62%)	125 (95%)	7 (5%)	0	100	100
77	Bl	131/166 (79%)	130 (99%)	1 (1%)	0	100	100
78	Bm	107/159 (67%)	102 (95%)	5 (5%)	0	100	100
79	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
80	Bo	92/124 (74%)	88 (96%)	4 (4%)	0	100	100
81	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
82	Bq	35/138 (25%)	34 (97%)	1 (3%)	0	100	100
83	Bt	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
84	Bu	137/205 (67%)	129 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
85	Bv	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
86	Bw	385/433 (89%)	359 (93%)	25 (6%)	1 (0%)	37	69
87	Bx	160/196 (82%)	154 (96%)	5 (3%)	1 (1%)	22	55
All	All	12706/16216 (78%)	12149 (96%)	542 (4%)	15 (0%)	50	79

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	BE	264	ILE
86	Bw	159	VAL
87	Bx	93	ILE
8	AJ	179	GLN
8	AJ	185	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/187 (100%)	168 (90%)	19 (10%)	6	24
3	AC	115/115 (100%)	101 (88%)	14 (12%)	4	19
4	AE	273/273 (100%)	245 (90%)	28 (10%)	6	23
5	AF	108/109 (99%)	99 (92%)	9 (8%)	9	32
6	AG	181/181 (100%)	169 (93%)	12 (7%)	14	38
7	AI	250/250 (100%)	236 (94%)	14 (6%)	17	43
8	AJ	119/181 (66%)	107 (90%)	12 (10%)	6	24
9	AK	102/102 (100%)	89 (87%)	13 (13%)	3	19
10	AL	92/92 (100%)	82 (89%)	10 (11%)	5	22
11	AN	92/114 (81%)	79 (86%)	13 (14%)	3	17
12	AO	159/205 (78%)	155 (98%)	4 (2%)	42	62
13	AP	97/97 (100%)	93 (96%)	4 (4%)	26	50
14	AQ	94/94 (100%)	87 (93%)	7 (7%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AR	89/89 (100%)	83 (93%)	6 (7%)	13	38
16	AU	77/77 (100%)	65 (84%)	12 (16%)	2	14
19	Aa	222/272 (82%)	207 (93%)	15 (7%)	13	38
20	Ab	113/162 (70%)	106 (94%)	7 (6%)	15	40
21	Ac	152/152 (100%)	138 (91%)	14 (9%)	7	28
22	Ad	149/149 (100%)	142 (95%)	7 (5%)	22	46
24	Af	86/160 (54%)	80 (93%)	6 (7%)	12	37
25	Ag	290/334 (87%)	268 (92%)	22 (8%)	11	34
26	Ah	95/95 (100%)	93 (98%)	2 (2%)	48	66
27	Ai	86/86 (100%)	80 (93%)	6 (7%)	12	37
28	Aj	182/184 (99%)	171 (94%)	11 (6%)	16	41
29	Ak	249/249 (100%)	227 (91%)	22 (9%)	8	30
30	Am	100/100 (100%)	90 (90%)	10 (10%)	6	24
31	An	66/66 (100%)	57 (86%)	9 (14%)	3	17
32	Ao	79/118 (67%)	74 (94%)	5 (6%)	15	40
33	Ap	168/168 (100%)	152 (90%)	16 (10%)	7	26
36	B0	92/115 (80%)	83 (90%)	9 (10%)	6	25
37	B1	219/229 (96%)	195 (89%)	24 (11%)	5	22
38	B2	164/228 (72%)	143 (87%)	21 (13%)	3	18
39	B3	110/147 (75%)	101 (92%)	9 (8%)	9	32
40	B4	42/114 (37%)	39 (93%)	3 (7%)	12	36
41	B5	99/163 (61%)	89 (90%)	10 (10%)	6	24
42	B6	45/60 (75%)	37 (82%)	8 (18%)	1	10
43	B7	41/78 (53%)	36 (88%)	5 (12%)	4	19
44	B8	87/162 (54%)	77 (88%)	10 (12%)	4	21
45	B9	36/77 (47%)	32 (89%)	4 (11%)	5	21
48	BD	193/248 (78%)	161 (83%)	32 (17%)	2	12
49	BE	263/290 (91%)	239 (91%)	24 (9%)	7	28
50	BF	217/251 (86%)	191 (88%)	26 (12%)	4	19
51	BI	88/228 (39%)	85 (97%)	3 (3%)	32	55
52	BJ	154/230 (67%)	142 (92%)	12 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BK	115/151 (76%)	109 (95%)	6 (5%)	19	44
54	BN	156/157 (99%)	138 (88%)	18 (12%)	4	21
55	BO	99/123 (80%)	88 (89%)	11 (11%)	5	21
56	BP	245/249 (98%)	208 (85%)	37 (15%)	2	14
57	BQ	189/210 (90%)	170 (90%)	19 (10%)	6	24
58	BR	132/143 (92%)	114 (86%)	18 (14%)	3	17
59	BS	123/153 (80%)	114 (93%)	9 (7%)	11	36
60	BT	206/243 (85%)	187 (91%)	19 (9%)	7	28
61	BU	118/127 (93%)	109 (92%)	9 (8%)	11	34
62	BV	136/178 (76%)	121 (89%)	15 (11%)	5	22
63	BW	144/180 (80%)	125 (87%)	19 (13%)	3	18
64	BX	119/134 (89%)	102 (86%)	17 (14%)	2	16
65	BY	183/192 (95%)	159 (87%)	24 (13%)	3	18
66	Ba	348/365 (95%)	310 (89%)	38 (11%)	5	22
67	Bb	310/328 (94%)	283 (91%)	27 (9%)	8	30
68	Bc	271/299 (91%)	253 (93%)	18 (7%)	14	38
69	Bd	92/181 (51%)	86 (94%)	6 (6%)	14	39
70	Be	100/108 (93%)	89 (89%)	11 (11%)	5	22
71	Bf	80/110 (73%)	70 (88%)	10 (12%)	3	19
72	Bg	128/136 (94%)	111 (87%)	17 (13%)	3	18
73	Bh	251/284 (88%)	226 (90%)	25 (10%)	6	24
74	Bi	218/281 (78%)	204 (94%)	14 (6%)	14	39
75	Bj	190/242 (78%)	176 (93%)	14 (7%)	11	35
76	Bk	119/181 (66%)	111 (93%)	8 (7%)	13	38
77	Bl	122/147 (83%)	104 (85%)	18 (15%)	2	15
78	Bm	103/145 (71%)	97 (94%)	6 (6%)	17	42
79	Bn	88/113 (78%)	77 (88%)	11 (12%)	3	19
80	Bo	74/97 (76%)	65 (88%)	9 (12%)	4	19
81	Bp	79/88 (90%)	74 (94%)	5 (6%)	15	40
82	Bq	36/114 (32%)	34 (94%)	2 (6%)	17	43
83	Bt	75/82 (92%)	62 (83%)	13 (17%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	Bu	126/169 (75%)	119 (94%)	7 (6%)	17	43
85	Bv	102/173 (59%)	96 (94%)	6 (6%)	16	41
86	Bw	340/373 (91%)	296 (87%)	44 (13%)	3	18
87	Bx	149/173 (86%)	135 (91%)	14 (9%)	7	27
All	All	11288/13510 (84%)	10215 (90%)	1073 (10%)	9	26

5 of 1073 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
75	Bj	264	LEU
77	Bl	138	THR
75	Bj	243	PHE
86	Bw	282	THR
39	B3	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 246 such sidechains are listed below:

Mol	Chain	Res	Type
49	BE	197	HIS
81	Bp	72	HIS
57	BQ	98	HIS
80	Bo	63	GLN
86	Bw	226	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	959/962 (99%)	308 (32%)	7 (0%)
17	AV	0/69	-	-
17	AY	0/69	-	-
18	AX	0/13	-	-
46	BA	1508/1570 (96%)	620 (41%)	30 (1%)
47	BB	0/51	-	-
All	All	2467/2734 (90%)	928 (37%)	37 (1%)

