

Summary of integrative structure determination of Integrative model of mTORC2-AKT1 (PDB ID: 9AAA | pdb_00009aaa)

1. Model Composition	
1.1. Entry composition	<ul style="list-style-type: none"> - MTOR: chain(s) A, B (2549 residues) - RICTOR: chain(s) C, D (1708 residues) - MLST8: chain(s) E, F (326 residues) - MSIN1: chain(s) G, H (522 residues) - AKT1: chain(s) I, J (480 residues)
1.2. Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: pdb_00009zbk - Experimental model, PDB: pdb_00007lc1 - De Novo model, AlphaFoldDB: AF-P31749-F1 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.17237325 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.17237325 - 3DEM volume, EMDB: EMD-44037 - 3DEM volume, Zenodo: 10.5281/zenodo.17237325
2. Representation	
2.1. Number of representations	1
2.2. Scale	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
2.3. Number of rigid and flexible segments	64, 66
3. Restraints	
3.1. Physical principles	Information about physical principles was not provided
3.2. Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 182 crosslinks - 1 unique CrossLinkRestraint: EDC, 19 crosslinks - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
4.2. Number of ensembles	1
4.3. Number of models in ensembles	1
4.4. Number of deposited models	1
4.5. Model precision	Not available
4.6. Data quality	Data quality has not been assessed
4.7. Model quality: assessment of excluded volume	Satisfaction: 99.95%
4.8. Fit to data used for modeling	Satisfaction of crosslinks: 77.50%
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	Sampling
5.2. Method type	Replica exchange monte carlo
5.4. Number of computed models	1
5.5. Software	<ul style="list-style-type: none">- IMP PMI module (version 2.21.0)- Integrative Modeling Platform (IMP) (version 2.21.0)