

# Integrative Structure Validation Report ?

February 18, 2025 - 08:36 AM PST

*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*

*pyHMMER Version 0.11.0*

PDB ID	9A34
PDB-Dev ID	PDBDEV_00000189
Structure Title	Model of E. coli OmpT by in-cell photo-crosslinking MS and deep learning
Structure Authors	Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J.
Deposited on	2023-02-03

*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](mailto:helpdesk@pdb-ihm.org)*

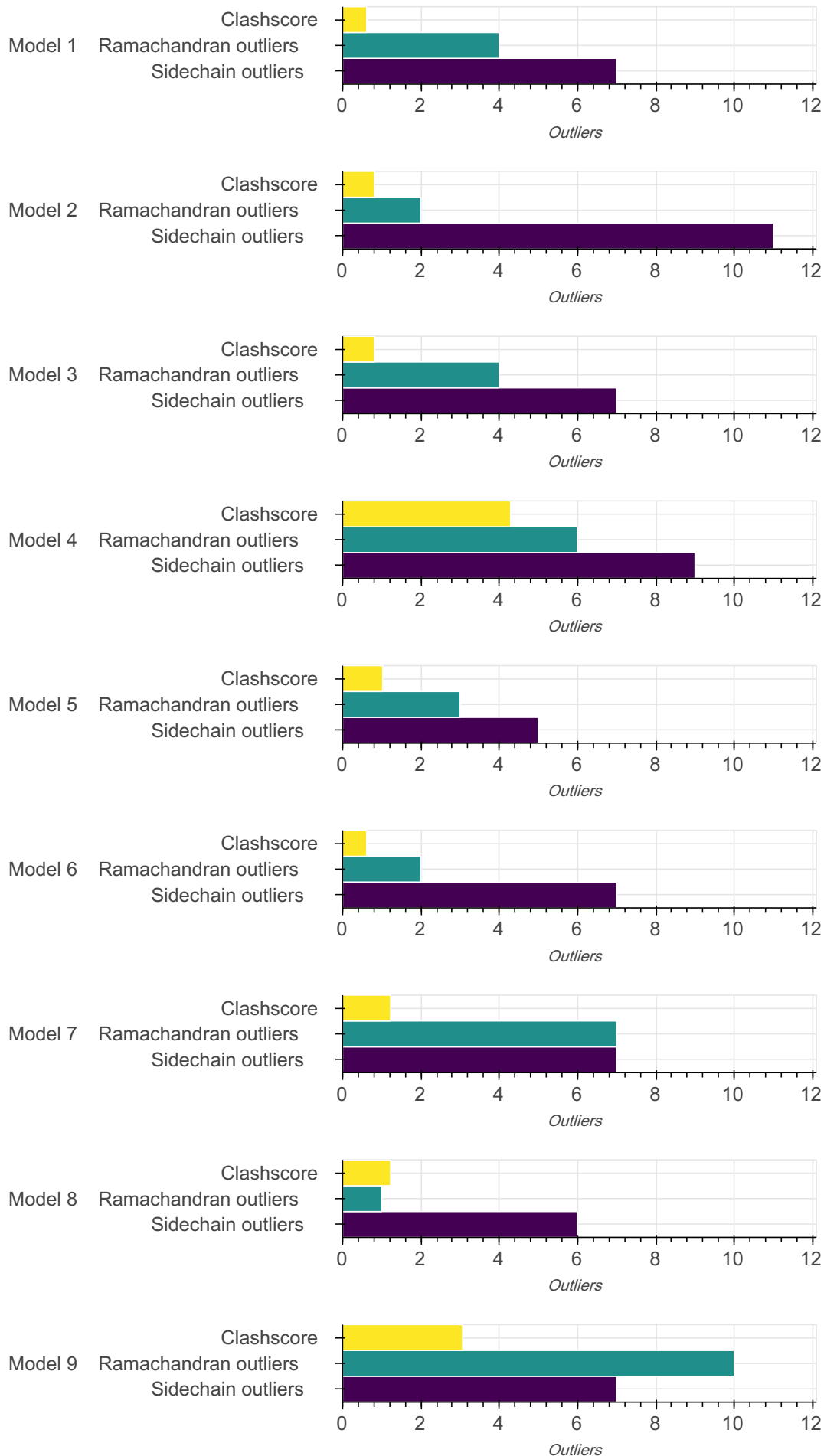
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

