



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:29 am GMT

PDB ID : 3J2C
EMDB ID: : EMD-5504
Title : Dissecting the in vivo assembly of the 30S ribosomal subunit reveals the role of RimM
Authors : Guo, Q.; Goto, S.; Chen, Y.; Muto, A.; Himeno, H.; Deng, H.; Lei, J.; Gao, N.
Deposited on : 2012-09-28
Resolution : 13.20 Å(reported)
Based on PDB ID : 3OFA

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

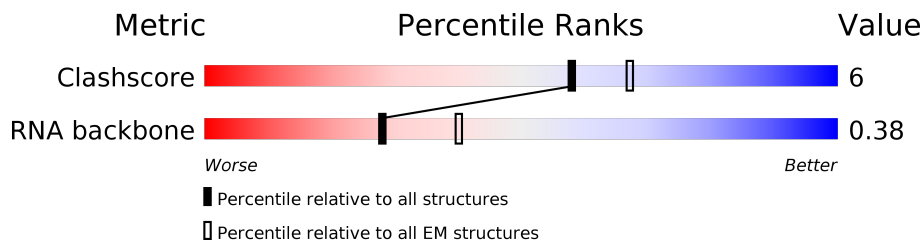
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

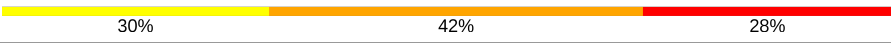
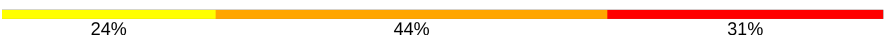

The reported resolution of this entry is 13.20 Å.

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	125131	1336
RNA backbone	3398	335

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	M	462	
2	N	927	
3	O	144	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49444 atoms, of which 16558 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 rRNA head domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	M	462	Total	C	H	N	O	P	0	0
			14865	4410	4987	1793	3214	461		

- Molecule 2 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	N	927	Total	C	H	N	O	P	0	0
			29941	8884	10017	3681	6433	926		

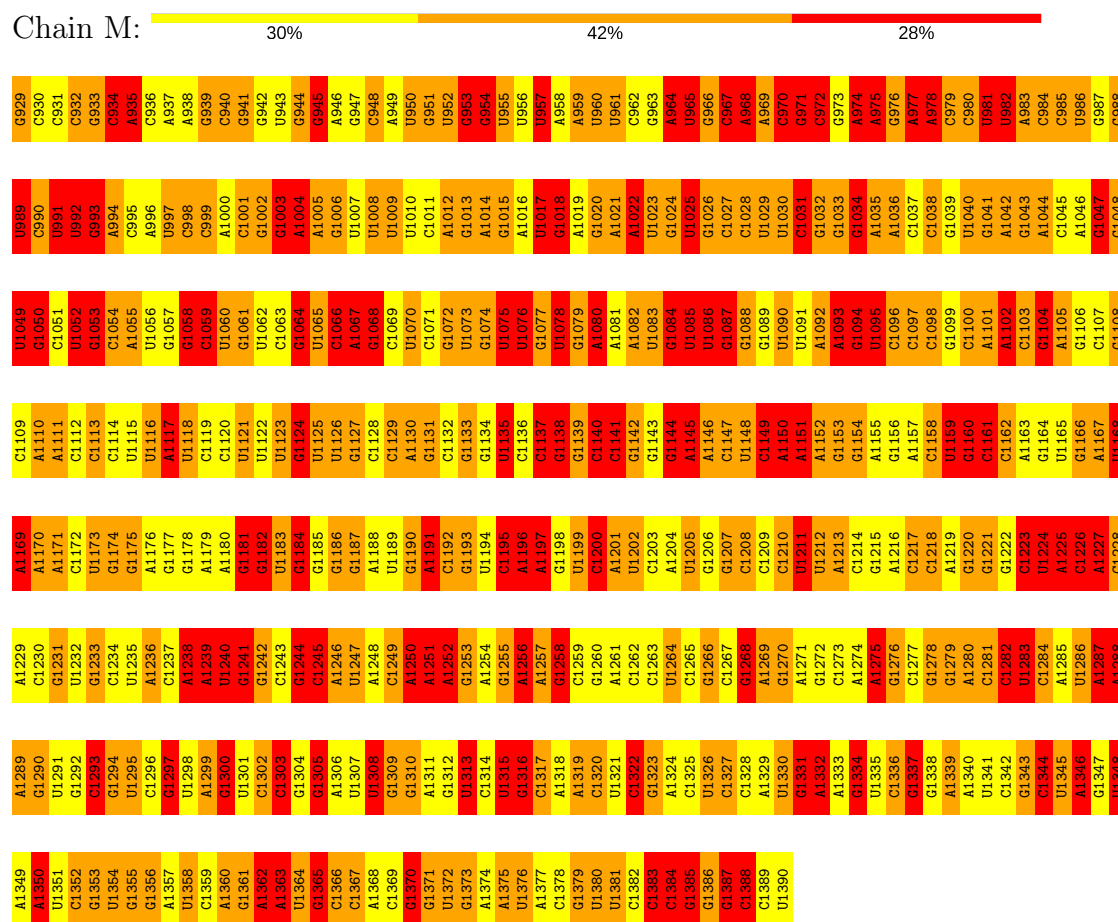
- Molecule 3 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	O	144	Total	C	H	N	O	P	0	0
			4638	1377	1554	562	1002	143		

