

Summary of integrative structure determination of Integrative structure of the human WDR76-SPIN1-Nucleosome complex (PDB ID: 9A8I, PDB-Dev ID: PDBDEV_00000382)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - WD repeat-containing protein 76: chain(s) A (626 residues) - Spindlin-1: chain(s) B (262 residues) - Histone H2A type 1: chain(s) C (130 residues) - Histone H2A type 1: chain(s) D (130 residues) - Histone H2B type 1-C/E/F/G/I: chain(s) E (126 residues) - Histone H2B type 1-C/E/F/G/I: chain(s) F (126 residues) - Histone H3.1: chain(s) G, H (136 residues) - Histone H4 : chain(s) I (103 residues) - Histone H4 : chain(s) J (103 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Zenodo: 10.5281/zenodo.11044599 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.11044599 - De Novo model, AlphaFoldDB: AF-Q9H967-F1 - Experimental model, PDB: 4H75 - Experimental model, PDB: 5GT0
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 20 residue(s) per bead
Number of rigid and flexible segments	11, 21
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 76 crosslinks - 1 unique CrossLinkRestraint: DSSO, 3 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	27314
Number of deposited models	1
Model precision (uncertainty of models)	24.00, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.65%

<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 14.10%
<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>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	750000
<i>Software</i>	<ul style="list-style-type: none">- IMP PMI module (version 2.16.0)- Integrative Modeling Platform (IMP) (version 2.16.0)