Full wwPDB Integrative Structure Validation Report

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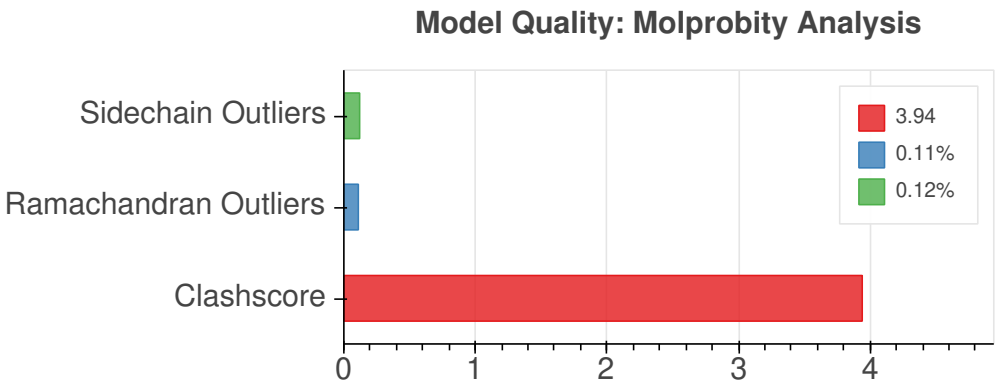
The following software were used in the production of this report:

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 C), 2nd best scoring model (domain C), 3rd best scoring model (domain C), 4th best scoring model (domain C), 5th best scoring model (domain C) respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	HSA_C	A	192
2	1	1	HSA_C	A	192
3	1	1	HSA_C	A	192
4	1	1	HSA_C	A	192
5	1	1	HSA_C	A	192

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	1-192: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 7680 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD2	1.089	0.93	84
CE2--HE2	1.088	0.93	64
CE1--HE1	1.089	0.93	84
CD1--HD1	1.089	0.93	64
CZ--HZ	1.088	0.93	44
NE--HE	1.01	0.86	34
N--H	1.008	0.86	914
NH2--HH21	1.01	0.86	34
NH1--HH11	1.009	0.86	34
NE2--HE2	1.009	0.86	19

NH1--HH12	1.009	0.86	34
NH2--HH22	1.008	0.86	34
NE2--HE21	1	0.86	39
ND2--HD21	0.999	0.86	29
NE2--HE22	0.999	0.86	39
ND2--HD22	0.998	0.86	29
CB--HB2	1.088	0.97	769
CG--HG3	1.087	0.97	339
CA--HA	1.088	0.97	939
CG--HG2	1.088	0.97	339
CD--HD3	1.088	0.97	189
CB--HB3	1.087	0.97	769
CD--HD2	1.088	0.97	189
SG--HG	1.328	1.2	59
CG--HG	1.089	0.97	84
CD2--HD21	1.089	0.97	84
CE--HE2	1.088	0.97	124
NZ--HZ2	1.009	0.89	114
CE--HE3	1.088	0.97	124
CG1--HG11	1.089	0.97	94
OG1--HG1	0.958	0.84	64
CD1--HD12	1.089	0.97	94
CB--HB	1.089	0.97	169
CG2--HG23	1.088	0.97	169
CE--HE1	1.089	0.97	9
CD1--HD11	1.089	0.97	94
CD2--HD22	1.089	0.97	84

CD2--HD23	1.089	0.97	84
CG2--HG22	1.088	0.97	169
NZ--HZ1	1.008	0.89	114
CG2--HG21	1.088	0.97	169
OH--HH	0.959	0.84	19
CG1--HG13	1.088	0.97	104
CB--HB1	1.089	0.97	84
OG--HG	0.959	0.84	44
NZ--HZ3	1.009	0.89	114
CD1--HD13	1.088	0.97	94
CG1--HG12	1.088	0.97	104
CA--HA2	1.089	0.97	19
CA--HA3	1.089	0.97	19
N--H1	1	0.89	4
N--H3	1	0.89	4
N--H2	1	0.89	4

There are 160 angle outliers in this entry.

Angle type	*Observed angle (°)*	*Ideal angle (°)*	*Number of outliers*
CA-CB-HB3	93.414	109	29
CB-CG-HG3	94.641	109	39
CB-CG-HG2	122.703	109	39
H1-N-H3	97.22	109.47	4
H2-N-H3	97.207	109.47	4
H1-N-H2	97.258	109.47	4
CZ-NE-HE	105.887	117.9	34

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	3.94	12
Model 2	2.63	8
Model 3	2.63	8
Model 4	2.63	8
Model 5	4.27	13

All 49 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	190	185	5	0
2	190	185	4	1
3	190	189	1	0
4	190	185	5	0
5	190	183	7	0

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
2	A:93	ASN

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	171	169	2	0
2	171	169	1	1
3	171	171	0	0
4	171	171	0	0
5	171	171	0	0

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
2	A:110	LYS

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model