Summary of integrative structure determination of Integrative model of the wild type yeast nuclear pore complex (PDB ID: 9A0F, PDB-Dev ID: PDBDEV_00000051)

1. Model Composition	
Entry composition	- Nup159: Chain V2 (1460 residues) - Nup157: Chain D2 (1391 residues) - Nsp1: Chain J2 (823 residues) - Nup120: Chain R2 (1037 residues) - Nsp1: Chain J1 (823 residues) - Nup84: Chain L1 (726 residues) - Nic96: Chain A2 (839 residues) - Sec13: Chain N2 (297 residues) - Sec13: Chain N1 (297 residues) - Nup120: Chain R1 (1037 residues) - Nup57: Chain H2 (541 residues) - Nup133: Chain K1 (1157 residues) - Nsp1: Chain J3 (823 residues) - Nup170: Chain d1 (1502 residues) - Nup145c: Chain M1 (712 residues) - Nup49: Chain I4 (472 residues) - Nup49: Chain I3 (472 residues) - Nup170: Chain d2 (1502 residues) - Seh1: Chain O1 (349 residues) - Nup157: Chain D1 (1391 residues) - Seh1: Chain O2 (349 residues) - Nup85: Chain P1 (744 residues) - Nic96: Chain A1 (839 residues) - Nup188: Chain B1 (1655 residues) - Nup82: Chain W2 (713 residues) - Nup57: Chain H1 (541 residues) - Nup188: Chain B2 (1655 residues) - Nup57: Chain H4 (541 residues) - Nsp1: Chain J4 (823 residues) - Nup49: Chain I2 (472 residues) - Nup192: Chain C1 (1683 residues) - Dyn2: Chain 91 (92 residues) - Nic96: Chain A4 (839 residues) - Nup133: Chain K2 (1157 residues) - Nup145c: Chain M2 (712 residues) - Nup85: Chain P2 (744 residues) - Nic96: Chain A3 (839 residues) - Nsp1: Chain J5 (823 residues) - Nup49: Chain I1 (472 residues) - Nup84: Chain L2 (726 residues) - Nup82: Chain W1 (713 residues) - Nup159: Chain V1 (1460 residues) - Dyn2: Chain 92 (92 residues) - Nup57: Chain H3 (541 residues) - Nup192: Chain C2 (1683 residues) - Nsp1: Chain J6 (823 residues)

Datasets used for modeling	- 3DEM volume, EMDB: EMD-10198 - 3DEM volume, File: 10.5281/zenodo.3820319 - 3DEM volume, File: 10.5281/zenodo.3820319 - Experimental model, PDB ID: 4XMM - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Integrative model, PDB-Dev: PDBDEV_00000010 - Integrative model, PDB-Dev: PDBDEV_00000010 - Integrative model, PDB-Dev: PDBDEV_00000010 - Other, File: https://doi.org/10.1038/nsmb1194
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 46

Flexible units	- K1: 1-1157 - L1: 1-726 - M1: 1-712 - N1: 1-297 - O1: 1-349 - P1: 1-744 - R1: 1-1037 - 91: 1-92 - W1: 1-713 - V1: 1-1460 - J1: 1-823 - 92: 1-92 - W2: 1-713 - V2: 1-1460 - J2: 1-823 - A1: 1-839 - B1: 1-1655 - D1: 1-1391 - H1: 1-541 - I1: 1-472 - J3: 1-823 - A2: 1-839 - C1: 1-1683 - H2: 1-541 - I2: 1-472 - J4: 1-823 - d1: 1-1502 - A3: 1-839 - C2: 1-1683 - H3: 1-541 - I3: 1-472 - J5: 1-823 - d2: 1-1502 - A4: 1-839 - B2: 1-1655 - D2: 1-1391 - H4: 1-541 - I4: 1-472 - J6: 1-823 - K2: 1-1157 - L2: 1-726 - M2: 1-712 - N2: 1-297 - O2: 1-349 - P2: 1-744 - R2: 1-1037
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM3DRestraint: None
4. Validation	
Number of ensembles	0

Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 721.14, Number of Ramachandran outliers = 1068, Number of sidechain outliers = 1409
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	Systematic fitting to EM maps with Global search from UCSF Chimera
Name	Systematic fitting of CR Y-complex, NR Y-complex, IR asymmetric unit and P-complex rigid bodies
2. Method	Monte Carlo simulated annealing optimization of multiple rigid bodies with IMP
Name	Monte Carlo simulated annealing optimization for CR Y-complex, NR Y-complex and IR asymmetric unit
Software	- Integrative Modeling Platform (IMP) (version 2.9.0) - UCSF Chimera (version 1.14)