5 of 928 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	A
1	AA	10	U
1	AA	11	G
1	AA	14	C
1	AA	18	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	BA	583	A
46	BA	1431	U
46	BA	653	C
46	BA	936	U
46	BA	112	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	Y5P	AY	69	-	14,19,20	2.70	2 (14%)	18,26,29	1.20	2 (11%)
47	P5P	BB	49	47	16,23,24	1.39	2 (12%)	14,33,36	2.02	2 (14%)
47	P5P	BB	10	47	16,23,24	1.30	3 (18%)	14,33,36	1.93	2 (14%)
17	Y5P	AY	10	-	14,19,20	2.65	2 (14%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	24	-	14,19,20	2.69	2 (14%)	18,26,29	1.03	1 (5%)
47	Y5P	BB	13	47	14,19,20	2.21	1 (7%)	18,26,29	1.22	1 (5%)
17	Y5P	AY	65	-	14,19,20	2.72	2 (14%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	71	-	14,19,20	2.67	2 (14%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	68	-	14,19,20	3.57	1 (7%)	18,26,29	0.80	1 (5%)
17	Y5P	AY	60	-	14,19,20	2.26	1 (7%)	18,26,29	0.98	1 (5%)
17	Y5P	AY	67	-	14,19,20	3.71	1 (7%)	18,26,29	0.92	0
47	P5P	BB	58	47	16,23,24	0.77	0	14,33,36	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	Y5P	BB	12	47	14,19,20	2.20	1 (7%)	18,26,29	0.96	1 (5%)
47	Y5P	BB	11	47	14,19,20	3.78	2 (14%)	18,26,29	0.75	0
47	P5P	BB	36	47	16,23,24	0.81	0	14,33,36	0.83	0
17	Y5P	AY	43	-	14,19,20	3.64	1 (7%)	18,26,29	0.83	1 (5%)
17	Y5P	AY	49	-	14,19,20	3.60	1 (7%)	18,26,29	0.83	2 (11%)
17	Y5P	AY	21	-	14,19,20	2.70	2 (14%)	18,26,29	1.04	1 (5%)
17	P5P	AY	35	-	16,23,24	0.81	0	14,33,36	0.79	0
17	P5P	AY	36	-	16,23,24	0.80	0	14,33,36	0.97	0
17	P5P	AY	76	46	16,23,24	0.75	0	14,33,36	0.77	1 (7%)
17	Y5P	AY	15	-	14,19,20	2.68	2 (14%)	18,26,29	1.12	2 (11%)
17	Y5P	AV	72	-	14,19,20	3.68	2 (14%)	18,26,29	0.81	0
47	Y5P	BB	44	47	14,19,20	2.42	1 (7%)	18,26,29	0.95	1 (5%)
17	Y5P	AV	63	-	14,19,20	2.67	2 (14%)	18,26,29	1.02	1 (5%)
47	P5P	BB	23	47	16,23,24	0.78	1 (6%)	14,33,36	1.48	2 (14%)
17	Y5P	AY	7	-	14,19,20	2.67	2 (14%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	57	-	14,19,20	2.69	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AY	55	-	14,19,20	2.52	1 (7%)	18,26,29	1.12	2 (11%)
17	Y5P	AY	66	-	14,19,20	2.29	1 (7%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	15	-	14,19,20	2.67	2 (14%)	18,26,29	0.99	1 (5%)
17	Y5P	AV	67	-	14,19,20	3.65	1 (7%)	18,26,29	0.89	0
17	Y5P	AV	68	-	14,19,20	3.65	1 (7%)	18,26,29	0.81	0
18	Y5P	AX	24	-	14,19,20	2.29	1 (7%)	18,26,29	0.92	1 (5%)
17	Y5P	AV	43	-	14,19,20	3.71	2 (14%)	18,26,29	0.75	0
17	Y5P	AV	11	-	14,19,20	3.56	1 (7%)	18,26,29	0.88	1 (5%)
17	Y5P	AY	22	-	14,19,20	2.67	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	11	-	14,19,20	3.63	1 (7%)	18,26,29	0.80	0
17	Y5P	AV	45	-	14,19,20	2.32	1 (7%)	18,26,29	0.94	1 (5%)
47	P5P	BB	66	47	16,23,24	0.79	0	14,33,36	0.80	0
17	P5P	AY	34	-	16,23,24	1.36	3 (18%)	14,33,36	2.02	2 (14%)
17	Y5P	AY	44	-	14,19,20	2.72	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	52	-	14,19,20	2.68	2 (14%)	18,26,29	1.10	1 (5%)
17	Y5P	AY	40	-	14,19,20	3.72	1 (7%)	18,26,29	0.84	2 (11%)
17	Y5P	AY	37	-	14,19,20	2.72	2 (14%)	18,26,29	1.05	1 (5%)
18	Y5P	AX	12	-	14,16,20	2.19	1 (7%)	18,22,29	1.00	1 (5%)
17	Y5P	AV	60	-	14,19,20	2.35	1 (7%)	18,26,29	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	Y5P	AY	72	-	14,19,20	3.64	2 (14%)	18,26,29	0.81	0
17	Y5P	AV	58	-	14,19,20	2.71	2 (14%)	18,26,29	1.09	1 (5%)
47	P5P	BB	32	47	16,23,24	0.80	0	14,33,36	0.83	0
17	Y5P	AY	6	-	14,19,20	2.67	2 (14%)	18,26,29	1.04	1 (5%)
18	Y5P	AX	16	-	14,19,20	2.34	1 (7%)	18,26,29	1.05	1 (5%)
18	Y5P	AX	18	-	14,19,20	3.69	1 (7%)	18,26,29	0.80	0
47	Y5P	BB	63	47	14,19,20	3.70	1 (7%)	18,26,29	0.82	1 (5%)
17	Y5P	AY	62	-	14,19,20	3.68	2 (14%)	18,26,29	0.86	1 (5%)
17	Y5P	AY	9	-	14,19,20	2.66	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	69	-	14,19,20	2.70	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AV	37	-	14,19,20	2.71	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	5	-	14,19,20	2.66	2 (14%)	18,26,29	1.08	1 (5%)
17	Y5P	AY	70	-	14,19,20	2.74	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	8	-	14,19,20	2.26	1 (7%)	18,26,29	1.01	1 (5%)
17	Y5P	AY	2	-	14,19,20	3.53	2 (14%)	18,26,29	0.81	1 (5%)
17	Y5P	AV	57	-	14,19,20	2.78	2 (14%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	40	-	14,19,20	3.75	1 (7%)	18,26,29	0.84	0
17	Y5P	AV	55	-	14,19,20	2.33	1 (7%)	18,26,29	1.05	1 (5%)
17	Y5P	AV	29	-	14,19,20	2.59	2 (14%)	18,26,29	1.16	1 (5%)
17	Y5P	AV	66	-	14,19,20	2.28	1 (7%)	18,26,29	1.01	1 (5%)
17	Y5P	AY	39	-	14,19,20	2.29	1 (7%)	18,26,29	1.02	1 (5%)
47	P5P	BB	9	47	16,23,24	0.76	0	14,33,36	0.82	0
17	Y5P	AV	41	-	14,19,20	3.91	1 (7%)	18,26,29	0.76	0
17	Y5P	AV	64	-	14,19,20	2.75	2 (14%)	18,26,29	1.02	1 (5%)
47	P5P	BB	14	47	16,23,24	0.76	0	14,33,36	0.86	0
17	Y5P	AV	3	-	14,19,20	3.74	1 (7%)	18,26,29	0.79	0
17	Y5P	AY	45	-	14,19,20	2.42	1 (7%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	51	-	14,19,20	2.29	1 (7%)	18,26,29	1.00	1 (5%)
47	P5P	BB	39	47	16,23,24	0.81	0	14,33,36	0.78	1 (7%)
17	Y5P	AY	29	-	14,19,20	2.67	2 (14%)	18,26,29	1.06	1 (5%)
47	P5P	BB	64	47	16,23,24	0.77	0	14,33,36	0.79	0
17	Y5P	AV	38	-	14,19,20	2.66	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AY	58	-	14,19,20	2.67	2 (14%)	18,26,29	1.10	1 (5%)
17	Y5P	AY	13	-	14,19,20	3.59	1 (7%)	18,26,29	0.82	2 (11%)
17	Y5P	AY	48	-	14,19,20	3.69	1 (7%)	18,26,29	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	Y5P	AV	61	-	14,19,20	3.66	1 (7%)	18,26,29	0.83	0
17	Y5P	AV	73	-	14,19,20	2.75	2 (14%)	18,26,29	1.33	3 (16%)
17	Y5P	AV	44	-	14,19,20	2.74	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AV	14	-	14,19,20	2.75	2 (14%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	39	-	14,19,20	2.39	1 (7%)	18,26,29	1.04	1 (5%)
47	Y5P	BB	34	47	14,19,20	2.29	1 (7%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	12	-	14,19,20	2.30	1 (7%)	18,26,29	0.99	1 (5%)
47	P5P	BB	37	47	16,23,24	0.82	0	14,33,36	0.94	0
47	P5P	BB	28	47	16,23,24	0.77	0	14,33,36	0.72	0
17	Y5P	AY	25	-	14,19,20	3.69	1 (7%)	18,26,29	0.80	1 (5%)
18	Y5P	AX	20	-	14,19,20	2.37	1 (7%)	18,26,29	1.02	1 (5%)
47	P5P	BB	38	47	16,23,24	0.82	0	14,33,36	0.82	0
17	Y5P	AY	38	-	14,19,20	2.69	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	6	-	14,19,20	2.67	2 (14%)	18,26,29	1.01	1 (5%)
17	Y5P	AV	26	-	14,19,20	2.71	2 (14%)	18,26,29	1.05	1 (5%)
47	P5P	BB	41	47	16,23,24	1.37	3 (18%)	14,33,36	2.11	2 (14%)
