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	9A14
PDB-Dev ID	PDBDEV_00000076
Structure Title	Structure of N4BP1 CUE domain from NMR chemical shifts
Structure Authors	Song W; Garnett J; Stieglitz B

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

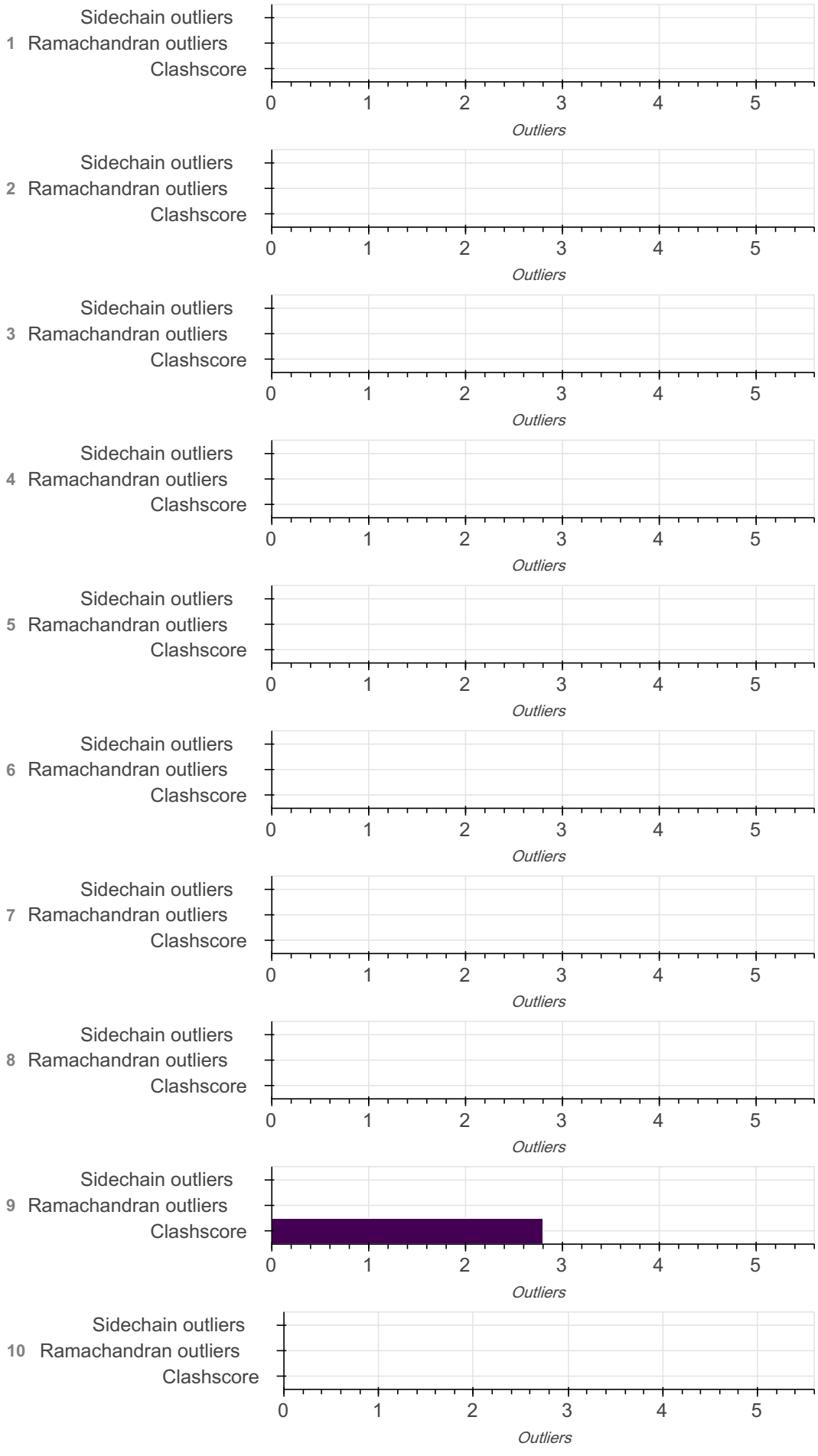
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


Sidechain outliers
1 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
2 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
3 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
4 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
5 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
6 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
7 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
8 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
9 Ramachandran outliers
Clashscore
0 1 2 3 4 5
Outliers
Sidechain outliers
10 Ramachandran outliers
Clashscore
0 1 2 3 4 5
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 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled S_08713, S_06192, S_15902, S_02507, S_08797, S_19499, S_19128, S_16128, S_00688, S_07018 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	N4BP1 CUE domain	A	A	44
2	1	1	N4BP1 CUE domain	A	A	44
3	1	1	N4BP1 CUE domain	A	A	44
4	1	1	N4BP1 CUE domain	A	A	44
5	1	1	N4BP1 CUE domain	A	A	44
6	1	1	N4BP1 CUE domain	A	A	44
7	1	1	N4BP1 CUE domain	A	A	44
8	1	1	N4BP1 CUE domain	A	A	44
9	1	1	N4BP1 CUE domain	A	A	44

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	1	1	N4BP1 CUE domain	A	A	44

Datasets used for modeling

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	50688

Representation

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-44

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	None	CS-ROSETTA modeling	None	20000	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	CS-ROSETTA	Not available	model building	https://csrosetta.bmrb.wisc.edu/submit

Data quality

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	0.00	0
2	0.00	0
3	0.00	0
4	0.00	0
5	0.00	0
6	0.00	0
7	0.00	0
8	0.00	0
9	2.80	2
10	0.00	0

All 2 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:43:LEU:O	A:44:ASP:O	0.425
9	A:34:ASP:C	A:34:ASP:OD1	0.408

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	42	42	0	0
2	42	42	0	0
3	42	42	0	0
4	42	42	0	0
5	42	42	0	0
6	42	42	0	0
7	42	42	0	0
8	42	42	0	0
9	42	42	0	0
10	42	42	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	39	39	0	0
2	39	39	0	0
3	39	39	0	0
4	39	39	0	0

Model ID	Analyzed	Favored	Allowed	Outliers
5	39	39	0	0
6	39	39	0	0
7	39	39	0	0
8	39	39	0	0
9	39	39	0	0
10	39	39	0	0

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling

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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