wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:31 PM BST

PDB ID	:	4V19
EMDB ID:	:	EMD-2787
Title	:	Structure of the large subunit of the mammalian mitoribosome, part 1 of 2
Authors	:	Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N.
Deposited on	:	2014-09-25
Resolution	:	3.40 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

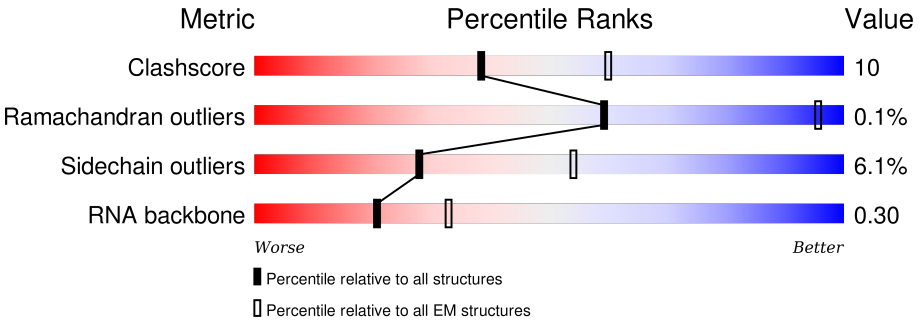
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=5%

Mol	Chain	Length	Quality of chain
1	0	148	56% 20% • 23%
2	1	256	73% 21% • 5%
3	2	252	58% 13% 29%
4	3	161	57% 16% • 27%
5	4	126	21% 14% 64%
6	5	188	43% 15% 41%
7	6	65	35% 35% • 26%
8	7	95	36% 9% • 52%

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Mol	Chain	Length	Quality of chain
9	8	188	36% 12% 49%
10	9	100	24% 13% 62%
11	A	1570	38% 37% 20%
12	B	62	42% 58%
13	C	3	33% 33% 33%
13	Z	3	100%
14	D	306	52% 25% 22%
15	E	348	64% 22% 12%
16	F	294	59% 25% 15%
17	I	268	25% 12% 63%
18	J	262	40% 24% 36%
19	K	192	48% 23% 26%
20	N	178	81% 17%
21	O	145	54% 23% 21%
22	P	296	67% 29%
23	Q	251	72% 14% 12%
24	R	169	63% 25% 9%
25	S	180	50% 28% 21%
26	T	292	55% 21% 23%
27	U	149	67% 25% 6%
28	V	209	52% 20% 26%
29	W	210	63% 14% 21%
30	X	150	61% 25% 11%
31	Y	216	66% 25% 6%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 69409 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	114	878	564	160	151	3	0	0

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	244	2036	1315	363	353	5	0	0

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	178	1544	990	289	259	6	0	0

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	118	968	622	178	165	3	0	0

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	45	381	239	77	62	3	0	0

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	110	902	553	181	162	6	0	0

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 11 is a RNA chain called MITORIBOSOMAL 16S RRNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127A	G	-	INSERTION	GB 4220565

- Molecule 12 is a RNA chain called MITORIBOSOMAL CP TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	62	Total	C	N	O	P	0	0
			1225	594	196	373	62		

- Molecule 13 is a RNA chain called TRNA.

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

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

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

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

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

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

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

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

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

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

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

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

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

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

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

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

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

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

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

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

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

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

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

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

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

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	224	Total	C	N	O	S	0	0
			1860	1189	324	338	9		

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

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

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

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

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

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

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

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

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

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

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	9	1	Total	Zn	0
			1	1	
32	5	1	Total	Zn	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	P	2	Total	Mg	0
			2	2	
33	Q	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
33	A	163	Total Mg 163 163	0
33	D	2	Total Mg 2 2	0
33	R	1	Total Mg 1 1	0

- Molecule 34 is water.

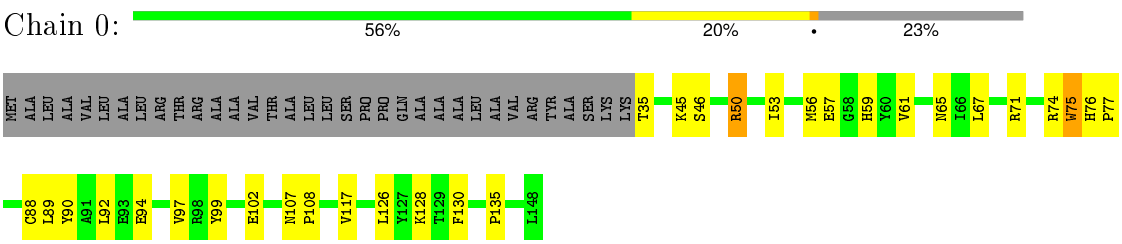
Mol	Chain	Residues	Atoms	AltConf
34	A	192	Total O 192 192	0
34	D	6	Total O 6 6	0
34	P	6	Total O 6 6	0

3 Residue-property plots (i)

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.

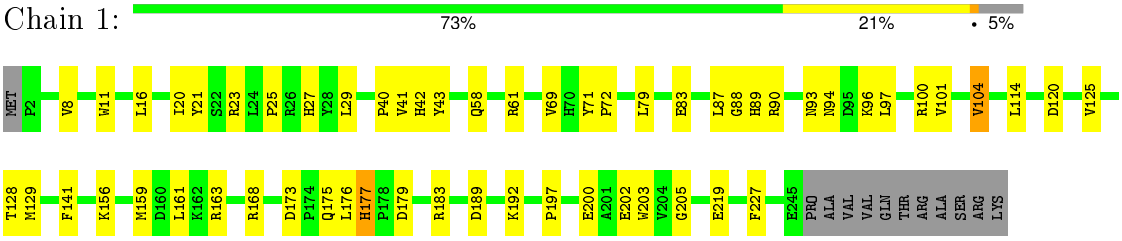
- Molecule 1: MITORIBOSOMAL PROTEIN BL27M, MRPL27

Chain 0:



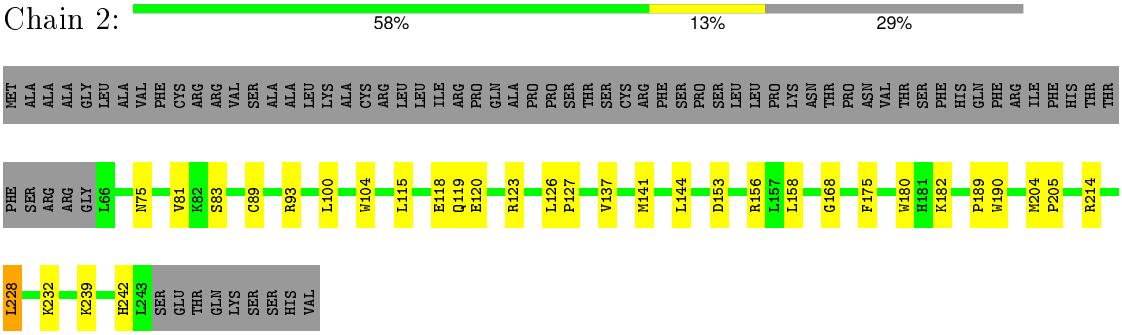
- Molecule 2: MITORIBOSOMAL PROTEIN BL28M, MRPL28

Chain 1:



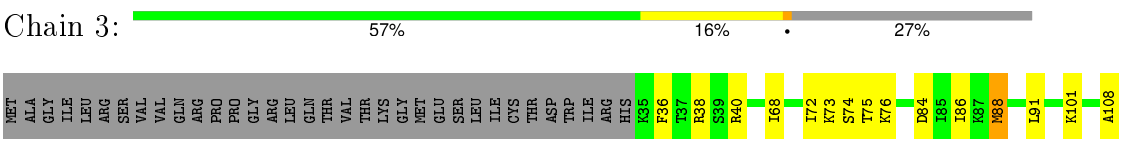
- Molecule 3: MITORIBOSOMAL PROTEIN UL29M, MRPL47

Chain 2:



