

**Summary of integrative structure determination of molecular architecture of the major membrane ring component, pom152, of the yeast nuclear pore complex (PDBDEV00000017)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	- pom152: Chain A (1337 residues)
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 5TVZ</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- 3DEM volume, EMDB ID: EMD-8543</li> <li>- 3DEM volume, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- 2DEM class average, EMDB ID: Not listed</li> <li>- SAS data, SASDBV9</li> <li>- SAS data, SASDBW9</li> <li>- SAS data, SASDBX9</li> <li>- SAS data, SASDBY9</li> <li>- SAS data, SASDBZ9</li> </ul>
<b>2. Representation</b>	
<a href="#">Atomic structural coverage</a>	64%
<a href="#">Number of rigid bodies, flexible units</a>	9, 9
<i>Rigid bodies</i>	- A: 379-472:Comparative model/None, 520-611:Comparative model/None, 616-714:Comparative model/None, 722-818:Comparative model/None, 824-918:Comparative model/None, 931-1026:Comparative model/None, 1036-1141:Comparative model/None, 1150-1229:Comparative model/None, 1244-1337:Comparative model/None.
<i>Flexible units</i>	- A: 1-378, 473-519, 612-615, 715-721, 819-823, 919-930, 1027-1035, 1142-1149, 1230-1243.
<a href="#">Resolution</a>	<ul style="list-style-type: none"> <li>- Rigid bodies: 1 residue per bead.</li> <li>- Flexible regions: N/A</li> </ul>
<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: Gaussian mixture models, 50</li> <li>- 6 unique EM2DRestraint: Number of micrographs: None, Image resolution: 50.0</li> <li>- 2 unique EM2DRestraint: Number of micrographs: None, Image resolution: 60.0</li> <li>- 5 unique SASRestraint: Assembly name: SAXS subassembly Fitting method: FoXS Multi-state: False</li> </ul>
<b>4. Validation</b>	
<a href="#">Sampling validation</a>	- Information related to sampling validation has not been provided
<a href="#">Clustering algorithm ,clustering feature</a>	Distance threshold-based clustering used if ensembles are deposited, dRMSD
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	364
<a href="#">Model precision (uncertainty of models)</a>	7.0Å
<a href="#">Quality of data</a>	<ul style="list-style-type: none"> <li>- SASDBV9: Rg from Gunier is 1.824nm and Rg from p(r) is 1.77nm</li> <li>- SASDBW9: Rg from Gunier is 2.787nm and Rg from p(r) is 2.71nm</li> <li>- SASDBY9: Rg from Gunier is 2.976nm and Rg from p(r) is 2.95nm</li> <li>- SASDBX9: Rg from Gunier is 2.636nm and Rg from p(r) is 2.78nm</li> <li>- SASDBZ9: Rg from Gunier is 4.629nm and Rg from p(r) is 4.34nm</li> </ul>
<a href="#">Model quality: assessment of atomic segments</a>	Not applicable
<a href="#">Model quality: assessment of excluded volume</a>	- Model-1: Number of violations-2089.0
<a href="#">Fit of the model to information used to compute it</a>	<ul style="list-style-type: none"> <li>- SASDBV9: Fit 1 with X<sup>2</sup> value 1.28</li> <li>- SASDBV9: Fit 2 with X<sup>2</sup> value 1.1</li> <li>- SASDBW9: Fit 1 with X<sup>2</sup> value 1.97</li> <li>- SASDBY9: Fit 1 with X<sup>2</sup> value 2.02</li> <li>- SASDBX9: Fit 1 with X<sup>2</sup> value 2.86</li> <li>- SASDBZ9: Fit 1 with X<sup>2</sup> value 1.94</li> </ul>
<a href="#">Fit of the model to information not used to compute it</a>	- Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<a href="#">Method</a>	Sampling
<a href="#">Name</a>	Replica exchange Monte Carlo
<a href="#">Details</a>	- Method details unspecified

Software

- Integrative Modeling Platform (IMP) (version develop-0a5706e202)
- IMP PMI module (version 67456c0)
- MODELLER (version 9.13)
- No location specified