

Integrative Structure Validation Report ?

February 18, 2025 - 08:37 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

PyMOL Version 2.5.0

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.
Deposited on	2023-08-25

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

We welcome your comments at helpdesk@pdb-ihm.org

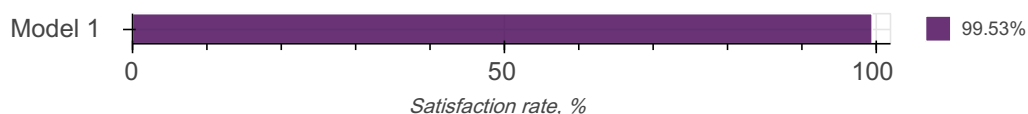
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

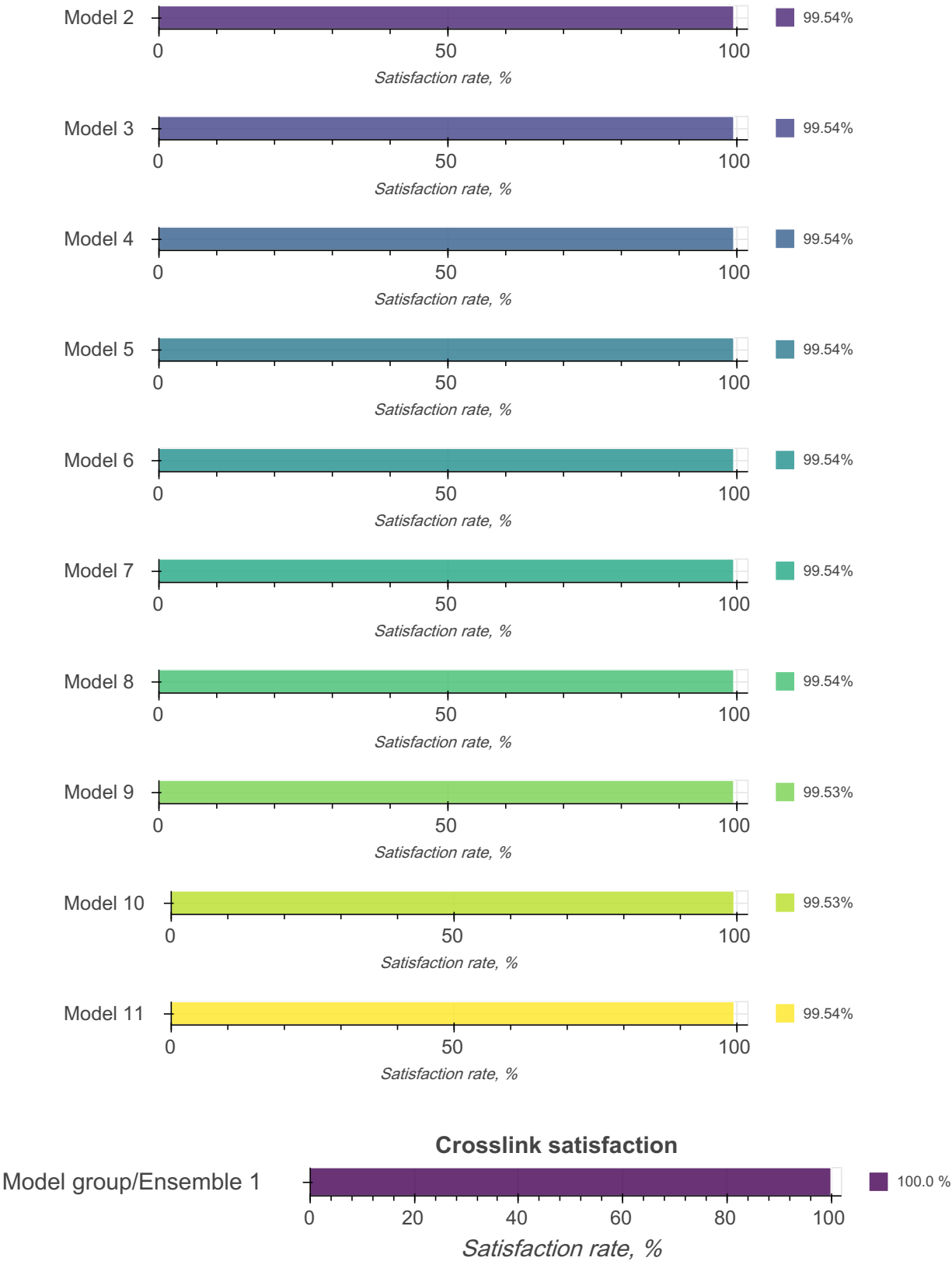
List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS 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 model(s). A total of 5 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-11	1	Nucleoporin POM152	A	1337	105-130, 144-167, 176-192, 200-212	1-104, 131-143, 168-175, 193-199, 213-250	18.70 / 32.00	Multiscale: Coarse-grained: 1 - 2 residue(s) per bead
				B					
		2	Nucleoporin POM34	C	299	44-86, 89-110, 122-150, 222-237	1-43, 87-88, 111-121, 151-221, 238-250	83.61 / 44.00	Multiscale: Coarse-grained: 1 - 2 residue(s) per bead
				D					