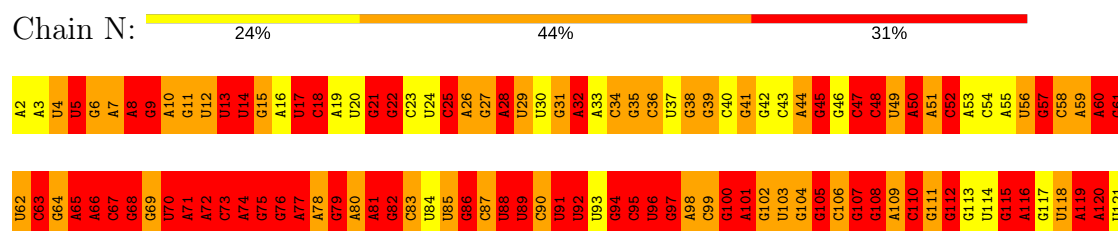
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 16S rRNA head domain



• Molecule 2: 16S rRNA body domain



- Molecule 3: 16S rRNA body domain

Response	Percentage
Yes, the U.S. is a democracy	32%
No, the U.S. is not a democracy	48%
Unsure	20%

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

G1511	U1512
A1513	G1514
G1515	G1516
G1517	A1518
A1519	C1520
C1521	U1522
G1523	C1524
G1525	G1526
U1527	U1528
G1529	G1530
A1531	U1532
C1533	A1534



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	44392	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	80000	Depositor
Image detector	4K*4K CCD Gatan 4000	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	M	3.43	1534/11053 (13.9%)	3.80	2624/17234 (15.2%)
2	N	3.44	3141/22318 (14.1%)	3.88	5510/34825 (15.8%)
3	O	3.32	455/3452 (13.2%)	3.95	849/5383 (15.8%)
All	All	3.43	5130/36823 (13.9%)	3.86	8983/57442 (15.6%)

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
1	M	0	236
2	N	0	522
3	O	0	78
All	All	0	836

The worst 5 of 5130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1502	A	N7-C5	-20.70	1.26	1.39
1	M	1251	A	N9-C4	18.33	1.48	1.37
2	N	124	C	N1-C6	-18.06	1.26	1.37
2	N	533	A	N7-C5	-17.64	1.28	1.39
2	N	350	G	C6-N1	17.60	1.51	1.39

The worst 5 of 8983 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1253	G	N1-C6-O6	26.96	136.07	119.90
3	O	1455	G	N1-C6-O6	26.35	135.71	119.90
3	O	1458	G	N1-C6-O6	25.20	135.02	119.90
1	M	1362	A	P-O3'-C3'	24.79	149.44	119.70
3	O	1405	G	C5-C6-O6	-24.61	113.83	128.60

There are no chirality outliers.

5 of 836 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	929	G	Sidechain
1	M	933	G	Sidechain
1	M	934	C	Sidechain
1	M	935	A	Sidechain
1	M	939	G	Sidechain

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	M	9878	4987	4986	67	0
2	N	19924	10017	10006	206	0
3	O	3084	1554	1553	14	0
All	All	32886	16558	16545	281	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 281 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:M:998:C:H42	1:M:1042:A:H61	1.38	0.71
2:N:50:A:H1'	2:N:52:C:C6	2.25	0.71
2:N:664:G:H22	2:N:741:G:H1	1.38	0.70
2:N:858:G:H1	2:N:869:G:H2'	1.55	0.70
2:N:411:A:H61	2:N:428:G:H1'	1.57	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	461/462 (99%)	152 (32%)	0
2	N	926/927 (99%)	255 (27%)	0
3	O	143/144 (99%)	31 (21%)	0
All	All	1530/1533 (99%)	438 (28%)	0

5 of 438 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	932	C
1	M	934	C
1	M	935	A
1	M	944	G
1	M	953	G

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.