

Summary of integrative structure determination of Integrative structure and functional anatomy of three spokes of a nuclear pore complex (PDB ID: 8ZZB, PDB-Dev ID: PDBDEV_00000011)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Nup84: chain(s) A, H, O, V, AC, AJ (726 residues) - Dyn2: chain(s) AQ, AR, AY, AZ, BG, BH (92 residues) - Nup82: chain(s) AS, AT, BA, BB, BI, BJ (713 residues) - Nup159: chain(s) AU, AV, BC, BD, BK, BL (1460 residues) - Nsp1: chain(s) AW, AX, BE, BF, BM, BN, BX, CB, CF, CJ, CN, CR, CV, CZ, DD, DH (823 residues) - Nup85: chain(s) B, I, P, W, AD, AK (744 residues) - Nic96: chain(s) BO, BS (839 residues) - Nsp1: chain(s) BP, BT (823 residues) - Nup49: chain(s) BQ, BU (472 residues) - Nup57: chain(s) BR, BV (541 residues) - Nic96: chain(s) BW, CA, CE, CI, CM, CQ, CU, CY, DC, DG (839 residues) - Nup49: chain(s) BY, CC, CG, CK, CO, CS, CW, DA, DE, DI (472 residues) - Nup57: chain(s) BZ, CD, CH, CL, CP, CT, CX, DB, DF, DJ (541 residues) - Nup120: chain(s) C, J, Q, X, AE, AL (1037 residues) - Nup133: chain(s) D, K, R, Y, AF, AM (1157 residues) - Nup157: chain(s) DK, DO, DS, DW, EA, EE (1391 residues) - Nup170: chain(s) DL, DP, DT, DX, EB, EF (1502 residues) - Nup188: chain(s) DM, DQ, DU, DY, EC, EG (1655 residues) - Nup192: chain(s) DN, DR, DV, DZ, ED, EH (1683 residues) - Nup145c: chain(s) E, L, S, Z, AG, AN (712 residues) - Nup53: chain(s) EI, EN, ES, EX, FC, FH (475 residues) - Nup59: chain(s) EJ, EO, ET, EY, FD, FI (528 residues) - Ndc1: chain(s) EK, EP, EU, EZ, FE, FJ (655 residues) - Pom34: chain(s) EL, EQ, EV, FA, FF, FK (299 residues) - Pom152: chain(s) EM, ER, EW, FB, FG, FL (1337 residues) - Seh1: chain(s) F, M, T, AA, AH, AO (349 residues) - Nup100: chain(s) FM, FN (959 residues) - Nup116: chain(s) FO, FP, FU, FV, GA, GB (1113 residues) - Gle1: chain(s) FR, FX, GD (538 residues) - Nup100: chain(s) FS, FT, FY, FZ (959 residues)

	<ul style="list-style-type: none"> - Sec13: chain(s) G, N, U, AB, AI, AP (297 residues) - Nup145: chain(s) GE, GF (1317 residues) - Nup1: chain(s) GG, GL, GQ (1076 residues) - Nup60: chain(s) GH, GI, GM, GN, GR, GS (539 residues) - Nup145: chain(s) GJ, GK, GO, GP (1317 residues) - Mlp1: chain(s) GT, GV, GX (1875 residues) - Mlp2: chain(s) GU, GW, GY (1679 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - 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 - 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, 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

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2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 100 residue(s) per bead
Number of rigid and flexible segments	24, 2496
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique EM3DRestraint: Assembly name: SAXS subassembly Fitting method: FoXS Multi-state: False - 1 unique CrossLinkRestraint: DSS, 509 crosslinks - 1 unique GeometricRestraint: Number of micrographs: 800, Image resolution: 35.0 - 1 unique EM2DRestraint: Gaussian mixture models - 1 unique SASRestraint: DSS, 508 crosslinks
4. Validation	

<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	5
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	1.00, Å
<i>Data quality</i>	<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 - 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
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.99%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 87.58%
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	500
2. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	3000
3. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	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)