

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	9A8U
Structure Title	Integrative structure of the epithelial desmosomal outer plaque
Structure Authors	Pasani, S.; Menon, K.S.; Shruthi, V.; Saltzberg, D.; Greenberg, C.H.; Viswanath, S.; Chemmama, I.; Webb, B.; Pellarin, R.; Echeverria, I.; Sali, A.; Russel, D.; Lasker, K.; Velquez-Muriel, J.; Tjioe, E.; Schneidman-Duhovny, D.; Peterson, B.
Deposited on	2024-08-24

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

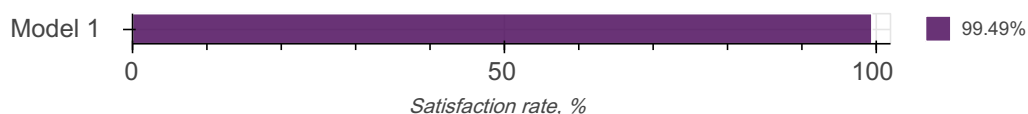
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 1 model(s). A total of 9 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	Plakophilin-1	A	726	-	1-726	100.00 / 100.00	Multiscale: Coarse-grained: 3 - 30 residue(s) per bead
				B					
				C					
				D					
		1	Plakophilin-1	E	726	244-387, 397-480, 509-700	-	57.85 / 100.00	Multiscale: Coarse-grained: 12 - 30 residue(s) per bead
				F					
				G					
		2	Junction plakoglobin	H	745	-	1-745	100.00 / 100.00	Multiscale: Coarse-grained: 2 - 30 residue(s) per bead
				I					
				J					
				K					
		3	Desmoplakin	L	584	-	1-584	100.00 / 100.00	Multiscale: Coarse-grained: 17 - 30 residue(s) per bead
				M					
				N					
				O					
		4	Desmocollin-1	P	180	-	1-180	100.00 / 100.00	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
				Q					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		5	Desmoglein-1	R	273	-	1-273	100.00 / 100.00	Multiscale: Coarse-grained: 8 - 30 residue(s) per bead
				S					

Datasets used for modeling ?

There are 9 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	EMDB	EMD-1703
2	Other	Not available	10.1242/jcs.112.23.4325
4	Comparative model	Zenodo	10.5281/zenodo.8035862
5	Comparative model	Zenodo	10.5281/zenodo.8035862
6	Yeast two-hybrid screening data	Not available	10.1242/jcs.112.23.4325
7	Other	Not available	10.1242/jcs.112.23.4325
3	Experimental model	PDB	3IFQ
8	Experimental model	PDB	1XM9
9	Experimental model	PDB	3R6N

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	2250000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.17.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.17.0	integrative model building	https://integrativemodeling.org

Data quality ?

Yeast two-hybrid screening

Validation for this section is under development.

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	96141	488	99.49

Fit of model to data used for modeling ?

Yeast two-hybrid screening

Validation for this section is under development.

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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