



wwPDB EM Map/Model Validation Report ⓘ

May 19, 2016 – 03:50 PM EDT

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)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

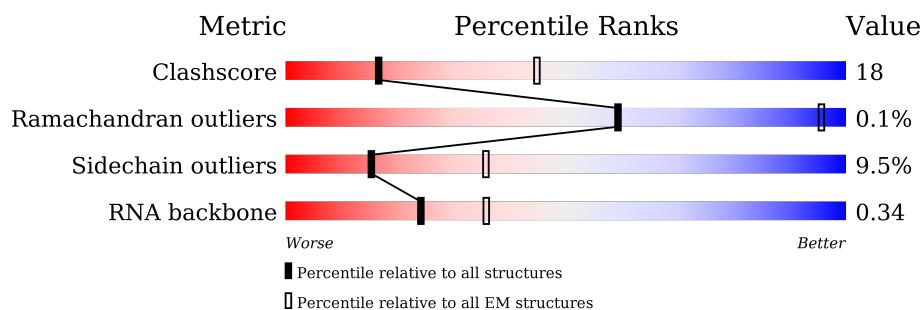
1 Overall quality at a glance

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.











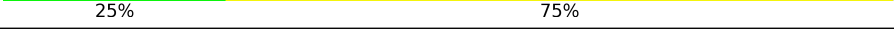

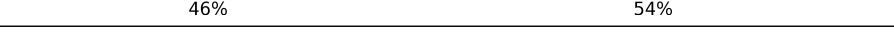
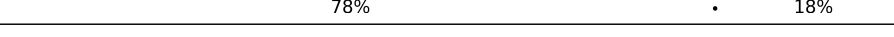

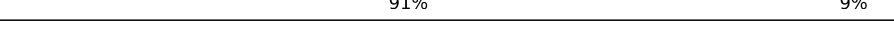
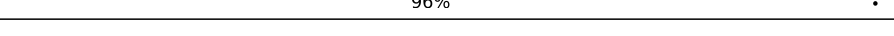
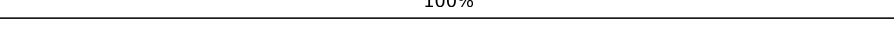
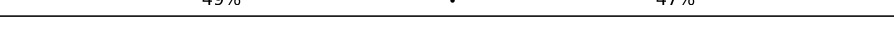

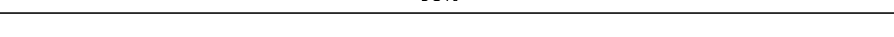






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AA	962	42% 43% 15%
2	AB	220	72% 25% .
3	AC	132	64% 33% .
4	AE	328	59% 37% .
5	AF	124	69% 27% . .
6	AG	208	69% 28% .
7	AI	311	67% 31% .
8	AJ	201	38% 24% . 36%

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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	


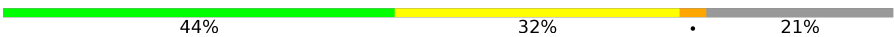



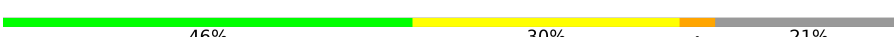




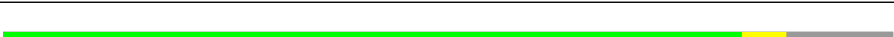


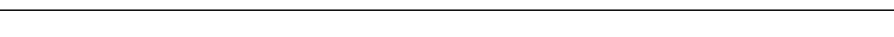
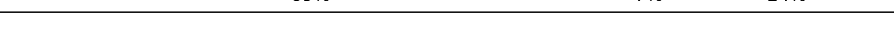
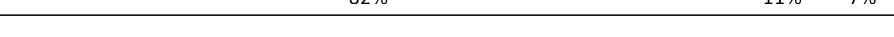



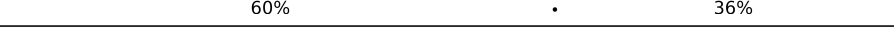





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Mol	Chain	Length	Quality of chain
33	Ap	188	
34	As	16	
35	Az	17	
36	B0	148	
37	B1	256	
38	B2	252	
39	B3	161	
40	B4	126	
41	B5	188	
42	B6	65	
43	B7	95	
44	B8	188	
45	B9	100	
46	BA	1570	
47	BB	51	
48	BD	306	
49	BE	348	
50	BF	294	
51	BI	268	
52	BJ	262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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	Y5P	AV	55	-	-	X	-
17	Y5P	AY	55	-	-	X	-
17	Y5P	AY	58	-	-	X	-

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 RRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 18 is a RNA chain called MRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 34 is a protein called UNASSIGNED HELICES.

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

- Molecule 35 is a protein called UNASSIGNED HELICES.

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 RRNA.

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	C	N	O	S	0	0
			2420	1554	426	430	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
61	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
85	Bv	131	Total	C	N	O	S	0	0
			1068	662	206	195	5		

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

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

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

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

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

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

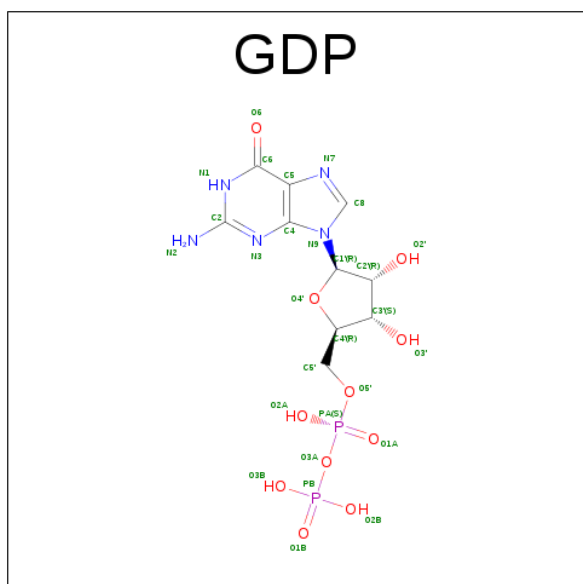
- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- 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
91	Ag	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 92 is water.

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

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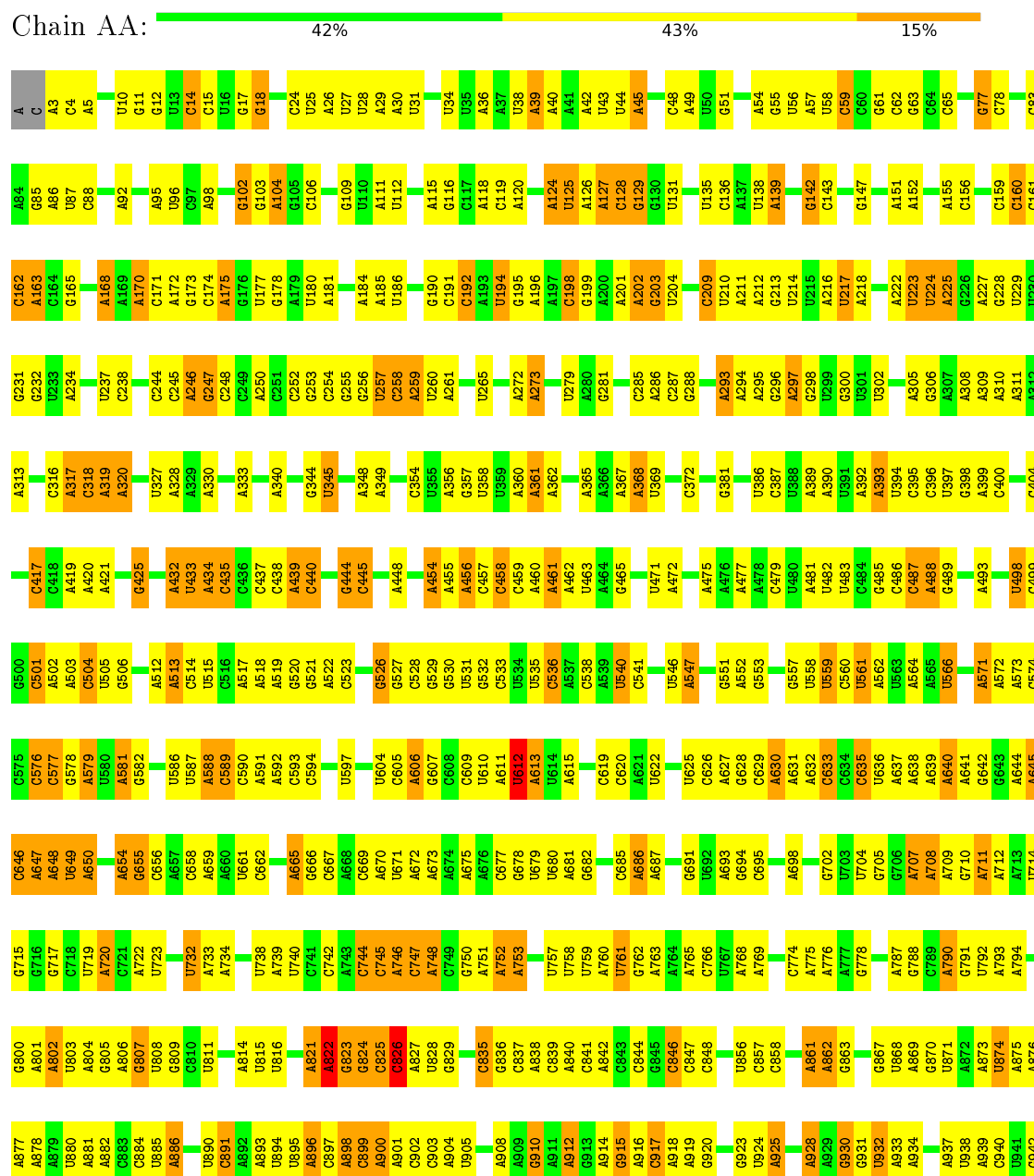
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Mol	Chain	Residues	Atoms		AltConf
92	B0	3	Total 3	O 3	0
92	B7	2	Total 2	O 2	0
92	B8	1	Total 1	O 1	0
92	BA	196	Total 196	O 196	0
92	BD	3	Total 3	O 3	0
92	BF	4	Total 4	O 4	0
92	BI	1	Total 1	O 1	0
92	BO	2	Total 2	O 2	0
92	BP	3	Total 3	O 3	0
92	BR	2	Total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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

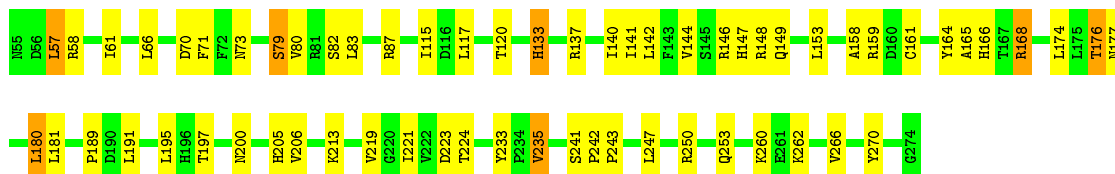
- Molecule 1: MITORIBOSOMAL 12S RRNA





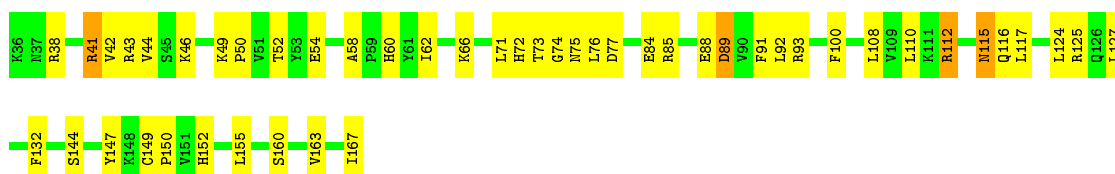
• Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2

Chain AB: 72% 25%



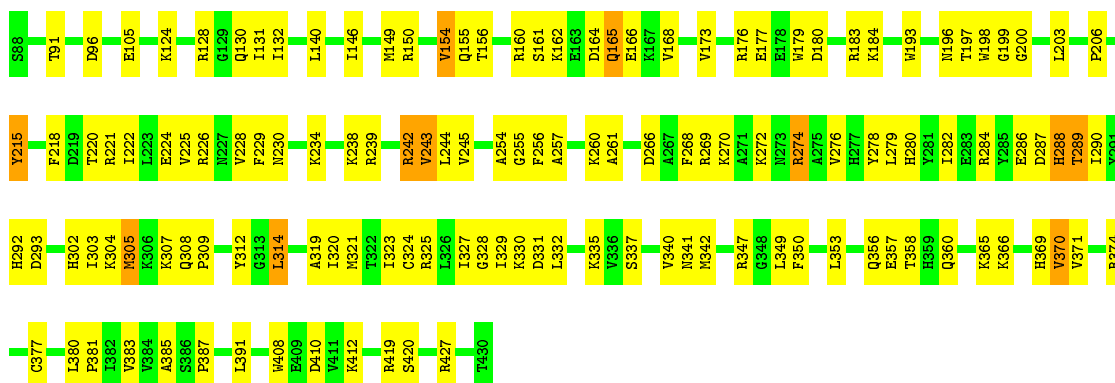
• Molecule 3: MITORIBOSOMAL PROTEIN US3M, MRPS24

Chain AC: 64% 33%



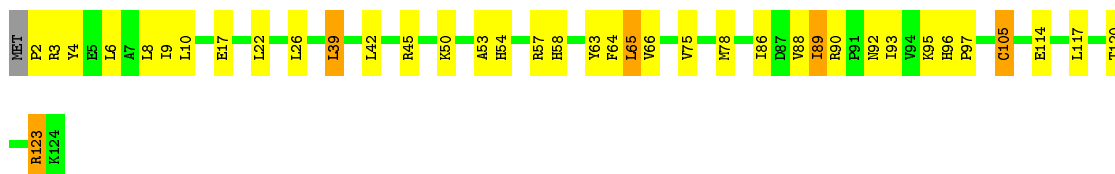
• Molecule 4: MITORIBOSOMAL PROTEIN US5M, MRPS5

