

Summary of integrative structure determination of Conformational ensemble of the PCASP and Ig3 domains of the Mucosa-associated lymphoid tissue lymphoma translocation protein 1 (MALT1(PCASP-Ig3)/339-719) at 298 K and 0.5 M NaCl (PDB ID: 9AAD | pdb_00009aad)

1. Model Composition	
1.1. Entry composition	Mucosa-associated lymphoid tissue lymphoma translocation protein 1: chain(s) A (388 residues)
1.2. Datasets used for modeling	- De Novo model, Not available - NMR data, BMRB: 52265
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	
4. Validation	
4.2. Number of ensembles	1
4.3. Number of models in ensembles	1000
4.4. Number of deposited models	20
4.5. Model precision	Not available
4.6. Data quality	Data quality has not been assessed
4.7. Model quality: assessment of atomic segments	- Clashscore: 0.00-1.45 - Ramachandran outliers: 1-11 - Sidechain outliers: 3-16
4.8. Fit to data used for modeling	Fit of model to information used to compute it has not been determined
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	Not available
5.3. Method description	Create starting structure

2. 5.1. Method name	Not available
5.3. Method description	Full-atom molecular dynamics, Charmm36 force field with cutoff correction were performed. After minimization and NVT, free dynamics in the NPT ensemble was launched for 4 microseconds.
3. 5.1. Method name	Not available
5.3. Method description	Relaxation parameters for the MD trajectory are calculated.
4. 5.1. Method name	Not available
5.3. Method description	Relaxation parameters for the MD trajectory are calculated.
5. 5.1. Method name	Not available
5.3. Method description	NMR data processed
6. 5.1. Method name	Not available
5.3. Method description	NMR data analysis
7. 5.1. Method name	Not available
5.3. Method description	NMR data analysis
5.5. Software	- Gromacs (version 2022.4) - wolfram mathematica (version Not available) - AlphaFold (version 2) - Python (version Not available) - TopSpin (version 4.3.0) - CcpNmr (version 2.4.2) - Dynamics Center (version 2.8.4) - MddNMR (version Not available)