Summary of integrative structure determination of Vimentin intermediate filament tetramer (PDB ID: 9A3R, PDB-Dev ID: PDBDEV_00000212)

1. Model Composition	
Entry composition	- Vimentin: Chain B (466 residues) - Vimentin: Chain D (466 residues) - Vimentin: Chain A (466 residues) - Vimentin: Chain C (466 residues)
Datasets used for modeling	- Mass Spectrometry data, Not available - 3DEM volume, EMDB: EMD-16844 - 3DEM volume, Not available - De Novo model, Not available - De Novo model, Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 4
Flexible units	- A: 1-466 - B: 1-466 - C: 1-466 - D: 1-466
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DST, 11 cross-links - 1 unique EM3DRestraint: Molecular dynamics flexible fitting
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 1.49, Number of Ramachandran outliers = 54, Number of sidechain outliers = 0

Model quality: assessment of excluded volume	Not applicable
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	Molecular dynamics flexible fitting
Name	Molecular dynamics flexible fitting
Description	The vimentin dimer starting model was fitted by molecular dynamics flexible fitting to an elongated version of the electron density map EMD-16844. Spatial restraints derived from chemical crosslinking and from an electron density map indicating the position of the vimentin tail domains were applied in the modelling procedure.
Number of computed models	1
Software	- AlphaFold (version 2.1.2) - ClusPro (version 2.0) - Namdinator (version Not available) - UCSF Chimera (version 1.15)