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	Zenodo	10.5281/zenodo.8226857
3	Crosslinking-MS data	Zenodo	10.5281/zenodo.8226857
4	De Novo model	Zenodo	10.5281/zenodo.8226857
5	De Novo model	Zenodo	10.5281/zenodo.8226857
1	3DEM volume	EMDB	EMD-41117

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	Sampling	Replica exchange monte carlo	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 ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

3DEM volume

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. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

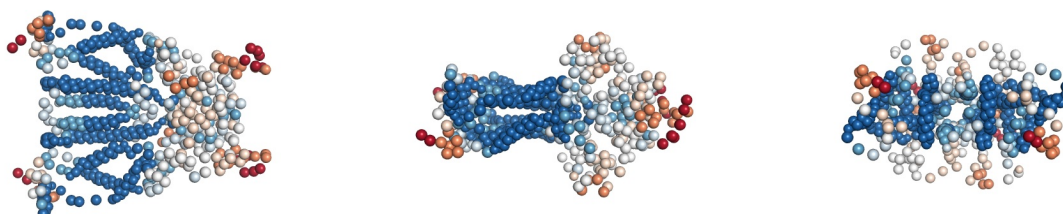
Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	241860	1128	99.53
2	241860	1112	99.54

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
3	241860	1118	99.54
4	241860	1108	99.54
5	241860	1108	99.54
6	241860	1114	99.54
7	241860	1119	99.54
8	241860	1118	99.54
9	241860	1137	99.53
10	241860	1130	99.53
11	241860	1122	99.54

PrISM precision analysis ?

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated.

PrISM analysis for Ensemble 1 (models deposited/total: 11/11).



Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

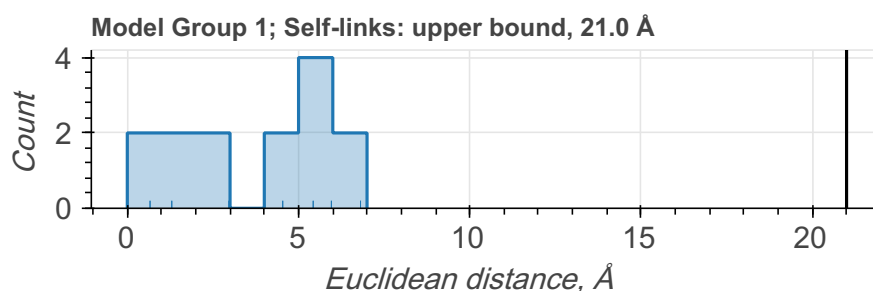
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". **Restraint group** represents a set of crosslinking restraints applied collectively in the modeling.

There are 14 crosslinking restraints combined in 4 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	coarse-grained	LYS	coarse-grained	upper bound	21.0	14

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



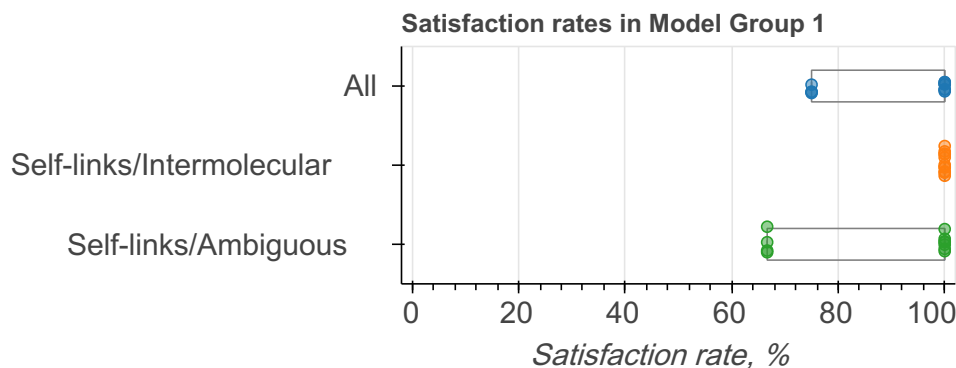
Satisfaction of restraints

Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=4)
1	1	1	11/11	All	100.00	0.00	4
				Self-links/Intermolecular	100.00	0.00	1
				Self-links/Ambiguous	100.00	0.00	3

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The 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 awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

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