

Table S1: Summary of Integrative Structure Determination of Complex of UbcH5c, RNF168-RING domain and the nucleosome (PDBDEV00000029)

1. Model Composition	
	<ul style="list-style-type: none"> - H3: Chain A (99 residues) - H3: Chain E (99 residues) - H4: Chain B (80 residues) - H4: Chain F (80 residues) - H2A N18S mutant: Chain C (107 residues) - H2A N18S mutant: Chain G (107 residues) - H2B S121A mutant: Chain D (95 residues) - H2B S121A mutant: Chain H (95 residues) - DNA strand 1: Chain I (147 residues) - DNA strand 2: Chain J (147 residues) - RNF168 RING domain: Chain K (91 residues) - UbcH5c: Chain L (153 residues) - H3: Chain A (99 residues) - H3: Chain E (99 residues) - H4: Chain B (80 residues) - H4: Chain F (80 residues) - H2A N18S mutant: Chain C (107 residues) - H2A N18S mutant: Chain G (107 residues) - H2B S121A mutant: Chain D (95 residues) - H2B S121A mutant: Chain H (95 residues) - DNA strand 1: Chain I (147 residues) - DNA strand 2: Chain J (147 residues) - RNF168 RING domain: Chain K (91 residues) - UbcH5c: Chain L (153 residues) - H3: Chain A (99 residues) - H3: Chain E (99 residues) - H4: Chain B (80 residues) - H4: Chain F (80 residues) - H2A N18S mutant: Chain C (107 residues) - H2A N18S mutant: Chain G (107 residues) - H2B S121A mutant: Chain D (95 residues) - H2B S121A mutant: Chain H (95 residues) - DNA strand 1: Chain I (147 residues) - DNA strand 2: Chain J (147 residues) - RNF168 RING domain: Chain K (91 residues) - UbcH5c: Chain L (153 residues) - H3: Chain A (99 residues) - H3: Chain E (99 residues) - H4: Chain B (80 residues) - H4: Chain F (80 residues) - H2A N18S mutant: Chain C (107 residues) - H2A N18S mutant: Chain G (107 residues) - H2B S121A mutant: Chain D (95 residues) - H2B S121A mutant: Chain H (95 residues) - DNA strand 1: Chain I (147 residues) - DNA strand 2: Chain J (147 residues) - RNF168 RING domain: Chain K (91 residues) - UbcH5c: Chain L (153 residues) - H3: Chain A (99 residues) - H3: Chain E (99 residues) - H4: Chain B (80 residues) - H4: Chain F (80 residues) - H2A N18S mutant: Chain C (107 residues) - H2A N18S mutant: Chain G (107 residues) - H2B S121A mutant: Chain D (95 residues) - H2B S121A mutant: Chain H (95 residues)

[Entry composition](#)

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Datasets used for modeling	<ul style="list-style-type: none"> - Integrative model, PDBDEV_00000028 - Experimental model, PDB ID: 1X23 - conserved E2-E3 interactions in RNF168, identified from aligned homologous structures, Not listed
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies , flexible units	0, 12
<i>Rigid regions</i>	<ul style="list-style-type: none"> - A: - - B: - - C: - - D: - - E: - - F: - - G: - - H: - - I: - - J: - - K: - - L: -
<i>Flexible units</i>	<ul style="list-style-type: none"> - 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.
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: 50 residues per bead.
3. Restraints	
Physical principles	Excluded volume and Sequence connectivity.
Experimental data	<ul style="list-style-type: none"> - 12 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.5 - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 4.0 - 2 unique DerivedDistanceRestraint: Upper Bound Distance: 9.0
4. Validation	
Sampling validation	1. Information related to sampling validation has not been provided
Clustering algorithm , clustering feature	distance threshold-based clustering, Not applicable

<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Quality of data</i>	1. Quality of input data has not be assessed
<i>Assessment of atomic regions</i>	
<i>Assessment of excluded volume</i>	
<i>Fit of the model to information used to compute it</i>	1. Fit of model to information used to compute it has not been determined
<i>Fit of the model to information not used to compute it</i>	1. Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>Method</i>	None
<i>Name</i>	None
<i>Details</i>	- Method details unspecified
<i>Software</i>	- HADDOCK (version 2.2) - No location specified