Summary of integrative structure determination of Escherichia coli sigma70 in apo form (PDB ID: 9A8C, PDB-Dev ID: PDBDEV_00000377)

1. Model Composition	
Entry composition	RNA polymerase sigma factor RpoD: chain(s) A (536 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD037183 - Experimental model, PDB: 6P1K
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 1 crosslinks - 1 unique CrossLinkRestraint: DMTMM, 1 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	4
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 43.31-62.59 - Ramachandran outliers: 8-9 - Sidechain outliers: 1-1
Fit to data used for modeling	Satisfaction of crosslinks: 100.00-100.00%
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. Name	Docking
2. Name	Docking

3. Name	Docking
Software	- PatchDock (version 1.3) - ChimeraX (version 1.2.5)