

Summary of integrative structure determination of Integrative model of SARS-CoV-2 Replicase polyprotein 1ab (PDB ID: 9A8D, PDB-Dev ID: PDBDEV_00000536)

1. Model Composition	
Entry composition	SARS-CoV-2 Replicase polyprotein 1ab: chain(s) A (638 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, PRIDE: PXD023487 - De Novo model, Not available - Comparative model, Not available - Experimental model, PDB: 3LD1
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 8
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 72 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
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 103.58 - Ramachandran outliers: 14 - Sidechain outliers: 13
Fit to data used for modeling	Satisfaction of crosslinks: 95.83%
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	Modeling with CombDock

<i>Description</i>	CombDock with AlphaFold2 domains and crosslinks as an input
<i>Software</i>	<ul style="list-style-type: none">- UCSF ChimeraX (version 1.2/v9)- CombDock (version Not available)