

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_0000063)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - DNA (30-MER): Chain B (30 residues) - Transcriptional enhancer factor TEF-3: Chain A (87 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Mass Spectrometry data, PRIDE: PXD012127 - Crosslinking-MS data, Linker name and number of cross-links: DSA, 7 cross-links - Experimental model, PDB ID: 5GZB - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - H/D exchange data, File: 10.17632/27zkz3v729.1
2. Representation	
Resolution	Atomic
Number of rigid bodies , flexible units	0, 2
Flexible units	<ul style="list-style-type: none"> - A: 1-87 - B: 1-30
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSA, 7 cross-links - 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)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
	<ul style="list-style-type: none"> - Model-1: Clashscore = 27.55, Number of Ramachandran outliers = 2, Number of sidechain outliers = 1

[Model quality: assessment of atomic segments](#)

- Model-2: Clashscore = 29.22, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0
- Model-3: Clashscore = 26.71, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0
- Model-4: Clashscore = 25.88, Number of Ramachandran outliers = 1, Number of sidechain outliers = 2
- Model-5: Clashscore = 27.96, Number of Ramachandran outliers = 2, Number of sidechain outliers = 2
- Model-6: Clashscore = 28.38, Number of Ramachandran outliers = 0, Number of sidechain outliers = 4
- Model-7: Clashscore = 30.88, Number of Ramachandran outliers = 4, Number of sidechain outliers = 1
- Model-8: Clashscore = 20.87, Number of Ramachandran outliers = 1, Number of sidechain outliers = 0
- Model-9: Clashscore = 30.88, Number of Ramachandran outliers = 1, Number of sidechain outliers = 1
- Model-10: Clashscore = 30.88, Number of Ramachandran outliers = 1, Number of sidechain outliers = 0
- Model-11: Clashscore = 33.39, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0
- Model-12: Clashscore = 29.63, Number of Ramachandran outliers = 4, Number of sidechain outliers = 1
- Model-13: Clashscore = 21.29, Number of Ramachandran outliers = 2, Number of sidechain outliers = 0
- Model-14: Clashscore = 27.55, Number of Ramachandran outliers = 1, Number of sidechain outliers = 2
- Model-15: Clashscore = 32.97, Number of Ramachandran outliers = 2, Number of sidechain outliers = 0
- Model-16: Clashscore = 28.8, Number of Ramachandran outliers = 5, Number of sidechain outliers = 2
- Model-17: Clashscore = 28.8, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0
- Model-18: Clashscore = 28.8, Number of Ramachandran outliers = 2, Number of sidechain outliers = 2
- Model-19: Clashscore = 27.96, Number of Ramachandran outliers = 1, Number of sidechain outliers = 0
- Model-20: Clashscore = 27.96, Number of Ramachandran outliers = 2, Number of sidechain outliers = 2
- Model-21: Clashscore = 31.72, Number of Ramachandran outliers = 2, Number of sidechain outliers = 1
- Model-22: Clashscore = 29.22, Number of Ramachandran outliers = 1, Number of sidechain outliers = 2
- Model-23: Clashscore = 26.29, Number of

	<p>Ramachandran outliers = 3, Number of sidechain outliers = 0</p> <p>- Model-24: Clashscore = 29.22, Number of Ramachandran outliers = 4, Number of sidechain outliers = 0</p> <p>- Model-25: Clashscore = 21.7, Number of Ramachandran outliers = 6, Number of sidechain outliers = 0</p>
<i>Model quality: assessment of excluded volume</i>	Not applicable
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<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	
<i>1. Method</i>	None
<i>Name</i>	homology modeling
<i>Number of computed models</i>	25
<i>2. Method</i>	None
<i>Name</i>	molecular docking
<i>Number of computed models</i>	200
<i>3. Method</i>	None
<i>Name</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)