

Summary of integrative structure determination of NMR-based structure of SARS-CoV-2 ORF6 accessory protein in liposomes (PDB ID: 9A8Y)

1. Model Composition	
Entry composition	SARS-CoV-2 ORF6 accessory protein: chain(s) A (61 residues)
Datasets used for modeling	- NMR data, BMRB: 52654
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
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: 0.00-1.92 - Ramachandran outliers: 0-0 - Sidechain outliers: 0-1
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	Model generation
Method	CS-Rosetta Fold and Dock (C2 Symmetry)

<i>Description</i>	Generation of 5000 Fold and Dock models
<i>Number of computed models</i>	5000
2. <i>Name</i>	Remove chain B
<i>Method</i>	None
<i>Description</i>	Remove the chain B of the dimer
<i>Number of computed models</i>	5000
<i>Software</i>	<ul style="list-style-type: none"> - CS-Rosetta (version 2.0) - Pymol (version 2.5) - Topspin (version 3.5, 4.0.9 and 4.1) - CCPNMR (version 3.2) - NMRbox (version Not available)