

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

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Nucleoporin Nup43: Chain X (380 residues) - Nuclear pore complex protein Nup85: Chain I (656 residues) - Nucleoporin SEH1: Chain P (360 residues) - Nucleoporin Nup37: Chain U (326 residues) - Nuclear pore complex protein Nup107: Chain R (926 residues) - Nucleoporin 153: Chain E (1462 residues) - Nuclear pore complex protein Nup50: Chain D (466 residues) - Nuclear pore complex protein Nup85: Chain J (656 residues) - Nucleoporin SEH1: Chain O (360 residues) - Nuclear pore complex protein Nup98-Nup96: Chain K (1816 residues) - Protein SEC13 homolog: Chain M (322 residues) - Nucleoporin TPR: Chain A (2431 residues) - Nucleoporin Nup43: Chain W (380 residues) - Nuclear pore complex protein Nup160: Chain G (1402 residues) - Nuclear pore complex protein Nup160: Chain H (1402 residues) - Nucleoporin TPR: Chain B (2431 residues) - Nuclear pore complex protein Nup98-Nup96: Chain L (1816 residues) - Nucleoporin 153: Chain F (1462 residues) - Nuclear pore complex protein Nup133: Chain T (1155 residues) - Protein SEC13 homolog: Chain N (322 residues) - Nucleoporin Nup37: Chain V (326 residues) - Nuclear pore complex protein Nup107: Chain Q (926 residues) - Nuclear pore complex protein Nup133: Chain S (1155 residues) - Nuclear pore complex protein Nup50: Chain C (466 residues)
<p>Datasets used for modeling</p>	<ul style="list-style-type: none"> - 3DEM volume, File: 10.5281/zenodo.13131753 - De Novo model, File: 10.5281/zenodo.13131753 - Comparative model, template PDB ID: Not available - 3DEM volume, File: 10.5281/zenodo.13131753 - Experimental model, PDB ID: 7r5j - 3DEM volume, EMDB: EMD-44379
2. Representation	
<p>Resolution</p>	<p>Coarse-grained: 1, 2, 3, 5, 13, 15 residue(s) per bead</p>

<i>Number of rigid bodies, flexible units</i>	74, 54
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - E: 36-57 - F: 36-57 - A: 96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690 - B: 96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690 - C: 151-204, 355-466 - D: 151-204, 355-466 - G: 1-1402 - H: 1-1402 - I: 1-656 - J: 1-656 - K: 1111-1159, 1194-1816 - L: 1111-1159, 1194-1816 - M: 1-302 - N: 1-302 - O: 1-324 - P: 1-324 - Q: 145-926 - R: 145-926 - S: 70-1155 - T: 70-1155 - U: 1-326 - V: 1-326 - W: 1-292, 327-380 - X: 1-292, 327-380

<i>Flexible units</i>	<ul style="list-style-type: none"> - E: 1-35, 58-428, 540-574 - F: 1-35, 58-428, 540-574 - A: 1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431 - B: 1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431 - C: 1-150, 205-354 - D: 1-150, 205-354 - G: - - H: - - I: - - J: - - K: - - L: - - M: - - N: - - O: - - P: - - Q: - - R: - - S: - - T: - - U: - - V: - - W: - - X: -
<i>Structural coverage (rigid bodies)</i>	79%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	- 1 unique GeometricRestraint: Bayesian EM restraint on Gaussian mixture models
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	21
<i>Number of deposited models</i>	22
<i>Model precision (uncertainty of models)</i>	41.9, Å
<i>Data quality</i>	Data quality has not been assessed

<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.96-99.96%
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	500
2. <u>Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	9569309
<u>Software</u>	<ul style="list-style-type: none"> - <u>IMP PMI module</u> (version 2.19.0) - <u>COCONUT</u> (version 1.0.0) - <u>Integrative Modeling Platform (IMP)</u> (version 2.18.0)