

Summary of integrative structure determination of Complex of RNF168-RING domain and the nucleosome (PDB ID: 8ZZS, PDB-Dev ID: PDBDEV_0000028)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - H2B: Chain H (95 residues) - H2B: Chain D (95 residues) - DNA strand 2: Chain J (147 residues) - H4: Chain F (80 residues) - H2A: Chain G (107 residues) - H2A: Chain C (107 residues) - H3: Chain E (99 residues) - RNF168 RING domain: Chain K (91 residues) - H3: Chain A (99 residues) - H4: Chain B (80 residues) - DNA strand 1: Chain I (147 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 2PYO - Experimental model, PDB ID: 4GB0 - Mutagenesis data, File: 10.1038/s41467-019-09756-z - NMR data, BMRB: 27786 - NMR data, BMRB: 27791 - NMR data, BMRB: 27792 - Crosslinking-MS data, Linker name and number of cross-links: BS3, 1 cross-links
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 11
Flexible units	<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
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 1 cross-links - 178 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	

<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	10
<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 6, Number of sidechain outliers = 35 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 6, Number of sidechain outliers = 30 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 3, Number of sidechain outliers = 29 - Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 9, Number of sidechain outliers = 45 - Model-5: Clashscore = 0.0, Number of Ramachandran outliers = 6, Number of sidechain outliers = 34 - Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 4, Number of sidechain outliers = 33 - Model-7: Clashscore = 0.0, Number of Ramachandran outliers = 4, Number of sidechain outliers = 31 - Model-8: Clashscore = 0.0, Number of Ramachandran outliers = 2, Number of sidechain outliers = 36 - Model-9: Clashscore = 0.0, Number of Ramachandran outliers = 7, Number of sidechain outliers = 31 - Model-10: Clashscore = 0.0, Number of Ramachandran outliers = 5, Number of sidechain outliers = 26
<i>Model quality: assessment of excluded volume</i>	Not applicable
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Method</i>	None
<i>Name</i>	None
<i>Software</i>	<ul style="list-style-type: none"> - HADDOCK (version 2.2) - JWALK (version 1.1)