17	Y5P	AV	59	-	14,19,20	2.37	1 (7%)	18,26,29	0.98	1 (5%)
17	Y5P	AV	62	-	14,19,20	3.63	1 (7%)	18,26,29	0.83	2 (11%)
47	Y5P	BB	31	47	14,19,20	3.79	1 (7%)	18,26,29	0.78	1 (5%)
47	Y5P	BB	65	47	14,19,20	2.35	1 (7%)	18,26,29	1.07	1 (5%)
47	P5P	BB	15	47	16,23,24	0.76	0	14,33,36	0.73	0
47	P5P	BB	50	47	16,23,24	0.83	0	14,33,36	0.86	0
17	Y5P	AV	27	-	14,19,20	2.76	2 (14%)	18,26,29	1.11	2 (11%)
17	Y5P	AV	5	-	14,19,20	2.73	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	30	-	14,19,20	2.71	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	1	-	14,16,20	2.69	2 (14%)	18,22,29	1.04	1 (5%)
17	Y5P	AY	31	-	14,19,20	2.71	2 (14%)	18,26,29	1.01	1 (5%)
47	Y5P	BB	33	47	14,19,20	3.76	1 (7%)	18,26,29	0.84	2 (11%)
17	Y5P	AY	71	-	14,19,20	2.72	2 (14%)	18,26,29	1.11	1 (5%)
47	Y5P	BB	43	47	14,19,20	3.60	1 (7%)	18,26,29	0.92	2 (11%)
17	Y5P	AV	28	-	14,19,20	2.68	2 (14%)	18,26,29	1.01	1 (5%)
47	P5P	BB	47	47	16,23,24	0.73	0	14,33,36	0.92	1 (7%)
17	Y5P	AV	75	-	14,19,20	3.69	1 (7%)	18,26,29	0.82	2 (11%)
17	Y5P	AV	31	-	14,19,20	2.70	2 (14%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	32	-	14,19,20	2.42	1 (7%)	18,26,29	0.97	1 (5%)
17	Y5P	AY	50	-	14,19,20	2.37	1 (7%)	18,26,29	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	Y5P	AV	21	-	14,19,20	2.79	2 (14%)	18,26,29	1.13	1 (5%)
17	Y5P	AY	51	-	14,19,20	2.22	1 (7%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	4	-	14,19,20	3.63	1 (7%)	18,26,29	0.85	1 (5%)
17	Y5P	AY	33	-	14,19,20	2.54	1 (7%)	18,26,29	1.02	1 (5%)
17	Y5P	AY	63	-	14,19,20	2.68	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	25	-	14,19,20	3.69	2 (14%)	18,26,29	0.77	0
17	Y5P	AY	26	-	14,19,20	2.76	2 (14%)	18,26,29	1.03	1 (5%)
47	P5P	BB	35	47	16,23,24	1.41	2 (12%)	14,33,36	2.02	2 (14%)
17	Y5P	AY	59	-	14,19,20	2.31	1 (7%)	18,26,29	0.97	1 (5%)
17	Y5P	AY	24	-	14,19,20	2.68	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AY	27	-	14,19,20	2.70	2 (14%)	18,26,29	1.18	2 (11%)
17	Y5P	AV	2	-	14,19,20	3.81	1 (7%)	18,26,29	0.72	0
17	Y5P	AY	73	-	14,19,20	2.79	2 (14%)	18,26,29	1.44	3 (16%)
17	Y5P	AV	42	-	14,19,20	3.84	1 (7%)	18,26,29	0.72	0
17	Y5P	AV	32	-	14,19,20	2.32	1 (7%)	18,26,29	0.96	1 (5%)
17	Y5P	AY	14	-	14,19,20	2.67	2 (14%)	18,26,29	0.98	1 (5%)
17	P5P	AV	34	-	16,23,24	1.47	3 (18%)	14,33,36	2.10	2 (14%)
47	P5P	BB	25	47	16,23,24	1.46	3 (18%)	14,33,36	2.01	3 (21%)
17	P5P	AV	76	46	16,23,24	0.71	0	14,33,36	0.78	1 (7%)
17	Y5P	AY	61	-	14,19,20	3.68	1 (7%)	18,26,29	0.83	1 (5%)
47	P5P	BB	7	47	16,23,24	1.33	3 (18%)	14,33,36	2.03	2 (14%)
47	P5P	BB	27	47	16,23,24	0.79	1 (6%)	14,33,36	0.89	0
17	Y5P	AY	30	-	14,19,20	2.68	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	33	-	14,19,20	2.71	1 (7%)	18,26,29	0.91	1 (5%)
47	Y5P	BB	53	47	14,19,20	3.68	1 (7%)	18,26,29	0.84	1 (5%)
18	Y5P	AX	19	-	14,19,20	2.41	1 (7%)	18,26,29	0.94	1 (5%)
17	Y5P	AV	4	-	14,19,20	3.72	1 (7%)	18,26,29	0.77	1 (5%)
18	Y5P	AX	21	-	14,19,20	3.83	1 (7%)	18,26,29	0.87	0
18	Y5P	AX	14	-	14,19,20	2.27	1 (7%)	18,26,29	0.96	1 (5%)
17	Y5P	AY	53	-	14,19,20	2.67	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	3	-	14,19,20	3.52	1 (7%)	18,26,29	0.91	2 (11%)
47	P5P	BB	30	47	16,23,24	1.33	2 (12%)	14,33,36	1.85	2 (14%)
17	Y5P	AV	8	-	14,19,20	2.32	1 (7%)	18,26,29	1.09	1 (5%)
17	Y5P	AY	28	-	14,19,20	2.69	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	52	-	14,19,20	2.65	2 (14%)	18,26,29	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	Y5P	AV	53	-	14,19,20	2.67	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AY	56	-	14,19,20	3.60	1 (7%)	18,26,29	0.79	1 (5%)
17	Y5P	AV	49	-	14,19,20	3.54	1 (7%)	18,26,29	0.82	1 (5%)
18	Y5P	AX	23	-	14,19,20	2.17	1 (7%)	18,26,29	0.99	1 (5%)
17	Y5P	AV	54	-	14,19,20	2.25	1 (7%)	18,26,29	1.00	1 (5%)
17	Y5P	AV	48	-	14,19,20	3.75	1 (7%)	18,26,29	0.94	1 (5%)
47	P5P	BB	46	47	16,23,24	1.27	2 (12%)	14,33,36	1.86	2 (14%)
17	Y5P	AY	41	-	14,19,20	3.70	1 (7%)	18,26,29	0.85	2 (11%)
17	Y5P	AY	64	-	14,19,20	2.74	2 (14%)	18,26,29	1.09	1 (5%)
47	Y5P	BB	61	47	14,19,20	2.21	1 (7%)	18,26,29	0.98	1 (5%)
47	P5P	BB	45	47	16,23,24	0.79	0	14,33,36	0.74	0
17	P5P	AV	36	-	16,23,24	0.82	0	14,33,36	0.77	1 (7%)
17	Y5P	AV	10	-	14,19,20	2.65	2 (14%)	18,26,29	1.10	1 (5%)
47	Y5P	BB	42	47	14,19,20	3.66	1 (7%)	18,26,29	0.87	1 (5%)
17	Y5P	AV	65	-	14,19,20	2.70	2 (14%)	18,26,29	1.04	1 (5%)
47	Y5P	BB	8	47	14,19,20	2.26	1 (7%)	18,26,29	1.06	1 (5%)
17	Y5P	AV	56	-	14,19,20	3.60	1 (7%)	18,26,29	0.79	1 (5%)
17	Y5P	AY	74	-	14,19,20	3.55	1 (7%)	18,26,29	0.79	0
17	Y5P	AY	42	-	14,19,20	3.61	1 (7%)	18,26,29	0.92	2 (11%)
17	Y5P	AY	23	-	14,19,20	2.69	2 (14%)	18,26,29	1.00	1 (5%)
47	Y5P	BB	26	47	14,19,20	3.65	1 (7%)	18,26,29	0.92	2 (11%)
47	Y5P	BB	6	47	14,19,20	2.36	1 (7%)	18,26,29	0.96	1 (5%)
17	Y5P	AV	12	-	14,19,20	2.16	1 (7%)	18,26,29	1.02	1 (5%)
47	P5P	BB	51	47	16,23,24	1.37	3 (18%)	14,33,36	2.00	2 (14%)
47	Y5P	BB	62	47	14,19,20	2.24	1 (7%)	18,26,29	1.00	1 (5%)
18	Y5P	AX	15	-	14,19,20	2.13	1 (7%)	18,26,29	1.03	1 (5%)
18	Y5P	AX	13	-	14,19,20	2.30	1 (7%)	18,26,29	0.98	1 (5%)
17	Y5P	AV	13	-	14,19,20	3.44	1 (7%)	18,26,29	0.86	2 (11%)
17	Y5P	AV	74	-	14,19,20	3.60	1 (7%)	18,26,29	0.84	0
17	Y5P	AV	7	-	14,19,20	2.62	2 (14%)	18,26,29	1.00	1 (5%)
47	Y5P	BB	40	47	14,19,20	2.39	1 (7%)	18,26,29	0.99	1 (5%)
17	Y5P	AV	1	-	14,16,20	2.63	2 (14%)	18,22,29	1.12	2 (11%)
17	Y5P	AV	9	-	14,19,20	2.66	2 (14%)	18,26,29	1.08	1 (5%)
18	Y5P	AX	17	-	14,19,20	2.47	1 (7%)	18,26,29	0.97	1 (5%)
17	Y5P	AV	23	-	14,19,20	2.66	2 (14%)	18,26,29	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	Y5P	BB	60	47	14,19,20	3.53	1 (7%)	18,26,29	0.92	2 (11%)
17	P5P	AV	35	-	16,23,24	0.83	1 (6%)	14,33,36	0.76	1 (7%)
47	P5P	BB	5	47	16,23,24	0.77	0	14,33,36	0.75	0
17	Y5P	AV	70	-	14,19,20	2.73	2 (14%)	18,26,29	1.04	1 (5%)
47	Y5P	BB	48	47	14,19,20	2.24	1 (7%)	18,26,29	1.00	1 (5%)
17	Y5P	AV	50	-	14,19,20	2.28	1 (7%)	18,26,29	0.99	1 (5%)
18	Y5P	AX	22	-	14,19,20	2.24	1 (7%)	18,26,29	1.12	1 (5%)
17	Y5P	AV	22	-	14,19,20	2.69	2 (14%)	18,26,29	1.07	1 (5%)
17	Y5P	AY	54	-	14,19,20	2.22	1 (7%)	18,26,29	1.03	1 (5%)
47	P5P	BB	24	47	16,23,24	0.88	1 (6%)	14,33,36	0.87	0
17	Y5P	AY	75	-	14,19,20	3.57	1 (7%)	18,26,29	0.82	1 (5%)
47	P5P	BB	59	47	16,23,24	1.37	3 (18%)	14,33,36	1.96	2 (14%)
47	P5P	BB	29	47	16,23,24	1.35	3 (18%)	14,33,36	2.08	2 (14%)
47	Y5P	BB	52	47	14,19,20	3.68	1 (7%)	18,26,29	0.81	1 (5%)

