Integrative Structure Validation Report

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

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

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

We welcome your comments at pdb-dev@mail.wwpdb.org

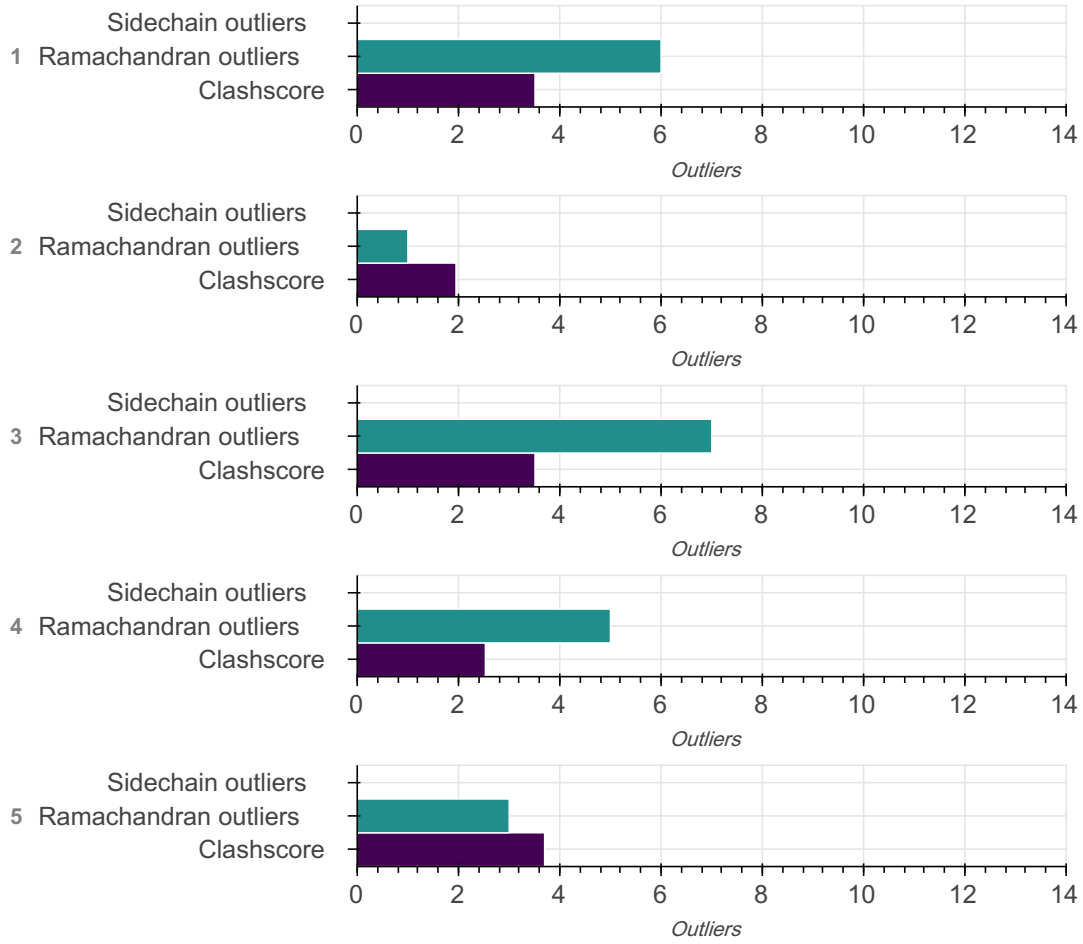
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 2 subunits in each model. A total of 20 datasets or restraints were 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	Chain ID [auth]	Total residues
1	1	1	GHSR	A	A	298

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

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

ID	Dataset type	Database name	Data access code
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

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

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

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

NMR

Validation for this section is under development.

Mutagenesis

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 13020 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.07	0.97	4
CG--HG2	1.07	0.97	1
CB--HB3	1.07	0.97	2
CD2--HD22	1.07	0.97	1
N--H2	0.99	0.89	1
CB--HB1	1.08	0.97	14
CB--HB3	1.08	0.97	92
CB--HB2	1.08	0.97	82
CG2--HG22	1.08	0.97	14
CG--HG3	1.08	0.97	19
CG--HG2	1.08	0.97	19
CD--HD2	1.08	0.97	8
CA--HA	1.08	0.97	127
CD1--HD13	1.08	0.97	15

