Full wwPDB Integrative Structure Validation Report

June 26, 2020 -- 12:01 PM

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

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000005
Molecule Name	Serum Albumin Domain A 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

Overall quality

Ensemble information

This entry consists of 0 distinct ensemble.

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.

Entry composition

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	HSA_A	A	197
2	1	1	HSA_A	A	197
3	1	1	HSA_A	A	197
4	1	1	HSA_A	A	197
5	1	1	HSA_A	A	197

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

Data quality

Model quality

Standard geometry

There are 7715 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD2	1.089	0.93	129
CD1--HD1	1.089	0.93	99
CE2--HE2	1.088	0.93	99
CE1--HE1	1.089	0.93	129
CZ--HZ	1.088	0.93	64
NE--HE	1.01	0.86	49
NH2--HH21	1.01	0.86	49
N--H	1.008	0.86	939
NH1--HH11	1.009	0.86	49
NE2--HE2	1.009	0.86	29
NH1--HH12	1.008	0.86	49
NH2--HH22	1.008	0.86	49
NE2--HE21	1.0	0.86	34
NE2--HE22	0.999	0.86	34
ND2--HD21	1.0	0.86	34
ND2--HD22	0.998	0.86	34
CD--HD2	1.089	0.97	174
CG--HG3	1.088	0.97	324

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD--HD3	1.088	0.97	174
CB--HB3	1.087	0.97	859
CA--HA	1.088	0.97	964
CG--HG2	1.089	0.97	324
CB--HB2	1.087	0.97	859
SG--HG	1.328	1.2	59
CE--HE2	1.087	0.97	94
CD1--HD12	1.088	0.97	114
CG--HG	1.089	0.97	104
NZ--HZ2	1.009	0.89	84
CG2--HG22	1.089	0.97	104
OG1--HG1	0.958	0.84	44
OH--HH	0.959	0.84	34
CG1--HG11	1.089	0.97	49
CD2--HD21	1.089	0.97	104
CG2--HG23	1.088	0.97	104
NZ--HZ1	1.009	0.89	84
CD1--HD11	1.089	0.97	114
CG1--HG13	1.088	0.97	59
CB--HB1	1.089	0.97	114
CE--HE3	1.089	0.97	94
CB--HB	1.089	0.97	104
CD2--HD22	1.089	0.97	104

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ3	1.008	0.89	84
OG--HG	0.959	0.84	24
CD2--HD23	1.089	0.97	104
CG1--HG12	1.088	0.97	59
CG2--HG21	1.088	0.97	104
CA--HA2	1.09	0.97	19
CE--HE1	1.09	0.97	9
CD1--HD13	1.088	0.97	114
CA--HA3	1.088	0.97	19
N--H3	1.0	0.89	4
N--H1	1.0	0.89	4
N--H2	1.0	0.89	4

There are 170 angle outliers in this entry.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB3	93.422	109.0	34
CB-CG-HG3	94.661	109.0	34
CB-CG-HG2	122.705	109.0	34
H2-N-H3	97.182	109.47	4
H1-N-H3	97.194	109.47	4
H1-N-H2	97.185	109.47	4
CZ-NE-HE	105.888	117.9	49

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	6.71	21
Model 2	3.84	12
Model 3	7.99	25
Model 4	6.39	20
Model 5	5.43	17

All 95 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	195	183	9	3
2	195	179	13	3
3	195	187	7	1
4	195	180	12	3
5	195	178	14	3

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:51	ALA
1	A:165	CYS
1	A:170	LYS
2	A:82	GLU
2	A:92	PRO
2	A:115	GLU

Model ID	Chain and res ID	Residue type
3	A:51	ALA
4	A:51	ALA
4	A:165	CYS
4	A:170	LYS
5	A:82	GLU
5	A:92	PRO
5	A:143	PRO

Torsion angles: 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	170	165	1	4
2	170	168	1	1
3	170	166	4	0
4	170	166	3	1
5	170	168	1	1

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:50	VAL
1	A:70	LEU
1	A:89	LYS
1	A:195	LYS
2	A:178	LEU
4	A:50	VAL

Model ID	Chain and res ID	Residue type
5	A:144	TYR

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model