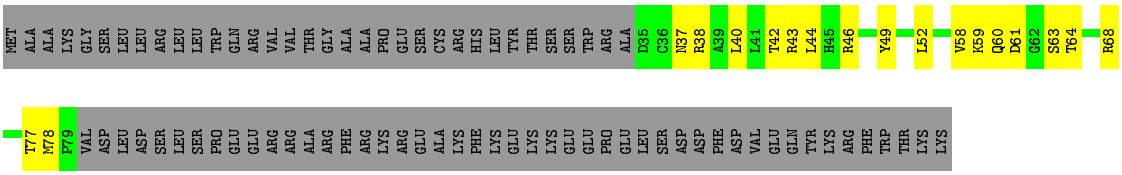
- Molecule 4: MITORIBOSOMAL PROTEIN UL30M, MRPL30

Chain 3:



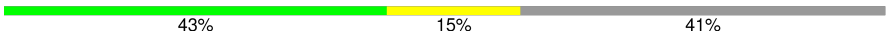
- Molecule 5: MITORIBOSOMAL PROTEIN BL31M, MRPL55

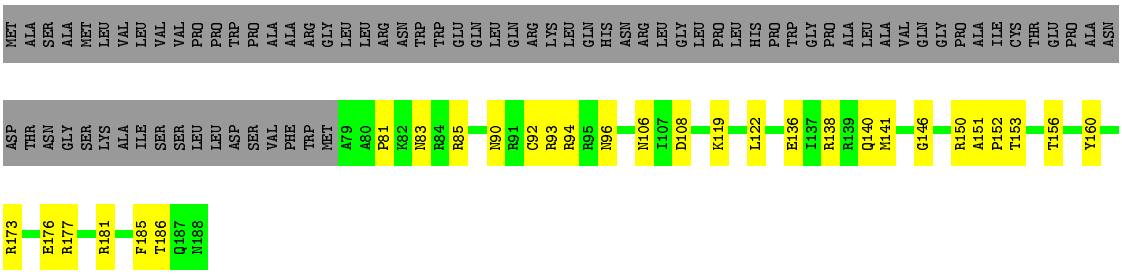
Chain 4:



- Molecule 6: MITORIBOSOMAL PROTEIN BL32M, MRPL32

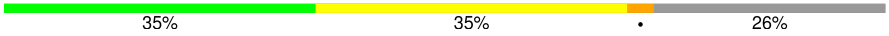
Chain 5:

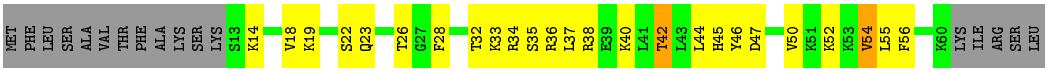




- Molecule 7: MITORIBOSOMAL PROTEIN BL33M, MRPL33

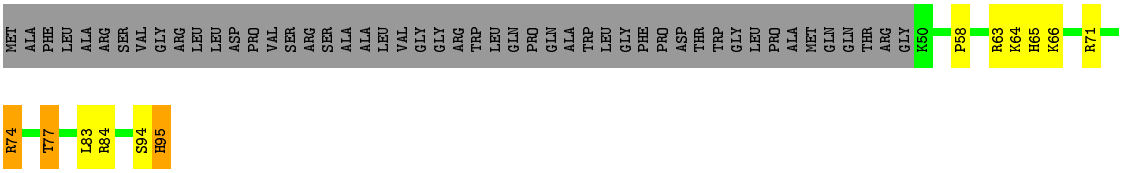
Chain 6:





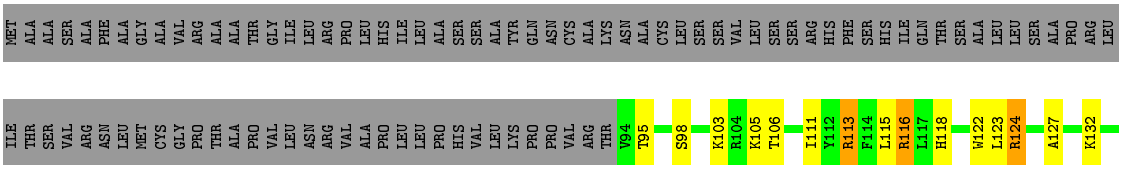
- Molecule 8: MITORIBOSOMAL PROTEIN BL34M, MRPL34

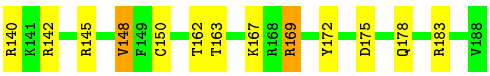
Chain 7:



- Molecule 9: MITORIBOSOMAL PROTEIN BL35M, MRPL35

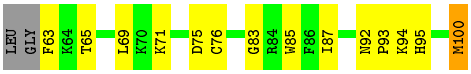
Chain 8:





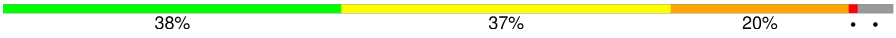
• Molecule 10: MITORIBOSOMAL PROTEIN BL36M, MRPL36

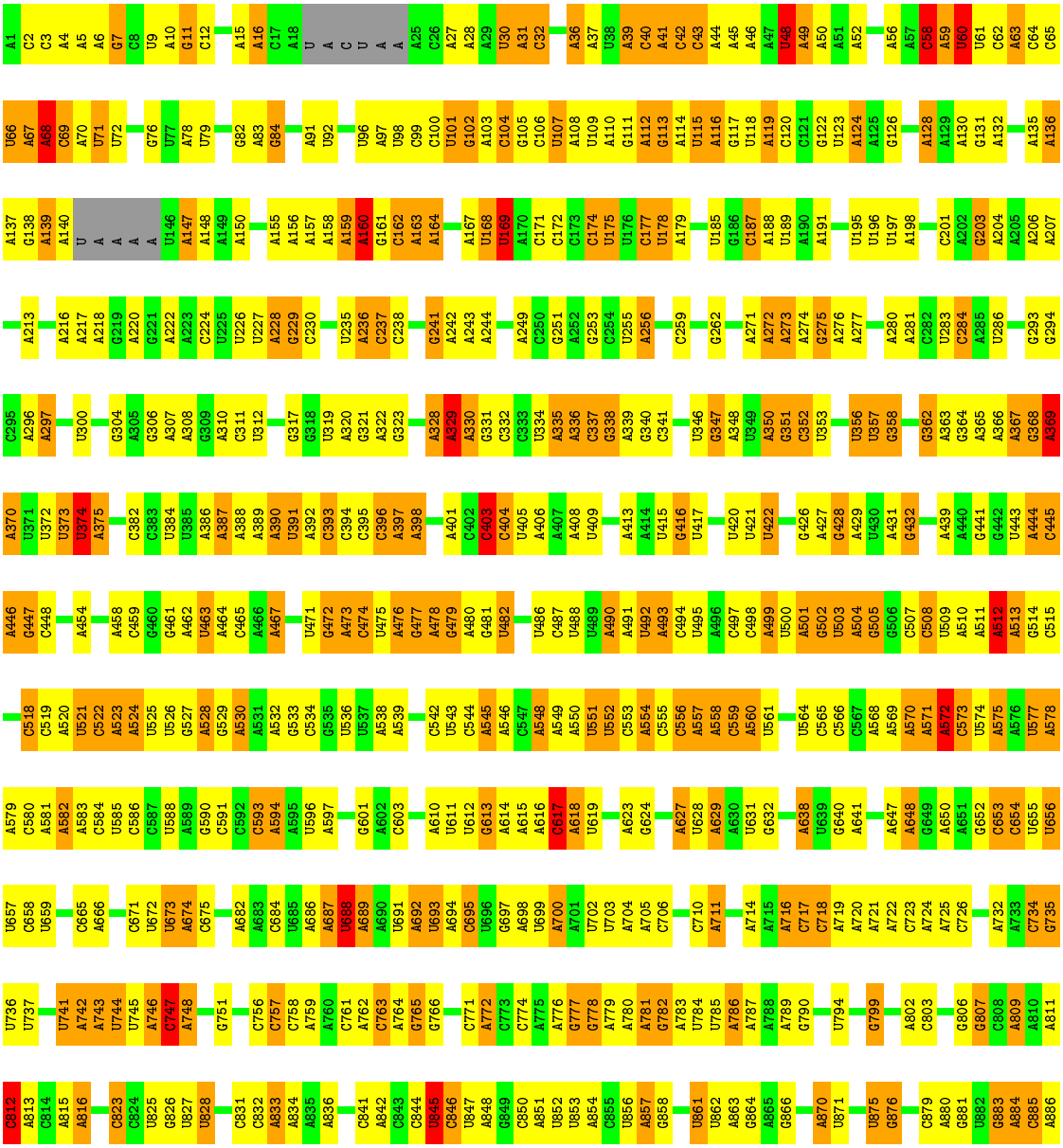
Chain 9:

