Integrative Structure Validation Report

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

IHMValidation Version 3.0
Python-IHM Version 2.5
MolProbity Version 4.5.2

PDB ID	9A3I | pdb_00009a3i
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.
Deposited on	2023-03-24

This is a PDB-IHM Structure Validation Report.

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.

1. Overview

1.1. Summary

This entry consists of 1 model(s). A total of 6 dataset(s) were used to build this entry.

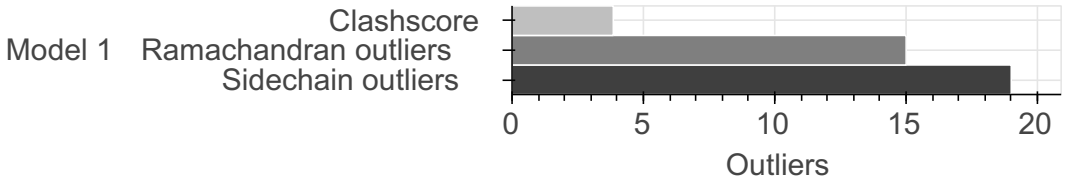
Name	Type	Count
Crosslinking-MS data	Experimental data	1
Experimental model	Starting model	2
Comparative model	Starting model	2

Name	Type	Count
De Novo model	Starting model	1

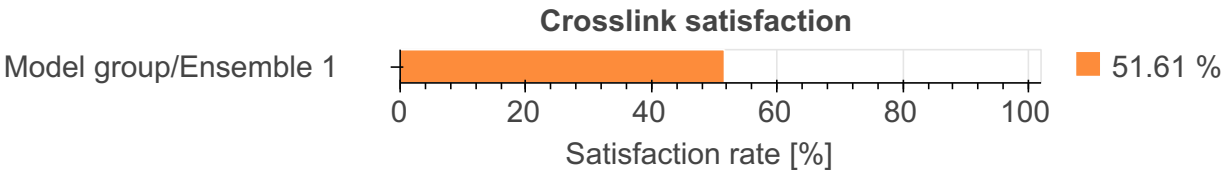
1.2. Overall quality

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



Fit to Data Used for Modeling



2. Model Details

2.1. Ensemble information

This entry consists of 0 distinct ensemble(s).

2.2. 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

2.3. 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	pdb_00006nbf
3	Experimental model	PDB	pdb_00006u1n
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	De Novo model	Not available	Not available

2.4. 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	Not available	Not available	Not available	Not available	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

3. Data quality

3.2. 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.

4. 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.

4.1b. MolProbity Analysis

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-partice or particle-atom pairs for which excluded volume was analysed.

