Summary of integrative structure determination of CS-Rosetta structure of engineered IgG-binding domain of protein G (GB) - model A1 (PDB ID: 9A1B, PDB-Dev ID: PDBDEV_00000083)

1. Model Composition	
Entry composition	Immunoglobulin G-binding protein G: chain(s) A (56 residues)
Datasets used for modeling	- NMR data, BMRB: 50907
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 0.00-5.43 - Ramachandran outliers: 0-0 - Sidechain outliers: 0-0
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	CS-Rosetta modeling
Method	?

Description	?
Number of computed models	?
Software	CS-Rosetta (version Not available)