

Integrative Structure Validation Report ?

March 13, 2025 - 12:43 PM 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	9A8N
PDB-Dev ID	PDBDEV_00000387
Structure Title	Modeling of Yeast 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	2024-07-07

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

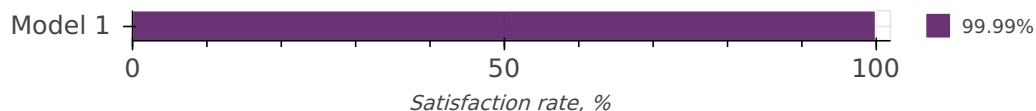
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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

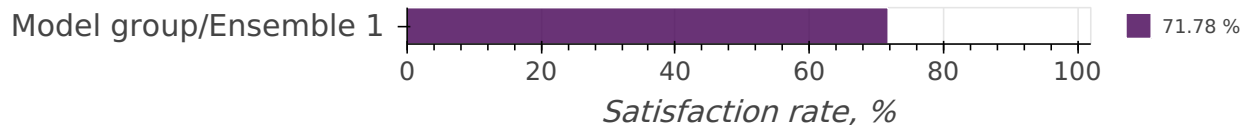
Overall quality ?

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



Crosslink satisfaction



Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 11 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

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	Unknown MLP Protein	A	1875	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875	100.00 / 54.99	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				B					
				C					
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					
				L					
				M					
				N					
				O					
				P					
		2	Nucleoporin NUP1	Q	1076	1-32, 85-104, 106-123	33-84, 105, 124-335	31.13 / 20.90	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				R					
				S					
				T					
				U					
				V					
				W					
				X					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		3	Nucleoporin NUP2	Y	720	83-136, 602-720	1-82, 137-601	100.00 / 24.03	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				Z					
				AA					
				AB					
				AC					
				AD					
				AE					
				AF					
				AG					
				AH					
				AI					
				AJ					
				AK					
				AL					
				AM					
				AN					
		4	Nucleoporin NUP60	AO	539	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105, 120, 141, 163-398, 505-539	80.33 / 20.79	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				AP					
				AQ					
				AR					
				AS					
				AT					
				AU					
				AV					
				AW					
				AX					
				AY					
				AZ					
				BA					
				BB					
				BC					
				BD					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		5	Nucleoporin NUP120	BE	1037	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037	100.00 / 97.01	Multiscale: Coarse-grained: 1 - 23 residue(s) per bead
				BF					
				BG					
				BH					
				BI					
				BJ					
				BK					
				BL					
				BM					
				BN					
				BO					
				BP					
				BQ					
				BR					
				BS					
				BT					
		6	Nucleoporin NUP85	BU	744	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450	100.00 / 90.73	Multiscale: Coarse-grained: 1 - 46 residue(s) per bead
				BW					
				BY					
				CA					
				CC					
				CE					
				CG					
				CI					
		6	Nucleoporin NUP85	BV	744	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744	100.00 / 90.05	Multiscale: Coarse-grained: 1 - 46 residue(s) per bead
				BX					
				BZ					
				CB					
				CD					
				CF					
				CH					
				CJ					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		7	Nucleoporin NUP145C	CK	712	119-712	1-118	100.00 / 83.43	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				CL					
				CM					
				CN					
				CO					
				CP					
				CQ					
				CR					
				CS					
				CT					
				CU					
				CV					
				CW					
				CX					
				CY					
				CZ					
		8	Protein transport protein SEC13	DA	297	8-157, 170-293	1-7, 158-169, 294-297	100.00 / 92.26	Multiscale: Coarse-grained: 1 - 12 residue(s) per bead
				DB					
				DC					
				DD					
				DE					
				DF					
				DG					
				DH					
				DI					
				DJ					
				DK					
				DL					
				DM					
				DN					
				DO					
				DP					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		9	Nucleoporin SEH1	DQ	349	1-248, 288-346	249-287, 347-349	100.00 / 87.97	Multiscale: Coarse-grained: 1 - 39 residue(s) per bead
				DR					
				DS					
				DT					
				DU					
				DV					
				DW					
				DX					
				DY					
				DZ					
				EA					
				EB					
				EC					
				ED					
				EE					
				EF					
		10	Nucleoporin NUP84	EG	726	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574	100.00 / 89.39	Multiscale: Coarse-grained: 1 - 22 residue(s) per bead
				EH					
				EI					
				EJ					
				EK					
				EL					
				EM					
				EN					
				EO					
				EP					
				EQ					
				ER					
				ES					
				ET					
				EU					
				EV					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		11	Nucleoporin NUP133	EW	1157	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157	100.00 / 91.79	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				EY					
				FA					
				FC					
				FE					
				FG					
				FI					
				FK					
		11	Nucleoporin NUP133	EX	1157	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157	100.00 / 89.02	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
				EZ					
				FB					
				FD					
				FF					
				FH					
				FJ					
				FL					

Datasets used for modeling ?

