Summary of integrative structure determination of Bovine adenylyl cyclase 8 in complex with the G protein heterodimer G beta gamma (PDB ID: 9A3T, PDB-Dev ID: PDBDEV_00000214)

1. Model Composition	
Entry composition	- Adenylate cyclase type 8: Chain A (890 residues) - Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2: Chain C (46 residues) - Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1: Chain B (339 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: PDH, 2 cross-links - Experimental model, PDB ID: 1XHM - Experimental model, PDB ID: 8BUZ
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 3
Flexible units	- A: 1-890 - B: 1-339 - C: 1-46
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: PDH, 2 cross-links - 1 unique CrossLinkRestraint: DMTMM, 1 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 11.51, Number of Ramachandran outliers = 11, Number of sidechain outliers = 125

Model quality: assessment of excluded volume	Not applicable
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. Method	Identification of crosslinked residues
Name	Crosslinked residues were identified from the acquired mass spectrometry data based on the presence of heavy/light pairs of linked peptides.
2. Method	Docking
Name	Accessible interaction space was assessed with DisVis, solvent accessible residues were determined with GetArea. The information from these steps was used for docking with HADDOCK.
Number of computed models	1
Software	- xQuest (version 2.1.5) - HADDOCK (version 2.4) - DisVis (version Not available) - GetArea (version Not available)