

**Summary of integrative structure determination of Integrative structure of transcriptional enhancer factor TEF-1 (PDB ID: 9A0Q, PDB-Dev ID: PDBDEV\_0000062)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	Transcriptional enhancer factor TEF-1: Chain A (87 residues)
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Mass Spectrometry data, PRIDE: PXD012127</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSA, 14 cross-links</li> <li>- Experimental model, PDB ID: 2HZD</li> <li>- Comparative model, template PDB ID: Not available</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of rigid bodies, flexible units</a>	0, 1
<a href="#">Flexible units</a>	A: 1-87
<a href="#">Structural coverage (rigid bodies)</a>	100%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: DSA, 14 cross-links
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	25
<a href="#">Model precision (uncertainty of models)</a>	Model precision can not be calculated with one structure
<a href="#">Data quality</a>	Data quality has not been assessed
	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 44.71, Number of Ramachandran outliers = 5, Number of sidechain outliers = 5</li> <li>- Model-2: Clashscore = 46.84, Number of Ramachandran outliers = 8, Number of sidechain outliers = 7</li> <li>- Model-3: Clashscore = 48.97, Number of Ramachandran outliers = 10, Number of sidechain outliers = 6</li> <li>- Model-4: Clashscore = 47.55, Number of Ramachandran outliers = 8, Number of sidechain outliers = 5</li> </ul>

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

outliers = 4

- Model-5: Clashscore = 49.68, Number of Ramachandran outliers = 7, Number of sidechain outliers = 4
- Model-6: Clashscore = 46.13, Number of Ramachandran outliers = 7, Number of sidechain outliers = 6
- Model-7: Clashscore = 51.1, Number of Ramachandran outliers = 7, Number of sidechain outliers = 7
- Model-8: Clashscore = 46.84, Number of Ramachandran outliers = 7, Number of sidechain outliers = 5
- Model-9: Clashscore = 46.84, Number of Ramachandran outliers = 5, Number of sidechain outliers = 4
- Model-10: Clashscore = 51.81, Number of Ramachandran outliers = 6, Number of sidechain outliers = 6
- Model-11: Clashscore = 41.87, Number of Ramachandran outliers = 5, Number of sidechain outliers = 4
- Model-12: Clashscore = 44.0, Number of Ramachandran outliers = 7, Number of sidechain outliers = 6
- Model-13: Clashscore = 48.26, Number of Ramachandran outliers = 8, Number of sidechain outliers = 6
- Model-14: Clashscore = 55.36, Number of Ramachandran outliers = 9, Number of sidechain outliers = 9
- Model-15: Clashscore = 43.29, Number of Ramachandran outliers = 8, Number of sidechain outliers = 6
- Model-16: Clashscore = 56.07, Number of Ramachandran outliers = 8, Number of sidechain outliers = 6
- Model-17: Clashscore = 44.71, Number of Ramachandran outliers = 11, Number of sidechain outliers = 4
- Model-18: Clashscore = 49.68, Number of Ramachandran outliers = 10, Number of sidechain outliers = 7
- Model-19: Clashscore = 65.29, Number of Ramachandran outliers = 6, Number of sidechain outliers = 8
- Model-20: Clashscore = 44.71, Number of Ramachandran outliers = 5, Number of sidechain outliers = 5
- Model-21: Clashscore = 56.07, Number of Ramachandran outliers = 10, Number of sidechain outliers = 7
- Model-22: Clashscore = 43.29, Number of Ramachandran outliers = 5, Number of sidechain outliers = 9
- Model-23: Clashscore = 44.71, Number of Ramachandran outliers = 8, Number of sidechain outliers = 7
- Model-24: Clashscore = 48.97, Number of Ramachandran outliers = 13, Number of sidechain outliers = 5
- Model-25: Clashscore = 62.46, Number of Ramachandran outliers = 9, Number of sidechain outliers = 7

<a href="#"><i>Model quality: assessment of excluded volume</i></a>	Not applicable
<a href="#"><i>Fit to data used for modeling</i></a>	Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#"><i>Method</i></a>	None
<a href="#"><i>Name</i></a>	homology modeling
<a href="#"><i>Number of computed models</i></a>	25
2. <a href="#"><i>Method</i></a>	None
<a href="#"><i>Name</i></a>	molecular dynamics
<a href="#"><i>Number of computed models</i></a>	100
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- <a href="#">MODELLER</a> (version 9.20)</li> <li>- <a href="#">Modeller</a> (version 9.24)</li> <li>- <a href="#">CNS</a> (version 1.3)</li> </ul>