There are 11 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
7	Crosslinking-MS data	Zenodo	10.5281/zenodo.13131753
8	Crosslinking-MS data	Zenodo	10.5281/zenodo.13131753
1	De Novo model	Zenodo	10.5281/zenodo.13131753
2	De Novo model	Zenodo	10.5281/zenodo.13131753
3	De Novo model	Zenodo	10.5281/zenodo.13131753
4	De Novo model	Zenodo	10.5281/zenodo.13131753
6	Experimental model	Zenodo	10.5281/zenodo.13131753
10	3DEM volume	Zenodo	10.5281/zenodo.13131753
11	3DEM volume	Zenodo	10.5281/zenodo.13131753
5	Experimental model	PDB	7N84

ID	Dataset type	Database name	Data access code
9	3DEM volume	EMDB	EMD-44377

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	1000	False	True
2	1	Sampling	Replica exchange monte carlo	None	15467933	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)	2.19.0	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	4672689456	234504	99.99

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.

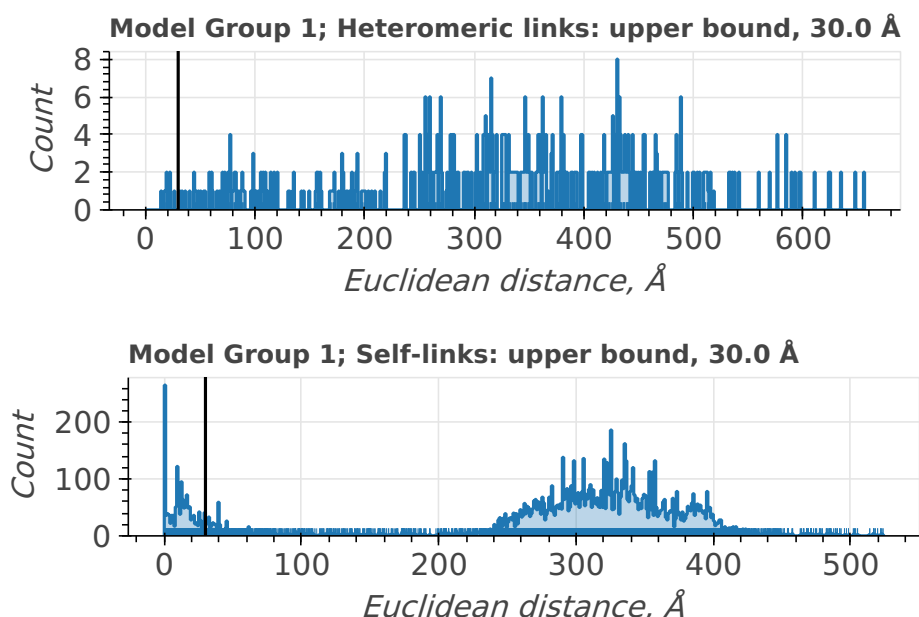
There are 12843 crosslinking restraints combined in 652 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	UNK	CA	UNK	CA	upper bound	30.0	4858
DSS	UNK	coarse-grained	UNK	coarse-grained	upper bound	30.0	6232
DSS	LYS	coarse-grained	UNK	coarse-grained	upper bound	30.0	190
DSS	LYS	CA	UNK	CA	upper bound	30.0	80
DSS	LYS	coarse-grained	LYS	coarse-grained	upper bound	30.0	1185
DSS	LYS	CA	LYS	CA	upper bound	30.0	198
DSS	HIS	coarse-grained	LYS	coarse-grained	upper bound	30.0	20
DSS	THR	coarse-grained	UNK	coarse-grained	upper bound	30.0	40
DSS	LYS	coarse-grained	THR	coarse-grained	upper bound	30.0	20

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	coarse-grained	MET	coarse-grained	upper bound	30.0	20

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.



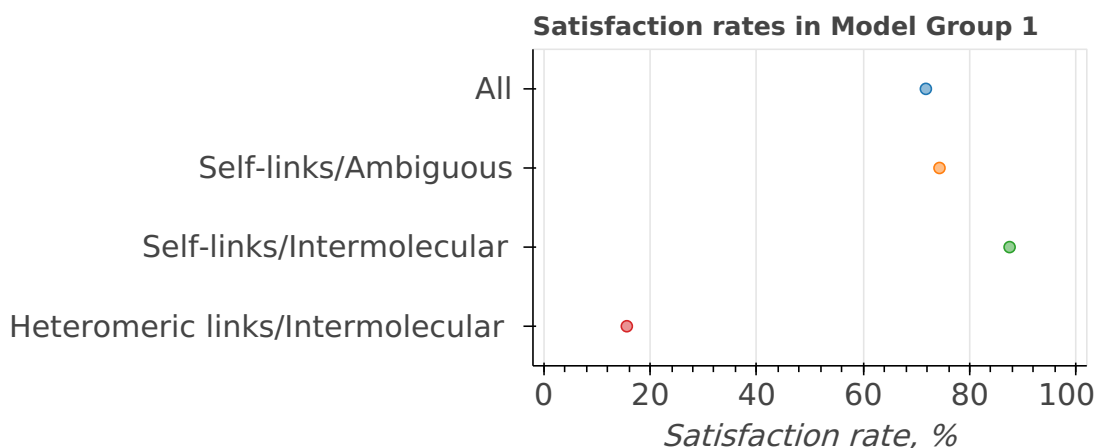
Satisfaction of restraints

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=652)
1	1	1	1/1	All	71.78	28.22	652
				Self-links/ Ambiguous	74.34	25.66	604
				Self-links/ Intermolecular	87.50	12.50	16
				Heteromeric links/ Intermolecular	15.62	84.38	32

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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