



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 3, 2019 – 07:53 PM EST

PDB ID : 5OOL
EMDB ID: : EMD-3842
Title : Structure of a native assembly intermediate of the human mitochondrial ribosome with unfolded interfacial rRNA
Authors : Brown, A.; Rathore, S.; Kimanius, D.; Aibara, S.; Bai, X.C.; Rorbach, J.; Amunts, A.; Ramakrishnan, V.
Deposited on : 2017-08-08
Resolution : 3.06 Å (reported)
Based on PDB ID : 3J9M

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

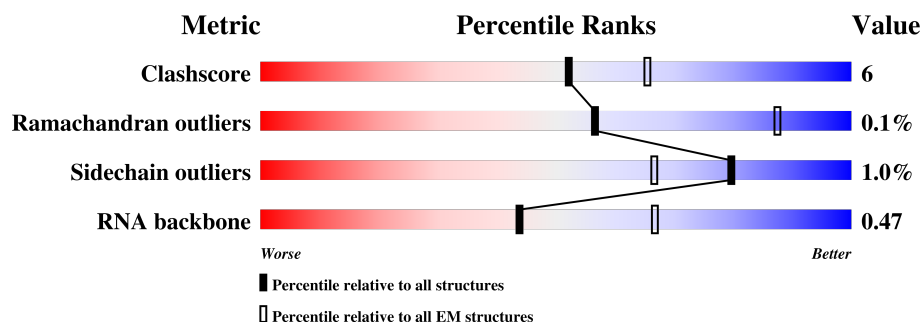
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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.






















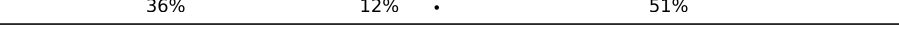
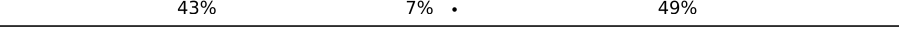




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	A	1559	53% 31% 8% 8%
2	B	69	46% 32% .. 19%
3	D	305	62% 14% . 23%
4	E	348	72% 15% . 13%
5	F	311	61% 18% . 20%
6	H	267	29% 7% 64%
7	I	261	43% 17% 39%
8	J	192	53% 20% 27%




















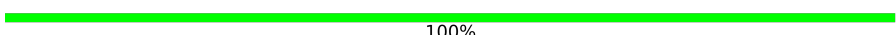

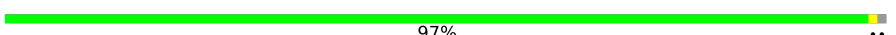

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Mol	Chain	Length	Quality of chain
9	K	178	 81% 17% ..
10	L	145	 66% 13% 21%
11	M	296	 79% 17% . .
12	N	251	 67% 15% 18%
13	O	175	 66% 21% 13%
14	P	180	 63% 14% . 22%
15	Q	292	 61% 14% 26%
16	R	149	 84% 9% . 6%
17	S	205	 60% 15% . 24%
18	T	206	 67% 14% 19%
19	U	153	 72% 17% . 9%
20	V	216	 77% 11% 11%
21	W	148	 60% 14% 26%
22	X	256	 77% 16% . 5%
23	Y	250	 61% 9% 30%
24	Z	161	 65% 10% 25%
25	0	188	 51% 7% 43%
26	1	65	 58% 22% 20%
27	2	92	 36% 12% . 51%
28	3	188	 43% 7% . 49%
29	4	103	 23% 13% 64%
30	5	423	 75% 16% 9%
31	6	380	 73% 12% 15%
32	7	338	 73% 12% 15%
33	8	206	 45% . 52%

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Mol	Chain	Length	Quality of chain
34	9	137	
35	a	142	
36	b	215	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	t	28	
54	u	234	
55	v	70	
56	w	156	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 98998 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	P	0	0
			30607	13732	5531	9903	1441		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	304	Total	C	N	O	S	0	0
			2396	1539	416	430	11		

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	95	Total	C	N	O	0	0
			784	498	152	134		

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	139	Total	C	N	O	S	0	0
			1154	734	220	197	3		

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	192	Total	C	N	O	S	0	0
			1575	1003	281	283	8		

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			333	212	71	47	3		

- Molecule 30 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 31 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 32 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 33 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 39 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 53 is a protein called Unknown protein or protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 54 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 55 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	v	69	Total	C	N	O	0	0
			588	372	116	100		

- Molecule 56 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

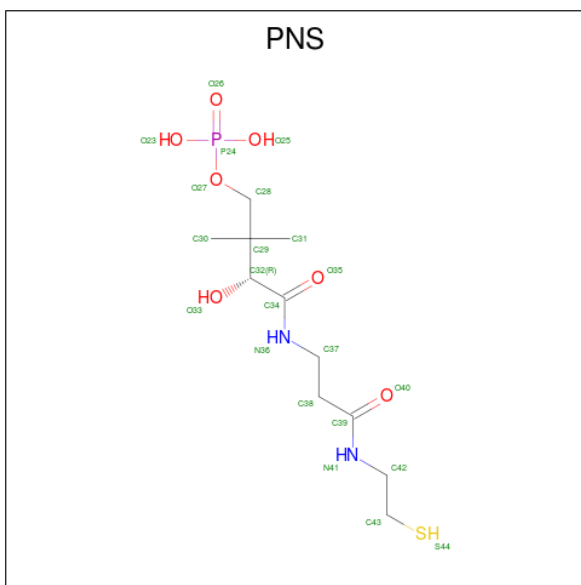
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	g	1	Total	Mg	0
			1	1	
57	D	1	Total	Mg	0
			1	1	
57	W	1	Total	Mg	0
			1	1	
57	A	87	Total	Mg	0
			87	87	
57	T	1	Total	Mg	0
			1	1	
57	M	1	Total	Mg	0
			1	1	

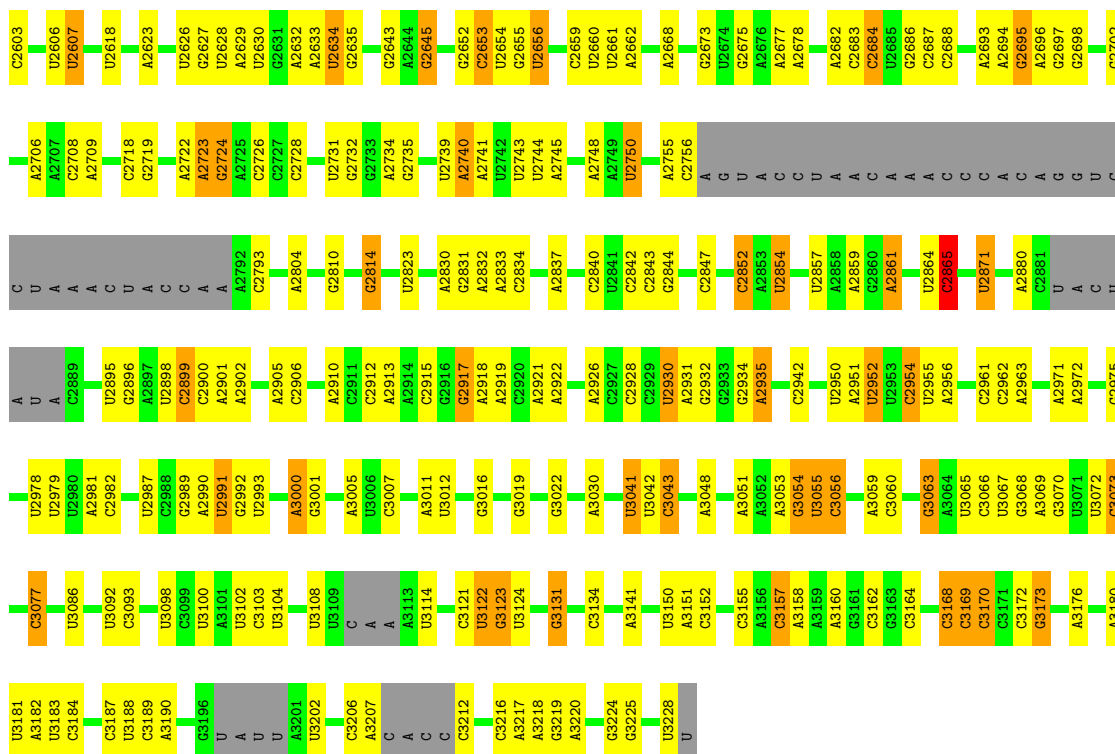
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	0	1	Total	Zn	0
			1	1	
58	I	1	Total	Zn	0
			1	1	
58	4	1	Total	Zn	0
			1	1	

