

Integrative Structure Validation Report ?

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

PDB ID	9A3S
PDB-Dev ID	PDBDEV_00000213
Structure Title	Implications of a multiscale structure of the yeast Nuclear Pore Complex
Structure Authors	Akey, C.A.; Echeverria, I.; Ouch, C.; Nudelman, I.; Shi, Y.; Wang, J.; Weiss, T.M.; Chait, B.T.; Sali, A.; Fernandez-Martinez, J.; Rout, M.P.

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

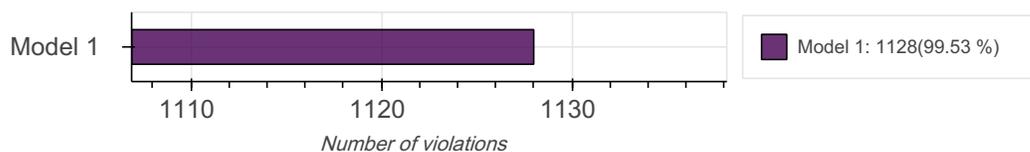
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

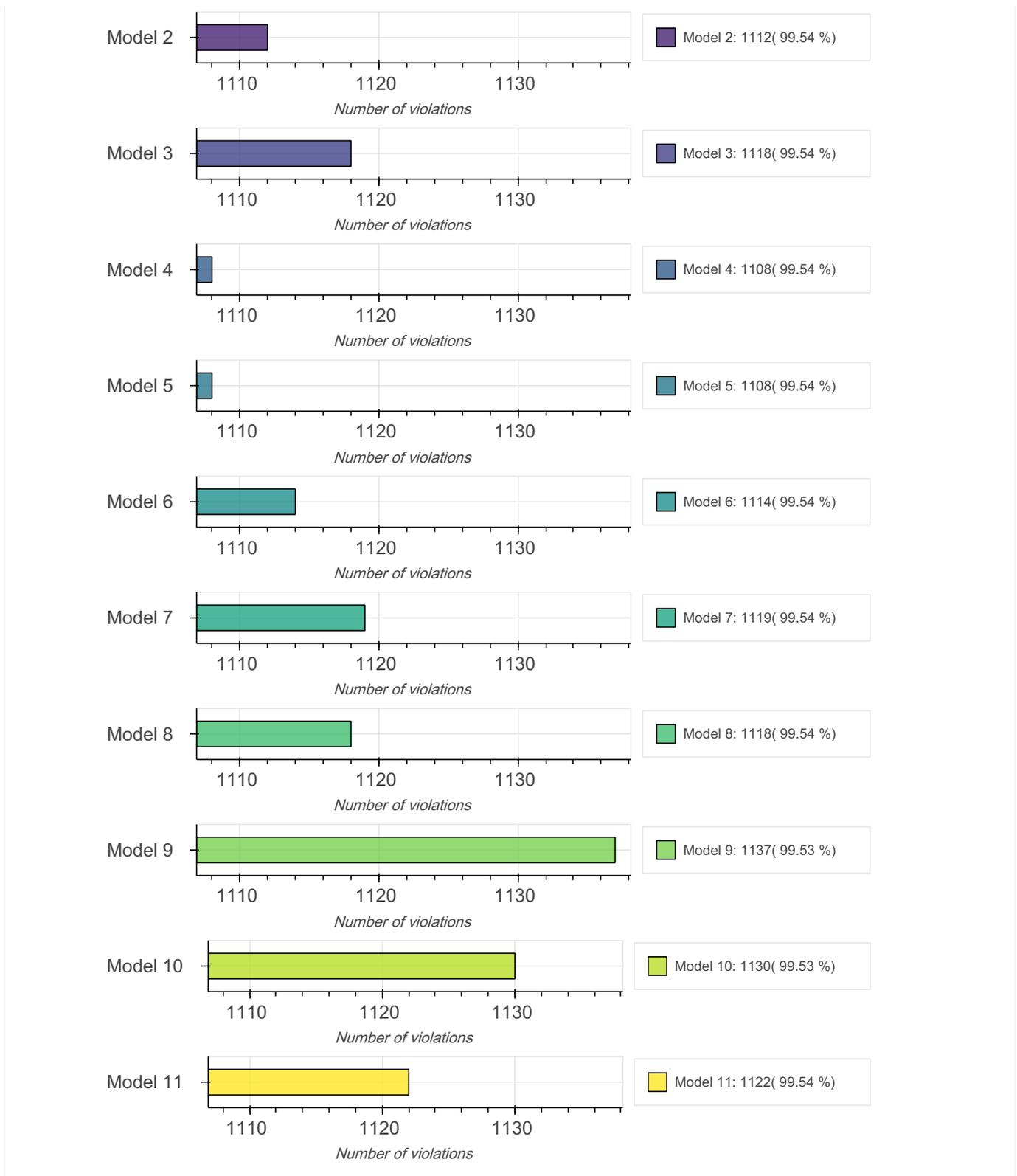
List of references used to build this report is available [here](#).

