

# Summary of integrative structure determination of Implications of a multiscale structure of the yeast Nuclear Pore Complex (PDB ID: 9A3S, PDB-Dev ID: PDBDEV\_00000213)

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Nucleoporin POM152: chain(s) A, B (1337 residues)</li> <li>- Nucleoporin POM34: chain(s) C, D (299 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- 3DEM volume, Zenodo: <a href="https://zenodo.org/record/10.5281/zenodo.8226857">10.5281/zenodo.8226857</a></li> <li>- Crosslinking-MS data, Zenodo: <a href="https://zenodo.org/record/10.5281/zenodo.8226857">10.5281/zenodo.8226857</a></li> <li>- De Novo model, Zenodo: <a href="https://zenodo.org/record/10.5281/zenodo.8226857">10.5281/zenodo.8226857</a></li> <li>- De Novo model, Zenodo: <a href="https://zenodo.org/record/10.5281/zenodo.8226857">10.5281/zenodo.8226857</a></li> <li>- 3DEM volume, EMD: <a href="https://emdb.ebi.ac.uk/emdb/EMD-41117">EMD-41117</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Multiscale: Coarse-grained: 1 - 2 residue(s) per bead
<a href="#">Number of <i>rigid</i> and <i>flexible</i> segments</a>	16, 20
<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 EM3DRestraint: DSSO, 36 crosslinks</li> <li>- 1 unique CrossLinkRestraint: Gaussian mixture models</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	11
<a href="#">Number of deposited models</a>	11
<a href="#">Model precision (uncertainty of models)</a>	9.52, Å
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of excluded volume</a>	Satisfaction: 99.53-99.54%
<a href="#">Fit to data used for modeling</a>	Satisfaction of crosslinks: 75.00-100.00%
<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>	

1. <a href="#">Name</a>	Sampling
<a href="#">Method</a>	Replica exchange monte carlo
<a href="#">Number of computed models</a>	6400000
<a href="#">Software</a>	<ul style="list-style-type: none"><li>- <a href="#">AlphaFold2</a> (version Not available)</li><li>- <a href="#">IMP PMI module</a> (version 20230908.develop.a93cf91143)</li><li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version 20230908.develop.a93cf91143)</li></ul>