Summary of integrative structure determination of 52-mer bacterial gasdermin pore model from Vitiosangium sp. (PDB ID: 9A84, PDB-Dev ID: PDBDEV_00000369)

1. Model Composition	
Entry composition	- Gasdermin bGSDM: Chain VA (234 residues) - Gasdermin bGSDM: Chain PA (234 residues) - Gasdermin bGSDM: Chain Y (234 residues) - Gasdermin bGSDM: Chain QA (234 residues) - Gasdermin bGSDM: Chain JA (234 residues) - Gasdermin bGSDM: Chain C (234 residues) - Gasdermin bGSDM: Chain O (234 residues) - Gasdermin bGSDM: Chain V (234 residues) - Gasdermin bGSDM: Chain NA (234 residues) - Gasdermin bGSDM: Chain SA (234 residues) - Gasdermin bGSDM: Chain KA (234 residues) - Gasdermin bGSDM: Chain XA (234 residues) - Gasdermin bGSDM: Chain B (234 residues) - Gasdermin bGSDM: Chain BA (234 residues) - Gasdermin bGSDM: Chain LA (234 residues) - Gasdermin bGSDM: Chain U (234 residues) - Gasdermin bGSDM: Chain AA (234 residues) - Gasdermin bGSDM: Chain TA (234 residues) - Gasdermin bGSDM: Chain N (234 residues) - Gasdermin bGSDM: Chain HA (234 residues) - Gasdermin bGSDM: Chain MA (234 residues) - Gasdermin bGSDM: Chain IA (234 residues) - Gasdermin bGSDM: Chain FA (234 residues) - Gasdermin bGSDM: Chain YA (234 residues) - Gasdermin bGSDM: Chain E (234 residues) - Gasdermin bGSDM: Chain R (234 residues) - Gasdermin bGSDM: Chain ZA (234 residues) - Gasdermin bGSDM: Chain G (234 residues) - Gasdermin bGSDM: Chain CA (234 residues) - Gasdermin bGSDM: Chain Q (234 residues) - Gasdermin bGSDM: Chain M (234 residues) - Gasdermin bGSDM: Chain UA (234 residues) - Gasdermin bGSDM: Chain GA (234 residues) - Gasdermin bGSDM: Chain X (234 residues) - Gasdermin bGSDM: Chain Z (234 residues) - Gasdermin bGSDM: Chain D (234 residues) - Gasdermin bGSDM: Chain K (234 residues) - Gasdermin bGSDM: Chain DA (234 residues) - Gasdermin bGSDM: Chain P (234 residues) - Gasdermin bGSDM: Chain EA (234 residues) - Gasdermin bGSDM: Chain OA (234 residues) - Gasdermin bGSDM: Chain WA (234 residues) - Gasdermin bGSDM: Chain L (234 residues) - Gasdermin bGSDM: Chain T (234 residues) - Gasdermin bGSDM: Chain H (234 residues) - Gasdermin bGSDM: Chain F (234 residues) - Gasdermin bGSDM: Chain I (234 residues) - Gasdermin bGSDM: Chain A (234 residues) - Gasdermin bGSDM: Chain W (234 residues) - Gasdermin bGSDM: Chain J (234 residues) - Gasdermin bGSDM: Chain S (234 residues) - Gasdermin bGSDM: Chain RA (234 residues)

Datasets used for modeling	- 2DEM class average, File: 10.5281/zenodo.10570209 - Experimental model, PDB ID: 8sl0
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 52

Flexible units	- AA: 1-234 - BA: 1-234 - CA: 1-234 - DA: 1-234 - EA: 1-234 - FA: 1-234 - GA: 1-234 - HA: 1-234 - IA: 1-234 - JA: 1-234 - KA: 1-234 - LA: 1-234 - MA: 1-234 - NA: 1-234 - OA: 1-234 - PA: 1-234 - QA: 1-234 - RA: 1-234 - SA: 1-234 - TA: 1-234 - UA: 1-234 - VA: 1-234 - WA: 1-234 - XA: 1-234 - YA: 1-234 - ZA: 1-234 - A: 1-234 - B: 1-234 - C: 1-234 - D: 1-234 - E: 1-234 - F: 1-234 - G: 1-234 - H: 1-234 - I: 1-234 - J: 1-234 - K: 1-234 - L: 1-234 - M: 1-234 - N: 1-234 - O: 1-234 - P: 1-234 - Q: 1-234 - R: 1-234 - S: 1-234 - T: 1-234 - U: 1-234 - V: 1-234 - W: 1-234 - X: 1-234 - Y: 1-234 - Z: 1-234
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	- 1 unique EM2DRestraint: Number of micrographs: 8930, Image resolution: 1.66
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 2.61, Number of Ramachandran outliers = 180, Number of sidechain outliers = 563
Model quality: assessment of excluded volume	Not applicable
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. Method	None
Name	None
Description	To make the 52-mer pore model, protomer models (PDB 8SL0) were realigned using a custom script and a geometric model based on the number of protomers observed in the major 2D classes (52). Protomers were realigned to preserve the inter-subunit hydrogen bonding pattern observed in the slinky-like oligomer.
Software	- Python (version v3.9.7) - MDAnalysis (version v2.4.2)