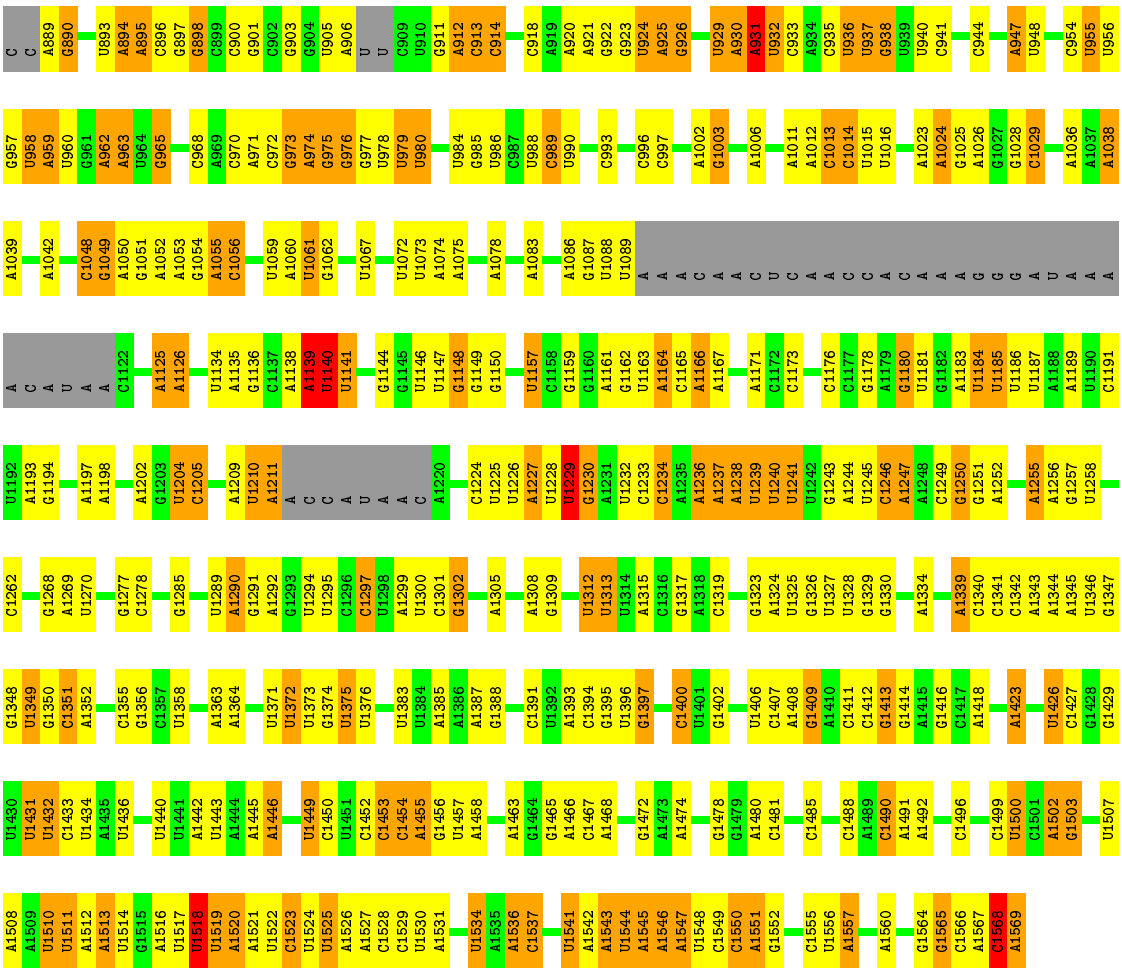


• Molecule 11: MITORIBOSOMAL 16S RRNA

Chain A:

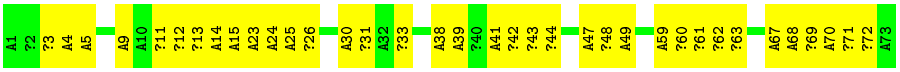






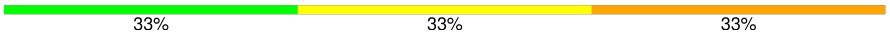
• Molecule 12: MITORIBOSOMAL CP TRNA

Chain B:



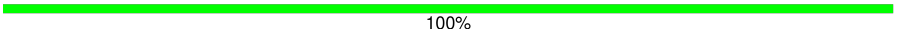
• Molecule 13: TRNA

Chain C:



• Molecule 13: TRNA

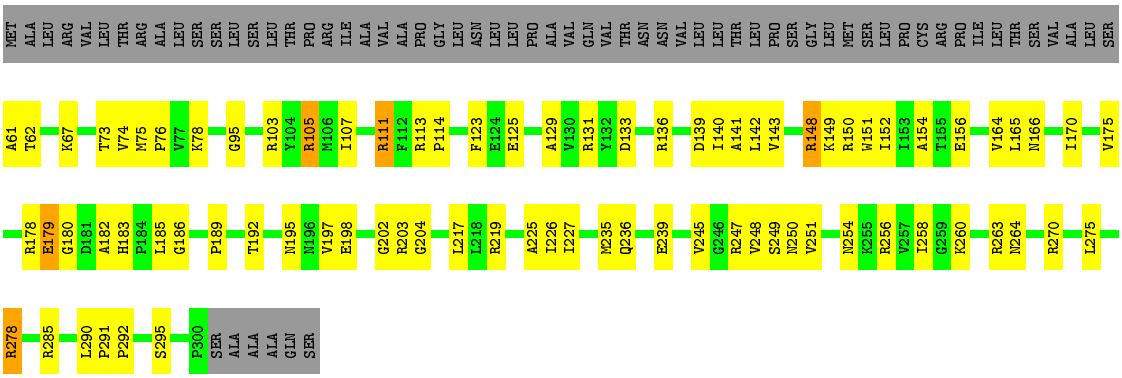
Chain Z:



There are no outlier residues recorded for this chain.