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA2	1.08	0.97	4
CG--HG	1.08	0.97	22
CD2--HD21	1.08	0.97	6
CG2--HG23	1.08	0.97	32
CA--HA3	1.08	0.97	8
CG1--HG12	1.08	0.97	8
CD2--HD23	1.08	0.97	4
CG1--HG11	1.08	0.97	8
CD--HD3	1.08	0.97	7
CD2--HD22	1.08	0.97	10
CB--HB	1.08	0.97	21
CG1--HG13	1.08	0.97	14
CE--HE1	1.08	0.97	1
CG2--HG21	1.08	0.97	14
CE--HE2	1.08	0.97	3
CD1--HD12	1.08	0.97	6
OG--HG	0.95	0.84	1
N--H3	1.00	0.89	2
CD1--HD11	1.08	0.97	4
SG--HG	1.31	1.20	1
OH--HH	0.95	0.84	1
CB--HB3	1.09	0.97	991
CB--HB1	1.09	0.97	96

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.09	0.97	1314
CG2--HG23	1.09	0.97	318
CD2--HD22	1.09	0.97	199
CB--HB2	1.09	0.97	1005
CG--HG3	1.09	0.97	272
CG1--HG12	1.09	0.97	257
CB--HB	1.09	0.97	329
CD1--HD13	1.09	0.97	270
CD2--HD23	1.09	0.97	206
CD--HD3	1.09	0.97	158
CG--HG2	1.09	0.97	272
CG--HG	1.09	0.97	188
CG1--HG13	1.09	0.97	251
CD2--HD21	1.09	0.97	204
CD1--HD12	1.09	0.97	279
N--H2	1.01	0.89	9
CD1--HD11	1.09	0.97	281
CG2--HG22	1.09	0.97	336
CG2--HG21	1.09	0.97	336
CA--HA3	1.09	0.97	67
OH--HH	0.96	0.84	48
CG1--HG11	1.09	0.97	182
CA--HA2	1.09	0.97	71

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD--HD2	1.09	0.97	167
CE--HE2	1.09	0.97	82
OG--HG	0.96	0.84	109
N--H1	1.01	0.89	10
CE--HE3	1.09	0.97	85
CE--HE1	1.09	0.97	29
N--H3	1.01	0.89	8
NZ--HZ2	1.01	0.89	55
OG1--HG1	0.96	0.84	85
NZ--HZ3	1.01	0.89	54
NZ--HZ1	1.01	0.89	55
CB--2HB	1.09	0.97	3
SG--HG	1.32	1.20	1
CD--HD3	1.10	0.97	55
CD--HD2	1.10	0.97	45
CB--2HB	1.10	0.97	2
CB--HB3	1.10	0.97	60
CA--HA	1.10	0.97	52
CG--HG2	1.10	0.97	58
CG--HG3	1.10	0.97	59
CB--HB2	1.10	0.97	58
NZ--HZ3	1.02	0.89	1
OH--HH	0.97	0.84	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
SG--HG	1.33	1.20	38
ND2--HD22	0.99	0.86	1
ND2--HD21	0.99	0.86	1
NE2--HE22	0.99	0.86	1
ND2--HD21	1.00	0.86	44
ND2--HD22	1.00	0.86	44
NE2--HE22	1.00	0.86	44
NE2--HE21	1.00	0.86	43
N--H	1.00	0.86	172
ND1--HD1	1.00	0.86	11
NH1--HH12	1.00	0.86	2
NH2--HH22	1.00	0.86	3
NH2--HH21	1.00	0.86	4
NH1--HH11	1.00	0.86	1
NE1--HE1	1.00	0.86	1
NE--HE	1.00	0.86	1
N--H	1.01	0.86	1279
NH2--HH21	1.01	0.86	98
NE1--HE1	1.01	0.86	34
NE2--HE21	1.01	0.86	2
CE1--HE1	1.08	0.93	8
NH1--HH12	1.01	0.86	103
NH2--HH22	1.01	0.86	102