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
17	Y5P	AY	69	-	-	2/7/33/34	0/2/2/2
47	P5P	BB	49	47	-	2/3/25/26	0/3/3/3
47	P5P	BB	10	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	10	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	24	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	13	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	65	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	71	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	68	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	60	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	67	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	58	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	12	47	-	3/7/33/34	0/2/2/2
47	Y5P	BB	11	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	36	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	43	-	-	4/7/33/34	0/2/2/2
17	Y5P	AY	49	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	21	-	-	3/7/33/34	0/2/2/2
17	P5P	AY	35	-	-	0/3/25/26	0/3/3/3
17	P5P	AY	36	-	-	0/3/25/26	0/3/3/3
17	P5P	AY	76	46	-	0/3/25/26	0/3/3/3
17	Y5P	AY	15	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	72	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	44	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	63	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	23	47	-	2/3/25/26	0/3/3/3
17	Y5P	AY	7	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	57	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	55	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	66	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	15	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	67	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	68	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	24	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	43	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	11	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	22	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	11	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	45	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	66	47	-	0/3/25/26	0/3/3/3
17	P5P	AY	34	-	-	2/3/25/26	0/3/3/3
17	Y5P	AY	44	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	52	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	40	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	37	-	-	4/7/33/34	0/2/2/2
18	Y5P	AX	12	-	-	3/6/30/34	0/2/2/2
17	Y5P	AV	60	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	72	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	58	-	-	4/7/33/34	0/2/2/2
47	P5P	BB	32	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	6	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	16	-	-	3/7/33/34	0/2/2/2
18	Y5P	AX	18	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	63	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	62	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	9	-	-	3/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	69	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	37	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	5	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	70	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	8	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	2	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	57	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	40	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	55	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	29	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	66	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	39	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	9	47	-	2/3/25/26	0/3/3/3
17	Y5P	AV	41	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	64	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	14	47	-	2/3/25/26	0/3/3/3
17	Y5P	AV	3	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	45	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	51	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	39	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	29	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	64	47	-	0/3/25/26	0/3/3/3
17	Y5P	AV	38	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	58	-	-	4/7/33/34	0/2/2/2
17	Y5P	AY	13	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	48	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	61	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	73	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	44	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	14	-	-	5/7/33/34	0/2/2/2
17	Y5P	AV	39	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	34	47	-	3/7/33/34	0/2/2/2
17	Y5P	AY	12	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	37	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	28	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	25	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	20	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	38	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	38	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	6	-	-	4/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	26	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	41	47	-	0/3/25/26	0/3/3/3
17	Y5P	AV	59	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	62	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	31	47	-	1/7/33/34	0/2/2/2
47	Y5P	BB	65	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	15	47	-	2/3/25/26	0/3/3/3
47	P5P	BB	50	47	-	0/3/25/26	0/3/3/3
17	Y5P	AV	27	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	5	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	30	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	1	-	-	1/6/30/34	0/2/2/2
17	Y5P	AY	31	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	33	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	71	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	43	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	28	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	47	47	-	0/3/25/26	0/3/3/3
17	Y5P	AV	75	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	31	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	32	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	50	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	21	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	51	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	4	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	33	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	63	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	25	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	26	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	35	47	-	2/3/25/26	0/3/3/3
17	Y5P	AY	59	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	24	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	27	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	2	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	73	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	42	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	32	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	14	-	-	1/7/33/34	0/2/2/2
17	P5P	AV	34	-	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	P5P	BB	25	47	-	2/3/25/26	0/3/3/3
17	P5P	AV	76	46	-	1/3/25/26	0/3/3/3
17	Y5P	AY	61	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	7	47	-	1/3/25/26	0/3/3/3
47	P5P	BB	27	47	-	0/3/25/26	0/3/3/3
17	Y5P	AY	30	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	33	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	53	47	-	1/7/33/34	0/2/2/2
18	Y5P	AX	19	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	4	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	21	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	14	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	53	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	3	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	30	47	-	0/3/25/26	0/3/3/3
17	Y5P	AV	8	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	28	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	52	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	53	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	56	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	49	-	-	3/7/33/34	0/2/2/2
18	Y5P	AX	23	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	54	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	48	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	46	47	-	3/3/25/26	0/3/3/3
17	Y5P	AY	41	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	64	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	61	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	45	47	-	0/3/25/26	0/3/3/3
17	P5P	AV	36	-	-	0/3/25/26	0/3/3/3
17	Y5P	AV	10	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	42	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	65	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	8	47	-	2/7/33/34	0/2/2/2
17	Y5P	AV	56	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	74	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	42	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	23	-	-	2/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	Y5P	BB	26	47	-	1/7/33/34	0/2/2/2
47	Y5P	BB	6	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	12	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	51	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	62	47	-	1/7/33/34	0/2/2/2
18	Y5P	AX	15	-	-	3/7/33/34	0/2/2/2
18	Y5P	AX	13	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	13	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	74	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	7	-	-	3/7/33/34	0/2/2/2
47	Y5P	BB	40	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	1	-	-	1/6/30/34	0/2/2/2
17	Y5P	AV	9	-	-	5/7/33/34	0/2/2/2
18	Y5P	AX	17	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	23	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	60	47	-	1/7/33/34	0/2/2/2
17	P5P	AV	35	-	-	0/3/25/26	0/3/3/3
47	P5P	BB	5	47	-	3/3/25/26	0/3/3/3
17	Y5P	AV	70	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	48	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	50	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	22	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	22	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	54	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	24	47	-	2/3/25/26	0/3/3/3
17	Y5P	AY	75	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	59	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	29	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	52	47	-	1/7/33/34	0/2/2/2

