Integrative Structure Validation Report

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

Integrative Modeling Validation Version 2.0
Python-IHM Version 1.8
MolProbity Version 4.5.2

PDB ID	8ZZ6
PDB-Dev ID	PDBDEV_00000006
Structure Title	Serum Albumin Domain B Structure
Structure Authors	Belsom A; Schneider M; Fischer L; Brock O; Rappsilber J
Deposited on	2017-11-01

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

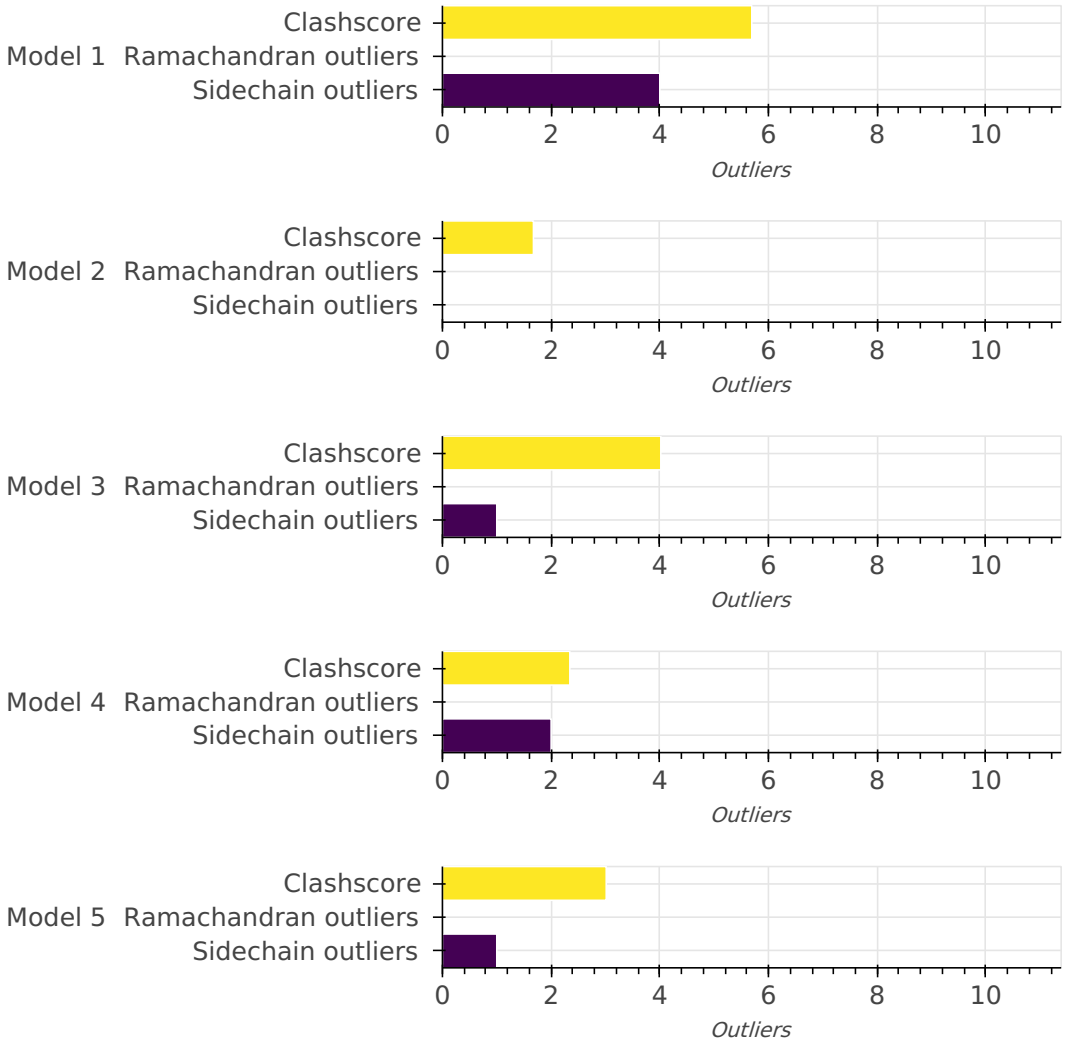
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

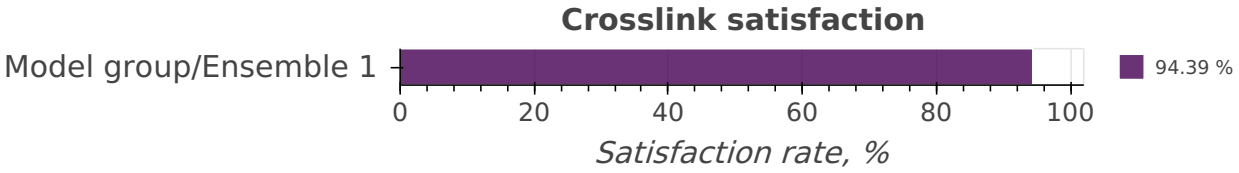
List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis





Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 5 model(s). A total of 2 datasets were used to build this entry.