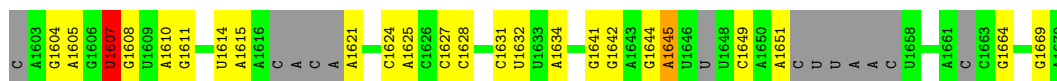
- Molecule 59 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



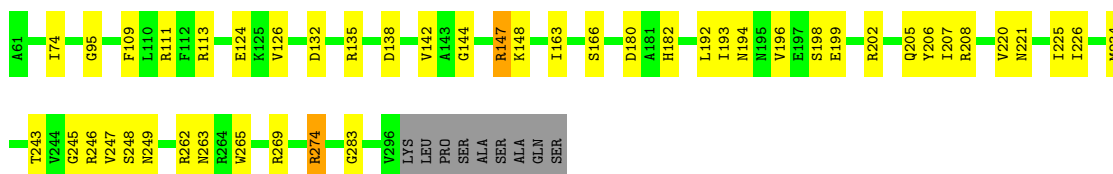
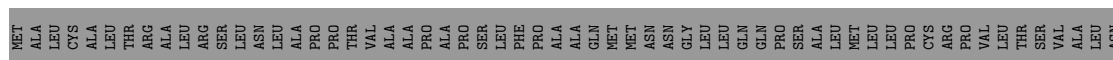
Mol	Chain	Residues	Atoms						AltConf
59	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	



• Molecule 2: mitochondrial tRNAVal

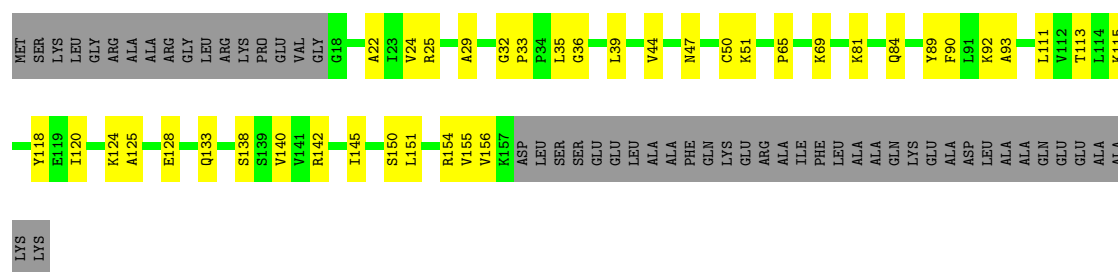


• Molecule 3: 39S ribosomal protein L2, mitochondrial



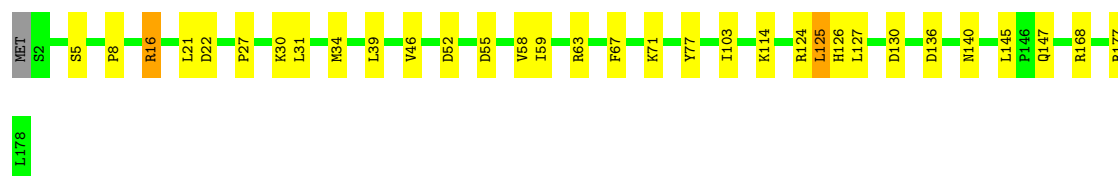
• Molecule 4: 39S ribosomal protein L3, mitochondrial





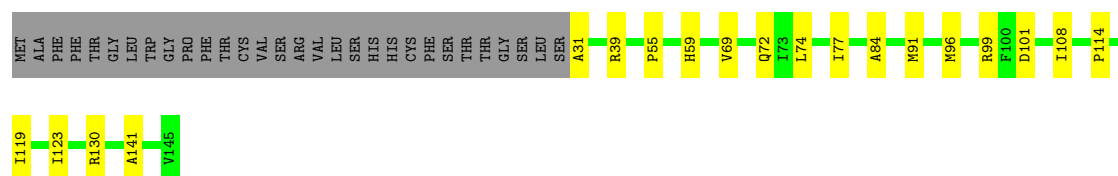
- Molecule 9: 39S ribosomal protein L13, mitochondrial

Chain K: 81% 17% ..



- Molecule 10: 39S ribosomal protein L14, mitochondrial

Chain L: 66% 13% 21%



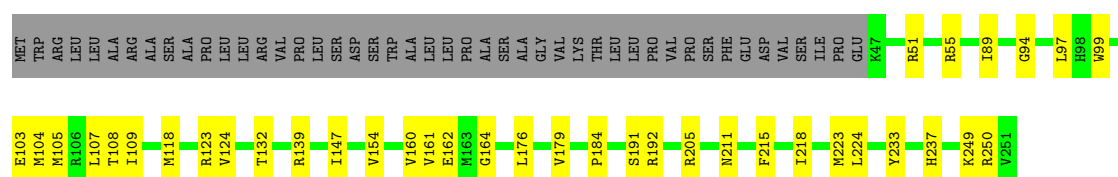
- Molecule 11: 39S ribosomal protein L15, mitochondrial

Chain M: 79% 17% ..

