



Full wwPDB Integrative Structure Validation Report

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

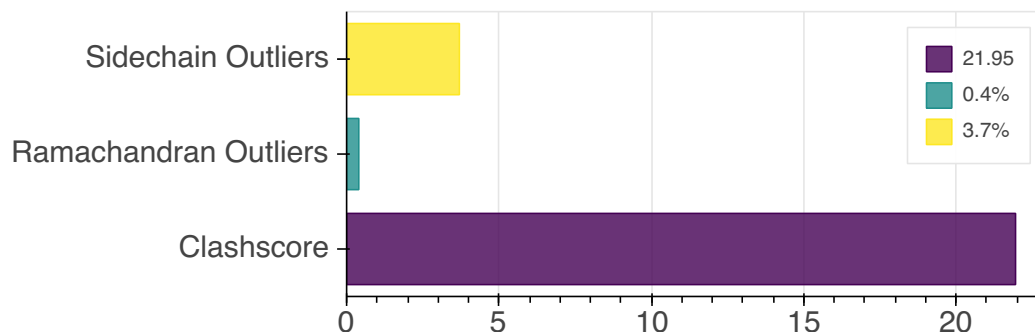
Molprobity : Version 4.4

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000014
Molecule Name	Structure of 16S rRNA complexed with methyltransferase A small subunit
Title	Integrative Modeling of Biomolecular Complexes: HADDOCKing with Cryo-Electron Microscopy Data.
Authors	van Zundert GCP;Melquiond ASJ;Bonvin AMJJ

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

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.

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

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	False
2	1	Semi-flexible SA in HADDOCK (it1)	Simulated annealing	400	False	False

Data quality

Model quality
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	0.86	12
NH2--HH22	0.999	0.86	12

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH21	1.0	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	0
C5'-O5'-HO5'	107.335	120.0	0

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.

Torsion angles: Protein backbone

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

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

Torsion angles: 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
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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

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model