Standard geometry: bond outliers

There are 53 bond length outliers in this entry (0.73% of 7273 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	9.78	1.52	1.72	1	1
C	467	SEP	O2P-P	4.83	1.51	1.61	1	1
C	478	SEP	O3P-P	4.82	1.51	1.61	1	1
C	493	SEP	O2P-P	4.81	1.51	1.61	1	1
C	463	SEP	O3P-P	4.80	1.51	1.61	1	1
C	478	SEP	O1P-P	4.79	1.51	1.61	1	1
C	463	SEP	O1P-P	4.79	1.51	1.61	1	1
C	467	SEP	O3P-P	4.79	1.51	1.61	1	1
C	467	SEP	O1P-P	4.79	1.51	1.61	1	1
C	493	SEP	O3P-P	4.79	1.51	1.61	1	1
C	493	SEP	O1P-P	4.79	1.51	1.61	1	1
C	463	SEP	O2P-P	4.78	1.51	1.61	1	1
C	478	SEP	O2P-P	4.76	1.51	1.61	1	1
C	493	SEP	OG-P	4.42	1.52	1.61	1	1
C	467	SEP	OG-P	4.42	1.52	1.61	1	1
C	463	SEP	OG-P	4.41	1.52	1.61	1	1
C	478	SEP	OG-P	4.40	1.52	1.61	1	1
C	476	HIS	CE1-NE2	4.37	1.36	1.32	1	1
A	295	HIS	CE1-NE2	4.36	1.36	1.32	1	1
B	32	HIS	CE1-NE2	4.35	1.36	1.32	1	1
A	353	HIS	CD2-NE2	4.33	1.33	1.37	1	1
A	353	HIS	CE1-NE2	4.33	1.36	1.32	1	1
C	197	HIS	CD2-NE2	4.33	1.33	1.37	1	1
C	281	HIS	CD2-NE2	4.32	1.33	1.37	1	1
C	117	HIS	CD2-NE2	4.32	1.33	1.37	1	1
B	25	HIS	CE1-NE2	4.32	1.36	1.32	1	1
C	88	HIS	CE1-NE2	4.32	1.36	1.32	1	1
C	476	HIS	CD2-NE2	4.30	1.33	1.37	1	1
C	114	HIS	CE1-NE2	4.30	1.36	1.32	1	1
A	198	HIS	CE1-NE2	4.30	1.36	1.32	1	1
A	30	HIS	CD2-NE2	4.29	1.33	1.37	1	1
C	197	HIS	CE1-NE2	4.29	1.36	1.32	1	1
A	295	HIS	CD2-NE2	4.28	1.33	1.37	1	1
C	416	HIS	CD2-NE2	4.28	1.33	1.37	1	1
A	30	HIS	CE1-NE2	4.27	1.36	1.32	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	117	HIS	CE1-NE2	4.27	1.36	1.32	1	1
C	88	HIS	CD2-NE2	4.26	1.33	1.37	1	1
A	159	HIS	CD2-NE2	4.26	1.33	1.37	1	1
B	9	HIS	CE1-NE2	4.26	1.36	1.32	1	1
B	9	HIS	CD2-NE2	4.26	1.33	1.37	1	1
B	32	HIS	CD2-NE2	4.26	1.33	1.37	1	1
C	281	HIS	CE1-NE2	4.25	1.36	1.32	1	1
A	219	HIS	CE1-NE2	4.25	1.36	1.32	1	1
A	219	HIS	CD2-NE2	4.24	1.33	1.37	1	1
A	210	HIS	CE1-NE2	4.24	1.36	1.32	1	1
B	25	HIS	CD2-NE2	4.23	1.33	1.37	1	1
A	210	HIS	CD2-NE2	4.23	1.33	1.37	1	1
A	111	HIS	CE1-NE2	4.23	1.36	1.32	1	1
C	416	HIS	CE1-NE2	4.23	1.36	1.32	1	1
A	111	HIS	CD2-NE2	4.23	1.33	1.37	1	1
C	114	HIS	CD2-NE2	4.22	1.33	1.37	1	1
A	198	HIS	CD2-NE2	4.21	1.33	1.37	1	1
A	159	HIS	CE1-NE2	4.21	1.36	1.32	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	3.85	55