Chain AE: 59% 37%

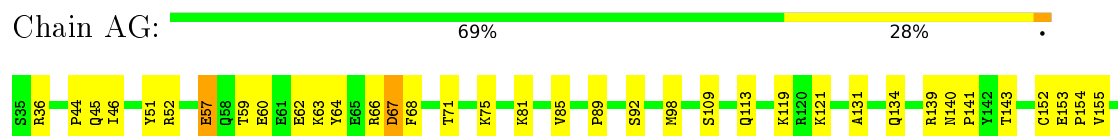


• Molecule 5: MITORIBOSOMAL PROTEIN BS6M, MRPS6

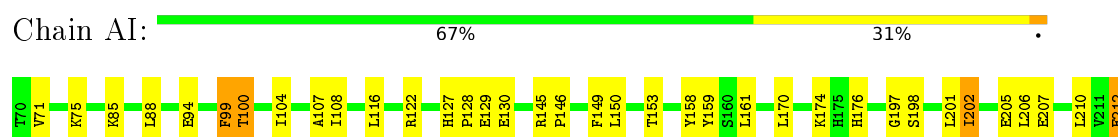
Chain AF: 69% 27%



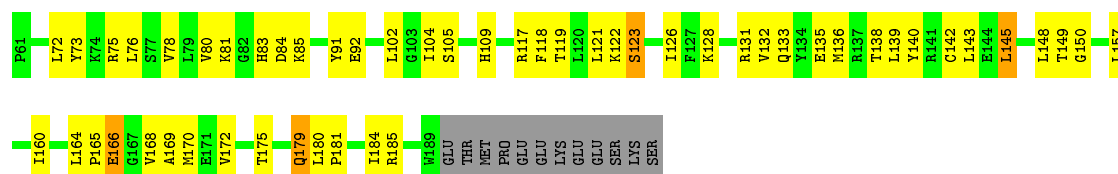
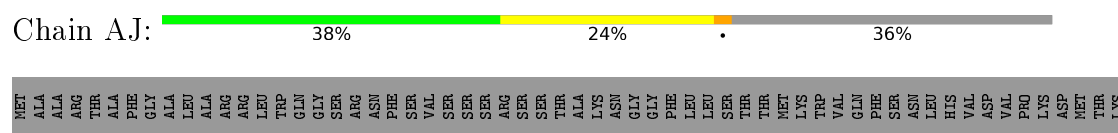
• Molecule 6: MITORIBOSOMAL PROTEIN US7M, MRPS7



- Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9



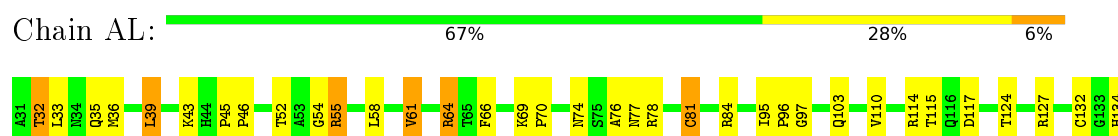
- Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10



- Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11



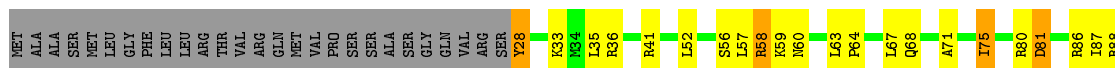
- Molecule 10: MITORIBOSOMAL PROTEIN US12M, MRPS12





- Molecule 11: MITORIBOSOMAL PROTEIN US14M, MRPS14

Chain AN: 48% 23% 8% 21%



- Molecule 12: MITORIBOSOMAL PROTEIN US15M, MRPS15

Chain AO: 56% 16% 27%



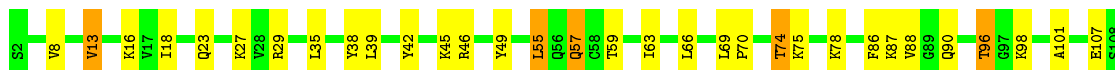
- Molecule 13: MITORIBOSOMAL PROTEIN BS16M, MRPS16

Chain AP: 72% 27% 1%



- Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17

Chain AQ: 70% 26% 5%

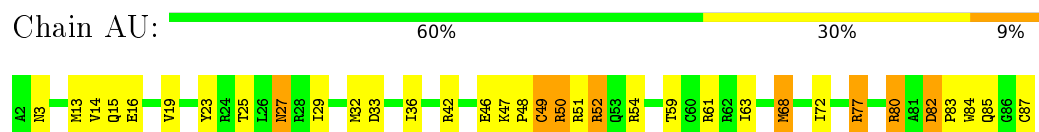


- Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

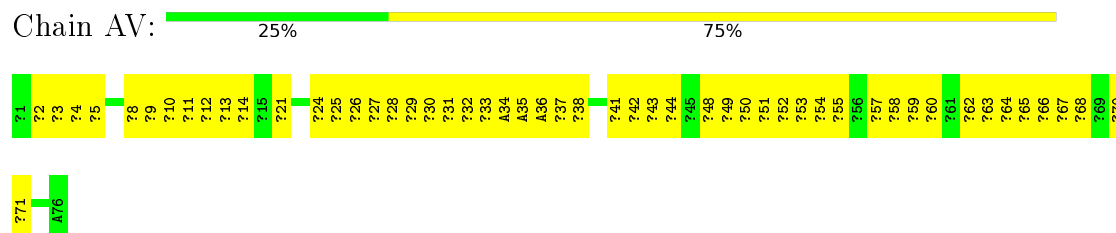
Chain AR: 70% 26% 4%



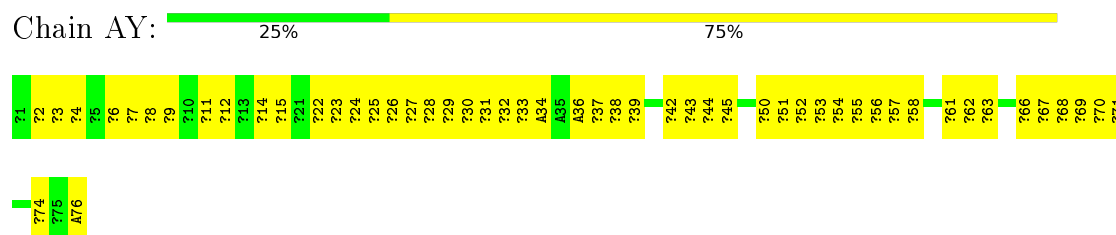
- Molecule 16: MITORIBOSOMAL PROTEIN BS21M, MRPS21



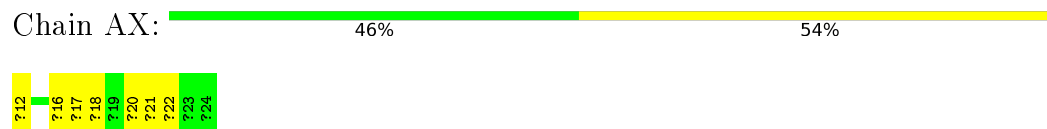
- Molecule 17: P-SITE AND A-SITE TRNA



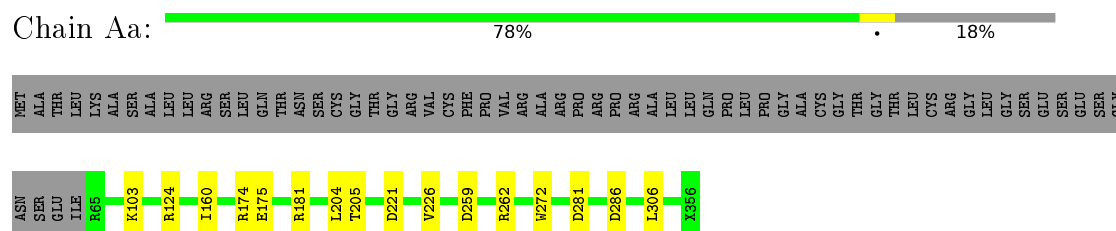
- Molecule 17: P-SITE AND A-SITE TRNA



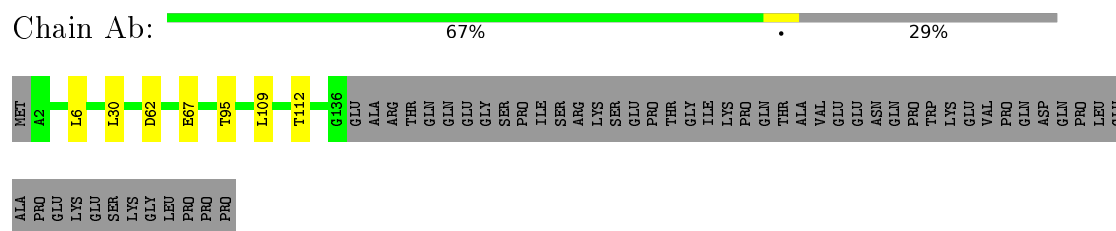
- Molecule 18: MRNA



- Molecule 19: MITORIBOSOMAL PROTEIN MS22, MRPS22



- Molecule 20: MITORIBOSOMAL PROTEIN MS23, MRPS23



- Molecule 21: MITORIBOSOMAL PROTEIN MS25, MRPS25

Chain Ac:  91% 9%



- Molecule 22: MITORIBOSOMAL PROTEIN MS26, MRPS26

Chain Ad:  96%



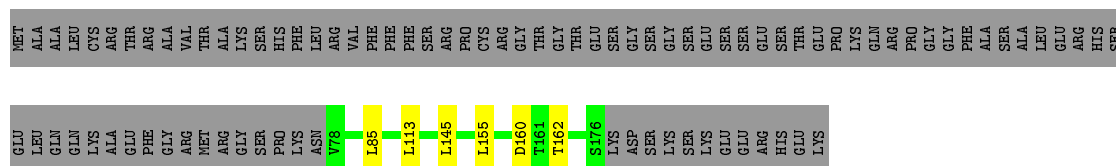
- Molecule 23: MITORIBOSOMAL PROTEIN MS27, MRPS27

Chain Ae:  100%


There are no outlier residues recorded for this chain.

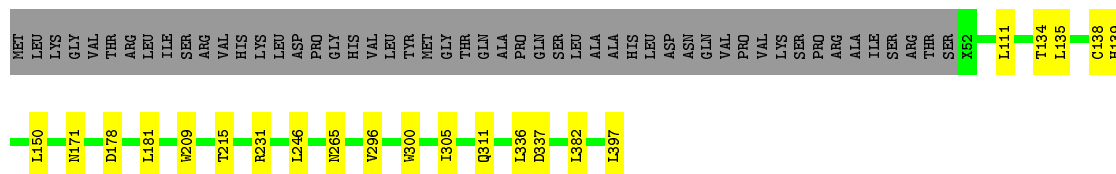
- Molecule 24: MITORIBOSOMAL PROTEIN MS28, MRPS28

Chain Af:  49% 47%



- Molecule 25: MITORIBOSOMAL PROTEIN MS29, MRPS29

Chain Ag:  82% 6% 13%



- Molecule 26: MITORIBOSOMAL PROTEIN MS31, MRPS31

Chain Ah:  98%



- Molecule 27: MITORIBOSOMAL PROTEIN MS33, MRPS33

Chain Ai:  94% 6%



- Molecule 28: MITORIBOSOMAL PROTEIN MS34, MRPS34

Chain Aj:  93% 5%



- Molecule 29: MITORIBOSOMAL PROTEIN MS35, MRPS35

Chain Ak:  92% 8%



- Molecule 30: MITORIBOSOMAL PROTEIN MS37, MRPS37

Chain Am:  91% 9%



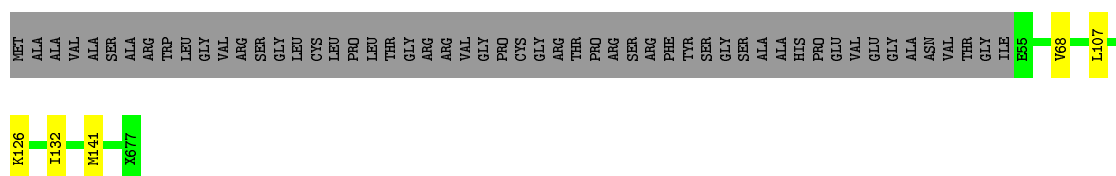
- Molecule 31: MITORIBOSOMAL PROTEIN MS38, MRPS38

Chain An:  88% 13%



- Molecule 32: MITORIBOSOMAL PROTEIN MS39, MRPS39

Chain Ao:  89% 10%



- Molecule 33: 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL

Chain Ap:  91% 9%



- Molecule 34: UNASSIGNED HELICES

Chain As:  100%

There are no outlier residues recorded for this chain.

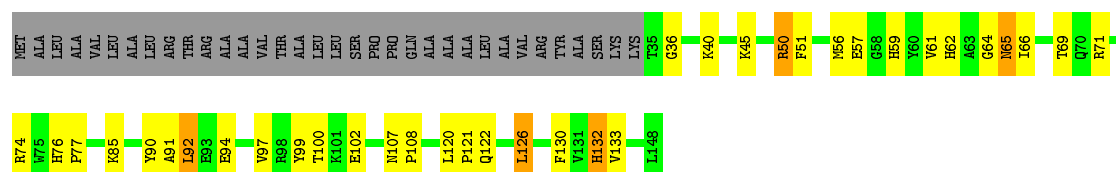
- Molecule 35: UNASSIGNED HELICES

Chain Az:  100%

There are no outlier residues recorded for this chain.