Representation

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-5	1	HSA_B	A	189	1-189	-	100.00 / 0.00	Atomic

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	Crosslinking-MS data	PRIDE	PXD001692
2	Predicted contacts	Zenodo	10.5281/zenodo.1035833

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Conformational search	Model-based search (MBS) in Rosetta	None	5000	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Rosetta MBS	Not available	Model Building	https://compbio.robotics.tu-berlin.de/rbo_aleph
2	EPC-map	Not available	Contact Predictor	https://compbio.robotics.tu-berlin.de/epsilon

Data quality

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully compliant dataset in the PRIDE Crosslinking database. Correspondence between crosslinking-MS and entry entities is established using pyHMMER. Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the PRIDE Crosslinking database.

Predicted contacts

Validation for this section is under development.

Model quality

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 34 bond length outliers in this entry (0.44% of 7680 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	178	PRO	N-CD	8.78	1.60	1.47	4	5
A	183	PRO	N-CD	8.33	1.59	1.47	2	5
A	102	PRO	N-CD	5.47	1.55	1.47	5	5
A	81	PRO	N-CD	5.38	1.55	1.47	4	5
A	98	PRO	N-CD	5.03	1.54	1.47	1	4
A	165	PRO	N-CD	4.90	1.54	1.47	5	5
A	138	PRO	N-CD	4.71	1.54	1.47	1	3
A	23	PRO	N-CD	4.06	1.53	1.47	1	2

Standard geometry: angle outliers

There are 55 bond angle outliers in this entry (0.53% of 10370 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	88	CYS	N-CA-CB	4.60	102.68	110.50	1	5
A	168	CYS	N-CA-CB	4.59	102.70	110.50	3	5
A	64	CYS	N-CA-CB	4.59	102.70	110.50	4	5

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	52	CYS	N-CA-CB	4.58	102.71	110.50	4	5
A	77	CYS	N-CA-CB	4.58	102.71	110.50	4	5
A	44	CYS	N-CA-CB	4.58	102.71	110.50	4	5
A	159	CYS	N-CA-CB	4.58	102.72	110.50	4	5
A	45	CYS	N-CA-CB	4.57	102.72	110.50	5	5
A	115	CYS	N-CA-CB	4.57	102.73	110.50	1	5
A	160	CYS	N-CA-CB	4.57	102.74	110.50	4	5
A	78	CYS	N-CA-CB	4.57	102.74	110.50	1	5

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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	5.69	17
2	1.67	5
3	4.02	12
4	2.34	7
5	3.01	9

There are 50 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are >= 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:49:LEU:O	A:52:CYS:SG	0.69	4	1
A:122:LYS:H	A:122:LYS:HD2	0.61	1	1
A:61:LYS:HA	A:64:CYS:SG	0.58	5	1
A:157:GLU:O	A:160:CYS:SG	0.57	3	1
A:50:LEU:O	A:50:LEU:HD23	0.56	4	1
A:37:LEU:O	A:37:LEU:HD23	0.53	1	1
A:41:HIS:HE1	A:52:CYS:SG	0.53	3	1
A:37:LEU:C	A:37:LEU:HD23	0.52	1	1
A:182:GLU:HB2	A:183:PRO:HD3	0.52	1	2
A:122:LYS:HD2	A:122:LYS:N	0.52	1	1
A:177:LYS:N	A:178:PRO:CD	0.52	3	3
A:122:LYS:CD	A:122:LYS:H	0.51	1	1
A:111:SER:O	A:115:CYS:SG	0.50	1	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:182:GLU:N	A:183:PRO:CD	0.49	4	4
A:85:LYS:O	A:88:CYS:SG	0.49	2	2
A:125:PHE:HD1	A:125:PHE:O	0.49	1	1
A:112:LYS:O	A:115:CYS:SG	0.49	4	2
A:74:LEU:O	A:78:CYS:SG	0.48	3	1
A:182:GLU:HB3	A:183:PRO:HD3	0.47	4	3
A:75:LYS:HA	A:78:CYS:SG	0.47	5	1
A:133:TYR:HD1	A:133:TYR:O	0.46	1	1
A:177:LYS:HB3	A:178:PRO:HD3	0.45	2	3
A:41:HIS:CE1	A:52:CYS:SG	0.45	3	1
A:84:GLU:O	A:88:CYS:SG	0.45	4	2
A:75:LYS:O	A:78:CYS:SG	0.45	5	1
A:164:ASP:O	A:168:CYS:SG	0.44	1	1
A:156:LEU:O	A:159:CYS:HB2	0.44	1	1
A:18:LEU:HD23	A:59:LEU:HD21	0.43	3	1
A:156:LEU:HA	A:156:LEU:HD12	0.43	1	1
A:125:PHE:C	A:125:PHE:CD1	0.43	1	1
A:50:LEU:CD2	A:50:LEU:O	0.42	4	1
A:155:THR:O	A:159:CYS:SG	0.42	3	1
A:2:LEU:O	A:2:LEU:HD23	0.41	5	1
A:41:HIS:HA	A:44:CYS:HB2	0.41	5	1
A:177:LYS:N	A:178:PRO:HD2	0.41	2	1
A:2:LEU:C	A:2:LEU:HD23	0.40	5	1

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	Analysed	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

Torsion angles : Protein sidechains

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

Model ID	Analysed	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

There are 6 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	18	LEU	3
A	50	LEU	1
A	59	LEU	1
A	74	LEU	1
A	130	LEU	1
A	156	LEU	1

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 107 crosslinking restraints combined in 107 restraint groups.

