Full wwPDB Integrative Structure Validation Report

November 05, 2019 -- 04:07 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
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

1. Overall quality at a glance

2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 10 unique models, with 11 subunits in each model. A total of 7 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 11 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	C	107
1	6	3	H2A	G	107
1	7	4	H2B	D	95
1	8	4	H2B	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
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	C	107
2	6	3	H2A	G	107
2	7	4	H2B	D	95
2	8	4	H2B	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
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	C	107
3	6	3	H2A	G	107
3	7	4	H2B	D	95
3	8	4	H2B	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
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	C	107
4	6	3	H2A	G	107
4	7	4	H2B	D	95
4	8	4	H2B	H	95
4	9	5	DNA strand 1	I	147
4	10	6	DNA strand 2	J	147
4	11	7	RNF168 RING domain	K	91
5	1	1	H3	A	99
5	2	1	H3	E	99

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

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

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

3.3 Datasets used for modeling

There are 7 unique datasets used to build the models 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

4. Representation

This entry has only one representation and includes 0 rigid bodies and 11 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.

5. Methodology and software

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

6. Data quality

7. Model quality

7.1 Standard geometry

There are 13530 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers

ND2--HD22	1.008	0.86	109
N--H	1.008	0.86	1609
NE2--HE2	1.008	0.86	39
NH1--HH12	1.008	0.86	89
CD2--HD2	1.078	0.93	199
CE1--HE1	1.078	0.93	199
CE2--HE2	1.078	0.93	159
NH1--HH11	1.009	0.86	89
ND2--HD21	1.009	0.86	109
NE2--HE22	1.009	0.86	99
CZ--HZ	1.079	0.93	49
NH2--HH22	1.009	0.86	89
NE2--HE21	1.008	0.86	99
NE--HE	1.009	0.86	89
CD1--HD1	1.078	0.93	159
NH2--HH21	1.009	0.86	89
CG--HG3	1.089	0.97	649
CA--HA	1.088	0.97	1659
CB--HB	1.088	0.97	149
CD--HD2	1.089	0.97	359
CB--HB2	1.088	0.97	1509
CD2--HD22	1.088	0.97	189
CE--HE1	1.088	0.97	59
CB--HB3	1.088	0.97	1509
CB--HB1	1.088	0.97	189
CG2--HG21	1.089	0.97	149
CA--HA2	1.089	0.97	179

CD2--HD21	1.088	0.97	189
CG--HG2	1.088	0.97	649
CA--HA3	1.089	0.97	179
CD--HD3	1.089	0.97	359
CD1--HD11	1.089	0.97	209
CD1--HD13	1.088	0.97	209
NZ--HZ3	1.009	0.89	49
CG1--HG12	1.089	0.97	79
CG2--HG22	1.088	0.97	149
N--H3	1.009	0.89	9
CG2--HG23	1.089	0.97	149
OG--HG	0.959	0.84	139
CE--HE2	1.089	0.97	109
CD1--HD12	1.089	0.97	209
CG1--HG11	1.089	0.97	59
NZ--HZ2	1.009	0.89	49
CG1--HG13	1.088	0.97	79
CD2--HD23	1.089	0.97	189
OG1--HG1	0.959	0.84	69
CE--HE3	1.089	0.97	109
NZ--HZ1	1.009	0.89	49
OH--HH	0.959	0.84	109
CG--HG	1.089	0.97	189
N--H2	1.009	0.89	9
N--H1	1.009	0.89	9

There are 316 angle outliers in this entry.

Angle type	*Observed angle (°)*	*Ideal angle (°)*	*Number of outliers*
C-N-H	112.269	124.3	122
HG2-CG-HG3	97.708	110	8
CG-CB-HB2	120.202	108	7
HD22-CD2-HD23	97.918	110	2
HG12-CG1-HG13	92.282	110	0
HB2-CB-HB3	97.993	110	31
HZ1-NZ-HZ3	122.371	109	2
CA-N-H	126.273	114	7
CB-OG1-HG1	93.037	110	0
CB-CA-HA	96.938	109	3
N-CA-HA	97.858	110	6
HD21-CD2-HD22	97.003	110	1
HB1-CB-HB2	96.99	110	5
CG-CB-HB3	95.827	108	7
HD2-CD-HD3	122.233	110	7
C-CA-HA	96.951	109	10
CE-NZ-HZ2	94.864	110	0
CA-CB-HB3	96.927	109	9
CA-CB-HB2	121.002	109	4
HD12-CD1-HD13	97.874	110	1
HD11-CD1-HD12	95.703	110	0
HG22-CG2-HG23	96.722	109	3
SD-CE-HE1	95.744	109	1
HG21-CG2-HG23	95.829	110	0
CB-CG-HG3	121.179	109	2
CB-CG1-HG11	122.984	109	0

