Summary of integrative structure determination of serum albumin domain b structure (PDBDEV00000006)

1. Model Composition	
Entry composition	- HSA_B: Chain A (189 residues)
Datasets used for modeling	- CX-MS data, Linker name and number of cross-links: sulfo-SDA, 107 cross-links - unspecified, Not listed
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	1, 0
Rigid bodies	- A: 1-189:None.
Flexible units	- A: -
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: sulfo-SDA, 107 cross-links
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, Not applicable
Number of ensembles	0
Number of models in ensembles	Not applicable
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Clashscore: 5.36, Ramachandran outliers: 0.0% , Sidechain outliers: 0.97%
Model quality: assessment of excluded volume	- Not applicable
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined

Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Conformational search
Name	Model-based search (MBS) in Rosetta
Details	- Method details unspecified
Software	- Rosetta MBS (version None) - EPC-map (version None) - No location specified