

Summary of integrative structure determination of Structural Basis for Mis18 Complex Assembly (PDB ID: 9A8G, PDB-Dev ID: PDBDEV_00000380)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Protein Mis18-alpha: chain(s) A, D, E, F (233 residues) - Protein Mis18-beta: chain(s) B, G (229 residues) - Mis18-binding protein 1: chain(s) C, H (130 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, EMDB: EMD-50218 - 3DEM volume, Not available - 3DEM volume, Not available - Crosslinking-MS data, PRIDE: PXD047345 - Experimental model, PDB: 7sfz - Experimental model, PDB: 7sfy - De Novo model, AlphaFoldDB: AF-Q9NYP9-F1 - De Novo model, AlphaFoldDB: AF-O43482-F1 - De Novo model, AlphaFoldDB: AF-Q6P0N0-F1
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 18
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 3 unique EM3DRestraint: manual - 1 unique CrossLinkRestraint: sulfo-SDA, 46 crosslinks - 1 unique CrossLinkRestraint: EDC, 185 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 49.39 - Ramachandran outliers: 7 - Sidechain outliers: 21
<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>Name</i>	docking
<i>Software</i>	<ul style="list-style-type: none"> - AlphaFold-Multimer (version 2.2) - CombDock (version Not available)