Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 06:45 PM

PDB ID	PDBDEV00000016
Molecule Name	Integrative structure-function mapping of the nucleoporin Nup133
Title	Integrative structure-function mapping of the nucleoporin Nup133 suggests a conserved mechanism for memb anchoring of the nuclear pore complex.
Authors	Kim SJ;Fernandez-Martinez J;Sampathkumar P;Martel A;Matsui T;Tsuruta H;Weiss TM;Shi Y;Markina-Inarrai A;Bonanno JB;Sauder JM;Burley SK;Chait BT;Almo SC;Rout MP;Sali A

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

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

1. Overall quality at a glance

2. Entry composition

There is 1 unique type of model in this entry. This entry contains 1 unique chain.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Nup133	A	1166

There are 6 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	HHpred	2.0.16	protein homology detection
2	PSIPRED	4.0	secondary structure prediction
3	DISOPRED	3	disorder prediction
4	Integrative Modeling Platform (IMP)	2.2	integrative model building
5	MODELLER	9.13	comparative modeling
6	AllosMod	None	sampling

There are 56 unique datasets used to build the model in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	SAS data	Not Listed	None
2	SAS data	Not Listed	None
3	SAS data	Not Listed	None
4	SAS data	Not Listed	None
5	SAS data	Not Listed	None
6	SAS data	Not Listed	None
7	SAS data	Not Listed	None
8	SAS data	Not Listed	None
9	SAS data	Not Listed	None
10	SAS data	Not Listed	None
11	SAS data	Not Listed	None
12	SAS data	Not Listed	None
13	SAS data	Not Listed	None
14	SAS data	Not Listed	None
15	SAS data	Not Listed	None
16	SAS data	Not Listed	None
17	SAS data	Not Listed	None
18	SAS data	Not Listed	None
19	SAS data	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	Not Listed	None

	average		
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	2DEM class average	Not Listed	None
36	2DEM class average	Not Listed	None
37	2DEM class average	Not Listed	None
38	2DEM class average	Not Listed	None
39	2DEM class average	Not Listed	None
40	2DEM class average	Not Listed	None
41	2DEM class average	Not Listed	None
42	2DEM class average	Not Listed	None
43	CX-MS data	Not Listed	None
44	Experimental model	PDB	3I4R
45	Experimental model	PDB	3KFO
46	Experimental model	PDB	4Q9T
47	Experimental model	PDB	2JO8
48	Experimental model	PDB	2QIW
49	Experimental model	PDB	3CIG
50	Experimental model	PDB	2ELO

51	Experimental model	PDB	3GUZ
52	Experimental model	PDB	2CIW
53	Experimental model	PDB	1A92
54	Experimental model	PDB	1GDJ
55	Experimental model	PDB	1X4O
56	Comparative model	Not Listed	None

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3. Data quality

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4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

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5. Fit of model and data

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6. Uncertaintiy of model