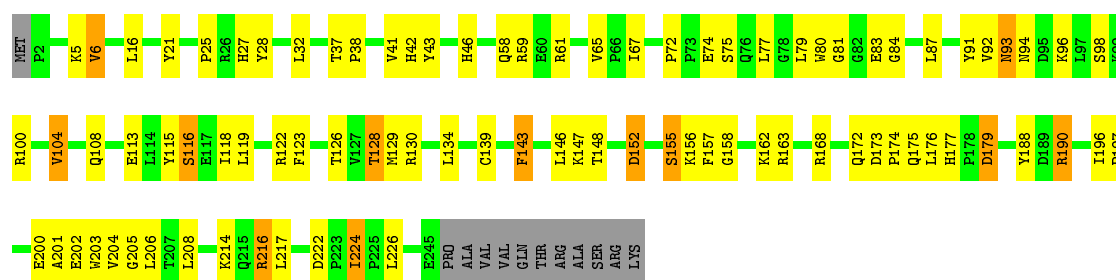
- Molecule 36: MITORIBOSOMAL PROTEIN BL27M, MRPL27

Chain B0:  53% 21% 23%



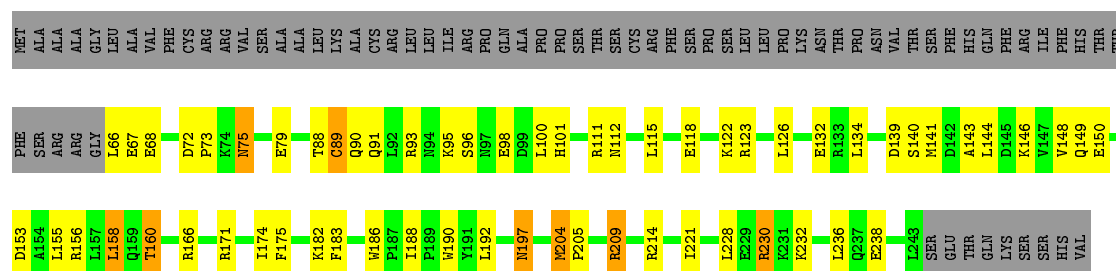
- Molecule 37: MITORIBOSOMAL PROTEIN BL28M, MRPL28

Chain B1:  61% 30% 5% 5%



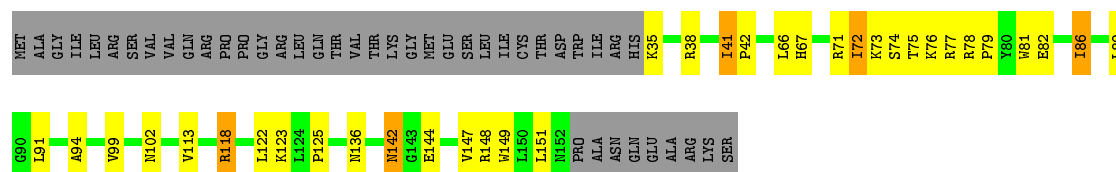
- Molecule 38: MITORIBOSOMAL PROTEIN UL29M, MRPL47

Chain B2:  46% 21% 29%

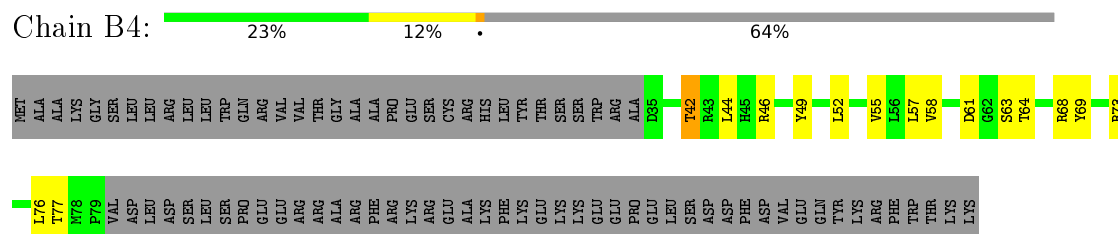


- Molecule 39: MITORIBOSOMAL PROTEIN UL30M, MRPL30

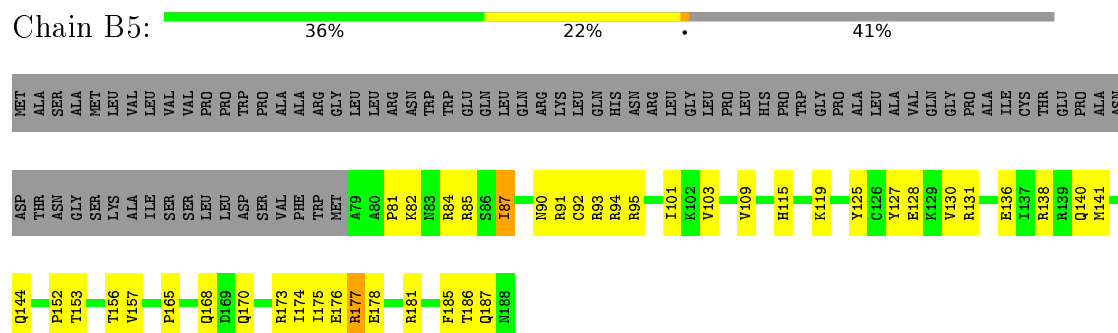
Chain B3:  52% 19% 27%



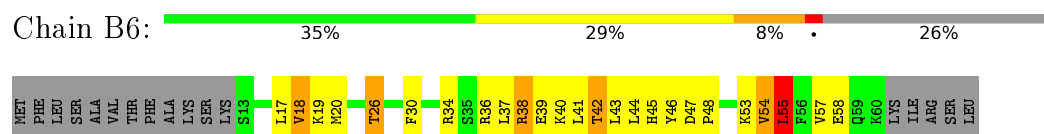
- Molecule 40: MITORIBOSOMAL PROTEIN BL31M, MRPL55



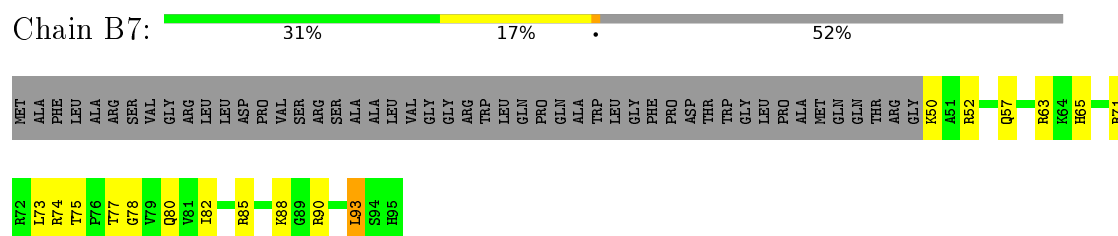
- Molecule 41: MITORIBOSOMAL PROTEIN BL32M, MRPL32



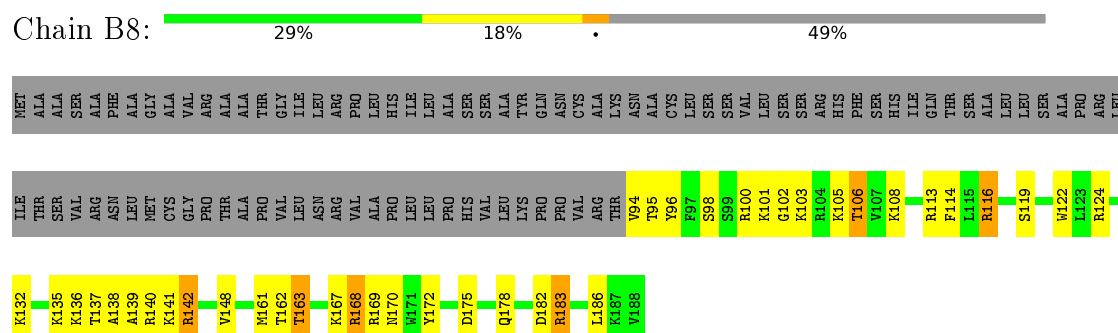
- Molecule 42: MITORIBOSOMAL PROTEIN BL33M, MRPL33



- Molecule 43: MITORIBOSOMAL PROTEIN BL34M, MRPL34



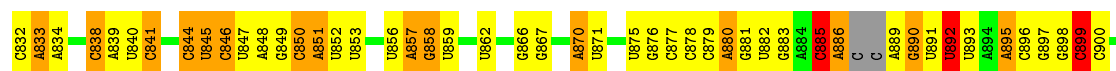
- Molecule 44: MITORIBOSOMAL PROTEIN BL35M, MRPL35

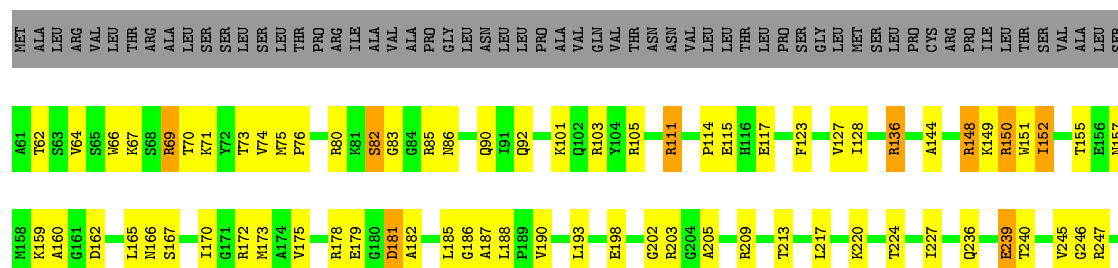


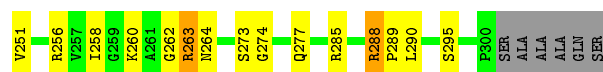
- Molecule 45: MITORIBOSOMAL PROTEIN BL36M, MRPL36



● Molecule 46: MITORIBOSOMAL 16S RRNA

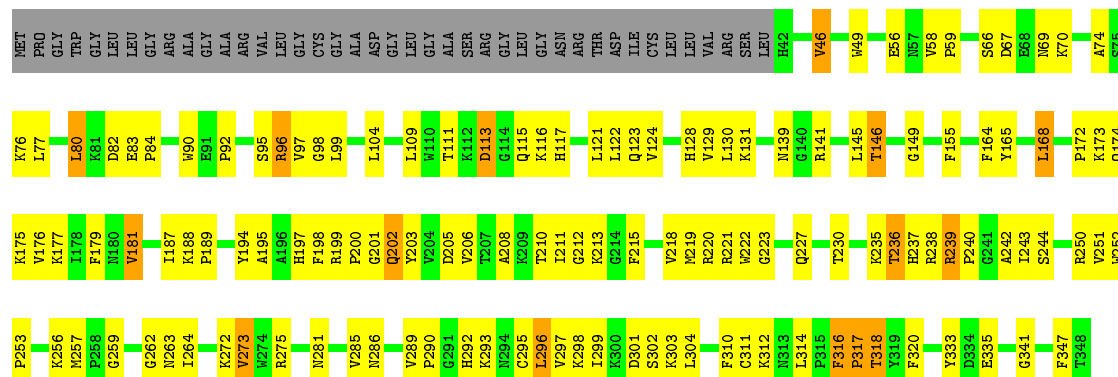


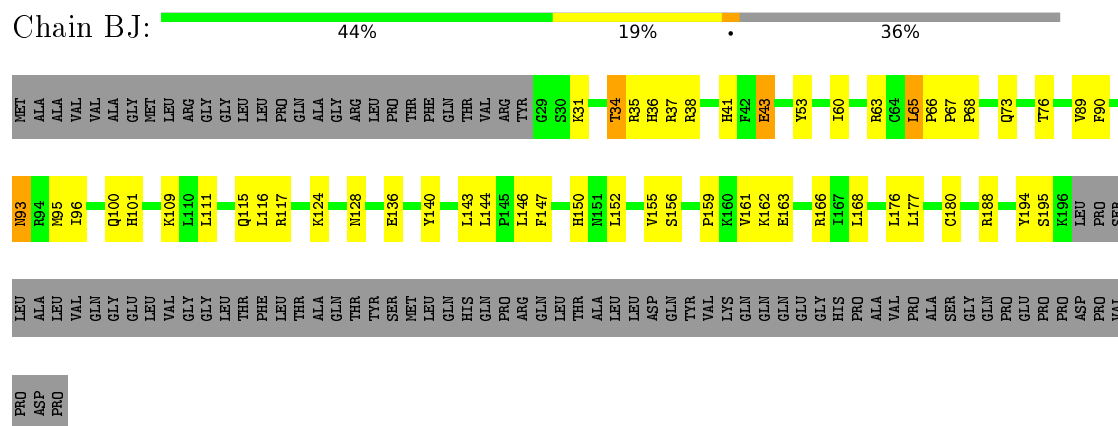




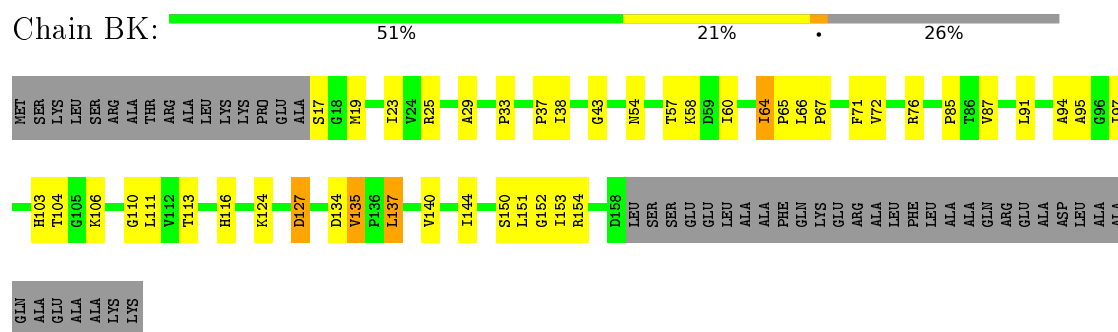
• Molecule 49: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain BE: 50% 34% 12%

