

## Summary of integrative structure determination of Integrative structure of human SNAPc-DNA (PDB ID: 9A8W)

<b>1. Model Composition</b>	
<a href="#"><u>Entry composition</u></a>	<ul style="list-style-type: none"> <li>- NT strand: Chain G (20 residues)</li> <li>- snRNA-activating protein complex subunit 3: Chain B (411 residues)</li> <li>- snRNA-activating protein complex subunit 2: Chain A (334 residues)</li> <li>- snRNA-activating protein complex subunit 4: Chain E (1519 residues)</li> <li>- snRNA-activating protein complex subunit 5: Chain C (98 residues)</li> <li>- T strand: Chain F (20 residues)</li> <li>- snRNA-activating protein complex subunit 1: Chain D (368 residues)</li> </ul>
<a href="#"><u>Datasets used for modeling</u></a>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, ID: PXD053341; Linker name and number of cross-links: SDA, 268 cross-links</li> <li>- 3DEM volume, File: 10.5281/zenodo.14009872</li> <li>- 3DEM volume, File: 10.5281/zenodo.14009872</li> <li>- De Novo model, MODEL ARCHIVE: ma-pgtjz</li> <li>- Experimental model, PDB ID: 9FS0</li> <li>- Experimental model, PDB ID: 7ZX8</li> <li>- Experimental model, PDB ID: 7XUR</li> <li>- 3DEM volume, EMDB: EMD-50730</li> </ul>
<b>2. Representation</b>	
<a href="#"><u>Resolution</u></a>	Coarse-grained: 1, 2, 3, 4, 5, 7, 9, 23 residue(s) per bead
<a href="#"><u>Number of rigid bodies, flexible units</u></a>	16, 16
<i>Rigid bodies</i>	<ul style="list-style-type: none"> <li>- B: 27-411</li> <li>- E: 122-163, 182-416, 424-541, 706-799, 806-859, 1304-1434</li> <li>- C: 3-52</li> <li>- D: 1-141, 162-234</li> <li>- A: 29-87, 97-160, 201-271, 304-334</li> <li>- F: 1-20</li> <li>- G: 1-20</li> </ul>
<i>Flexible units</i>	<ul style="list-style-type: none"> <li>- B: 1-26</li> <li>- E: 41-121, 164-181, 417-423, 542-705, 800-805, 860-1303, 1435-1519</li> <li>- C: 1-2, 53-98</li> <li>- D: 142-161, 235-368</li> <li>- A: 1-28, 88-96, 161-200, 272-303</li> <li>- F: -</li> <li>- G: -</li> </ul>
<a href="#"><u>Structural coverage (rigid bodies)</u></a>	58%

<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: SDA, 268 cross-links</li> <li>- 1 unique EM3DRestraint: Gaussian mixture models</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	5766
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	None, Å
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of excluded volume</a>	Satisfaction: 99.71-99.71%
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<b>1. Method</b>	Sampling
<a href="#">Name</a>	Replica exchange monte carlo
<a href="#">Number of computed models</a>	320000
<a href="#">Software</a>	<ul style="list-style-type: none"> <li>- <a href="#">IMP PMI module</a> (version 2.20.0)</li> <li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version 2.20.0)</li> <li>- <a href="#">AlphaPulldown</a> (version 0.30.7)</li> <li>- <a href="#">AlphaFold2</a> (version 2.3.2)</li> </ul>