The worst 5 of 274 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	41	Y5P	C4-N3	-14.48	1.33	1.46
18	AX	21	Y5P	C4-N3	-14.19	1.33	1.46
17	AV	42	Y5P	C4-N3	-14.17	1.33	1.46
17	AV	2	Y5P	C4-N3	-14.02	1.33	1.46
47	BB	31	Y5P	C4-N3	-13.97	1.33	1.46

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AV	34	P5P	C6-N1-C2	6.97	125.83	115.84
47	BB	7	P5P	C6-N1-C2	6.76	125.52	115.84
47	BB	41	P5P	C6-N1-C2	6.69	125.43	115.84
17	AY	34	P5P	C6-N1-C2	6.68	125.41	115.84
47	BB	49	P5P	C6-N1-C2	6.54	125.20	115.84

There are no chirality outliers.

5 of 295 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AV	76	P5P	C4'-C5'-O5'-P
17	AY	34	P5P	O4'-C4'-C5'-O5'
47	BB	5	P5P	C3'-C4'-C5'-O5'
47	BB	5	P5P	O4'-C4'-C5'-O5'
47	BB	15	P5P	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 358 ligands modelled in this entry, 357 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
91	GDP	Ag	500	-	24,30,30	1.06	2 (8%)	30,47,47	1.26	4 (13%)

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
91	GDP	Ag	500	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Ag	500	GDP	O4'-C1'	2.45	1.44	1.41
91	Ag	500	GDP	C5-C4	2.23	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	Ag	500	GDP	C3'-C2'-C1'	3.01	105.51	100.98
91	Ag	500	GDP	C8-N7-C5	2.41	107.58	102.99
91	Ag	500	GDP	C5-C6-N1	2.20	117.84	113.95
91	Ag	500	GDP	PA-O3A-PB	-2.16	125.42	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

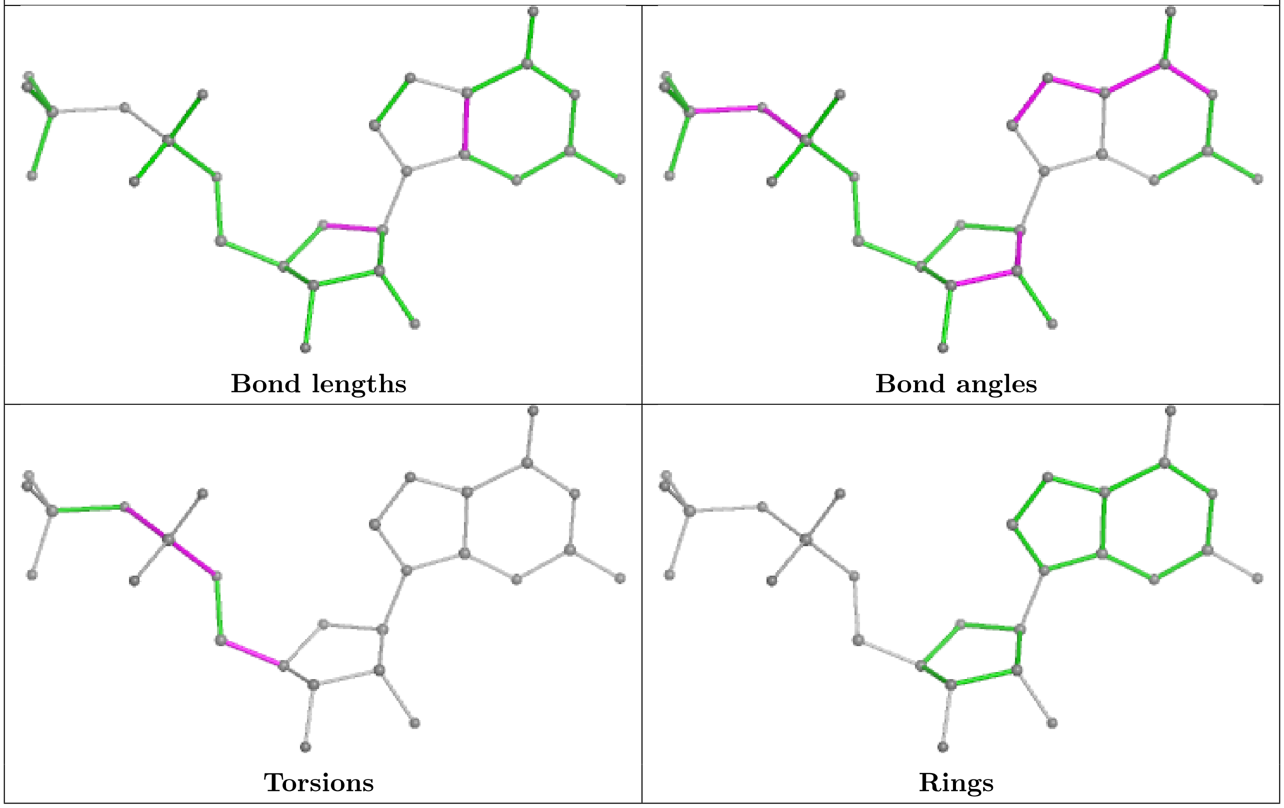
Mol	Chain	Res	Type	Atoms
91	Ag	500	GDP	C5'-O5'-PA-O1A
91	Ag	500	GDP	C5'-O5'-PA-O2A
91	Ag	500	GDP	O4'-C4'-C5'-O5'
91	Ag	500	GDP	C3'-C4'-C5'-O5'
91	Ag	500	GDP	PB-O3A-PA-O2A

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 GDP Ag 500



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	Ao	26
88	Bz	4
23	Ae	4
17	AY	3
47	BB	2
17	AV	2
7	AI	1
4	AE	1

The worst 5 of 43 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	36:UNK	C	99:UNK	N	56.86
1	Bz	425:UNK	C	601:UNK	N	55.59
1	Ae	262:UNK	C	263:UNK	N	42.03
1	Ae	309:UNK	C	354:UNK	N	28.87
1	Bz	106:UNK	C	300:UNK	N	28.46

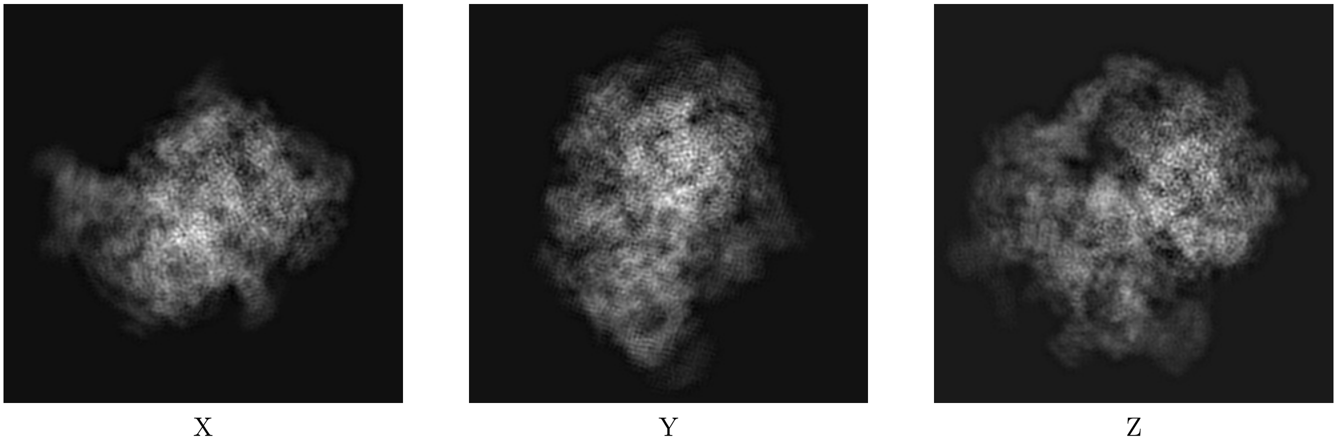
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2914. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

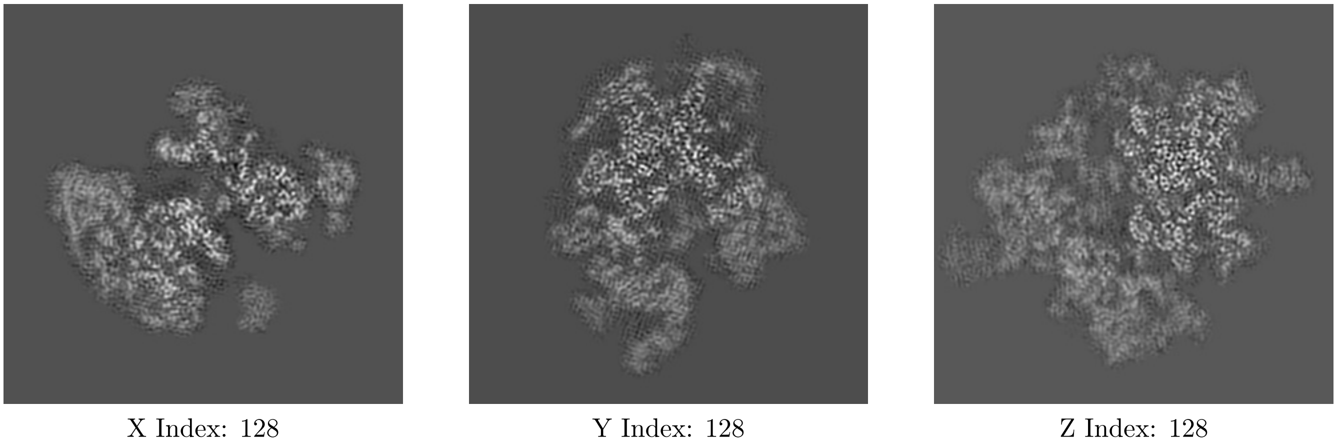
6.1.1 Primary map


X
Y
Z

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

6.2 Central slices (i)

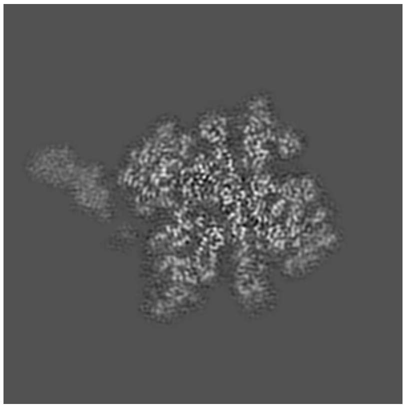
6.2.1 Primary map

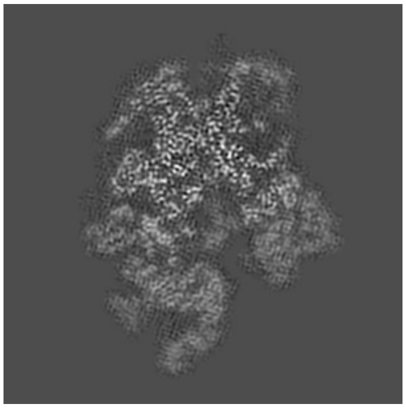

X Index: 128
Y Index: 128
Z Index: 128

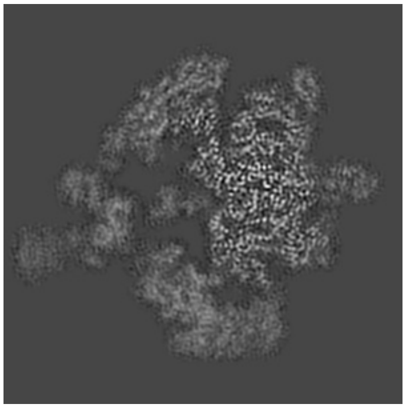
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map


