wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

PDB ID	:	3IY8
EMDB ID:	:	EMD-5113
Title	:	Leishmania tarentolae Mitonchondrial Ribosome small subunit
Authors	:	Sharma, M.R.; Booth, T.M.; Simpson, L.; Maslov, D.A.; Agrawal, R.K.
Deposited on	:	2009-04-16
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

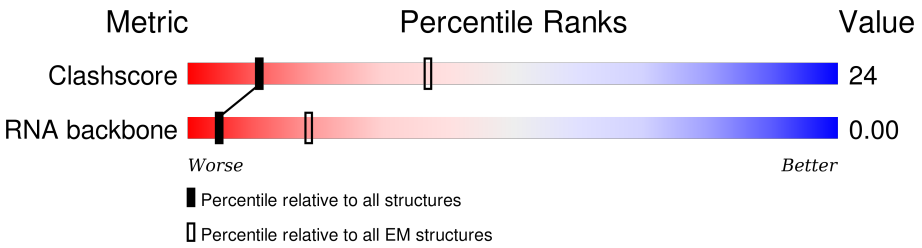
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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	540	94% 6%
2	E	150	99% .
3	F	100	97% .
4	H	129	93% 7%
5	I	127	100%
6	K	117	92% 8%
7	L	123	94% 6%
8	O	88	97% .
9	P	82	98% .
10	Q	80	95% 5%

Continued on next page...

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Mol	Chain	Length	Quality of chain
11	R	55	96%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 1591 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 small subunit.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	P		
1	A	540	540	540	0	540

- Molecule 2 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	E	150	150	150	0	150

- Molecule 3 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	F	100	100	100	0	100

- Molecule 4 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
4	H	129	129	129	0	129

- Molecule 5 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
5	I	127	127	127	0	127

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
6	K	117	117	117	0	117

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
7	L	123	123	123	0	123

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
8	O	88	88	88	0	88

- Molecule 9 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
9	P	82	82	82	0	82

- Molecule 10 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
10	Q	80	80	80	0	80

- Molecule 11 is a protein called 30S ribosomal protein S18.

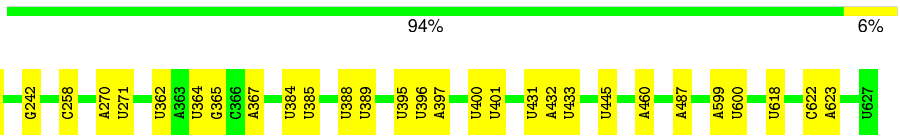
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
11	R	55	55	55	0	55

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.

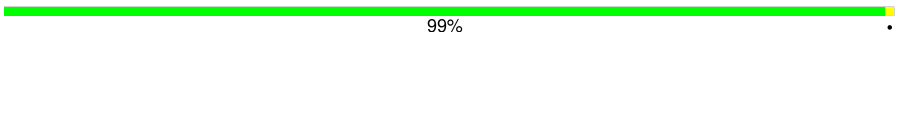
- Molecule 1: Leishmania tarentolae mitochondrial small subunit

Chain A:



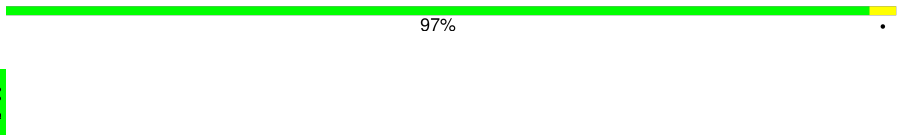
- Molecule 2: 30S ribosomal protein S5

Chain E:



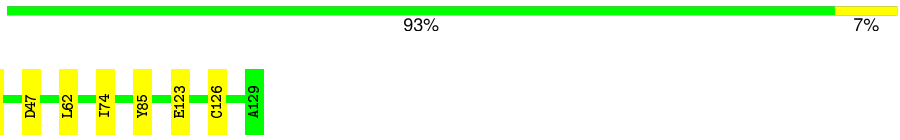
- Molecule 3: 30S ribosomal protein S6

Chain F:



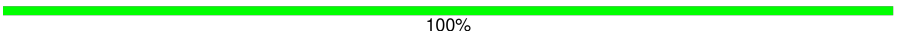
- Molecule 4: 30S ribosomal protein S8

Chain H:



- Molecule 5: 30S ribosomal protein S9

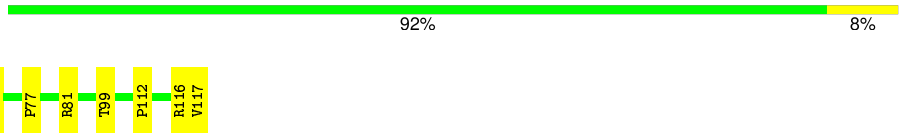
Chain I:



There are no outlier residues recorded for this chain.

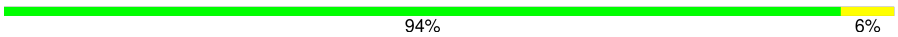
- Molecule 6: 30S ribosomal protein S11

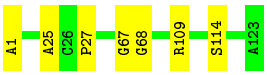
Chain K:



- Molecule 7: 30S ribosomal protein S12

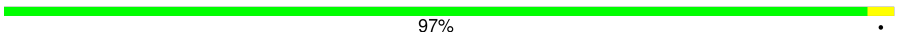
Chain L:

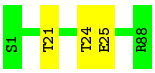




- Molecule 8: 30S ribosomal protein S15

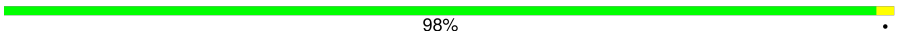
Chain O:





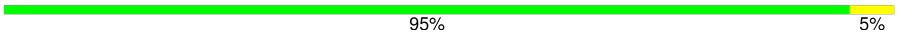
- Molecule 9: 30S ribosomal protein S16

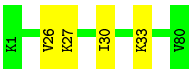
Chain P:



- Molecule 10: 30S ribosomal protein S17

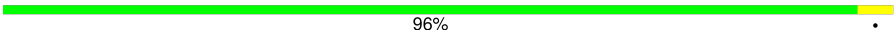
Chain Q:





- Molecule 11: 30S ribosomal protein S18

Chain R:



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 (i)

5.1 Standard geometry (i)

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 (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	A	540	0	0	34	0
2	E	150	0	0	1	0
3	F	100	0	0	3	0
4	H	129	0	0	10	0
5	I	127	0	0	0	0
6	K	117	0	0	9	0
7	L	123	0	0	7	0
8	O	88	0	0	3	0
9	P	82	0	0	2	0
10	Q	80	0	0	4	0
11	R	55	0	0	2	0
All	All	1591	0	0	38	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 24.

The worst 5 of 38 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)
1:A:242:G:P	7:L:67:GLY:CA	2.11	1.39
1:A:389:U:P	6:K:99:THR:CA	2.12	1.38
1:A:622:C:P	6:K:81:ARG:CA	2.10	1.37
1:A:271:U:P	7:L:25:ALA:CA	2.20	1.30
1:A:367:A:P	4:H:12:ARG:CA	2.20	1.29

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/540	-	-

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 (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)

There are no ligands in this entry.

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.