

**Summary of integrative structure determination of Comprehensive structure and functional adaptations of the yeast nuclear pore complex (PDB ID: 9A1P, PDB-Dev ID: PDBDEV\_0000097)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Nsp1: Chain A (823 residues)</li> <li>- Nup49: Chain C (472 residues)</li> <li>- Nup57: Chain K (541 residues)</li> <li>- Nup49: Chain I (472 residues)</li> <li>- Nup59: Chain X (528 residues)</li> <li>- Nup188: Chain N (1655 residues)</li> <li>- Nic96: Chain Q (839 residues)</li> <li>- Nsp1: Chain D (823 residues)</li> <li>- Nup170: Chain Y (1502 residues)</li> <li>- Nup157: Chain 1 (1391 residues)</li> <li>- Nic96: Chain S (839 residues)</li> <li>- Nup170: Chain 0 (1502 residues)</li> <li>- Nup49: Chain L (472 residues)</li> <li>- Nup59: Chain V (528 residues)</li> <li>- Nup192: Chain O (1683 residues)</li> <li>- Nsp1: Chain J (823 residues)</li> <li>- Nup53: Chain W (475 residues)</li> <li>- Nic96: Chain R (839 residues)</li> <li>- Nup192: Chain M (1683 residues)</li> <li>- Nup57: Chain E (541 residues)</li> <li>- Nic96: Chain T (839 residues)</li> <li>- Nup49: Chain F (472 residues)</li> <li>- Nup57: Chain B (541 residues)</li> <li>- Nup57: Chain H (541 residues)</li> <li>- Nsp1: Chain G (823 residues)</li> <li>- Nup157: Chain Z (1391 residues)</li> <li>- Nup53: Chain U (475 residues)</li> <li>- Nup188: Chain P (1655 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSS, 114 cross-links</li> <li>- 3DEM volume, EMDB: EMDB-24232</li> <li>- Experimental model, PDB ID: 7N85</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Coarse-grained: 1 residue(s) per bead
Number of <a href="#">rigid bodies</a> , <a href="#">flexible units</a>	28, 0

<i>Rigid bodies</i>	<ul style="list-style-type: none"> <li>- Z: 1-1391</li> <li>- 1: 1-1391</li> <li>- Y: 1-1502</li> <li>- O: 1-1502</li> <li>- U: 1-475</li> <li>- W: 1-475</li> <li>- V: 1-528</li> <li>- X: 1-528</li> <li>- A: 1-823</li> <li>- D: 1-823</li> <li>- G: 1-823</li> <li>- J: 1-823</li> <li>- B: 1-541</li> <li>- E: 1-541</li> <li>- H: 1-541</li> <li>- K: 1-541</li> <li>- C: 1-472</li> <li>- F: 1-472</li> <li>- I: 1-472</li> <li>- L: 1-472</li> <li>- N: 1-1655</li> <li>- P: 1-1655</li> <li>- M: 1-1683</li> <li>- O: 1-1683</li> <li>- Q: 1-839</li> <li>- R: 1-839</li> <li>- S: 1-839</li> <li>- T: 1-839</li> </ul>
<a href="#"><i>Structural coverage (rigid bodies)</i></a>	100%
<b>3. Restraints</b>	
<a href="#"><i>Physical principles</i></a>	Information about physical principles was not provided
<a href="#"><i>Experimental data</i></a>	- 1 unique CrossLinkRestraint: DSS, 114 cross-links
<b>4. Validation</b>	
<a href="#"><i>Number of ensembles</i></a>	1
<a href="#"><i>Number of models in ensembles</i></a>	10
<a href="#"><i>Number of deposited models</i></a>	10
<a href="#"><i>Model precision (uncertainty of models)</i></a>	None, Å
<a href="#"><i>Data quality</i></a>	Data quality has not been assessed
<a href="#"><i>Model quality: assessment of excluded volume</i></a>	Satisfaction: 100.00-100.00%
<a href="#"><i>Fit to data used for modeling</i></a>	Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined

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<b>5. Methodology and Software</b>	
<i>1. Method</i>	Production sampling
<i><a href="#">Name</a></i>	Enumeration
<i><a href="#">Number of computed models</a></i>	1200
<i><a href="#">Software</a></i>	- <a href="#">PSIPRED</a> (version 4.0) - <a href="#">Integrative Modeling Platform (IMP)</a> (version 2.2)