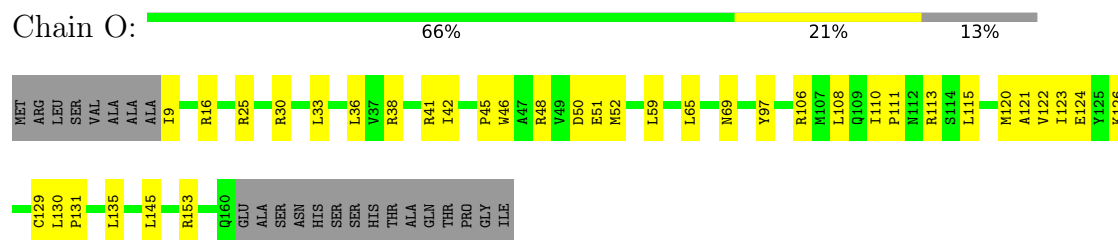


- Molecule 12: 39S ribosomal protein L16, mitochondrial

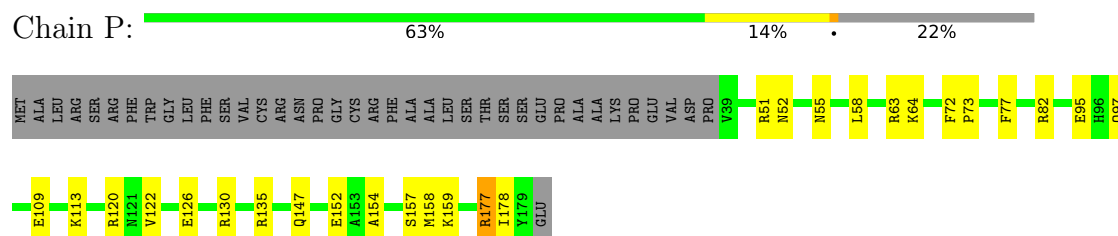
Chain N: 67% 15% 18%



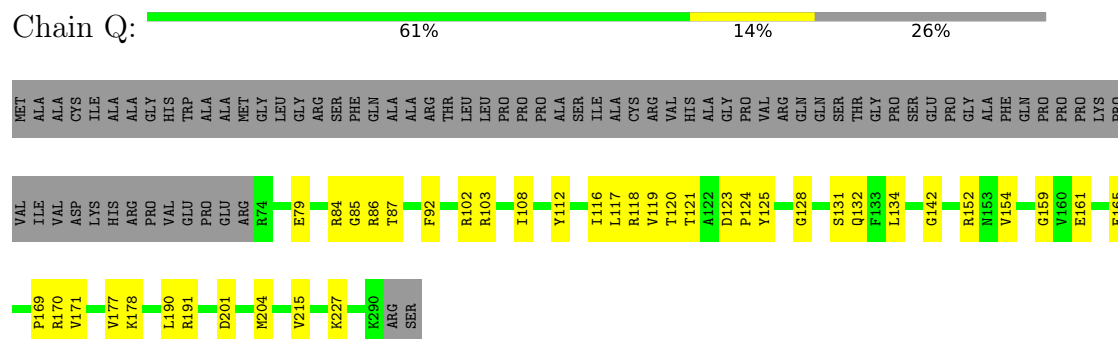
- Molecule 13: 39S ribosomal protein L17, mitochondrial



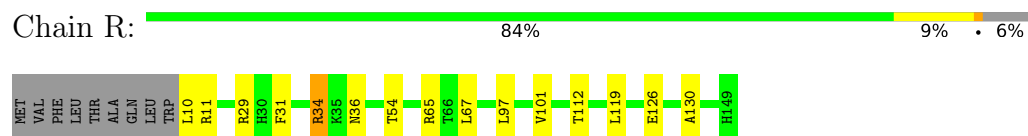
- Molecule 14: 39S ribosomal protein L18, mitochondrial



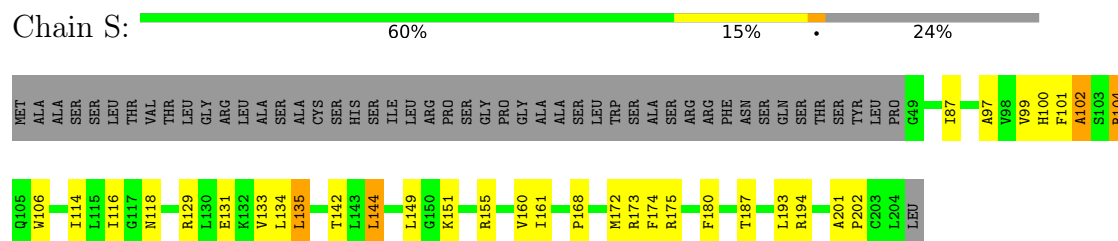
- Molecule 15: 39S ribosomal protein L19, mitochondrial



- Molecule 16: 39S ribosomal protein L20, mitochondrial

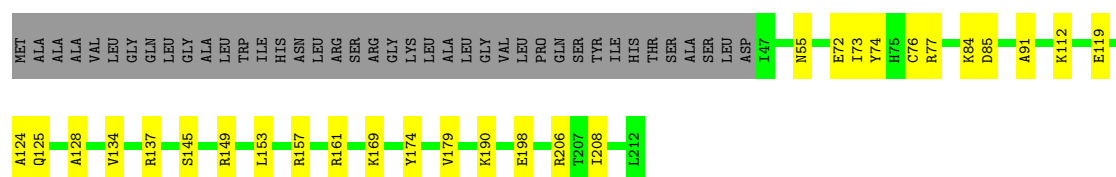


- Molecule 17: 39S ribosomal protein L21, mitochondrial



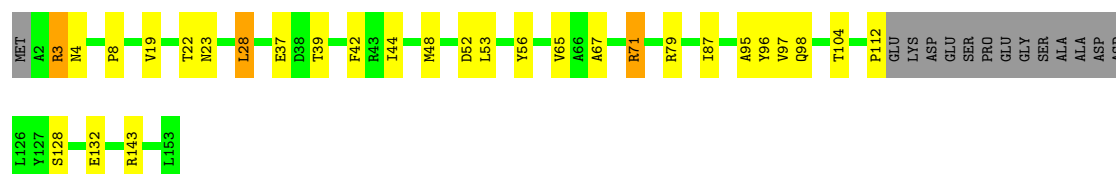
- Molecule 18: 39S ribosomal protein L22, mitochondrial





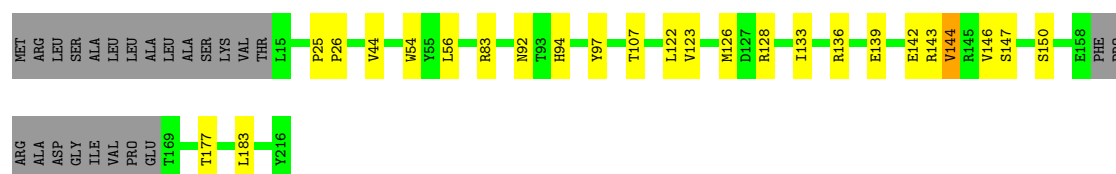
- Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U: 72% 17% 9%



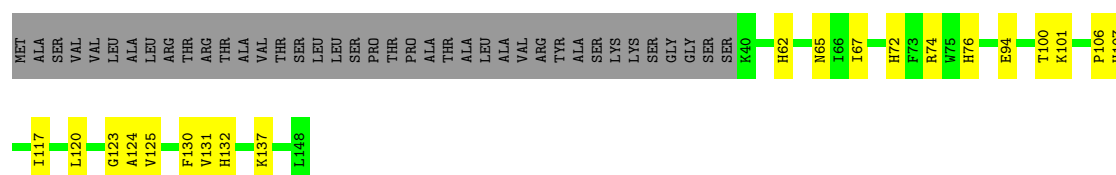
- Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V: 77% 11% 11%