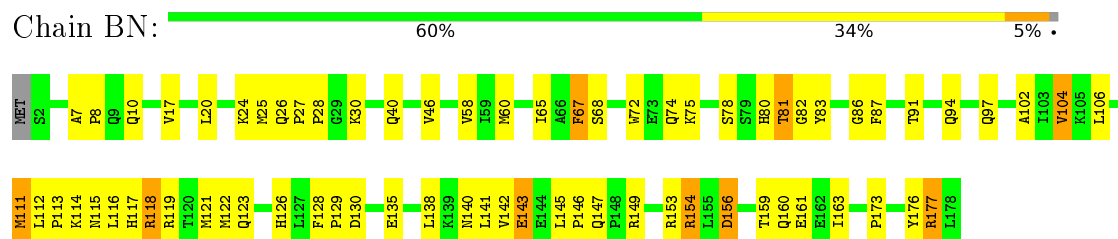




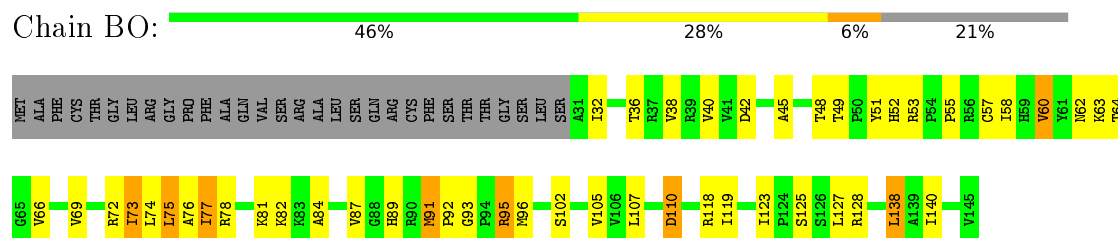
- Molecule 53: MITORIBOSOMAL PROTEIN UL11M, MRPL11



- Molecule 54: MITORIBOSOMAL PROTEIN UL13M, MRPL13

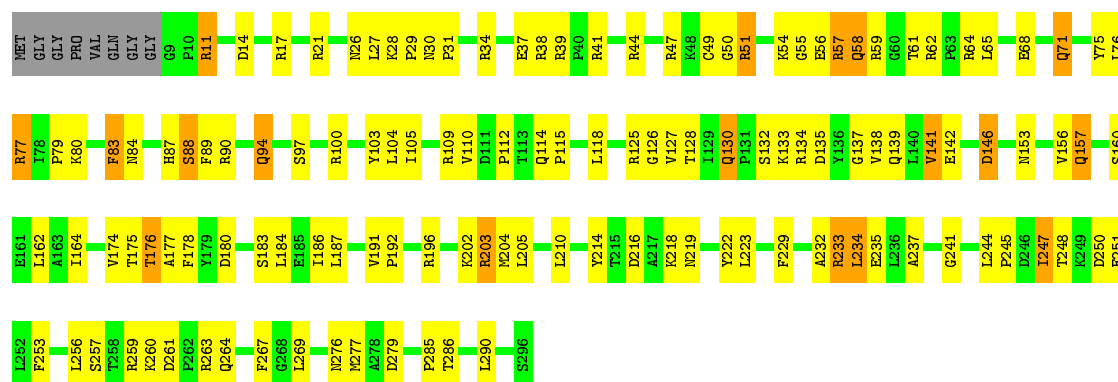


- Molecule 55: MITORIBOSOMAL PROTEIN UL14M, MRPL14



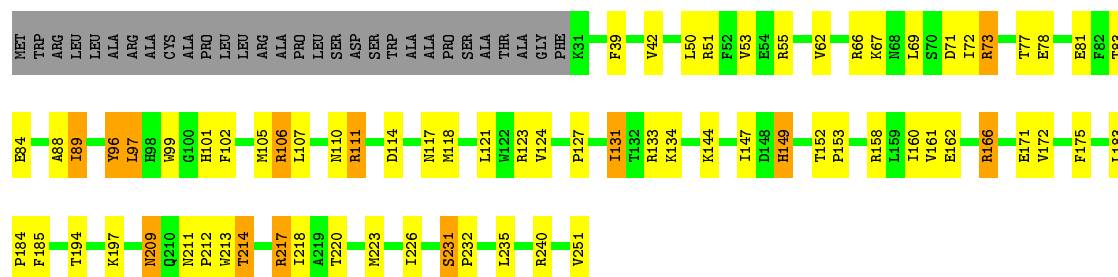
- Molecule 56: MITORIBOSOMAL PROTEIN UL15M, MRPL15





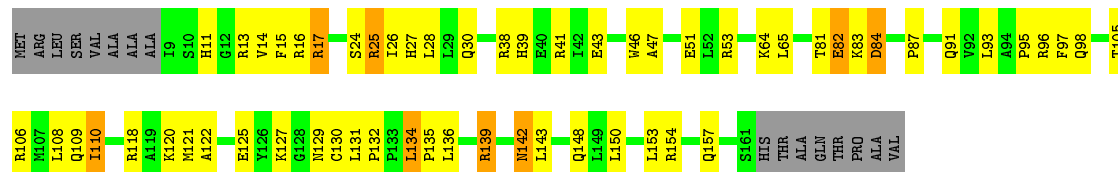
• Molecule 57: MITORIBOSOMAL PROTEIN UL16M, MRPL16

Chain BQ: 59% 24% 5% 12%



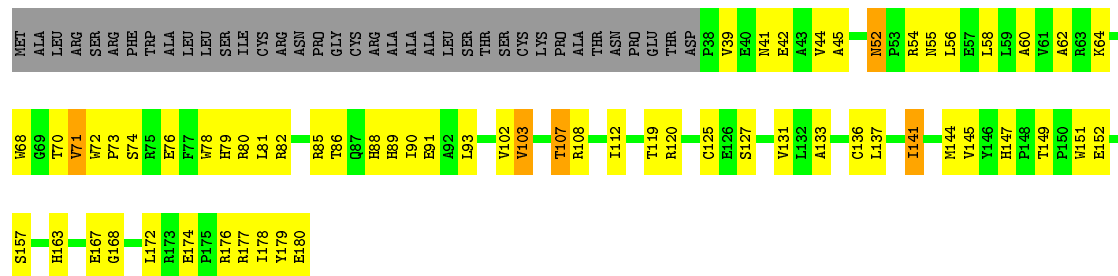
• Molecule 58: MITORIBOSOMAL PROTEIN BL17M, MRPL17

Chain BR: 56% 30% 5% 9%



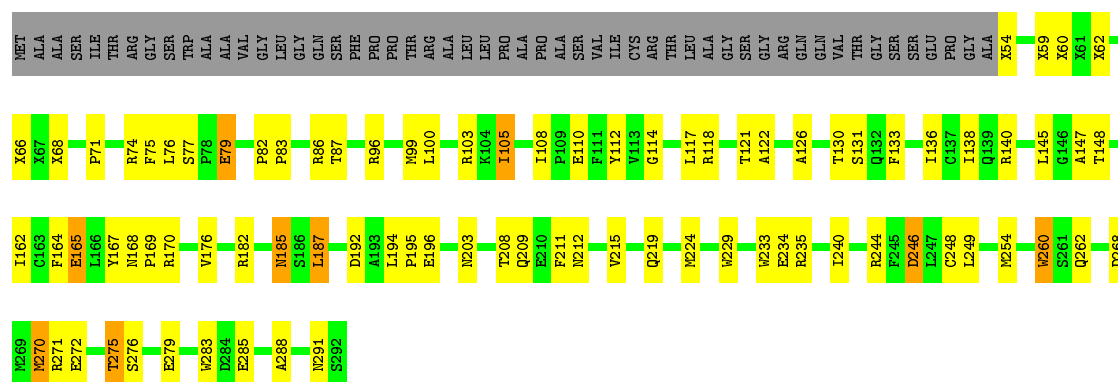
• Molecule 59: MITORIBOSOMAL PROTEIN UL18M, MRPL18

Chain BS: 44% 32% 21% 3%



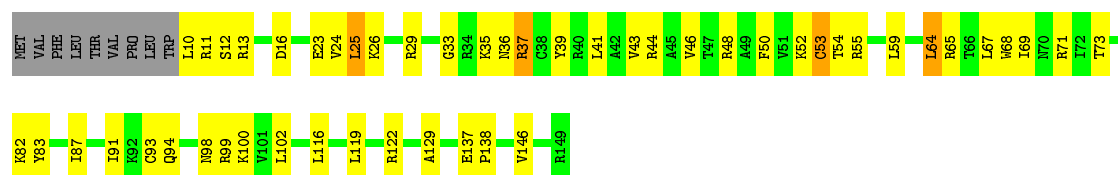
• Molecule 60: MITORIBOSOMAL PROTEIN BL19M, MRPL19

Chain BT: 53% 26% 18% 3%



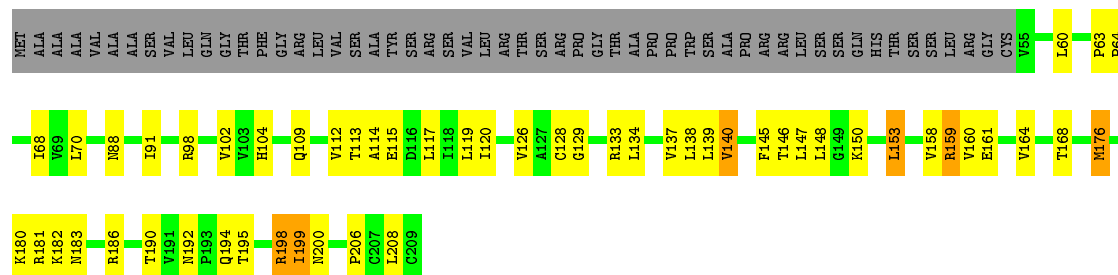
- Molecule 61: MITORIBOSOMAL PROTEIN BL20M, MRPL20

Chain BU: 60% 31% 6%



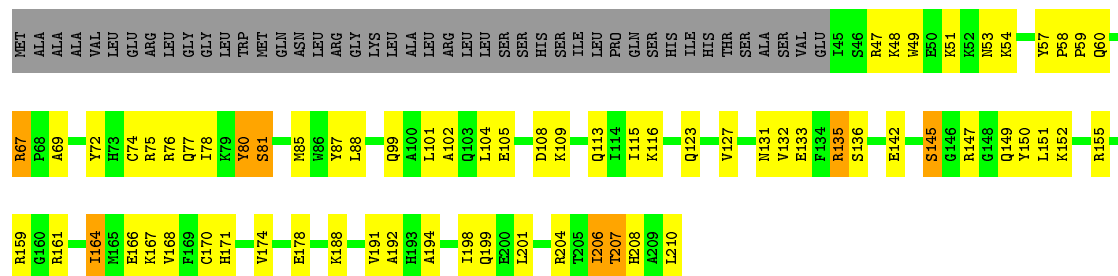
- Molecule 62: MITORIBOSOMAL PROTEIN BL21M, MRPL21

Chain BV: 48% 23% 26%



- Molecule 63: MITORIBOSOMAL PROTEIN UL22M, MRPL22

Chain BW: 46% 30% 21%

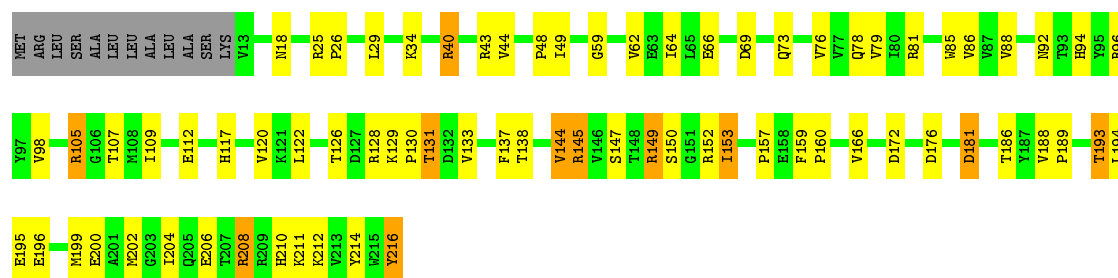


- Molecule 64: MITORIBOSOMAL PROTEIN UL23M, MRPL23


Chain BX: 51% 33% 5% 11%

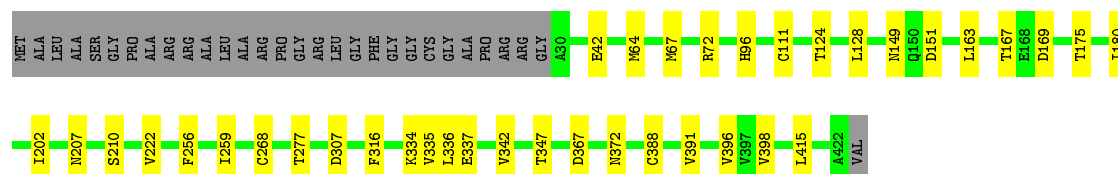
- Molecule 65: MITORIBOSOMAL PROTEIN UL24M, MRPL24

Chain BY: 



