Integrative Structure Validation Report

March 27, 2025 - 10:12 AM PDT

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	9A3L
PDB-Dev ID	PDBDEV_00000206
Structure Title	Parathyroid hormone receptor type 1 in complex with a long-acting parathyroid hormone analog and arrestin 2 (6tko-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.
Deposited on	2023-03-24

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

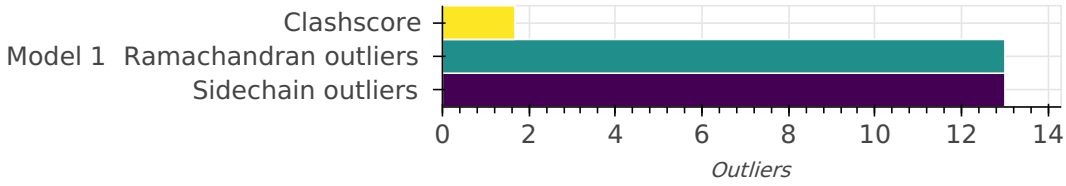
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

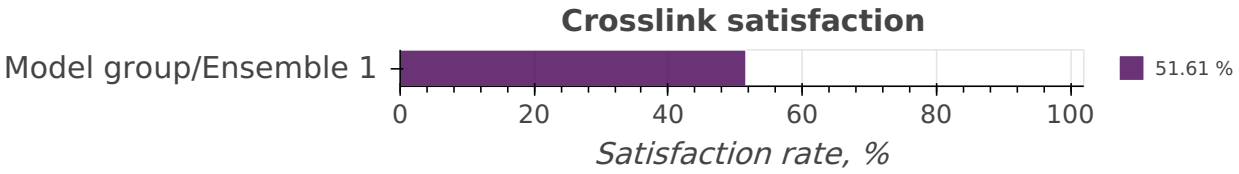
List of references used to build this report is available here.

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 1 model(s). A total of 6 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	1	Arrestin2	A	357	-	1-357	100.00 / 100.00	Atomic
		2	Long-acting parathyroid hormone analog	B	32	-	1-32	100.00 / 100.00	Atomic
		3	PTH1R	C [P]	504	-	1-504	100.00 / 100.00	Atomic

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	6TKO
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	De Novo model	Not available	Not available

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

At the moment, data validation is only available for crosslinking-MS data deposited as a fully compliant dataset in the PRIDE Crosslinking database. Correspondence between crosslinking-MS and entry entities is established using pyHMMER. Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the PRIDE Crosslinking database.