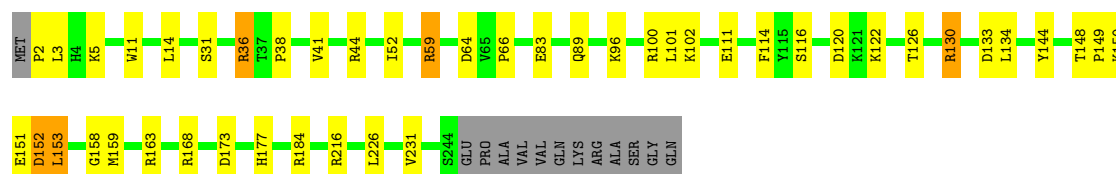
- Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W: 60% 14% 26%



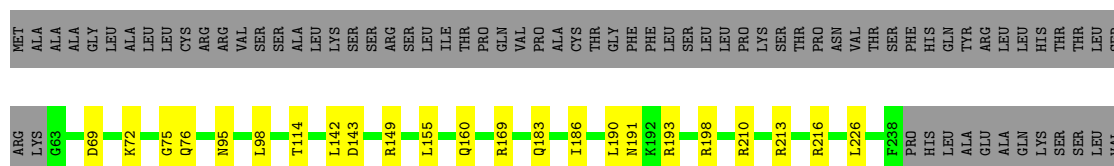
- Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X: 77% 16% 5%



- Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y: 61% 9% 30%



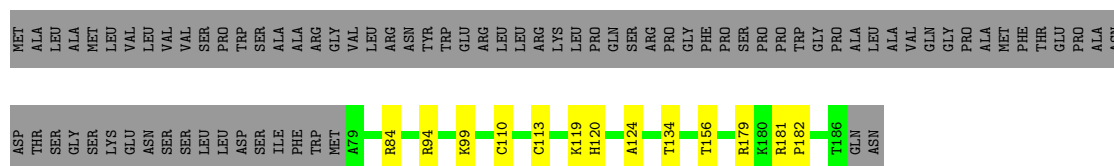
- Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z: 65% 10% 25%



- Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0: 51% 7% 43%



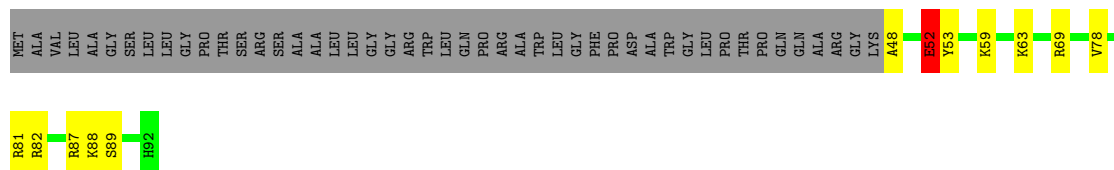
- Molecule 26: 39S ribosomal protein L33, mitochondrial

Chain 1: 58% 22% 20%



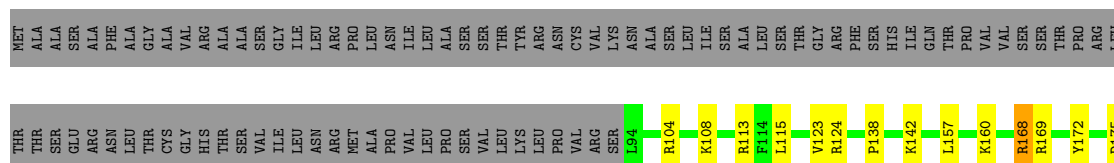
- Molecule 27: 39S ribosomal protein L34, mitochondrial

Chain 2: 36% 12% 51%



- Molecule 28: 39S ribosomal protein L35, mitochondrial

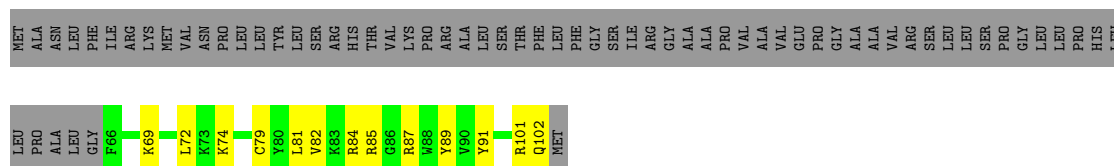
Chain 3: 43% 7% 49%





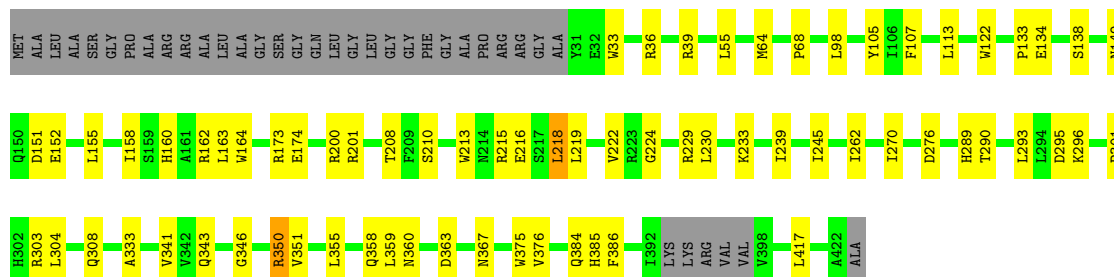
- Molecule 29: 39S ribosomal protein L36, mitochondrial

Chain 4: 23% 13% 64%



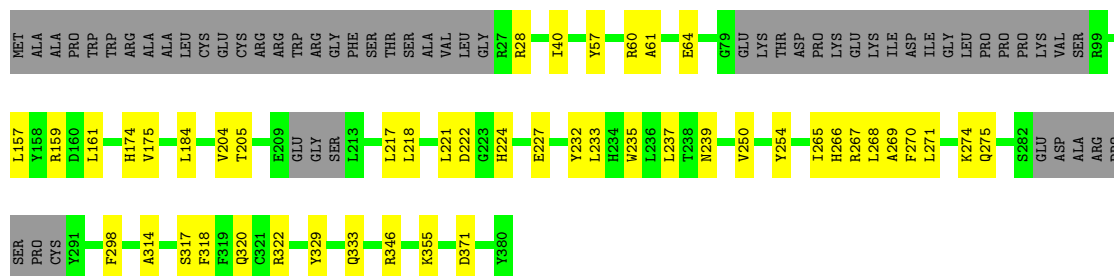
- Molecule 30: 39S ribosomal protein L37, mitochondrial

Chain 5: 75% 16% 9%



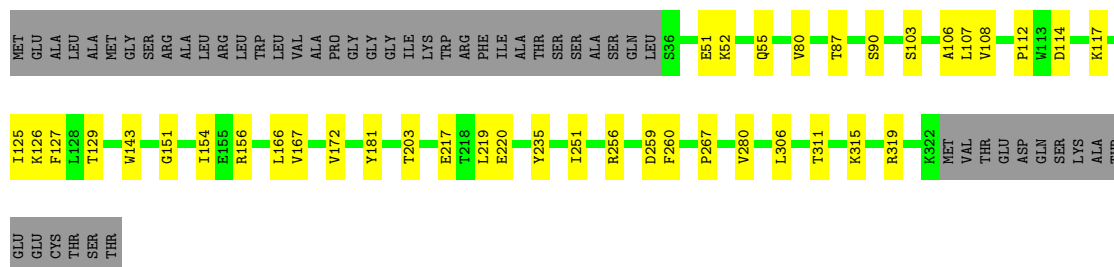
- Molecule 31: 39S ribosomal protein L38, mitochondrial

