

**Summary of integrative structure determination of Serum Albumin Domain B Structure
(PDB ID: 8ZZ6, PDB-Dev ID: PDBDEV_0000006)**

1. Model Composition	
Entry composition	HSA_B: Chain A (189 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: sulfo-SDA, 107 cross-links - Other, File: 10.5281/zenodo.1035833
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	1, 0
Rigid bodies	A: 1-189:None
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: sulfo-SDA, 107 cross-links - 95 unique PredictedContactRestraint: Distance: 8.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	5
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Model-1: Clashscore = 5.69, Number of Ramachandran outliers = 0, Number of sidechain outliers = 4 - Model-2: Clashscore = 1.67, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-3: Clashscore = 4.02, Number of Ramachandran outliers = 0, Number of sidechain outliers = 1 - Model-4: Clashscore = 2.34, Number of Ramachandran outliers = 0, Number of sidechain outliers = 2 - Model-5: Clashscore = 3.01, Number of Ramachandran outliers = 0, Number of sidechain outliers = 1
<i>Model quality: assessment of excluded volume</i>	Not applicable
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Method</i>	Conformational search
<i>Name</i>	Model-based search (MBS) in Rosetta
<i>Number of computed models</i>	5000
<i>Software</i>	<ul style="list-style-type: none"> - Rosetta MBS (version Not available) - EPC-map (version Not available)