

Summary of integrative structure determination of Molecular architecture of the major membrane ring component, Pom152, of the yeast nuclear pore complex (PDB ID: 8ZZH, PDB-Dev ID: PDBDEV_00000017)

1. Model Composition	
<u>Entry composition</u>	pom152: Chain A (1337 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 5TVZ - Comparative model, template PDB ID: Not available - 3DEM volume, EMDB: EMD-8543 - 3DEM volume, File: 10.5281/zenodo.1231518 - 2DEM class average, File: 10.5281/zenodo.1231518 - SAS data, SASBDB: SASDBV9 - SAS data, SASBDB: SASDBW9 - SAS data, SASBDB: SASDBX9 - SAS data, SASBDB: SASDBY9 - SAS data, SASBDB: SASDBZ9
2. Representation	
<u>Resolution</u>	Coarse-grained: 1, 2, 5, 15 residue(s) per bead
<u>Number of rigid bodies, flexible units</u>	9, 9
<u>Rigid bodies</u>	A: 379-472, 520-611, 616-714, 722-818, 824-918, 931-1026, 1036-1141, 1150-1229, 1244-1337
<u>Flexible units</u>	A: 1-378, 473-519, 612-615, 715-721, 819-823, 919-930, 1027-1035, 1142-1149, 1230-1243
<u>Structural coverage (rigid bodies)</u>	64%

3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique EM3DRestraint: Gaussian mixture models - 6 unique EM2DRestraint: Number of micrographs: None, Image resolution: 50.0 - 2 unique EM2DRestraint: Number of micrographs: None, Image resolution: 60.0 - 5 unique SASRestraint: Assembly name: SAXS subassembly Fitting method: FoXS Multi-state: False
4. Validation	
<u>Number of ensembles</u>	1
<u>Number of models in ensembles</u>	364
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	7.0, Å
<u>Data quality</u>	<ul style="list-style-type: none"> - SASDBV9: Rg from Gunier is 1.77nm and Rg from p(r) is 1.82nm - SASDBW9: Rg from Gunier is 2.71nm and Rg from p(r) is 2.79nm - SASDBX9: Rg from Gunier is 2.78nm and Rg from p(r) is 2.64nm - SASDBY9: Rg from Gunier is 2.95nm and Rg from p(r) is 2.98nm - SASDBZ9: Rg from Gunier is 4.34nm and Rg from p(r) is 4.63nm
<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.46-99.46%
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<u>1. Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	100000
<u>Software</u>	<ul style="list-style-type: none"> - Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0) - MODELLER (version 9.13)