

**Summary of integrative structure determination of A metastable contact and structural disorder in the estrogen receptor transactivation domain (PDB ID: 8ZZR, PDB-Dev ID: PDBDEV\_0000027)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	Estrogen receptor: Chain A (184 residues)
<a href="#">Datasets used for modeling</a>	- SAS data, SASBDB: SASDEE2 - Other, File: 10.1016/j.str.2018.10.026
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
Number of <a href="#">rigid bodies</a> , <a href="#">flexible units</a>	1, 0
<a href="#">Rigid bodies</a>	A: 1-184:None
<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 SASRestraint: Assembly name: Complete assembly Fitting method: ? Multi-state: False
<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>	10
<a href="#">Model precision (uncertainty of models)</a>	Model precision can not be calculated with one structure
<a href="#">Data quality</a>	SASDEE2: Rg from Guinier is 3.0nm and Rg from p(r) is 3.11nm

<p><a href="#"><i>Model quality: assessment of atomic segments</i></a></p>	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10</li> <li>- Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 4, Number of sidechain outliers = 2</li> <li>- Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 3, Number of sidechain outliers = 6</li> <li>- Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 2, Number of sidechain outliers = 6</li> <li>- Model-5: Clashscore = 0.0, Number of Ramachandran outliers = 7, Number of sidechain outliers = 15</li> <li>- Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 6, Number of sidechain outliers = 8</li> <li>- Model-7: Clashscore = 0.0, Number of Ramachandran outliers = 4, Number of sidechain outliers = 12</li> <li>- Model-8: Clashscore = 0.0, Number of Ramachandran outliers = 6, Number of sidechain outliers = 7</li> <li>- Model-9: Clashscore = 0.0, Number of Ramachandran outliers = 7, Number of sidechain outliers = 8</li> <li>- Model-10: Clashscore = 0.0, Number of Ramachandran outliers = 4, Number of sidechain outliers = 7</li> </ul>
<p><a href="#"><i>Model quality: assessment of excluded volume</i></a></p>	<p>Not applicable</p>
<p><a href="#"><i>Fit to data used for modeling</i></a></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><a href="#"><i>Fit to data used for validation</i></a></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p><b>5. Methodology and Software</b></p>	
<p>1. <a href="#"><i>Method</i></a></p>	<p>Modeling estrogen receptor N-terminal domain</p>
<p><a href="#"><i>Name</i></a></p>	<p>?</p>
<p><a href="#"><i>Software</i></a></p>	<p><a href="#">iSPOT</a> (version Not available)</p>