

Summary of integrative structure determination of Modeling of Mouse NPC basket (PDB ID: 9A8L, PDB-Dev ID: PDBDEV_00000385)

| 1. Model Composition | |
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| <p>Entry composition</p> | <ul style="list-style-type: none"> - Nucleoprotein TPR: chain(s) A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P (2431 residues) - Nucleoporin 153: chain(s) AG, AH, AI, AJ, AK, AL, AM, AN, AO, AP, AQ, AR, AS, AT, AU, AV (1462 residues) - Nuclear pore complex protein Nup160: chain(s) AW, AX, AY, AZ, BA, BB, BC, BD, BE, BF, BG, BH, BI, BJ, BK, BL (1402 residues) - Nuclear pore complex protein Nup85: chain(s) BM, BN, BO, BP, BQ, BR, BS, BT, BU, BV, BW, BX, BY, BZ, CA, CB (656 residues) - Nuclear pore complex protein Nup98-Nup96: chain(s) CC, CD, CE, CF, CG, CH, CI, CJ, CK, CL, CM, CN, CO, CP, CQ, CR (1816 residues) - Protein SEC13 homolog: chain(s) CS, CT, CU, CV, CW, CX, CY, CZ, DA, DB, DC, DD, DE, DF, DG, DH (322 residues) - Nucleoporin SEH1: chain(s) DI, DJ, DK, DL, DM, DN, DO, DP, DQ, DR, DS, DT, DU, DV, DW, DX (360 residues) - Nuclear pore complex protein Nup107: chain(s) DY, DZ, EA, EB, EC, ED, EE, EF, EG, EH, EI, EJ, EK, EL, EM, EN (926 residues) - Nuclear pore complex protein Nup133: chain(s) EO, EP, EQ, ER, ES, ET, EU, EV, EW, EX, EY, EZ, FA, FB, FC, FD (1155 residues) - Nucleoporin Nup37: chain(s) FE, FF, FG, FH, FI, FJ, FK, FL, FM, FN, FO, FP, FQ, FR, FS, FT (326 residues) - Nucleoporin Nup43: chain(s) FU, FV, FW, FX, FY, FZ, GA, GB, GC, GD, GE, GF, GG, GH, GI, GJ (380 residues) - Nuclear pore complex protein Nup50: chain(s) Q, R, S, T, U, V, W, X, Y, Z, AA, AB, AC, AD, AE, AF (466 residues) |
| <p>Datasets used for modeling</p> | <ul style="list-style-type: none"> - De Novo model, Zenodo: 10.5281/zenodo.13131753 - Comparative model, Zenodo: 10.5281/zenodo.13131753 - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - Experimental model, PDB: 7r5j - 3DEM volume, EMDB: EMD-44379 |
| 2. Representation | |
| <p>Number of representations</p> | 1 |
| <p>Scale</p> | Multiscale: Coarse-grained: 1 - 50 residue(s) per bead |
| <p>Number of rigid and flexible segments</p> | 592, 432 |

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| 3. Restraints | |
| <i>Physical principles</i> | Information about physical principles was not provided |
| <i>Experimental data</i> | - 1 unique EM3DRestraint: Bayesian EM restraint on Gaussian mixture models |
| 4. Validation | |
| <i>Number of ensembles</i> | 1 |
| <i>Number of models in ensembles</i> | 1 |
| <i>Number of deposited models</i> | 1 |
| <i>Model precision (uncertainty of models)</i> | 41.90, Å |
| <i>Data quality</i> | Data quality has not been assessed |
| <i>Model quality: assessment of excluded volume</i> | Satisfaction: 100.00% |
| <i>Fit to data used for modeling</i> | Fit of model to information used to compute it has not been determined |
| <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> | 9569309 |
| <i>Software</i> | <ul style="list-style-type: none"> - IMP PMI module (version 2.19.0) - COCONUT (version 1.0.0) - Integrative Modeling Platform (IMP) (version 2.19.0) |