

# Integrative Structure Validation Report

November 26, 2024 - 06:07 PM PST

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

*Python-IHM Version 1.3*

*Integrative Modeling Validation Version 1.2.1*

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.; Velzquez-Muriel, J.; Tjioe, E.; Schneidman-Duhovny, D.; Peterson, B.

*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)*

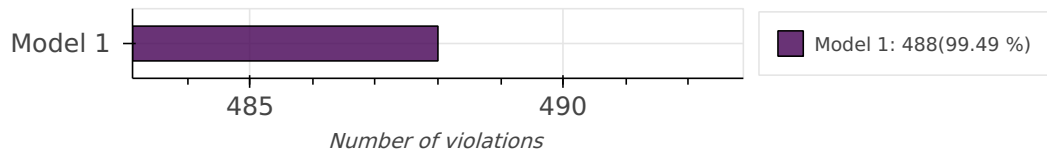
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 19 subunits in each model. A total of 9 datasets or restraints were used to build this entry. Each model is represented by 9 rigid bodies and 16 flexible or non-rigid units.*

## Entry composition ?

*There is 1 unique type of models in this entry. This model is titled Cluster 0/None.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Plakophilin-1	A	A	726
1	2	1	Plakophilin-1	B	B	726
1	3	1	Plakophilin-1	C	C	726
1	4	1	Plakophilin-1	D	D	726
1	5	1	Plakophilin-1	E	E	726
1	6	1	Plakophilin-1	F	F	726
1	7	1	Plakophilin-1	G	G	726
1	8	2	Junction plakoglobin	H	H	745
1	9	2	Junction plakoglobin	I	I	745
1	10	2	Junction plakoglobin	J	J	745

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	11	2	Junction plakoglobin	K	K	745
1	12	3	Desmoplakin	L	L	584
1	13	3	Desmoplakin	M	M	584
1	14	3	Desmoplakin	N	N	584
1	15	3	Desmoplakin	O	O	584
1	16	4	Desmocollin-1	P	P	180
1	17	4	Desmocollin-1	Q	Q	180
1	18	5	Desmoglein-1	R	R	273
1	19	5	Desmoglein-1	S	S	273

### 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	File	10.1242/jcs.112.23.4325
4	Comparative model	File	10.5281/zenodo.8035862
5	Comparative model	File	10.5281/zenodo.8035862
6	Yeast two-hybrid screening data	File	10.1242/jcs.112.23.4325
7	Other	File	10.1242/jcs.112.23.4325
3	Experimental model	PDB	3IFQ
8	Experimental model	PDB	1XM9
9	Experimental model	PDB	3R6N

## Representation ?

*This entry has only one representation and includes 9 rigid bodies and 16 flexible units.*

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-726
B	-	1-726
C	-	1-726
D	-	1-726
E	244-387, 397-480, 509-700	-
F	244-387, 397-480, 509-700	-
G	244-387, 397-480, 509-700	-
H	-	1-745
I	-	1-745
J	-	1-745
K	-	1-745
L	-	1-584
M	-	1-584
N	-	1-584
O	-	1-584
P	-	1-180
Q	-	1-180
R	-	1-273
S	-	1-273

## 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	Replica exchange monte carlo	Sampling	None	2250000	False	True

*There are 2 software packages reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">IMP PMI module</a>	2.17.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
2	<a href="#">Integrative Modeling Platform (IMP)</a>	2.17.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>

## Data quality ?

### 3DEM volume

Validation for this section is under development.

### Yeast two-hybrid screening

Validation for this section is under development.

## Model quality ?

For models with atomic structures, molprobit 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.*

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.49	488.0

### Fit of model to data used for modeling ?

#### 3DEM volume

Validation for this section is under development.

#### Yeast two-hybrid screening

Validation for this section is under development.

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### Fit of model to data used for validation ?

Validation for this section is under development.

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#### *Acknowledgements*

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