

Summary of integrative structure determination of Elliptical 52-mer bacterial gasdermin pore model from *Vitiosangium* sp. (PDB ID: 9A86, PDB-Dev ID: PDBDEV_0000371)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Gasdermin bGSDM: Chain G (234 residues) - Gasdermin bGSDM: Chain P (234 residues) - Gasdermin bGSDM: Chain B (234 residues) - Gasdermin bGSDM: Chain HA (234 residues) - Gasdermin bGSDM: Chain EA (234 residues) - Gasdermin bGSDM: Chain LA (234 residues) - Gasdermin bGSDM: Chain DA (234 residues) - Gasdermin bGSDM: Chain F (234 residues) - Gasdermin bGSDM: Chain R (234 residues) - Gasdermin bGSDM: Chain V (234 residues) - Gasdermin bGSDM: Chain T (234 residues) - Gasdermin bGSDM: Chain AA (234 residues) - Gasdermin bGSDM: Chain U (234 residues) - Gasdermin bGSDM: Chain OA (234 residues) - Gasdermin bGSDM: Chain X (234 residues) - Gasdermin bGSDM: Chain XA (234 residues) - Gasdermin bGSDM: Chain SA (234 residues) - Gasdermin bGSDM: Chain TA (234 residues) - Gasdermin bGSDM: Chain VA (234 residues) - Gasdermin bGSDM: Chain ZA (234 residues) - Gasdermin bGSDM: Chain FA (234 residues) - Gasdermin bGSDM: Chain A (234 residues) - Gasdermin bGSDM: Chain H (234 residues) - Gasdermin bGSDM: Chain JA (234 residues) - Gasdermin bGSDM: Chain BA (234 residues) - Gasdermin bGSDM: Chain YA (234 residues) - Gasdermin bGSDM: Chain K (234 residues) - Gasdermin bGSDM: Chain GA (234 residues) - Gasdermin bGSDM: Chain CA (234 residues) - Gasdermin bGSDM: Chain MA (234 residues) - Gasdermin bGSDM: Chain QA (234 residues) - Gasdermin bGSDM: Chain L (234 residues) - Gasdermin bGSDM: Chain NA (234 residues) - Gasdermin bGSDM: Chain W (234 residues) - Gasdermin bGSDM: Chain O (234 residues) - Gasdermin bGSDM: Chain J (234 residues) - Gasdermin bGSDM: Chain KA (234 residues) - Gasdermin bGSDM: Chain IA (234 residues) - Gasdermin bGSDM: Chain N (234 residues) - Gasdermin bGSDM: Chain M (234 residues) - Gasdermin bGSDM: Chain PA (234 residues) - Gasdermin bGSDM: Chain UA (234 residues) - Gasdermin bGSDM: Chain Z (234 residues) - Gasdermin bGSDM: Chain I (234 residues) - Gasdermin bGSDM: Chain D (234 residues) - Gasdermin bGSDM: Chain Y (234 residues) - Gasdermin bGSDM: Chain Q (234 residues) - Gasdermin bGSDM: Chain WA (234 residues) - Gasdermin bGSDM: Chain RA (234 residues) - Gasdermin bGSDM: Chain E (234 residues) - Gasdermin bGSDM: Chain C (234 residues) - Gasdermin bGSDM: Chain S (234 residues)

<i>Datasets used for modeling</i>	<ul style="list-style-type: none">- 2DEM class average, File: 10.5281/zenodo.10570209- Experimental model, PDB ID: 8sl0- 3DEM volume, EMDB: EMD-43510
2. Representation	
<i>Resolution</i>	Atomic
<i>Number of <i>rigid bodies</i>, <i>flexible units</i></i>	0, 52

<i>Flexible units</i>	<ul style="list-style-type: none"> - 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
<u><i>Structural coverage (rigid bodies)</i></u>	100%
3. Restraints	
<u><i>Physical principles</i></u>	Information about physical principles was not provided
<u><i>Experimental data</i></u>	

4. Validation	
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	Model-1: Clashscore = 48.93, Number of Ramachandran outliers = 156, Number of sidechain outliers = 104
<i>Model quality: assessment of excluded volume</i>	Not applicable
<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>Method</i>	None
<i>Name</i>	None
<i>Description</i>	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) and the eccentricity of a cryo-EM map of an oval pore (0.86, EMD-43510). Protomers were realigned to preserve the inter-subunit hydrogen bonding pattern observed in the slinky-like oligomer.
<i>Software</i>	- Python (version v3.9.7) - MDAnalysis (version v2.4.2)