Integrative Structure Validation Report July 22, 2024 - 04:53 PM PDT

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

Python-IHM Version 1.3 Integrative Modeling Validation Version 1.2

PDB ID	9A2C
PDB-Dev ID	PDBDEV_00000155
Structure Title	Integrative structure of the human NuDe complex
Structure Authors	Arvindekar S; Jackman MJ; Low JKK; Landsberg MJ; Mackay JP; Viswanath S

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

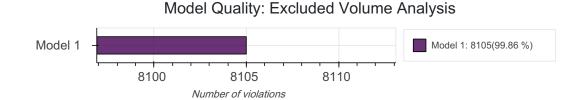
We welcome your comments at pdb-dev@mail.wwpdb.org

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 o

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.



IM Structure Validation Report

Ensemble information @

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 10 subunits in each model. A total of 19 datasets or restraints were used to build this entry. Each model is represented by 21 rigid bodies and 37 flexible or non-rigid units.

Entry composition?

There is 1 unique type of models in this entry. This model is titled Cluster 0/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	MTA1	А	A	715
1	2	1	MTA1	В	В	715
1	3	2	HDAC1	С	С	482
1	4	2	HDAC1	D	D	482
1	5	3	RBBP4	E	E	425
1	6	3	RBBP4	F	F	425
1	7	3	RBBP4	G	G	425
1	8	3	RBBP4	Н	н	425
1	9	4	MBD3	I	I	291
1	10	5	P66A	J	J	633

Datasets used for modeling ?

There are 19 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
15	Crosslinking-MS data	PRIDE	PXD010111
16	Crosslinking-MS data	PRIDE	PXD010111
17	Crosslinking-MS data	PRIDE	PXD010111
2	Comparative model	File	10.5281/zenodo.6674232
4	De Novo model	File	10.5281/zenodo.6674232
6	Comparative model	File	10.5281/zenodo.6674232
9	Comparative model	File	10.5281/zenodo.6674232
10	De Novo model	File	10.5281/zenodo.6674232
11	Comparative model	File	10.5281/zenodo.6674232
14	Experimental model	PDB	2L2L
19	3DEM volume	File	10.5281/zenodo.6674232
3	Experimental model	PDB	4BKX
7	Experimental model	PDB	5FXY
8	Experimental model	PDB	4PBZ
12	Experimental model	PDB	6CC8
1	Experimental model	PDB	2FVU
5	Experimental model	PDB	2GAT
13	Experimental model	PDB	2L2L
18	3DEM volume	EMDB	EMD-22904

Representation ?

This entry has only one representation and includes 21 rigid bodies and 37 flexible units

Chain ID	Rigid bodies	Non-rigid segments
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Chain ID	Rigid bodies	Non-rigid segments
н	10-411	1-9, 90-102, 164-165, 176-179, 212-213, 412-425
E	2-411	1-1, 90-113, 412-425
F	2-411	1-1, 90-113, 412-425
G	10-411	1-9, 90-102, 164-165, 176-179, 212-213, 412-425
В	1-164, 165-333, 334-353, 389-431, 468-546, 670-691	229-236, 354-388, 432-467, 519-528, 547-669, 692-715
A	1-164, 165-333, 334-353, 389-431, 468-546, 670-691	229-236, 354-388, 432-467, 519-528, 547-669, 692-715
D	8-376	1-7, 377-482
С	8-376	1-7, 377-482
I	1-71, 221-249	72-220, 250-291
J	137-178	136-136

Methodology and software

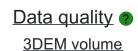
This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	1000000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.16.0	integrative model building	https://integrativemodeling.org

ID	Software name	Software version	Software classification	Software location
2	Integrative Modeling Platform (IMP)	2.16.0	integrative model building	https://integrativemodeling.org



Validation for this section is under development.

Crossl	inl	kin	a-	MS

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.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below.

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.86	8105.0

Fit of model to data used for modeling @

3DEM volume

Validation for this section is under development.

Crosslinking-MS

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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