X Index: 159

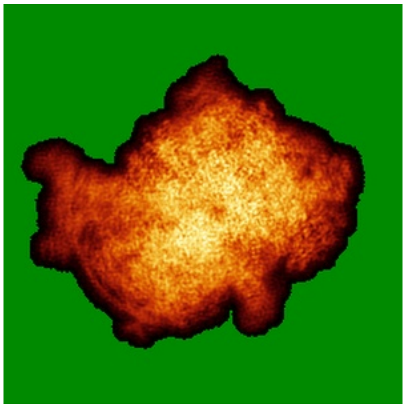

Y Index: 128

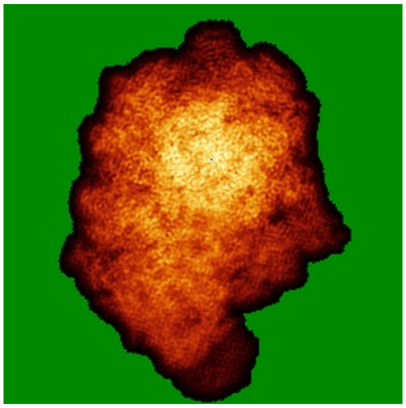

Z Index: 138

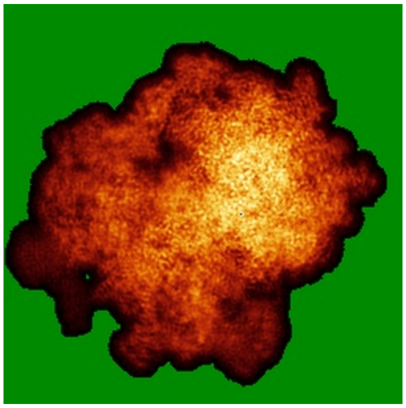
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

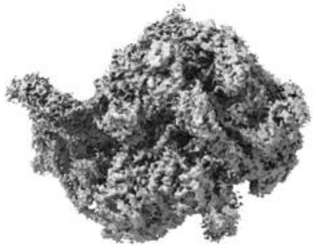

Y


Z

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

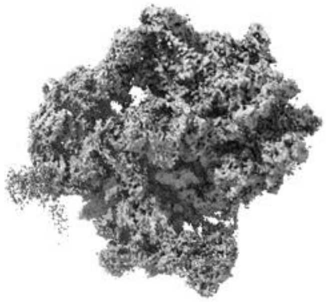
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

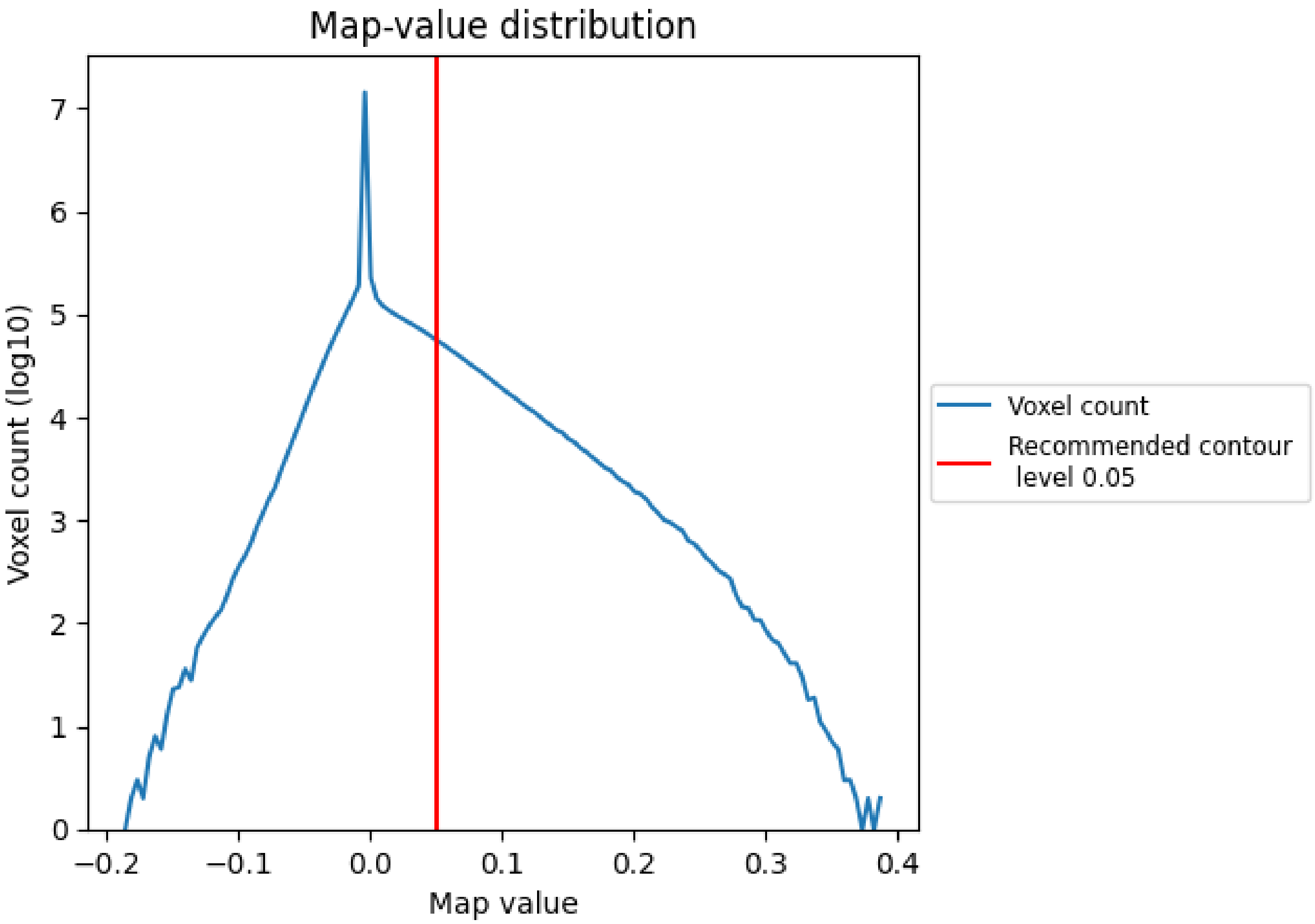
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

