

Full wwPDB Integrative Structure Validation Report

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

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

1. Overall quality at a glance

2. Entry composition

There is 1 unique type of model in this entry. Model has 2 chains respectively.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	GHSR	Α	298
1	Ghrelin	В	17

There is 1 software package 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 in this entry.

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

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

4.1 Too-close contacts	
4.2 Torsion angles	
4.2.1 Protein backbone	
4.2.2 Protein sidechains	
5. Fit of model and data	
6. Uncertaintiy of model	