

Summary of integrative structure determination of Integrative model of Nup116 knockout (at 37C) yeast nuclear pore complex (PDB ID: 9A0H, PDB-Dev ID: PDBDEV_00000053)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - Seh1: Chain O1 (349 residues) - Nup84: Chain L1 (726 residues) - Nup120: Chain R1 (1037 residues) - Nup157: Chain D1 (1391 residues) - Nic96: Chain A1 (839 residues) - Sec13: Chain N1 (297 residues) - Nup145c: Chain M1 (712 residues) - Nup188: Chain B1 (1655 residues) - Nup85: Chain P1 (744 residues) - Nup133: Chain K1 (1157 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - 3DEM volume, EMDB: EMD-10661 - 3DEM volume, File: 10.5281/zenodo.3820319 - 3DEM volume, File: 10.5281/zenodo.3820319 - Integrative model, PDB-Dev: PDBDEV_00000051 - Integrative model, PDB-Dev: PDBDEV_00000051 - Other, File: https://doi.org/10.1038/nsmb1194 - Other, File: https://doi.org/10.1038/nature26003
2. Representation	
<u>Resolution</u>	Atomic
<u>Number of rigid bodies, flexible units</u>	0, 10
<u>Flexible units</u>	<ul style="list-style-type: none"> - A1: 1-839 - B1: 1-1655 - D1: 1-1391 - K1: 1-1157 - L1: 1-726 - M1: 1-712 - N1: 1-297 - O1: 1-349 - P1: 1-744 - R1: 1-1037
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	- 1 unique InnerSurfaceGeometricRestraint: None
4. Validation	
<u>Number of ensembles</u>	0
<u>Number of models in ensembles</u>	Not applicable

<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	Model precision can not be calculated with one structure
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 566.51, Number of Ramachandran outliers = 264, Number of sidechain outliers = 399
<u>Model quality: assessment of excluded volume</u>	Not applicable
<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>	Monte Carlo simulated annealing optimization of multiple rigid bodies with IMP
<u>Name</u>	Monte Carlo simulated annealing optimization for NR Y-complex and IR asymmetric unit (outer nuclear copy)
<u>Software</u>	Integrative Modeling Platform (IMP) (version 2.9.0)