

**Summary of integrative structure determination of Structure of the Nup84 sub-complex of the Nuclear Pore Complex (PDB ID: 8ZZ1, PDB-Dev ID: PDBDEV\_00000001)**

1. Model Composition	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Nup84: chain(s) A (726 residues)</li> <li>- Nup85: chain(s) B (744 residues)</li> <li>- Nup120: chain(s) C (1037 residues)</li> <li>- Nup133: chain(s) D (1157 residues)</li> <li>- Nup145c: chain(s) E (712 residues)</li> <li>- Seh1: chain(s) F (349 residues)</li> <li>- Sec13: chain(s) G (297 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB: <a href="#">3JRO</a></li> <li>- Experimental model, PDB: <a href="#">3F3F</a></li> <li>- Experimental model, PDB: <a href="#">3IKO</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">3CQC</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">4LCT</a></li> <li>- Experimental model, PDB: <a href="#">2QX5</a></li> <li>- Experimental model, PDB: <a href="#">3EWE</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">3F7F</a></li> <li>- Experimental model, PDB: <a href="#">3HXR</a></li> <li>- Experimental model, PDB: <a href="#">4FHN</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">4Q9T</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">3I4R</a></li> <li>- Experimental model, PDB: <a href="#">3KFO</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">3BG1</a></li> <li>- Experimental model, PDB: <a href="#">3BG0</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Experimental model, PDB: <a href="#">3F3F</a></li> <li>- Experimental model, PDB: <a href="#">2PM7</a></li> <li>- Crosslinking-MS data, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- Crosslinking-MS data, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> <li>- EM raw micrographs, Zenodo: <a href="#">10.5281/zenodo.58025</a></li> <li>- 2DEM class average, Zenodo: <a href="#">10.5281/zenodo.1218053</a></li> </ul>
2. Representation	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Multiscale: Coarse-grained: 1 - 20 residue(s) per bead

<i>Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments</i>	40, 42
<b>3. Restraints</b>	
<i><a href="#">Physical principles</a></i>	Information about physical principles was not provided
<i><a href="#">Experimental data</a></i>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: DSS, 164 crosslinks</li> <li>- 1 unique CrossLinkRestraint: EDC, 127 crosslinks</li> <li>- 1 unique EM2DRestraint: Number of micrographs: 800, Image resolution: 30.0</li> </ul>
<b>4. Validation</b>	
<i><a href="#">Number of ensembles</a></i>	2
<i><a href="#">Number of models in ensembles</a></i>	1257, 1010
<i><a href="#">Number of deposited models</a></i>	2
<i><a href="#">Model precision (uncertainty of models)</a></i>	<ul style="list-style-type: none"> <li>- 15.40, Å</li> <li>- 12.70, Å</li> </ul>
<i><a href="#">Data quality</a></i>	Data quality has not been assessed
<i><a href="#">Model quality: assessment of excluded volume</a></i>	Satisfaction: 99.88-99.88%
<i><a href="#">Fit to data used for modeling</a></i>	Satisfaction of crosslinks: 74.91-74.91%
<i><a href="#">Fit to data used for validation</a></i>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <i><a href="#">Name</a></i>	Sampling
<i><a href="#">Method</a></i>	Replica exchange monte carlo
<i><a href="#">Number of computed models</a></i>	500
2. <i><a href="#">Name</a></i>	Sampling
<i><a href="#">Method</a></i>	Replica exchange monte carlo
<i><a href="#">Number of computed models</a></i>	5000
<i><a href="#">Software</a></i>	<ul style="list-style-type: none"> <li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version develop-0a5706e202)</li> <li>- <a href="#">IMP PMI module</a> (version 67456c0)</li> <li>- <a href="#">HHpred</a> (version 2.0.16)</li> <li>- <a href="#">PSIPRED</a> (version 4.0)</li> <li>- <a href="#">DISOPRED</a> (version 3)</li> <li>- <a href="#">MODELLER</a> (version 9.12)</li> </ul>