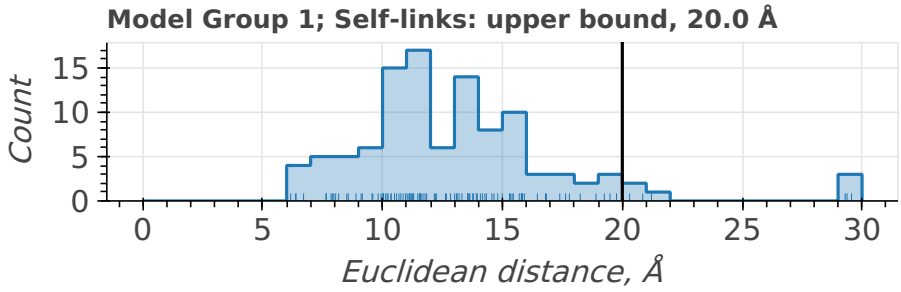
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
sulfo-SDA	ASP	CA	THR	CA	upper bound	20.0	4
sulfo-SDA	LEU	CA	SER	CA	upper bound	20.0	1
sulfo-SDA	PHE	CA	THR	CA	upper bound	20.0	2
sulfo-SDA	GLU	CA	THR	CA	upper bound	20.0	2
sulfo-SDA	GLU	CA	LYS	CA	upper bound	20.0	9
sulfo-SDA	ASP	CA	TYR	CA	upper bound	20.0	2
sulfo-SDA	LYS	CA	PHE	CA	upper bound	20.0	5
sulfo-SDA	LEU	CA	LYS	CA	upper bound	20.0	6
sulfo-SDA	LEU	CA	TYR	CA	upper bound	20.0	6
sulfo-SDA	GLY	CA	THR	CA	upper bound	20.0	2

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
sulfo-SDA	ASN	CA	THR	CA	upper bound	20.0	3
sulfo-SDA	GLY	CA	LYS	CA	upper bound	20.0	2
sulfo-SDA	HIS	CA	LYS	CA	upper bound	20.0	3
sulfo-SDA	ILE	CA	LYS	CA	upper bound	20.0	3
sulfo-SDA	ALA	CA	TYR	CA	upper bound	20.0	4
sulfo-SDA	LYS	CA	THR	CA	upper bound	20.0	3
sulfo-SDA	PRO	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	PHE	CA	SER	CA	upper bound	20.0	3
sulfo-SDA	GLN	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	GLU	CA	TYR	CA	upper bound	20.0	3
sulfo-SDA	SER	CA	VAL	CA	upper bound	20.0	2
sulfo-SDA	ASP	CA	LYS	CA	upper bound	20.0	3
sulfo-SDA	ARG	CA	THR	CA	upper bound	20.0	1
sulfo-SDA	ALA	CA	SER	CA	upper bound	20.0	2
sulfo-SDA	LYS	CA	TYR	CA	upper bound	20.0	3
sulfo-SDA	LYS	CA	SER	CA	upper bound	20.0	2
sulfo-SDA	PHE	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	ALA	CA	LYS	CA	upper bound	20.0	4
sulfo-SDA	LYS	CA	VAL	CA	upper bound	20.0	3
sulfo-SDA	HIS	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	LYS	CA	PRO	CA	upper bound	20.0	1
sulfo-SDA	ARG	CA	LYS	CA	upper bound	20.0	2
sulfo-SDA	ARG	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	HIS	CA	SER	CA	upper bound	20.0	2
sulfo-SDA	ILE	CA	SER	CA	upper bound	20.0	2
sulfo-SDA	SER	CA	TRP	CA	upper bound	20.0	1
sulfo-SDA	TYR	CA	VAL	CA	upper bound	20.0	1
sulfo-SDA	THR	CA	VAL	CA	upper bound	20.0	1
sulfo-SDA	LYS	CA	LYS	CA	upper bound	20.0	1
sulfo-SDA	ALA	CA	THR	CA	upper bound	20.0	1
sulfo-SDA	ASP	CA	SER	CA	upper bound	20.0	2
sulfo-SDA	ARG	CA	SER	CA	upper bound	20.0	1
sulfo-SDA	GLY	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	ASN	CA	TYR	CA	upper bound	20.0	1
sulfo-SDA	GLU	CA	SER	CA	upper bound	20.0	1

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
sulfo-SDA	GLN	CA	LYS	CA	upper bound	20.0	1

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



Satisfaction of restraints

Satisfaction of restraints is calculated on a restraint group (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=107)
1	1	1	5/5	All	94.39	5.61	107
				Self-links/ Intramolecular	94.39	5.61	107

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.

Predicted contacts

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgments

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