

**Summary of integrative structure determination of SARS-CoV-2 nsp7-8 polyprotein
(PDB ID: 9A1T, PDB-Dev ID: PDBDEV_00000119)**

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| 1. Model Composition | |
| Entry composition | SARS-CoV-2 nsp7-8 polyprotein: Chain A (283 residues) |
| Datasets used for modeling | <ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 46 cross-links - H/D exchange data, PRIDE: PXD033698 - SAS data, SASBDB: SASDPY2 - Experimental model, PDB ID: 6YHU - De Novo model, Not available |
| 2. Representation | |
| Resolution | Atomic |
| Number of rigid bodies, flexible units | 0, 3 |
| Flexible units | A: 3-82, 161-277, 83-160 |
| Structural coverage (rigid bodies) | 100% |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | <ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 46 cross-links - 1 unique SASRestraint: Assembly name: SARS-CoV-2 nsp7-8 polyprotein Fitting method: CRY SOL Multi-state: False |
| 4. Validation | |
| Number of ensembles | 0 |
| Number of models in ensembles | Not applicable |
| Number of deposited models | 10 |
| Model precision (uncertainty of models) | Model precision can not be calculated with one structure |
| Data quality | |

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| <p><i>Model quality: assessment of atomic segments</i></p> | <ul style="list-style-type: none"> - Model-1: Clashscore = 11.56, Number of Ramachandran outliers = 19, Number of sidechain outliers = 37 - Model-2: Clashscore = 3.4, Number of Ramachandran outliers = 38, Number of sidechain outliers = 24 - Model-3: Clashscore = 3.63, Number of Ramachandran outliers = 26, Number of sidechain outliers = 36 - Model-4: Clashscore = 5.44, Number of Ramachandran outliers = 18, Number of sidechain outliers = 27 - Model-5: Clashscore = 1.81, Number of Ramachandran outliers = 25, Number of sidechain outliers = 26 - Model-6: Clashscore = 2.72, Number of Ramachandran outliers = 15, Number of sidechain outliers = 20 - Model-7: Clashscore = 19.71, Number of Ramachandran outliers = 19, Number of sidechain outliers = 36 - Model-8: Clashscore = 24.47, Number of Ramachandran outliers = 47, Number of sidechain outliers = 35 - Model-9: Clashscore = 5.67, Number of Ramachandran outliers = 48, Number of sidechain outliers = 33 - Model-10: Clashscore = 12.46, Number of Ramachandran outliers = 21, Number of sidechain outliers = 31 |
| <p><i>Model quality: assessment of excluded volume</i></p> | <p>Not applicable</p> |
| <p><i>Fit to data used for modeling</i></p> | <p>Fit of model to information used to compute it has not been determined</p> |
| <p><i>Fit to data used for validation</i></p> | <p>Fit of model to information not used to compute it has not been determined</p> |
| <p>5. Methodology and Software</p> | |
| <p><i>1. Method</i></p> | <p>Integrative modeling</p> |
| <p><i>Name</i></p> | <p>None</p> |
| <p><i>Software</i></p> | <p>I-TASSER (version Not available)</p> |