

Summary of integrative structure determination of Integrative structure of transcriptional enhancer factor TEF-1 (PDB ID: 9A0Q, PDB-Dev ID: PDBDEV_00000062)

1. Model Composition	
Entry composition	Transcriptional enhancer factor TEF-1: chain(s) A (87 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: 2HZD - Comparative model, Not available
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: DSA, 14 crosslinks
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: 41.87-65.29 - Ramachandran outliers: 5-13 - Sidechain outliers: 4-9
Fit to data used for modeling	Satisfaction of crosslinks: 78.57-92.86%
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	None
Method	homology modeling
Number of computed models	25
2. Name	None
Method	molecular dynamics
Number of computed models	100
Software	<ul style="list-style-type: none">- MODELLER (version 9.20)- Modeller (version 9.24)- CNS (version 1.3)