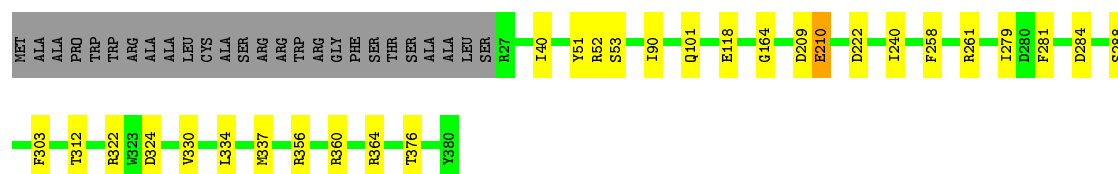
- Molecule 66: MITORIBOSOMAL PROTEIN ML37, MRPL37

Chain Ba:  84% 9% 7%

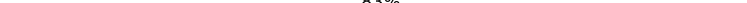


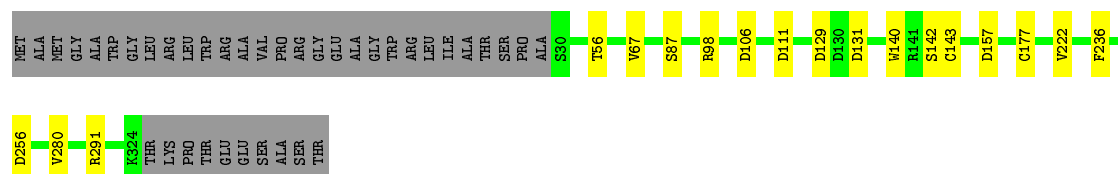
- Molecule 67: MITORIBOSOMAL PROTEIN ML38, MRPL38

Chain Bb: 86% 7% 7%



- Molecule 68: MITORIBOSOMAL PROTEIN ML39, MRPL39

Chain Bc: 



- Molecule 69: MITORIBOSOMAL PROTEIN ML40, MRPL40

[illegible]

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|
| MET | GLY | LEU | LEU | SER | GLY | ALA | ALA | ARG | ALA | LEU | VAL | ARG | GLY | ALA | S23 | R28 | V60 | L63 | F66 | R67 | L68 | V72 | E78 | T106 | H111 | Q127 | F135 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|

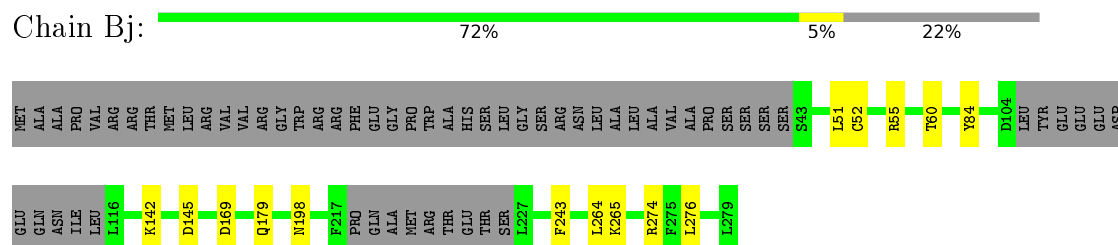
- [illegible]

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | T2 | T6 | T12 | S13 | V14 | R21 | L33 | S34 | R41 | R68 | P69 | C70 | H90 | S93 | S108 | V112 | K117 | P118 | F119 | S125 | I126 | Q149 | ASP | PRO | ALA | PRO | ALA | ALA | GLN | VAL | GLN | ALA | GLN |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

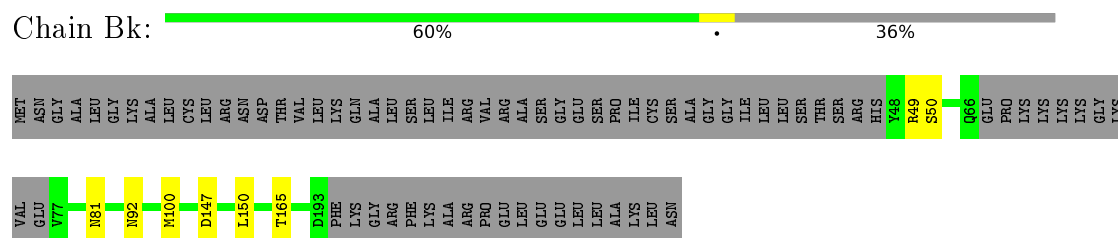
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| MET | ALA | SER | GLY | LEU | VAL | ARG | LEU | GLN | TRP | GLY | PRO | ARG | ARG | LEU | LEU | LEU | ALA | PRO | ALA | ALA | PRO | THR | LEU | ALA | ALA | PRO | PRO | VAL | ARG | GLY | A31 | K32 | K33 | L51 | K52 | C53 | R78 | T82 | F83 | S84 | C96 | Y97 | I98 | D121 | F145 | V153 | L191 | L213 | R216 |
| M231 | S251 | R259 | S263 | L267 | T288 | V289 | E293 | E294 | L301 | F307 | P319 | LYS | GLU | GLU | HIS | VAL | ALA | ALA | GLU | LYS | THR | ILE | THR | ALA | SER | | | | | | | | | | | | | | | | | | | | | | | | |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| F445 | T165 | H74 | D175 | V181 | Q196 | T221 | R230 | D237 | V242 | L243 | E244 | S258 | I276 | Q297 | G10 | G11 | V12 | H13 | P14 | G15 | P16 | P17 | A18 | A19 | A20 | A21 | A22 | SER | | | | | | | | | | | | | | | |
| MET | ALA | VAL | THR | ARG | LEU | CYS | PRO | VAL | LEU | TRP | SER | ARG | PRO | VAL | THR | GLN | SER | THR | ALA | VAL | VAL | PRO | VAL | ARG | THR | LYS | ARG | PHE | THR | PRO | THR | TYR | GLN | PRO | LYS | LYS | SER | GLU | LYS | GLY | P56 | R74 | T100 |

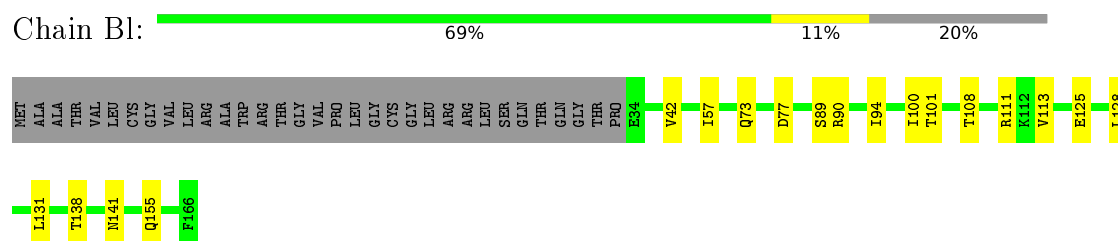
- Molecule 75: MITORIBOSOMAL PROTEIN ML46, MRPL46



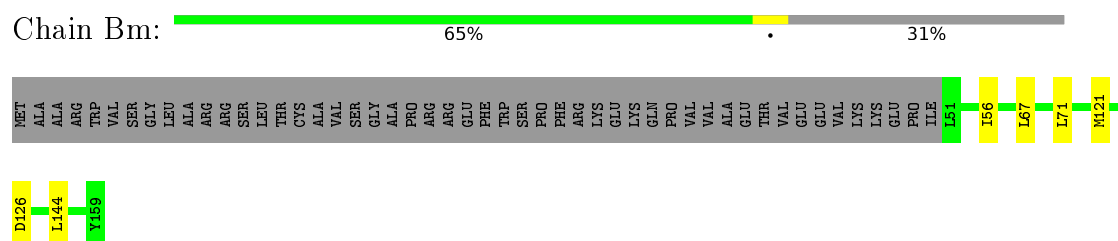
- Molecule 76: MITORIBOSOMAL PROTEIN ML48, MRPL48



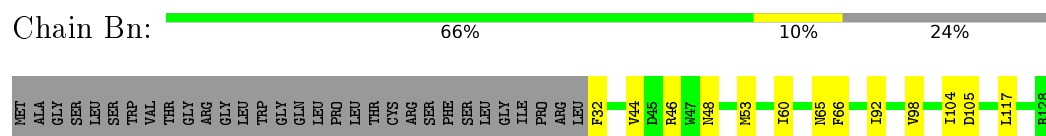
- Molecule 77: MITORIBOSOMAL PROTEIN ML49, MRPL49



- Molecule 78: MITORIBOSOMAL PROTEIN ML50, MRPL50

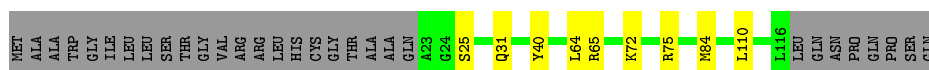


- Molecule 79: MITORIBOSOMAL PROTEIN ML51, MRPL51



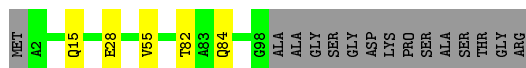
- Molecule 80: MITORIBOSOMAL PROTEIN ML52, MRPL52





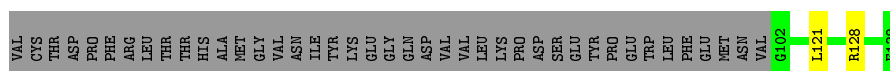
- Molecule 81: MITORIBOSOMAL PROTEIN ML53, MRPL53

Chain Bp: 82% 13%



- Molecule 82: MITORIBOSOMAL PROTEIN ML54, MRPL54

Chain Bq: 25% 73%



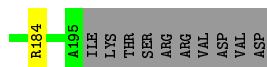
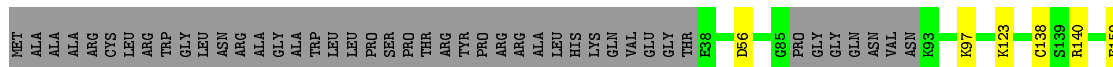
- Molecule 83: MITORIBOSOMAL PROTEIN ML63, MRPL57

Chain Bt: 78% 14% 8%



- Molecule 84: MITORIBOSOMAL PROTEIN ML62, MRPL58

Chain Bu: 70% 26%



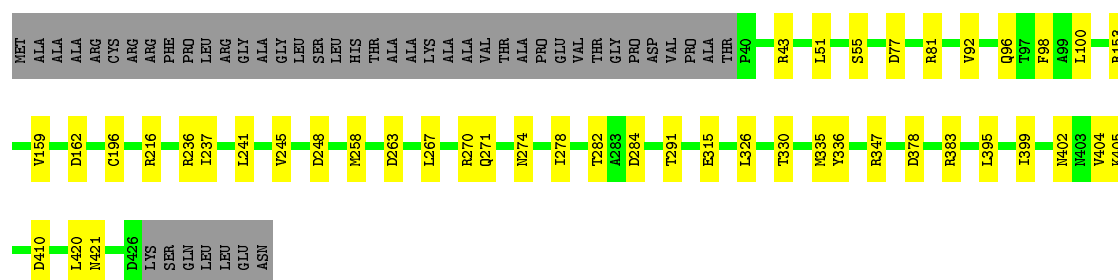
- Molecule 85: MITORIBOSOMAL PROTEIN ML64, MRPL59

Chain Bv: 56% 41%



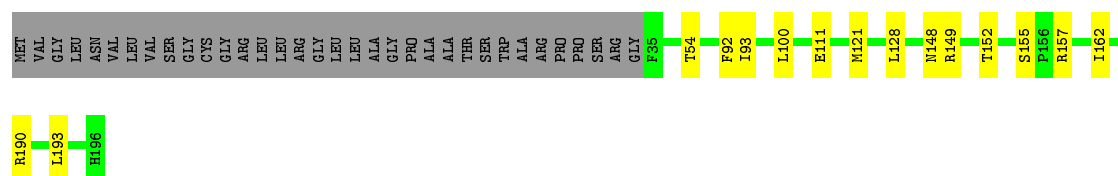
- Molecule 86: MITORIBOSOMAL PROTEIN ML65, MRPS30

Chain Bw: 79% 10% 11%



- Molecule 87: MITORIBOSOMAL PROTEIN ML66, MRPS18A

Chain Bx: 75% 8% 17%



- Molecule 88: UNASSIGNED SECONDARY STRUCTURE ELEMENTS

Chain Bz: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, Y5P, ZN, P5P, MG

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 > 2$	RMSZ	# $ Z > 2$
1	AA	0.47	2/22852 (0.0%)	1.00	23/35580 (0.1%)
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
2	AB	0.35	0/1804	0.52	0/2445
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
3	AC	0.32	0/1105	0.53	0/1496
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
38	B2	0.42	0/1582	0.56	0/2118
39	B3	0.49	0/993	0.66	0/1341
4	AE	0.34	0/2673	0.52	0/3591
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%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >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
5	AF	0.36	0/1008	0.59	0/1358
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
6	AG	0.34	0/1763	0.49	0/2368
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
7	AI	0.32	0/2455	0.45	0/3291
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%)
8	AJ	0.36	0/1091	0.56	0/1474
80	Bo	0.45	0/762	0.59	0/1022
81	Bp	0.32	0/752	0.54	0/1013
82	Bq	0.32	0/346	0.44	0/463

