

Summary of integrative structure determination of Modeling of Yeast NPC basket (PDB ID: 9A8N, PDB-Dev ID: PDBDEV_00000387)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Unknown MLP Protein: chain(s) A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P (1875 residues) - Nucleoporin NUP60: chain(s) AO, AP, AQ, AR, AS, AT, AU, AV, AW, AX, AY, AZ, BA, BB, BC, BD (539 residues) - Nucleoporin NUP120: chain(s) BE, BF, BG, BH, BI, BJ, BK, BL, BM, BN, BO, BP, BQ, BR, BS, BT (1037 residues) - Nucleoporin NUP85: chain(s) BU, BW, BY, CA, CC, CE, CG, CI (744 residues) - Nucleoporin NUP85: chain(s) BV, BX, BZ, CB, CD, CF, CH, CJ (744 residues) - Nucleoporin NUP145C: chain(s) CK, CL, CM, CN, CO, CP, CQ, CR, CS, CT, CU, CV, CW, CX, CY, CZ (712 residues) - Protein transport protein SEC13: chain(s) DA, DB, DC, DD, DE, DF, DG, DH, DI, DJ, DK, DL, DM, DN, DO, DP (297 residues) - Nucleoporin SEH1: chain(s) DQ, DR, DS, DT, DU, DV, DW, DX, DY, DZ, EA, EB, EC, ED, EE, EF (349 residues) - Nucleoporin NUP84: chain(s) EG, EH, EI, EJ, EK, EL, EM, EN, EO, EP, EQ, ER, ES, ET, EU, EV (726 residues) - Nucleoporin NUP133: chain(s) EW, EY, FA, FC, FE, FG, FI, FK (1157 residues) - Nucleoporin NUP133: chain(s) EX, EZ, FB, FD, FF, FH, FJ, FL (1157 residues) - Nucleoporin NUP1: chain(s) Q, R, S, T, U, V, W, X (1076 residues) - Nucleoporin NUP2: chain(s) Y, Z, AA, AB, AC, AD, AE, AF, AG, AH, AI, AJ, AK, AL, AM, AN (720 residues)
<p>Datasets used for modeling</p>	<ul style="list-style-type: none"> - Crosslinking-MS data, Zenodo: 10.5281/zenodo.13131753 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - Experimental model, Zenodo: 10.5281/zenodo.13131753 - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - Experimental model, PDB: 7N84 - 3DEM volume, EMDB: EMD-44377

2. Representation	
<i>Number of representations</i>	1
<i>Scale</i>	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
<i>Number of <i>rigid</i> and <i>flexible</i> segments</i>	912, 1000
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: DSS, 164 crosslinks - 1 unique GeometricRestraint: DSS, 539 crosslinks - 1 unique CrossLinkRestraint: 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>	57.20, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.99%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 71.78%
<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>	1000
2. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	15467933

[Software](#)

- [IMP PMI module](#) (version 2.19.0)
- [COCONUT](#) (version 1.0.0)
- [Integrative Modeling Platform \(IMP\)](#) (version 2.19.0)