wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:43 PM BST

PDB ID	:	3IY9
EMDB ID:	:	EMD-5113
Title	:	Leishmania Tarentolae Mitochondrial Large Ribosomal Subunit Model
Authors	:	Sharma, M.R.; Booth, T.M.; Simpson, L.; Maslov, D.A.; Agrawal, R.K.
Deposited on	:	2009-04-20
Resolution	:	14.10 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

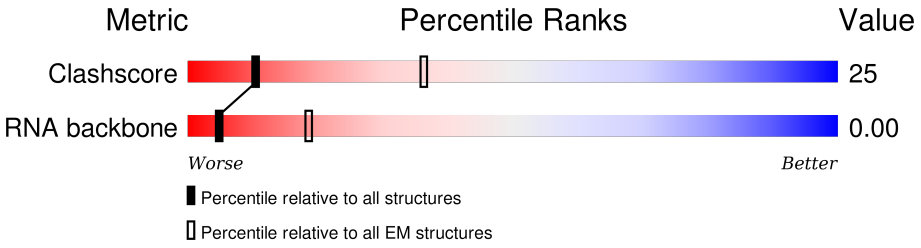
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 14.10 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
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	A	1027	94% 6%
2	B	136	100%
3	C	209	94% 6%
4	D	175	98% .
5	H	60	100%
6	G	145	98% .
7	J	140	96% .
8	K	121	99% .
9	L	144	93% 7%
10	I	118	97% .

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Mol	Chain	Length	Quality of chain
11	S	116	95% 5%
12	Q	117	93% 7%
13	R	103	96%
14	M	110	95% 5%
15	T	99	97%
16	N	96	94% 6%
17	O	69	90% 10%
18	X	63	100%
19	Y	58	97%
20	P	52	100%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 3158 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 Leishmania Tarentolae Mitochondrial Large Ribosomal Subunit.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	1027	Total P 1027 1027	0	1027

- Molecule 2 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	B	136	Total C 136 136	0	136

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	C	209	Total C 209 209	0	209

- Molecule 4 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	D	175	Total C 175 175	0	175

- Molecule 5 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	H	60	Total C 60 60	0	60

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	G	145	Total C 145 145	0	145

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	J	140	Total C 140 140	0	140

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	K	121	Total C 121 121	0	121

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	L	144	Total C 144 144	0	144

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	I	118	Total C 118 118	0	118

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	S	116	Total C 116 116	0	116

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	Q	117	Total C 117 117	0	117

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	R	103	Total C 103 103	0	103

- Molecule 14 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	M	110	Total C 110 110	0	110

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	T	99	Total C 99 99	0	99

- Molecule 16 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	N	96	Total C 96 96	0	96

- Molecule 17 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	O	69	Total C 69 69	0	69

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	AltConf	Trace
18	X	63	Total C 63 63	0	63

- Molecule 19 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	AltConf	Trace
19	Y	58	Total C 58 58	0	58

- Molecule 20 is a protein called 39S ribosomal protein L33, mitochondrial.

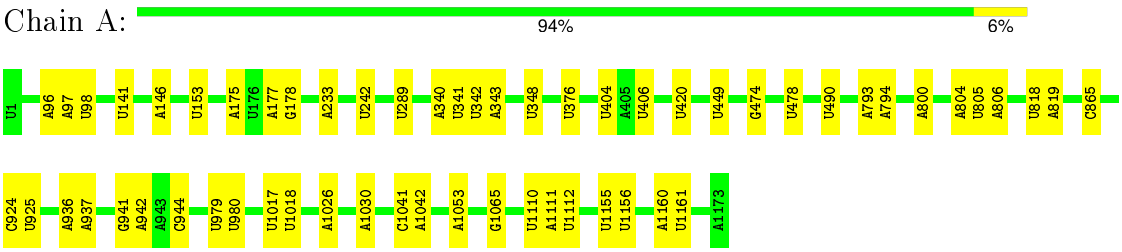
Mol	Chain	Residues	Atoms	AltConf	Trace
20	P	52	Total C 52 52	0	52

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: Leishmania Tarentolae Mitochondrial Large Ribosomal Subunit

Chain A:



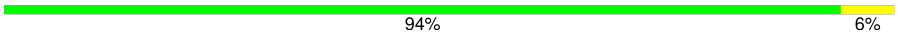
- Molecule 2: 39S ribosomal protein L2, mitochondrial

Chain B:

There are no outlier residues recorded for this chain.

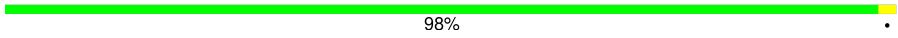
- Molecule 3: 50S ribosomal protein L3

Chain C:



- Molecule 4: 39S ribosomal protein L4, mitochondrial

Chain D:



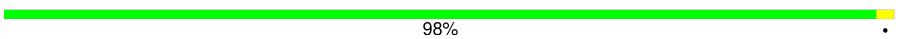
- Molecule 5: 50S ribosomal protein L9

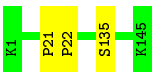
Chain H:

There are no outlier residues recorded for this chain.

