Materials Design Analysis Reporting (MDAR) Checklist for Authors

The MDAR framework establishes a minimum set of requirements in transparent reporting applicable to studies in the life sciences (see Statement of Task: doi:10.31222/osf.io/9sm4x.). The MDAR checklist is a tool for authors, editors and others seeking to adopt the MDAR framework for transparent reporting in manuscripts and other outputs. Please refer to the MDAR Elaboration Document for additional context for the MDAR framework.

Materials

Antibodies	Yes (indicate where provided: page no/section/legend)	n/a
For commercial reagents, provide supplier name, catalogue number and RRID, if available.		n.a.

Cell materials	Yes (indicate where provided: page no/section/legend)	n/a
Cell lines: Provide species information, strain. Provide accession number in repository **OR** supplier name, catalog number, clone number, **OR** RRID		n.a.
Primary cultures: Provide species, strain, sex of origin, genetic modification status.		n.a.

Experimental animals	Yes (indicate where provided: page no/section/legend)	n/a
Laboratory animals: Provide species, strain, sex, age, genetic modification status. Provide accession number in repository **OR** supplier name, catalog number, clone number, **OR** RRID		n.a.
Animal observed in or captured from the field: Provide species, sex and age where possible		n.a.
Model organisms: Provide Accession number in repository (where relevant) **OR** RRID		n.a.

Plants and microbes	Yes (indicate where provided: page no/section/legend)	n/a
Plants: provide species and strain, unique accession number if available, and source (including location for collected wild specimens)		n.a.
Microbes: provide species and strain, unique accession number if available, and source	Supplementary Materials, Materials and methods, page 2: *Mycoplasma pneumoniae* strain M129 (ATCC 29342)	

Human research participants	Yes (indicate where provided: page no/section/legend)	n/a
Identify authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		n.a.
Provide statement confirming informed consent obtained from study participants.		n.a.
Report on age and sex for all study participants.		n.a.

Design

Study protocol	Yes (indicate where provided: page no/section/legend)	n/a
For clinical trials, provide the trial registration number **OR** cite DOI in manuscript.		n.a.

Laboratory protocol	Yes (indicate where provided: page no/section/legend)	n/a
Provide DOI or other citation details if detailed step-by-step protocols are available.		n.a.

Experimental study design (statistics details)	Yes (indicate where provided: page no/section/legend)	n/a
State whether and how the following have been done**, or** if they were not carried out.		
Sample size determination	Cryo-electron tomography and CLMS: No statistical methods were used to predetermine sample size	
Randomisation	Cryo-electron tomography and CLMS: experiments were not randomized. Integrative modelling: detailed in "Integrative structure modeling: representation and sampling" section in methods. Supplementary Materials, Materials and methods, page 11.	
Blinding	Cryo-electron tomography, CLMS and integrative modeling: investigators were not blinded to allocation during experiments and outcome assessment	
Inclusion/exclusion criteria	Cryo-electron tomography: no data was excluded. CLMS: no data collected was excluded. Integrative modeling: no data was excluded.	

Sample definition and in-laboratory replication	Yes (indicate where provided: page no/section/legend)	n/a
State number of times the experiment was replicated in laboratory	CLMS: two datasets with two different crosslinkers were collected for CLMS data and handled separately for statistical tests. These are not technical replicates but analyze cells from replicated cultures. Supplementary Materials, Materials and methods, page 3. Cryo-electron tomography: 500 tomograms, equivalent to 500 single cells, were acquired: 352 for native, untreated cells, 65 for Cm-treated and 83 for PUM-treated cells. Supplementary Materials, Materials and methods, page 7. Integrative modelling: 20 independent replicates. Detailed in "Integrative structure modeling: representation and sampling" section in methods. Supplementary Materials, Materials and methods, page 12.	

Define whether data describe technical or biological replicates	CLMS: two datasets with two different crosslinkers were collected for CLMS data and handled separately for statistical tests. These are not technical replicates but analyze cells from replicated cultures. Supplementary Materials, Materials and methods, page 2. Cryo-electron tomography: 500 tomograms, equivalent to 500 single cells, were acquired on the following number of grids representing independent biological replicates: 6 for untreated cells, 1 for Cm-treated and 1 for PUM-treated cells. Supplementary Materials, Materials and methods, page 7. Integrative Modeling: Technical replicates. "Integrative structure modeling: representation and sampling" section in methods. Supplementary Materials, Materials and methods, page 12.	

