

Full wwPDB Integrative Structure Validation Report

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PDB ID	PDBDEV00000006
Molecule Name	Serum Albumin Domain B Structure
Title	Serum Albumin Domain Structures in Human Blood Serum by Mass Spectrometry and Computational E
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The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobit : 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_B	A	189

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
