

Summary of integrative structure determination of CS-Rosetta structure of engineered IgG-binding domain of protein G (GB) - model B1 (PDB ID: 9A1C, PDB-Dev ID: PDBDEV_00000084)

1. Model Composition	
Entry composition	Immunoglobulin G-binding protein G: Chain A (56 residues)
Datasets used for modeling	NMR data, BMRB: 50910
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 1
Flexible units	A: 1-56
Structural coverage (rigid bodies)	100%
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)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 3.67, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-5: Clashscore = 1.22, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-7: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-8: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-9: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-10: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>
<p><i>Fit to data used for modeling</i></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><i>Fit to data used for validation</i></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p>5. Methodology and Software</p>	
<p>1. <i>Method</i></p>	<p>CS-Rosetta modeling</p>
<p><i>Name</i></p>	<p>?</p>
<p><i>Description</i></p>	<p>?</p>
<p><i>Number of computed models</i></p>	<p>?</p>
<p><i>Software</i></p>	<p>CS-Rosetta (version Not available)</p>