Full wwPDB Integrative Structure Validation Report

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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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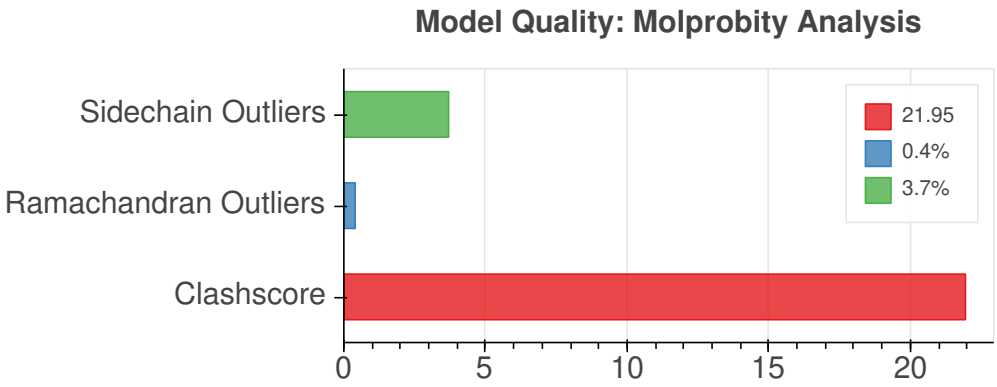
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 2 subunits in each model. A total of 4 datasets or restraints was used to build this entry. Each model is represented by 20 rigid bodies and 19 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled it1 ensemble/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	16Srna	A	1530
1	2	2	ksga	B	252

3.3 Datasets used for modeling

There are 4 unique datasets used to build the models 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

4. Representation

This entry has only one representation and includes 20 rigid bodies and 19 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
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.	755-769, 777-780, 786-789, 797-799, 887-888, 894-898, 1508-1516.

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.	1-2, 98-105, 107-107, 124-128, 131-131, 137-139, 141-144, 162-162, 167-173, 198-212, 215-215, 229-235.

5. Methodology and software

Step number	*Protocol ID*	*Method name*	*Method type*	*Number of computed models*	*Multi state modeling*	*Multi scale modeling*
1	1	Rigid-body minimization in HADDOCK (it0)	Rigid-body minimization	10000	False	True
2	1	Semi-flexible SA in HADDOCK (it1)	Simulated annealing	400	False	True

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

6. Data quality

7. Model quality

7.1 Standard geometry

There are 15655 bond outliers in this entry.

Bond type	*Observed distance (Å)*	*Ideal distance (Å)*	*Number of outliers*
C6--H6	1.089	0.93	603
C5--H5	1.089	0.93	603
C2--H2	1.089	0.93	355
NZ--HZ3	1.04	0.89	7
N--H3	1.041	0.89	0
N6--H61	1.009	0.86	355
C8--H8	1.079	0.93	805
N4--H42	1.009	0.86	320
N2--H21	1.009	0.86	449
N1--H1	1.004	0.86	449
N2--H22	1.009	0.86	449
N4--H41	1.009	0.86	320
NZ--HZ1	1.039	0.89	7
N6--H62	1.008	0.86	355
N3--H3	1.008	0.86	282
NZ--HZ2	1.039	0.89	7
N--H1	1.04	0.89	0
N--H2	1.039	0.89	0
NH1--HH11	1	0.86	12
NH2--HH22	0.999	0.86	12
NH2--HH21	1	0.86	12
NH1--HH12	0.999	0.86	12
SG--HG	1.325	1.2	1
C2'--H2'	1.089	0.97	1409

C1'--H1'	1.089	0.97	1409
C4'--H4'	1.089	0.97	1409
C5'--H5'	1.088	0.97	1409
C5'--H5''	1.088	0.97	1409
C3'--H3'	1.087	0.97	1409
N--H	0.978	0.86	231
NE2--HE22	0.979	0.86	13
OG--HG	0.959	0.84	11
OH--HH	0.959	0.84	7
OG1--HG1	0.959	0.84	11
NE2--HE2	0.98	0.86	4
NE--HE	0.979	0.86	12
ND2--HD21	0.979	0.86	14
NE2--HE21	0.979	0.86	13
ND2--HD22	0.979	0.86	14
ND1--HD1	0.98	0.86	4
O5'--HO5'	0.96	0.84	0
O3'--HO3'	0.96	0.84	0
O2'--HO2'	0.955	0.84	1409

There are 2 angle outliers in this entry.

Angle type	*Observed angle (°)*	*Ideal angle (°)*	*Number of outliers*
C3'-O3'-HO3'	107.296	120	0
C5'-O5'-HO5'	107.335	120	0

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
Model 1	21.95	1085

All 1085 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	250	246	3	1

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	V:130	THR

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	216	194	14	8

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	V:17	GLN
1	V:21	ASN
1	V:37	LYS
1	V:81	LEU
1	V:91	ASP
1	V:155	LYS

1	V:205	LYS
1	V:231	ASN

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model