

# Full wwPDB Integrative Structure Validation Report

June 26, 2020 -- 11:58 AM

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

Integrative Modeling Validation Package: Version 1.0

PDB ID	PDBDEV_00000001
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 heptameric 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;Chait BT



### **Ensemble information**

This entry consists of 2 distinct ensembles.

### **Entry composition**

There are 2 unique types of models in this entry. These models are titled Cluster 1/Best scoring model, Cluster 2/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	Nup84	А	726
1	2	2	Nup85	В	744
1	3	3	Nup120	С	1037
1	4	4	Nup133	D	1157
1	5	5	Nup145c	Е	712
1	6	6	Seh1	F	349
1	7	7	Sec13	G	297
2	1	1	Nup84	А	726
2	2	2	Nup85	В	744
2	3	3	Nup120	С	1037
2	4	4	Nup133	D	1157
2	5	5	Nup145c	E	712
2	6	6	Seh1	F	349
2	7	7	Sec13	G	297

### Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	500	False	True
2	1	Replica exchange monte carlo	Sampling	5000	False	True

### **Data quality**

## **Model quality**

#### Excluded volume satisfaction

Excluded volume satisfaction for the models in the entry are listed below.

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.88	10899.0
2	99.88	10935.0

### Fit of model to data used for modeling

Fit of model to data not used for modeling

# Uncertainty of data and model

4 of 4			