# 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*** | |
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| *Entry composition* | - Ghrelin: Chain B (17 residues)<br>- GHSR: Chain A (298 residues) |
| *Datasets used for modeling* | - Comparative model, template PDB ID: Not available<br>- De Novo model, Not available<br>- Mutagenesis data, Not available<br>- NMR data, BMRB: 27600<br>- Experimental model, PDB ID: 1u19<br>- Experimental model, PDB ID: 2rh1<br>- Experimental model, PDB ID: 2y03<br>- Experimental model, PDB ID: 3eml<br>- Experimental model, PDB ID: 3odu<br>- Experimental model, PDB ID: 3pbl<br>- Experimental model, PDB ID: 3rze<br>- Experimental model, PDB ID: 3uon<br>- Experimental model, PDB ID: 3vw2<br>- Experimental model, PDB ID: 4daj<br>- Experimental model, PDB ID: 4djh<br>- Experimental model, PDB ID: 4dkl<br>- Experimental model, PDB ID: 4ea3<br>- Experimental model, PDB ID: 4ej4<br>- Experimental model, PDB ID: 4iar<br>- Experimental model, PDB ID: 4ib4 |
| ***2. Representation*** | |
| *Resolution* | Atomic |
| *Number of rigid bodies, flexible units* | 0, 2 |
| *Flexible units* | - A: 40-337<br>- B: 1-17 |
| *Structural coverage (rigid bodies)* | 100% |
| ***3. Restraints*** | |
| *Physical principles* | Information about physical principles was not provided |
| *Experimental data* | - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 3.0<br>- 4 unique DerivedDistanceRestraint: Upper Bound Distance: 5.0 |
| ***4. Validation*** | |
| *Number of ensembles* | 0 |
| *Number of models in ensembles* | Not applicable |

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| *Number of deposited models* | 5 |
| *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 = 3.51, Number of Ramachandran outliers = 6, Number of sidechain outliers = 0<br>- Model-2: Clashscore = 1.95, Number of Ramachandran outliers = 1, Number of sidechain outliers = 0<br>- Model-3: Clashscore = 3.51, Number of Ramachandran outliers = 7, Number of sidechain outliers = 0<br>- Model-4: Clashscore = 2.53, Number of Ramachandran outliers = 5, Number of sidechain outliers = 0<br>- Model-5: Clashscore = 3.7, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0 |
| *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* | Comparative Modeling |
| *Name* | Multiple Template Comparative Modeling |
| *Number of computed models* | 15000 |
| *2. Method* | Flexible Peptide Docking |
| *Name* | Ab initio folding and docking of peptide |
| *Number of computed models* | 10000 |
| *3. Method* | Comparative Modeling |
| *Name* | Multiple Template Comparative Modeling |
| *Number of computed models* | 1000 |
| *4. Method* | Flexible Peptide Docking |
| *Name* | Ab initio folding and docking of peptide |
| *Number of computed models* | 10000 |

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| *5. Method* | Comparative Modeling |
| *Name* | Multiple Template Comparative Modeling |
| *Number of computed models* | 1000 |
| *6. Method* | Flexible Peptide Docking |
| *Name* | Ab initio folding and docking of peptide |
| *Number of computed models* | 5000 |
| *7. Method* | Comparative Modeling |
| *Name* | Multiple Template Comparative Modeling |
| *Number of computed models* | 1000 |
| *Software* | ROSETTA (version Rosetta version 3.6) |