

Integrative Structure Validation Report ?

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	8ZZO
PDB-Dev ID	PDBDEV_00000024
Structure Title	Structural Model of Ghrelin Bound to its G Protein-Coupled Receptor
Structure Authors	Brian J. Bender; Gerrit Vortmeier; Stefan Ernicke; Mathias Bosse; Anette Kaiser; Sylvia Els-Heindl; Ulrike Krug; Annette Beck-Sickinger; Jens Meiler; Daniel Huster
Deposited on	2018-08-30

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

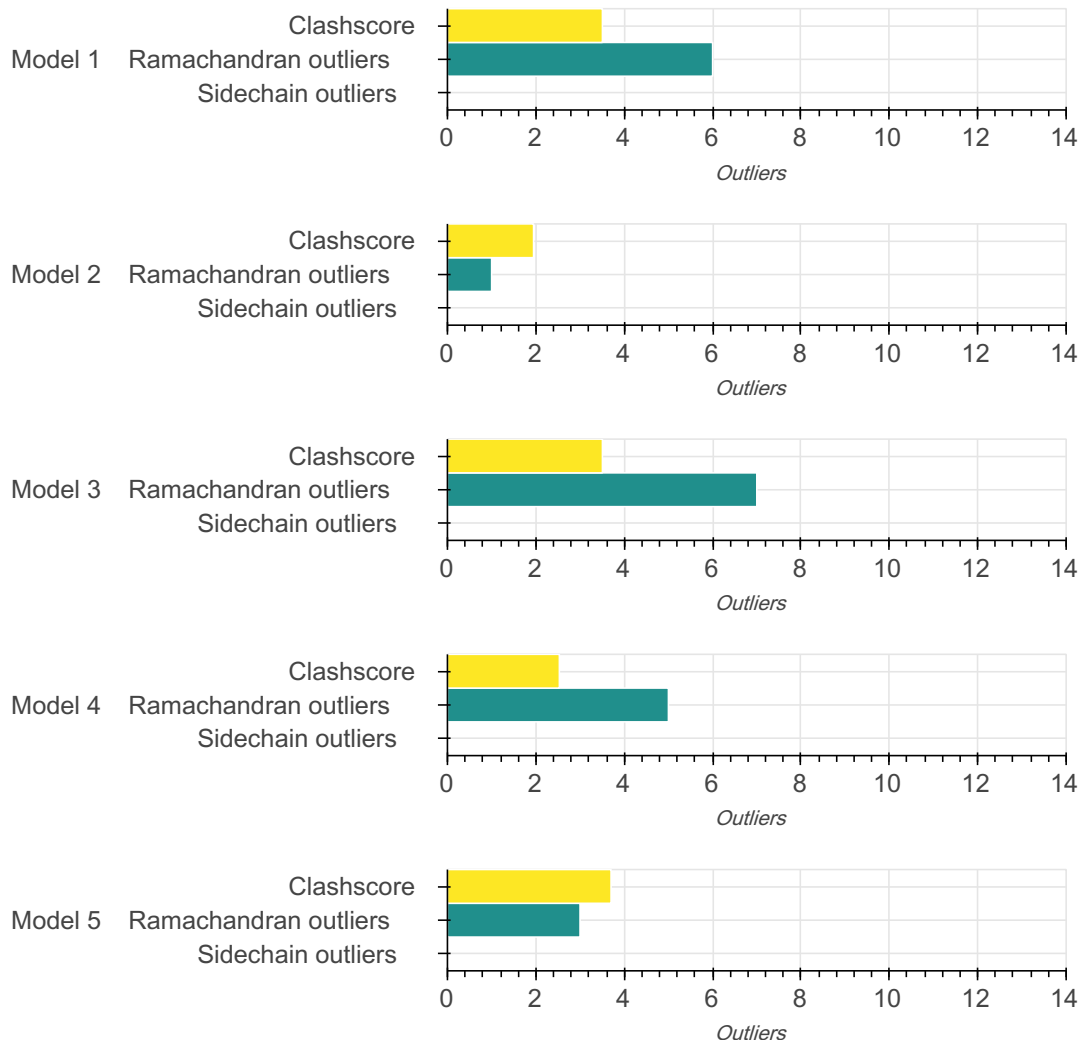
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 5 model(s). A total of 20 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-5	1	GHSR	A	366	-	40-337	81.42 / 100.00	Atomic
		2	Ghrelin	B	28	-	1-17	60.71 / 100.00	Atomic

