Full RCSB Integrative Structure Validation Report

March 04, 2021 -- 12:11 PM

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

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000020
Molecule Name	Structure of the S. cerevisiae nuclear pore complex cytoplasmic mRNA export platform, Nup82
Title	Structure and Function of the Nuclear Pore Complex Cytoplasmic mRNA Export Platform.
Authors	Fernandez-Martinez J;Kim SJ;Shi Y;Upla P;Pellarin R;Gagnon M;Chemmama IE;Wang J;Nudelman I;Zhang W;Williams R;Rice WJ;Stokes DL;Zenklusen D;Chait BT;Sali A;Rout MP

Overall quality

Model quality: Excluded Volume Analysis
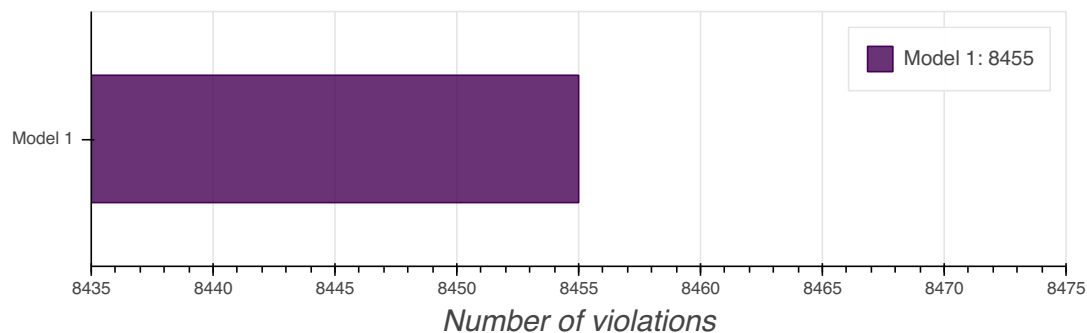
Ensemble information

This entry consists of 1 distinct ensemble.

Entry composition

There is 1 unique type of model in this entry.This model is titled Cluster 0/None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	Dyn2	A	92
1	2	1	Dyn2	B	92
1	3	2	Nup82	C	713
1	4	2	Nup82	D	713
1	5	3	Nup159	E	1460
1	6	3	Nup159	F	1460
1	7	4	Nsp1	G	823
1	8	4	Nsp1	H	823
1	9	5	Nup116	I	1113
1	10	5	Nup116	J	1113

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling

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1	1	Replica exchange monte carlo	Sampling	1000	False	True
2	1	Replica exchange monte carlo	Sampling	1350000	False	True
3	1	Replica exchange monte carlo	Sampling	10000	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	99.84	8455.0

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model