Chain 6: 73% 12% 15%



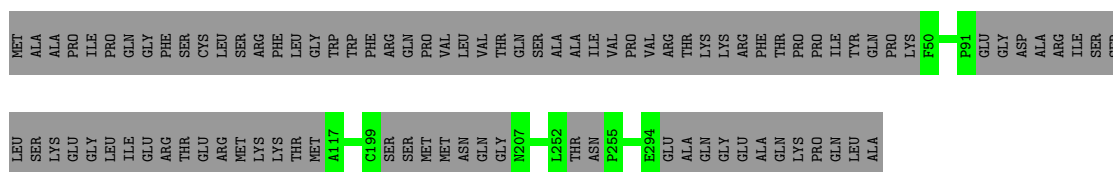
- Molecule 32: 39S ribosomal protein L39, mitochondrial

Chain 7: 73% 12% 15%




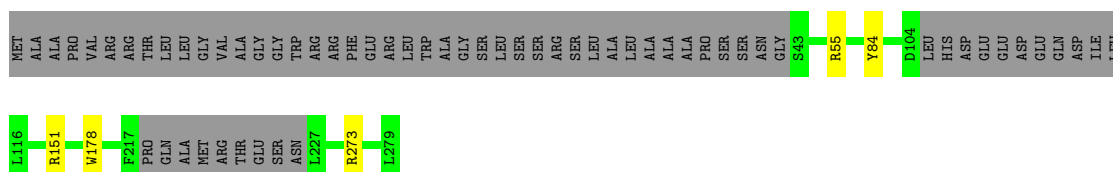
- Molecule 38: 39S ribosomal protein L45, mitochondrial

Chain d:  69% 31%



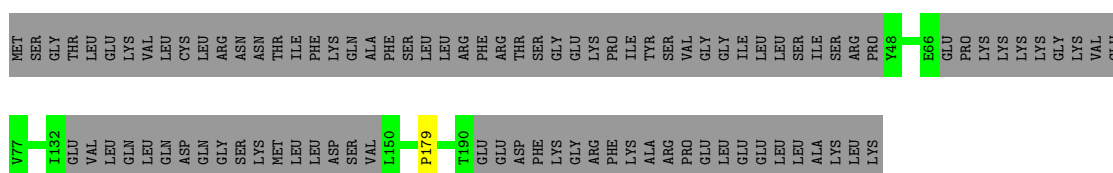
- Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:  76% 22%




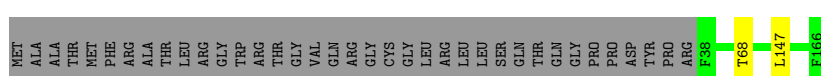
- Molecule 40: 39S ribosomal protein L48, mitochondrial

Chain f:  54% 45%



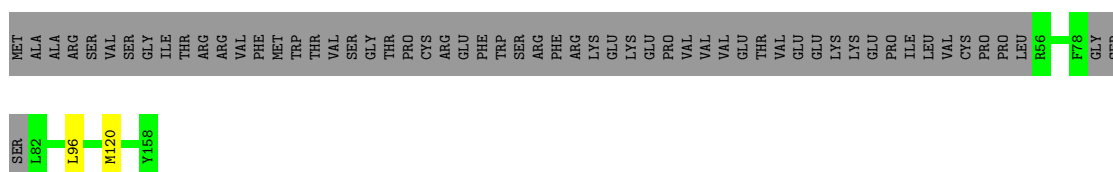
- Molecule 41: 39S ribosomal protein L49, mitochondrial

Chain g:  77% 22%



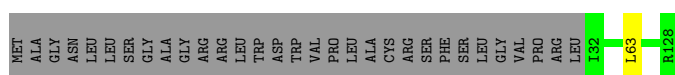
- Molecule 42: 39S ribosomal protein L50, mitochondrial

Chain h:  62% 37%



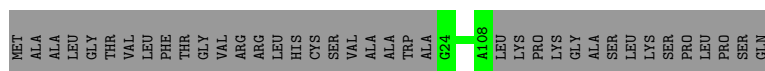
- Molecule 43: 39S ribosomal protein L51, mitochondrial

Chain i:  75% 24%



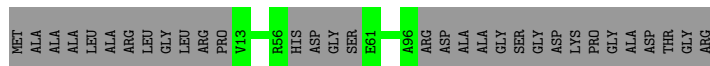
- Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain j:  69% 31%



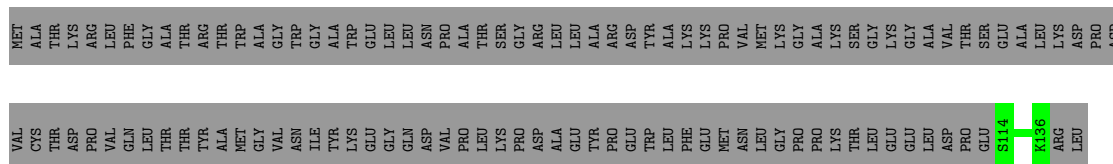
- Molecule 45: 39S ribosomal protein L53, mitochondrial

Chain k:  71% 29%



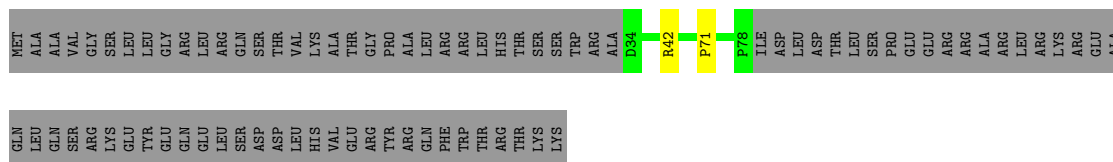
- Molecule 46: 39S ribosomal protein L54, mitochondrial

Chain 1: 17% 83%



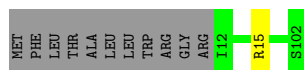
- Molecule 47: 39S ribosomal protein L55, mitochondrial

Chain m: 34% . 65%



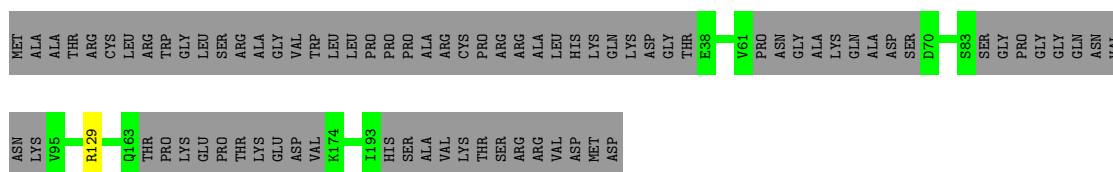
- Molecule 48: Ribosomal protein 63, mitochondrial

Chain o: 88% • 11%



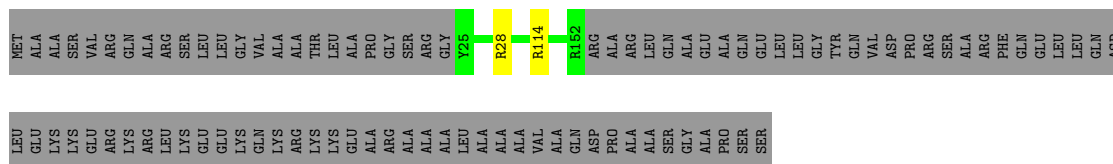
- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p: 61% 38%



