Integrative Structure Validation Report July 22, 2024 - 04:34 PM PDT

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	9A1L			
PDB-Dev ID	PDBDEV_00000093			
Structure Title	N4BP1 CUE domain in complex with ubiquitin			
Structure Authors	Fornili A; Pandini A; 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

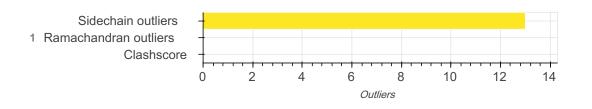
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 2 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 2 rigid bodies and 9 flexible or non-rigid units.

Entry composition?

There is 1 unique type of models in this entry. This model is titled None/Best scoring model.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	N4BP1 CUE domain	А	А	47
1	2	2	Ubiquitin	В	В	76

Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Integrative model	PDB-Dev	PDBDEV_00000076
2	Experimental model	PDB	1UBQ
3	Other	Not available	Not available

Representation ?

This entry has only one representation and includes 2 rigid bodies and 9 flexible units

Chain ID	Rigid bodies	Non-rigid segments		
А	1-47	7-25, 27-28, 37-47		
В	1-76	4-13, 27-27, 34-34, 36-36, 39-51, 66-76		

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	Rigid-body minimization in HADDOCK (it0)	Rigid-body minimization	None	1000	False	True
2	1	Semi-flexible SA in HADDOCK (it1)	Simulated annealing	None	200	False	True
3	1	Water refinement in HADDOCK (itw)	Refinement	None	200	False	True

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	Not available	model building	http://haddock.science.uu.nl/services/HADDOCK/

Data quality ?

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 216 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2HE22	0.97	0.86	1
ND2HD22	0.98	0.86	3
NHN	0.98	0.86	104
NE2HE22	0.98	0.86	7
ND2HD21	0.98	0.86	2
OG1HG1	0.96	0.84	5
NE2HE21	0.98	0.86	6
ОННН	0.96	0.84	2
NE2HE2	0.98	0.86	2
OGHG	0.96	0.84	4
NEHE	0.98	0.86	2
NHN	0.99	0.86	12
OGHG	0.97	0.84	2
NEHE	0.99	0.86	2
NE2HE21	0.99	0.86	1
ND2HD21	0.99	0.86	1
OG1HG1	0.97	0.84	1
ND1HD1	0.99	0.86	1
NHN	1.00	0.86	1

Bond type	Observed distance (Å)	ldeal distance (Å)	Number of outliers
NE2HE21	1.00	0.86	1
OG1HG1	0.98	0.84	2
NEHE	1.00	0.86	1
NZHZ2	1.04	0.89	10
NZHZ1	1.04	0.89	8
NZHZ3	1.04	0.89	8
NZHZ3	1.05	0.89	3
NZHZ1	1.05	0.89	3
NZHZ2	1.05	0.89	1
NH2HH21	1.03	0.86	1
NH2HH22	1.04	0.86	4
NH1HH11	1.04	0.86	5
NH1HH12	1.04	0.86	5
NH2HH21	1.04	0.86	1
NH2HH21	1.05	0.86	3
NH2HH22	1.06	0.86	1

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

All 0 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	119	113	6	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	108	87	8	13

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	А	5	0THR
1	А	19	0SER
1	А	47	0ASP
1	В	6	0LYS
1	В	14	0THR
1	В	18	0GLU
1	В	20	0SER
1	В	21	0ASP
1	В	22	0THR
1	В	39	0ASP
1	В	40	0GLN
1	В	57	0SER
1	В	66	0THR

Fit of model to data used for modeling ②

Fit of model to data used for validation ②

Validation for this section is under development.

Acknowledgements

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