Summary of integrative structure determination of Modeling hLINE1 ORF2p (PDB ID: 9A3Q, PDB-Dev ID: PDBDEV_00000211)

1. Model Composition	
Entry composition	ORF2: Chain A (1275 residues)
Datasets used for modeling	- 3DEM volume, File: 10.5281/zenodo.10377421 - Crosslinking-MS data, Linker name and number of cross-links: BS3, 15 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BS3, 11 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BS3, 30 cross-links - 2DEM class average, File: 10.5281/zenodo.10377421 - 2DEM class average, File: 10.5281/zenodo.10377421 - 2DEM class average, File: 10.5281/zenodo.10377421 - De Novo model, AlphaFoldDB: O00370 - 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	
Resolution	Coarse-grained: 1 residue(s) per bead
Number of rigid bodies, flexible units	15, 14
Rigid bodies	A: 8-237, 250-258, 260-277, 284-310, 313-352, 353-359, 362-370, 375-381, 393-849, 857-862, 864-868, 873-955, 960-1030, 1033-1061, 1068-1275
Flexible units	A: 1-7, 238-249, 259-259, 278-283, 311-312, 360-361, 371-374, 382-392, 850-856, 863-863, 869-872, 956-959, 1031-1032, 1062-1067
Structural coverage (rigid bodies)	95%
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	- 1 unique EM2DRestraint: Number of micrographs: None, Image resolution: 20.0 - 1 unique EM3DRestraint: Gaussian mixture models - 1 unique CrossLinkRestraint: BS3, 15 cross-links - 1 unique CrossLinkRestraint: BS3, 11 cross-links - 1 unique CrossLinkRestraint: BS3, 30 cross-links - 15 unique PredictedContactRestraint: Distance: 27.0
4. Validation	
Number of ensembles	1
Number of models in ensembles	1383
Number of deposited models	159
Model precision (uncertainty of models)	12.871, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.60-99.61%
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. Method	Sampling
Name	AlphaFold2
Description	Modeling of full-length ORF2p with AlphaFold2 using varying alignment depth. Details of the simulations are availabel in the ModelArchive entry ma-fejd6
2. Method	Sampling
Name	Molecular Dynamics simulations
Description	Details of molecular dynamics simulations are available ModelArchive entries
3. Method	Sampling
Name	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo
Description	20 replicas; 3 runs; 10000 models per run
Number of computed models	30000

4. Method	Refinement
Name	Steepest descent
Description	Conversion of a Ca-model to a full backbone model
Number of computed models	159
5. Method	Refinement
Name	SCWRL
Description	Conversion of a backbone model to afull-atom model
Number of computed models	159
6. Method	Refinement
Name	Geometry optimization
Description	Conversion of a backbone model to a full-atom model
Number of computed models	159
Software	- 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)