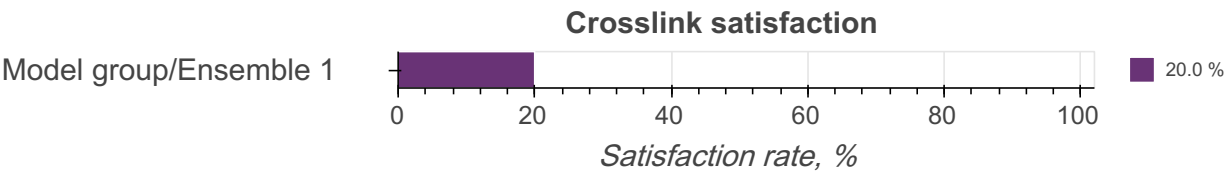
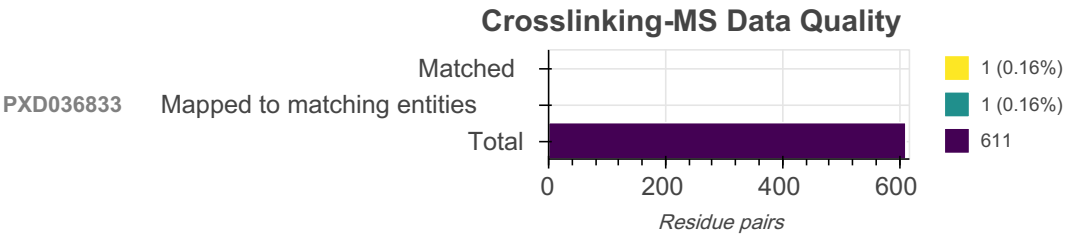
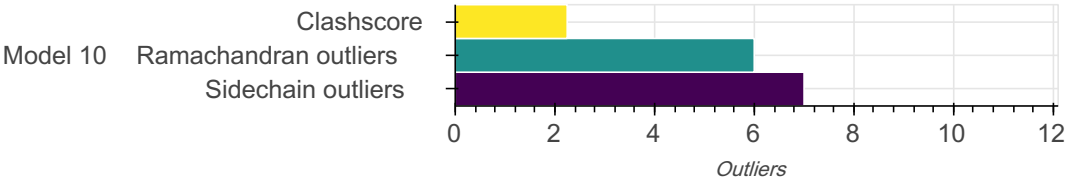
*List of references used to build this report is available [here](#).*

## 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 10 model(s). A total of 1 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	1-10	1	P09169	A	317	-	1-317	100.00 / 0.00	Atomic

Datasets used for modeling ?

There is 1 unique dataset used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	jPOSTrepo	JPST001851

## 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	AlphaLink	AlphaLink with 10 msa subsamples	None	10	False	False

*There is 1 software package reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">AlphaLink</a>	1.00	model building	<a href="https://github.com/lhatsk/AlphaLink">https://github.com/lhatsk/AlphaLink</a>

## 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 ([PRIDE ID](#)) [PXD036833](#)

Number of entities in the crosslinking-MS dataset: 1102

Number of entities in the entry: 1

Matching entities:

Entity ID	Molecule name	Crosslinking-MS Entity ID	E-value	Exact match
1	P09169	dbseq_P09169_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A34	5	5 (100.00%)	1 (20.00%)
PXD036833	611	1 (0.16%)	1 (0.16%)

