Summary of integrative structure determination of Integrative structure and functional anatomy of a single spoke of a nuclear pore complex (PDB ID: 8ZZA, PDB-Dev ID: PDBDEV_00000010)

1. Model Composition	
Entry composition	- Nup84: chain(s) A, H (726 residues) - Nic96: chain(s) AE, AI (839 residues) - Nup49: chain(s) AG, AK (472 residues) - Nup57: chain(s) AH, AL (541 residues) - Nup157: chain(s) AM, AQ (1391 residues) - Nup170: chain(s) AN, AR (1502 residues) - Nup188: chain(s) AO, AS (1655 residues) - Nup192: chain(s) AP, AT (1683 residues) - Nup53: chain(s) AU, AZ (475 residues) - Nup59: chain(s) AV, BA (528 residues) - Ndc1: chain(s) AW, BB (655 residues) - Pom34: chain(s) AX, BC (299 residues) - Pom152: chain(s) AY, BD (1337 residues) - Nup85: chain(s) B, I (744 residues) - Nup100: chain(s) BE, BF (959 residues) - Nup116: chain(s) BG, BH (1113 residues) - Gle1: chain(s) BJ (538 residues) - Nup145: chain(s) BK, BL (1317 residues) - Nup1: chain(s) BM (1076 residues) - Nup60: chain(s) BN, BO (539 residues) - Mlp1: chain(s) BP (1875 residues) - Mlp2: chain(s) BQ (1679 residues) - Nup120: chain(s) C, J (1037 residues) - Nup133: chain(s) D, K (1157 residues) - Nup145c: chain(s) E, L (712 residues) - Seh1: chain(s) F, M (349 residues) - Sec13: chain(s) G, N (297 residues) - Dyn2: chain(s) O, P (92 residues) - Nup82: chain(s) Q, R (713 residues) - Nup159: chain(s) S, T (1460 residues) - Nsp1: chain(s) U, V, AF, AJ (823 residues) - Nic96: chain(s) W, AA (839 residues) - Nsp1: chain(s) X, AB (823 residues) - Nup49: chain(s) Y, AC (472 residues) - Nup57: chain(s) Z, AD (541 residues)
	- Integrative model, Not available: 10.1016/j.cell.2016.10.028 - Integrative model, Zenodo: 10.5281/zenodo.1194547 - Experimental model, PDB: 5CWS - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Experimental model, PDB: 2QX5 - Experimental model, Zenodo: 10.5281/zenodo.1194547 - Experimental model, Zenodo: 10.5281/zenodo.1194547 - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Comparative model, Zenodo: 10.5281/zenodo.1194547

Datasets used for modeling	- Comparative model, Zenodo: 10.5281/zenodo.1194547 - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Integrative model, Not available: 10.1016/j.str.2017.01.006 - Integrative model, Zenodo: 10.5281/zenodo.1194547 - Experimental model, PDB: 3NF5 - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Comparative model, Zenodo: 10.5281/zenodo.1194547 - Experimental model, PDB: 3KEP - Experimental model, Zenodo: 10.5281/zenodo.1194547 - Mass Spectrometry data, Zenodo: 10.5281/zenodo.1149746 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.1194547 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.1194547 - EM raw micrographs, EMPIAR: EMPIAR-10155 - 3DEM volume, EMDB: EMD-7321 - 3DEM volume, Zenodo: 10.5281/zenodo.1194547 - SAS data, SASBDB: SASDBV9 - SAS data, SASBDB: SASDBW9 - SAS data, SASBDB: SASDBZ9 - SAS data, SASBDB: SASDBX9 - SAS data, SASBDB: SASDBY9 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547 - SAS data, Zenodo: 10.5281/zenodo.1194547

	- EM raw micrographs, EMPIAR: EMPIAR-10162 - 2DEM class average, Zenodo: 10.5281/zenodo.1194547 - 2DEM class average, Zenodo: 10.5281/zenodo.1194547
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 100 residue(s) per bead
Number of rigid and flexible segments	24, 816
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM2DRestraint: Number of micrographs: 800, Image resolution: 35.0 - 1 unique GeometricRestraint: Assembly name: SAXS subassembly Fitting method: FoXS Multi-state: False - 1 unique CrossLinkRestraint: DSS, 505 crosslinks - 1 unique SASRestraint: Gaussian mixture models - 1 unique EM3DRestraint: DSS, 509 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	5
Number of deposited models	1
Model precision (uncertainty of models)	1.00, Å
Data quality	- 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 - SASDBZ9: Rg from Gunier is 4.34nm and Rg from p(r) is 4.63nm - 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
Model quality: assessment of excluded volume	Satisfaction: 99.98%
Fit to data used for modeling	Satisfaction of crosslinks: 87.52%

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. Name	Sampling
Method	Replica exchange monte carlo
Number of computed models	500
2. Name	Sampling
Method	Replica exchange monte carlo
Number of computed models	3000
3. Name	Sampling
Method	Replica exchange monte carlo
Number of computed models	1000
Software	- Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0) - HHpred (version 2.0.16) - PSIPRED (version 4.0) - DISOPRED (version 3) - DomPred (version Not available) - COILS/PCOILS (version Not available) - EMAN2 (version 2.2) - RELION (version 1.4) - SGD (version Not available) - HeliQuest (version Not available) - MODELLER (version 9.15) - MODELLER (version 9.13)