

**Summary of integrative structure determination of Integrative model of the nuclear pore complex  
from Schizosaccharomyces pombe (PDB ID: 9A1M | pdb\_00009a1m, PDB-Dev ID:  
PDBDEV\_00000094 )**

1. Model Composition	
<a href="#">1.1. Entry composition</a>	<ul style="list-style-type: none"> <li>- Nup184: chain(s) B, B1, B2, B3, B4, B5, B6, B7, B8, B9, B10, B11, B12, B13, B14, B15 (1564 residues)</li> <li>- Nup186: chain(s) C, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15 (1647 residues)</li> <li>- Nup155: chain(s) D, D1, D2, D3, D4, D5, D6, D7, D8, D9, D10, D11, D12, D13, D14, D15, D16, D17, D18, D19, D20, D21, D22, D23, D24, D25, D26, D27, D28, D29, D30, D31 (1315 residues)</li> <li>- Nup44: chain(s) H, H1, H2, H3, H4, H5, H6, H7, H8, H9, H10, H11, H12, H13, H14, H15, H16, H17, H18, H19, H20, H21, H22, H23, H24, H25, H26, H27, H28, H29, H30, H31 (403 residues)</li> <li>- Nup45: chain(s) I, I1, I2, I3, I4, I5, I6, I7, I8, I9, I10, I11, I12, I13, I14, I15, I16, I17, I18, I19, I20, I21, I22, I23, I24, I25, I26, I27, I28, I29, I30, I31 (425 residues)</li> <li>- Nsp1: chain(s) J, J1, J2, J3, J4, J5, J6, J7, J8, J9, J10, J11, J12, J13, J14, J15, J16, J17, J18, J19, J20, J21, J22, J23, J24, J25, J26, J27, J28, J29, J30, J31 (598 residues)</li> <li>- Nup107: chain(s) L, L1, L2, L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15 (813 residues)</li> <li>- Nup189c: chain(s) M, M1, M2, M3, M4, M5, M6, M7, M8, M9, M10, M11, M12, M13, M14, M15, M16, M17, M18, M19, M20, M21, M22, M23 (844 residues)</li> <li>- Sec13: chain(s) N, N1, N2, N3, N4, N5, N6, N7, N8, N9, N10, N11, N12, N13, N14, N15, N16, N17, N18, N19, N20, N21, N22, N23 (297 residues)</li> <li>- Seh1: chain(s) O, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23 (339 residues)</li> <li>- Nup85: chain(s) P, P1, P2, P3, P4, P5, P6, P7, P8, P9, P10, P11, P12, P13, P14, P15, P16, P17, P18, P19, P20, P21, P22, P23 (675 residues)</li> <li>- Nup132: chain(s) Q, Q1, Q2, Q3, Q4, Q5, Q6, Q7, Q8, Q9, Q10, Q11, Q12, Q13, Q14, Q15 (1162 residues)</li> <li>- Nup120: chain(s) R, R1, R2, R3, R4, R5, R6, R7, R8, R9, R10, R11, R12, R13, R14, R15, R16, R17, R18, R19, R20, R21, R22, R23 (1136 residues)</li> <li>- Nup37: chain(s) S, S1, S2, S3, S4, S5, S6, S7, S8, S9, S10, S11, S12, S13, S14, S15, S16, S17, S18, S19, S20, S21, S22, S23 (391 residues)</li> <li>- Ely5: chain(s) T, T1, T2, T3, T4, T5, T6, T7, T8, T9, T10, T11, T12, T13, T14, T15, T16, T17, T18, T19, T20, T21, T22, T23 (298 residues)</li> <li>- Nup97: chain(s) Y, Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8, Y9, Y10, Y11, Y12, Y13, Y14, Y15, Y16, Y17, Y18, Y19, Y20, Y21, Y22, Y23, Y24, Y25, Y26, Y27, Y28, Y29, Y30, Y31 (851 residues)</li> </ul>

<a href="#">1.2. Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- 3DEM volume, EMDB: <a href="#">EMD-11373</a></li> <li>- 3DEM volume, Zenodo: <a href="#">10.5281/zenodo.5585949</a></li> <li>- Experimental model, PDB: <a href="#">pdb_00004gg2</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.5585949</a></li> <li>- Other, Not available: <a href="https://doi.org/10.1038/nsmb1194">https://doi.org/10.1038/nsmb1194</a></li> <li>- Other, Not available: <a href="https://doi.org/10.1038/nature15381">https://doi.org/10.1038/nature15381</a></li> </ul>
<b>2. Representation</b>	
<a href="#">2.1. Number of representations</a>	1
<a href="#">2.2. Scale</a>	Atomic
<a href="#">2.3. Number of rigid and flexible segments</a>	664, 0
<b>3. Restraints</b>	
<a href="#">3.1. Physical principles</a>	Information about physical principles was not provided
<a href="#">3.2. Experimental data</a>	
<b>4. Validation</b>	
<a href="#">4.2. Number of ensembles</a>	0
<a href="#">4.3. Number of models in ensembles</a>	Not applicable
<a href="#">4.4. Number of deposited models</a>	1
<a href="#">4.5. Model precision</a>	Not available
<a href="#">4.6. Data quality</a>	EMD-11373: resolution is 22.00 Å
<a href="#">4.7. Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 0.00</li> <li>- Ramachandran outliers: 4824</li> <li>- Sidechain outliers: 12720</li> </ul>
<a href="#">4.8. Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">4.9. Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">5.1. Method name</a>	Systematic fitting to EM maps with Global search from UCSF Chimera as implemented in Assemblin
<a href="#">5.2. Method type</a>	Systematic fitting of CR and NR subunits and IR asymmetric unit using Assemblin and UCSF Chimera
2. <a href="#">5.1. Method name</a>	Modeling the cytoplasmic side
<a href="#">5.2. Method type</a>	Global optimization with Assemblin starting from systematic fitting results

3. <a href="#"><i>5.1. Method name</i></a>	Modeling the nuclear ring
<a href="#"><i>5.2. Method type</i></a>	Global optimization with Assemblin starting from systematic fitting results
4. <a href="#"><i>5.1. Method name</i></a>	Modeling the inner ring
<a href="#"><i>5.2. Method type</i></a>	Refinement optimization with Assemblin starting from the fitted comparative model
5. <a href="#"><i>5.1. Method name</i></a>	Modeling the full nuclear pore complex from models of the individual rings
<a href="#"><i>5.2. Method type</i></a>	Refinement optimization with Assemblin
<a href="#"><i>5.5. Software</i></a>	<ul style="list-style-type: none"> <li>- <a href="#">Assemblin</a> (version 0.99beta)</li> <li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version 2.15.0)</li> <li>- <a href="#">UCSF Chimera</a> (version 1.14)</li> </ul>