Integrative Structure Validation Report

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A0V
PDB-Dev ID	PDBDEV_00000067
Structure Title	Hybrid NMR-SAXS structure of a trans-cleaving VS ribozyme
Structure Authors	Dagenais P; Desjardins G; Legault P

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

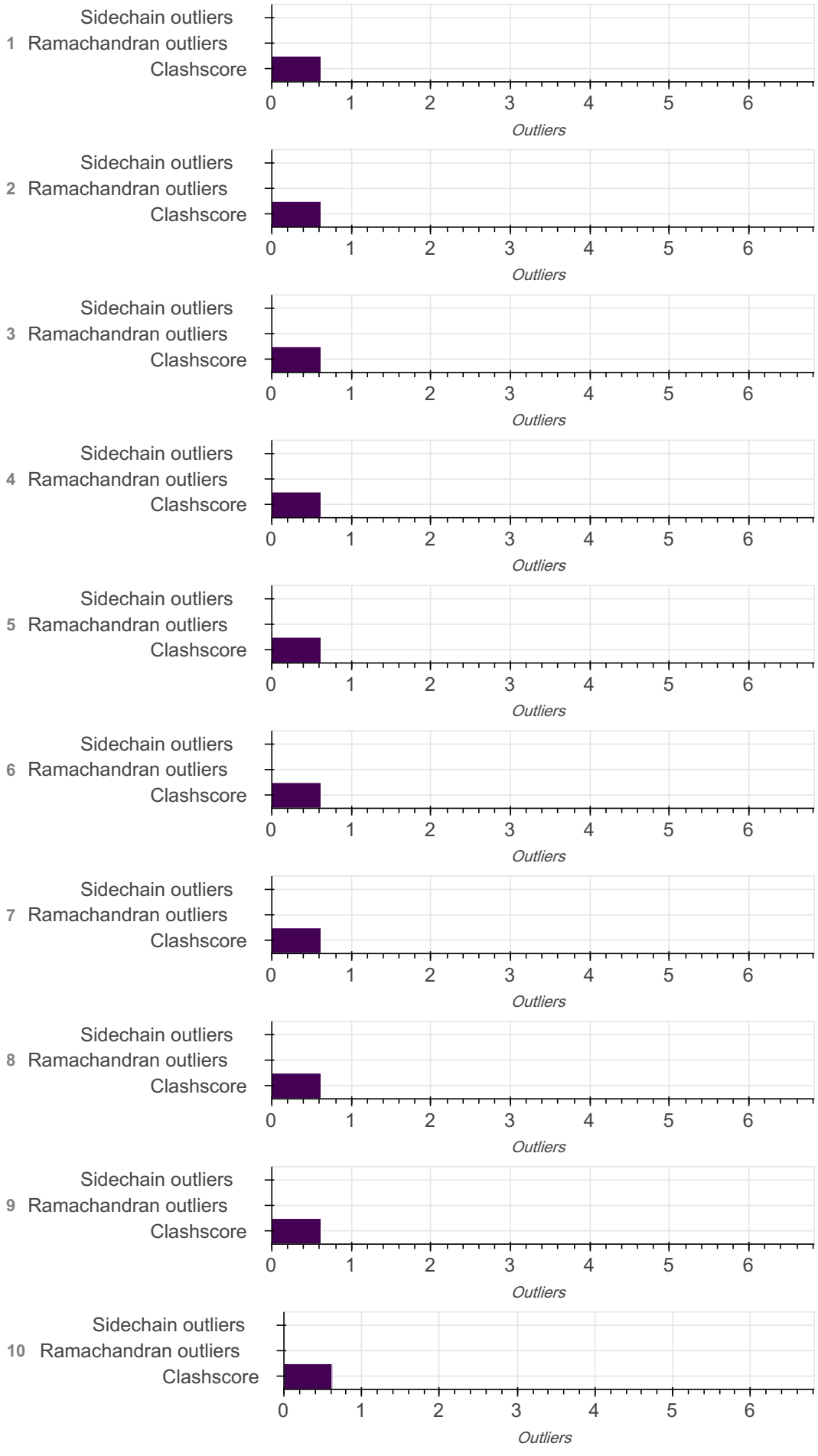
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis


1
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
1
2
3
4
5
6
Outliers

Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 unique models, with 1 subunits in each model. A total of 12 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 15 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled Best scoring model, 2nd best scoring model, 3rd best scoring model, 4th best scoring model, 5th best scoring model, 6th best scoring model, 7th best scoring model, 8th best scoring model, 9th best scoring model, 10th best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
2	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
3	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
4	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
5	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
6	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
7	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
8	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101
9	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	1	1	Neurospora Varkud Satellite Ribozyme	A	A	101

Datasets used for modeling

There are 12 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	25654
2	NMR data	BMRB	25163
3	NMR data	BMRB	17292
4	NMR data	BMRB	50637
5	SAS data	SASBDB	SASDKU3
6	SAS data	SASBDB	SASDKV3
7	SAS data	SASBDB	SASDKW3
8	SAS data	SASBDB	SASDKY3
9	Experimental model	PDB	2N3Q
10	Experimental model	PDB	2MTJ
11	Experimental model	PDB	2L5Z
12	Experimental model	PDB	1YN1

Representation

This entry has only one representation and includes 0 rigid bodies and 15 flexible units

Chain ID	Rigid bodies	Non-rigid segments

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-13, 14-18, 19-20, 21-22, 23-27, 28-31, 32-42, 43-46, 47-54, 55-65, 66-70, 71-80, 81-87, 88-100, 101-101

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	fragment assembly	_	_	_	False	False
2	1	refinement	_	_	_	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	QRNAS	Not available	refinement	http://genesilico.pl/software/stand-alone/qrnas
2	Pymol	Not available	model building	https://pymol.org/2/
3	Crysol	Not available	data processing	https://www.embl-hamburg.de/biosaxs/crysol.html

Data quality

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

NMR

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

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
1	0.62	2
2	0.62	2
3	0.62	2
4	0.62	2
5	0.62	2
6	0.62	2
7	0.62	2
8	0.62	2
9	0.62	2
10	0.62	2

All 20 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	0	0	0	0
2	0	0	0	0
3	0	0	0	0

Model ID	Analyzed	Favored	Allowed	Outliers
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0
7	0	0	0	0
8	0	0	0	0
9	0	0	0	0
10	0	0	0	0

Detailed list of outliers are tabulated below.

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	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0
7	0	0	0	0
8	0	0	0	0
9	0	0	0	0
10	0	0	0	0

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

NMR

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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