CG-CD2-HD23	121.251	109	1
NZ-CE-HE2	121.714	108	0
HD21-CD2-HD23	96.708	110	1
N-CA-HA2	96.384	110	0
HE2-CE-HE3	96.468	110	0
CB-CG-HG2	121.139	109	2
CD-CG-HG2	121.262	108	0
CB-CG2-HG22	97.308	110	1
HG11-CG1-HG13	97.438	110	3
SD-CE-HE2	121.941	109	0
HE1-CE-HE3	97.073	110	0
CZ-CE2-HE2	107.364	120.2	0
HG11-CG1-HG12	97.195	110	0
CZ-OH-HH	122.334	110	1
HH21-NH2-HH22	107.333	120	0
HB1-CB-HB3	97.473	110	1
OG-CB-HB2	121.604	109	0
CD-CG-HG3	97.925	110	2
N-CD-HD3	121.548	109	0
CG-CD1-HD12	121.475	109	0
N-CD-HD2	121.456	109	0
CG-CD2-HD22	121.003	109	1
CD2-CG-HG	95.7	108	0
CZ-NH2-HH22	107.711	120	0
CG2-CB-HB	95.715	108	0
HZ2-NZ-HZ3	121.179	109	1
OG-CB-HB3	96.789	109	0

CB-CG2-HG23	121.082	109	1
CG-CD-HD3	121.18	109	0
HD11-CD1-HD13	97.867	110	0
C-CA-HA3	96.869	109	0
HA2-CA-HA3	96.936	109	1
CZ-NH1-HH11	107.88	120	0
CG-ND2-HD21	107.932	120	0
CA-CB-HB1	121.049	109	0
NZ-CE-HE3	120.023	108	0

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	*Clash score*	*Number of clashes*
Model 1	0.00	0
Model 10	0.00	0
Model 2	0.00	0
Model 3	0.00	0
Model 4	0.00	0
Model 5	0.00	0
Model 6	0.00	0
Model 7	0.00	0
Model 8	0.00	0
Model 9	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	182	147	32	3
2	182	150	28	4
3	182	169	10	3
4	182	154	26	2
5	182	161	14	7
6	182	153	23	6
7	182	159	19	4
8	182	153	23	6
9	182	156	19	7
10	182	155	23	4

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:55	PRO
1	A:74	GLY
1	A:136	PRO
2	A:21	1ASN
2	A:35	1LEU
2	A:55	1PRO
2	A:129	1PRO
3	A:55	PRO
3	A:72	VAL
3	A:124	HIS
4	A:55	PRO
4	A:99	PRO

5	A:10	SER
5	A:11	GLY
5	A:14	LEU
5	A:55	PRO
5	A:76	THR
5	A:117	LEU
5	A:144	ALA
6	A:55	PRO
6	A:70	ALA
6	A:103	VAL
6	A:126	GLN
6	A:146	PRO
6	A:163	GLU
7	A:44	LEU
7	A:47	SER
7	A:55	PRO
7	A:110	LEU
8	A:32	LYS
8	A:55	PRO
8	A:79	PRO
8	A:86	ALA
8	A:90	GLY
8	A:144	ALA
9	A:55	PRO
9	A:57	GLY
9	A:69	ASN
9	A:70	ALA

9	A:88	ALA
9	A:96	GLY
9	A:126	GLN
10	A:42	VAL
10	A:55	PRO
10	A:57	GLY
10	A:141	VAL

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	147	123	14	10
2	147	133	12	2
3	147	132	9	6
4	147	125	16	6
5	147	108	24	15
6	147	126	13	8
7	147	116	19	12
8	147	119	21	7
9	147	124	15	8
10	147	119	21	7

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:2	THR
1	A:18	ILE
1	A:26	LEU

1	A:72	VAL
1	A:109	MET
1	A:116	GLN
1	A:151	ARG
1	A:165	LEU
1	A:168	THR
1	A:184	TYR
2	A:106	SER
2	A:177	GLU
3	A:17	GLN
3	A:26	LEU
3	A:33	ILE
3	A:99	PRO
3	A:102	SER
3	A:140	THR
4	A:12	MET
4	A:51	VAL
4	A:91	SER
4	A:97	PHE
4	A:112	HIS
4	A:140	THR
5	A:14	LEU
5	A:39	LEU
5	A:42	VAL
5	A:43	TYR
5	A:60	TYR
5	A:97	PHE

5	A:103	VAL
5	A:117	LEU
5	A:120	PHE
5	A:135	GLU
5	A:154	SER
5	A:164	ARG
5	A:168	THR
5	A:169	ASN
5	A:181	GLU
6	A:4	THR
6	A:52	TYR
6	A:85	GLU
6	A:110	LEU
6	A:134	ASN
6	A:140	THR
6	A:165	LEU
6	A:177	GLU
7	A:1	MET
7	A:4	THR
7	A:31	LEU
7	A:35	LEU
7	A:45	ASP
7	A:91	SER
7	A:126	GLN
7	A:128	VAL
7	A:132	LEU
7	A:165	LEU

7	A:180	LYS
7	A:183	ARG
8	A:44	LEU
8	A:72	VAL
8	A:108	LEU
8	A:140	THR
8	A:143	GLU
8	A:159	GLN
8	A:168	THR
9	A:6	HIS
9	A:15	LEU
9	A:19	GLN
9	A:104	SER
9	A:126	GLN
9	A:127	GLN
9	A:174	MET
9	A:178	SER
10	A:35	LEU
10	A:39	LEU
10	A:42	VAL
10	A:78	LEU
10	A:100	LEU
10	A:129	PRO
10	A:176	MET

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model