

Full wwPDB Integrative Structure Validation Report

September 06, 2019 -- 02:06 PM

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| PDB ID | PDBDEV00000020 |
| Molecule Name | Structure of the <i>S. cerevisiae</i> nuclear pore complex cytoplasmic mRNA export platform, Nup82 |
| Title | Structure and Function of the Nuclear Pore Complex Cytoplasmic mRNA Export Platform. |
| Authors | Fernandez-Martinez J;Kim SJ;Shi Y;Upla P;Pellarin R;Gagnon M;Chemmam IE;Wang J;Nudelman I;Zhang W;Williams R;Rice WJ;Stokes DL;Zenklusen D;Chait BT;Sali A;Rout MP |

The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobit : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There are 4 unique types of models in this entry. Models have 10,1,1,1 chains respectively.

| Molecule ID | Molecule Name | Chain ID | Total Residues |
|-------------|---------------|----------|----------------|
| 1 | Dyn2 | A | 92 |
| 1 | Nup82 | B | 92 |
| 1 | Nup159 | C | 713 |
| 1 | Nsp1 | D | 713 |
| 1 | Nup116 | E | 1460 |
| 1 | Dyn2 | F | 1460 |
| 1 | Nup82 | G | 823 |
| 1 | Nup159 | H | 823 |
| 1 | Nsp1 | I | 1113 |
| 1 | Nup116 | J | 1113 |

There are 9 software packages reported in this entry.

| ID | Software Name | Software Version | Software Classification |
|----|-------------------------------------|--------------------|--------------------------------|
| 1 | Integrative Modeling Platform (IMP) | develop-0a5706e202 | integrative model building |
| 2 | IMP PMI module | 67456c0 | integrative model building |
| 3 | HHpred | 2.0.16 | protein homology detection |
| 4 | PSIPRED | 4.0 | secondary structure prediction |
| 5 | DISOPRED | 3 | disorder prediction |
| 6 | DomPred | None | domain prediction |
| 7 | COILS/PCOILS | None | coiled-coil prediction |
| 8 | Multicoil2 | None | coiled-coil prediction |
| 9 | MODELLER | 9.15 | comparative modeling |

There are 37 unique datasets used to build the model in this entry.

| ID | Dataset Type | Database Name | Data Access Code |
|----|--------------------|---------------|------------------|
| 1 | Experimental model | PDB | 4DS1 |
| 2 | Experimental model | PDB | 3PBP |
| 3 | Experimental model | PDB | 5CWS |
| 4 | Comparative model | Not Listed | None |
| 5 | Comparative model | Not Listed | None |
| 6 | Comparative model | Not Listed | None |
| 7 | Comparative model | Not Listed | None |
| 8 | Comparative model | Not Listed | None |
| 9 | Comparative model | Not Listed | None |
| 10 | Experimental model | PDB | 1XIP |
| 11 | CX-MS data | Not Listed | None |
| 12 | CX-MS data | Not Listed | None |
| 13 | CX-MS data | Not Listed | None |
| 14 | 2DEM class average | Not Listed | None |
| 15 | 2DEM class average | Not Listed | None |
| 16 | 2DEM class | Not Listed | None |

| | | | |
|----|--------------------|------------|------|
| | average | | |
| 17 | 2DEM class average | Not Listed | None |
| 18 | 2DEM class average | Not Listed | None |
| 19 | 2DEM class average | Not Listed | None |
| 20 | 2DEM class average | Not Listed | None |
| 21 | 2DEM class average | Not Listed | None |
| 22 | 2DEM class average | Not Listed | None |
| 23 | 2DEM class average | Not Listed | None |
| 24 | 2DEM class average | Not Listed | None |
| 25 | 2DEM class average | Not Listed | None |
| 26 | 2DEM class average | Not Listed | None |
| 27 | 2DEM class average | Not Listed | None |
| 28 | 2DEM class average | Not Listed | None |
| 29 | 2DEM class average | Not Listed | None |
| 30 | 2DEM class average | Not Listed | None |
| 31 | 2DEM class average | Not Listed | None |
| 32 | 2DEM class average | Not Listed | None |
| 33 | 2DEM class average | Not Listed | None |
| 34 | 2DEM class average | Not Listed | None |
| 35 | SAS data | Not Listed | None |
| 36 | SAS data | Not Listed | None |
| 37 | SAS data | Not Listed | None |

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertainty of model
