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	
Entry composition	- 30SsubunitF: Chain T (153 residues) - Q50295: Chain C (327 residues) - 30SsubunitL: Chain W (119 residues) - P75581: Chain I (108 residues) - 30Ssubunitj: Chain AE (77 residues) - 30SsubunitJ: Chain U (118 residues) - 30SsubunitN: Chain Y (84 residues) - P75090: Chain R (144 residues) - longRNAR1: Chain O (46 residues) - DNA1N: Chain N (39 residues) - 30SsubunitR: Chain AC (83 residues) - 30SsubunitO: Chain Z (80 residues) - P78013: Chain D (1391 residues) - P46775: Chain K (205 residues) - P41205: Chain J (273 residues) - Q50295: Chain B (327 residues) - P75560: Chain H (294 residues) - P75049: Chain F (320 residues) - 30SsubunitQ: Chain AB (71 residues) - P75271: Chain E (1290 residues) - 30SsubunitE: Chain S (92 residues) - Q50304: Chain L (142 residues) - longRNAR1: Chain P (46 residues) - 30SsubunitP: Chain AA (83 residues) - P75179: Chain M (132 residues) - DNA1T: Chain Q (39 residues) - P75591: Chain A (540 residues) - 30SsubunitK: Chain V (135 residues) - Q50301: Chain G (219 residues) - 30SsubunitT: Chain AD (1544 residues) - 30SsubunitM: Chain X (60 residues) - 30SsubunitZ: Chain AF (77 residues)

Datasets used for modeling	- Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 6flq - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3j9w - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: DSS, 379 cross-links - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 104 cross-links - 3DEM volume, EMDB: EMD-10680 - 3DEM volume, File: 10.5281/zenodo.3837625 - Experimental model, PDB ID: 6FLQ - Experimental model, PDB ID: 6C6U - Experimental model, PDB ID: 3J9W
2. Representation	
Resolution	Coarse-grained: 1, 2, 3, 5, 6, 8, 9 residue(s) per bead
Number of rigid bodies, flexible units	39, 47

Rigid bodies	- A: 12-141, 145-212, 216-364 - B: 29-233, 234-239, 266-325 - C: 29-233, 234-325 - D: 14-980, 990-998, 1006-1356 - E: 14-1280 - F: 7-146 - G: 70-212 - H: 20-241 - I: 12-107 - J: 2-206 - K: 2-202 - L: 10-142 - M: 6-132 - N: 1-38 - O: 1-9 - P: 37-46 - Q: 2-39 - R: 9-74 - S: 1-92 - T: 1-153 - U: 1-118 - V: 1-135 - W: 1-119 - X: 1-60 - Y: 1-84 - Z: 1-80 - AA: 1-83 - AB: 1-71 - AC: 1-83 - AD: 1-1544 - AE: 1-77 - AF: 1-77

Flexible units	- A: 1-11, 142-144, 213-215, 365-540 - B: 1-28, 240-265, 326-327 - C: 1-28, 240-265, 326-327 - D: 1-13, 225-342, 398-498, 981-989, 999-1005, 1357-1391 - E: 1-13, 137-237, 266-272, 658-690, 836-848, 1027-1047, 1056-1056, 1064-1068, 1117-1120, 1281-1290 - F: 1-6, 48-91, 147-150 - G: 1-69, 213-219 - H: 1-19, 242-294 - I: 1-11, 108-108 - J: 1-1, 207-273 - K: 1-1, 203-205 - L: 1-9 - M: 1-5 - N: 16-24, 39-39 - O: 10-11 - P: - - Q: 1-1 - R: 1-8, 75-85 - S: - - T: - - U: - - V: - - W: - - X: - - Y: - - Z: - - AA: - - AB: - - AC: - - AD: - - AE: - - AF: -
Structural coverage (rigid bodies)	87%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSS, 379 cross-links - 1 unique CrossLinkRestraint: DSSO, 104 cross-links - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
Number of ensembles	1
Number of models in ensembles	20131
Number of deposited models	1
Model precision (uncertainty of models)	None, Å
Data quality	Data quality has not been assessed

Model quality: assessment of excluded volume	Satisfaction: 99.95-99.95%
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	Replica exchange monte carlo
Number of computed models	14400000
Software	- 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)