

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

PDB ID	PDBDEV00000029
Molecule Name	Complex of Ubch5c, RNF168-RING domain and the nucleosome
Title	Structural basis of specific H2A K13/K15 ubiquitination by RNF168
Authors	Horn V;Uckelmann M;Zhang H;Eerland J;Aarsman I;le Paige UB;Davidovich C;Sixma TK;van Ingen H

The following softwares were used in the production of this report:

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

1. Overall quality at a glance

2. Entry composition

There are 2 unique types of models in this entry. The entry contains 12 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	H3	A	99
1	H4	E	99
1	H2A N18S mutant	B	80
1	H2B S121A mutant	F	80
1	DNA strand 1	C	107
1	DNA strand 2	G	107
1	RNF168 RING domain	D	95
1	Ubch5c	H	95
1	H3	I	147
1	H4	J	147
1	H2A N18S mutant	K	91

1	H2B S121A mutant	L	153
---	------------------	---	-----

There are 1 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	HADDOCK	2.2	molecular docking

There are 3 unique datasets used to build the model(s) in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Integrative model	None	PDBDEV_00000028
2	Experimental model	PDB	1X23
3	unspecified	Not Listed	None

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

6. Uncertainty of model
