

Summary of integrative structure determination of Type I Amyloid beta Fibril MEMMI ensemble (PDB ID: 9A8E, PDB-Dev ID: PDBDEV_00000378)

1. Model Composition	
Entry composition	Amyloid-beta protein 42: 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 (42 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 7q4b - 3DEM volume, Zenodo: 10.5281/zenodo.14766466 - 3DEM volume, EMDB: EMD-13800
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 24
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM3DRestraint: Gaussian mixture model
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00-2.13 - Ramachandran outliers: 0-5 - Sidechain outliers: 10-15
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. Name	None
Description	All the necessary input files for the ensemble generation are available at https://zenodo.org/records/14766466 in the SIMULATION zip file.
Software	<ul style="list-style-type: none">- gmmconvert (version Not available)- Gromacs (version GROMACS-2020.5)- Plumed (version PLUMED.2.6.0-dev)