

**Summary of integrative structure determination of serum albumin domain a structure  
(PDBDEV00000005)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	- HSA_A: Chain A (197 residues)
<a href="#">Datasets used for modeling</a>	- CX-MS data, Linker name and number of cross-links: sulfo-SDA, 320 cross-links - unspecified, 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: 1-197: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 CrossLinkRestraint: sulfo-SDA, 320 cross-links
<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>	- Quality of input data has not be assessed
<a href="#">Model quality: assessment of atomic segments</a>	Clashscore: 6.71, Ramachandran outliers: 1.33% , Sidechain outliers: 0.82%
<a href="#">Model quality: assessment of excluded volume</a>	- Not applicable
<a href="#">Fit of the model to information used to compute it</a>	- Fit of model to information used to compute it has not been determined

<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>	Conformational search
<a href="#"><i>Name</i></a>	Model-based search (MBS) in Rosetta
<a href="#"><i>Details</i></a>	- Method details unspecified
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"><li>- Rosetta MBS (version None)</li><li>- EPC-map (version None)</li><li>- No location specified</li></ul>