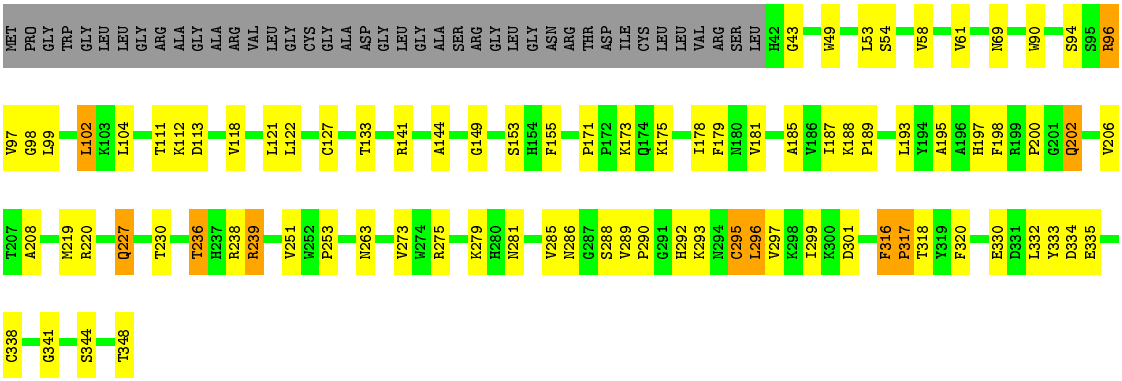
• Molecule 14: MITORIBOSOMAL PROTEIN UL2M, MRPL2

Chain D:



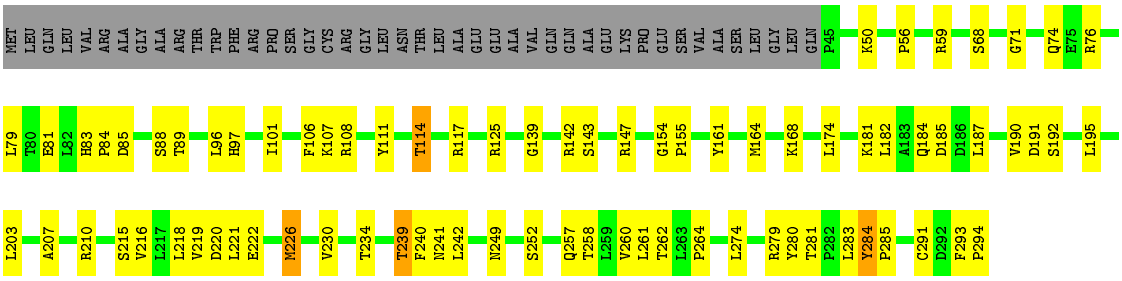
• Molecule 15: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain E:



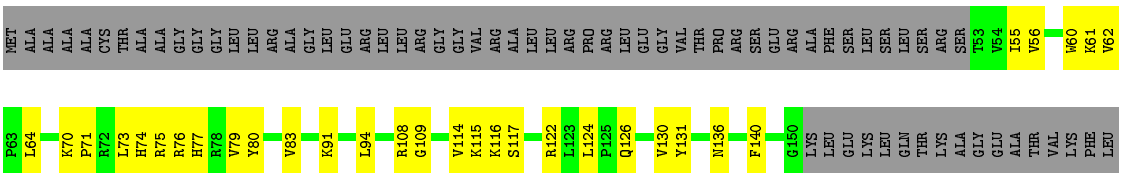
• Molecule 16: MITORIBOSOMAL PROTEIN UL4M, MRPL4

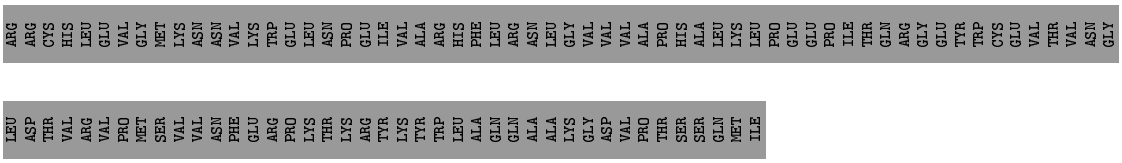
Chain F:



• Molecule 17: MITORIBOSOMAL PROTEIN BL9M, MRPL9

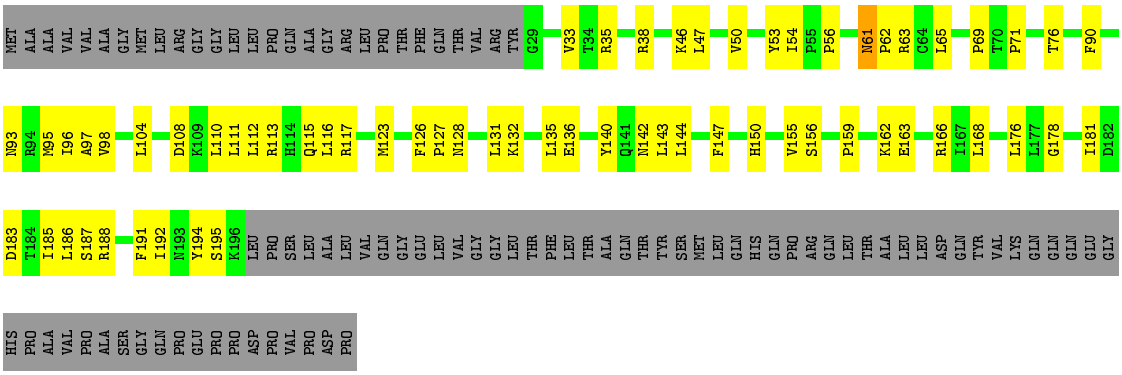
Chain I:





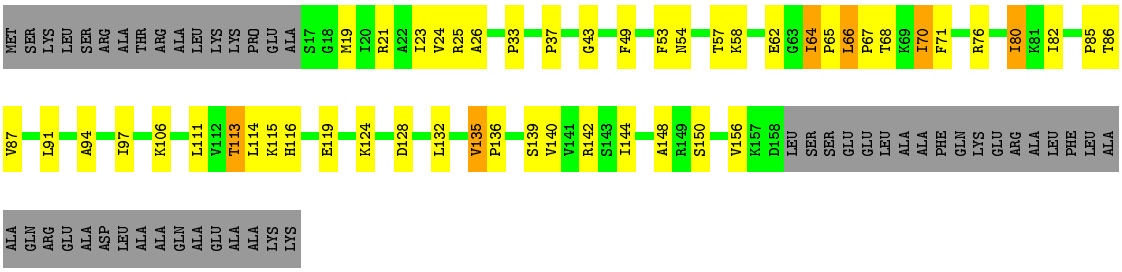
• Molecule 18: MITORIBOSOMAL PROTEIN UL10M, MRPL10

Chain J:



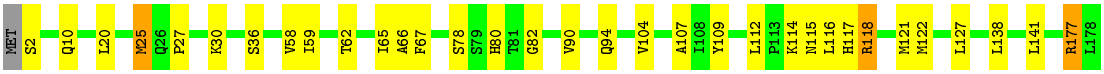
• Molecule 19: MITORIBOSOMAL PROTEIN UL11M, MRPL11

Chain K:



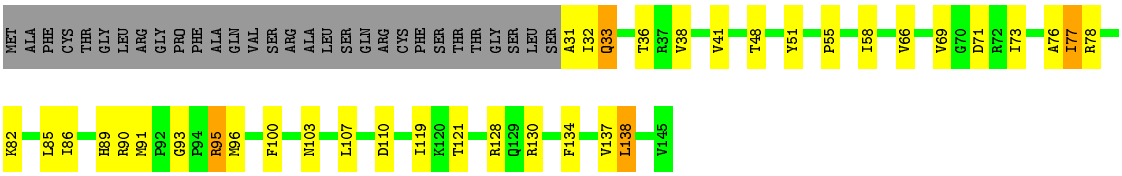
• Molecule 20: MITORIBOSOMAL PROTEIN UL13M, MRPL13

Chain N:



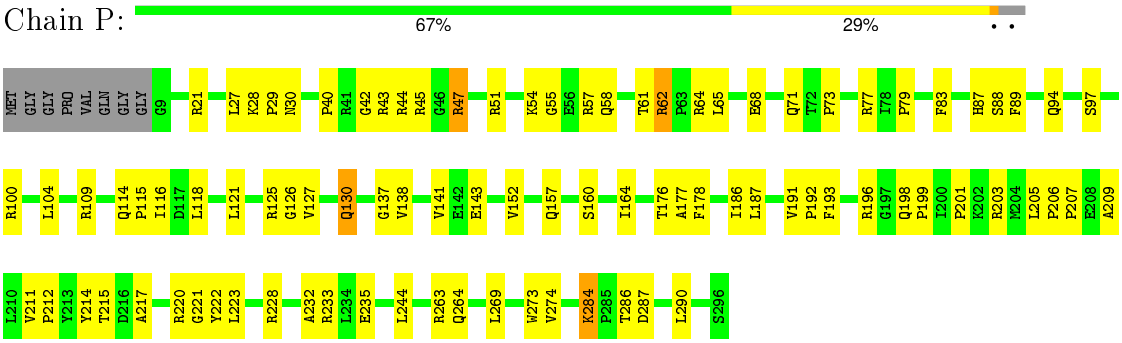
• Molecule 21: MITORIBOSOMAL PROTEIN UL14M, MRPL14

