Summary of integrative structure determination of Structure of 16S rRNA complexed with methyltransferase A small subunit (PDB ID: 8ZZE | pdb_00008zze, PDB-Dev ID: PDBDEV_00000014)

1. Model Composition	
1.1. Entry composition	- 16Srna: chain(s) A (1530 residues) - ksga: chain(s) B [V] (252 residues)
1.2. Datasets used for modeling	- Experimental model, PDB: pdb_00004adv - Mutagenesis data, Not available: 10.1074/jbc.M111.318121 - 3DEM volume, EMDB: EMD-2017 - DNA footprinting data, Not available: 10.1038/nsmb.1408
2. Representation	
2.1. Number of representations	1
2.2. Scale	Atomic
2.3. Number of rigid and flexible segments	20, 19
3. Restraints	
3.1. Physical principles	Information about physical principles was not provided
3.2. Experimental data	- 6 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0 - 2 unique EM3DRestraint: Local refinement
4. Validation	
4.2. Number of ensembles	0
4.3. Number of models in ensembles	Not applicable
4.4. Number of deposited models	1
4.5. Model precision	Not available
4.6. Data quality	EMD-2017: resolution is 13.50 Å
4.7. Model quality: assessment of atomic segments	- Clashscore: 21.89 - Ramachandran outliers: 1 - Sidechain outliers: 8
4.8. Fit to data used for modeling	- 3DEM q-score(s): 0.07 - 3DEM atom inclusion score(s): 0.83
4.9. Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	

1. 5.1. Method name	Rigid-body minimization
5.2. Method type	Rigid-body minimization in HADDOCK (it0)
5.4. Number of computed models	10000
2. 5.1. Method name	Simulated annealing
5.2. Method type	Semi-flexible SA in HADDOCK (it1)
5.4. Number of computed models	400
5.5. Software	- HADDOCK (version 2.3) - POWERFIT (version 2.0)