WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB Integrative Structure Validation Report

November 07, 2019 -- 03:20 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 software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

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1. Overall quality at a glance

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2. Ensemble information

This entry consists of 0 distinct ensemble.

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3. Model composition

3.1 Summary

This entry consists of 10 unique models, with 12 subunits in each model. A total of 3 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 12 flexible or non-rigid units.

3.2 Entry composition

There are 10 unique types of models in this entry.These models are titled Best Scoring Model cluster 1, no.2 Scoring Model cluster 1, no.3 Scoring Model cluster 1, no.4 Scoring Model cluster 1, no.5 Scoring Model cluster 1, no.6 Scoring Model cluster 1, no.7 Scoring Model cluster 1, no.8 Scoring Model cluster 1, no.9 Scoring Model cluster 1, no.10 Scoring Model cluster 1 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	H3	A	99
1	2	1	H3	E	99
1	3	2	H4	B	80
1	4	2	H4	F	80
1	5	3	H2A N18S mutant	C	107
1	6	3	H2A N18S mutant	G	107
1	7	4	H2B S121A mutant	D	95
1	8	4	H2B S121A mutant	H	95
1	9	5	DNA strand 1	I	147
1	10	6	DNA strand 2	J	147
1	11	7	RNF168 RING domain	K	91
1	12	8	UbcH5c	L	153
2	1	1	H3	A	99
2	2	1	H3	E	99
2	3	2	H4	B	80
2	4	2	H4	F	80
2	5	3	H2A N18S mutant	C	107
2	6	3	H2A N18S mutant	G	107
2	7	4	H2B S121A mutant	D	95
2	8	4	H2B S121A mutant	H	95
2	9	5	DNA strand 1	I	147
2	10	6	DNA strand 2	J	147
2	11	7	RNF168 RING domain	K	91
2	12	8	UbcH5c	L	153
3	1	1	H3	A	99
3	2	1	H3	E	99
3	3	2	H4	B	80
3	4	2	H4	F	80

3	5	3	H2A N18S mutant	C	107
3	6	3	H2A N18S mutant	G	107
3	7	4	H2B S121A mutant	D	95
3	8	4	H2B S121A mutant	H	95
3	9	5	DNA strand 1	I	147
3	10	6	DNA strand 2	J	147
3	11	7	RNF168 RING domain	K	91
3	12	8	UbcH5c	L	153
4	1	1	H3	A	99
4	2	1	H3	E	99
4	3	2	H4	B	80
4	4	2	H4	F	80
4	5	3	H2A N18S mutant	C	107
4	6	3	H2A N18S mutant	G	107
4	7	4	H2B S121A mutant	D	95
4	8	4	H2B S121A mutant	H	95
4	9	5	DNA strand 1	I	147
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4	11	7	RNF168 RING domain	K	91
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5	1	1	H3	A	99
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7	1	1	H3	A	99
7	2	1	H3	E	99
7	3	2	H4	B	80
7	4	2	H4	F	80
7	5	3	H2A N18S mutant	C	107
7	6	3	H2A N18S mutant	G	107
7	7	4	H2B S121A mutant	D	95
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8	3	2	H4	B	80
8	4	2	H4	F	80
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10	12	8	UbcH5c	L	153

3.3 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	None	PDBDEV_00000028
2	Experimental model	PDB	1X23
3	unspecified	Not listed	None

4. Representation

This entry has only one representation and includes 0 rigid bodies and 12 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-99.
B	-	1-80.
C	-	1-107.
D	-	1-95.
E	-	1-99.
F	-	1-80.
G	-	1-107.
H	-	1-95.
I	-	1-147.
J	-	1-147.
K	-	1-91.
L	-	1-153.

5. Methodology and software

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	2.2	molecular docking	http://haddock.science.uu.nl/service

6. Data quality

7. Model quality

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model