

**Summary of integrative structure determination of Integrative structure of the human WDR76-SPIN1-Nucleosome complex (PDB ID: 9A8I, PDB-Dev ID: PDBDEV\_00000382)**

<b>1. Model Composition</b>	
<i>Entry composition</i>	<ul style="list-style-type: none"> <li>- Histone H2A type 1: Chain D (130 residues)</li> <li>- Histone H3.1: Chain H (136 residues)</li> <li>- WD repeat-containing protein 76: Chain A (626 residues)</li> <li>- Histone H2B type 1-C/E/F/G/I: Chain F (126 residues)</li> <li>- Histone H4 : Chain I (103 residues)</li> <li>- Histone H2B type 1-C/E/F/G/I: Chain E (126 residues)</li> <li>- Histone H2A type 1: Chain C (130 residues)</li> <li>- Histone H4 : Chain J (103 residues)</li> <li>- Histone H3.1: Chain G (136 residues)</li> <li>- Spindlin-1: Chain B (262 residues)</li> </ul>
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSSO, 76 cross-links</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSSO, 3 cross-links</li> <li>- De Novo model, AlphaFoldDB: AF-Q9H967-F1</li> <li>- Experimental model, PDB ID: 4H75</li> <li>- Experimental model, PDB ID: 5GT0</li> </ul>
<b>2. Representation</b>	
<i>Resolution</i>	Coarse-grained: 1, 2, 3, 4, 13 residue(s) per bead
<i>Number of rigid bodies, flexible units</i>	11, 21
<i>Rigid bodies</i>	<ul style="list-style-type: none"> <li>- F: 28-125</li> <li>- E: 32-125</li> <li>- H: 37-135</li> <li>- D: 14-119</li> <li>- C: 13-118</li> <li>- G: 37-135</li> <li>- J: 24-102</li> <li>- I: 17-102</li> <li>- A: 245-276, 288-626</li> <li>- B: 45-259</li> </ul>
<i>Flexible units</i>	<ul style="list-style-type: none"> <li>- F: 1-27, 126-126</li> <li>- E: 1-31, 126-126</li> <li>- H: 1-36, 136-136</li> <li>- D: 1-13, 120-130</li> <li>- C: 1-12, 119-130</li> <li>- G: 1-36, 136-136</li> <li>- J: 1-23, 103-103</li> <li>- I: 1-16, 103-103</li> <li>- A: 1-244, 277-287</li> <li>- B: 1-44, 195-210, 260-262</li> </ul>

<u>Structural coverage (rigid bodies)</u>	71%
<b>3. Restraints</b>	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: DSSO, 76 cross-links</li> <li>- 1 unique CrossLinkRestraint: DSSO, 3 cross-links</li> </ul>
<b>4. Validation</b>	
<u>Number of ensembles</u>	1
<u>Number of models in ensembles</u>	27314
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	24.0, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.65-99.65%
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<u>1. Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	750000
<u>Software</u>	<ul style="list-style-type: none"> <li>- <a href="#">IMP PMI module</a> (version 2.16.0)</li> <li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version 2.16.0)</li> </ul>