

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

PDB ID	PDBDEV00000014
Molecule Name	Structure of 16S rRNA complexed with methyltransferase A small subunit
Title	Integrative Modeling of Biomolecular Complexes: HADDOCKing with Cryo-Electron Microscopy Data.
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The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobrity : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There are 1 unique types of models in this entry. The entry contains 4 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	16Srna	A	1530
1	ksga	B	252

There are 2 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	HADDOCK	2.3	molecular docking
2	POWERFIT	2.0	em fitter

There are 4 unique datasets used to build the model(s) in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Experimental model	PDB	4ADV
2	Mutagenesis data	Not Listed	None

3	3DEM volume	EMDB	EMD-2017
4	unspecified	Not Listed	None

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertainty of model
