

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	9A3I
PDB-Dev ID	PDBDEV_00000203
Structure Title	Parathyroid hormone receptor type 1 in complex with a long-acting parathyroid hormone analog and arrestin 2 (6u1n-based template)
Structure Authors	Aydin, Y.; Bottke, T.; Lam, J.H.; Ernicke, S.; Fortmann, A.; Tretbar, M.; Zarzycka, B.; Gurevich, V.V.; Katritch, V.; Coin, I.

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

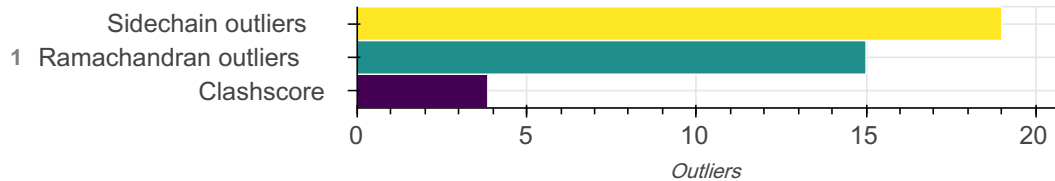
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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 1 unique models, with 3 subunits in each model. A total of 6 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 3 flexible or non-rigid units.

Entry composition ?

There is 1 unique type of models in this entry. This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Arrestin2	A	A	357
1	2	2	Long-acting parathyroid hormone analog	B	B	32
1	3	3	PTH1R	C	P	504

Datasets used for modeling ?

There are 6 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	Not available	Not available
2	Experimental model	PDB	6NBF
3	Experimental model	PDB	6U1N

ID	Dataset type	Database name	Data access code
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	De Novo model	Not available	Not available

Representation ?

This entry has only one representation and includes 0 rigid bodies and 3 flexible units

Chain ID	Rigid bodies	Non-rigid segments
C	-	1-504
A	-	1-357
B	-	1-32

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	None	None	None	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	ICM-Pro	v.3.9.2c	Model building	https://www.molsoft.com/icm_pro.html

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Model quality ?

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

Standard geometry: bond outliers ?

There are 7118 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	1.09	0.98	4
CB--HB3	1.09	0.97	666
CB--HB2	1.09	0.97	666
CE--HE3	1.09	0.97	73
CG--HG2	1.09	0.97	255
CG--HG3	1.09	0.97	255
CG1--HG12	1.09	0.97	113
CD1--HD13	1.09	0.97	132
CD2--HD23	1.09	0.97	93
CA--HA	1.09	0.97	833
CG1--HG13	1.09	0.97	113
CE--HE2	1.09	0.97	73
CA--HA3	1.09	0.97	51
CG2--HG22	1.09	0.97	166
CA--HA2	1.09	0.97	51
CD--HD3	1.09	0.97	162
CD2--HD22	1.09	0.97	93
CG--HG	1.09	0.97	93
CG2--HG23	1.09	0.97	166

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD11	1.09	0.97	132
CB--HB1	1.09	0.97	71
CG1--HG11	1.09	0.97	74
CG2--HG21	1.09	0.97	166
CB--HB	1.09	0.97	167
CD1--HD12	1.09	0.97	132
CD--HD2	1.09	0.97	162
CD2--HD21	1.09	0.97	93
CE--HE1	1.09	0.97	16
CB--2HB	1.09	0.97	4
CG2--2HG2	1.09	0.97	1
CG2--1HG2	1.09	0.97	1
CG2--3HG2	1.09	0.97	1
NZ--HZ3	1.01	0.89	57
NZ--HZ2	1.01	0.89	57
NZ--HZ1	1.01	0.89	57
SG--HG	1.33	1.20	13
NH2--HH22	1.00	0.86	56
N--H	1.00	0.86	831
NH1--HH12	1.00	0.86	56
NH2--HH21	1.00	0.86	56
NH1--HH11	1.00	0.86	56
NE--HE	1.00	0.86	56

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE21	1.00	0.86	23
ND1--HD1	1.00	0.86	18
ND2--HD21	1.00	0.86	30
ND2--HD22	1.00	0.86	30
NE2--HE22	1.00	0.86	23
NE1--HE1	1.00	0.86	15
CE1--HE1	1.09	0.93	97
OG1--HG1	1.00	0.84	53
CE2--HE2	1.09	0.93	79
CZ--HZ	1.09	0.93	42
CE3--HE3	1.09	0.93	15
CD2--HD2	1.09	0.93	97
CD1--HD1	1.09	0.93	94
CH2--HH2	1.09	0.93	15
OG--HG	1.00	0.84	47
CZ3--HZ3	1.09	0.93	15
OH--HH	1.00	0.84	37
CZ2--HZ2	1.09	0.93	15