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 available	Not available
2	De Novo model	Not available	Not available
3	Mutagenesis data	Not available	Not available
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

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Comparative Modeling	Multiple Template Comparative Modeling	None	15000	False	False
2	1	Flexible Peptide Docking	Ab initio folding and docking of peptide	None	10000	False	False
3	1	Comparative Modeling	Multiple Template Comparative Modeling	None	1000	False	False
4	1	Flexible Peptide Docking	Ab initio folding and docking of peptide	None	10000	False	False
5	1	Comparative Modeling	Multiple Template Comparative Modeling	None	1000	False	False
6	1	Flexible Peptide Docking	Ab initio folding and docking of peptide	None	5000	False	False
7	1	Comparative Modeling	Multiple Template Comparative Modeling	None	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/RosettaCommons

Data quality ?

Mutagenesis

Validation for this section is under development.

NMR

Validation for this section is under development.

Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

There are 8 bond length outliers in this entry (0.06% of 12945 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	2	SER	C-N	6.20	1.42	1.33	3	3
B	3	OCS	N-CA	6.09	1.57	1.46	2	1
B	3	OCS	C-N	5.90	1.41	1.33	5	3
B	3	OCS	CA-CB	4.31	1.62	1.53	5	1

Standard geometry: angle outliers ?

There are 41 bond angle outliers in this entry (0.23% of 17605 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	2	SER	C-N-CA	29.67	68.29	121.70	5	5
B	3	OCS	CA-C-N	27.49	61.23	116.20	2	5
B	3	OCS	O-C-N	21.19	89.10	123.00	3	4
B	3	OCS	CA-C-O	20.01	154.82	120.80	1	5
B	3	OCS	C-CA-CB	10.69	89.79	110.10	3	3
A	99	ASP	CA-CB-CG	5.72	118.32	112.60	2	1
B	3	OCS	N-CA-C	5.62	95.28	111.00	5	2
A	102	ARG	NE-CZ-NH2	5.59	114.17	119.20	5	1
A	172	PHE	CA-CB-CG	5.41	119.21	113.80	2	1
A	108	PRO	CA-N-CD	5.30	104.58	112.00	5	1
A	309	PHE	CA-CB-CG	5.11	108.69	113.80	2	1
A	54	PHE	CA-CB-CG	5.10	118.90	113.80	3	1
A	312	PHE	CA-CB-CG	4.98	118.78	113.80	5	1
B	2	SER	O-C-N	4.91	130.86	123.00	4	3
A	279	PHE	CA-CB-CG	4.63	109.17	113.80	1	1
A	194	ASP	C-N-CA	4.54	129.88	121.70	5	1
A	194	ASP	CA-C-O	4.53	113.11	120.80	5	1
A	194	ASP	O-C-N	4.24	116.22	123.00	5	1
A	319	ASN	CA-C-N	4.05	122.98	116.90	4	2
A	324	ASN	CA-CB-CG	4.04	108.56	112.60	2	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	3.51	18
2	1.95	10

