

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

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - 16Srna: chain(s) A (1530 residues) - ksga: chain(s) B [V] (252 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 4ADV - 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	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	20, 19
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 6 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0 - 2 unique EM3DRestraint: Local refinement
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 21.89 - Ramachandran outliers: 1 - Sidechain outliers: 8
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
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. <i>Name</i>	Rigid-body minimization
<i>Method</i>	Rigid-body minimization in HADDOCK (it0)
<i>Number of computed models</i>	10000
2. <i>Name</i>	Simulated annealing
<i>Method</i>	Semi-flexible SA in HADDOCK (it1)
<i>Number of computed models</i>	400
<i>Software</i>	- HADDOCK (version 2.3) - POWERFIT (version 2.0)