

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	<ul style="list-style-type: none"> - Adenylate cyclase type 8: chain(s) A (890 residues) - Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1: chain(s) B (339 residues) - Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2: chain(s) C (46 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, PRIDE: PXD040374 - Experimental model, PDB: 1XHM - Experimental model, PDB: 8BUZ
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 3
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: PDH, 2 crosslinks - 1 unique CrossLinkRestraint: DMTMM, 1 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 11.50 - Ramachandran outliers: 11 - Sidechain outliers: 125
Fit to data used for modeling	Satisfaction of crosslinks: 100.00%
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. <i>Name</i>	Identification of crosslinked residues
2. <i>Name</i>	Docking
<i>Method</i>	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.
<i>Number of computed models</i>	1
<i>Software</i>	<ul style="list-style-type: none"> - xQuest (version 2.1.5) - HADDOCK (version 2.4) - DisVis (version Not available) - GetArea (version Not available)