Integrative Structure Validation Report

February 27, 2025 - 12:16 PM PST

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	9A1B
PDB-Dev ID	PDBDEV_00000083
Structure Title	CS-Rosetta structure of engineered IgG-binding domain of protein G (GB) - model A1
Structure Authors	He Y; Chen Y; Ruan B; Choi EJ; Chen Y; Motabar D; Solomon T; Simmerman R; Kauffman T; Gallagher DT; Bryan PN; Orban J
Deposited on	2021-04-21

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

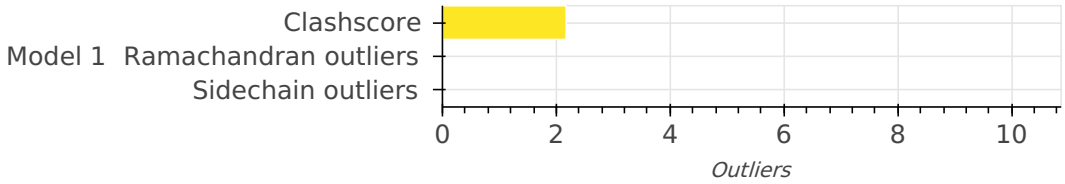
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

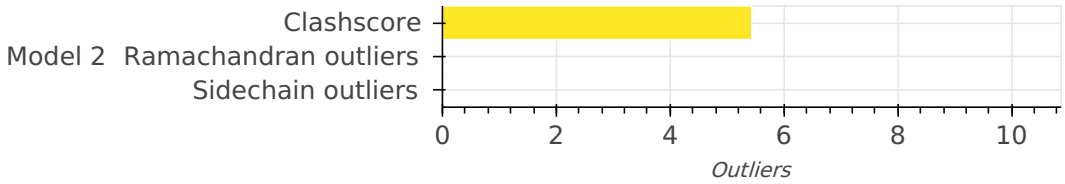
List of references used to build this report is available here.

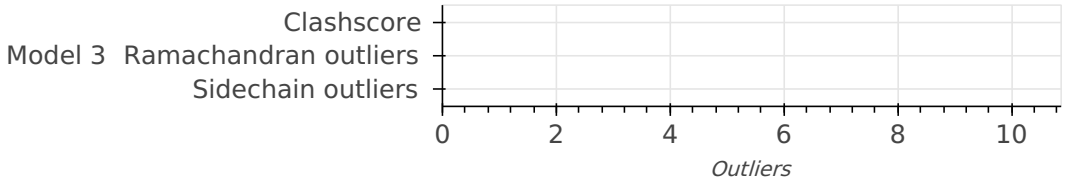
Overall quality

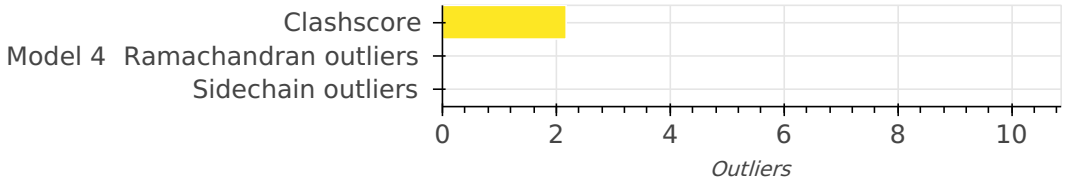
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