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

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
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Model ID	Clash score	Number of clashes
1	3.85	55

All 55 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:327:LEU:O	A:328:VAL:HG13	0.836
1	C:459:ARG:O	C:460:LYS:C	0.746
1	A:337:ASP:O	A:338:LEU:CB	0.713
1	A:42:LEU:C	A:42:LEU:HD13	0.653
1	A:337:ASP:O	A:338:LEU:CG	0.651
1	C:165:TYR:C	C:165:TYR:CD2	0.628
1	A:337:ASP:O	A:338:LEU:HB2	0.620
1	C:62:TYR:N	C:63:PRO:HD2	0.587
1	A:204:ASP:C	A:204:ASP:OD1	0.570
1	C:71:ALA:N	C:72:PRO:CD	0.570
1	A:339:ALA:O	A:340:SER:HB3	0.562
1	C:165:TYR:CD2	C:166:THR:N	0.561
1	C:469:SER:O	C:470:TYR:CB	0.553
1	A:203:LEU:N	A:203:LEU:HD12	0.551
1	A:202:SER:C	A:203:LEU:HD12	0.540
1	C:305:LEU:N	C:306:PRO:CD	0.531
1	C:391:PHE:O	C:392:GLY:C	0.531
1	C:339:VAL:N	C:340:PRO:CD	0.530
1	A:337:ASP:O	A:338:LEU:HG	0.524
1	A:15:ASN:OD1	A:16:GLY:N	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:87:PHE:HA	A:88:PRO:C	0.497
1	A:5:GLY:O	A:6:THR:HB	0.472
1	A:76:ARG:O	C:366:THR:HG23	0.467
1	C:62:TYR:N	C:63:PRO:CD	0.466
1	A:66:GLU:CD	A:66:GLU:N	0.465
1	A:42:LEU:HD13	A:43:VAL:N	0.463
1	C:469:SER:O	C:470:TYR:HB2	0.462
1	C:62:TYR:HB3	C:63:PRO:HD3	0.461
1	A:339:ALA:O	A:340:SER:CB	0.456
1	A:328:VAL:HG11	A:342:ASP:HB3	0.454
1	C:321:ALA:O	C:322:ASN:C	0.447
1	A:25:ARG:NH1	C:477:TPO:HG21	0.445
1	A:13:SER:HB2	A:14:PRO:CD	0.442
1	A:13:SER:OG	A:15:ASN:OD1	0.442
1	C:123:ASP:C	C:123:ASP:OD1	0.440
1	C:369:GLY:O	C:370:ARG:CB	0.440
1	A:61:PHE:C	A:61:PHE:CD1	0.439
1	A:50:GLU:HG2	A:51:ARG:N	0.438
1	A:150:CYS:O	A:151:ALA:HB2	0.430
1	A:203:LEU:CD1	A:203:LEU:N	0.430
1	A:327:LEU:C	A:328:VAL:HG22	0.429
1	C:264:TYR:O	C:268:THR:HG23	0.422
1	C:47:SER:O	C:48:THR:C	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	C:1:ASP:C	C:1:ASP:OD1	0.419
1	A:42:LEU:C	A:42:LEU:CD1	0.418
1	A:61:PHE:CZ	A:317:ILE:HD11	0.415
1	C:388:MET:N	C:389:PRO:CD	0.414
1	A:327:LEU:O	A:328:VAL:CG1	0.414
1	A:59:CYS:SG	A:142:VAL:HG13	0.412
1	C:388:MET:HB2	C:389:PRO:HD3	0.409
1	A:13:SER:HB2	A:14:PRO:HD2	0.407
1	C:490:LEU:CB	C:491:PRO:HA	0.407
1	A:38:ASP:N	A:38:ASP:OD1	0.407
1	A:48:LEU:N	A:48:LEU:HD22	0.406
1	C:487:GLY:O	C:488:LEU:C	0.406

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	859	791	53	15

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	Analysed	Favored	Allowed	Outliers
1	761	696	46	19

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	6	THR

Model ID	Chain	Residue ID	Residue type
1	A	30	HIS
1	A	40	VAL
1	A	50	GLU
1	A	66	GLU
1	A	81	VAL
1	A	142	VAL
1	A	155	GLU
1	A	204	ASP
1	A	224	THR
1	A	227	THR
1	A	327	LEU
1	A	328	VAL
1	A	329	VAL
1	A	335	LEU
1	C	373	THR
1	C	455	LEU
1	C	469	SER
1	C	490	LEU

Fit of model to data used for modeling

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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