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE--HE	1.01	0.86	98
NH1--HH11	1.01	0.86	102
CD1--HD1	1.08	0.93	10
NE2--HE2	1.01	0.86	9
CD2--HD2	1.08	0.93	14
CZ--HZ	1.08	0.93	11
CE2--HE2	1.08	0.93	5
CZ2--HZ2	1.08	0.93	1
CH2--HH2	1.08	0.93	2
CA--HA	1.12	0.97	1
N--H	1.02	0.86	53
CZ--HZ	1.09	0.93	119
CE1--HE1	1.09	0.93	192
CH2--HH2	1.09	0.93	33
CD1--HD1	1.09	0.93	205
CE2--HE2	1.09	0.93	175
NE--HE	1.02	0.86	6
NH2--HH21	1.02	0.86	3
CZ3--HZ3	1.09	0.93	35
NH1--HH11	1.02	0.86	2
CD2--HD2	1.09	0.93	186
CZ2--HZ2	1.09	0.93	34
CE3--HE3	1.09	0.93	35

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.14	0.97	2
N--H	1.03	0.86	1

Standard geometry: angle outliers

There are 54 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	68.29	1
C-N-CA	121.70	71.61	1
C-N-CA	121.70	71.92	1
CA-C-N	116.20	61.23	1
CA-C-N	116.20	61.96	1
CA-C-N	116.20	65.18	1
O-C-N	123.00	89.10	1
CA-C-O	120.80	154.82	1
CA-C-N	116.20	76.95	1
CA-C-N	116.20	77.33	1
C-N-CA	121.70	88.99	1
CA-C-O	120.80	151.16	1
O-C-N	123.00	94.89	1
C-N-CA	121.70	91.30	1
O-C-N	123.00	96.01	1
CA-C-O	120.80	146.25	1
CA-C-O	120.80	145.93	1
CA-C-O	120.80	145.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	89.79	1
C-CA-CB	110.10	91.93	1
CA-CB-CG	112.60	118.32	1
N-CA-C	111.00	95.28	1
NE-CZ-NH2	119.20	114.17	1
CA-CB-CG	113.80	119.21	1
O-C-N	123.00	131.51	1
CA-N-CD	112.00	104.58	1
CA-CB-CG	113.80	108.69	1
CA-CB-CG	113.80	118.90	1
CA-CB-CG	113.80	118.78	1
O-C-N	123.00	130.86	1
CA-CB-CG	113.80	109.17	1
C-N-CA	121.70	129.88	1
CA-C-O	120.80	113.11	1
O-C-N	123.00	130.22	1
O-C-N	123.00	116.22	1
C-CA-CB	110.10	102.08	1
N-CA-C	111.00	99.36	1
O-C-N	123.00	129.53	1
CA-C-N	116.90	122.98	1
CA-CB-CG	112.60	108.56	1
CA-C-N	116.90	122.92	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	112.00	124.30	1
N-CA-HA	124.17	110.00	1
C-N-H	109.37	124.30	1
N-CA-HA	126.93	110.00	1
CA-N-H	136.98	114.00	1
CB-CA-HA	132.18	109.00	1
CA-N-H	138.94	114.00	1
CA-N-H	141.32	114.00	1
CA-N-H	144.40	114.00	1
CA-N-H	145.72	114.00	1
C-N-H	89.84	124.30	1
C-N-H	87.18	124.30	1
C-N-H	83.81	124.30	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
1	3.51	18
2	1.95	10
3	3.51	18
4	2.53	13
5	3.70	19