There are 55 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)
A:327:LEU:O	A:328:VAL:HG13	0.84	1	1
C:459:ARG:O	C:460:LYS:C	0.75	1	1
A:337:ASP:O	A:338:LEU:CB	0.71	1	1
A:42:LEU:C	A:42:LEU:HD13	0.65	1	1
A:337:ASP:O	A:338:LEU:CG	0.65	1	1
C:165:TYR:C	C:165:TYR:CD1	0.63	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:337:ASP:O	A:338:LEU:HB2	0.62	1	1
C:62:TYR:N	C:63:PRO:HD2	0.59	1	1
A:204:ASP:C	A:204:ASP:OD1	0.57	1	1
C:71:ALA:N	C:72:PRO:CD	0.57	1	1
A:339:ALA:O	A:340:SER:HB3	0.56	1	1
C:165:TYR:CD1	C:166:THR:N	0.56	1	1
C:469:SER:O	C:470:TYR:CB	0.55	1	1
A:203:LEU:N	A:203:LEU:HD12	0.55	1	1
A:202:SER:C	A:203:LEU:HD12	0.54	1	1
C:305:LEU:N	C:306:PRO:CD	0.53	1	1
C:391:PHE:O	C:392:GLY:C	0.53	1	1
C:339:VAL:N	C:340:PRO:CD	0.53	1	1
A:337:ASP:O	A:338:LEU:HG	0.52	1	1
A:15:ASN:OD1	A:16:GLY:N	0.50	1	1
A:87:PHE:HA	A:88:PRO:C	0.50	1	1
A:5:GLY:O	A:6:THR:HB	0.47	1	1
A:76:ARG:O	C:366:THR:HG23	0.47	1	1
C:62:TYR:N	C:63:PRO:CD	0.47	1	1
A:66:GLU:CD	A:66:GLU:N	0.47	1	1
A:42:LEU:HD13	A:43:VAL:N	0.46	1	1
C:469:SER:O	C:470:TYR:HB2	0.46	1	1
C:62:TYR:HB3	C:63:PRO:HD3	0.46	1	1
A:339:ALA:O	A:340:SER:CB	0.46	1	1
A:328:VAL:HG11	A:342:ASP:HB3	0.45	1	1
C:321:ALA:O	C:322:ASN:C	0.45	1	1
A:25:ARG:NH1	C:477:TPO:HG21	0.45	1	1
A:13:SER:HB2	A:14:PRO:CD	0.44	1	1
A:13:SER:OG	A:15:ASN:OD1	0.44	1	1
C:123:ASP:C	C:123:ASP:OD1	0.44	1	1
C:369:GLY:O	C:370:ARG:CB	0.44	1	1
A:61:PHE:C	A:61:PHE:CD1	0.44	1	1
A:50:GLU:HG2	A:51:ARG:N	0.44	1	1
A:150:CYS:O	A:151:ALA:HB2	0.43	1	1
A:203:LEU:CD1	A:203:LEU:N	0.43	1	1
A:327:LEU:C	A:328:VAL:HG22	0.43	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
C:264:TYR:O	C:268:THR:HG23	0.42	1	1
C:47:SER:O	C:48:THR:C	0.42	1	1
C:1:ASP:C	C:1:ASP:OD1	0.42	1	1
A:42:LEU:C	A:42:LEU:CD1	0.42	1	1
A:61:PHE:CZ	A:317:ILE:HD11	0.41	1	1
C:388:MET:N	C:389:PRO:CD	0.41	1	1
A:327:LEU:O	A:328:VAL:CG1	0.41	1	1
A:59:CYS:SG	A:142:VAL:HG13	0.41	1	1
C:388:MET:HB2	C:389:PRO:HD3	0.41	1	1
A:13:SER:HB2	A:14:PRO:HD2	0.41	1	1
C:490:LEU:CB	C:491:PRO:HA	0.41	1	1
A:38:ASP:N	A:38:ASP:OD1	0.41	1	1
A:48:LEU:N	A:48:LEU:HD22	0.41	1	1
C:487:GLY:O	C:488:LEU:C	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	859	791	53	15

There are 15 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	THR	1
A	328	VAL	1
A	333	GLY	1
A	338	LEU	1
A	340	SER	1
C	149	THR	1
C	322	ASN	1
C	331	GLY	1
C	366	THR	1
C	370	ARG	1
C	392	GLY	1
C	459	ARG	1
C	460	LYS	1

Chain	Res	Type	Models (Total)
C	482	VAL	1
C	486	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	761	696	46	19

There are 19 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	THR	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	1

5. Fit to Data Used for Modeling Assessment

5.2. Crosslinking-MS

5.2.1. Restraint types

This table summarizes information about crosslinker(s) used for data generation, and how crosslinking information was translated into

actual modeling restraints. 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.

