

# 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	9A8L
PDB-Dev ID	PDBDEV_00000385
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	2024-07-02

*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](mailto:helpdesk@pdb-ihm.org)*

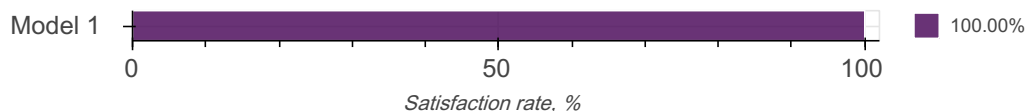
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 1 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	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					
				C					
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					
				L					
				M					
				N					
				O					
				P					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	Nuclear pore complex protein Nup50	Q	466	151-204, 355-466	1-150, 205-354	100.00 / 35.62	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				R					
				S					
				T					
				U					
				V					
				W					
				X					
				Y					
				Z					
				AA					
				AB					
				AC					
				AD					
				AE					
				AF					
		3	Nucleoporin 153	AG	1462	36-57	1-35, 58-428, 540-574	31.67 / 4.75	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				AH					
				AI					
				AJ					
				AK					
				AL					
				AM					
				AN					
				AO					
				AP					
				AQ					
				AR					
				AS					
				AT					
				AU					
				AV					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	Nuclear pore complex protein Nup160	AW	1402	1-1402	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				AX					
				AY					
				AZ					
				BA					
				BB					
				BC					
				BD					
				BE					
				BF					
				BG					
				BH					
				BI					
				BJ					
				BK					
				BL					
		5	Nuclear pore complex protein Nup85	BM	656	1-656	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				BN					
				BO					
				BP					
				BQ					
				BR					
				BS					
				BT					
				BU					
				BV					
				BW					
				BX					
				BY					
				BZ					
				CA					
				CB					

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	CC	1816	1111-1159, 1194-1816	-	37.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				CD					
				CE					
				CF					
				CG					
				CH					
				CI					
				CJ					
				CK					
				CL					
				CM					
				CN					
				CO					
				CP					
				CQ					
				CR					
		7	Protein SEC13 homolog	CS	322	1-302	-	93.79 / 100.00	Coarse-grained: 1 residue(s) per bead
				CT					
				CU					
				CV					
				CW					
				CX					
				CY					
				CZ					
				DA					
				DB					
				DC					
				DD					
				DE					
				DF					
				DG					
				DH					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		8	Nucleoporin SEH1	DI	360	1-324	-	90.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				DJ					
				DK					
				DL					
				DM					
				DN					
				DO					
				DP					
				DQ					
				DR					
				DS					
				DT					
				DU					
				DV					
				DW					
				DX					
		9	Nuclear pore complex protein Nup107	DY	926	145-926	-	84.45 / 100.00	Coarse-grained: 1 residue(s) per bead
				DZ					
				EA					
				EB					
				EC					
				ED					
				EE					
				EF					
				EG					
				EH					
				EI					
				EJ					
				EK					
				EL					
				EM					
				EN					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		10	Nuclear pore complex protein Nup133	EO	1155	70-1155	-	94.03 / 100.00	Coarse-grained: 1 residue(s) per bead
				EP					
				EQ					
				ER					
				ES					
				ET					
				EU					
				EV					
				EW					
				EX					
				EY					
				EZ					
				FA					
				FB					
				FC					
				FD					
		11	Nucleoporin Nup37	FE	326	1-326	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
				FF					
				FG					
				FH					
				FI					
				FJ					
				FK					
				FL					
				FM					
				FN					
				FO					
				FP					
				FQ					
				FR					
				FS					
				FT					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		12	Nucleoporin Nup43	FU	380	1-292, 327-380	-	91.05 / 100.00	Coarse-grained: 1 residue(s) per bead
				FV					
				FW					
				FX					
				FY					
				FZ					
				GA					
				GB					
				GC					
				GD					
				GE					
				GF					
				GG					
				GH					
				GI					
				GJ					

### 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
1	De Novo model	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.13131753">10.5281/zenodo.13131753</a>
3	Comparative model	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.13131753">10.5281/zenodo.13131753</a>
5	3DEM volume	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.13131753">10.5281/zenodo.13131753</a>
6	3DEM volume	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.13131753">10.5281/zenodo.13131753</a>
2	Experimental model	PDB	<a href="https://www.rcsb.org/structure/7r5j">7r5j</a>
4	3DEM volume	EMDB	<a href="https://www.ebi.ac.uk/emdb/EMD-44379">EMD-44379</a>

### 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	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
3	COCONUT	1.0.0	Coiled-coil model building	<a href="https://github.com/neeleshsoni21/COCONUT">https://github.com/neeleshsoni21/COCONUT</a>
2	Integrative Modeling Platform (IMP)	2.19.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>

## 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	7031971936	316896	100.00

## 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.

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### *Acknowledgments*

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*Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.*

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