

Integrative Structure Validation Report ?

February 18, 2025 - 08:46 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

PDB ID	9A8K
PDB-Dev ID	PDBDEV_00000384
Structure Title	Modeling of Mouse NPC basket
Structure Authors	Singh, D.; Soni, N.; Hutchings, J.; Echeverria, I.; Shaikh, F.; Duquette, M.; Suslov, S.; Li, Z.; van Eeuwen, T.; Molloy, K.; Shi, Y.; Wang, J.; Guo, Q.; Chait, B.T.; Fernandez-Martinez, J.; Rout, M.P.; Sali, A.; Villa, E.
Deposited on	2024-06-27

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

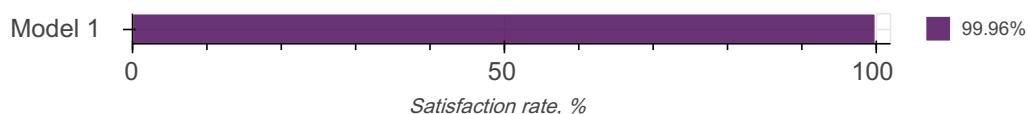
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

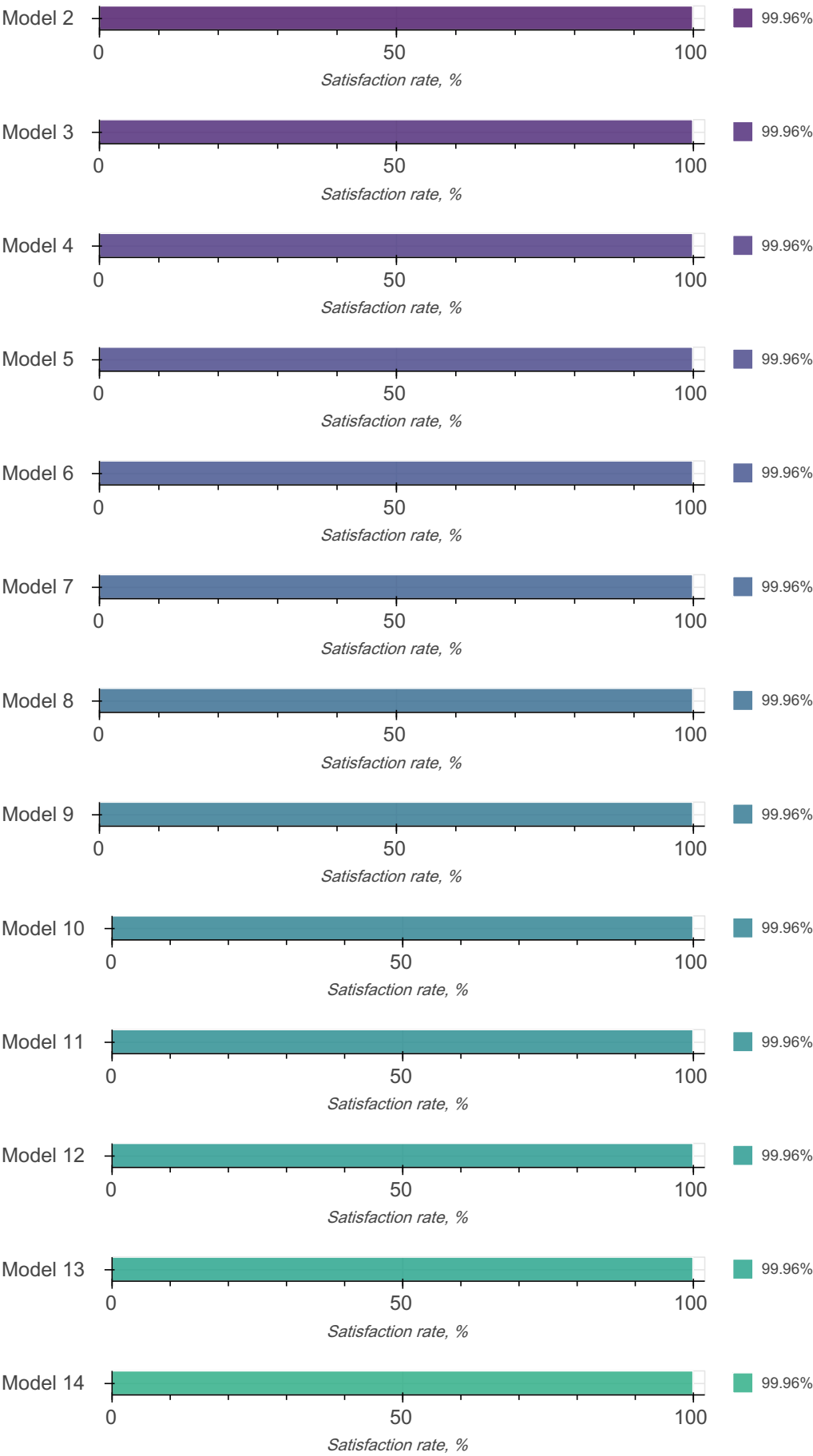
List of references used to build this report is available [here](#).

