# Summary of integrative structure determination of Serum Albumin Domain B Structure (PDB ID: 8ZZ6, PDB-Dev ID: PDBDEV_00000006)

| ***1. Model Composition*** | |
|---|---|
| *Entry composition* | HSA_B: chain(s) A (189 residues) |
| *Datasets used for modeling* | - Crosslinking-MS data, PRIDE: PXD001692<br>- 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 CrossLinkRestraint: sulfo-SDA, 107 crosslinks<br>- 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)* | Not available |
| *Data quality* | Data quality has not been assessed |
| *Model quality: assessment of atomic segments* | - Clashscore: 1.67-5.69<br>- Ramachandran outliers: 0-0<br>- Sidechain outliers: 0-4 |
| *Fit to data used for modeling* | Satisfaction of crosslinks: 85.98-92.52% |
| *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 |

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|---|---|
| *Method* | Model-based search (MBS) in Rosetta |
| *Number of computed models* | 5000 |
| *Software* | - Rosetta MBS (version Not available)<br>- EPC-map (version Not available) |