

**Summary of integrative structure determination of Escherichia coli sigma70 in apo form  
(PDB ID: 9A8C, PDB-Dev ID: PDBDEV\_00000377)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	RNA polymerase sigma factor RpoD: Chain A (536 residues)
<a href="#">Datasets used for modeling</a>	- Crosslinking-MS data, Linker name and number of cross-links: BS3, 1 cross-links - Experimental model, PDB ID: 6P1K
<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: 1-536
<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 CrossLinkRestrict: BS3, 1 cross-links - 1 unique CrossLinkRestrict: DMTMM, 1 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>	4
<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

<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 62.61, Number of Ramachandran outliers = 8, Number of sidechain outliers = 1</li> <li>- Model-2: Clashscore = 56.24, Number of Ramachandran outliers = 8, Number of sidechain outliers = 1</li> <li>- Model-3: Clashscore = 43.32, Number of Ramachandran outliers = 9, Number of sidechain outliers = 1</li> <li>- Model-4: Clashscore = 61.34, Number of Ramachandran outliers = 8, Number of sidechain outliers = 1</li> </ul>
<a href="#">Model quality: assessment of excluded volume</a>	Not applicable
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">Method</a>	Docking
<a href="#">Name</a>	None
2. <a href="#">Method</a>	Docking
<a href="#">Name</a>	None
3. <a href="#">Method</a>	Docking
<a href="#">Name</a>	None
<a href="#">Software</a>	<ul style="list-style-type: none"> <li>- <a href="#">PatchDock</a> (version 1.3)</li> <li>- <a href="#">ChimeraX</a> (version 1.2.5)</li> </ul>