- Molecule 6: 39S ribosomal protein L11, mitochondrial

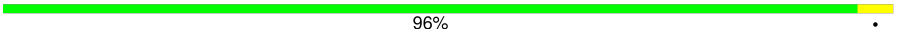
Chain G:





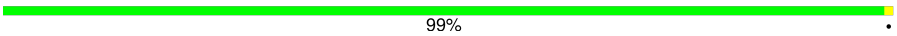
• Molecule 7: 50S ribosomal protein L13

Chain J:



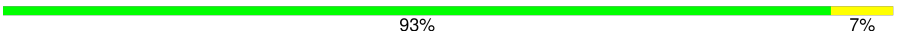
• Molecule 8: 50S ribosomal protein L14

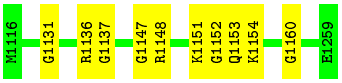
Chain K:



• Molecule 9: 50S ribosomal protein L15

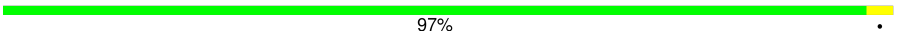
Chain L:

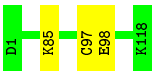




• Molecule 10: 39S ribosomal protein L16, mitochondrial

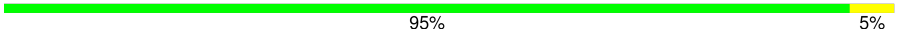
Chain I:





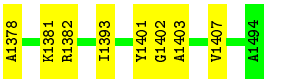
• Molecule 11: 39S ribosomal protein L17, mitochondrial

Chain S:



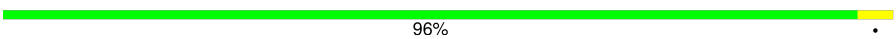
• Molecule 12: 50S ribosomal protein L20

Chain Q:



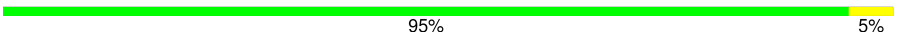
• Molecule 13: 50S ribosomal protein L21

Chain R:



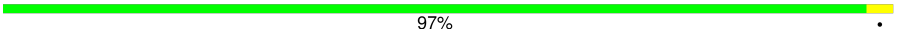
- Molecule 14: 39S ribosomal protein L22, mitochondrial

Chain M:



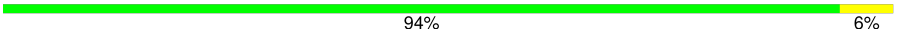
- Molecule 15: 50S ribosomal protein L23

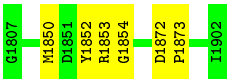
Chain T:



- Molecule 16: 39S ribosomal protein L24, mitochondrial

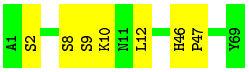
Chain N:





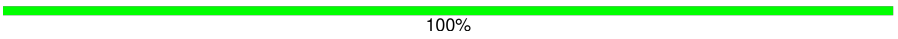
- Molecule 17: 39S ribosomal protein L27, mitochondrial

Chain O:



- Molecule 18: 50S ribosomal protein L29

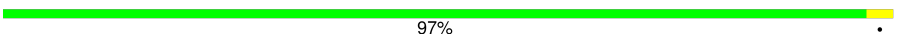
Chain X:

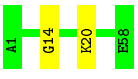


There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L30

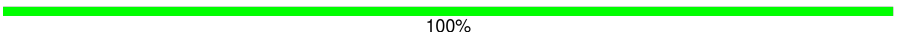
Chain Y:





- Molecule 20: 39S ribosomal protein L33, mitochondrial

Chain P:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	53475	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each Micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	50000	Depositor
Image detector	Kodak S0163 film	Depositor

5 Model quality

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	1027	0	0	61	0
2	B	136	0	0	0	0
3	C	209	0	0	15	0
4	D	175	0	0	3	0
5	H	60	0	0	0	0
6	G	145	0	0	2	0
7	J	140	0	0	7	0
8	K	121	0	0	1	0
9	L	144	0	0	11	0
10	I	118	0	0	3	0
11	S	116	0	0	8	0
12	Q	117	0	0	8	0
13	R	103	0	0	3	0
14	M	110	0	0	5	0
15	T	99	0	0	4	0
16	N	96	0	0	5	0
17	O	69	0	0	6	0
18	X	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	58	0	0	2	0
20	P	52	0	0	0	0
All	All	3158	0	0	78	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 25.

The worst 5 of 78 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:C:442:GLY:CA	11:S:3:ARG:CA	2.04	1.36
1:A:1160:A:P	3:C:438:SER:CA	2.17	1.32
1:A:98:U:P	14:M:1613:LEU:CA	2.19	1.29
15:T:1738:VAL:CA	16:N:1850:MET:CA	2.10	1.26
1:A:376:U:P	6:G:135:SER:CA	2.23	1.26

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/1027	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.