Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

PDB ID	PDBDEV00000001
Molecule Name	Structure of the Nup84 sub-complex of the Nuclear Pore Complex
Title	Structural characterization by cross-linking reveals the detailed architecture of a coatomer-related heptamer module from the nuclear pore complex.
Authors	Shi Y;Fernandez-Martinez J;Tjioe E;Pellarin R;Kim SJ;Williams R;Schneidman-Duhovny D;Sali A;Rout MP;(

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 are 1 unique types of models in this entry. The entry contains 7 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Nup84	A	726
1	Nup85	B	744
1	Nup120	C	1037
1	Nup133	D	1157
1	Nup145c	E	712
1	Seh1	F	349
1	Sec13	G	297

There are 6 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	MODELLER	9.12	comparative modeling

There are 28 unique datasets used to build the model(s) in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Experimental model	PDB	3JRO
2	Experimental model	PDB	3F3F
3	Experimental model	PDB	3IKO
4	Comparative model	Not Listed	None
5	Experimental model	PDB	3CQC
6	Comparative model	Not Listed	None
7	Experimental model	PDB	4LCT
8	Experimental model	PDB	2QX5
9	Experimental model	PDB	3EWE
10	Comparative model	Not Listed	None
11	Experimental model	PDB	3F7F
12	Experimental model	PDB	3HXR
13	Experimental model	PDB	4FHN
14	Comparative model	Not Listed	None
15	Experimental model	PDB	4Q9T
16	Comparative model	Not Listed	None
17	Experimental model	PDB	3I4R
18	Experimental model	PDB	3KFO
19	Comparative model	Not Listed	None
20	Experimental model	PDB	3BG1
21	Experimental model	PDB	3BG0
22	Comparative model	Not Listed	None
23	Experimental model	PDB	3F3F

24	Experimental model	PDB	2PM7
25	CX-MS data	Not Listed	None
26	CX-MS data	Not Listed	None
27	EM raw micrographs	Not Listed	None
28	2DEM class average	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. Uncertaintiy of model