

Summary of integrative structure determination of Integrative structure of the epithelial desmosomal outer plaque (PDB ID: 9A8U)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Plakophilin-1: chain(s) A, B, C, D (726 residues) - Plakophilin-1: chain(s) E, F, G (726 residues) - Junction plakoglobin: chain(s) H, I, J, K (745 residues) - Desmoplakin: chain(s) L, M, N, O (584 residues) - Desmocollin-1: chain(s) P, Q (180 residues) - Desmoglein-1: chain(s) R, S (273 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, EMDB: EMD-1703 - Other, Not available: 10.1242/jcs.112.23.4325 - Comparative model, Zenodo: 10.5281/zenodo.8035862 - Comparative model, Zenodo: 10.5281/zenodo.8035862 - Yeast two-hybrid screening data, Not available: 10.1242/jcs.112.23.4325 - Other, Not available: 10.1242/jcs.112.23.4325 - Experimental model, PDB: 3IFQ - Experimental model, PDB: 1XM9 - Experimental model, PDB: 3R6N
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
Number of rigid and flexible segments	9, 16
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
Number of ensembles	1
Number of models in ensembles	24866
Number of deposited models	1
Model precision (uncertainty of models)	67.00, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.49%

<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	2250000
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version 2.17.0) - Integrative Modeling Platform (IMP) (version 2.17.0)