

**Summary of integrative structure determination of Dipeptide repeat designed model, 4x DPR2, verified with CD and NMR data. (PDB ID: 9A8B, PDB-Dev ID: PDBDEV\_00000376)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	ACE-ZTR-PRO-ZTR-PRO-ZTR-PRO-ZTR-PRO-NME peptide: chain(s) A (10 residues)
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- NMR data, BMRB: <a href="#">52499</a></li> <li>- Other, Not available</li> <li>- NMR data, BMRB: <a href="#">52504</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	0, 1
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	
<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>	1
<a href="#">Model precision (uncertainty of models)</a>	Not available
<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>- Clashscore: 0.00</li> <li>- Ramachandran outliers: 0</li> <li>- Sidechain outliers: 0</li> </ul>
<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="#">Name</a>	None

<a href="#"><i>Description</i></a>	Computational model produced with in-house monomer and dimer sampling protocols using AIMnet(SMD)-D4 for energy minimizations and scoring.
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"><li>- <a href="#">PDBStat</a> (version 5.21)</li><li>- <a href="#">Poky</a> (version build 20220114)</li><li>- <a href="#">AIMNet</a> (version AIMNet(SMD)-D4)</li><li>- <a href="#">Cambridge Structural Database (CSD)</a></li><li>- <a href="#">ConfGen</a> (version Not available)</li><li>- <a href="#">SciPy</a> (version Not available)</li></ul>