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
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
9	AK	0.35	0/1021	0.60	0/1381
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
49	BE	0	1
57	BQ	0	1
60	BT	0	1
67	Bb	0	2
79	Bn	0	1
83	Bt	0	1
9	AK	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(°)	Ideal(°)
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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20411	0	10345	323	0
2	AB	1762	0	1774	43	0
3	AC	1075	0	1087	33	0
4	AE	2621	0	2640	91	0
5	AF	990	0	1025	36	0
6	AG	1721	0	1747	41	0
7	AI	2498	0	2473	79	0
8	AJ	1067	0	1101	42	0
9	AK	1001	0	1037	39	0
10	AL	840	0	890	26	0
11	AN	858	0	883	41	0
12	AO	1448	0	1536	29	0
13	AP	932	0	951	25	0
14	AQ	853	0	913	35	0
15	AR	784	0	813	29	0
16	AU	734	0	745	28	0
17	AV	1251	0	823	70	0
17	AY	1251	0	824	78	0
18	AX	231	0	157	7	0
19	Aa	2296	0	2317	0	0
20	Ab	1101	0	1118	0	0
21	Ac	1367	0	1385	0	0
22	Ad	1467	0	1466	0	0
23	Ae	2016	0	2028	0	0
24	Af	778	0	791	0	0
25	Ag	2774	0	2810	0	0
26	Ah	876	0	832	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Ai	824	0	842	0	0
28	Aj	1777	0	1788	0	0
29	Ak	2222	0	2270	0	0
30	Am	930	0	959	0	0
31	An	639	0	709	0	0
32	Ao	3028	0	3081	0	0
33	Ap	1551	0	1519	0	0
34	As	96	0	98	0	0
35	Az	102	0	104	0	0
36	B0	878	0	896	31	0
37	B1	2036	0	2058	57	0
38	B2	1544	0	1580	46	0
39	B3	968	0	1018	29	0
40	B4	381	0	400	8	0
41	B5	902	0	916	37	0
42	B6	391	0	429	23	0
43	B7	387	0	413	14	0
44	B8	833	0	883	38	0
45	B9	335	0	359	16	0
46	BA	32233	0	16311	642	0
47	BB	1008	0	555	29	0
48	BD	1860	0	1923	69	0
49	BE	2420	0	2418	108	0
50	BF	2011	0	2049	82	0
51	BI	805	0	845	26	0
52	BJ	1361	0	1448	37	0
53	BK	1081	0	1146	35	0
54	BN	1444	0	1437	50	0
55	BO	896	0	946	39	0
56	BP	2312	0	2373	112	0
57	BQ	1792	0	1832	51	0
58	BR	1240	0	1260	46	0
59	BS	1168	0	1159	50	0
60	BT	1950	0	1969	62	0
61	BU	1159	0	1228	49	0
62	BV	1231	0	1278	43	0
63	BW	1374	0	1405	47	0
64	BX	1120	0	1133	48	0
65	BY	1663	0	1665	57	0
66	Ba	3173	0	3153	0	0
67	Bb	2952	0	2840	0	0
68	Bc	2408	0	2415	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	Bd	832	0	828	0	0
70	Be	968	0	968	0	0
71	Bf	852	0	834	0	0
72	Bg	1167	0	1173	0	0
73	Bh	2319	0	2332	0	0
74	Bi	1979	0	1974	0	0
75	Bj	1775	0	1797	0	0
76	Bk	1087	0	1080	0	0
77	Bl	1097	0	1080	0	0
78	Bm	893	0	878	0	0
79	Bn	837	0	860	0	0
80	Bo	747	0	748	0	0
81	Bp	742	0	749	0	0
82	Bq	336	0	342	0	0
83	Bt	780	0	792	0	0
84	Bu	1208	0	1227	0	0
85	Bv	1068	0	1032	0	0
86	Bw	3126	0	3153	0	0
87	Bx	1325	0	1354	0	0
88	Bz	564	0	574	0	0
89	AA	146	0	0	0	0
89	Ag	1	0	0	0	0
89	B0	1	0	0	0	0
89	B2	1	0	0	0	0
89	BA	195	0	0	0	0
89	BD	2	0	0	0	0
89	BE	1	0	0	0	0
89	BP	1	0	0	0	0
89	BR	2	0	0	0	0
89	BX	1	0	0	0	0
90	AR	1	0	0	0	0
90	Ac	1	0	0	0	0
90	Ap	1	0	0	0	0
90	B5	1	0	0	0	0
90	B9	1	0	0	0	0
90	Bx	1	0	0	0	0
91	Ag	28	0	12	0	0
92	AA	114	0	0	7	0
92	Ag	4	0	0	0	0
92	B0	3	0	0	0	0
92	B7	2	0	0	0	0
92	B8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BA	196	0	0	12	0
92	BD	3	0	0	0	0
92	BF	4	0	0	0	0
92	BI	1	0	0	0	0
92	BO	2	0	0	0	0
92	BP	3	0	0	2	0
92	BR	2	0	0	0	0
92	BU	1	0	0	0	0
92	BW	4	0	0	0	0
All	All	167915	0	141408	2642	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 2642 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AV:54:Y5P:N3	17:AV:58:Y5P:H5	1.56	1.20
92:AA:8117:HOH:O	17:AV:29:Y5P:H4A	1.44	1.17
44:B8:142:ARG:NH1	46:BA:1191:C:OP2	1.90	1.05
53:BK:124:LYS:NZ	53:BK:127:ASP:OD2	1.89	1.05
55:BO:72:ARG:HH11	55:BO:72:ARG:HB2	1.22	1.02

There are no symmetry-related clashes.

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AE	324/328 (99%)	305 (94%)	18 (6%)	1 (0%)	46	83
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%)	12	58
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
16	AU	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
19	Aa	243/356 (68%)	238 (98%)	4 (2%)	1 (0%)	39	80
20	Ab	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	Ac	167/169 (99%)	157 (94%)	9 (5%)	1 (1%)	30	74
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%)	39	80
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	19	66
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
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%)	26	72
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%)	46	83
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Bh	287/332 (86%)	269 (94%)	18 (6%)	0	100	100
74	Bi	240/312 (77%)	227 (95%)	12 (5%)	1 (0%)	39	80
75	Bj	211/279 (76%)	198 (94%)	12 (6%)	1 (0%)	34	77
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
85	Bv	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
86	Bw	385/433 (89%)	359 (93%)	25 (6%)	1 (0%)	46	83
87	Bx	160/196 (82%)	154 (96%)	5 (3%)	1 (1%)	30	74
All	All	12706/16216 (78%)	12149 (96%)	542 (4%)	15 (0%)	59	90

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%)	9	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	115/115 (100%)	101 (88%)	14 (12%)	6	34
4	AE	273/273 (100%)	245 (90%)	28 (10%)	9	42
5	AF	108/109 (99%)	99 (92%)	9 (8%)	14	52
6	AG	181/181 (100%)	169 (93%)	12 (7%)	21	62
7	AI	250/250 (100%)	236 (94%)	14 (6%)	26	67
8	AJ	119/181 (66%)	107 (90%)	12 (10%)	9	43
9	AK	102/102 (100%)	89 (87%)	13 (13%)	5	32
10	AL	92/92 (100%)	82 (89%)	10 (11%)	8	40
11	AN	92/114 (81%)	79 (86%)	13 (14%)	4	29
12	AO	159/205 (78%)	155 (98%)	4 (2%)	55	83
13	AP	97/97 (100%)	93 (96%)	4 (4%)	37	74
14	AQ	94/94 (100%)	87 (93%)	7 (7%)	17	57
15	AR	89/89 (100%)	83 (93%)	6 (7%)	20	62
16	AU	77/77 (100%)	65 (84%)	12 (16%)	3	24
19	Aa	222/272 (82%)	207 (93%)	15 (7%)	20	61
20	Ab	113/162 (70%)	106 (94%)	7 (6%)	23	64
21	Ac	152/152 (100%)	138 (91%)	14 (9%)	11	48
22	Ad	149/149 (100%)	142 (95%)	7 (5%)	32	72
24	Af	86/160 (54%)	80 (93%)	6 (7%)	19	60
25	Ag	290/334 (87%)	268 (92%)	22 (8%)	16	56
26	Ah	95/95 (100%)	93 (98%)	2 (2%)	61	86
27	Ai	86/86 (100%)	80 (93%)	6 (7%)	19	60
28	Aj	182/184 (99%)	171 (94%)	11 (6%)	24	65
29	Ak	249/249 (100%)	227 (91%)	22 (9%)	12	50
30	Am	100/100 (100%)	90 (90%)	10 (10%)	9	43
31	An	66/66 (100%)	57 (86%)	9 (14%)	5	30
32	Ao	79/118 (67%)	74 (94%)	5 (6%)	22	63
33	Ap	168/168 (100%)	152 (90%)	16 (10%)	11	46
36	B0	92/115 (80%)	83 (90%)	9 (10%)	10	44
37	B1	219/229 (96%)	195 (89%)	24 (11%)	8	39
38	B2	164/228 (72%)	143 (87%)	21 (13%)	5	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	B3	110/147 (75%)	101 (92%)	9 (8%)	14	53
40	B4	42/114 (37%)	39 (93%)	3 (7%)	18	59
41	B5	99/163 (61%)	89 (90%)	10 (10%)	9	43
42	B6	45/60 (75%)	37 (82%)	8 (18%)	2	17
43	B7	41/78 (53%)	36 (88%)	5 (12%)	6	34
44	B8	87/162 (54%)	77 (88%)	10 (12%)	7	37
45	B9	36/77 (47%)	32 (89%)	4 (11%)	8	39
48	BD	193/248 (78%)	161 (83%)	32 (17%)	3	20
49	BE	263/290 (91%)	239 (91%)	24 (9%)	12	48
50	BF	217/251 (86%)	191 (88%)	26 (12%)	6	34
51	BI	88/228 (39%)	85 (97%)	3 (3%)	44	79
52	BJ	154/230 (67%)	142 (92%)	12 (8%)	16	55
53	BK	115/151 (76%)	109 (95%)	6 (5%)	29	69
54	BN	156/157 (99%)	138 (88%)	18 (12%)	7	37
55	BO	99/123 (80%)	88 (89%)	11 (11%)	8	39
56	BP	245/249 (98%)	208 (85%)	37 (15%)	3	25
57	BQ	189/210 (90%)	170 (90%)	19 (10%)	9	43
58	BR	132/143 (92%)	114 (86%)	18 (14%)	5	30
59	BS	123/153 (80%)	114 (93%)	9 (7%)	17	58
60	BT	206/243 (85%)	187 (91%)	19 (9%)	11	48
61	BU	118/127 (93%)	109 (92%)	9 (8%)	16	56
62	BV	136/178 (76%)	121 (89%)	15 (11%)	8	39
63	BW	144/180 (80%)	125 (87%)	19 (13%)	5	31
64	BX	119/134 (89%)	102 (86%)	17 (14%)	4	28
65	BY	183/192 (95%)	159 (87%)	24 (13%)	5	31
66	Ba	348/365 (95%)	310 (89%)	38 (11%)	8	40
67	Bb	310/328 (94%)	283 (91%)	27 (9%)	13	50
68	Bc	271/299 (91%)	253 (93%)	18 (7%)	21	62
69	Bd	92/181 (51%)	86 (94%)	6 (6%)	21	62
70	Be	100/108 (93%)	89 (89%)	11 (11%)	8	39
71	Bf	80/110 (73%)	70 (88%)	10 (12%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	Bg	128/136 (94%)	111 (87%)	17 (13%)	5	31
73	Bh	251/284 (88%)	226 (90%)	25 (10%)	9	43
74	Bi	218/281 (78%)	204 (94%)	14 (6%)	22	63
75	Bj	190/242 (78%)	176 (93%)	14 (7%)	17	57
76	Bk	119/181 (66%)	111 (93%)	8 (7%)	20	62
77	Bl	122/147 (83%)	104 (85%)	18 (15%)	4	26
78	Bm	103/145 (71%)	97 (94%)	6 (6%)	25	66
79	Bn	88/113 (78%)	77 (88%)	11 (12%)	6	33
80	Bo	74/97 (76%)	65 (88%)	9 (12%)	6	34
81	Bp	79/88 (90%)	74 (94%)	5 (6%)	22	63
82	Bq	36/114 (32%)	34 (94%)	2 (6%)	26	67
83	Bt	75/82 (92%)	62 (83%)	13 (17%)	2	18
84	Bu	126/169 (75%)	119 (94%)	7 (6%)	26	67
85	Bv	102/173 (59%)	96 (94%)	6 (6%)	24	66
86	Bw	340/373 (91%)	296 (87%)	44 (13%)	5	32
87	Bx	149/173 (86%)	135 (91%)	14 (9%)	11	47
All	All	11288/13510 (84%)	10215 (90%)	1073 (10%)	15	46

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

Mol	Chain	Res	Type
49	BE	311	CYS
56	BP	286	THR
83	Bt	25	ARG
50	BF	129	VAL
54	BN	122	MET