Chain O:



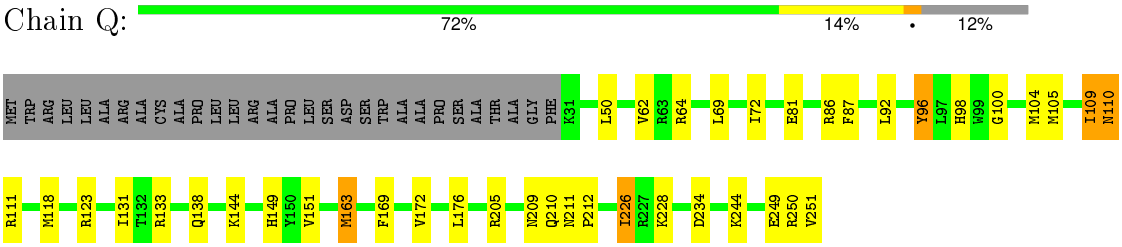
• Molecule 22: MITORIBOSOMAL PROTEIN UL15M, MRPL15

Chain P:



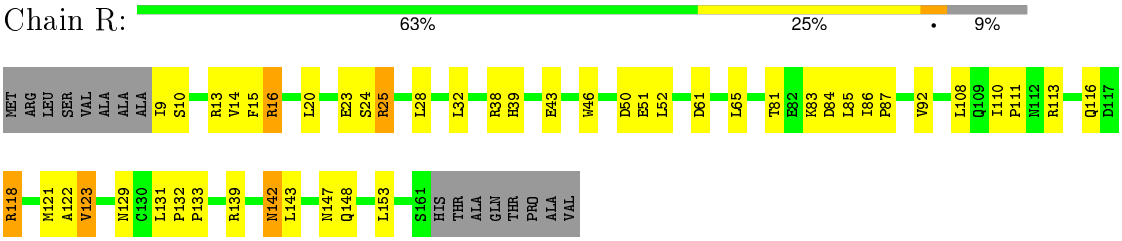
• Molecule 23: MITORIBOSOMAL PROTEIN UL16M, MRPL16

Chain Q:



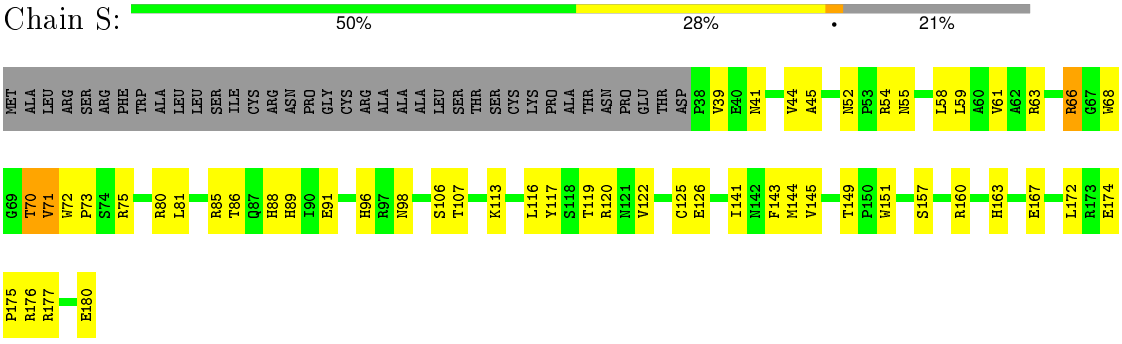
• Molecule 24: MITORIBOSOMAL PROTEIN BL17M, MRPL17

Chain R:



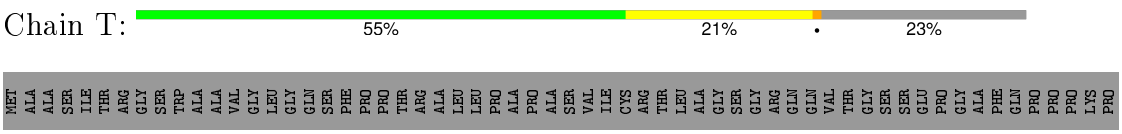
• Molecule 25: MITORIBOSOMAL PROTEIN UL18M, MRPL18

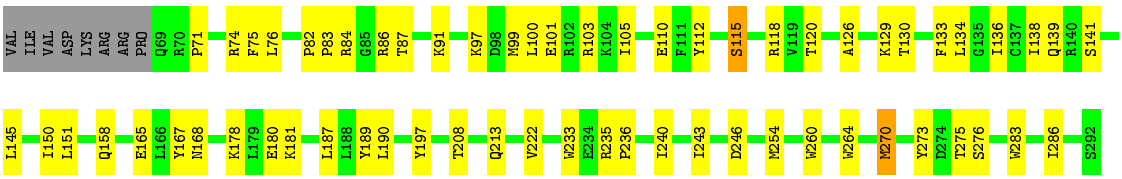
Chain S:



• Molecule 26: MITORIBOSOMAL PROTEIN BL19M, MRPL19

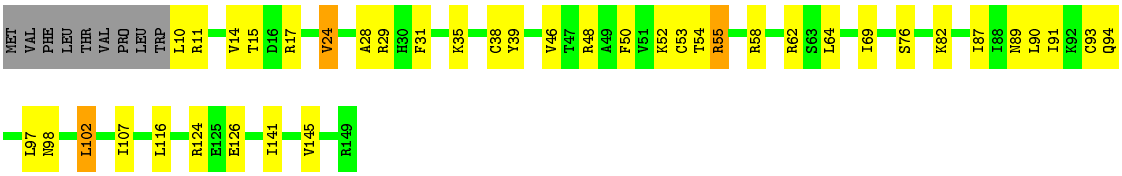
Chain T:





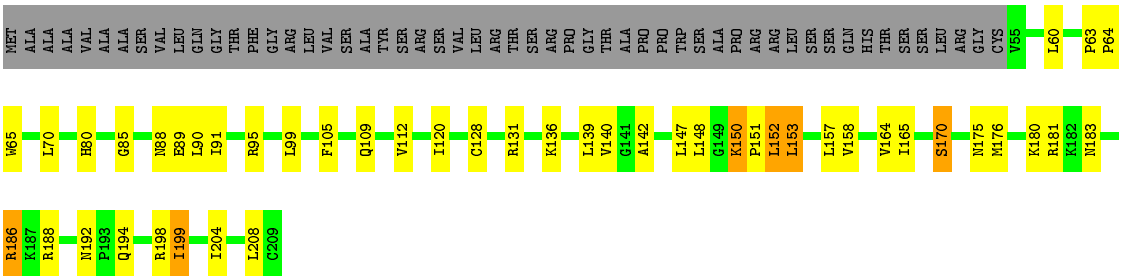
• Molecule 27: MITORIBOSOMAL PROTEIN BL20M, MRPL20

Chain U:



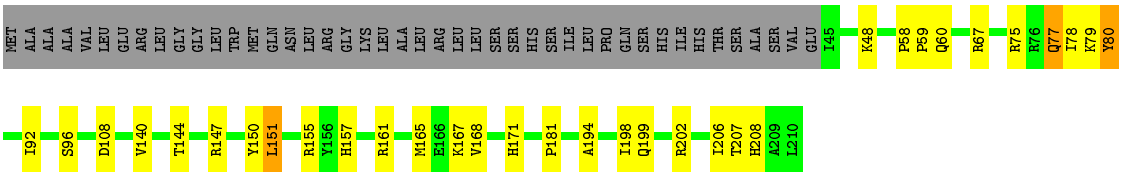
• Molecule 28: MITORIBOSOMAL PROTEIN BL21M, MRPL21

Chain V:



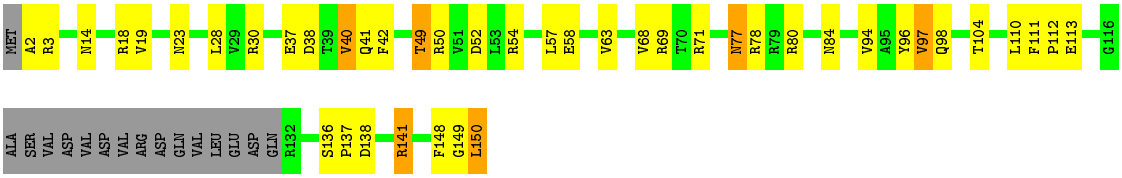
• Molecule 29: MITORIBOSOMAL PROTEIN UL22M, MRPL22

Chain W:



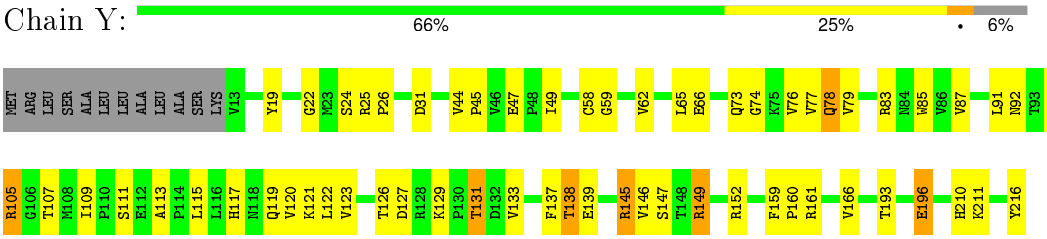
• Molecule 30: MITORIBOSOMAL PROTEIN UL23M, MRPL23

Chain X:



• Molecule 31: MITORIBOSOMAL PROTEIN UL24M, MRPL24

Chain Y:


66%
25%
6%
MET ARG LEU SER ALA LEU LEU ALA LEU ALA SER LYS V13 Y19 G22 M23 S24 R25 P26 D31 V44 P45 Y46 E47 P48 I49 C58 G59 V62 L65 E66 Q73 G74 K75 V76 V77 Q78 V79 H83 N84 W85 V86 V87 L91 N92 T93 H94 V98
R105 G106 T107 M108 I109 P110 S111 E112 A113 P114 L115 L116 H117 N118 Q119 V120 K121 L122 V123 T126 D127 R128 K129 P130 T131 D132 V133 F137 T138 E139 R145 V146 S147 T148 R149 R152 F159 P160 R161 V166 T193 E196 H210 K211 Y216

4 Experimental information (i)

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 ($e^-/Å^2$)	2000	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: 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	0	0.43	0/901	0.59	0/1217
10	9	0.47	0/342	0.57	0/450
11	A	0.62	2/36094 (0.0%)	1.06	72/56186 (0.1%)
13	C	0.50	0/68	1.01	0/103
13	Z	0.32	0/68	0.86	0/103
14	D	0.38	0/1898	0.58	0/2555
15	E	0.38	0/2493	0.61	0/3387
16	F	0.42	0/2069	0.58	0/2816
17	I	0.35	0/819	0.52	0/1101
18	J	0.35	0/1392	0.55	0/1881
19	K	0.35	0/1099	0.49	0/1480
2	1	0.35	0/2093	0.51	0/2835
20	N	0.40	0/1487	0.57	0/2017
21	O	0.36	0/912	0.56	0/1231
22	P	0.40	0/2368	0.60	0/3198
23	Q	0.39	0/1838	0.57	0/2475
24	R	0.39	0/1262	0.57	0/1700
25	S	0.36	0/1197	0.55	0/1624
26	T	0.35	0/1903	0.54	0/2567
27	U	0.46	0/1179	0.61	0/1578
28	V	0.40	0/1256	0.58	0/1706
29	W	0.42	0/1407	0.57	0/1891
3	2	0.36	0/1582	0.52	0/2118
30	X	0.37	0/1149	0.59	0/1554
31	Y	0.35	0/1704	0.54	0/2310
4	3	0.41	0/993	0.59	0/1341
5	4	0.29	0/388	0.57	0/523
6	5	0.38	0/917	0.53	0/1227
7	6	0.35	0/396	0.54	0/526
8	7	0.45	0/395	0.55	0/524
9	8	0.48	0/853	0.60	0/1136
All	All	0.52	2/72522 (0.0%)	0.87	72/105360 (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
15	E	0	2
28	V	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1255	A	N9-C4	-6.05	1.34	1.37
11	A	490	A	C8-N7	5.63	1.35	1.31

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	374	U	N1-C2-O2	8.42	128.70	122.80
11	A	374	U	N3-C2-O2	-8.24	116.43	122.20
11	A	48	U	N3-C2-O2	-7.50	116.95	122.20
11	A	593	C	C6-N1-C2	-7.38	117.35	120.30
11	A	1413	G	C4-N9-C1'	7.14	135.78	126.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	E	316	PHE	Peptide
15	E	43	GLY	Peptide
28	V	150	LYS	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	0	878	0	896	20	0
2	1	2036	0	2058	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	1544	0	1580	26	0
4	3	968	0	1018	23	0
5	4	381	0	400	9	0
6	5	902	0	916	22	0
7	6	391	0	429	18	0
8	7	387	0	413	10	0
9	8	833	0	883	17	0
10	9	335	0	359	11	0
11	A	32233	0	16310	440	0
12	B	1225	0	675	29	0
13	C	62	0	34	1	0
13	Z	62	0	34	0	0
14	D	1860	0	1923	58	0
15	E	2420	0	2418	63	0
16	F	2011	0	2049	50	0
17	I	805	0	845	21	0
18	J	1361	0	1449	46	0
19	K	1081	0	1146	36	0
20	N	1444	0	1437	22	0
21	O	896	0	946	25	0
22	P	2312	0	2373	63	0
23	Q	1792	0	1832	31	0
24	R	1240	0	1260	40	0
25	S	1168	0	1159	46	0
26	T	1860	0	1875	45	0
27	U	1159	0	1228	35	0
28	V	1231	0	1278	35	0
29	W	1374	0	1405	20	0
30	X	1120	0	1133	27	0
31	Y	1663	0	1665	50	0
32	5	1	0	0	0	0
32	9	1	0	0	0	0
33	A	163	0	0	0	0
33	D	2	0	0	0	0
33	P	2	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
34	A	192	0	0	5	0
34	D	6	0	0	0	0
34	P	6	0	0	4	0
All	All	69409	0	53426	1171	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 10.

The worst 5 of 1171 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)
11:A:346:U:H4'	11:A:347:G:H5'	1.53	0.91
27:U:54:THR:HG21	28:V:176:MET:H	1.38	0.88
14:D:111:ARG:HH11	14:D:182:ALA:HB2	1.40	0.86
16:F:262:THR:HG22	16:F:264:PRO:HD2	1.59	0.85
18:J:156:SER:HB3	18:J:159:PRO:HB3	1.59	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	112/148 (76%)	110 (98%)	2 (2%)	0	100	100
2	1	242/256 (94%)	235 (97%)	7 (3%)	0	100	100
3	2	176/252 (70%)	167 (95%)	9 (5%)	0	100	100
4	3	116/161 (72%)	113 (97%)	3 (3%)	0	100	100
5	4	43/126 (34%)	42 (98%)	1 (2%)	0	100	100
6	5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
7	6	46/65 (71%)	44 (96%)	2 (4%)	0	100	100
8	7	44/95 (46%)	44 (100%)	0	0	100	100
9	8	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
10	9	36/100 (36%)	36 (100%)	0	0	100	100
14	D	238/306 (78%)	230 (97%)	8 (3%)	0	100	100
15	E	305/348 (88%)	279 (92%)	24 (8%)	2 (1%)	26	70
16	F	248/294 (84%)	237 (96%)	10 (4%)	1 (0%)	39	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	I	96/268 (36%)	87 (91%)	9 (9%)	0	100	100
18	J	166/262 (63%)	158 (95%)	8 (5%)	0	100	100
19	K	140/192 (73%)	133 (95%)	7 (5%)	0	100	100
20	N	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
21	O	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
22	P	286/296 (97%)	275 (96%)	11 (4%)	0	100	100
23	Q	219/251 (87%)	217 (99%)	2 (1%)	0	100	100
24	R	151/169 (89%)	148 (98%)	3 (2%)	0	100	100
25	S	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	26	70
26	T	222/292 (76%)	215 (97%)	6 (3%)	1 (0%)	34	75
27	U	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
28	V	153/209 (73%)	148 (97%)	5 (3%)	0	100	100
29	W	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
30	X	130/150 (87%)	125 (96%)	5 (4%)	0	100	100
31	Y	202/216 (94%)	191 (95%)	11 (5%)	0	100	100
All	All	4303/5694 (76%)	4135 (96%)	163 (4%)	5 (0%)	59	89