Ethics	**Yes (indicate where provided: page no/section/legend)**	**n/a**
Studies involving human participants: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		n.a.
Studies involving experimental animals: State details of authority granting ethics approval (IRB or equivalent committee(s), provide reference number for approval.		n.a.
Studies involving specimen and field samples: State if relevant permits obtained, provide details of authority approving study; if none were required, explain why.		n.a.

Dual Use Research of Concern (DURC)	**Yes (indicate where provided: page no/section/legend)**	**n/a**
If study is subject to dual use research of concern, state the authority granting approval and reference number for the regulatory approval		n.a.

Analysis

Attrition	Yes (indicate where provided: page	n/a
State if sample or data point from the analysis is excluded, and whether the criteria for exclusion were determined and specified in advance.		n.a.

Statistics	Yes (indicate where provided: page no/section/legend)	n/a
Describe statistical tests used and justify choice of tests.	Box plot and analysis in MATLAB were used to describe the distribution of cell sample thickness and particle number picked per tomogram: described in Supplementary Materials, Fig. S5, panel C and F, and figure legend, page 22. Target decoy analysis was used to assess error in the CLMS data: Described in materials and methods. Supplementary Materials, Materials and methods, page 4. Integrative modeling and model fitting: Described in "Integrative structure modeling: scoring and analysis" section in methods Supplementary Materials, Materials and methods, page 12-13. Also in the legend to Fig. S21.	

Data Availability	Yes (indicate where provided: page	n/a
State whether newly created datasets are available, including protocols for access or restriction on access.	Newly created datasets will be made available upon publication. Accession codes are listed in the 'Data and materials availability' section, page 11 of the main manuscript.	
If data are publicly available, provide accession number in repository or DOI or URL.	EM densities have been deposited in the EMDataBank (URL: https://www.ebi.ac.uk/pdbe/emdb/) with the following accession numbers: EMD-10677, 10678, 10679, 10680, 10681, 10682, 10683, 10684, 10685, 10686, 10687. CLMS data are available via ProteomeXchange (URL: https://www.ebi.ac.uk/pride/archive/) with identifiers PXD017711 (DSSO) and PXD017695 (DSS). Integrative model is available in PDB-dev (URL: https://pdb-dev.wwpdb.org/) with accession code: PDBDEV_00000049. Homology models are deposited in the ModelArchive (URL https://modelarchive.org/) with accession numbers: : ma-mrryl, ma-7ov95, ma-eeo9f, ma-8tn6v	
If publicly available data are reused, provide accession number in repository or DOI or URL, where possible.	Published structures on PDB: URL: All publicly available data used to generate models is described with database names and accession numbers in table S4.	

Code Availability	Yes (indicate where provided: page	n/a
For all newly generated code and software essential for replicating the main findings of the study:		n.a.
State whether the code or software is available.	Yes	
If code is publicly available, provide accession number in repository, or DOI or URL.	Integrative modeling code is available in Zenodo under the doi https://doi.org/10.5281/zenodo.3829334 .	

Reporting

Adherence to community standards	Yes (indicate where provided: page no/section/legend)	n/a
MDAR framework recommends adoption of discipline-specific guidelines, established and endorsed through community initiatives. Journals have their own policy about requiring specific guidelines and recommendations to complement MDAR.	The crosslinking MS community is currently in discussions regarding reporting standards, and no recommendations yet exist. However, the data presented here is in line with what is being discussed, with correct false discovery rate estimation and upload of all data to online repositories. The cryo-ET community does not have formal stablished checklists. The maps and models have been deposited to public repositories according to the accepted highest standards in the community. Integrative modeling and model selection were performed in accordance to published specifications by the authors of the IMP software, as described in methods section.	
State if relevant guidelines (eg., ICMJE, MIBBI, ARRIVE) have been followed, and whether a checklist (eg., CONSORT, PRISMA, ARRIVE) is provided with the manuscript.		n.a.