

Summary of integrative structure determination of Modeling hLINE1 ORF2p (PDB ID: 9A3Q, PDB-Dev ID: PDBDEV_0000211)

1. Model Composition	
<i>Entry composition</i>	ORF2: chain(s) A (1275 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - 3DEM volume, Zenodo: 10.5281/zenodo.10377421 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.10377421 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.10377421 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.10377421 - 2DEM class average, Zenodo: 10.5281/zenodo.10377421 - 2DEM class average, Zenodo: 10.5281/zenodo.10377421 - 2DEM class average, Zenodo: 10.5281/zenodo.10377421 - De Novo model, AlphaFoldDB: AF-O00370-F1 - De Novo model, MODEL ARCHIVE: ma-fejd6 - De Novo model, MODEL ARCHIVE: ma-joo4d - De Novo model, MODEL ARCHIVE: ma-lzyrq - De Novo model, MODEL ARCHIVE: ma-xlzzy - De Novo model, MODEL ARCHIVE: ma-9wovj - Mass Spectrometry data, PRIDE: PXD038615 - EM raw micrographs, EMPIAR: EMPIAR-11556 - 3DEM volume, EMDB: 40856
2. Representation	
<i>Number of representations</i>	1
<i>Scale</i>	Coarse-grained: 1 residue(s) per bead
<i>Number of rigid and flexible segments</i>	15, 14
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique EM2DRestraint: Number of micrographs: None, Image resolution: 20.0 - 1 unique EM3DRestraint: Gaussian mixture models - 1 unique CrossLinkRestraint: BS3, 15 crosslinks - 1 unique CrossLinkRestraint: BS3, 11 crosslinks - 1 unique CrossLinkRestraint: BS3, 30 crosslinks - 15 unique PredictedContactRestraint: Distance: 27.0

4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	1383
<i>Number of deposited models</i>	159
<i>Model precision (uncertainty of models)</i>	12.87, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.60-99.61%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 85.71-92.86%
<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>	Sampling
<i>Description</i>	Modeling of full-length ORF2p with AlphaFold2 using varying alignment depth. Details of the simulations are available in the ModelArchive entry ma-fejd6
2. <i>Name</i>	Sampling
<i>Description</i>	Details of molecular dynamics simulations are available ModelArchive entries
3. <i>Name</i>	Sampling
<i>Method</i>	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo
<i>Description</i>	20 replicas; 3 runs; 10000 models per run
<i>Number of computed models</i>	30000
4. <i>Name</i>	Refinement
<i>Method</i>	Steepest descent
<i>Description</i>	Conversion of a Ca-model to a full backbone model
<i>Number of computed models</i>	159
5. <i>Name</i>	Refinement
<i>Method</i>	SCWRL

<i>Description</i>	Conversion of a backbone model to a full-atom model
<i>Number of computed models</i>	159
6. <i>Name</i>	Refinement
<i>Method</i>	Geometry optimization
<i>Description</i>	Conversion of a backbone model to a full-atom model
<i>Number of computed models</i>	159
<i>Software</i>	<ul style="list-style-type: none"> - Sampcon (version 2.18.0) - ColabFold (version 1.3.0) - GROMACS (version 2022.3) - IMP PMI module (version 2.19.0) - PULCHRA (version 3.04) - SCWRL4.0 (version 4.0) - Integrative Modeling Platform (IMP) (version 2.19.0)