# Full wwPDB Integrative Structure Validation Report

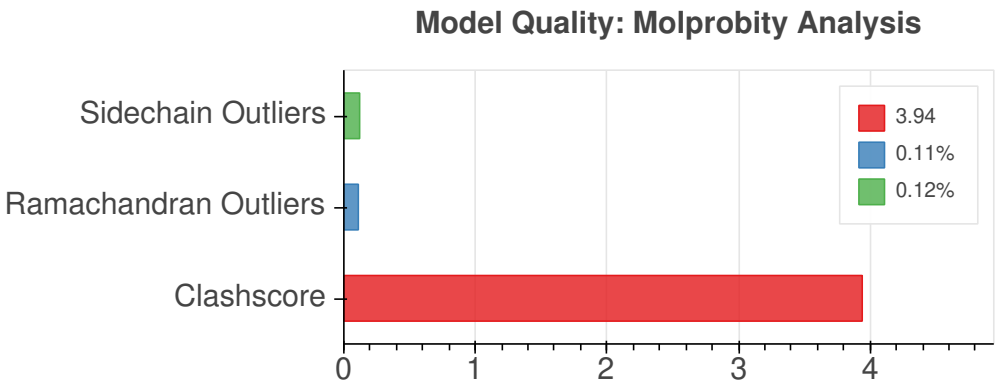
## November 05, 2019 -- 04:07 PM

| ***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 |
| Authors | Belsom A;Schneider M;Fischer L;Brock O;Rappsilber J |

**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