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

Mol	Chain	Res	Type
42	B6	45	HIS
54	BN	74	GLN
84	Bu	103	HIS
49	BE	156	HIS
50	BF	201	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	294	G
46	BA	446	A
46	BA	1423	A
46	BA	347	G
46	BA	350	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	AV	1	-	15,16,20	3.46	3 (20%)	18,22,29	2.87	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	Y5P	AV	10	-	14,19,20	3.59	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	11	-	14,19,20	4.79	3 (21%)	18,26,29	1.84	1 (5%)
17	Y5P	AV	12	-	14,19,20	3.10	2 (14%)	18,26,29	2.99	2 (11%)
17	Y5P	AV	13	-	14,19,20	4.65	3 (21%)	18,26,29	1.80	1 (5%)
17	Y5P	AV	14	-	14,19,20	3.65	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AV	15	-	14,19,20	3.60	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AV	2	-	14,19,20	5.10	3 (21%)	18,26,29	1.56	1 (5%)
17	Y5P	AV	21	-	14,19,20	3.69	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AV	22	-	14,19,20	3.61	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	23	-	14,19,20	3.59	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	24	-	14,19,20	3.62	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	25	-	14,19,20	4.96	3 (21%)	18,26,29	1.57	1 (5%)
17	Y5P	AV	26	-	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	27	-	14,19,20	3.66	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AV	28	-	14,19,20	3.61	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AV	29	-	14,19,20	3.55	3 (21%)	18,26,29	2.88	2 (11%)
17	Y5P	AV	3	-	14,19,20	5.02	3 (21%)	18,26,29	1.59	1 (5%)
17	Y5P	AV	30	-	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	31	-	14,19,20	3.62	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	32	-	14,19,20	3.28	2 (14%)	18,26,29	2.88	2 (11%)
17	Y5P	AV	33	-	14,19,20	3.73	2 (14%)	18,26,29	2.39	2 (11%)
17	P5P	AV	34	-	16,23,24	1.48	2 (12%)	15,33,36	2.00	2 (13%)
17	P5P	AV	35	-	16,23,24	0.77	1 (6%)	15,33,36	0.76	0
17	P5P	AV	36	-	16,23,24	0.74	0	15,33,36	0.77	0
17	Y5P	AV	37	-	14,19,20	3.64	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	38	-	14,19,20	3.59	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AV	39	-	14,19,20	3.35	2 (14%)	18,26,29	2.90	2 (11%)
17	Y5P	AV	4	-	14,19,20	5.00	3 (21%)	18,26,29	1.66	1 (5%)
17	Y5P	AV	40	-	14,19,20	5.04	3 (21%)	18,26,29	1.66	1 (5%)
17	Y5P	AV	41	-	14,19,20	5.23	3 (21%)	18,26,29	1.61	1 (5%)
17	Y5P	AV	42	-	14,19,20	5.13	3 (21%)	18,26,29	1.60	1 (5%)
17	Y5P	AV	43	-	14,19,20	4.99	3 (21%)	18,26,29	1.61	1 (5%)
17	Y5P	AV	44	-	14,19,20	3.65	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	45	-	14,19,20	3.28	2 (14%)	18,26,29	2.62	2 (11%)
17	Y5P	AV	48	-	14,19,20	5.03	3 (21%)	18,26,29	1.73	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	Y5P	AV	49	-	14,19,20	4.77	3 (21%)	18,26,29	1.72	1 (5%)
17	Y5P	AV	5	-	14,19,20	3.64	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AV	50	-	14,19,20	3.25	3 (21%)	18,26,29	2.79	2 (11%)
17	Y5P	AV	51	-	14,19,20	3.25	2 (14%)	18,26,29	2.73	2 (11%)
17	Y5P	AV	52	-	14,19,20	3.62	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AV	53	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	54	-	14,19,20	3.20	2 (14%)	18,26,29	2.95	2 (11%)
17	Y5P	AV	55	-	14,19,20	3.28	2 (14%)	18,26,29	2.73	2 (11%)
17	Y5P	AV	56	-	14,19,20	4.85	3 (21%)	18,26,29	1.67	1 (5%)
17	Y5P	AV	57	-	14,19,20	3.67	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AV	58	-	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	59	-	14,19,20	3.33	3 (21%)	18,26,29	2.89	2 (11%)
17	Y5P	AV	6	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	60	-	14,19,20	3.32	2 (14%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	61	-	14,19,20	4.92	3 (21%)	18,26,29	1.67	1 (5%)
17	Y5P	AV	62	-	14,19,20	4.87	3 (21%)	18,26,29	1.82	1 (5%)
17	Y5P	AV	63	-	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	64	-	14,19,20	3.66	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	65	-	14,19,20	3.62	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AV	66	-	14,19,20	3.24	2 (14%)	18,26,29	2.72	2 (11%)
17	Y5P	AV	67	-	14,19,20	4.91	3 (21%)	18,26,29	1.66	1 (5%)
17	Y5P	AV	68	-	14,19,20	4.91	3 (21%)	18,26,29	1.65	1 (5%)
17	Y5P	AV	69	-	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	7	-	14,19,20	3.57	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AV	70	-	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	71	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	72	-	14,19,20	4.96	3 (21%)	18,26,29	1.56	1 (5%)
17	Y5P	AV	73	-	14,19,20	3.66	3 (21%)	18,26,29	2.96	4 (22%)
17	Y5P	AV	74	-	14,19,20	4.86	3 (21%)	18,26,29	1.64	1 (5%)
17	Y5P	AV	75	-	14,19,20	4.94	2 (14%)	18,26,29	1.68	1 (5%)
17	P5P	AV	76	-	16,23,24	0.67	0	15,33,36	0.75	1 (6%)
17	Y5P	AV	8	-	14,19,20	3.26	2 (14%)	18,26,29	3.08	2 (11%)
17	Y5P	AV	9	-	14,19,20	3.59	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	AX	12	-	15,16,20	3.04	2 (13%)	18,22,29	2.94	2 (11%)
18	Y5P	AX	13	-	14,19,20	3.26	3 (21%)	18,26,29	2.91	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	AX	14	-	14,19,20	3.23	3 (21%)	18,26,29	2.70	2 (11%)
18	Y5P	AX	15	-	14,19,20	3.07	3 (21%)	18,26,29	2.95	2 (11%)
18	Y5P	AX	16	-	14,19,20	3.29	3 (21%)	18,26,29	2.93	2 (11%)
18	Y5P	AX	17	-	14,19,20	3.43	2 (14%)	18,26,29	2.88	2 (11%)
18	Y5P	AX	18	-	14,19,20	4.96	3 (21%)	18,26,29	1.62	1 (5%)
18	Y5P	AX	19	-	14,19,20	3.38	3 (21%)	18,26,29	2.80	2 (11%)
18	Y5P	AX	20	-	14,19,20	3.32	2 (14%)	18,26,29	2.87	2 (11%)
18	Y5P	AX	21	-	14,19,20	5.12	3 (21%)	18,26,29	1.61	1 (5%)
18	Y5P	AX	22	-	14,19,20	3.18	3 (21%)	18,26,29	2.92	2 (11%)
18	Y5P	AX	23	-	14,19,20	3.11	3 (21%)	18,26,29	2.97	2 (11%)
18	Y5P	AX	24	-	14,19,20	3.26	3 (21%)	18,26,29	2.72	2 (11%)
17	Y5P	AY	1	-	15,16,20	3.49	3 (20%)	18,22,29	2.84	2 (11%)
17	Y5P	AY	10	-	14,19,20	3.58	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	11	-	14,19,20	4.89	3 (21%)	18,26,29	1.65	1 (5%)
17	Y5P	AY	12	-	14,19,20	3.25	2 (14%)	18,26,29	2.89	2 (11%)
17	Y5P	AY	13	-	14,19,20	4.83	3 (21%)	18,26,29	1.80	1 (5%)
17	Y5P	AY	14	-	14,19,20	3.59	3 (21%)	18,26,29	2.81	2 (11%)
17	Y5P	AY	15	-	14,19,20	3.60	3 (21%)	18,26,29	2.88	3 (16%)
17	Y5P	AY	2	-	14,19,20	4.77	3 (21%)	18,26,29	1.76	1 (5%)
17	Y5P	AY	21	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	22	-	14,19,20	3.61	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	23	-	14,19,20	3.60	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	24	-	14,19,20	3.60	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AY	25	-	14,19,20	4.95	3 (21%)	18,26,29	1.77	1 (5%)
17	Y5P	AY	26	-	14,19,20	3.67	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	27	-	14,19,20	3.63	3 (21%)	18,26,29	2.88	3 (16%)
17	Y5P	AY	28	-	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	29	-	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	3	-	14,19,20	4.75	2 (14%)	18,26,29	1.86	1 (5%)
17	Y5P	AY	30	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	31	-	14,19,20	3.62	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	32	-	14,19,20	3.38	2 (14%)	18,26,29	2.78	2 (11%)
17	Y5P	AY	33	-	14,19,20	3.53	2 (14%)	18,26,29	2.63	2 (11%)
17	P5P	AY	34	-	16,23,24	1.36	2 (12%)	15,33,36	1.97	3 (20%)
17	P5P	AY	35	-	16,23,24	0.73	0	15,33,36	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	P5P	AY	36	-	16,23,24	0.74	0	15,33,36	1.02	0
17	Y5P	AY	37	-	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	38	-	14,19,20	3.61	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	39	-	14,19,20	3.24	2 (14%)	18,26,29	2.97	2 (11%)
17	Y5P	AY	4	-	14,19,20	4.89	3 (21%)	18,26,29	1.82	1 (5%)
17	Y5P	AY	40	-	14,19,20	4.99	2 (14%)	18,26,29	1.82	1 (5%)
17	Y5P	AY	41	-	14,19,20	4.97	3 (21%)	18,26,29	1.80	1 (5%)
17	Y5P	AY	42	-	14,19,20	4.86	3 (21%)	18,26,29	1.87	1 (5%)
17	Y5P	AY	43	-	14,19,20	4.90	3 (21%)	18,26,29	1.82	1 (5%)
17	Y5P	AY	44	-	14,19,20	3.64	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	45	-	14,19,20	3.38	2 (14%)	18,26,29	2.95	2 (11%)
17	Y5P	AY	48	-	14,19,20	4.96	3 (21%)	18,26,29	1.69	1 (5%)
17	Y5P	AY	49	-	14,19,20	4.84	3 (21%)	18,26,29	1.77	1 (5%)
17	Y5P	AY	5	-	14,19,20	3.59	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	50	-	14,19,20	3.33	2 (14%)	18,26,29	2.93	2 (11%)
17	Y5P	AY	51	-	14,19,20	3.16	2 (14%)	18,26,29	3.05	2 (11%)
17	Y5P	AY	52	-	14,19,20	3.58	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AY	53	-	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	54	-	14,19,20	3.16	2 (14%)	18,26,29	3.04	2 (11%)
17	Y5P	AY	55	-	14,19,20	3.53	3 (21%)	18,26,29	2.83	3 (16%)
17	Y5P	AY	56	-	14,19,20	4.86	3 (21%)	18,26,29	1.71	1 (5%)
17	Y5P	AY	57	-	14,19,20	3.62	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	58	-	14,19,20	3.61	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AY	59	-	14,19,20	3.26	2 (14%)	18,26,29	2.87	2 (11%)
17	Y5P	AY	6	-	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	60	-	14,19,20	3.21	2 (14%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	61	-	14,19,20	4.94	3 (21%)	18,26,29	1.78	1 (5%)
17	Y5P	AY	62	-	14,19,20	4.94	3 (21%)	18,26,29	1.86	1 (5%)
17	Y5P	AY	63	-	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	64	-	14,19,20	3.64	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AY	65	-	14,19,20	3.63	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AY	66	-	14,19,20	3.23	2 (14%)	18,26,29	2.88	2 (11%)
17	Y5P	AY	67	-	14,19,20	4.98	3 (21%)	18,26,29	1.65	1 (5%)
17	Y5P	AY	68	-	14,19,20	4.82	3 (21%)	18,26,29	1.75	1 (5%)
17	Y5P	AY	69	-	14,19,20	3.63	3 (21%)	18,26,29	2.90	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	Y5P	AY	7	-	14,19,20	3.59	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	70	-	14,19,20	3.66	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	71	-	14,19,20	3.64	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AY	72	-	14,19,20	4.91	3 (21%)	18,26,29	1.51	1 (5%)
17	Y5P	AY	73	-	14,19,20	3.70	3 (21%)	18,26,29	3.00	4 (22%)
17	Y5P	AY	74	-	14,19,20	4.80	3 (21%)	18,26,29	1.62	1 (5%)
17	Y5P	AY	75	-	14,19,20	4.82	3 (21%)	18,26,29	1.70	1 (5%)
17	P5P	AY	76	-	16,23,24	0.69	0	15,33,36	0.75	0
17	Y5P	AY	8	-	14,19,20	3.20	2 (14%)	18,26,29	2.94	2 (11%)
17	Y5P	AY	9	-	14,19,20	3.60	3 (21%)	18,26,29	2.83	2 (11%)
47	P5P	BB	10	47	16,23,24	1.28	3 (18%)	15,33,36	1.90	3 (20%)
47	Y5P	BB	11	47	14,19,20	5.08	3 (21%)	18,26,29	1.56	1 (5%)
47	Y5P	BB	12	47	14,19,20	3.15	2 (14%)	18,26,29	2.78	2 (11%)
47	Y5P	BB	13	47	14,19,20	3.14	2 (14%)	18,26,29	3.06	2 (11%)
47	P5P	BB	14	47	16,23,24	0.69	0	15,33,36	0.94	0
47	P5P	BB	15	47	16,23,24	0.69	0	15,33,36	0.70	0
47	P5P	BB	23	47	16,23,24	0.74	1 (6%)	15,33,36	2.05	3 (20%)
47	P5P	BB	24	47	16,23,24	0.86	1 (6%)	15,33,36	0.90	0
47	P5P	BB	25	47	16,23,24	1.43	3 (18%)	15,33,36	2.09	3 (20%)
47	Y5P	BB	26	47	14,19,20	4.91	3 (21%)	18,26,29	1.88	1 (5%)
47	P5P	BB	27	47	16,23,24	0.71	0	15,33,36	1.04	1 (6%)
47	P5P	BB	28	47	16,23,24	0.70	0	15,33,36	0.69	0
47	P5P	BB	29	47	16,23,24	1.34	2 (12%)	15,33,36	2.07	3 (20%)
47	P5P	BB	30	47	16,23,24	1.31	2 (12%)	15,33,36	1.75	2 (13%)
47	Y5P	BB	31	47	14,19,20	5.08	3 (21%)	18,26,29	1.73	1 (5%)
47	P5P	BB	32	47	16,23,24	0.74	0	15,33,36	0.81	0
47	Y5P	BB	33	47	14,19,20	5.04	3 (21%)	18,26,29	1.77	1 (5%)
47	Y5P	BB	34	47	14,19,20	3.26	3 (21%)	18,26,29	2.71	2 (11%)
47	P5P	BB	35	47	16,23,24	1.40	2 (12%)	15,33,36	1.96	2 (13%)
47	P5P	BB	36	47	16,23,24	0.73	0	15,33,36	0.90	0
47	P5P	BB	37	47	16,23,24	0.75	0	15,33,36	1.08	1 (6%)
47	P5P	BB	38	47	16,23,24	0.76	0	15,33,36	0.84	0
47	P5P	BB	39	47	16,23,24	0.74	0	15,33,36	0.76	0
47	Y5P	BB	40	47	14,19,20	3.34	2 (14%)	18,26,29	2.73	2 (11%)
47	P5P	BB	41	47	16,23,24	1.36	3 (18%)	15,33,36	2.02	2 (13%)
47	Y5P	BB	42	47	14,19,20	4.92	3 (21%)	18,26,29	1.71	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	Y5P	BB	43	47	14,19,20	4.84	3 (21%)	18,26,29	1.77	1 (5%)
47	Y5P	BB	44	47	14,19,20	3.38	2 (14%)	18,26,29	2.65	2 (11%)
47	P5P	BB	45	47	16,23,24	0.73	0	15,33,36	0.77	0
47	P5P	BB	46	47	16,23,24	1.26	3 (18%)	15,33,36	1.74	2 (13%)
47	P5P	BB	47	47	16,23,24	0.67	0	15,33,36	0.92	1 (6%)
47	Y5P	BB	48	47	14,19,20	3.18	2 (14%)	18,26,29	2.92	2 (11%)
47	P5P	BB	49	47	16,23,24	1.38	2 (12%)	15,33,36	1.96	2 (13%)
47	P5P	BB	5	47	16,23,24	0.71	0	15,33,36	0.75	0
47	P5P	BB	50	47	16,23,24	0.76	0	15,33,36	0.87	0
47	P5P	BB	51	47	16,23,24	1.35	2 (12%)	15,33,36	1.91	2 (13%)
47	Y5P	BB	52	47	14,19,20	4.95	3 (21%)	18,26,29	1.75	1 (5%)
47	Y5P	BB	53	47	14,19,20	4.95	3 (21%)	18,26,29	1.75	1 (5%)
47	P5P	BB	58	47	16,23,24	0.70	0	15,33,36	0.73	0
47	P5P	BB	59	47	16,23,24	1.35	2 (12%)	15,33,36	1.87	2 (13%)
47	Y5P	BB	6	47	14,19,20	3.31	2 (14%)	18,26,29	2.77	2 (11%)
47	Y5P	BB	60	47	14,19,20	4.75	3 (21%)	18,26,29	1.85	1 (5%)
47	Y5P	BB	61	47	14,19,20	3.15	2 (14%)	18,26,29	2.75	2 (11%)
47	Y5P	BB	62	47	14,19,20	3.20	2 (14%)	18,26,29	2.93	2 (11%)
47	Y5P	BB	63	47	14,19,20	4.98	3 (21%)	18,26,29	1.72	1 (5%)
47	P5P	BB	64	47	16,23,24	0.70	0	15,33,36	0.81	0
47	Y5P	BB	65	47	14,19,20	3.30	2 (14%)	18,26,29	2.93	2 (11%)
47	P5P	BB	66	47	16,23,24	0.73	0	15,33,36	0.77	0
47	P5P	BB	7	47	16,23,24	1.32	2 (12%)	15,33,36	1.92	2 (13%)
47	Y5P	BB	8	47	14,19,20	3.19	2 (14%)	18,26,29	3.04	2 (11%)
47	P5P	BB	9	47	16,23,24	0.70	0	15,33,36	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	1	-	-	0/6/30/34	0/2/2/2
17	Y5P	AV	10	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	11	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	12	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	13	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	14	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	15	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	2	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	21	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	22	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	23	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	24	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	25	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	26	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	27	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	28	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	29	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	3	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	30	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	31	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	32	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	33	-	-	0/7/33/34	0/2/2/2
17	P5P	AV	34	-	-	0/3/25/26	0/3/3/3
17	P5P	AV	35	-	-	0/3/25/26	0/3/3/3
17	P5P	AV	36	-	-	0/3/25/26	0/3/3/3
17	Y5P	AV	37	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	38	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	39	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	4	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	40	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	41	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	42	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	43	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	44	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	45	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	48	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	49	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	5	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	50	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	51	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	52	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	53	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	54	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	55	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	56	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	57	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	58	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	59	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	6	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	60	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	61	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	62	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	63	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	64	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	65	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	66	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	67	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	68	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	69	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	7	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	70	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	71	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	72	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	73	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	74	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	75	-	-	0/7/33/34	0/2/2/2
17	P5P	AV	76	-	-	0/3/25/26	0/3/3/3
17	Y5P	AV	8	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	9	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	12	-	-	0/6/30/34	0/2/2/2
18	Y5P	AX	13	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	14	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	15	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	16	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	17	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	18	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	19	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	20	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	21	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	22	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	23	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	24	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	1	-	-	0/6/30/34	0/2/2/2
17	Y5P	AY	10	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	11	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	12	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	13	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	14	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	15	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	2	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	21	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	22	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	23	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	24	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	25	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	26	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	27	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	28	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	29	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	3	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	30	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	31	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	32	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	33	-	-	0/7/33/34	0/2/2/2
17	P5P	AY	34	-	-	0/3/25/26	0/3/3/3
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	Y5P	AY	37	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	38	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	39	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	4	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	40	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	41	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	42	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	43	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	44	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	45	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	48	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	49	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	5	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	50	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	51	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	52	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	53	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	54	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	55	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	56	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	57	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	58	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	59	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	6	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	60	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	61	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	62	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	63	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	64	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	65	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	66	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	67	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	68	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	69	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	7	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	70	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	71	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	72	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	73	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	74	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	75	-	-	0/7/33/34	0/2/2/2
17	P5P	AY	76	-	-	0/3/25/26	0/3/3/3
17	Y5P	AY	8	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	9	-	-	0/7/33/34	0/2/2/2
47	P5P	BB	10	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	11	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	12	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	13	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	14	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	15	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	23	47	-	1/3/25/26	0/3/3/3
47	P5P	BB	24	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	25	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	26	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	27	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	28	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	29	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	30	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	31	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	32	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	33	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	34	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	35	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	36	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	37	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	38	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	39	47	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	Y5P	BB	40	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	41	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	42	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	43	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	44	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	45	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	46	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	47	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	48	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	49	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	5	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	50	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	51	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	52	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	53	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	58	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	59	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	6	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	60	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	61	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	62	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	63	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	64	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	65	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	66	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	7	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	8	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	9	47	-	0/3/25/26	0/3/3/3