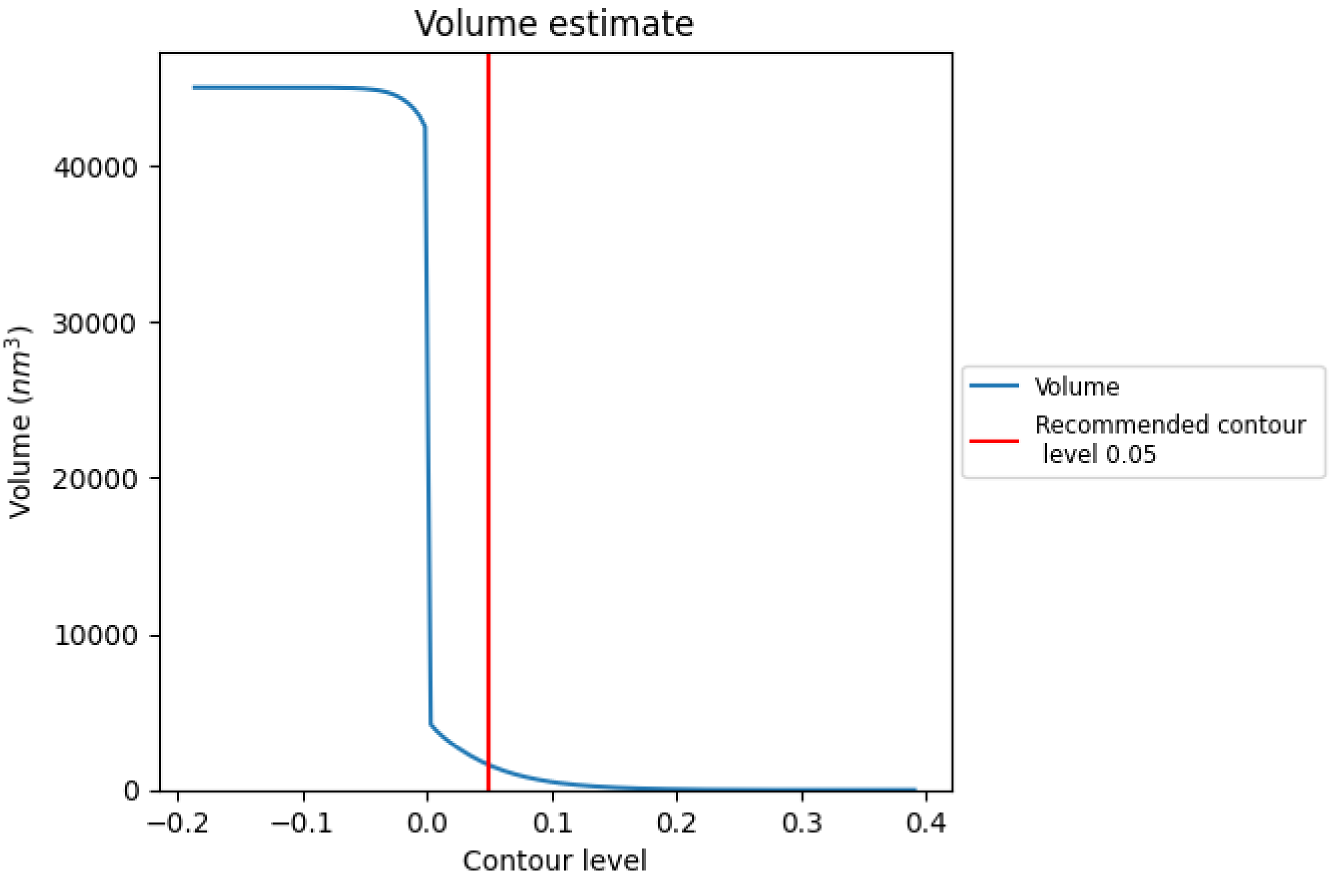
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

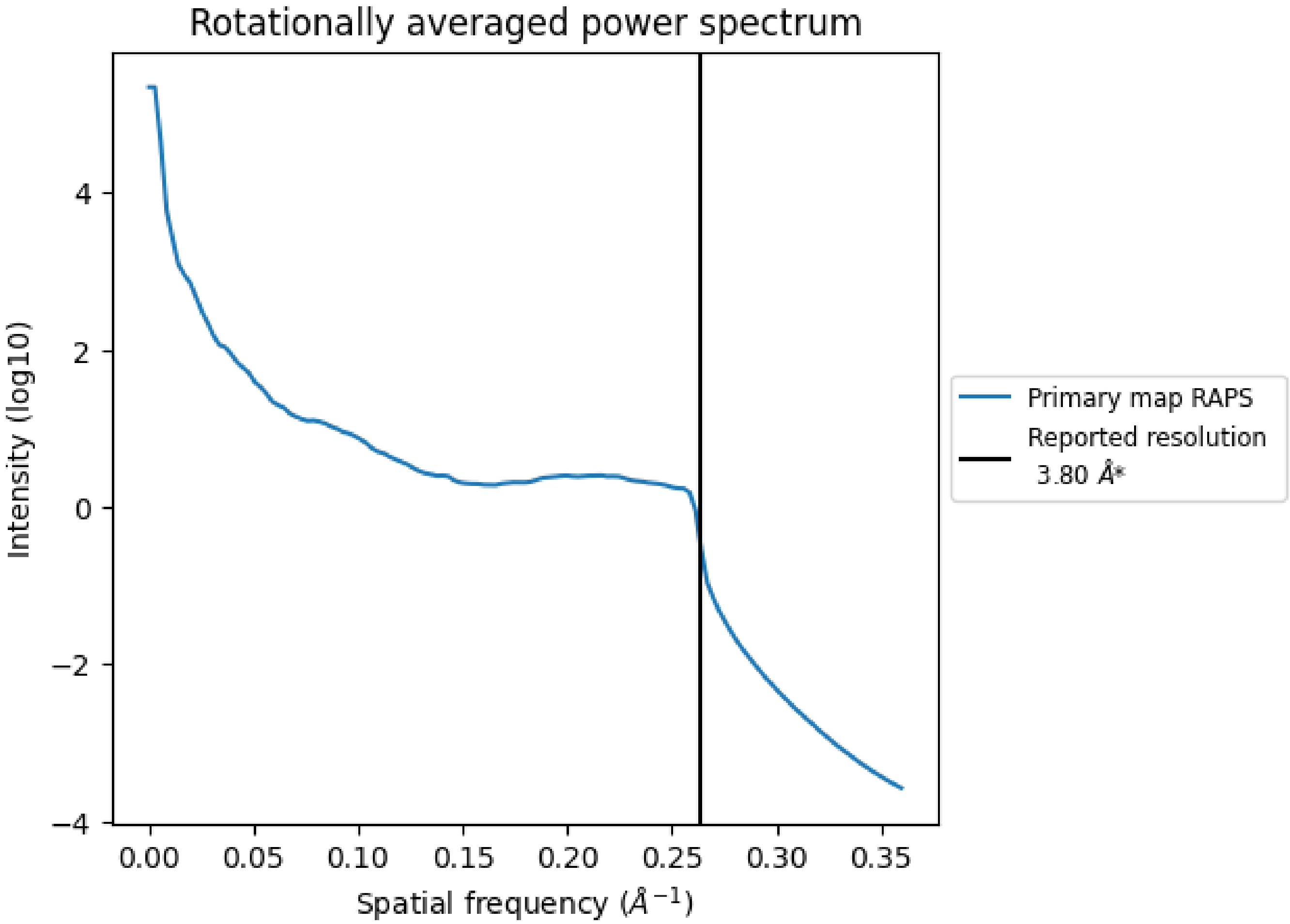
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1591 nm^3; this corresponds to an approximate mass of 1437 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

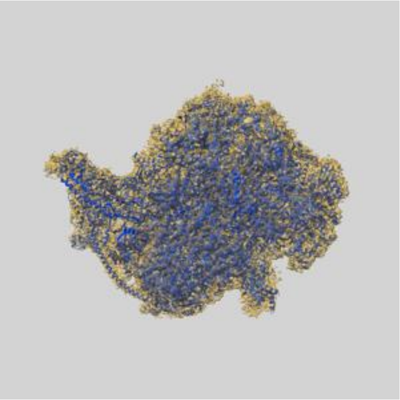
8 Fourier-Shell correlation ⓘ

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

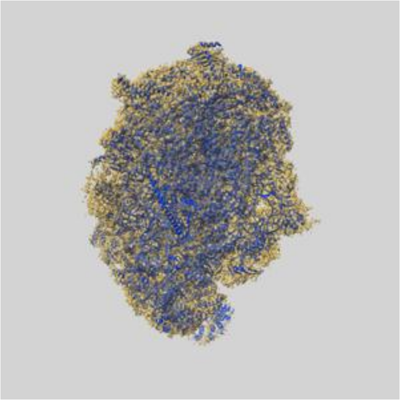
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-2914 and PDB model 5AJ4. Per-residue inclusion information can be found in section 3 on page 23.

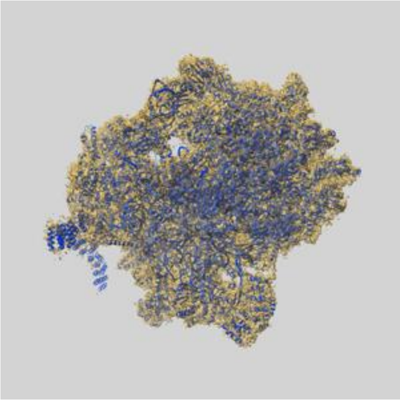
9.1 Map-model overlay ⓘ



X



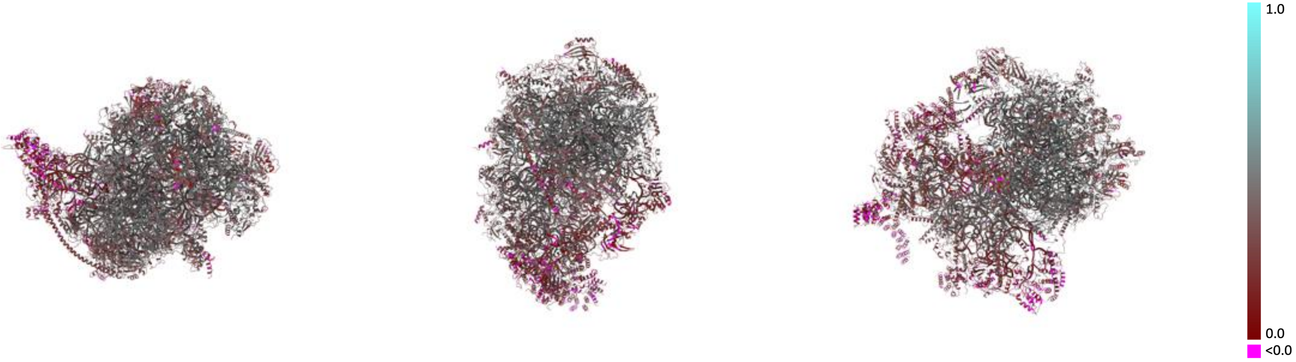
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