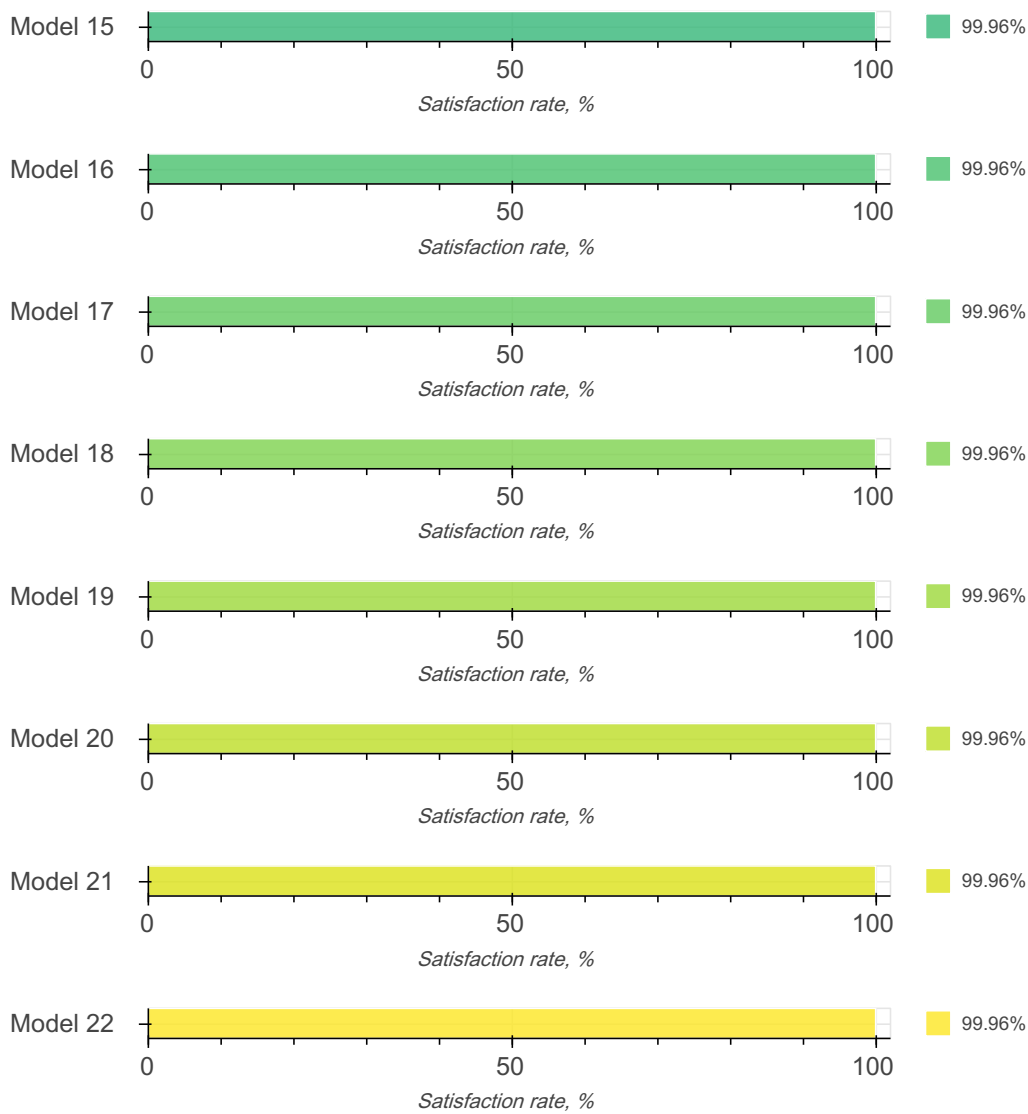
Overall quality ?

