

Integrative Structure Validation Report ?

March 27, 2025 - 10:05 AM PDT

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

PDB ID	9A1P
PDB-Dev ID	PDBDEV_00000097
Structure Title	Comprehensive structure and functional adaptations of the yeast nuclear pore complex
Structure Authors	Akey CW; Singh D; Ouch C; Echeverria I; Nudelman I; Varberg JM; Yu Z; Fang F; Shi Y; Wang J; Salzberg D; Song K; Xu C; Gumbart JC; Suslov S; Unruh J; Jaspersen SL; Chait BT; Sali A; Fernandez-Martinez J; Ludtke SJ; Villa E; Rout MP
Deposited on	2021-11-19

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

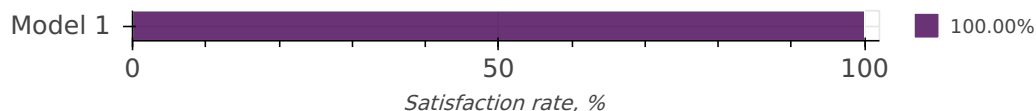
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

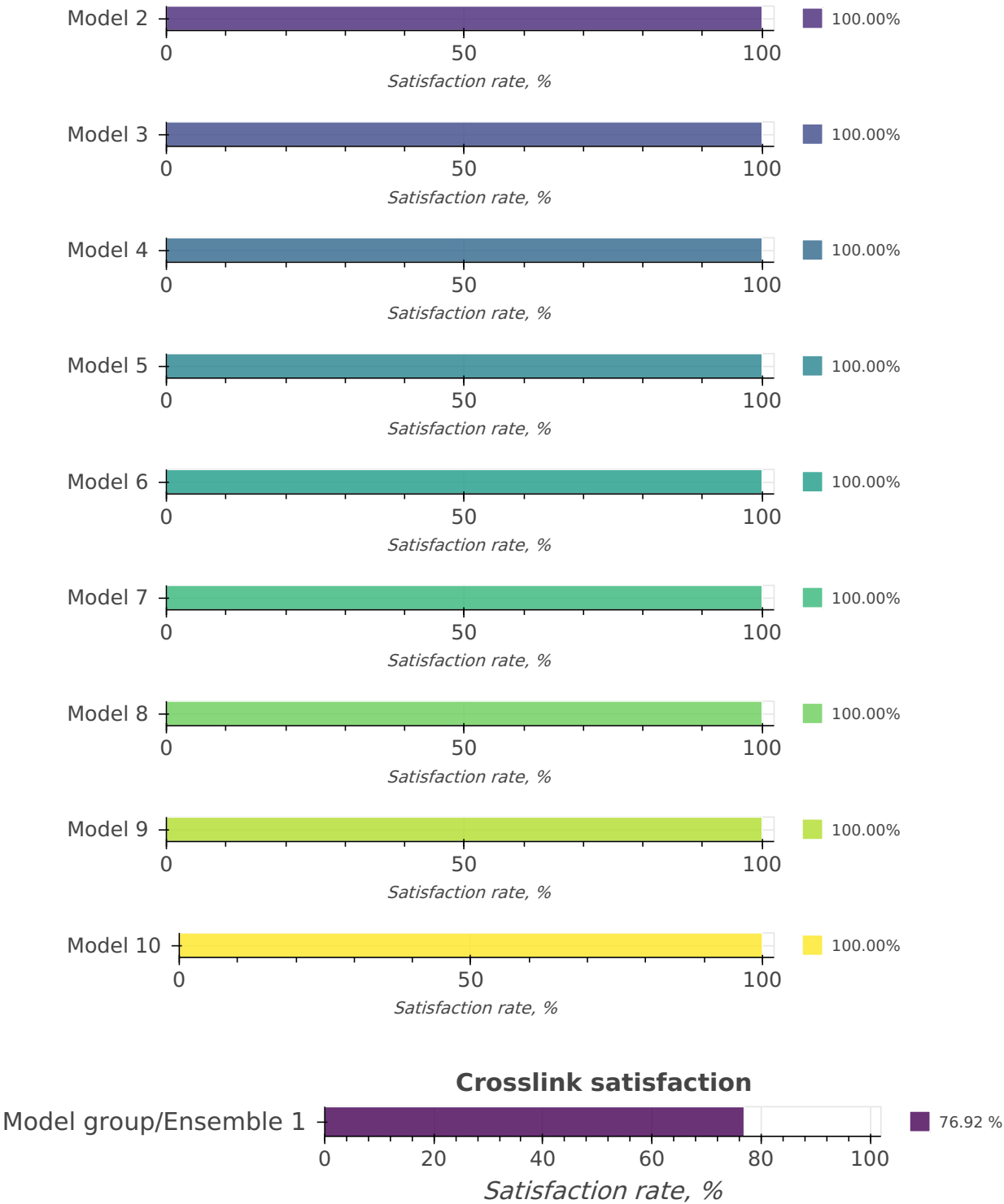
List of references used to build this report is available [here](#).

