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 Biology
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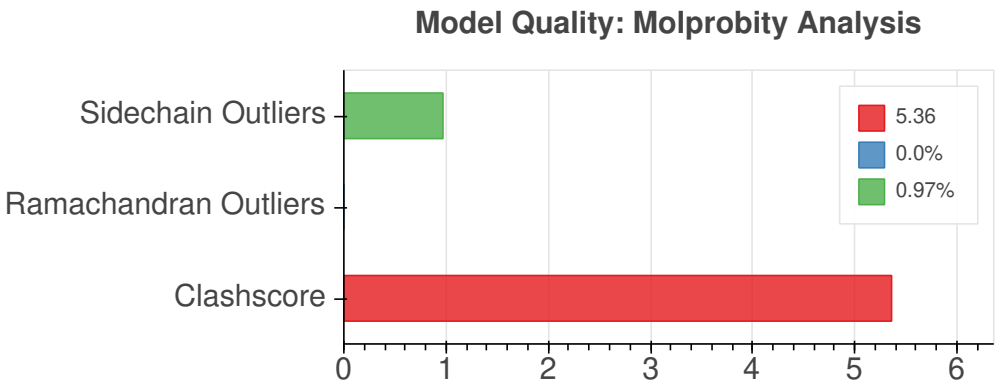
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 5 unique models, with 1 subunits in each model. A total of 2 datasets or restraints was used to build this entry. Each model is represented by 1 rigid bodies and 0 flexible or non-rigid units.

3.2 Entry composition

There are 5 unique types of models in this entry.These models are titled Best scoring model (domain B), 2nd best scoring model (domain B), 3rd best scoring model (domain B), 4th best scoring model (domain B), 5th best scoring model (domain B) respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	HSA_B	A	189
2	1	1	HSA_B	A	189
3	1	1	HSA_B	A	189
4	1	1	HSA_B	A	189
5	1	1	HSA_B	A	189

3.3 Datasets used for modeling

There are 2 unique datasets used to build the models in this entry.

ID	*Dataset type*	*Database name*	*Data access code*
1	CX-MS data	PRIDE	PXD001692
2	unspecified	Not listed	None

4. Representation

This entry has only one representation and includes 1 rigid bodies and 0 flexible units.

Chain ID	*Rigid bodies*	*Non-rigid segments*
A	1-189:None.	-

5. Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Model-based search (MBS) in Rosetta	Conformational search	5000	False	True

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

6. Data quality

7. Model quality

7.1 Standard geometry

There are 7400 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD2	1.089	0.93	104
CE2--HE2	1.088	0.93	79
CD1--HD1	1.088	0.93	84
CE1--HE1	1.089	0.93	104
CH2--HH2	1.089	0.93	4
CZ2--HZ2	1.089	0.93	4
CZ3--HZ3	1.089	0.93	4
CZ--HZ	1.088	0.93	44
CE3--HE3	1.088	0.93	4
NE--HE	1.011	0.86	34

NH2--HH21	1.01	0.86	34
N--H	1.008	0.86	899
NE2--HE2	1.009	0.86	24
NH1--HH11	1.009	0.86	34
NH1--HH12	1.009	0.86	34
NE1--HE1	1.009	0.86	4
NH2--HH22	1.008	0.86	34
NE2--HE21	1	0.86	24
ND2--HD21	0.999	0.86	19
NE2--HE22	0.999	0.86	24
ND2--HD22	0.998	0.86	19
CG--HG2	1.088	0.97	304
CG--HG3	1.088	0.97	304
CB--HB2	1.087	0.97	819
CB--HB3	1.087	0.97	819
CD--HD2	1.089	0.97	164
CD--HD3	1.089	0.97	164
CA--HA	1.088	0.97	929
SG--HG	1.328	1.2	54
NZ--HZ2	1.009	0.89	89
CD2--HD21	1.089	0.97	104
CA--HA2	1.089	0.97	14
CG1--HG11	1.089	0.97	59
CG1--HG13	1.089	0.97	79
NZ--HZ1	1.009	0.89	89
CE--HE2	1.088	0.97	99
OG1--HG1	0.96	0.84	29

CD2--HD23	1.089	0.97	104
CD1--HD12	1.089	0.97	124
OG--HG	0.959	0.84	49
CD2--HD22	1.089	0.97	104
CD1--HD11	1.089	0.97	124
CG1--HG12	1.088	0.97	79
CG2--HG23	1.088	0.97	109
CG--HG	1.089	0.97	104
CB--HB	1.088	0.97	109
CE--HE3	1.088	0.97	99
NZ--HZ3	1.009	0.89	89
OH--HH	0.959	0.84	34
CG2--HG21	1.088	0.97	109
CB--HB1	1.088	0.97	104
CG2--HG22	1.088	0.97	109
CE--HE1	1.09	0.97	9
CA--HA3	1.088	0.97	14
CD1--HD13	1.088	0.97	124
N--H1	1	0.89	4
N--H3	1	0.89	4
N--H2	1	0.89	4

There are 119 angle outliers in this entry.

Angle type	***Observed angle (°)***	***Ideal angle (°)***	***Number of outliers***
CA-CB-HB3	93.397	109	19
CB-CG-HG3	94.637	109	24
CB-CG-HG2	122.721	109	24
H1-N-H3	97.224	109.47	4

H2-N-H3	97.206	109.47	4
H1-N-H2	97.229	109.47	4
CZ-NE-HE	105.873	117.9	33

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	*Clash score*	*Number of clashes*
Model 1	5.36	16
Model 2	1.67	5
Model 3	4.02	12
Model 4	2.01	6
Model 5	2.68	8

All 47 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	187	184	3	0
2	187	186	1	0
3	187	186	1	0
4	187	182	5	0
5	187	185	2	0

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	165	157	4	4
2	165	165	0	0
3	165	161	3	1
4	165	162	1	2
5	165	163	1	1

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:18	LEU
1	A:74	LEU
1	A:130	LEU
1	A:156	LEU
3	A:59	LEU
4	A:18	LEU
4	A:50	LEU
5	A:18	LEU

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model