Summary of integrative structure determination of structure of the s. cerevisiae nuclear pore complex cytoplasmic mrna export platform, nup82 (PDBDEV00000020)

1. Model Composition	
Entry composition	- Nsp1: Chain H (823 residues) - Nup159: Chain F (1460 residues) - Nup82: Chain D (713 residues) - Nup159: Chain E (1460 residues) - Nup116: Chain I (1113 residues) - Dyn2: Chain B (92 residues) - Nsp1: Chain G (823 residues) - Nup116: Chain J (1113 residues) - Dyn2: Chain A (92 residues) - Nup82: Chain C (713 residues)
Datasets used for modeling	- Experimental model, PDB ID: 4DS1 - Experimental model, PDB ID: 3PBP - Experimental model, PDB ID: 5CWS - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Comparative model, template PDB ID: Not listed - Experimental model, PDB ID: 1XIP - CX-MS data, Linker name and number of cross-links: DSS, 240 cross-links - CX-MS data, Linker name and number of cross-links: DSS, 109 cross-links - CX-MS data, Linker name and number of cross-links: EDC, 81 cross-links - 2DEM class average, EMDB ID: Not listed - SAS data, Not listed - SAS data, Not listed - SAS data, Not listed
2. Representation	
Atomic structural coverage	37%
Number of rigid bodies, flexible units	38, 42

Rigid bodies	- A: 7-92:Experimental model/4DS1. - B: 7-92:Experimental model/4DS1. - C: 7-16:Experimental model/3PBP, 23-120:Experimental model/3PBP, 123-452:Experimental model/3PBP, 522-612:Comparative model/None, 625-669:Comparative model/None, 678-713:Comparative model/None. - D: 7-16:Experimental model/3PBP, 23-120:Experimental model/3PBP, 123-452:Experimental model/3PBP, 522-612:Comparative model/None, 625-669:Comparative model/None, 678-713:Comparative model/None. - E: 2-347:Experimental model/1XIP, 362-381:Experimental model/1XIP, 1117-1126:Experimental model/4DS1, 1211-1239:Comparative model/None, 1266-1321:Comparative model/None, 1332-1372:Comparative model/None, 1382-1412:Comparative model/None, 1429-1456:Experimental model/3PBP. - F: 2-347:Experimental model/1XIP, 362-381:Experimental model/1XIP, 1117-1126:Experimental model/4DS1, 1211-1239:Comparative model/None, 1266-1321:Comparative model/None, 1332-1372:Comparative model/None, 1382-1412:Comparative model/None, 1429-1456:Experimental model/3PBP. - G: 637-727:Comparative model/None, 742-778:Comparative model/None, 788-823:Comparative model/None. - H: 637-727:Comparative model/None, 742-778:Comparative model/None, 788-823:Comparative model/None. - I: 966-1111:Experimental model/3PBP. - J: 966-1111:Experimental model/3PBP.
Flexible units	- A: 1-6. - B: 1-6. - C: 1-6, 17-22, 121-122, 453-521, 613-624, 670-677. - D: 1-6, 17-22, 121-122, 453-521, 613-624, 670-677. - E: 1-1, 348-361, 382-1116, 1127-1210, 1240-1265, 1322-1331, 1373-1381, 1413-1428, 1457-1460. - F: 1-1, 348-361, 382-1116, 1127-1210, 1240-1265, 1322-1331, 1373-1381, 1413-1428, 1457-1460. - G: 1-636, 728-741, 779-787. - H: 1-636, 728-741, 779-787. - I: 1-965, 1112-1113. - J: 1-965, 1112-1113.
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, 240 cross-links - 1 unique CrossLinkRestraint: DSS, 109 cross-links - 1 unique CrossLinkRestraint: EDC, 81 cross-links - 21 unique EM2DRestraint: Number of micrographs: None, Image resolution: 35.0 - 3 unique SASRestraint: Assembly name: SAXS subassembly Fitting method: FoXS Multi-state: False
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	1
Number of models in ensembles	370
Model precision (uncertainty of models)	9.0Å
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Not applicable
Model quality: assessment of excluded volume	- Model-1: Number of violations-8455.0
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	- 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 unspecified
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) - DomPred (version None) - COILS/PCOILS (version None) - Multicoil2 (version None) - MODELLER (version 9.15) - No location specified