

PDB

# Full RCSB Integrative Structure Validation Report

July 09, 2021 -- 12:25 PM

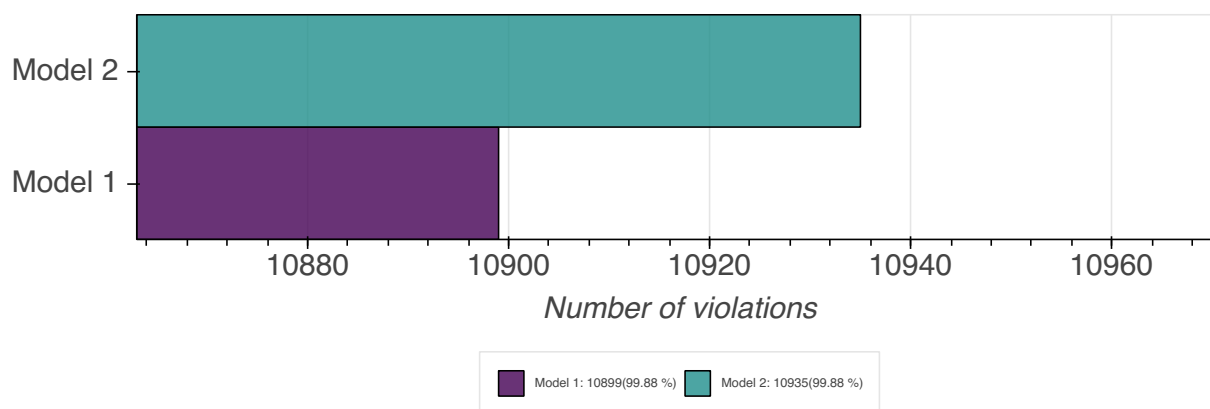
The following software were used in the production of this report:

*Integrative Modeling Validation Package : Version 1.0*

<b>PDB ID</b>	<b>PDBDEV_00000001</b>
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

## Overall quality

### Model quality: Excluded Volume Analysis



### 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	A	726
1	2	2	Nup85	B	744
1	3	3	Nup120	C	1037
1	4	4	Nup133	D	1157
1	5	5	Nup145c	E	712
1	6	6	Seh1	F	349
1	7	7	Sec13	G	297
2	1	1	Nup84	A	726
2	2	2	Nup85	B	744
2	3	3	Nup120	C	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