

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

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 1 unique types of models in this entry. The entry contains 13 chains.

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(s) 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
