Integrative Structure Validation Report

March 27, 2025 - 10:03 AM PDT

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

Integrative Modeling Validation Version 2.0
Python-IHM Version 1.8
MolProbity Version 4.5.2
ATSAS Version 3.2.1 (r14885)

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
Deposited on	2020-12-14

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

We welcome your comments at helpdesk@pdb-ihm.org

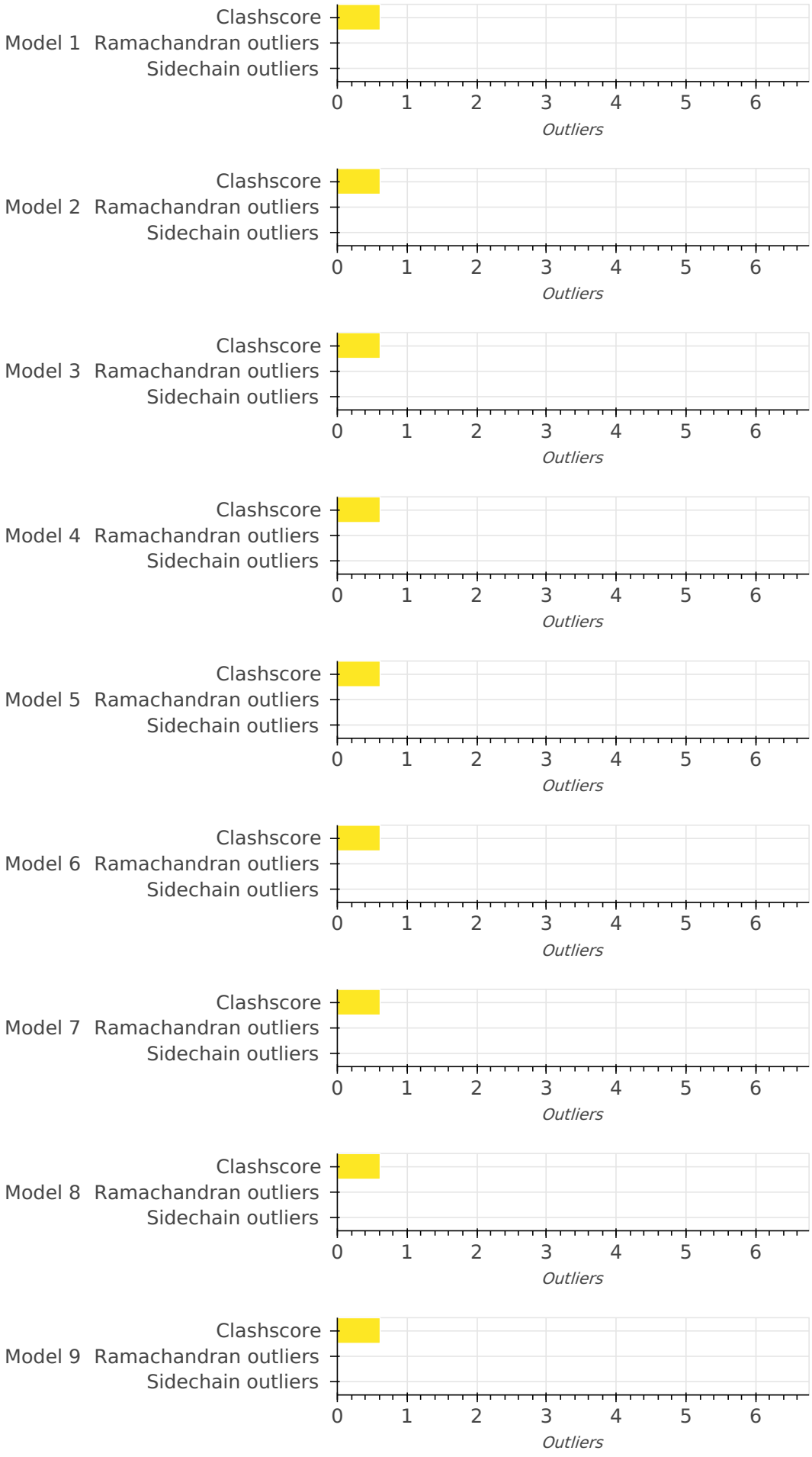
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

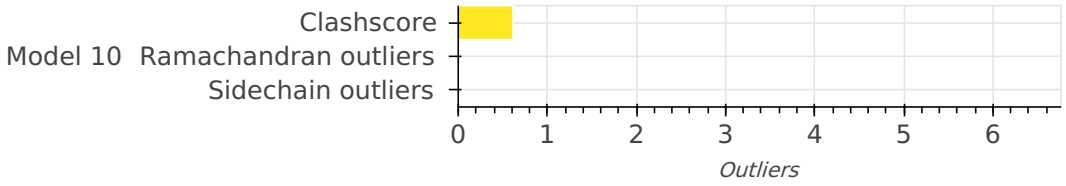
List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS 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


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



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 model(s). A total of 12 datasets were used to build this entry.