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 63 bond length outliers in this entry (0.86% of 7323 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	477	TPO	OG1-P	9.76	1.52	1.72	1	1
C	467	SEP	O2P-P	4.85	1.51	1.61	1	1
C	478	SEP	O1P-P	4.85	1.51	1.61	1	1
C	463	SEP	O1P-P	4.83	1.51	1.61	1	1
C	467	SEP	O1P-P	4.82	1.51	1.61	1	1
C	493	SEP	O1P-P	4.81	1.51	1.61	1	1
C	493	SEP	O2P-P	4.80	1.51	1.61	1	1
C	463	SEP	O2P-P	4.79	1.51	1.61	1	1
C	467	SEP	O3P-P	4.79	1.51	1.61	1	1
C	478	SEP	O3P-P	4.78	1.51	1.61	1	1
C	463	SEP	O3P-P	4.78	1.51	1.61	1	1
C	493	SEP	O3P-P	4.77	1.51	1.61	1	1
C	478	SEP	O2P-P	4.75	1.52	1.61	1	1
C	493	SEP	OG-P	4.41	1.52	1.61	1	1
C	467	SEP	OG-P	4.40	1.52	1.61	1	1
C	478	SEP	OG-P	4.39	1.52	1.61	1	1
C	463	SEP	OG-P	4.37	1.52	1.61	1	1
C	476	HIS	CE1-NE2	4.36	1.36	1.32	1	1
C	394	HIS	CE1-NE2	4.34	1.36	1.32	1	1
A	198	HIS	CE1-NE2	4.34	1.36	1.32	1	1
C	199	HIS	CE1-NE2	4.34	1.36	1.32	1	1
A	353	HIS	CD2-NE2	4.33	1.33	1.37	1	1
C	197	HIS	CE1-NE2	4.33	1.36	1.32	1	1
A	111	HIS	CE1-NE2	4.32	1.36	1.32	1	1
C	416	HIS	CE1-NE2	4.32	1.36	1.32	1	1
A	219	HIS	CE1-NE2	4.31	1.36	1.32	1	1
C	114	HIS	CE1-NE2	4.31	1.36	1.32	1	1
B	9	HIS	CE1-NE2	4.31	1.36	1.32	1	1
A	219	HIS	CD2-NE2	4.30	1.33	1.37	1	1
C	117	HIS	CE1-NE2	4.30	1.36	1.32	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	32	HIS	CE1-NE2	4.30	1.36	1.32	1	1
C	394	HIS	CD2-NE2	4.30	1.33	1.37	1	1
A	111	HIS	CD2-NE2	4.29	1.33	1.37	1	1
B	25	HIS	CE1-NE2	4.29	1.36	1.32	1	1
A	210	HIS	CE1-NE2	4.29	1.36	1.32	1	1
C	197	HIS	CD2-NE2	4.29	1.33	1.37	1	1
A	30	HIS	CD2-NE2	4.28	1.33	1.37	1	1
C	476	HIS	CD2-NE2	4.28	1.33	1.37	1	1
C	281	HIS	CD2-NE2	4.28	1.33	1.37	1	1
C	134	HIS	CD2-NE2	4.28	1.33	1.37	1	1
C	199	HIS	CD2-NE2	4.27	1.33	1.37	1	1
A	30	HIS	CE1-NE2	4.27	1.36	1.32	1	1
C	16	HIS	CD2-NE2	4.27	1.33	1.37	1	1
C	114	HIS	CD2-NE2	4.26	1.33	1.37	1	1
B	25	HIS	CD2-NE2	4.26	1.33	1.37	1	1
A	159	HIS	CE1-NE2	4.26	1.36	1.32	1	1
C	190	HIS	CE1-NE2	4.26	1.36	1.32	1	1
A	295	HIS	CD2-NE2	4.25	1.33	1.37	1	1
C	16	HIS	CE1-NE2	4.25	1.36	1.32	1	1
C	88	HIS	CE1-NE2	4.24	1.36	1.32	1	1
A	295	HIS	CE1-NE2	4.24	1.36	1.32	1	1
B	9	HIS	CD2-NE2	4.24	1.33	1.37	1	1
A	198	HIS	CD2-NE2	4.24	1.33	1.37	1	1
C	190	HIS	CD2-NE2	4.24	1.33	1.37	1	1
A	353	HIS	CE1-NE2	4.24	1.36	1.32	1	1
A	210	HIS	CD2-NE2	4.23	1.33	1.37	1	1
C	117	HIS	CD2-NE2	4.23	1.33	1.37	1	1
C	88	HIS	CD2-NE2	4.21	1.33	1.37	1	1
C	134	HIS	CE1-NE2	4.21	1.36	1.32	1	1
C	416	HIS	CD2-NE2	4.21	1.33	1.37	1	1
A	159	HIS	CD2-NE2	4.21	1.33	1.37	1	1
C	281	HIS	CE1-NE2	4.19	1.36	1.32	1	1
B	32	HIS	CD2-NE2	4.16	1.33	1.37	1	1

Standard geometry: angle outliers

There are no bond angle outliers.

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	1.68	24

There are 24 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)
C:459:ARG:O	C:460:LYS:C	0.69	1	1
C:436:CYS:O	C:437:ASN:C	0.65	1	1
C:436:CYS:O	C:437:ASN:O	0.63	1	1
C:62:TYR:N	C:63:PRO:HD2	0.60	1	1
A:42:LEU:C	A:42:LEU:HD13	0.57	1	1
C:71:ALA:N	C:72:PRO:CD	0.57	1	1
A:327:LEU:O	A:328:VAL:HG13	0.55	1	1
C:339:VAL:N	C:340:PRO:CD	0.54	1	1
C:365:GLU:O	C:366:THR:CB	0.53	1	1
C:305:LEU:N	C:306:PRO:CD	0.52	1	1
C:369:GLY:O	C:370:ARG:CB	0.51	1	1
C:455:LEU:O	C:456:ASP:C	0.51	1	1
A:203:LEU:N	A:203:LEU:HD12	0.48	1	1
C:62:TYR:N	C:63:PRO:CD	0.48	1	1
A:15:ASN:OD1	A:16:GLY:N	0.48	1	1
C:165:TYR:C	C:165:TYR:CD1	0.47	1	1
C:365:GLU:O	C:366:THR:HB	0.47	1	1
A:87:PHE:HA	A:88:PRO:C	0.46	1	1
C:501:THR:OG1	C:502:THR:N	0.43	1	1
C:388:MET:N	C:389:PRO:CD	0.42	1	1
C:467:SEP:O	C:468:TYR:C	0.42	1	1
C:62:TYR:HB3	C:63:PRO:HD3	0.42	1	1
C:165:TYR:CD1	C:166:THR:N	0.41	1	1
A:15:ASN:C	A:15:ASN:OD1	0.41	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	874	811	50	13

