

Summary of integrative structure determination of Modeling of Mouse NPC basket (PDB ID: 9A8K, PDB-Dev ID: PDBDEV_00000384)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Nucleoprotein TPR: chain(s) A, B (2431 residues) - Nuclear pore complex protein Nup50: chain(s) C, D (466 residues) - Nucleoporin 153: chain(s) E, F (1462 residues) - Nuclear pore complex protein Nup160: chain(s) G, H (1402 residues) - Nuclear pore complex protein Nup85: chain(s) I, J (656 residues) - Nuclear pore complex protein Nup98-Nup96: chain(s) K, L (1816 residues) - Protein SEC13 homolog: chain(s) M, N (322 residues) - Nucleoporin SEH1: chain(s) O, P (360 residues) - Nuclear pore complex protein Nup107: chain(s) Q, R (926 residues) - Nuclear pore complex protein Nup133: chain(s) S, T (1155 residues) - Nucleoporin Nup37: chain(s) U, V (326 residues) - Nucleoporin Nup43: chain(s) W, X (380 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - Comparative model, Zenodo: 10.5281/zenodo.13131753 - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - Experimental model, PDB: 7r5j - 3DEM volume, EMDB: EMD-44379
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
Number of <i>rigid</i> and <i>flexible</i> segments	74, 54
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM3DRestraint: Bayesian EM restraint on Gaussian mixture models
4. Validation	
Number of ensembles	1
Number of models in ensembles	21

<i>Number of deposited models</i>	22
<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: 99.96-99.96%
<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 2.18.0)