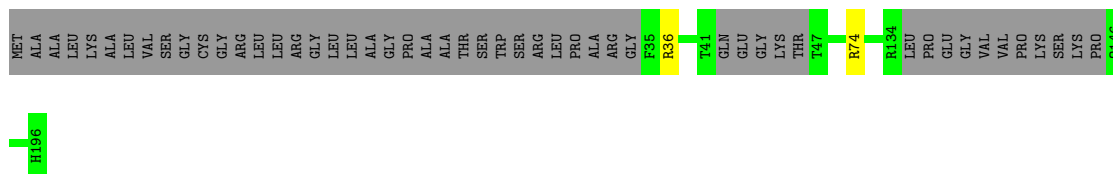
- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  57% 42%




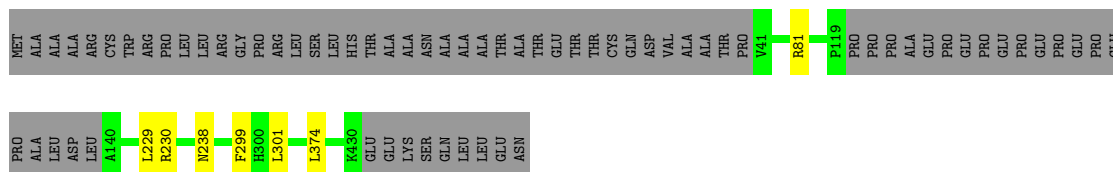
- Molecule 51: 39S ribosomal protein S18a, mitochondrial

Chain r:  73% 26%



- Molecule 52: 39S ribosomal protein S30, mitochondrial

Chain s:  83% 16%



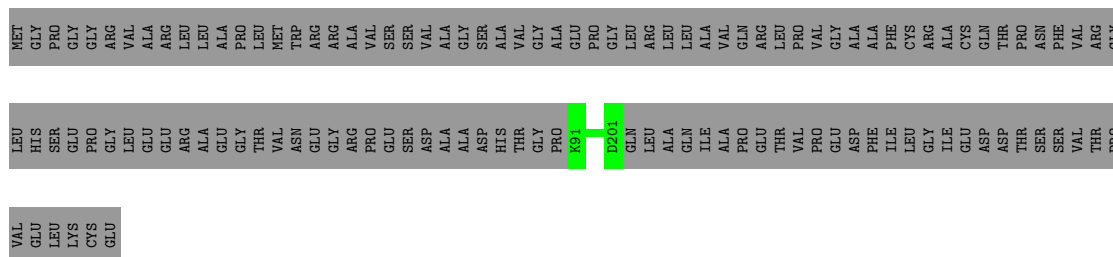
- Molecule 53: Unknown protein or protein extension

Chain t:  100%

There are no outlier residues recorded for this chain.

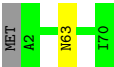
- Molecule 54: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:  47% 53%



- Molecule 55: MIEF1 upstream open reading frame protein

Chain v:  97% ..



● Molecule 56: Acyl carrier protein, mitochondrial



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134685	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	130841	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.93	2/34235 (0.0%)	1.20	300/53263 (0.6%)
10	L	0.45	0/904	0.62	0/1218
11	M	0.54	0/2359	0.68	1/3185 (0.0%)
12	N	0.42	0/1697	0.57	0/2281
13	O	0.49	0/1269	0.68	0/1708
14	P	0.40	0/1173	0.60	0/1588
15	Q	0.44	0/1846	0.62	0/2487
16	R	0.59	0/1174	0.70	3/1572 (0.2%)
17	S	0.52	0/1276	0.67	1/1729 (0.1%)
18	T	0.54	0/1402	0.60	0/1886
19	U	0.47	0/1183	0.65	1/1600 (0.1%)
2	B	0.45	0/1328	1.16	4/2056 (0.2%)
20	V	0.42	0/1616	0.54	0/2189
21	W	0.56	0/881	0.61	0/1188
22	X	0.40	0/2090	0.59	2/2825 (0.1%)
23	Y	0.47	0/1552	0.58	1/2079 (0.0%)
24	Z	0.49	0/1003	0.60	0/1354
25	0	0.50	0/895	0.61	0/1201
26	1	0.42	0/438	0.72	0/583
27	2	0.53	0/373	0.68	0/496
28	3	0.60	0/852	0.63	1/1136 (0.1%)
29	4	0.58	0/341	0.61	0/451
3	D	0.42	0/1879	0.57	0/2527
30	5	0.40	0/3250	0.62	1/4429 (0.0%)
31	6	0.42	0/2726	0.59	1/3715 (0.0%)
32	7	0.42	0/2391	0.56	0/3234
33	8	0.31	0/855	0.50	0/1152
34	9	0.43	0/972	0.56	0/1306
35	a	0.48	0/709	0.56	0/963
36	b	0.54	0/1202	0.62	0/1626
37	c	0.45	0/2264	0.59	1/3059 (0.0%)
38	d	0.39	0/1790	0.56	0/2423

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	e	0.27	0/1797	0.56	2/2422 (0.1%)
4	E	0.51	0/2465	0.62	1/3344 (0.0%)
40	f	0.34	0/931	0.54	0/1259
41	g	0.54	0/1102	0.65	1/1503 (0.1%)
42	h	0.39	0/847	0.60	1/1150 (0.1%)
43	i	0.57	0/849	0.70	1/1135 (0.1%)
44	j	0.42	0/698	0.53	0/940
45	k	0.31	0/635	0.60	0/855
46	l	0.30	0/226	0.47	0/299
47	m	0.26	0/379	0.60	0/510
48	o	0.45	0/792	0.59	0/1064
49	p	0.33	0/1071	0.55	0/1433
5	F	0.54	0/2071	0.66	0/2817
50	q	0.36	0/1107	0.52	0/1498
51	r	0.45	0/1238	0.58	0/1676
52	s	0.45	0/3114	0.64	4/4225 (0.1%)
54	u	0.37	0/949	0.60	0/1281
55	v	0.31	0/597	0.53	0/796
56	w	0.29	0/647	0.57	0/871
6	H	0.40	0/798	0.62	0/1073
7	I	0.33	0/1308	0.65	3/1761 (0.2%)
8	J	0.29	0/1077	0.55	0/1452
9	K	0.51	0/1495	0.63	0/2029
All	All	0.65	2/104118 (0.0%)	0.87	330/147902 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1828	A	N9-C4	-8.72	1.32	1.37
1	A	1994	A	N9-C4	-5.08	1.34	1.37