There are 13 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	THR	1
A	159	HIS	1
A	328	VAL	1
A	333	GLY	1
C	149	THR	1
C	331	GLY	1
C	366	THR	1
C	370	ARG	1
C	374	ARG	1
C	437	ASN	1
C	459	ARG	1
C	460	LYS	1
C	482	VAL	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	766	714	39	13

There are 13 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	30	HIS	1
A	40	VAL	1
A	50	GLU	1
A	204	ASP	1
A	327	LEU	1
A	328	VAL	1
A	329	VAL	1
A	335	LEU	1
A	338	LEU	1
C	268	THR	1

Chain	Res	Type	Models (Total)
C	370	ARG	1
C	373	THR	1
C	495	ARG	1

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 136 crosslinking restraints combined in 136 restraint groups.

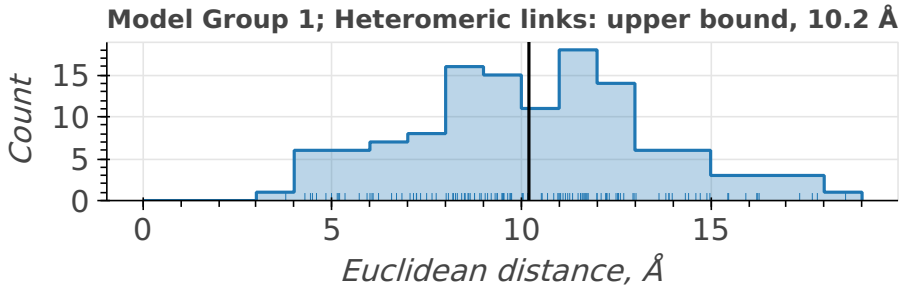
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BrEtY	ALA	CB	TYR	CB	upper bound	10.2	1
BrEtY	ALA	CB	ASP	CB	upper bound	10.2	1
BrEtY	ALA	CB	LYS	CB	upper bound	10.2	3
BrEtY	ALA	CB	LEU	CB	upper bound	10.2	1
BrEtY	ALA	CB	VAL	CB	upper bound	10.2	1
BrEtY	ALA	CB	HIS	CB	upper bound	10.2	1
BrEtY	ALA	CB	ASN	CB	upper bound	10.2	1
BrEtY	CYS	CB	THR	CB	upper bound	10.2	1
BrEtY	ASP	CB	CYS	CB	upper bound	10.2	2
BrEtY	CYS	CB	PHE	CB	upper bound	10.2	1
BrEtY	CYS	CB	LYS	CB	upper bound	10.2	1
BrEtY	ASP	CB	ASP	CB	upper bound	10.2	1
BrEtY	ASP	CB	PHE	CB	upper bound	10.2	1
BrEtY	ASP	CB	LYS	CB	upper bound	10.2	1
BrEtY	ASP	CB	VAL	CB	upper bound	10.2	1
BrEtY	ASP	CB	GLU	CB	upper bound	10.2	1
BrEtY	GLU	CB	GLU	CB	upper bound	10.2	1
BrEtY	GLU	CB	PHE	CB	upper bound	10.2	1
BrEtY	GLU	CB	LYS	CB	upper bound	10.2	1
BrEtY	GLU	CB	LEU	CB	upper bound	10.2	1
BrEtY	GLU	CB	VAL	CB	upper bound	10.2	1