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	E	202	GLN
15	E	317	PRO
26	T	270	MET
16	F	291	CYS
25	S	45	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	92/115 (80%)	82 (89%)	10 (11%)	8 34
2	1	219/229 (96%)	209 (95%)	10 (5%)	33 72
3	2	164/228 (72%)	160 (98%)	4 (2%)	57 85
4	3	110/147 (75%)	107 (97%)	3 (3%)	52 83
5	4	42/114 (37%)	38 (90%)	4 (10%)	11 41
6	5	99/163 (61%)	96 (97%)	3 (3%)	48 81
7	6	45/60 (75%)	41 (91%)	4 (9%)	12 45
8	7	41/78 (53%)	36 (88%)	5 (12%)	6 28
9	8	87/162 (54%)	75 (86%)	12 (14%)	4 23
10	9	36/77 (47%)	34 (94%)	2 (6%)	26 66
14	D	193/248 (78%)	186 (96%)	7 (4%)	42 78
15	E	263/290 (91%)	246 (94%)	17 (6%)	21 61
16	F	217/251 (86%)	200 (92%)	17 (8%)	16 52
17	I	88/228 (39%)	84 (96%)	4 (4%)	34 73
18	J	154/230 (67%)	145 (94%)	9 (6%)	25 65
19	K	115/151 (76%)	107 (93%)	8 (7%)	19 58
20	N	156/157 (99%)	148 (95%)	8 (5%)	29 69
21	O	99/123 (80%)	91 (92%)	8 (8%)	15 51
22	P	245/249 (98%)	231 (94%)	14 (6%)	25 65
23	Q	189/210 (90%)	179 (95%)	10 (5%)	28 67
24	R	132/143 (92%)	122 (92%)	10 (8%)	16 54
25	S	123/153 (80%)	118 (96%)	5 (4%)	37 75
26	T	206/258 (80%)	197 (96%)	9 (4%)	35 73
27	U	118/127 (93%)	109 (92%)	9 (8%)	16 54
28	V	136/178 (76%)	127 (93%)	9 (7%)	21 61
29	W	144/180 (80%)	135 (94%)	9 (6%)	22 62
30	X	119/134 (89%)	110 (92%)	9 (8%)	16 54
31	Y	183/192 (95%)	170 (93%)	13 (7%)	18 58
All	All	3815/4875 (78%)	3583 (94%)	232 (6%)	28 63

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	J	61	ASN
21	O	73	ILE
30	X	77	ASN
18	J	116	LEU
19	K	128	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
17	I	136	ASN
22	P	84	ASN
30	X	41	GLN
18	J	41	HIS
21	O	103	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1508/1570 (96%)	726 (48%)	29 (1%)
12	B	0/62	-	-
13	C	2/3 (66%)	2 (100%)	0
13	Z	2/3 (66%)	0	0
All	All	1512/1638 (92%)	728 (48%)	29 (1%)

5 of 728 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	4	A
11	A	5	A
11	A	7	G
11	A	11	G
11	A	12	C

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	569	A
11	A	583	A
11	A	1431	U
11	A	572	A
11	A	617	C

