

Summary of integrative structure determination of Fibrillar adhesin CdrA from *Pseudomonas aeruginosa* Downfield (PDB ID: 9AAQ | pdb_00009aaq)

1. Model Composition	
1.1. Entry composition	Filamentous haemagglutinin FhaB/tRNA nuclease CdiA-like TPS domain-containing protein: chain(s) A (1668 residues)
1.2. Datasets used for modeling	- 3DEM volume, EMDB: EMD-49677 - NMR data, Other: 10.5281/zenodo.14994263 - De Novo model, AlphaFoldDB: AF-Q9HVG6-F1 - 3DEM volume, EMDB: EMD-49679 - NMR data, Zenodo: 10.5281/zenodo.14994263 - NMR data, Zenodo: 10.5281/zenodo.14994263 - NMR data, Zenodo: 10.5281/zenodo.14994263 - NMR data, Zenodo: 10.5281/zenodo.14994263 - NMR data, Zenodo: 10.5281/zenodo.14994263
2. Representation	
2.1. Number of representations	1
2.2. Scale	Atomic
2.3. Number of rigid and flexible segments	0, 1
3. Restraints	
3.1. Physical principles	Information about physical principles was not provided
3.2. Experimental data	- 2 unique EM3DRestraint: Real-Space refine into 3D cryo EM map - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 5.6-7.6 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 5.7-7.7 - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 5.2-7.2
4. Validation	
4.2. Number of ensembles	0
4.3. Number of models in ensembles	Not applicable
4.4. Number of deposited models	1
4.5. Model precision	Not available
4.6. Data quality	- EMD-49677: resolution is 6.00 Å - EMD-49679: resolution is 11.00 Å
4.7. Model quality: assessment of atomic segments	- Clashscore: 37.27 - Ramachandran outliers: 9 - Sidechain outliers: 5

4.8. Fit to data used for modeling	- 3DEM q-score(s): 0.00-0.00 - 3DEM atom inclusion score(s): 0.00-0.00
4.9. 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. 5.1. Method name	Initial Modeling
5.3. Method description	N*-terminal domain and each repeat module were modeled individually
2. 5.1. Method name	Energy Minimization with Tinker 8
5.2. Method type	Energy minimization
5.3. Method description	All simulations were performed in the gas phase at a dielectric of 80 and without charges. We performed energy minimization in Cartesian coordinate space using limited memory BFGS quasi-Newton nonlinear optimization with the Amber99sb force field to an RMS gradient convergence of 1 kcal mol ⁻¹ Å ⁻¹ . We restrained the phi and psi angles +/- 5 degrees relative to the TALOS-N value for the identified residues with a force constant of 125 kcal Å ⁻² . For repeat modules where the residue identity varied, we did not include a restraint. We additionally included longer-distance restraints between V14-G16 (6.6 Å), R46-A48 (6.7 Å) and L29-Y69 (6.2 Å) +/- 1 Å with a force constant of 100 kcal Å ⁻² . As the sequence is not identical between all residues, the residue location varied slightly, but distances were maintained. All other values were maintained from the AlphaFold model.
3. 5.1. Method name	TALOS-N to determine torsion angles
5.3. Method description	Determination of torsion (phi/psi) angles from chemical shift information from solid-state NMR.
4. 5.1. Method name	Geometry Minimization in Phenix
5.3. Method description	Phenix geometry-minimization to fix rotamers and Ramachandran angles
5. 5.1. Method name	Model Validation
5.2. Method type	Validation:
5.3. Method description	MolProbity to compare torsion angles from chemical shift data and final PDB file

5.5. Software

- [AlphaFold 3](#) (version Not available)
- [TALOS-N](#) (version Not available)
- [Tinker 8](#) (version Not available)
- [Phenix](#) (version 1.21.2)
- [MolProbity](#) (version 4.5.2)
- [UCSF ChimeraX](#) (version 1.10.1)
- [cryoSPARC](#) (version 4.7.1)