

Summary of integrative structure determination of Structure of the *S. cerevisiae* nuclear pore complex cytoplasmic mRNA export platform, Nup82 (PDB ID: 8ZZK, PDB-Dev ID: PDBDEV_0000020)

| 1. Model Composition | |
|---|---|
| <p>Entry composition</p> | <ul style="list-style-type: none"> - Nup82: Chain C (713 residues) - Nup159: Chain F (1460 residues) - Dyn2: Chain A (92 residues) - Nup82: Chain D (713 residues) - Nup159: Chain E (1460 residues) - Dyn2: Chain B (92 residues) - Nup116: Chain J (1113 residues) - Nsp1: Chain H (823 residues) - Nup116: Chain I (1113 residues) - Nsp1: Chain G (823 residues) |
| <p>Datasets used for modeling</p> | <ul style="list-style-type: none"> - Experimental model, PDB ID: 4DS1 - Experimental model, PDB ID: 3PBP - Experimental model, PDB ID: 5CWS - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 1XIP - Crosslinking-MS data, Linker name and number of cross-links: DSS, 240 cross-links - Crosslinking-MS data, Linker name and number of cross-links: DSS, 109 cross-links - Crosslinking-MS data, Linker name and number of cross-links: EDC, 81 cross-links - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 - 2DEM class average, File: 10.5281/zenodo.1256259 |

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| 2. Representation | |
| Resolution | Coarse-grained: 1, 2, 3, 7, 8, 9, 17 residue(s) per bead |
| <i>Number of rigid bodies, flexible units</i> | 38, 42 |
| <i>Rigid bodies</i> | <ul style="list-style-type: none"> - A: 7-92 - B: 7-92 - C: 7-16, 23-120, 123-452, 522-612, 625-669, 678-713 - D: 7-16, 23-120, 123-452, 522-612, 625-669, 678-713 - E: 2-347, 362-381, 1117-1126, 1211-1239, 1266-1321, 1332-1372, 1382-1412, 1429-1456 - F: 2-347, 362-381, 1117-1126, 1211-1239, 1266-1321, 1332-1372, 1382-1412, 1429-1456 - G: 637-727, 742-778, 788-823 - H: 637-727, 742-778, 788-823 - I: 966-1111 - J: 966-1111 |
| <i>Flexible units</i> | <ul style="list-style-type: none"> - 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 |
| Structural coverage (rigid bodies) | 37% |

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| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | <ul style="list-style-type: none"> - 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 | |
| Number of ensembles | 1 |
| Number of models in ensembles | 370 |
| Number of deposited models | 1 |
| Model precision (uncertainty of models) | 9.0, Å |
| Data quality | Data quality has not been assessed |
| Model quality: assessment of excluded volume | Satisfaction: 99.84-99.84% |
| 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 | |
| 1. Method | Sampling |
| Name | Replica exchange monte carlo |
| Number of computed models | 1000 |
| 2. Method | Sampling |
| Name | Replica exchange monte carlo |
| Number of computed models | 1350000 |
| 3. Method | Sampling |
| Name | Replica exchange monte carlo |
| Number of computed models | 10000 |

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 Not available)
- [COILS/PCOILS](#) (version Not available)
- [Multicoil2](#) (version Not available)
- [MODELLER](#) (version 9.15)