### 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 no bond length outliers.*

#### Standard geometry: angle outliers ?

*There are 77 bond angle outliers in this entry (0.22% of 34940 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	2	ARG	C-N-CA	7.22	134.70	121.70	7	2
A	61	GLN	OE1-CD-NE2	6.04	116.56	122.60	4	8
A	229	ASN	OD1-CG-ND2	5.87	116.73	122.60	10	4
A	63	ASP	CA-CB-CG	5.84	118.44	112.60	5	4
A	29	PRO	C-N-CA	5.73	132.01	121.70	10	4
A	8	ILE	C-N-CA	5.39	131.40	121.70	10	1
A	1	MET	C-N-CA	5.38	131.38	121.70	7	2
A	155	GLN	OE1-CD-NE2	5.30	117.30	122.60	2	8
A	16	ILE	C-N-CA	5.26	131.16	121.70	4	1
A	289	ASN	OD1-CG-ND2	4.93	117.67	122.60	5	1
A	179	ASP	O-C-N	4.93	115.12	123.00	1	1
A	104	GLN	OE1-CD-NE2	4.83	117.77	122.60	2	8
A	125	GLN	OE1-CD-NE2	4.82	117.78	122.60	9	1
A	179	ASP	C-N-CA	4.78	130.31	121.70	1	1
A	31	ASN	OD1-CG-ND2	4.64	117.96	122.60	7	2
A	30	ASP	CA-CB-CG	4.61	117.21	112.60	8	2
A	44	LYS	CG-CD-CE	4.58	100.76	111.30	4	1
A	53	GLU	C-N-CA	4.46	129.73	121.70	4	1
A	179	ASP	CA-C-N	4.43	125.06	116.20	1	1
A	176	PHE	C-N-CA	4.38	129.58	121.70	9	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	83	GLN	OE1-CD-NE2	4.30	118.30	122.60	10	9
A	100	ASN	OD1-CG-ND2	4.27	118.33	122.60	5	3
A	45	THR	CA-CB-CG2	4.26	117.74	110.50	7	1
A	147	ARG	NE-CZ-NH2	4.24	123.02	119.20	7	1
A	175	GLY	C-N-CA	4.18	129.22	121.70	4	1
A	147	ARG	NH1-CZ-NH2	4.16	113.89	119.30	10	1
A	9	VAL	N-CA-CB	4.14	104.45	111.50	10	1
A	2	ARG	O-C-N	4.13	116.39	123.00	7	1
A	288	HIS	CB-CG-CD2	4.12	125.84	131.20	10	2
A	178	ASP	CA-CB-CG	4.08	116.68	112.60	7	2
A	142	ASN	OD1-CG-ND2	4.01	118.59	122.60	4	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	0.61	3
2	0.82	4
3	0.82	4
4	4.29	21
5	1.02	5
6	0.61	3
7	1.23	6
8	1.23	6
9	3.06	15
10	2.25	11

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

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:101:MET:HE1	A:190:ILE:HD12	0.77	9	2
A:101:MET:HE2	A:121:HIS:CD2	0.71	9	2
A:9:VAL:HG12	A:11:THR:HG23	0.68	3	2
A:25:LEU:HD22	A:27:PHE:CZ	0.64	4	1
A:168:TYR:CZ	A:181:GLY:HA3	0.63	1	1
A:101:MET:CE	A:163:ALA:HB2	0.61	10	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:25:LEU:HD11	A:263:PRO:HA	0.60	7	1
A:62:LEU:HD11	A:101:MET:SD	0.59	10	1
A:64:TRP:CZ2	A:101:MET:SD	0.57	4	2
A:101:MET:CE	A:121:HIS:CD2	0.57	4	2
A:64:TRP:CH2	A:101:MET:SD	0.57	9	2
A:59:VAL:HG12	A:107:MET:CE	0.57	9	1
A:183:PHE:CE1	A:188:ARG:CZ	0.56	7	1
A:44:LYS:HE2	A:46:LYS:HE2	0.56	2	6
A:228:ASP:OD2	A:302:ILE:HD11	0.56	10	1
A:62:LEU:HD21	A:64:TRP:HE1	0.56	4	1
A:57:ARG:NH2	A:107:MET:SD	0.54	9	1
A:237:LYS:HA	A:289:ASN:HD21	0.52	4	1
A:30:ASP:HA	A:317:PHE:O	0.52	10	3
A:25:LEU:HD22	A:80:LEU:HD11	0.51	8	1
A:101:MET:HE3	A:163:ALA:HB2	0.50	10	1
A:237:LYS:HE2	A:239:ILE:HD11	0.50	4	1
A:198:MET:HG2	A:224:VAL:HG22	0.49	8	2
A:226:SER:CB	A:248:GLN:HE22	0.49	4	1
A:45:THR:HG22	A:64:TRP:HB2	0.49	7	3
A:188:ARG:HH21	A:191:GLY:HA3	0.49	10	3
A:50:TYR:CD1	A:280:LYS:HE2	0.49	8	1
A:168:TYR:CE1	A:181:GLY:HA3	0.49	1	1
A:25:LEU:HD22	A:27:PHE:CE2	0.47	4	1
A:132:PHE:CZ	A:134:LEU:HG	0.47	1	1
A:47:GLU:HB3	A:62:LEU:HB3	0.47	4	1
A:195:ARG:NH2	A:197:LYS:HE2	0.47	6	1
A:224:VAL:HB	A:248:GLN:HB2	0.47	4	1
A:278:ASN:HB3	A:302:ILE:H	0.47	4	1
A:126:LEU:HD13	A:161:PHE:CE2	0.46	9	1
A:9:VAL:CG1	A:11:THR:HG23	0.46	3	1
A:132:PHE:CE2	A:156:GLU:HB3	0.46	2	1
A:283:THR:HB	A:300:ALA:HB2	0.44	2	2
A:58:LYS:HE3	A:60:SER:HB2	0.44	4	1
A:247:ASP:HB2	A:279:LYS:HZ3	0.44	5	1
A:128:TYR:CZ	A:160:SER:HB2	0.44	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:151:MET:HE3	A:204:THR:HB	0.44	5	1
A:101:MET:CE	A:190:ILE:HD12	0.44	9	1
A:27:PHE:CZ	A:147:ARG:HD2	0.43	4	1
A:237:LYS:CE	A:239:ILE:HD11	0.43	4	1
A:64:TRP:CZ3	A:101:MET:CE	0.43	10	1
A:126:LEU:HD13	A:161:PHE:CE1	0.43	4	1
A:64:TRP:CZ3	A:101:MET:HE2	0.43	10	1
A:29:PRO:HA	A:79:ASP:O	0.43	4	1
A:44:LYS:HE2	A:46:LYS:CE	0.42	4	1
A:64:TRP:CZ2	A:192:TYR:HB2	0.42	10	1
A:58:LYS:HE3	A:115:TRP:CH2	0.42	8	1
A:64:TRP:CH2	A:101:MET:CE	0.42	10	1
A:107:MET:HE3	A:115:TRP:CH2	0.42	6	1
A:25:LEU:HD11	A:263:PRO:CA	0.42	7	1
A:116:THR:HB	A:171:SER:HB3	0.42	7	1
A:241:TYR:CE2	A:285:LEU:HD12	0.41	9	2
A:29:PRO:HG3	A:82:PRO:HD3	0.40	4	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	315	289	22	4
2	315	299	14	2
3	315	293	18	4
4	315	294	15	6
5	315	297	15	3
6	315	298	15	2
7	315	295	13	7
8	315	293	21	1
9	315	288	17	10
10	315	296	13	6

