

Summary of integrative structure determination of Equilibrated 52-mer bacterial gasdermin pore model from *Vitiosangium* sp. (PDB ID: 9A85, PDB-Dev ID: PDBDEV_00000370)

1. Model Composition	
Entry composition	Gasdermin bGSMD: chain(s) A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z, AA [a], BA [b], CA [c], DA [d], EA [e], FA [f], GA [g], HA [h], IA [i], JA [j], KA [k], LA [l], MA [m], NA [n], OA [o], PA [p], QA [q], RA [r], SA [s], TA [t], UA [u], VA [v], WA [w], XA [x], YA [y], ZA [z] (234 residues)
Datasets used for modeling	- Experimental model, PDB: 8sl0 - Integrative model, PDB: 9A84
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 52
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 0.95 - Ramachandran outliers: 322 - Sidechain outliers: 367
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined

5. Methodology and Software	
1. <i>Name</i>	None
<i>Description</i>	This model is derivative of PDB 9A84 and the protocol is therefore highly similar. However, this particular model resulted from allowing the PDB 9A84 model to equilibrate in an MD simulation with backbone positions restrained, but the rest was allowed to move such that key features (i.e., the palmitoyl) entered more natural conformations.
<i>Software</i>	<ul style="list-style-type: none">- Python (version v3.9.7)- MDAnalysis (version v2.4.2)- Gromacs (version v2022.4)- Charmm (version Not available)