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2523	C	N1-C2-O2	13.60	127.06	118.90
1	A	2724	G	C5-N7-C8	-12.62	97.99	104.30
1	A	2724	G	N7-C8-N9	11.97	119.09	113.10
1	A	2523	C	C2-N1-C1'	11.52	131.48	118.80
1	A	2322	C	N1-C2-O2	10.81	125.38	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	30607	0	15549	183	0
2	B	1191	0	607	8	0
3	D	1842	0	1891	45	0
4	E	2396	0	2402	36	0
5	F	2013	0	2044	38	0
6	H	784	0	832	12	0
7	I	1283	0	1368	30	0
8	J	1061	0	1141	24	0
9	K	1451	0	1448	20	0
10	L	889	0	941	14	0
11	M	2305	0	2378	33	0
12	N	1654	0	1681	22	0
13	O	1245	0	1283	24	0
14	P	1148	0	1148	17	0
15	Q	1805	0	1841	33	0
16	R	1153	0	1214	12	0
17	S	1251	0	1322	36	0
18	T	1368	0	1410	18	0
19	U	1154	0	1154	21	0
20	V	1575	0	1583	18	0
21	W	859	0	888	13	0
22	X	2035	0	2054	49	0
23	Y	1517	0	1561	15	0
24	Z	978	0	1030	11	0
25	0	880	0	902	9	0
26	1	433	0	475	6	0
27	2	367	0	393	14	0
28	3	831	0	883	12	0
29	4	333	0	352	9	0
30	5	3156	0	3138	48	0
31	6	2640	0	2464	33	0
32	7	2334	0	2343	25	0
33	8	836	0	844	4	0
34	9	947	0	949	18	0
35	a	686	0	658	0	0
36	b	1178	0	1180	0	0
37	c	2217	0	2220	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	d	1741	0	1727	0	0
39	e	1762	0	1767	0	0
40	f	915	0	917	0	0
41	g	1067	0	1056	0	0
42	h	827	0	806	0	0
43	i	827	0	857	0	0
44	j	684	0	673	0	0
45	k	627	0	636	0	0
46	l	221	0	227	0	0
47	m	372	0	387	0	0
48	o	771	0	774	0	0
49	p	1058	0	1083	0	0
50	q	1076	0	1049	0	0
51	r	1203	0	1220	0	0
52	s	3036	0	3022	0	0
53	t	140	0	30	0	0
54	u	927	0	921	0	0
55	v	588	0	604	0	0
56	w	638	0	636	0	0
57	A	87	0	0	0	0
57	D	1	0	0	0	0
57	M	1	0	0	0	0
57	T	1	0	0	0	0
57	W	1	0	0	0	0
57	g	1	0	0	0	0
58	0	1	0	0	0	0
58	4	1	0	0	0	0
58	I	1	0	0	0	0
59	v	21	0	21	0	0
All	All	98998	0	83984	760	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 6.

The worst 5 of 760 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)
3:D:109:PHE:CD1	3:D:208:ARG:NH1	1.70	1.59
3:D:109:PHE:CG	3:D:208:ARG:NH1	1.71	1.59
3:D:109:PHE:CD2	3:D:208:ARG:NH1	2.11	1.19
3:D:109:PHE:CE1	3:D:208:ARG:NH1	2.13	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:52:GLU:HG2	27:2:53:TYR:N	1.55	1.14

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	
3	D	234/305 (77%)	223 (95%)	11 (5%)	0	100	100
4	E	302/348 (87%)	287 (95%)	15 (5%)	0	100	100
5	F	248/311 (80%)	233 (94%)	15 (6%)	0	100	100
6	H	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
7	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
8	J	138/192 (72%)	125 (91%)	13 (9%)	0	100	100
9	K	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
10	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
11	M	285/296 (96%)	270 (95%)	15 (5%)	0	100	100
12	N	203/251 (81%)	193 (95%)	10 (5%)	0	100	100
13	O	150/175 (86%)	146 (97%)	4 (3%)	0	100	100
14	P	139/180 (77%)	130 (94%)	9 (6%)	0	100	100
15	Q	215/292 (74%)	201 (94%)	14 (6%)	0	100	100
16	R	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
17	S	154/205 (75%)	148 (96%)	5 (3%)	1 (1%)	27	60
18	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
19	U	135/153 (88%)	125 (93%)	10 (7%)	0	100	100
20	V	188/216 (87%)	179 (95%)	8 (4%)	1 (0%)	31	64
21	W	107/148 (72%)	104 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	X	241/256 (94%)	235 (98%)	6 (2%)	0	100	100
23	Y	174/250 (70%)	169 (97%)	5 (3%)	0	100	100
24	Z	118/161 (73%)	112 (95%)	6 (5%)	0	100	100
25	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
26	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
27	2	43/92 (47%)	41 (95%)	1 (2%)	1 (2%)	7	27
28	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
29	4	35/103 (34%)	35 (100%)	0	0	100	100
30	5	383/423 (90%)	368 (96%)	15 (4%)	0	100	100
31	6	316/380 (83%)	304 (96%)	12 (4%)	0	100	100
32	7	285/338 (84%)	265 (93%)	20 (7%)	0	100	100
33	8	97/206 (47%)	91 (94%)	6 (6%)	0	100	100
34	9	113/137 (82%)	106 (94%)	7 (6%)	0	100	100
35	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
36	b	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
37	c	271/332 (82%)	263 (97%)	8 (3%)	0	100	100
38	d	203/306 (66%)	193 (95%)	10 (5%)	0	100	100
39	e	211/279 (76%)	184 (87%)	27 (13%)	0	100	100
40	f	110/212 (52%)	101 (92%)	8 (7%)	1 (1%)	19	52
41	g	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
42	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
43	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
44	j	83/123 (68%)	83 (100%)	0	0	100	100
45	k	76/112 (68%)	70 (92%)	6 (8%)	0	100	100
46	l	21/138 (15%)	20 (95%)	1 (5%)	0	100	100
47	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	7	27
48	o	89/102 (87%)	86 (97%)	2 (2%)	1 (1%)	16	46
49	p	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
50	q	126/222 (57%)	125 (99%)	1 (1%)	0	100	100
51	r	140/196 (71%)	135 (96%)	5 (4%)	0	100	100
52	s	366/439 (83%)	351 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	u	109/234 (47%)	103 (94%)	6 (6%)	0	100	100
55	v	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
56	w	77/156 (49%)	70 (91%)	7 (9%)	0	100	100
All	All	8042/11129 (72%)	7635 (95%)	401 (5%)	6 (0%)	56	84

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	S	102	ALA
27	2	52	GLU
47	m	71	PRO
48	o	15	ARG
20	V	144	VAL