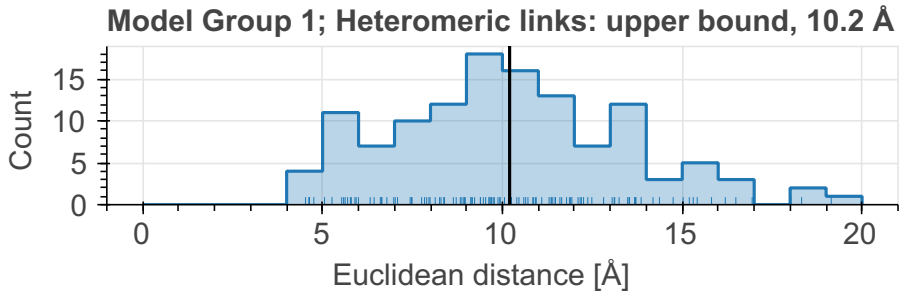
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BrEtY	ALA	CB	TYR	CB	upper bound	10.20	1
BrEtY	ALA	CB	ASP	CB	upper bound	10.20	1
BrEtY	ALA	CB	LYS	CB	upper bound	10.20	3
BrEtY	ALA	CB	LEU	CB	upper bound	10.20	1
BrEtY	ALA	CB	VAL	CB	upper bound	10.20	1
BrEtY	ALA	CB	HIS	CB	upper bound	10.20	1
BrEtY	ALA	CB	ASN	CB	upper bound	10.20	1
BrEtY	CYS	CB	THR	CB	upper bound	10.20	1
BrEtY	ASP	CB	CYS	CB	upper bound	10.20	2
BrEtY	CYS	CB	PHE	CB	upper bound	10.20	1
BrEtY	CYS	CB	LYS	CB	upper bound	10.20	1
BrEtY	ASP	CB	ASP	CB	upper bound	10.20	1
BrEtY	ASP	CB	PHE	CB	upper bound	10.20	1
BrEtY	ASP	CB	LYS	CB	upper bound	10.20	1
BrEtY	ASP	CB	VAL	CB	upper bound	10.20	1
BrEtY	ASP	CB	GLU	CB	upper bound	10.20	1
BrEtY	GLU	CB	GLU	CB	upper bound	10.20	1
BrEtY	GLU	CB	PHE	CB	upper bound	10.20	1
BrEtY	GLU	CB	LYS	CB	upper bound	10.20	1
BrEtY	GLU	CB	LEU	CB	upper bound	10.20	1
BrEtY	GLU	CB	VAL	CB	upper bound	10.20	1
BrEtY	PHE	CB	TYR	CB	upper bound	10.20	1
BrEtY	ASP	CB	GLY	CB	upper bound	10.20	1
BrEtY	GLY	CB	PHE	CB	upper bound	10.20	1
BrEtY	GLY	CB	VAL	CB	upper bound	10.20	1
BrEtY	GLY	CB	LYS	CB	upper bound	10.20	5
BrEtY	ASN	CB	GLY	CB	upper bound	10.20	1
BrEtY	GLY	CB	PRO	CB	upper bound	10.20	1
BrEtY	ARG	CB	GLY	CB	upper bound	10.20	2
BrEtY	LEU	CB	LYS	CB	upper bound	10.20	3
BrEtY	ARG	CB	LEU	CB	upper bound	10.20	8

