Integrative Structure Validation Report ?

July 22, 2024 - 03:46 PM PDT

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

PDB ID	8ZZK
PDB-Dev ID	PDBDEV_00000020
Structure Title	Structure of the S. cerevisiae nuclear pore complex cytoplasmic mRNA export platform, Nup82
Structure 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 ?

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis

Model 1: 8455(99.84 %)

Number of violations
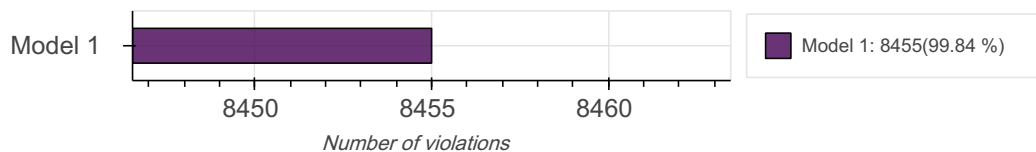
Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 10 subunits in each model. A total of 37 datasets or restraints were used to build this entry. Each model is represented by 38 rigid bodies and 42 flexible or non-rigid units.

Entry composition ?

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

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

Datasets used for modeling ?

There are 37 unique datasets used to build the models in this entry.

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ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4DS1
2	Experimental model	PDB	3PBP
3	Experimental model	PDB	5CWS
4	Comparative model	File	10.5281/zenodo.1256259
5	Comparative model	File	10.5281/zenodo.1256259
6	Comparative model	File	10.5281/zenodo.1256259
7	Comparative model	File	10.5281/zenodo.1256259
8	Comparative model	File	10.5281/zenodo.1256259
9	Comparative model	File	10.5281/zenodo.1256259
10	Experimental model	PDB	1XIP
11	Crosslinking-MS data	File	10.5281/zenodo.1256259
12	Crosslinking-MS data	File	10.5281/zenodo.1256259
13	Crosslinking-MS data	File	10.5281/zenodo.1256259
14	2DEM class average	File	10.5281/zenodo.1256259
15	2DEM class average	File	10.5281/zenodo.1256259
16	2DEM class average	File	10.5281/zenodo.1256259
17	2DEM class average	File	10.5281/zenodo.1256259
18	2DEM class average	File	10.5281/zenodo.1256259
19	2DEM class average	File	10.5281/zenodo.1256259
20	2DEM class average	File	10.5281/zenodo.1256259
21	2DEM class average	File	10.5281/zenodo.1256259
22	2DEM class average	File	10.5281/zenodo.1256259
23	2DEM class average	File	10.5281/zenodo.1256259

ID	Dataset type	Database name	Data access code
24	2DEM class average	File	10.5281/zenodo.1256259
25	2DEM class average	File	10.5281/zenodo.1256259
26	2DEM class average	File	10.5281/zenodo.1256259
27	2DEM class average	File	10.5281/zenodo.1256259
28	2DEM class average	File	10.5281/zenodo.1256259
29	2DEM class average	File	10.5281/zenodo.1256259
30	2DEM class average	File	10.5281/zenodo.1256259
31	2DEM class average	File	10.5281/zenodo.1256259
32	2DEM class average	File	10.5281/zenodo.1256259
33	2DEM class average	File	10.5281/zenodo.1256259
34	2DEM class average	File	10.5281/zenodo.1256259
35	SAS data	File	10.5281/zenodo.1256259
36	SAS data	File	10.5281/zenodo.1256259
37	SAS data	File	10.5281/zenodo.1256259

Representation ?

This entry has only one representation and includes 38 rigid bodies and 42 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	7-92	1-6
B	7-92	1-6
C	7-16, 23-120, 123-452, 522-612, 625-669, 678-713	1-6, 17-22, 121-122, 453-521, 613-624, 670-677

Chain ID	Rigid bodies	Non-rigid segments
D	7-16, 23-120, 123-452, 522-612, 625-669, 678-713	1-6, 17-22, 121-122, 453-521, 613-624, 670-677
E	2-347, 362-381, 1117-1126, 1211-1239, 1266-1321, 1332-1372, 1382-1412, 1429-1456	1-1, 348-361, 382-1116, 1127-1210, 1240-1265, 1322-1331, 1373-1381, 1413-1428, 1457-1460
F	2-347, 362-381, 1117-1126, 1211-1239, 1266-1321, 1332-1372, 1382-1412, 1429-1456	1-1, 348-361, 382-1116, 1127-1210, 1240-1265, 1322-1331, 1373-1381, 1413-1428, 1457-1460
G	637-727, 742-778, 788-823	1-636, 728-741, 779-787
H	637-727, 742-778, 788-823	1-636, 728-741, 779-787
I	966-1111	1-965, 1112-1113
J	966-1111	1-965, 1112-1113

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	1000	False	True
2	1	Replica exchange monte carlo	Sampling	None	1350000	False	True
3	1	Replica exchange monte carlo	Sampling	None	10000	False	True

There are 9 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.org
3	HHpred	2.0.16	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred
4	PSIPRED	4.0	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
5	DISOPRED	3	disorder prediction	http://bioinf.cs.ucl.ac.uk/psipred/?disopred=1
6	DomPred	Not available	domain prediction	http://bioinf.cs.ucl.ac.uk/psipred/?dompred=1
7	COILS/PCOILS	Not available	coiled-coil prediction	https://toolkit.tuebingen.mpg.de/pcoils
8	Multicoil2	Not available	coiled-coil prediction	http://groups.csail.mit.edu/cb/multicoil2/cgi-bin/multicoil2.cgi
9	MODELLER	9.15	comparative modeling	https://salilab.org/modeller/

Data quality ?

2DEM class average

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

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 ?

2DEM class average

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.