

Summary of integrative structure determination of structural model of ghrelin bound to its g protein-coupled receptor (PDBDEV00000024)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - GHSR: Chain A (298 residues) - Ghrelin: Chain B (17 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 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
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: - - B: -
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 40-337. - B: 1-17.
Resolution	<ul style="list-style-type: none"> - Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.0 - 4 unique DerivedDistanceRestraint: Upper Bound Distance: 5.0
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided

<i>Clustering algorithm ,clustering feature</i>	Distance threshold-based clustering used if ensembles are deposited, Not applicable
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Quality of data</i>	- Quality of input data has not be assessed
<i>Model quality: assessment of atomic segments</i>	Clashscore: 3.31, Ramachandran outliers: 1.68% , Sidechain outliers: 0.0%
<i>Model quality: assessment of excluded volume</i>	- Not applicable
<i>Fit of the model to information used to compute it</i>	- Fit of model to information used to compute it has not been determined
<i>Fit of the model to information not used to compute it</i>	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>Method</i>	Comparative Modeling
<i>Name</i>	Multiple Template Comparative Modeling
<i>Details</i>	- Method details unspecified
<i>Software</i>	- ROSETTA (version Rosetta version 3.6) - No location specified