

**Summary of integrative structure determination of a metastable contact and structural disorder in the estrogen receptor transactivation domain (PDBDEV00000027)**

<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, SASDEE2 - Hydroxyl radical protein footprinting, Not listed
<b>2. Representation</b>	
<a href="#">Atomic structural coverage</a>	100%
<a href="#">Number of rigid bodies, flexible units</a>	1, 0
<a href="#">Rigid bodies</a>	- A: 1-184:None.
<a href="#">Flexible units</a>	- A: -
<a href="#">Resolution</a>	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
<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="#">Sampling validation</a>	- Information related to sampling validation has not been provided
<a href="#">Clustering algorithm ,clustering feature</a>	Distance threshold-based clustering used if ensembles are deposited, Not applicable
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Model precision (uncertainty of models)</a>	Model precision can not be calculated with one structure
<a href="#">Quality of data</a>	- SASDEE2: Rg from Gunier is 3.11nm and Rg from p(r) is 3.0nm
<a href="#">Model quality: assessment of atomic segments</a>	Clashscore: 0.0, Ramachandran outliers: 2.56% , Sidechain outliers: 5.51%
<a href="#">Model quality: assessment of excluded volume</a>	- Not applicable
<a href="#">Fit of the model to information used to compute it</a>	- SASDEE2: Fit 1 with X <sup>2</sup> value 0.14 - SASDEE2: Fit 2 with X <sup>2</sup> value 0.34 - SASDEE2: Fit 3 with X <sup>2</sup> value 0.51

<a href="#"><i>Fit of the model to information not used to compute it</i></a>	- Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<a href="#"><i>Method</i></a>	Modeling estrogen receptor N-terminal domain
<a href="#"><i>Name</i></a>	?
<a href="#"><i>Details</i></a>	- Method details unspecified
<a href="#"><i>Software</i></a>	- iSPOT (version None) - No location specified