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BrEtY	LEU	CB	PRO	CB	upper bound	10.20	1
BrEtY	LYS	CB	MET	CB	upper bound	10.20	1
BrEtY	ASN	CB	ASP	CB	upper bound	10.20	2
BrEtY	ASN	CB	PHE	CB	upper bound	10.20	1
BrEtY	ASN	CB	LYS	CB	upper bound	10.20	2
BrEtY	ASN	CB	VAL	CB	upper bound	10.20	2
BrEtY	ASN	CB	LEU	CB	upper bound	10.20	1
BrEtY	ARG	CB	ASN	CB	upper bound	10.20	2
BrEtY	LYS	CB	PRO	CB	upper bound	10.20	4
BrEtY	ARG	CB	PRO	CB	upper bound	10.20	8
BrEtY	GLN	CB	PHE	CB	upper bound	10.20	1
BrEtY	GLN	CB	LYS	CB	upper bound	10.20	1
BrEtY	ARG	CB	ASP	CB	upper bound	10.20	1
BrEtY	ARG	CB	PHE	CB	upper bound	10.20	2
BrEtY	ARG	CB	LYS	CB	upper bound	10.20	5
BrEtY	ARG	CB	VAL	CB	upper bound	10.20	4
BrEtY	ARG	CB	HIS	CB	upper bound	10.20	1
BrEtY	ARG	CB	ARG	CB	upper bound	10.20	4
BrEtY	HIS	CB	SEP	CB	upper bound	10.20	2
BrEtY	LYS	CB	SEP	CB	upper bound	10.20	5
BrEtY	PRO	CB	SEP	CB	upper bound	10.20	3
BrEtY	LYS	CB	SER	CB	upper bound	10.20	7
BrEtY	PRO	CB	SER	CB	upper bound	10.20	3
BrEtY	HIS	CB	SER	CB	upper bound	10.20	1
BrEtY	SER	CB	SER	CB	upper bound	10.20	1
BrEtY	ASN	CB	SEP	CB	upper bound	10.20	1
BrEtY	ARG	CB	SEP	CB	upper bound	10.20	2
BrEtY	ASP	CB	THR	CB	upper bound	10.20	1
BrEtY	PHE	CB	THR	CB	upper bound	10.20	2
BrEtY	LYS	CB	THR	CB	upper bound	10.20	2
BrEtY	LEU	CB	THR	CB	upper bound	10.20	1
BrEtY	THR	CB	VAL	CB	upper bound	10.20	1
BrEtY	LYS	CB	TPO	CB	upper bound	10.20	2
BrEtY	ARG	CB	THR	CB	upper bound	10.20	1
BrEtY	LYS	CB	VAL	CB	upper bound	10.20	2

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BrEtY	LYS	CB	TYR	CB	upper bound	10.20	4
BrEtY	ASN	CB	TYR	CB	upper bound	10.20	2
BrEtY	PRO	CB	TYR	CB	upper bound	10.20	2

Distograms of individual restraints

Distograms (i.e., histogram plots of distances) provide an overview of distributions of distances between residues for which chemical crosslinks were identified. The shift of the distogram relative to the threshold value may indicate a poor model. 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.



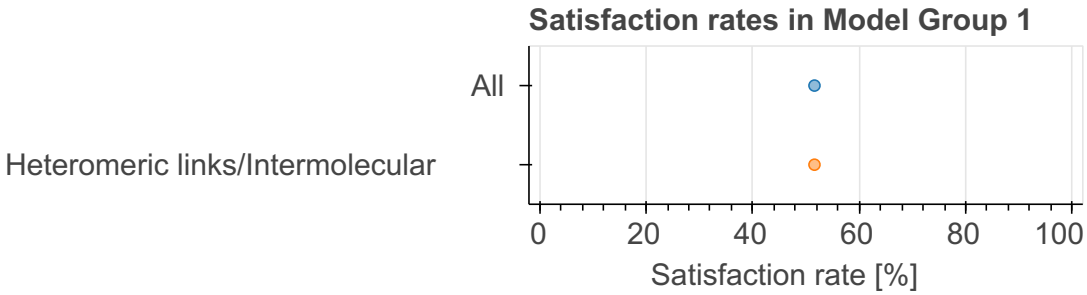
5.2.2. Satisfaction of restraints

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.



6. Fit to Data Used for Validation Assessment

Validation for this section is under development.

Acknowledgments

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