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

1. Model Composition	
Entry composition	- pom152: Chain A (1337 residues)
Datasets used for modeling	- Experimental model, PDB ID: 5TVZ - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - 3DEM volume, EMDB ID: EMD-8543 - 3DEM volume, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - 2DEM class average, EMDB ID: Not listed - SAS data, SASDBV9 - SAS data, SASDBW9 - SAS data, SASDBX9 - SAS data, SASDBY9 - SAS data, SASDBZ9
2. Representation	
Atomic structural coverage	64%
Number of rigid bodies, flexible units	9, 9
Rigid bodies	- 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.
Flexible units	- A: 1-378, 473-519, 612-615, 715-721, 819-823, 919-930, 1027-1035, 1142-1149, 1230-1243.
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	- 1 unique EM3DRestraint: Gaussian mixture models, 50 - 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	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, dRMSD
Number of ensembles	1
Number of models in ensembles	364
Model precision (uncertainty of models)	7.0Å
Quality of data	- SASDBY9: Rg from Gunier is 2.976nm and Rg from p(r) is 2.95nm - SASDBV9: Rg from Gunier is 1.824nm and Rg from p(r) is 1.77nm - SASDBZ9: Rg from Gunier is 4.629nm and Rg from p(r) is 4.34nm - SASDBW9: Rg from Gunier is 2.787nm and Rg from p(r) is 2.71nm - SASDBX9: Rg from Gunier is 2.636nm and Rg from p(r) is 2.78nm
Model quality: assessment of atomic segments	Not applicable
Model quality: assessment of excluded volume	- Model-1: Number of violations-2089.0
Fit of the model to information used to compute it	- SASDBY9: Fit 1 with X^2 value 2.02 - SASDBV9: Fit 1 with X^2 value 1.28 - SASDBV9: Fit 2 with X^2 value 1.1 - SASDBZ9: Fit 1 with X^2 value 1.94 - SASDBW9: Fit 1 with X^2 value 1.97 - SASDBX9: Fit 1 with X^2 value 2.86
Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Sampling
Name	Replica exchange Monte Carlo
Details	- Method details unspecified

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