Full wwPDB Integrative Structure Validation Report

September 06, 2019 -- 02:06 PM

PDB ID	PDBDEV00000028
Molecule Name	Complex of RNF168-RING domain and the nucleosome
Title	Structural basis of specific H2A K13/K15 ubiquitination by RNF168
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The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobity : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There is 1 unique type of model in this entry. Model has 11 chains respectively.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	H3	A	99
1	H4	E	99
1	H2A	B	80
1	H2B	F	80
1	DNA strand 1	C	107
1	DNA strand 2	G	107
1	RNF168 RING domain	D	95
1	H3	H	95
1	H4	I	147
1	H2A	J	147
1	H2B	K	91

There are 2 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	HADDOCK	2.2	molecular docking
2	JWALK	1.1	XL-MS validation

There are 7 unique datasets used to build the model in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Experimental model	PDB	2PYO
2	Experimental model	PDB	4GB0
3	Mutagenesis data	Not Listed	None
4	NMR data	BMRB	27786
5	NMR data	BMRB	27791
6	NMR data	BMRB	27792
7	CX-MS data	PRIDE	PXD012723

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

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6. Uncertaintiy of model