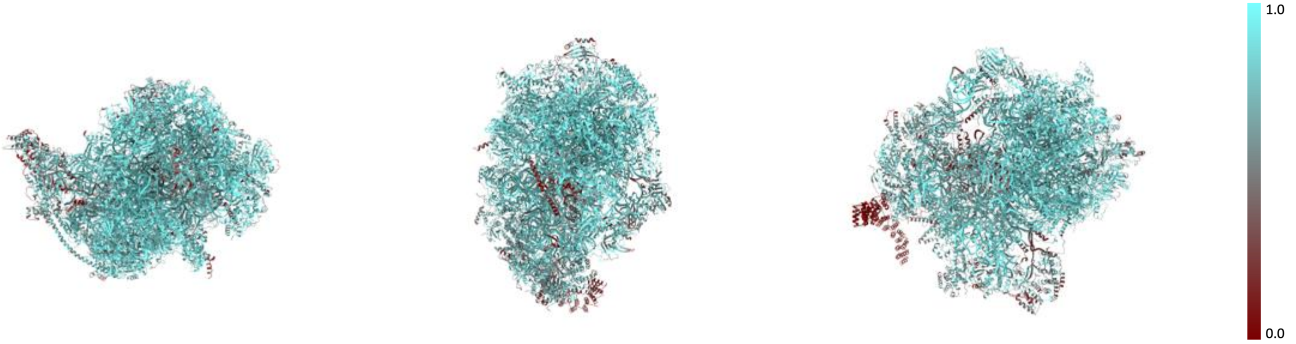
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

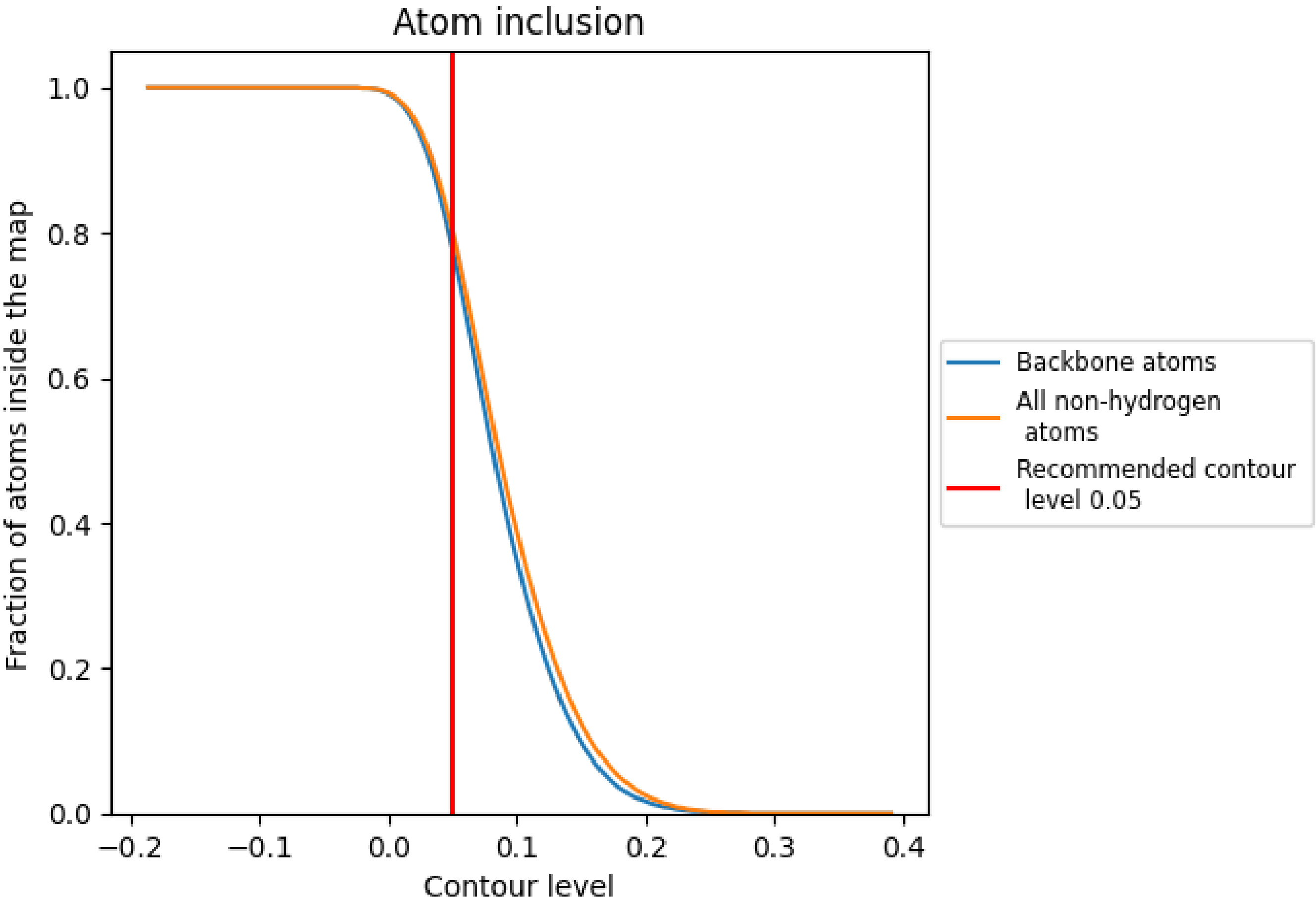
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.3580
AA	0.9200	0.3580
AB	0.7920	0.3500
AC	0.7490	0.3540
AE	0.7070	0.3400
AF	0.7510	0.3610
AG	0.6430	0.2620
AI	0.7100	0.2850
AJ	0.7180	0.2990
AK	0.8160	0.3670
AL	0.7460	0.3790
AN	0.7890	0.3120
AO	0.7150	0.3430
AP	0.7240	0.2080
AQ	0.7940	0.3420
AR	0.7900	0.3810
AU	0.7950	0.3760
AV	0.6410	0.2940
AX	0.7490	0.4000
AY	0.4840	0.2070
Aa	0.6410	0.1880
Ab	0.6870	0.2790
Ac	0.7380	0.3080
Ad	0.7310	0.2440
Ae	0.5250	0.1220
Af	0.7290	0.3360
Ag	0.6800	0.1920
Ah	0.6970	0.2250
Ai	0.7280	0.2650
Aj	0.5360	0.1580
Ak	0.6560	0.2400
Am	0.6970	0.3340
An	0.7910	0.4160
Ao	0.2110	0.1440
Ap	0.7260	0.2400

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Chain	Atom inclusion	Q-score
As	0.0730	-0.0030
Az	0.7550	0.2900
B0	0.9010	0.4720
B1	0.8310	0.4060
B2	0.8590	0.4290
B3	0.8860	0.4520
B4	0.8340	0.2750
B5	0.8490	0.4260
B6	0.1900	0.1820
B7	0.9080	0.4800
B8	0.8970	0.4840
B9	0.9250	0.4600
BA	0.9540	0.4350
BB	0.8950	0.2640
BD	0.8810	0.4570
BE	0.8710	0.4320
BF	0.8920	0.4530
BI	0.7290	0.3510
BJ	0.6380	0.2690
BK	0.4930	0.1750
BN	0.8910	0.4580
BO	0.8690	0.4550
BP	0.8990	0.4400
BQ	0.8740	0.4420
BR	0.8780	0.4480
BS	0.8560	0.3790
BT	0.8230	0.4230
BU	0.8710	0.4490
BV	0.8490	0.4390
BW	0.8590	0.4720
BX	0.8510	0.4360
BY	0.6230	0.3490
Ba	0.8690	0.4050
Bb	0.8340	0.3330
Bc	0.8180	0.3520
Bd	0.7260	0.2320
Be	0.8260	0.3880
Bf	0.7790	0.4070
Bg	0.8900	0.4590
Bh	0.8320	0.3890
Bi	0.5600	0.2960
Bj	0.7040	0.1810

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Chain	Atom inclusion	Q-score
Bk	0.7420	0.3210
Bl	0.8990	0.4350
Bm	0.7690	0.3240
Bn	0.8900	0.4730
Bo	0.8610	0.4180
Bp	0.5970	0.2170
Bq	0.6390	0.2510
Bt	0.8870	0.4650
Bu	0.5420	0.2520
Bv	0.5470	0.2740
Bw	0.8630	0.4070
Bx	0.8200	0.3960
Bz	0.3940	0.2010