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

62 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	$\#\|Z\|>2$
12	P5P	B	1	12	21,24,24	1.37	2 (9%)	21,36,36	1.71	3 (14%)
12	P5P	B	10	12	16,23,24	1.29	3 (18%)	15,33,36	1.88	3 (20%)
12	Y5P	B	11	12	14,19,20	4.94	3 (21%)	18,26,29	1.71	1 (5%)
12	Y5P	B	12	12	14,19,20	3.17	2 (14%)	18,26,29	2.85	2 (11%)
12	Y5P	B	13	12	14,19,20	3.30	2 (14%)	18,26,29	3.16	2 (11%)
12	P5P	B	14	12	16,23,24	0.73	0	15,33,36	0.82	0
12	P5P	B	15	12	16,23,24	0.74	0	15,33,36	0.80	1 (6%)
12	Y5P	B	2	12	14,19,20	3.21	2 (14%)	18,26,29	2.85	2 (11%)
12	P5P	B	23	12	16,23,24	0.81	0	15,33,36	0.89	0
12	P5P	B	24	12	16,23,24	0.76	0	15,33,36	0.79	0
12	P5P	B	25	12	16,23,24	1.33	3 (18%)	15,33,36	2.13	3 (20%)
12	Y5P	B	26	12	14,19,20	4.80	3 (21%)	18,26,29	1.88	1 (5%)
12	P5P	B	27	12	16,23,24	0.72	0	15,33,36	1.08	1 (6%)
12	P5P	B	28	12	16,23,24	0.78	0	15,33,36	0.71	0
12	P5P	B	29	12	16,23,24	1.37	2 (12%)	15,33,36	2.13	3 (20%)
12	Y5P	B	3	12	14,19,20	3.24	2 (14%)	18,26,29	3.16	2 (11%)
12	P5P	B	30	12	16,23,24	1.33	3 (18%)	15,33,36	1.89	3 (20%)
12	Y5P	B	31	12	14,19,20	5.02	3 (21%)	18,26,29	1.68	1 (5%)
12	P5P	B	32	12	16,23,24	0.73	0	15,33,36	0.80	0
12	Y5P	B	33	12	14,19,20	4.99	3 (21%)	18,26,29	1.68	1 (5%)
12	Y5P	B	34	12	14,19,20	3.20	2 (14%)	18,26,29	2.83	2 (11%)
12	P5P	B	35	12	16,23,24	1.50	2 (12%)	15,33,36	1.76	2 (13%)
12	P5P	B	36	12	16,23,24	0.75	0	15,33,36	0.95	0
12	P5P	B	37	12	16,23,24	0.74	0	15,33,36	0.81	0
12	P5P	B	38	12	16,23,24	0.71	0	15,33,36	0.96	0
12	P5P	B	39	12	16,23,24	0.72	0	15,33,36	0.91	1 (6%)
12	P5P	B	4	12	16,23,24	0.74	0	15,33,36	0.73	0
12	Y5P	B	40	12	14,19,20	3.33	2 (14%)	18,26,29	2.86	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	P5P	B	41	12	16,23,24	1.31	2 (12%)	15,33,36	1.76	2 (13%)
12	Y5P	B	42	12	14,19,20	4.84	3 (21%)	18,26,29	1.78	1 (5%)
12	Y5P	B	43	12	14,19,20	5.06	3 (21%)	18,26,29	1.65	1 (5%)
12	Y5P	B	44	12	14,19,20	3.14	2 (14%)	18,26,29	2.76	2 (11%)
12	P5P	B	45	12	16,23,24	0.73	0	15,33,36	0.79	0
12	P5P	B	46	12	16,23,24	1.31	3 (18%)	15,33,36	1.87	2 (13%)
12	P5P	B	47	12	16,23,24	0.75	1 (6%)	15,33,36	0.87	1 (6%)
12	Y5P	B	48	12	14,19,20	3.28	2 (14%)	18,26,29	2.82	2 (11%)
12	P5P	B	49	12	16,23,24	1.43	2 (12%)	15,33,36	1.96	2 (13%)
12	P5P	B	5	12	16,23,24	0.73	0	15,33,36	0.81	1 (6%)
12	P5P	B	50	12	16,23,24	0.77	0	15,33,36	0.82	0
12	P5P	B	51	12	16,23,24	1.40	2 (12%)	15,33,36	1.93	2 (13%)
12	Y5P	B	52	12	14,19,20	4.82	3 (21%)	18,26,29	1.83	1 (5%)
12	Y5P	B	53	12	14,19,20	4.87	3 (21%)	18,26,29	1.82	1 (5%)
12	P5P	B	58	12	16,23,24	0.73	0	15,33,36	0.76	0
12	P5P	B	59	12	16,23,24	1.41	2 (12%)	15,33,36	1.93	2 (13%)
12	Y5P	B	6	12	14,19,20	3.22	2 (14%)	18,26,29	2.93	2 (11%)
12	Y5P	B	60	12	14,19,20	4.75	3 (21%)	18,26,29	1.83	1 (5%)
12	Y5P	B	61	12	14,19,20	3.21	3 (21%)	18,26,29	2.85	2 (11%)
12	Y5P	B	62	12	14,19,20	3.21	2 (14%)	18,26,29	2.92	2 (11%)
12	Y5P	B	63	12	14,19,20	4.87	3 (21%)	18,26,29	1.78	1 (5%)
12	P5P	B	64	12	16,23,24	0.72	0	15,33,36	0.85	0
12	Y5P	B	65	12	14,19,20	3.23	2 (14%)	18,26,29	2.94	2 (11%)
12	P5P	B	66	12	16,23,24	0.77	1 (6%)	15,33,36	0.69	0
12	P5P	B	67	12	16,23,24	0.75	0	15,33,36	0.86	1 (6%)
12	P5P	B	68	12	16,23,24	0.74	0	15,33,36	0.80	0
12	Y5P	B	69	12	14,19,20	4.78	3 (21%)	18,26,29	1.73	1 (5%)
12	P5P	B	7	12	16,23,24	1.40	2 (12%)	15,33,36	2.00	2 (13%)
12	P5P	B	70	12	16,23,24	0.73	0	15,33,36	0.73	0
12	Y5P	B	71	12	14,19,20	4.85	3 (21%)	18,26,29	1.76	1 (5%)
12	Y5P	B	72	12	14,19,20	4.87	3 (21%)	18,26,29	1.73	1 (5%)
12	P5P	B	73	12	16,23,24	0.75	1 (6%)	15,33,36	0.63	0
12	Y5P	B	8	12	14,19,20	3.11	2 (14%)	18,26,29	3.20	2 (11%)
12	P5P	B	9	12	16,23,24	0.77	0	15,33,36	0.72	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
12	P5P	B	1	12	-	0/6/26/26	0/3/3/3
12	P5P	B	10	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	11	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	12	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	13	12	-	0/7/33/34	0/2/2/2
12	P5P	B	14	12	-	0/3/25/26	0/3/3/3
12	P5P	B	15	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	2	12	-	0/7/33/34	0/2/2/2
12	P5P	B	23	12	-	0/3/25/26	0/3/3/3
12	P5P	B	24	12	-	0/3/25/26	0/3/3/3
12	P5P	B	25	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	26	12	-	0/7/33/34	0/2/2/2
12	P5P	B	27	12	-	0/3/25/26	0/3/3/3
12	P5P	B	28	12	-	0/3/25/26	0/3/3/3
12	P5P	B	29	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	3	12	-	0/7/33/34	0/2/2/2
12	P5P	B	30	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	31	12	-	0/7/33/34	0/2/2/2
12	P5P	B	32	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	33	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	34	12	-	0/7/33/34	0/2/2/2
12	P5P	B	35	12	-	0/3/25/26	0/3/3/3
12	P5P	B	36	12	-	0/3/25/26	0/3/3/3
12	P5P	B	37	12	-	0/3/25/26	0/3/3/3
12	P5P	B	38	12	-	0/3/25/26	0/3/3/3
12	P5P	B	39	12	-	0/3/25/26	0/3/3/3
12	P5P	B	4	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	40	12	-	0/7/33/34	0/2/2/2
12	P5P	B	41	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	42	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	43	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	44	12	-	0/7/33/34	0/2/2/2
12	P5P	B	45	12	-	0/3/25/26	0/3/3/3
12	P5P	B	46	12	-	0/3/25/26	0/3/3/3
12	P5P	B	47	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	48	12	-	0/7/33/34	0/2/2/2
12	P5P	B	49	12	-	0/3/25/26	0/3/3/3
12	P5P	B	5	12	-	0/3/25/26	0/3/3/3
12	P5P	B	50	12	-	0/3/25/26	0/3/3/3
12	P5P	B	51	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	52	12	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	Y5P	B	53	12	-	0/7/33/34	0/2/2/2
12	P5P	B	58	12	-	0/3/25/26	0/3/3/3
12	P5P	B	59	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	6	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	60	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	61	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	62	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	63	12	-	0/7/33/34	0/2/2/2
12	P5P	B	64	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	65	12	-	0/7/33/34	0/2/2/2
12	P5P	B	66	12	-	0/3/25/26	0/3/3/3
12	P5P	B	67	12	-	0/3/25/26	0/3/3/3
12	P5P	B	68	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	69	12	-	0/7/33/34	0/2/2/2
12	P5P	B	7	12	-	0/3/25/26	0/3/3/3
12	P5P	B	70	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	71	12	-	0/7/33/34	0/2/2/2
12	Y5P	B	72	12	-	0/7/33/34	0/2/2/2
12	P5P	B	73	12	-	0/3/25/26	0/3/3/3
12	Y5P	B	8	12	-	0/7/33/34	0/2/2/2
12	P5P	B	9	12	-	0/3/25/26	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	43	Y5P	C4-N3	-18.44	1.33	1.46
12	B	31	Y5P	C4-N3	-18.38	1.33	1.46
12	B	33	Y5P	C4-N3	-18.26	1.33	1.46
12	B	11	Y5P	C4-N3	-18.00	1.33	1.46
12	B	63	Y5P	C4-N3	-17.70	1.34	1.46

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	8	Y5P	N1-C2-N3	-12.59	113.87	125.85
12	B	13	Y5P	N1-C2-N3	-12.57	113.89	125.85
12	B	3	Y5P	N1-C2-N3	-12.46	114.00	125.85
12	B	6	Y5P	N1-C2-N3	-11.66	114.76	125.85
12	B	65	Y5P	N1-C2-N3	-11.60	114.82	125.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

36 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	11	Y5P	1	0
12	B	12	Y5P	1	0
12	B	13	Y5P	1	0
12	B	14	P5P	1	0
12	B	15	P5P	1	0
12	B	23	P5P	3	0
12	B	24	P5P	1	0
12	B	25	P5P	3	0
12	B	26	Y5P	1	0
12	B	3	Y5P	1	0
12	B	30	P5P	1	0
12	B	31	Y5P	1	0
12	B	33	Y5P	1	0
12	B	38	P5P	2	0
12	B	39	P5P	2	0
12	B	4	P5P	2	0
12	B	41	P5P	1	0
12	B	42	Y5P	2	0
12	B	43	Y5P	1	0
12	B	44	Y5P	1	0
12	B	47	P5P	2	0
12	B	48	Y5P	1	0
12	B	49	P5P	1	0
12	B	5	P5P	1	0
12	B	59	P5P	1	0
12	B	60	Y5P	2	0
12	B	61	Y5P	2	0
12	B	62	Y5P	2	0
12	B	63	Y5P	2	0
12	B	67	P5P	1	0
12	B	68	P5P	1	0
12	B	69	Y5P	2	0
12	B	70	P5P	1	0
12	B	71	Y5P	1	0
12	B	72	Y5P	1	0
12	B	9	P5P	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 171 ligands modelled in this entry, 171 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no chain breaks in this entry.