

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

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| PDB ID | PDBDEV00000007 |
| Molecule Name | Serum Albumin Domain C Structure |
| Title | Serum Albumin Domain Structures in Human Blood Serum by Mass Spectrometry and Computational E |
| Authors | Belsom A;Schneider M;Fischer L;Brock O;Rappsilber J |

The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobitry : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There are 1 unique types of models in this entry. The entry contains 1 chains.

| Molecule ID | Molecule Name | Chain ID | Total Residues |
|-------------|---------------|----------|----------------|
| 1 | HSA_C | A | 192 |

There are 2 software packages reported in this entry.

| ID | Software Name | Software Version | Software Classification |
|----|---------------|------------------|-------------------------|
| 1 | Rosetta MBS | None | Model Building |
| 2 | EPC-map | None | Contact Predictor |

There are 2 unique datasets used to build the model(s) in this entry.

| ID | Dataset Type | Database Name | Data Access Code |
|----|--------------|---------------|------------------|
| 1 | CX-MS data | PRIDE | PXD001692 |
| 2 | unspecified | Not Listed | None |

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertainty of model