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 10 model(s). A total of 3 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	1-10	2	Nup170	0	1502	1-1502	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				Y					
		1	Nup157	1	1391	1-1391	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				Z					
		5	Nsp1	A	823	1-823	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				D					
				G					
				J					
		6	Nup57	B	541	1-541	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				E					
				H					
				K					
		7	Nup49	C	472	1-472	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				F					
				I					
				L					
		9	Nup192	M	1683	1-1683	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				O					
		8	Nup188	N	1655	1-1655	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				P					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		10	Nic96	Q	839	1-839	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				R					
				S					
				T					
		3	Nup53	U	475	1-475	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				W					
		4	Nup59	V	528	1-528	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				X					

Datasets used for modeling ?

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	Zenodo	10.5281/zenodo.5662389
2	3DEM volume	EMDB	EMD-24232
3	Experimental model	PDB	7N85

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	Production sampling	Enumeration	None	1200	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	PSIPRED	4.00	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
2	Integrative Modeling Platform (IMP)	2.20	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	7541209455	124879	100.00
2	7541209455	124879	100.00
3	7541209455	124879	100.00
4	7541209455	124879	100.00
5	7541209455	124879	100.00
6	7541209455	124879	100.00
7	7541209455	124879	100.00

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
8	7541209455	124879	100.00
9	7541209455	124879	100.00
10	7541209455	124879	100.00

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

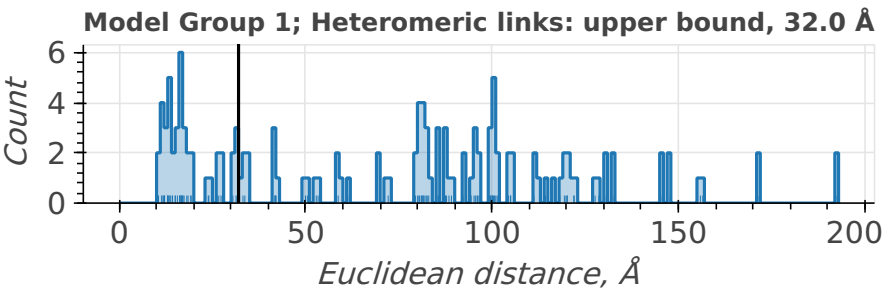
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

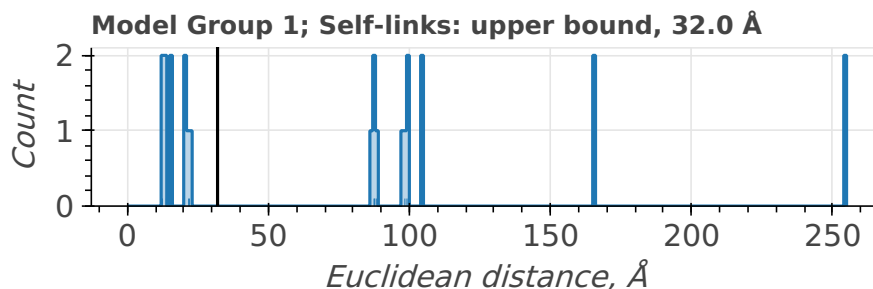
There are 1284 crosslinking restraints combined in 114 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	ALA	CA	LYS	CA	upper bound	32.0	692
DSS	LYS	CA	LYS	CA	upper bound	32.0	512
DSS	ALA	CA	ALA	CA	upper bound	32.0	80

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.





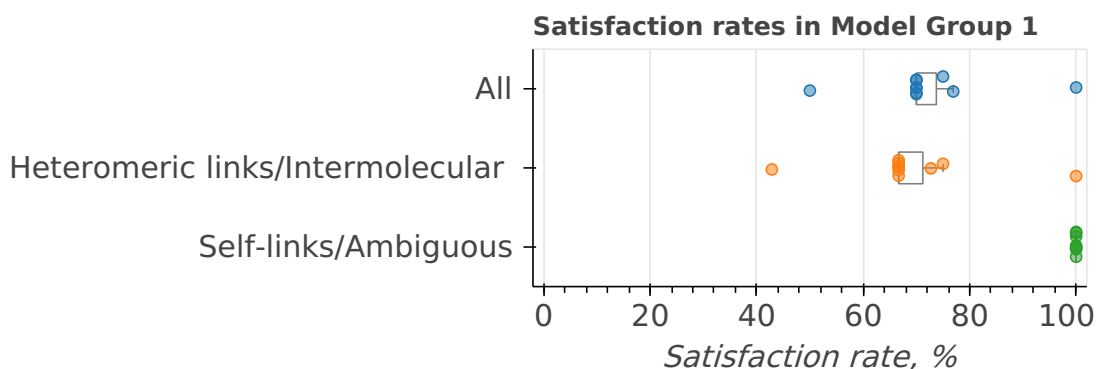
Satisfaction of restraints

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=114)
1	1	1	10/10	All	76.92	23.08	13
				Heteromeric links/ Intermolecular	72.73	27.27	11
				Self-links/ Ambiguous	100.00	0.00	2

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

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