Integrative Structure Validation Report July 22, 2024 - 04:25 PM PDT

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

Python-IHM Version 1.3 MolProbity Version 4.5.2 Integrative Modeling Validation Version 1.2

PDB ID	9A1C
PDB-Dev ID	PDBDEV_00000084
Structure Title	CS-Rosetta structure of engineered IgG-binding domain of protein G (GB) - model B1
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

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

We welcome your comments at pdb-dev@mail.wwpdb.org

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

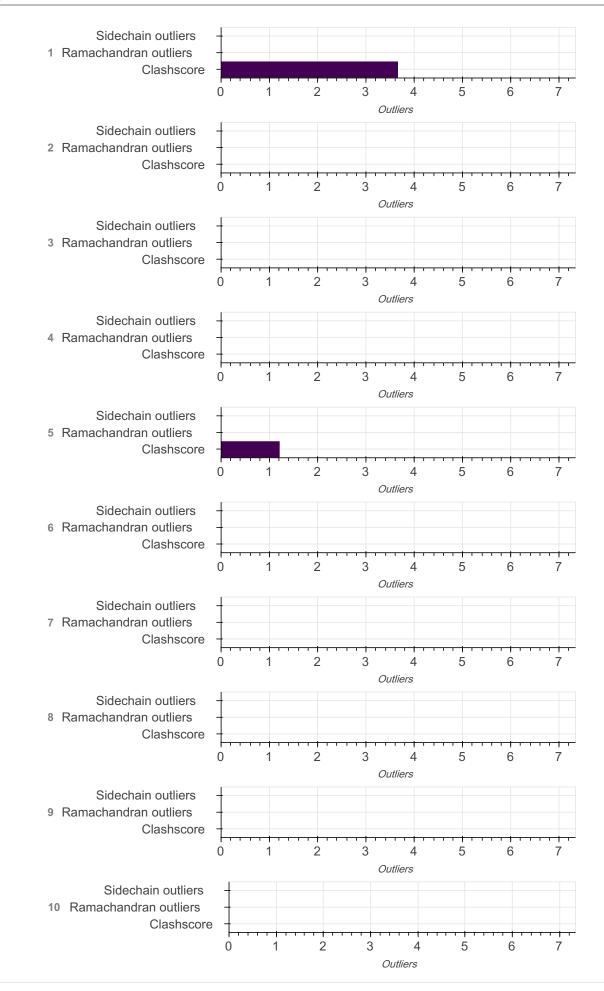
List of references used to build this report is available here.

Overall quality o

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS 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

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IM Structure Validation Report

Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 10 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition?

There are 10 unique types of models in this entry. These models are titled None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Immunoglobulin G-binding protein G	А	А	56
2	1	1	Immunoglobulin G-binding protein G	А	А	56
3	1	1	Immunoglobulin G-binding protein G	A	A	56
4	1	1	Immunoglobulin G-binding protein G	A	A	56
5	1	1	Immunoglobulin G-binding protein G	A	А	56
6	1	1	Immunoglobulin G-binding protein G	A	А	56
7	1	1	Immunoglobulin G-binding protein G	A	А	56
8	1	1	Immunoglobulin G-binding protein G	А	А	56
9	1	1	Immunoglobulin G-binding protein G	А	А	56

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	1	1	Immunoglobulin G-binding protein G	А	А	56

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	50910

Representation ?

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-56

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

<u>NMR</u>

Validation for this section is under development.

r models with stomic str	Model quali	
uctures, excluded volume		ed. For models with coarse-grained or multi-scale
	Standard geometry: bo	ond outliers?
ond length outliers can no	t be evaluated for this model Standard geometry: ar	gle outliers?
ond angle outliers do not	exist or can not be evaluated for this i	nodel
	Too-close contain	acts
÷		vsis. All-atom clashscore is defined as the number of able below contains clashscores for all the models in
Model ID	Clash score	Number of clashes
1	3.67	3
2	0.00	0
3	0.00	0
4	0.00	0
5	1.22	1
6	0.00	0
7	0.00	0
	0.00	0
8	0.00	
8 9	0.00	0

All 4 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
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Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:44:THR:OG1	A:53:THR:OG1	0.519
1	A:27:LEU:C	A:27:LEU:HD23	0.505
1	A:12:LEU:N	A:12:LEU:HD23	0.434
5	A:27:LEU:C	A:27:LEU:HD23	0.490

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	54	52	2	0
2	54	54	0	0
3	54	52	2	0
4	54	54	0	0
5	54	53	1	0
6	54	53	1	0
7	54	54	0	0
8	54	52	2	0
9	54	53	1	0
10	54	52	2	0

Detailed list of outliers are tabulated below.

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	41	41	0	0
2	41	41	0	0

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Model ID	Analyzed	Favored	Allowed	Outliers
3	41	41	0	0
4	41	41	0	0
5	41	41	0	0
6	41	41	0	0
7	41	41	0	0
8	41	41	0	0
9	41	41	0	0
10	41	41	0	0

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling @

<u>NMR</u>

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgements

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