Summary of integrative structure determination of structure of the nup84 sub-complex of the nuclear pore complex (PDBDEV_00000001)

1. Model Composition	
Entry composition	- Nup133: Chain D (1157 residues) - Nup84: Chain A (726 residues) - Nup120: Chain C (1037 residues) - Sec13: Chain G (297 residues) - Nup85: Chain B (744 residues) - Nup145c: Chain E (712 residues) - Seh1: Chain F (349 residues)
Datasets used for modeling	- 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 - CX-MS data, Linker name and number of cross-links: DSS, 164 cross-links - CX-MS data, Linker name and number of cross-links: EDC, 127 cross-links - EM raw micrographs, EMDB ID: Not available - 2DEM class average, EMDB ID: Not available
2. Representation	
Atomic structural coverage	84%
Number of rigid bodies, flexible units	40, 42

Rigid bodies	- A: 7-20:Comparative model/None, 27-80:Comparative model/None, 96-126:Comparative model/None, 136-364:Comparative model/None, 372-483:Comparative model/None, 506-562:Comparative model/None, 575-726:Comparative model/None. - B: 67-122:Comparative model/None, 135-427:Comparative model/None, 461-529:Comparative model/None, 533-602:Comparative model/None, 620-671:Comparative model/None, 680-743:Comparative model/None. - C: 1-29:Comparative model/None, 53-212:Comparative model/None, 221-305:Comparative model/None, 311-429:Comparative model/None, 440-710:Comparative model/None, 711-712:Comparative model/None, 727-781:Comparative model/None, 805-892:Comparative model/None, 903-910:Comparative model/None, 921-1010:Comparative model/None, 1023-1037:Comparative model/None. - D: 56-78:Comparative model/None, 86-125:Comparative model/None, 133-144:Comparative model/None, 162-184:Comparative model/None, 193-200:Comparative model/None, 206-249:Comparative model/None, 258-480:Comparative model/None, 490-763:Comparative model/None, 772-1155:Comparative model/None. - E: 126-144:Comparative model/None, 151-175:Comparative model/None, 182-553:Comparative model/None. - F: 1-248:Experimental model/3F3F, 288-346:Experimental model/3F3F. - G: 2-158:Experimental model/2PM7, 166-296:Experimental model/2PM7.
Flexible units	- 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.
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 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	
Sampling validation	- Information related to sampling validation has not been provided

Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, dRMSD
Number of ensembles	2
Number of models in ensembles	1257, 1010
Model precision (uncertainty of models)	15.4Å, 12.7Å
Data quality	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	
Model quality: assessment of excluded volume	- Model-1: Number of violations = 10899.0 - Model-2: Number of violations = 10935.0
Fit to data used for modeling	- Fit of model to information used to compute it has not been determined
Fit to data used for validation	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Sampling
Name	Replica exchange Monte Carlo
Details	- Method details not available
Software	- 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)