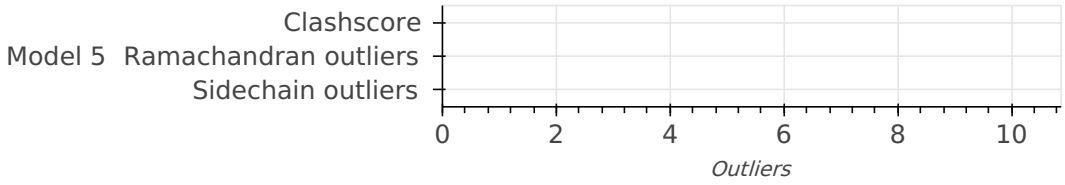
Model Quality: MolProbity Analysis

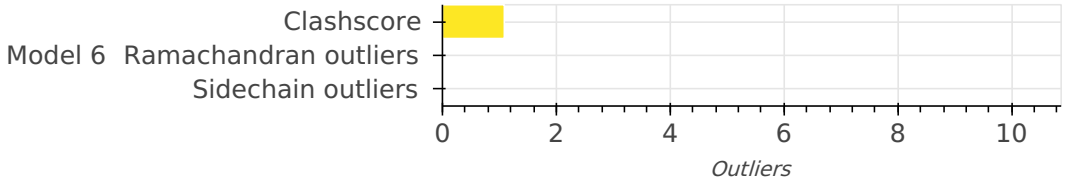

Clashscore
Model 1 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers

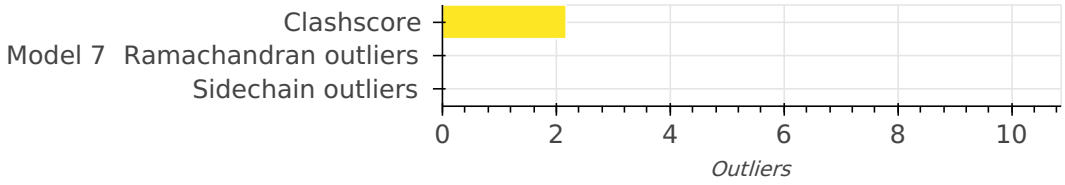

Clashscore
Model 2 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers

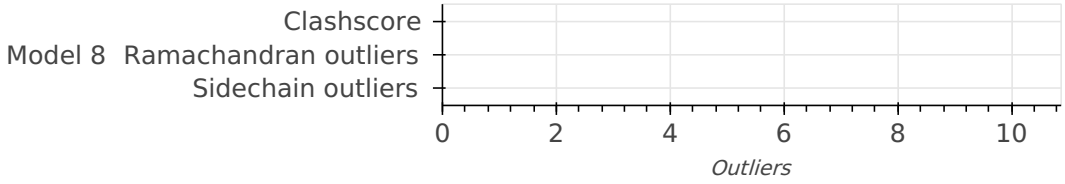

Clashscore
Model 3 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers

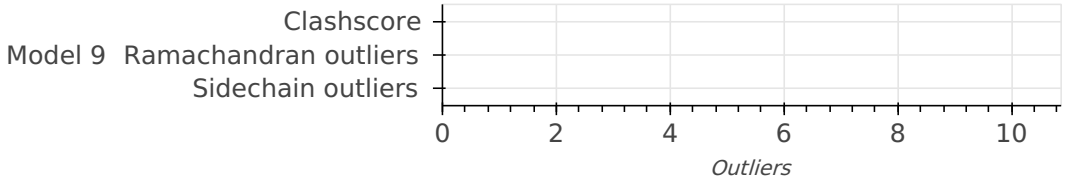

Clashscore
Model 4 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers

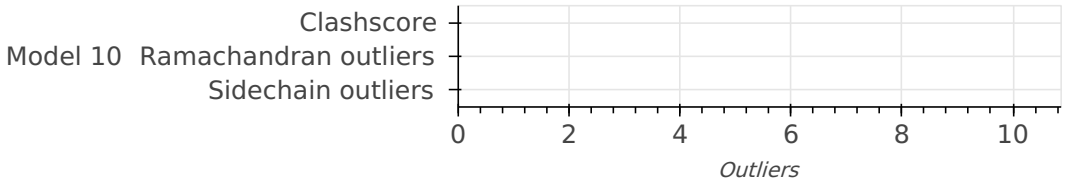

Clashscore
Model 5 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers


Clashscore
Model 6 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers


Clashscore
Model 7 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers


Clashscore
Model 8 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers


Clashscore
Model 9 Ramachandran outliers
Sidechain outliers
0 2 4 6 8 10
Outliers



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 model(s). A total of 1 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	1-10	1	Immunoglobulin G-binding protein G	A	56	-	1-56	100.00 / 0.00	Atomic

Datasets used for modeling

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	50907

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	CS-Rosetta modeling	–	–	–	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	CS-Rosetta	Not available	model building	https://spin.niddk.nih.gov/bax/software/CSROSETTA/

Data quality

NMR

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 no bond length outliers.

Standard geometry: angle outliers

There are no bond angle outliers.

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	2.17	2
2	5.43	5
3	0.00	0
4	2.17	2
5	0.00	0
6	1.09	1
7	2.17	2
8	0.00	0

Model ID	Clash score	Number of clashes
9	0.00	0
10	0.00	0

There are 12 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:9:LEU:O	A:9:LEU:HD23	0.71	2	1
A:9:LEU:C	A:9:LEU:HD23	0.62	2	1
A:50:LEU:O	A:50:LEU:HD23	0.60	4	4
A:50:LEU:C	A:50:LEU:HD23	0.59	4	5
A:9:LEU:C	A:9:LEU:CD2	0.47	2	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	54	54	0	0
2	54	54	0	0
3	54	54	0	0
4	54	54	0	0
5	54	54	0	0
6	54	53	1	0
7	54	54	0	0
8	54	54	0	0
9	54	54	0	0
10	54	54	0	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	46	46	0	0
2	46	45	1	0
3	46	46	0	0
4	46	46	0	0
5	46	46	0	0
6	46	45	1	0

Model ID	Analysed	Favored	Allowed	Outliers
7	46	46	0	0
8	46	46	0	0
9	46	46	0	0
10	46	45	1	0

Fit of model to data used for modeling

NMR

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the PDB-IHM team (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the RCSB PDB (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the Sali lab contributed model validation metrics and software packages.

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