All 78 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:3:OCS:C	B:3:OCS:CD	0.661
1	B:3:OCS:CD	B:3:OCS:O	0.597
1	A:243:ARG:HA	A:243:ARG:NE	0.536
1	B:2:SER:O	B:3:OCS:CB	0.529
1	A:187:GLU:O	A:190:THR:OG1	0.510
1	B:8:GLU:N	B:8:GLU:OE1	0.498
1	B:3:OCS:CE2	B:3:OCS:O	0.489
1	A:313:TYR:C	A:313:TYR:CD2	0.466
1	A:101:VAL:O	A:101:VAL:HG12	0.460
1	A:223:LEU:HB2	A:224:PRO:HD3	0.455
1	A:319:ASN:HB3	A:320:PRO:CD	0.448
1	A:40:ALA:N	A:41:PRO:CD	0.442
1	A:276:TRP:CD1	A:276:TRP:N	0.436
1	A:319:ASN:HB3	A:320:PRO:HD3	0.417
1	A:277:LEU:HB3	A:278:PRO:HD3	0.413
1	B:5:LEU:C	B:5:LEU:HD12	0.409
1	A:103:LEU:HB3	A:306:LEU:HD21	0.407
1	A:243:ARG:HA	A:243:ARG:HE	0.400
2	B:3:OCS:C	B:3:OCS:CD	1.095
2	B:3:OCS:C	B:3:OCS:CE2	0.729
2	B:3:OCS:N	B:3:OCS:OE1	0.492
2	A:193:TRP:CD1	A:193:TRP:N	0.459
2	B:2:SER:O	B:3:OCS:CB	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:64:THR:O	A:330:TYR:OH	0.457
2	A:276:TRP:NE1	A:315:SER:OG	0.449
2	A:241:ARG:C	A:241:ARG:HD2	0.436
2	A:283:ARG:HG3	B:2:SER:O	0.425
2	A:189:GLY:O	A:191:ASP:N	0.402
3	A:283:ARG:NH1	B:2:SER:OG	0.733
3	A:312:PHE:HD1	A:312:PHE:O	0.636
3	A:312:PHE:C	A:312:PHE:CD1	0.630
3	A:312:PHE:C	A:312:PHE:HD1	0.510
3	A:276:TRP:CD1	A:276:TRP:N	0.480
3	B:12:VAL:HA	B:15:ARG:HG2	0.474
3	A:102:ARG:HA	A:102:ARG:NE	0.450
3	A:313:TYR:C	A:313:TYR:CD2	0.447
3	A:295:LEU:O	A:296:GLU:HB2	0.435
3	A:223:LEU:HB2	A:224:PRO:HD3	0.432
3	A:96:MET:HB2	A:97:PRO:HD3	0.424
3	A:305:ASN:O	A:308:SER:OG	0.423
3	A:184:VAL:O	A:185:GLU:HB2	0.418
3	A:41:PRO:O	A:43:LEU:N	0.418
3	A:312:PHE:CD1	A:312:PHE:O	0.414
3	A:187:GLU:N	A:187:GLU:OE1	0.411
3	A:319:ASN:HB3	A:320:PRO:CD	0.407
3	A:298:ALA:HA	B:8:GLU:HG2	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:11:ARG:C	B:11:ARG:HD3	0.566
4	A:313:TYR:C	A:313:TYR:CD2	0.501
4	A:319:ASN:HB3	A:320:PRO:CD	0.500
4	B:2:SER:O	B:3:OCS:CB	0.495
4	A:96:MET:HB3	A:97:PRO:HD3	0.487
4	A:93:PHE:CD1	A:93:PHE:N	0.472
4	A:319:ASN:HB3	A:320:PRO:HD3	0.444
4	A:102:ARG:HA	A:102:ARG:NE	0.434
4	A:277:LEU:HB3	A:278:PRO:HD3	0.432
4	A:223:LEU:HB2	A:224:PRO:HD3	0.430
4	A:140:GLU:HA	A:140:GLU:OE1	0.420
4	A:40:ALA:N	A:41:PRO:HD2	0.414
4	A:318:ILE:O	A:319:ASN:C	0.411
5	A:102:ARG:HA	A:102:ARG:NE	0.542
5	A:313:TYR:C	A:313:TYR:CD2	0.535
5	A:199:ARG:NH1	A:199:ARG:O	0.532
5	A:93:PHE:CD1	A:93:PHE:N	0.505
5	B:5:LEU:C	B:5:LEU:HD12	0.500
5	A:199:ARG:HD3	A:199:ARG:N	0.486
5	A:276:TRP:CD1	A:276:TRP:N	0.468
5	A:102:ARG:HA	A:102:ARG:HE	0.465
5	A:107:ARG:HB3	A:108:PRO:HD2	0.441
5	B:1:GLY:HA2	B:2:SER:HA	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:103:LEU:HB3	A:306:LEU:HD21	0.425
5	A:194:ASP:C	A:194:ASP:OD1	0.421
5	A:223:LEU:HB2	A:224:PRO:HD3	0.421
5	A:117:LYS:HG2	A:182:VAL:O	0.410
5	B:5:LEU:O	B:5:LEU:HD12	0.408
5	A:319:ASN:HB3	A:320:PRO:CD	0.406
5	A:191:ASP:HA	A:192:PRO:HD3	0.405
5	A:277:LEU:HB3	A:278:PRO:HD3	0.401
5	A:279:PHE:CD1	A:279:PHE:N	0.401

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	308	294	8	6
2	308	297	10	1
3	308	290	11	7
4	308	293	10	5
5	308	295	10	3

Detailed list of outliers are tabulated below.

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
2	277	276	1	0

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

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling

NMR

Validation for this section is under development.

Mutagenesis

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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