

## Summary of integrative structure determination of SARS-CoV-2 nsp7-8 polyprotein (PDB ID: 9A1T, PDB-Dev ID: PDBDEV\_00000119)

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	SARS-CoV-2 nsp7-8 polyprotein: chain(s) A (283 residues)
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, PRIDE: <a href="#">PXD033748</a></li> <li>- H/D exchange data, PRIDE: <a href="#">PXD033698</a></li> <li>- SAS data, SASBDB: <a href="#">SASDPY2</a></li> <li>- Experimental model, PDB: <a href="#">6YHU</a></li> <li>- De Novo model, Not available</li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
<a href="#">Number of <i>rigid</i> and <i>flexible</i> segments</a>	0, 5
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: DSSO, 46 crosslinks</li> <li>- 1 unique SASRestraint: Assembly name: SARS-CoV-2 nsp7-8 polyprotein Fitting method: CRY SOL Multi-state: False</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	10
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	
<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 1.81-24.47</li> <li>- Ramachandran outliers: 15-48</li> <li>- Sidechain outliers: 20-37</li> </ul>
<a href="#">Fit to data used for modeling</a>	Satisfaction of crosslinks: 60.87-78.26%
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	

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1. <a href="#">Name</a>	Integrative modeling
<a href="#">Software</a>	<a href="#">I-TASSER</a> (version Not available)