

Summary of integrative structure determination of Structural Model of Ghrelin Bound to its G Protein-Coupled Receptor (PDB ID: 8ZZO, PDB-Dev ID: PDBDEV_00000024)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - GHSR: chain(s) A (366 residues) - Ghrelin: chain(s) B (28 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Comparative model, Not available - De Novo model, Not available - Mutagenesis data, Not available - NMR data, BMRB: 27600 - Experimental model, PDB: 1u19 - Experimental model, PDB: 2rh1 - Experimental model, PDB: 2y03 - Experimental model, PDB: 3eml - Experimental model, PDB: 3odu - Experimental model, PDB: 3pbl - Experimental model, PDB: 3rze - Experimental model, PDB: 3uon - Experimental model, PDB: 3vw2 - Experimental model, PDB: 4daj - Experimental model, PDB: 4djh - Experimental model, PDB: 4dkl - Experimental model, PDB: 4ea3 - Experimental model, PDB: 4ej4 - Experimental model, PDB: 4iar - Experimental model, PDB: 4ib4
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
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	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	5
Model precision (uncertainty of models)	Not available

<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 1.95-3.70 - Ramachandran outliers: 1-7 - Sidechain outliers: 0-0
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Comparative Modeling
<i>Method</i>	Multiple Template Comparative Modeling
<i>Number of computed models</i>	15000
2. <i>Name</i>	Flexible Peptide Docking
<i>Method</i>	Ab initio folding and docking of peptide
<i>Number of computed models</i>	10000
3. <i>Name</i>	Comparative Modeling
<i>Method</i>	Multiple Template Comparative Modeling
<i>Number of computed models</i>	1000
4. <i>Name</i>	Flexible Peptide Docking
<i>Method</i>	Ab initio folding and docking of peptide
<i>Number of computed models</i>	10000
5. <i>Name</i>	Comparative Modeling
<i>Method</i>	Multiple Template Comparative Modeling
<i>Number of computed models</i>	1000
6. <i>Name</i>	Flexible Peptide Docking
<i>Method</i>	Ab initio folding and docking of peptide
<i>Number of computed models</i>	5000
7. <i>Name</i>	Comparative Modeling
<i>Method</i>	Multiple Template Comparative Modeling
<i>Number of computed models</i>	1000

[Software](#)[ROSETTA](#) (version Rosetta version 3.6)