

Summary of integrative structure determination of Serum Albumin Domain A Structure (PDB ID: 8ZZ5, PDB-Dev ID: PDBDEV_00000005)

1. Model Composition	
Entry composition	HSA_A: chain(s) A (197 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD001692 - Predicted contacts, Zenodo: 10.5281/zenodo.1035833
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	1, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestrict: sulfo-SDA, 320 crosslinks - 99 unique PredictedContactRestrict: 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)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 3.84-8.31 - Ramachandran outliers: 1-3 - Sidechain outliers: 0-4
Fit to data used for modeling	Satisfaction of crosslinks: 68.75-82.19%
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	Conformational search

<i>Method</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)