

Summary of integrative structure determination of Integrative structure and functional anatomy of eight spokes of a nuclear pore complex (PDB ID: 8ZZC, PDB-Dev ID: PDBDEV_00000012)

| 1. Model Composition | |
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| <p>Entry composition</p> | <ul style="list-style-type: none"> - Nup84: chain(s) A, H, BR, BY, CF, CM, CT, DA, DH, DO, DV, EC, EJ, EQ, EX, FE (726 residues) - Nic96: chain(s) AE, AI, JT, JU, KB, KC, KJ, KK, KR, KS, KZ, LA, LH, LI, LP, LQ (839 residues) - Nup49: chain(s) AG, AK, JX, JY, KF, KG, KN, KO, KV, KW, LD, LE, LL, LM, LT, LU (472 residues) - Nup57: chain(s) AH, AL, JZ, KA, KH, KI, KP, KQ, KX, KY, LF, LG, LN, LO, LV, LW (541 residues) - Nup157: chain(s) AM, AQ, LX, MB, MF, MJ, MN, MR, MV, MZ, ND, NH, NL, NP, NT, NX (1391 residues) - Nup170: chain(s) AN, AR, LY, MC, MG, MK, MO, MS, MW, NA, NE, NI, NM, NQ, NU, NY (1502 residues) - Nup188: chain(s) AO, AS, LZ, MD, MH, ML, MP, MT, MX, NB, NF, NJ, NN, NR, NV, NZ (1655 residues) - Nup192: chain(s) AP, AT, MA, ME, MI, MM, MQ, MU, MY, NC, NG, NK, NO, NS, NW, OA (1683 residues) - Nup53: chain(s) AU, AZ, OB, OG, OL, OQ, OV, PA, PF, PK, PP, PU, PZ, QE, QJ, QO (475 residues) - Nup59: chain(s) AV, BA, OC, OH, OM, OR, OW, PB, PG, PL, PQ, PV, QA, QF, QK, QP (528 residues) - Ndc1: chain(s) AW, BB, OD, OI, ON, OS, OX, PC, PH, PM, PR, PW, QB, QG, QL, QQ (655 residues) - Pom34: chain(s) AX, BC, OE, OJ, OO, OT, OY, PD, PI, PN, PS, PX, QC, QH, QM, QR (299 residues) - Pom152: chain(s) AY, BD, OF, OK, OP, OU, OZ, PE, PJ, PO, PT, PY, QD, QI, QN, QS (1337 residues) - Nup85: chain(s) B, I, BS, BZ, CG, CN, CU, DB, DI, DP, DW, ED, EK, ER, EY, FF (744 residues) - Nup100: chain(s) BE, BF, QT, QU, QZ, RA, RF, RG, RL, RM, RR, RS, RX, RY, SD, SE (959 residues) - Nup116: chain(s) BG, BH, QV, QW, RB, RC, RH, RI, RN, RO, RT, RU, RZ, SA, SF, SG (1113 residues) - Gle1: chain(s) BJ, QY, RE, RK, RQ, RW, SC, SI (538 residues) - Nup145: chain(s) BK, BL, SJ, SK, SO, SP, ST, SU, SY, SZ, TD, TE, TI, TJ, TN, TO (1317 residues) - Nup1: chain(s) BM, SN, SS, SX, TC, TH, TM, TR (1076 residues) - Nup60: chain(s) BN, BO, SL, SM, SQ, SR, SV, SW, TA, TB, TF, TG, TK, TL, TP, TQ (539 residues) |

