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

Entry composition	 Dyn2: Chain A (92 residues) Nsp1: Chain G (823 residues) Nup82: Chain C (713 residues) Nup159: Chain F (1460 residues) Dyn2: Chain B (92 residues) Nup116: Chain J (1113 residues) Nup116: Chain I (1113 residues) Nup82: Chain D (713 residues) Nup82: Chain E (1460 residues) Nsp1: Chain H (823 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 - 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 - 2DEM class average, EMDB ID: No
2. Representation	
Atomic structural coverage	37%

	- A: 7-92:Experimental model/4DS1 B: 7-92:Experimental model/4DS1.
Rigid bodies	- 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, 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/None, 1429-1456:Experimental model/3PBP G: 637-727:Comparative model/None, 1382-1412:Comparative model/None, 1266-1321: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 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	- CX-MS Fit of medioid: model # 1, percentage satisfied 77.44%
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	
<u>Method</u>	Sampling
<u>Name</u>	Replica exchange Monte Carlo
<u>Details</u>	- Method details unspecified
<u>Software</u>	- 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