Full wwPDB Integrative Structure Validation Report

November 07, 2019 -- 03:09 PM

PDB ID	*PDBDEV00000024*
Molecule Name	Structural Model of Ghrelin Bound to its G Protein-Coupled Receptor
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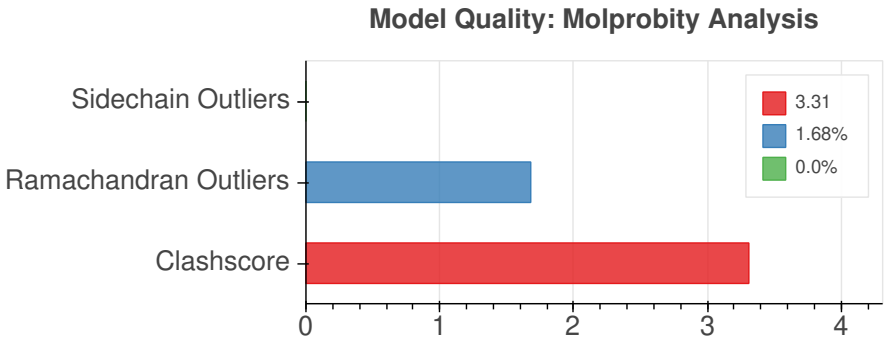
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 5 unique models, with 2 subunits in each model. A total of 20 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 2 flexible or non-rigid units.

3.2 Entry composition

There are 5 unique types of models in this entry.These models are titled Best scoring model, 2nd Best scoring model, 3rd Best scoring model, 4th Best scoring model, 5th Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	GHSR	A	298
1	2	2	Ghrelin	B	17
2	1	1	GHSR	A	298
2	2	2	Ghrelin	B	17
3	1	1	GHSR	A	298
3	2	2	Ghrelin	B	17
4	1	1	GHSR	A	298
4	2	2	Ghrelin	B	17
5	1	1	GHSR	A	298
5	2	2	Ghrelin	B	17

3.3 Datasets used for modeling

There are 20 unique datasets used to build the models 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

4. Representation

This entry has only one representation and includes 0 rigid bodies and 2 flexible units.

Chain ID	*Rigid bodies*	*Non-rigid segments*
A	-	40-337.
B	-	1-17.

5. Methodology and software

Step number	*Protocol ID*	*Method name*	*Method type*	*Number of computed models*	*Multi state modeling*	*Multi scale modeling*
1	1	Multiple Template Comparative Modeling	Comparative Modeling	15000	False	False
2	1	Ab initio folding and docking of peptide	Flexible Peptide Docking	10000	False	False
3	1	Multiple Template Comparative Modeling	Comparative Modeling	1000	False	False
4	1	Ab initio folding and docking of peptide	Flexible Peptide Docking	10000	False	False
5	1	Multiple Template Comparative Modeling	Comparative Modeling	1000	False	False

6	1	Ab initio folding and docking of peptide	Flexible Peptide Docking	5000	False	False
7	1	Multiple Template Comparative Modeling	Comparative Modeling	1000	False	False

There is 1 software package reported in this entry.

ID	*Software name*	*Software version*	*Software classification*	*Software location*
1	ROSETTA	Rosetta version 3.6	protein structure prediction and docking	https://github.com/RosettaCo

6. Data quality

7. Model quality

7.1 Standard geometry

There are 13020 bond outliers in this entry.

Bond type	*Observed distance (Å)*	*Ideal distance (Å)*	*Number of outliers*
N--H	0.998	0.86	1504
CD2--HD2	1.079	0.93	199
CZ3--HZ3	1.086	0.93	34
CD1--HD1	1.078	0.93	214
CE1--HE1	1.076	0.93	199
CE2--HE2	1.083	0.93	179
CH2--HH2	1.085	0.93	34
CZ2--HZ2	1.084	0.93	34
CE3--HE3	1.087	0.93	34
CZ--HZ	1.08	0.93	129
NE--HE	1.005	0.86	104
NH2--HH21	1.003	0.86	104
NH1--HH11	1.005	0.86	104

CA--HA	1.07	0.97	1499
NE1--HE1	1.005	0.86	34
NH2--HH22	1.003	0.86	104
NH1--HH12	1.001	0.86	104
NE2--HE2	1.009	0.86	8
NE2--HE21	0.997	0.86	44
ND2--HD22	0.995	0.86	44
NE2--HE22	0.995	0.86	44
ND2--HD21	0.995	0.86	44
ND1--HD1	0.998	0.86	10
CG--HG3	1.076	0.97	349
CB--HB2	1.076	0.97	1144
CG--HG2	1.072	0.97	349
CB--HB3	1.073	0.97	1144
CD--HD2	1.077	0.97	219
CD--HD3	1.082	0.97	219
SG--HG	1.315	1.2	39
OH--HH	0.955	0.84	49
NZ--HZ3	1.008	0.89	54
CB--2HB	1.095	0.97	4
OG1--HG1	0.958	0.84	84
NZ--HZ2	1.008	0.89	54
OG--HG	0.954	0.84	109
CE--HE2	1.082	0.97	84
CD1--HD12	1.083	0.97	284
CD2--HD21	1.079	0.97	209
CB--HB	1.082	0.97	349
CD1--HD11	1.084	0.97	284
CG1--HG12	1.081	0.97	264
CG1--HG11	1.081	0.97	189
NZ--HZ1	1.009	0.89	54

CG2--HG22	1.076	0.97	349
CD2--HD22	1.073	0.97	209
CB--HB1	1.076	0.97	109
CE--HE3	1.088	0.97	84
CD2--HD23	1.081	0.97	209
CG2--HG23	1.079	0.97	349
CG--HG	1.078	0.97	209
CA--HA2	1.077	0.97	74
CG1--HG13	1.082	0.97	264
CG2--HG21	1.082	0.97	349
CE--HE1	1.082	0.97	29
CD1--HD13	1.077	0.97	284
N--H1	1.007	0.89	9
N--H3	1.004	0.89	9
CA--HA3	1.08	0.97	74
N--H2	0.994	0.89	9

There are 13 angle outliers in this entry.

Angle type	*Observed angle (°)*	*Ideal angle (°)*	*Number of outliers*
C-N-H	111.996	124.3	4
CA-N-H	136.984	114	4
CB-CA-HA	132.177	109	0
N-CA-HA	124.17	110	1

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	*Clash score*	*Number of clashes*
Model 1	3.31	17
Model 2	1.75	9
Model 3	3.51	18

Model 4	2.34	12
Model 5	3.70	19

All 75 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	310	296	8	6
2	309	295	11	3
3	309	290	11	8
4	309	293	10	6
5	309	296	10	3

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:144	ALA
1	A:145	ILE
1	A:185	GLU
1	A:194	ASP
1	A:204	ALA
1	A:292	PRO
2	A:190	THR
2	B:4	PHE
2	A:41	PRO
3	A:42	LEU
3	A:185	GLU
3	A:191	ASP
3	A:204	ALA
3	A:291	GLU
3	B:2	SER

3	B:4	PHE
3	B:7	PRO
4	A:204	ALA
4	A:292	PRO
4	A:319	ASN
4	B:5	LEU
4	B:11	ARG
4	A:41	PRO
5	A:108	PRO
5	A:195	THR
5	B:4	PHE

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	277	277	0	0
2	277	276	1	0
3	277	276	1	0
4	277	276	1	0
5	277	276	1	0

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model