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| | <p>residues)</p> <ul style="list-style-type: none"> - Mlp1: chain(s) BP, TS, TU, TW, TY, UA, UC, UE (1875 residues) - Mlp2: chain(s) BQ, TT, TV, TX, TZ, UB, UD, UF (1679 residues) - Nup120: chain(s) C, J, BT, CA, CH, CO, CV, DC, DJ, DQ, DX, EE, EL, ES, EZ, FG (1037 residues) - Nup133: chain(s) D, K, BU, CB, CI, CP, CW, DD, DK, DR, DY, EF, EM, ET, FA, FH (1157 residues) - Nup145c: chain(s) E, L, BV, CC, CJ, CQ, CX, DE, DL, DS, DZ, EG, EN, EU, FB, FI (712 residues) - Seh1: chain(s) F, M, BW, CD, CK, CR, CY, DF, DM, DT, EA, EH, EO, EV, FC, FJ (349 residues) - Sec13: chain(s) G, N, BX, CE, CL, CS, CZ, DG, DN, DU, EB, EI, EP, EW, FD, FK (297 residues) - Dyn2: chain(s) O, P, FL, FM, FT, FU, GB, GC, GJ, GK, GR, GS, GZ, HA, HH, HI (92 residues) - Nup82: chain(s) Q, R, FN, FO, FV, FW, GD, GE, GL, GM, GT, GU, HB, HC, HJ, HK (713 residues) - Nup159: chain(s) S, T, FP, FQ, FX, FY, GF, GG, GN, GO, GV, GW, HD, HE, HL, HM (1460 residues) - Nsp1: chain(s) U, V, AF, AJ, FR, FS, FZ, GA, GH, GI, GP, GQ, GX, GY, HF, HG, HN, HO, JV, JW, KD, KE, KL, KM, KT, KU, LB, LC, LJ, LK, LR, LS (823 residues) - Nsp1: chain(s) U, V, X, AB, AF, AJ, FR, FS, FZ, GA, GH, GI, GP, GQ, GX, GY, HF, HG, HN, HO, HR, HS, HZ, IA, IH, II, IP, IQ, IX, IY, JF, JG, JN, JO, JV, JW, KD, KE, KL, KM, KT, KU, LB, LC, LJ, LK, LR, LS (823 residues) - Nic96: chain(s) W, AA, HP, HQ, HX, HY, IF, IG, IN, IO, IV, IW, JD, JE, JL, JM (839 residues) - Nsp1: chain(s) X, AB, HR, HS, HZ, IA, IH, II, IP, IQ, IX, IY, JF, JG, JN, JO (823 residues) - Nup49: chain(s) Y, AC, AG, AK, HT, HU, IB, IC, IJ, IK, IR, IS, IZ, JA, JH, JI, JP, JQ, JX, JY, KF, KG, KN, KO, KV, KW, LD, LE, LL, LM, LT, LU (472 residues) - Nup49: chain(s) Y, AC, HT, HU, IB, IC, IJ, IK, IR, IS, IZ, JA, JH, JI, JP, JQ (472 residues) - Nup57: chain(s) Z, AD, AH, AL, HV, HW, ID, IE, IL, IM, IT, IU, JB, JC, JJ, JK, JR, JS, JZ, KA, KH, KI, KP, KQ, KX, KY, LF, LG, LN, LO, LV, LW (541 residues) - Nup57: chain(s) Z, AD, HV, HW, ID, IE, IL, IM, IT, IU, JB, JC, JJ, JK, JR, JS (541 residues) |
| | <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 |

Datasets used for modeling

- Comparative model, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
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- Comparative model, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- Integrative model, Not available: [10.1016/j.str.2017.01.006](https://doi.org/10.1016/j.str.2017.01.006)
- Integrative model, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- Experimental model, PDB: [3NF5](https://www.rcsb.org/structure/3NF5)
- Comparative model, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- Comparative model, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- Experimental model, PDB: [3KEP](https://www.rcsb.org/structure/3KEP)
- Experimental model, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- Mass Spectrometry data, Zenodo: [10.5281/zenodo.1149746](https://zenodo.org/record/1149746)
- Crosslinking-MS data, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
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- EM raw micrographs, EMPIAR: [EMPIAR-10155](https://www.ebi.ac.uk/EMPIAR/EMPIAR-10155)
- 3DEM volume, EMD: [EMD-7321](https://www.ebi.ac.uk/EMD/EMD-7321)
- 3DEM volume, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- SAS data, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
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- SAS data, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
- SAS data, SASBDB: [SASDBV9](https://www.rcsb.org/structure/SASDBV9)
- SAS data, SASBDB: [SASDBW9](https://www.rcsb.org/structure/SASDBW9)
- SAS data, SASBDB: [SASDBZ9](https://www.rcsb.org/structure/SASDBZ9)
- SAS data, SASBDB: [SASDBX9](https://www.rcsb.org/structure/SASDBX9)
- SAS data, SASBDB: [SASDBY9](https://www.rcsb.org/structure/SASDBY9)
- SAS data, Zenodo: [10.5281/zenodo.1194547](https://zenodo.org/record/1194547)
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| 2. Representation | |
| <i>Number of representations</i> | 2 |
| <i>Scale</i> | <ul style="list-style-type: none"> - Multiscale: Coarse-grained: 1 - 100 residue(s) per bead - Multiscale: Coarse-grained: 18 - 20 residue(s) per bead |
| <i>Number of rigid and flexible segments</i> | <ul style="list-style-type: none"> - 192, 6528 - 0, 200 |
| 3. Restraints | |
| <i>Physical principles</i> | Information about physical principles was not provided |
| <i>Experimental data</i> | <ul style="list-style-type: none"> - 1 unique EM3DRestraint: Number of micrographs: 800, Image resolution: 35.0 - 1 unique GeometricRestraint: DSS, 509 crosslinks - 1 unique SASRestraint: Gaussian mixture models - 1 unique CrossLinkRestraint: Assembly name: SAXS subassembly Fitting method: FoXS Multi-state: False - 1 unique EM2DRestraint: DSS, 508 crosslinks |
| 4. Validation | |
| <i>Number of ensembles</i> | 2 |
| <i>Number of models in ensembles</i> | 5, 1000 |
| <i>Number of deposited models</i> | 2 |
| <i>Model precision (uncertainty of models)</i> | <ul style="list-style-type: none"> - 1.00, Å - 1.00, Å |

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| <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: 100.00-100.00% |
| <i>Fit to data used for modeling</i> | Satisfaction of crosslinks: 87.52% |
| <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 |
| 4. <i>Name</i> | Sampling |
| <i>Method</i> | Brownian dynamics |
| <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)