Integrative Structure Validation Report October 24, 2024 - 10:36 AM 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	9A8I
PDB-Dev ID	PDBDEV_00000382
Structure Title	Integrative structure of the human WDR76-SPIN1-Nucleosome complex
Structure Authors	Xingyu Liu; Ying Zhang; Zhihui Wen; Yan Hao; Charles A.S. Banks; Joseph Cesare; Saikat Bhattacharya; Shreyas Arvindekar; Jeffrey J. Lange; Brian D. Slaughter; Jay R. Unruh; Shruthi Viswanath; Laurence Florens; Jerry L. Workman; Michael P. Washburn

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.

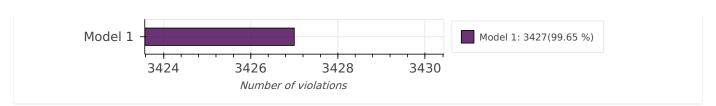
List of references used to build this report is available here.

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: Excluded Volume Analysis

2 of 5



Ensemble information ()

This entry consists of 1 distinct ensemble(s).

Summary 7

This entry consists of 1 unique models, with 10 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 11 rigid bodies and 21 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	WD repeat-containing protein 76	A	А	626
1	2	2	Spindlin-1	В	В	262
1	3	3	Histone H2A type 1	С	С	130
1	4	3	Histone H2A type 1	D	D	130
1	5	4	Histone H2B type 1- C/E/F/G/I	Е	Е	126
1	6	4	Histone H2B type 1- C/E/F/G/I	F	F	126
1	7	5	Histone H3.1	G	G	136
1	8	5	Histone H3.1	Н	н	136
1	9	6	Histone H4	I	I	103
1	10	6	Histone H4	J	J	103

Datasets used for modeling @ There are 5 unique datasets used to build the models in this entry. ID Data access code **Dataset type Database name** 4 Crosslinking-MS data MASSIVE MSV000086749 5 MASSIVE Crosslinking-MS data MSV000086828 1 De Novo model AlphaFoldDB AF-Q9H967-F1 2 PDB Experimental model 4H75 3 Experimental model PDB 5GT0

Representation (

This entry has only one representation and includes 11 rigid bodies and 21 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
F	28-125	1-27, 126-126
E	32-125	1-31, 126-126
Н	37-135	1-36, 136-136
D	14-119	1-13, 120-130
С	13-118	1-12, 119-130
G	37-135	1-36, 136-136
J	24-102	1-23, 103-103
I	17-102	1-16, 103-103
А	245-276, 288-626	1-244, 277-287
В	45-259	1-44, 195-210, 260-262

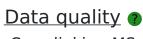
Methodology and software

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	750000	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
2	Integrative Modeling Platform (IMP)	2.16.0	integrative model building	https://integrativemodeling.org



Crosslinking-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	99.65	3427.0

Fit of model to data used for modeling

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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