Summary of integrative structure determination of structure of 16s rrna complexed with methyltransferase a small subunit (PDBDEV00000014)

1. Model Composition	
Entry composition	- 16Srna: Chain A (1530 residues) - ksga: Chain B (252 residues)
Datasets used for modeling	- Experimental model, PDB ID: 4ADV - Mutagenesis data, Not listed - 3DEM volume, EMDB ID: EMD-2017 - unspecified, Not listed
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	20, 19
Rigid bodies	- A: 1-754:Experimental model/4ADV, 770-776:Experimental model/4ADV, 781-785:Experimental model/4ADV, 790-796:Experimental model/4ADV, 800-886:Experimental model/4ADV, 889-893:Experimental model/4ADV, 899-1507:Experimental model/4ADV, 1517-1530:Experimental model/4ADV. - B: 3-97:Experimental model/4ADV, 106-106:Experimental model/4ADV, 108-123:Experimental model/4ADV, 129-130:Experimental model/4ADV, 132-136:Experimental model/4ADV, 140-140:Experimental model/4ADV, 145-161:Experimental model/4ADV, 163-166:Experimental model/4ADV, 174-197:Experimental model/4ADV, 213-214:Experimental model/4ADV, 216-228:Experimental model/4ADV, 236-252:Experimental model/4ADV.
Flexible units	- A: 755-769, 777-780, 786-789, 797-799, 887-888, 894-898, 1508-1516. - B: 1-2, 98-105, 107-107, 124-128, 131-131, 137-139, 141-144, 162-162, 167-173, 198-212, 215-215, 229-235.
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 6 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0 - 1 unique EM3DRestraint: Local refinement, None
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, Not applicable

Number of ensembles	0
Number of models in ensembles	Not applicable
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Clashscore: 21.95, Ramachandran outliers: 0.4% , Sidechain outliers: 3.7%
Model quality: assessment of excluded volume	- Not applicable
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Rigid-body minimization
Name	Rigid-body minimization in HADDOCK (it0)
Details	- Method details unspecified
Software	- HADDOCK (version 2.3) - POWERFIT (version 2.0) - No location specified