## Summary of integrative structure determination of serum albumin domain c structure (PDBDEV00000007)

1. Model Composition	
Entry composition	- HSA_C: Chain A (192 residues)
Datasets used for modeling	- CX-MS data, Linker name and number of cross-links: sulfo-SDA, 248 cross-links - unspecified, Not listed
2. Representation	
Atomic structural coverage	100%
Number of <u>rigid bodies</u> , <u>flexible units</u>	1, 0
Rigid bodies	- A: 1-192: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, 248 crosslinks
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: 3.94, Ramachandran outliers: 0.11%, Sidechain outliers: 0.12%
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	
<u>Method</u>	Conformational search
<u>Name</u>	Model-based search (MBS) in Rosetta
<u>Details</u>	- Method details unspecified
<u>Software</u>	- Rosetta MBS (version None) - EPC-map (version None) - No location specified