Representation

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-10	1	Neurospora Varkud Satellite Ribozyme	A	101	-	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	100.00 / 100.00	Atomic

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

ID	Dataset type	Database name	Data access code
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

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

There are no bond length outliers.

Standard geometry: angle outliers

There are 254 bond angle outliers in this entry (0.68% of 37540 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	84	G	C4'-O4'-C1'	7.23	102.67	109.90	3	10
A	19	C	O4'-C1'-C2'	6.66	100.94	107.60	2	10
A	39	U	C5'-C4'-C3'	5.62	107.57	116.00	5	3
A	17	C	C5'-C4'-C3'	5.53	107.71	116.00	2	10
A	66	G	C5'-C4'-C3'	5.37	107.95	116.00	1	6
A	25	U	C5'-C4'-C3'	5.11	108.34	116.00	4	10
A	82	C	O4'-C1'-C2'	5.05	102.55	107.60	9	3
A	26	C	C5'-C4'-C3'	5.05	108.43	116.00	6	10
A	37	A	C5'-C4'-C3'	4.94	108.58	116.00	2	10
A	70	C	C4'-O4'-C1'	4.89	105.01	109.90	9	3
A	94	A	C5'-C4'-C3'	4.88	108.68	116.00	9	10
A	16	C	C5'-C4'-C3'	4.83	108.75	116.00	2	10
A	9	C	C4'-O4'-C1'	4.79	105.11	109.90	2	1
A	52	U	C5'-C4'-C3'	4.70	108.95	116.00	2	4
A	70	C	C5'-C4'-C3'	4.70	108.95	116.00	4	10
A	39	U	C4'-O4'-C1'	4.68	105.22	109.90	2	1
A	51	A	O4'-C4'-C3'	4.66	108.66	104.00	10	6
A	4	G	C5'-C4'-C3'	4.62	109.07	116.00	9	10
A	7	A	C3'-C2'-C1'	4.62	105.92	101.30	2	4
A	87	C	C3'-C2'-C1'	4.58	106.08	101.50	7	4
A	26	C	O4'-C1'-C2'	4.54	103.06	107.60	8	6
A	87	C	C4'-C3'-O3'	4.54	106.20	113.00	4	6
A	94	A	O4'-C1'-C2'	4.42	103.18	107.60	4	10
A	25	U	C3'-C2'-C1'	4.42	105.72	101.30	4	4
A	53	U	C5'-C4'-C3'	4.38	109.42	116.00	8	10
A	39	U	C4'-C3'-C2'	4.30	98.30	102.60	1	3

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	36	G	C5'-C4'-C3'	4.22	109.67	116.00	5	10
A	66	G	OP1-P-OP2	4.22	106.94	119.60	2	4
A	91	A	C4'-O4'-C1'	4.22	105.48	109.70	9	10
A	39	U	OP1-P-OP2	4.20	107.00	119.60	1	6
A	70	C	O4'-C1'-N1	4.16	114.73	108.50	4	3
A	69	A	O3'-C3'-C2'	4.15	107.47	113.70	9	3
A	50	G	C4'-O4'-C1'	4.10	105.60	109.70	1	4
A	50	G	C5'-C4'-C3'	4.08	109.88	116.00	9	6
A	48	G	C4'-O4'-C1'	4.07	105.63	109.70	10	5
A	19	C	OP1-P-OP2	4.07	107.40	119.60	4	10
A	70	C	C3'-C2'-C1'	4.05	105.35	101.30	9	1
A	52	U	O4'-C1'-C2'	4.05	103.55	107.60	2	4
A	87	C	C5'-C4'-C3'	4.02	109.97	116.00	4	2
A	26	C	C2'-C1'-N1	4.02	118.03	112.00	5	2
A	9	C	C4'-C3'-C2'	4.01	98.59	102.60	2	1

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 atomic 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

There are 20 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are >= 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:30:G:H22	A:44:U:H3	0.49	6	10
A:30:G:H1	A:44:U:H3	0.42	2	10

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	Analysed	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

Torsion angles : Protein sidechains

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

Model ID	Analysed	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

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.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the PDB-IHM team (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the RCSB PDB (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the Sali lab contributed model validation metrics and software packages.

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