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	
3	D	190/245 (78%)	188 (99%)	2 (1%)	76	90
4	E	259/290 (89%)	257 (99%)	2 (1%)	83	92
5	F	217/262 (83%)	211 (97%)	6 (3%)	47	76
6	H	86/228 (38%)	86 (100%)	0	100	100
7	I	145/232 (62%)	144 (99%)	1 (1%)	85	93
8	J	113/150 (75%)	113 (100%)	0	100	100
9	K	155/156 (99%)	152 (98%)	3 (2%)	60	82
10	L	98/124 (79%)	97 (99%)	1 (1%)	78	90
11	M	245/249 (98%)	240 (98%)	5 (2%)	58	82
12	N	172/211 (82%)	170 (99%)	2 (1%)	74	89
13	O	133/150 (89%)	132 (99%)	1 (1%)	83	92
14	P	123/155 (79%)	120 (98%)	3 (2%)	52	78
15	Q	199/256 (78%)	199 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	141/180 (78%)	139 (99%)	2 (1%)	69	87
18	T	146/176 (83%)	146 (100%)	0	100	100
19	U	124/135 (92%)	122 (98%)	2 (2%)	65	86
20	V	172/191 (90%)	171 (99%)	1 (1%)	87	94
21	W	89/119 (75%)	89 (100%)	0	100	100
22	X	219/229 (96%)	214 (98%)	5 (2%)	53	79
23	Y	159/223 (71%)	156 (98%)	3 (2%)	60	82
24	Z	111/147 (76%)	111 (100%)	0	100	100
25	0	97/164 (59%)	96 (99%)	1 (1%)	78	90
26	1	49/60 (82%)	46 (94%)	3 (6%)	20	51
27	2	39/72 (54%)	38 (97%)	1 (3%)	49	77
28	3	88/166 (53%)	87 (99%)	1 (1%)	76	90
29	4	36/89 (40%)	36 (100%)	0	100	100
30	5	348/368 (95%)	343 (99%)	5 (1%)	69	87
31	6	265/332 (80%)	264 (100%)	1 (0%)	92	96
32	7	263/303 (87%)	262 (100%)	1 (0%)	92	96
33	8	91/190 (48%)	90 (99%)	1 (1%)	76	90
34	9	99/112 (88%)	99 (100%)	0	100	100
35	a	78/133 (59%)	77 (99%)	1 (1%)	71	88
36	b	130/186 (70%)	129 (99%)	1 (1%)	83	92
37	c	241/288 (84%)	239 (99%)	2 (1%)	83	92
38	d	193/274 (70%)	193 (100%)	0	100	100
39	e	188/236 (80%)	185 (98%)	3 (2%)	65	86
40	f	101/188 (54%)	101 (100%)	0	100	100
41	g	119/148 (80%)	118 (99%)	1 (1%)	83	92
42	h	95/148 (64%)	94 (99%)	1 (1%)	76	90
43	i	86/110 (78%)	86 (100%)	0	100	100
44	j	68/97 (70%)	68 (100%)	0	100	100
45	k	71/90 (79%)	71 (100%)	0	100	100
46	l	23/116 (20%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m	40/113 (35%)	39 (98%)	1 (2%)	50	78
48	o	78/87 (90%)	78 (100%)	0	100	100
49	p	117/181 (65%)	116 (99%)	1 (1%)	81	91
50	q	110/178 (62%)	108 (98%)	2 (2%)	62	83
51	r	133/169 (79%)	131 (98%)	2 (2%)	67	86
52	s	326/381 (86%)	323 (99%)	3 (1%)	81	91
54	u	105/200 (52%)	105 (100%)	0	100	100
55	v	59/60 (98%)	58 (98%)	1 (2%)	63	85
56	w	73/136 (54%)	72 (99%)	1 (1%)	69	87
All	All	7223/9609 (75%)	7150 (99%)	73 (1%)	80	90

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	X	130	ARG
26	1	34	ARG
51	r	74	ARG
23	Y	198	ARG
26	1	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
20	V	92	ASN
33	8	143	GLN
52	s	343	GLN
21	W	76	HIS
30	5	289	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1425/1559 (91%)	377 (26%)	17 (1%)
2	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1476/1628 (90%)	392 (26%)	18 (1%)

5 of 392 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1674	A
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2245	A
1	A	2457	A
1	A	2905	A
1	A	2186	C
1	A	2243	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 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	$\# Z > 2$
59	PNS	v	101	55,56	13,20,21	2.43	5 (38%)	18,26,29	1.32	2 (11%)

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
59	PNS	v	101	55,56	-	12/24/26/27	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	v	101	PNS	C39-N41	5.24	1.45	1.33
59	v	101	PNS	C34-N36	5.08	1.44	1.33
59	v	101	PNS	O27-C28	-3.36	1.40	1.44
59	v	101	PNS	O40-C39	-2.25	1.18	1.23
59	v	101	PNS	O35-C34	-2.20	1.19	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	v	101	PNS	C38-C37-N36	-2.38	107.20	111.88
59	v	101	PNS	C37-C38-C39	-2.06	108.92	112.36

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

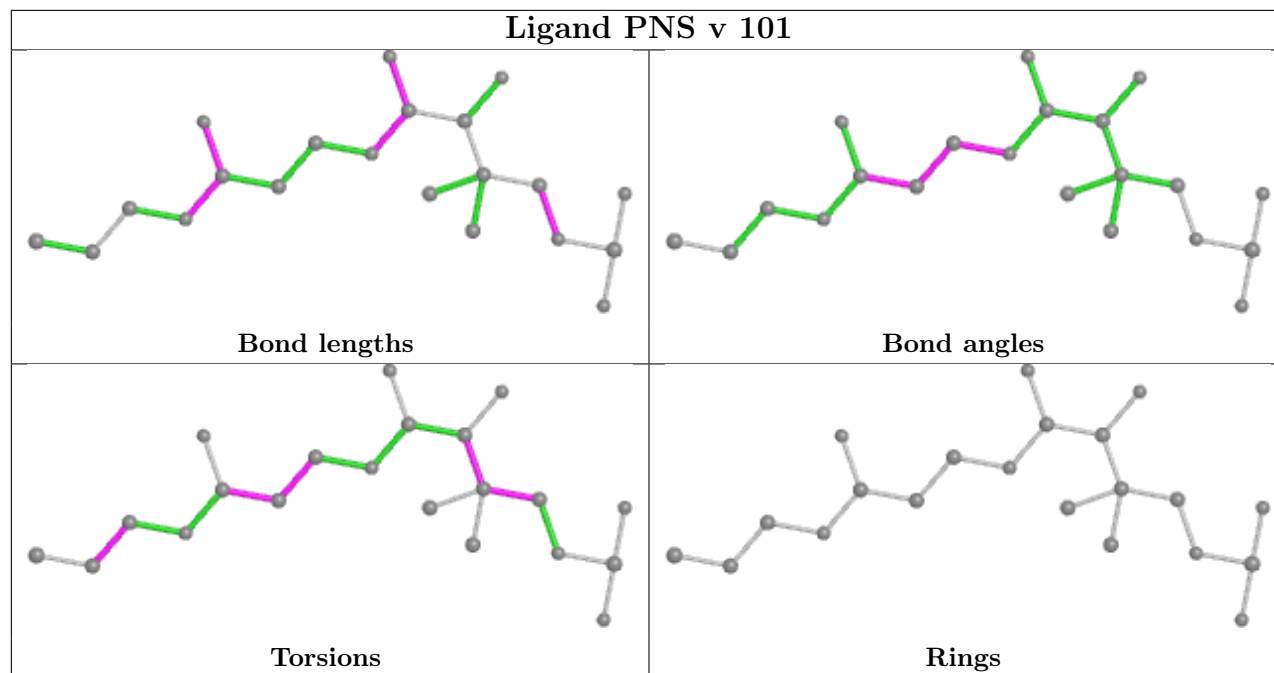
Mol	Chain	Res	Type	Atoms
59	v	101	PNS	C28-C29-C32-O33
59	v	101	PNS	C28-C29-C32-C34
59	v	101	PNS	C31-C29-C32-O33
59	v	101	PNS	C31-C29-C32-C34
59	v	101	PNS	N36-C37-C38-C39

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.