

Summary of integrative structure determination of Integrative structure of transcriptional enhancer factor TEF-1 bound to C-MYC exon (PDB ID: 9A0R, PDB-Dev ID: PDBDEV_00000063)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Transcriptional enhancer factor TEF-3: chain(s) A (87 residues) - DNA (30-MER): chain(s) B (30 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Mass Spectrometry data, PRIDE: PXD012127 - Crosslinking-MS data, Not available: 10.17632/27zkz3v729.1 - Experimental model, PDB: 5GZB - Comparative model, Not available - Comparative model, Not available - H/D exchange data, Not available: 10.17632/27zkz3v729.1
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSA, 7 crosslinks - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 2.5
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	25
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 20.87-33.39 - Ramachandran outliers: 0-6 - Sidechain outliers: 0-4
Fit to data used for modeling	Satisfaction of crosslinks: 71.43-100.00%

<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	
1. <i>Name</i>	None
<i>Method</i>	homology modeling
<i>Number of computed models</i>	25
2. <i>Name</i>	None
<i>Method</i>	molecular docking
<i>Number of computed models</i>	200
3. <i>Name</i>	None
<i>Method</i>	molecular dynamics
<i>Number of computed models</i>	300
<i>Software</i>	<ul style="list-style-type: none"> - MODELLER (version 9.20) - Make-na (version Not available) - Modeller (version 9.24) - Haddock (version 2.2) - CNS (version 1.3)