

Summary of integrative structure determination of Complex of RNF168-RING domain and the nucleosome (PDB ID: 8ZZS, PDB-Dev ID: PDBDEV_00000028)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - H3: chain(s) A, E (99 residues) - H4: chain(s) B, F (80 residues) - H2A: chain(s) C, G (107 residues) - H2B: chain(s) D, H (95 residues) - DNA strand 1: chain(s) I (147 residues) - DNA strand 2: chain(s) J (147 residues) - RNF168 RING domain: chain(s) K (91 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 2PYO - Experimental model, PDB: 4GB0 - Mutagenesis data, Not available: 10.1038/s41467-019-09756-z - NMR data, BMRB: 27786 - NMR data, BMRB: 27791 - NMR data, BMRB: 27792 - Crosslinking-MS data, PRIDE: PXD012723
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 11
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 1 crosslinks - 178 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 12.55-15.12 - Ramachandran outliers: 2-9 - Sidechain outliers: 26-45
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 100.00-100.00%
<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>Name</i>	None
<i>Software</i>	<ul style="list-style-type: none"> - HADDOCK (version 2.2) - JWALK (version 1.1)