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BrEtY	PHE	CB	TYR	CB	upper bound	10.2	1
BrEtY	ASP	CB	GLY	CB	upper bound	10.2	1
BrEtY	GLY	CB	PHE	CB	upper bound	10.2	1
BrEtY	GLY	CB	VAL	CB	upper bound	10.2	1
BrEtY	GLY	CB	LYS	CB	upper bound	10.2	5
BrEtY	ASN	CB	GLY	CB	upper bound	10.2	1
BrEtY	GLY	CB	PRO	CB	upper bound	10.2	1
BrEtY	ARG	CB	GLY	CB	upper bound	10.2	2
BrEtY	LEU	CB	LYS	CB	upper bound	10.2	3
BrEtY	ARG	CB	LEU	CB	upper bound	10.2	8
BrEtY	LEU	CB	PRO	CB	upper bound	10.2	1
BrEtY	LYS	CB	MET	CB	upper bound	10.2	1
BrEtY	ASN	CB	ASP	CB	upper bound	10.2	2
BrEtY	ASN	CB	PHE	CB	upper bound	10.2	1
BrEtY	ASN	CB	LYS	CB	upper bound	10.2	2
BrEtY	ASN	CB	VAL	CB	upper bound	10.2	2
BrEtY	ASN	CB	LEU	CB	upper bound	10.2	1
BrEtY	ARG	CB	ASN	CB	upper bound	10.2	2
BrEtY	LYS	CB	PRO	CB	upper bound	10.2	4
BrEtY	ARG	CB	PRO	CB	upper bound	10.2	8
BrEtY	GLN	CB	PHE	CB	upper bound	10.2	1
BrEtY	GLN	CB	LYS	CB	upper bound	10.2	1
BrEtY	ARG	CB	ASP	CB	upper bound	10.2	1
BrEtY	ARG	CB	PHE	CB	upper bound	10.2	2
BrEtY	ARG	CB	LYS	CB	upper bound	10.2	5
BrEtY	ARG	CB	VAL	CB	upper bound	10.2	4
BrEtY	ARG	CB	HIS	CB	upper bound	10.2	1
BrEtY	ARG	CB	ARG	CB	upper bound	10.2	4
BrEtY	HIS	CB	SEP	CB	upper bound	10.2	2
BrEtY	LYS	CB	SEP	CB	upper bound	10.2	5
BrEtY	PRO	CB	SEP	CB	upper bound	10.2	3
BrEtY	LYS	CB	SER	CB	upper bound	10.2	7
BrEtY	PRO	CB	SER	CB	upper bound	10.2	3
BrEtY	HIS	CB	SER	CB	upper bound	10.2	1
BrEtY	SER	CB	SER	CB	upper bound	10.2	1

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BrEtY	ASN	CB	SEP	CB	upper bound	10.2	1
BrEtY	ARG	CB	SEP	CB	upper bound	10.2	2
BrEtY	ASP	CB	THR	CB	upper bound	10.2	1
BrEtY	PHE	CB	THR	CB	upper bound	10.2	2
BrEtY	LYS	CB	THR	CB	upper bound	10.2	2
BrEtY	LEU	CB	THR	CB	upper bound	10.2	1
BrEtY	THR	CB	VAL	CB	upper bound	10.2	1
BrEtY	LYS	CB	TPO	CB	upper bound	10.2	2
BrEtY	ARG	CB	THR	CB	upper bound	10.2	1
BrEtY	LYS	CB	VAL	CB	upper bound	10.2	2
BrEtY	LYS	CB	TYR	CB	upper bound	10.2	4
BrEtY	ASN	CB	TYR	CB	upper bound	10.2	2
BrEtY	PRO	CB	TYR	CB	upper bound	10.2	2

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



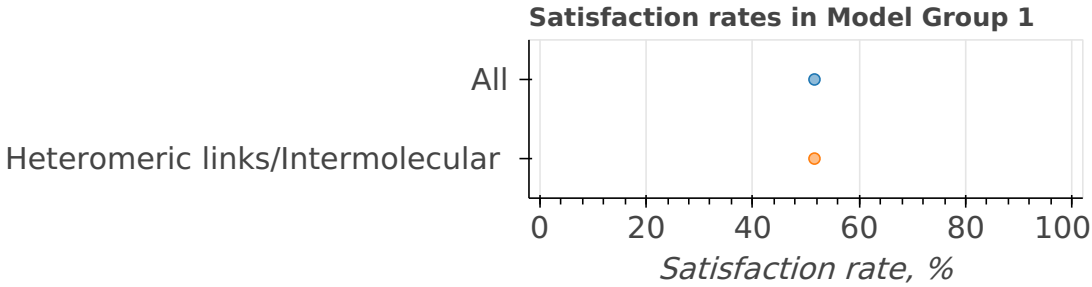
Satisfaction of restraints

Satisfaction of restraints is calculated on a restraint group (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=136)
1	1	1	1/1	All	51.61	48.39	124
				Heteromeric links/ Intermolecular	51.61	48.39	124

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Fit of model to data used for validation

Validation for this section is under development.

Acknowledgments

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