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 22 model(s). A total of 6 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	1-22	1	Nucleoprotein TPR	A	2431	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431	100.00 / 51.79	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				B					
		2	Nuclear pore complex protein Nup50	C	466	151-204, 355-466	1-150, 205-354	100.00 / 35.62	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				D					
		3	Nucleoporin 153	E	1462	36-57	1-35, 58-428, 540-574	31.67 / 4.75	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				F					
		4	Nuclear pore complex protein Nup160	G	1402	1-1402	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				H					
		5	Nuclear pore complex protein Nup85	I	656	1-656	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				J					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		6	Nuclear pore complex protein Nup98-Nup96	K	1816	1111-1159, 1194-1816	-	37.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				L					
		7	Protein SEC13 homolog	M	322	1-302	-	93.79 / 100.00	Coarse-grained: 1 residue(s) per bead
				N					
		8	Nucleoporin SEH1	O	360	1-324	-	90.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				P					
		9	Nuclear pore complex protein Nup107	Q	926	145-926	-	84.45 / 100.00	Coarse-grained: 1 residue(s) per bead
				R					
		10	Nuclear pore complex protein Nup133	S	1155	70-1155	-	94.03 / 100.00	Coarse-grained: 1 residue(s) per bead
				T					
		11	Nucleoporin Nup37	U	326	1-326	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				V					
		12	Nucleoporin Nup43	W	380	1-292, 327-380	-	91.05 / 100.00	Coarse-grained: 1 residue(s) per bead
				X					

Datasets used for modeling ?

There are 6 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
6	3DEM volume	Zenodo	10.5281/zenodo.13131753
1	De Novo model	Zenodo	10.5281/zenodo.13131753
3	Comparative model	Zenodo	10.5281/zenodo.13131753

ID	Dataset type	Database name	Data access code
5	3DEM volume	Zenodo	10.5281/zenodo.13131753
2	Experimental model	PDB	7r5j
4	3DEM volume	EMDB	EMD-44379

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	500	False	True
2	1	Sampling	Replica exchange monte carlo	None	9569309	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.19.0	integrative model building	https://integrativemodeling.org
3	COCONUT	1.0.0	Coiled-coil model building	https://github.com/neeleshsoni21/COCONUT
2	Integrative Modeling Platform (IMP)	2.18.0	integrative model building	https://integrativemodeling.org

Data quality ?

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	109868076	39412	99.96
2	109868076	39409	99.96
3	109868076	39694	99.96
4	109868076	39195	99.96
5	109868076	39325	99.96
6	109868076	39716	99.96
7	109868076	39884	99.96
8	109868076	39444	99.96
9	109868076	39381	99.96
10	109868076	39327	99.96
11	109868076	39609	99.96
12	109868076	39418	99.96
13	109868076	39437	99.96
14	109868076	39295	99.96
15	109868076	39387	99.96
16	109868076	39399	99.96
17	109868076	39414	99.96
18	109868076	39381	99.96
19	109868076	39123	99.96
20	109868076	39195	99.96
21	109868076	39336	99.96
22	109868076	39412	99.96

Fit of model to data used for modeling ?

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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