Table S1: Summary of Integrative Structure Determination of Structural Model of Ghrelin Bound to its G Protein-Coupled Receptor (PDBDEV00000024)

1. Model Composition	
Entry composition	- GHSR: Chain A (298 residues) - Ghrelin: Chain B (17 residues) - GHSR: Chain A (298 residues) - Ghrelin: Chain B (17 residues) - GHSR: Chain A (298 residues) - Ghrelin: Chain B (17 residues) - GHSR: Chain A (298 residues) - Ghrelin: Chain B (17 residues) - GHSR: Chain A (298 residues) - Ghrelin: Chain B (17 residues)
Datasets used for modeling	- Comparative model, template PDB ID: Not listed - De Novo model, Not listed - Mutagenesis data, Not listed - NMR data, 27600 - Experimental model, PDB ID: 1u19 - Experimental model, PDB ID: 2rh1 - Experimental model, PDB ID: 2y03 - Experimental model, PDB ID: 3eml - Experimental model, PDB ID: 3odu - Experimental model, PDB ID: 3pbl - Experimental model, PDB ID: 3rze - Experimental model, PDB ID: 3uon - Experimental model, PDB ID: 3vw2 - Experimental model, PDB ID: 4daj - Experimental model, PDB ID: 4djh - Experimental model, PDB ID: 4dkl - Experimental model, PDB ID: 4ea3 - Experimental model, PDB ID: 4ej4 - Experimental model, PDB ID: 4iar - Experimental model, PDB ID: 4ib4
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	0, 2
Rigid regions	- A: - - B: -
Flexible units	- A: 40-337. - B: 1-17.
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: 50 residues per bead.
3. Restraints	
Physical principles	Excluded volume and Sequence connectivity.
Experimental data	- 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.0

	- 4 unique DerivedDistanceRestraint: Upper Bound Distance: 5.0
4. Validation	
Sampling validation	1. Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	distance threshold-based clustering, Not applicable
Number of ensembles	0
Number of models in ensembles	Not applicable
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Quality of data	1. Quality of input data has not be assessed
Assessment of atomic regions	Clashscore: 3.31, Ramachandran outliers: 1.68, Sidechain outliers: 0.0
Assessment of excluded volume	1. Not applicable
Fit of the model to information used to compute it	1. Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	1. Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Comparative Modeling
Name	Multiple Template Comparative Modeling
Details	- Method details unspecified
Software	- ROSETTA (version Rosetta version 3.6) - No location specified