

Summary of integrative structure determination of Structure of the Nup84 sub-complex of the Nuclear Pore Complex (PDB ID: 8ZZ1, PDB-Dev ID: PDBDEV_00000001)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - Sec13: Chain G (297 residues) - Nup85: Chain B (744 residues) - Nup84: Chain A (726 residues) - Nup133: Chain D (1157 residues) - Seh1: Chain F (349 residues) - Nup120: Chain C (1037 residues) - Nup145c: Chain E (712 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 3JRO - Experimental model, PDB ID: 3F3F - Experimental model, PDB ID: 3IKO - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3CQC - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 4LCT - Experimental model, PDB ID: 2QX5 - Experimental model, PDB ID: 3EWE - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3F7F - Experimental model, PDB ID: 3HXR - Experimental model, PDB ID: 4FHN - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 4Q9T - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3I4R - Experimental model, PDB ID: 3KFO - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3BG1 - Experimental model, PDB ID: 3BG0 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3F3F - Experimental model, PDB ID: 2PM7 - Crosslinking-MS data, Linker name and number of cross-links: DSS, 164 cross-links - Crosslinking-MS data, Linker name and number of cross-links: EDC, 127 cross-links - EM raw micrographs, File: 10.5281/zenodo.58025 - 2DEM class average, File: 10.5281/zenodo.1218053
2. Representation	
<u>Resolution</u>	Coarse-grained: 1, 2, 3, 4, 7, 8 residue(s) per bead
<u>Number of rigid bodies, flexible units</u>	40, 42

<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: 7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726 - B: 67-122, 135-427, 461-529, 533-602, 620-671, 680-743 - C: 1-29, 53-212, 221-305, 311-429, 440-710, 711-712, 727-781, 805-892, 903-910, 921-1010, 1023-1037 - D: 56-78, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155 - E: 126-144, 151-175, 182-553 - F: 1-248, 288-346 - G: 2-158, 166-296
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574 - B: 1-66, 123-134, 428-460, 530-532, 603-619, 672-679, 744-744 - C: 30-52, 213-220, 306-310, 430-439, 713-726, 782-804, 893-902, 911-920, 1011-1022 - D: 1-55, 79-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157 - E: 1-125, 145-150, 176-181, 554-712 - F: 249-287, 347-349 - G: 1-1, 159-165, 297-297
<u>Structural coverage (rigid bodies)</u>	84%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 164 cross-links - 1 unique CrossLinkRestraint: EDC, 127 cross-links - 1 unique EM2DRestraint: Number of micrographs: 800, Image resolution: 30.0
4. Validation	
<u>Number of ensembles</u>	2
<u>Number of models in ensembles</u>	1257, 1010
<u>Number of deposited models</u>	2
<u>Model precision (uncertainty of models)</u>	15.4, Å, 12.7, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.88-99.88%
<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>	5000
<u>Software</u>	<ul style="list-style-type: none"> - Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0) - HHpred (version 2.0.16) - PSIPRED (version 4.0) - DISOPRED (version 3) - MODELLER (version 9.12)