Full wwPDB Integrative Structure Validation Report

July 06, 2020 -- 09:30 PM

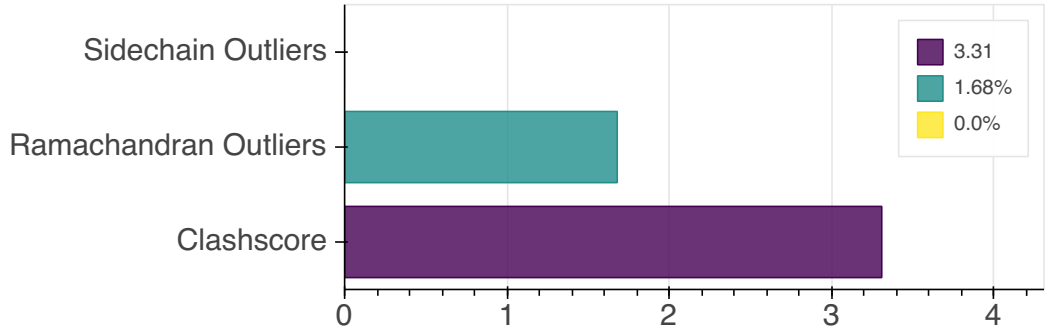
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000024
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;Annette Beck-Sickinger;Jens Meiler;Daniel Huster

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

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.

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

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

Data quality

Model quality

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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
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	114.0	4
CB-CA-HA	132.177	109.0	0
N-CA-HA	124.17	110.0	1

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 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.

Torsion angles: Protein backbone

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

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

Model ID	Chain and res ID	Residue type
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

Torsion angles: 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

Model ID	Analyzed	Favored	Allowed	Outliers
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

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model