W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB Integrative Structure Validation Report

June 29, 2020 -- 10:06 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

Overall quality

Model quality: Excluded Volume Analysis

Legend:
- Model 1: 10899
- Model 2: 10935

X-axis: Number of violations
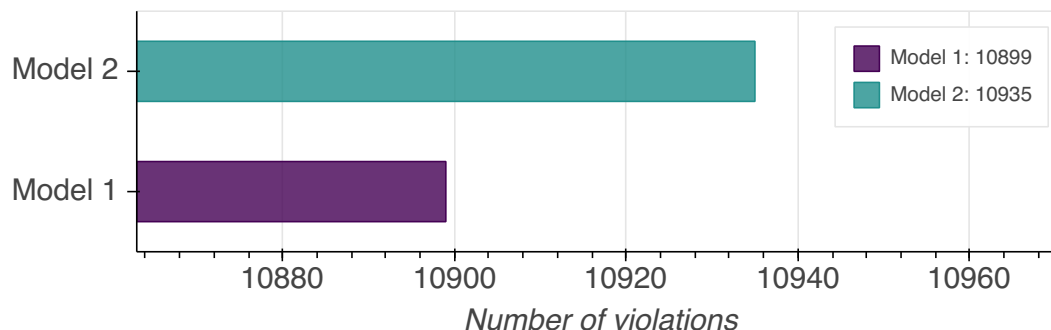
Ensemble information

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

Full wwPDB IM Structure Validation Report