

Summary of integrative structure determination of In-cell architecture of an actively transcribing-translating expressome from *M. pneumoniae* (PDB ID: 9A0D, PDB-Dev ID: PDBDEV_00000049)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - P75591: chain(s) A (540 residues) - 30SsubunitP: chain(s) AA (83 residues) - 30SsubunitQ: chain(s) AB (71 residues) - 30SsubunitR: chain(s) AC (83 residues) - 30SsubunitT: chain(s) AD (1544 residues) - 30Ssubunitj: chain(s) AE (77 residues) - 30SsubunitZ: chain(s) AF (77 residues) - Q50295: chain(s) B (327 residues) - Q50295: chain(s) C (327 residues) - P78013: chain(s) D (1391 residues) - P75271: chain(s) E (1290 residues) - P75049: chain(s) F (150 residues) - Q50301: chain(s) G (219 residues) - P75560: chain(s) H (294 residues) - P75581: chain(s) I (108 residues) - P41205: chain(s) J (273 residues) - P46775: chain(s) K (205 residues) - Q50304: chain(s) L (142 residues) - P75179: chain(s) M (132 residues) - DNA1N: chain(s) N (39 residues) - longRNAR1: chain(s) O (46 residues) - longRNAR1: chain(s) P (46 residues) - DNA1T: chain(s) Q (39 residues) - P75090: chain(s) R (85 residues) - 30SsubunitE: chain(s) S (92 residues) - 30SsubunitF: chain(s) T (153 residues) - 30Ssubunitj: chain(s) U (118 residues) - 30SsubunitK: chain(s) V (135 residues) - 30SsubunitL: chain(s) W (119 residues) - 30SsubunitM: chain(s) X (60 residues) - 30SsubunitN: chain(s) Y (84 residues) - 30SsubunitO: chain(s) Z (80 residues)

<p><i>Datasets used for modeling</i></p>	<ul style="list-style-type: none"> - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Experimental model, PDB: 6flq - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Experimental model, PDB: 3j9w - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Comparative model, Zenodo: 10.5281/zenodo.3837625 - Crosslinking-MS data, PRIDE: PXD017695 - Crosslinking-MS data, PRIDE: PXD017711 - 3DEM volume, EMDB: EMD-10680 - 3DEM volume, Zenodo: 10.5281/zenodo.3837625 - Experimental model, PDB: 6FLQ - Experimental model, PDB: 6C6U - Experimental model, PDB: 3J9W
2. Representation	
<i>Number of representations</i>	1
<i>Scale</i>	Multiscale: Coarse-grained: 1 - 25 residue(s) per bead
<i>Number of rigid and flexible segments</i>	39, 47
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 CrossLinkRestraint: DSS, 379 crosslinks - 1 unique CrossLinkRestraint: DSSO, 104 crosslinks - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	20131
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.95%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 85.39%
<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	
<i>1. Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	14400000
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version 2.12.0) - Integrative Modeling Platform (IMP) (version 2.12.0) - SWISS-MODEL (version 2019-11-21) - MODELLER (version 9.21) - SWISS-MODEL (version 2.0.0) - SWISS-MODEL (version 1.3.0)