The worst 5 of 486 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	41	Y5P	C4-N3	-19.22	1.33	1.46
18	AX	21	Y5P	C4-N3	-18.84	1.33	1.46
17	AV	42	Y5P	C4-N3	-18.82	1.33	1.46
17	AV	2	Y5P	C4-N3	-18.61	1.33	1.46
47	BB	31	Y5P	C4-N3	-18.55	1.33	1.46

The worst 5 of 322 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AV	8	Y5P	N1-C2-N3	-12.27	114.18	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	BB	13	Y5P	N1-C2-N3	-12.16	114.28	125.85
17	AY	51	Y5P	N1-C2-N3	-12.09	114.35	125.85
17	AY	54	Y5P	N1-C2-N3	-12.08	114.36	125.85
47	BB	8	Y5P	N1-C2-N3	-12.06	114.38	125.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	BB	23	P5P	P-O5'-C5'-C4'

There are no ring outliers.

141 monomers are involved in 183 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	10	Y5P	2	0
17	AV	11	Y5P	2	0
17	AV	12	Y5P	1	0
17	AV	13	Y5P	1	0
17	AV	14	Y5P	1	0
17	AV	2	Y5P	2	0
17	AV	21	Y5P	1	0
17	AV	24	Y5P	2	0
17	AV	25	Y5P	3	0
17	AV	26	Y5P	2	0
17	AV	27	Y5P	4	0
17	AV	28	Y5P	6	0
17	AV	29	Y5P	4	0
17	AV	3	Y5P	1	0
17	AV	30	Y5P	3	0
17	AV	31	Y5P	2	0
17	AV	32	Y5P	1	0
17	AV	33	Y5P	1	0
17	AV	34	P5P	1	0
17	AV	35	P5P	1	0
17	AV	36	P5P	2	0
17	AV	37	Y5P	5	0
17	AV	38	Y5P	4	0
17	AV	4	Y5P	1	0
17	AV	41	Y5P	1	0
17	AV	42	Y5P	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	43	Y5P	6	0
17	AV	44	Y5P	4	0
17	AV	48	Y5P	2	0
17	AV	49	Y5P	1	0
17	AV	5	Y5P	1	0
17	AV	50	Y5P	1	0
17	AV	51	Y5P	2	0
17	AV	52	Y5P	2	0
17	AV	53	Y5P	2	0
17	AV	54	Y5P	6	0
17	AV	55	Y5P	7	0
17	AV	57	Y5P	5	0
17	AV	58	Y5P	4	0
17	AV	59	Y5P	2	0
17	AV	60	Y5P	2	0
17	AV	62	Y5P	2	0
17	AV	63	Y5P	4	0
17	AV	64	Y5P	3	0
17	AV	65	Y5P	1	0
17	AV	66	Y5P	3	0
17	AV	67	Y5P	4	0
17	AV	68	Y5P	1	0
17	AV	70	Y5P	1	0
17	AV	71	Y5P	1	0
17	AV	8	Y5P	1	0
17	AV	9	Y5P	2	0
18	AX	12	Y5P	1	0
18	AX	16	Y5P	1	0
18	AX	17	Y5P	1	0
18	AX	18	Y5P	2	0
18	AX	20	Y5P	1	0
18	AX	21	Y5P	3	0
18	AX	22	Y5P	1	0
17	AY	11	Y5P	2	0
17	AY	12	Y5P	1	0
17	AY	14	Y5P	6	0
17	AY	15	Y5P	1	0
17	AY	2	Y5P	1	0
17	AY	22	Y5P	6	0
17	AY	23	Y5P	1	0
17	AY	24	Y5P	3	0
17	AY	25	Y5P	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	26	Y5P	3	0
17	AY	27	Y5P	1	0
17	AY	28	Y5P	2	0
17	AY	29	Y5P	2	0
17	AY	3	Y5P	3	0
17	AY	30	Y5P	2	0
17	AY	31	Y5P	3	0
17	AY	32	Y5P	4	0
17	AY	33	Y5P	2	0
17	AY	34	P5P	2	0
17	AY	36	P5P	2	0
17	AY	37	Y5P	3	0
17	AY	38	Y5P	3	0
17	AY	39	Y5P	2	0
17	AY	4	Y5P	1	0
17	AY	42	Y5P	1	0
17	AY	43	Y5P	2	0
17	AY	44	Y5P	1	0
17	AY	45	Y5P	1	0
17	AY	50	Y5P	1	0
17	AY	51	Y5P	1	0
17	AY	52	Y5P	1	0
17	AY	53	Y5P	1	0
17	AY	54	Y5P	6	0
17	AY	55	Y5P	14	0
17	AY	56	Y5P	1	0
17	AY	57	Y5P	3	0
17	AY	58	Y5P	11	0
17	AY	6	Y5P	3	0
17	AY	61	Y5P	1	0
17	AY	62	Y5P	2	0
17	AY	63	Y5P	1	0
17	AY	66	Y5P	1	0
17	AY	67	Y5P	3	0
17	AY	68	Y5P	4	0
17	AY	69	Y5P	2	0
17	AY	7	Y5P	2	0
17	AY	70	Y5P	2	0
17	AY	71	Y5P	2	0
17	AY	74	Y5P	2	0
17	AY	76	P5P	1	0
17	AY	8	Y5P	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	9	Y5P	6	0
47	BB	11	Y5P	1	0
47	BB	12	Y5P	1	0
47	BB	13	Y5P	2	0
47	BB	23	P5P	1	0
47	BB	24	P5P	4	0
47	BB	25	P5P	3	0
47	BB	26	Y5P	1	0
47	BB	28	P5P	1	0
47	BB	29	P5P	3	0
47	BB	30	P5P	3	0
47	BB	31	Y5P	1	0
47	BB	32	P5P	1	0
47	BB	33	Y5P	2	0
47	BB	34	Y5P	1	0
47	BB	36	P5P	1	0
47	BB	37	P5P	2	0
47	BB	38	P5P	2	0
47	BB	39	P5P	2	0
47	BB	43	Y5P	2	0
47	BB	44	Y5P	3	0
47	BB	45	P5P	1	0
47	BB	46	P5P	1	0
47	BB	47	P5P	1	0
47	BB	48	Y5P	1	0
47	BB	61	Y5P	2	0
47	BB	62	Y5P	3	0
47	BB	63	Y5P	1	0
47	BB	65	Y5P	2	0
47	BB	66	P5P	2	0
47	BB	9	P5P	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	1.41	3 (12%)	26,47,47	1.94	6 (23%)

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	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Ag	500	GDP	O4'-C1'	2.28	1.44	1.41
91	Ag	500	GDP	C5-C4	3.69	1.48	1.40
91	Ag	500	GDP	C6-C5	4.46	1.50	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	Ag	500	GDP	C5-C6-N1	-4.35	117.84	123.52
91	Ag	500	GDP	N3-C2-N1	-3.65	122.59	127.56
91	Ag	500	GDP	C6-C5-C4	-3.11	117.30	120.86
91	Ag	500	GDP	C2'-C1'-N9	-2.02	108.05	113.47
91	Ag	500	GDP	O4'-C1'-N9	2.01	111.90	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
4	AE	1
7	AI	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