

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

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| PDB ID | PDBDEV00000024 |
| Molecule Name | Structural Model of Ghrelin Bound to its G Protein-Coupled Receptor |
| Title | Structural Model of Ghrelin Bound to it G Protein-Coupled Receptor |
| Authors | Brian J. Bender;Gerrit Vortmeier;Stefan Ernicke;Mathias Bosse;Anette Kaiser;Sylvia Els-Heindl;Ulrike Krug;Beck-Sickinger;Jens Meiler;Daniel Huster |

The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobit : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There are 1 unique types of models in this entry. The entry contains 2 chains.

| Molecule ID | Molecule Name | Chain ID | Total Residues |
|-------------|---------------|----------|----------------|
| 1 | GHSR | A | 298 |
| 1 | Ghrelin | B | 17 |

There are 1 software packages reported in this entry.

| ID | Software Name | Software Version | Software Classification |
|----|---------------|---------------------|--|
| 1 | ROSETTA | Rosetta version 3.6 | protein structure prediction and docking |

There are 20 unique datasets used to build the model(s) in this entry.

| ID | Dataset Type | Database Name | Data Access Code |
|----|-------------------|---------------|------------------|
| 1 | Comparative model | Not Listed | None |
| 2 | De Novo model | Not Listed | None |

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|----|--------------------|------------|-------|
| 3 | Mutagenesis data | Not Listed | None |
| 4 | NMR data | BMRB | 27600 |
| 5 | Experimental model | PDB | 1u19 |
| 6 | Experimental model | PDB | 2rh1 |
| 7 | Experimental model | PDB | 2y03 |
| 8 | Experimental model | PDB | 3eml |
| 9 | Experimental model | PDB | 3odu |
| 10 | Experimental model | PDB | 3pbl |
| 11 | Experimental model | PDB | 3rze |
| 12 | Experimental model | PDB | 3uon |
| 13 | Experimental model | PDB | 3vw2 |
| 14 | Experimental model | PDB | 4daj |
| 15 | Experimental model | PDB | 4djh |
| 16 | Experimental model | PDB | 4dkl |
| 17 | Experimental model | PDB | 4ea3 |
| 18 | Experimental model | PDB | 4ej4 |
| 19 | Experimental model | PDB | 4iar |
| 20 | Experimental model | PDB | 4ib4 |

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertainty of model