Model ID	Clash score	Number of clashes
3	3.51	18
4	2.53	13
5	3.70	19

There are 78 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:3:OCS:C	B:3:OCS:CD	1.09	2	2
A:283:ARG:NH1	B:2:SER:OG	0.73	3	1
B:3:OCS:C	B:3:OCS:CE2	0.73	2	1
A:312:PHE:HD1	A:312:PHE:O	0.64	3	1
A:312:PHE:C	A:312:PHE:CD1	0.63	3	1
B:3:OCS:CD	B:3:OCS:O	0.60	1	1
B:11:ARG:C	B:11:ARG:HD3	0.57	4	1
A:102:ARG:HA	A:102:ARG:NE	0.54	5	3
A:243:ARG:HA	A:243:ARG:NE	0.54	1	1
A:313:TYR:C	A:313:TYR:CD1	0.54	5	4
A:199:ARG:NH1	A:199:ARG:O	0.53	5	1
B:2:SER:O	B:3:OCS:CB	0.53	1	3
A:187:GLU:O	A:190:THR:OG1	0.51	1	1
A:312:PHE:C	A:312:PHE:HD1	0.51	3	1
A:93:PHE:CD1	A:93:PHE:N	0.51	5	2
A:319:ASN:HB3	A:320:PRO:CD	0.50	4	4
B:5:LEU:C	B:5:LEU:HD12	0.50	5	2
B:8:GLU:N	B:8:GLU:OE1	0.50	1	1
B:3:OCS:N	B:3:OCS:OE1	0.49	2	1
B:3:OCS:CE2	B:3:OCS:O	0.49	1	1
A:96:MET:HB3	A:97:PRO:HD3	0.49	4	1
A:199:ARG:HD3	A:199:ARG:N	0.49	5	1
A:276:TRP:CD1	A:276:TRP:N	0.48	3	3
B:12:VAL:HA	B:15:ARG:HG2	0.47	3	1
A:102:ARG:HA	A:102:ARG:HE	0.47	5	1
A:101:VAL:O	A:101:VAL:HG12	0.46	1	1
A:193:TRP:CD1	A:193:TRP:N	0.46	2	1
A:64:THR:O	A:330:TYR:OH	0.46	2	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:223:LEU:HB2	A:224:PRO:HD3	0.46	1	4
A:276:TRP:NE1	A:315:SER:OG	0.45	2	1
A:319:ASN:HB3	A:320:PRO:HD3	0.44	4	2
A:40:ALA:N	A:41:PRO:CD	0.44	1	1
A:107:ARG:HB3	A:108:PRO:HD2	0.44	5	1
A:241:ARG:C	A:241:ARG:HD2	0.44	2	1
A:295:LEU:O	A:296:GLU:HB2	0.43	3	1
A:277:LEU:HB3	A:278:PRO:HD3	0.43	4	3
B:1:GLY:HA2	B:2:SER:HA	0.43	5	1
A:103:LEU:HB3	A:306:LEU:HD21	0.42	5	2
A:283:ARG:HG3	B:2:SER:O	0.42	2	1
A:96:MET:HB2	A:97:PRO:HD3	0.42	3	1
A:305:ASN:O	A:308:SER:OG	0.42	3	1
A:194:ASP:C	A:194:ASP:OD1	0.42	5	1
A:140:GLU:HA	A:140:GLU:OE1	0.42	4	1
A:184:VAL:O	A:185:GLU:HB2	0.42	3	1
A:41:PRO:O	A:43:LEU:N	0.42	3	1
A:312:PHE:CD1	A:312:PHE:O	0.41	3	1
A:40:ALA:N	A:41:PRO:HD2	0.41	4	1
A:187:GLU:N	A:187:GLU:OE1	0.41	3	1
A:318:ILE:O	A:319:ASN:C	0.41	4	1
A:117:LYS:HG2	A:182:VAL:O	0.41	5	1
B:5:LEU:O	B:5:LEU:HD12	0.41	5	1
A:191:ASP:HA	A:192:PRO:HD3	0.41	5	1
A:298:ALA:HA	B:8:GLU:HG2	0.40	3	1
A:189:GLY:O	A:191:ASP:N	0.40	2	1
A:279:PHE:CD1	A:279:PHE:N	0.40	5	1
A:243:ARG:HA	A:243:ARG:HE	0.40	1	1

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	Analysed	Favored	Allowed	Outliers
1	308	294	8	6
2	308	297	10	1
3	308	290	11	7

Model ID	Analysed	Favored	Allowed	Outliers
4	308	293	10	5
5	308	295	10	3

There are 17 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	204	ALA	3
A	41	PRO	2
A	185	GLU	2
A	292	PRO	2
A	42	LEU	1
A	108	PRO	1
A	144	ALA	1
A	145	ILE	1
A	190	THR	1
A	191	ASP	1
A	194	ASP	1
A	195	THR	1
A	291	GLU	1
A	319	ASN	1
B	5	LEU	1
B	7	PRO	1
B	11	ARG	1

Torsion angles : Protein sidechains ?

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

Model ID	Analysed	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

Fit of model to data used for modeling ?

Mutagenesis

Validation for this section is under development.

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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