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





Ensemble information

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 11 unique models, with 4 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 16 rigid bodies and 20 flexible or non-rigid units.

Entry composition ?

There are 11 unique types of models in this entry. These models are titled None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Nucleoporin POM152	A	A	1337
1	2	1	Nucleoporin POM152	B	B	1337
1	3	2	Nucleoporin POM34	C	C	299
1	4	2	Nucleoporin POM34	D	D	299
2	1	1	Nucleoporin POM152	A	A	1337
2	2	1	Nucleoporin POM152	B	B	1337
2	3	2	Nucleoporin POM34	C	C	299
2	4	2	Nucleoporin POM34	D	D	299
3	1	1	Nucleoporin POM152	A	A	1337
3	2	1	Nucleoporin POM152	B	B	1337
3	3	2	Nucleoporin POM34	C	C	299

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	4	2	Nucleoporin POM34	D	D	299
4	1	1	Nucleoporin POM152	A	A	1337
4	2	1	Nucleoporin POM152	B	B	1337
4	3	2	Nucleoporin POM34	C	C	299
4	4	2	Nucleoporin POM34	D	D	299
5	1	1	Nucleoporin POM152	A	A	1337
5	2	1	Nucleoporin POM152	B	B	1337
5	3	2	Nucleoporin POM34	C	C	299
5	4	2	Nucleoporin POM34	D	D	299
6	1	1	Nucleoporin POM152	A	A	1337
6	2	1	Nucleoporin POM152	B	B	1337
6	3	2	Nucleoporin POM34	C	C	299
6	4	2	Nucleoporin POM34	D	D	299
7	1	1	Nucleoporin POM152	A	A	1337
7	2	1	Nucleoporin POM152	B	B	1337

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
7	3	2	Nucleoporin POM34	C	C	299
7	4	2	Nucleoporin POM34	D	D	299
8	1	1	Nucleoporin POM152	A	A	1337
8	2	1	Nucleoporin POM152	B	B	1337
8	3	2	Nucleoporin POM34	C	C	299
8	4	2	Nucleoporin POM34	D	D	299
9	1	1	Nucleoporin POM152	A	A	1337
9	2	1	Nucleoporin POM152	B	B	1337
9	3	2	Nucleoporin POM34	C	C	299
9	4	2	Nucleoporin POM34	D	D	299
10	1	1	Nucleoporin POM152	A	A	1337
10	2	1	Nucleoporin POM152	B	B	1337
10	3	2	Nucleoporin POM34	C	C	299
10	4	2	Nucleoporin POM34	D	D	299
11	1	1	Nucleoporin POM152	A	A	1337

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
11	2	1	Nucleoporin POM152	B	B	1337
11	3	2	Nucleoporin POM34	C	C	299
11	4	2	Nucleoporin POM34	D	D	299

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	3DEM volume	File	10.5281/zenodo.8226857
3	Crosslinking-MS data	File	10.5281/zenodo.8226857
4	De Novo model	AlphaFoldDB	AF-P39685-F1
5	De Novo model	AlphaFoldDB	AF-Q12445-F1
1	3DEM volume	EMDB	EMD-41117

Representation

This entry has only one representation and includes 16 rigid bodies and 20 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	105-130, 144-167, 176-192, 200-212	1-104, 131-143, 168-175, 193-199, 213-250
B	105-130, 144-167, 176-192, 200-212	1-104, 131-143, 168-175, 193-199, 213-250
C	44-86, 89-110, 122-150, 222-237	1-43, 87-88, 111-121, 151-221, 238-250
D	44-86, 89-110, 122-150, 222-237	1-43, 87-88, 111-121, 151-221, 238-250

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	6400000	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaFold2	Not available	structure prediction	https://alphafold.ebi.ac.uk/
2	IMP PMI module	20230908.develop.a93cf91143	integrative model building	https://integrativemodeling.org
3	Integrative Modeling Platform (IMP)	20230908.develop.a93cf91143	integrative model building	https://integrativemodeling.org

Data quality ?

3DEM volume

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobtity 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
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Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.53	1128.0
2	99.54	1112.0
3	99.54	1118.0
4	99.54	1108.0
5	99.54	1108.0
6	99.54	1114.0
7	99.54	1119.0
8	99.54	1118.0
9	99.53	1137.0
10	99.53	1130.0
11	99.54	1122.0

Fit of model to data used for modeling ?

3DEM volume

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.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-

2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.

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