There are 25 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	25	LEU	5



Chain	Res	Type	Models (Total)
A	16	ILE	4
A	18	SER	4
A	22	THR	3
A	30	ASP	3
A	178	ASP	3
A	17	SER	2
A	19	PHE	2
A	21	SER	2
A	176	PHE	2
A	2	ARG	1
A	3	ALA	1
A	6	LEU	1
A	7	GLY	1
A	8	ILE	1
A	11	THR	1
A	14	ILE	1
A	15	ALA	1
A	20	ALA	1
A	24	THR	1
A	54	GLU	1
A	107	MET	1
A	177	ARG	1
A	180	ILE	1
A	296	SER	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	264	254	3	7
2	264	248	5	11
3	264	252	5	7
4	264	249	6	9
5	264	251	8	5
6	264	255	2	7

Model ID	Analysed	Favored	Allowed	Outliers
7	264	253	4	7
8	264	252	6	6
9	264	250	7	7
10	264	250	7	7

There are 25 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	5	LEU	9
A	12	THR	9
A	10	LEU	7
A	6	LEU	6
A	24	THR	6
A	247	ASP	6
A	22	THR	4
A	25	LEU	3
A	28	THR	3
A	45	THR	3
A	17	SER	2
A	33	ASN	2
A	1	MET	1
A	8	ILE	1
A	11	THR	1
A	16	ILE	1
A	30	ASP	1
A	57	ARG	1
A	85	SER	1
A	105	ASP	1
A	124	THR	1
A	151	MET	1
A	157	SER	1
A	171	SER	1
A	313	LEU	1

Fit of model to data used for modeling ?

## Fit of model(s) to crosslinking-MS data

### Restraint types

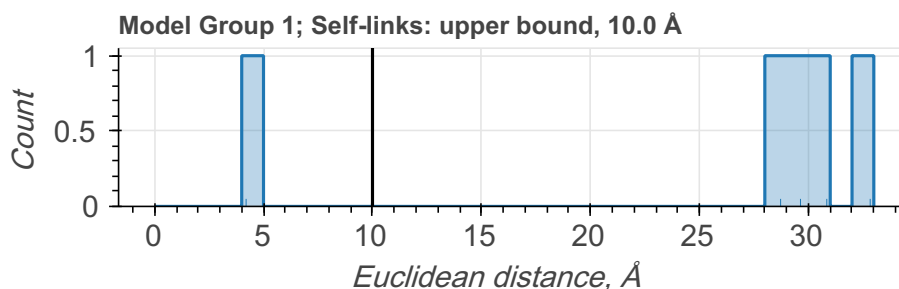
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 5 crosslinking restraints combined in 5 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	GLY	CA	LEU	CA	upper bound	10.0	2
L-Photo-Leucine	ALA	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	LEU	CA	upper bound	10.0	1

### 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.



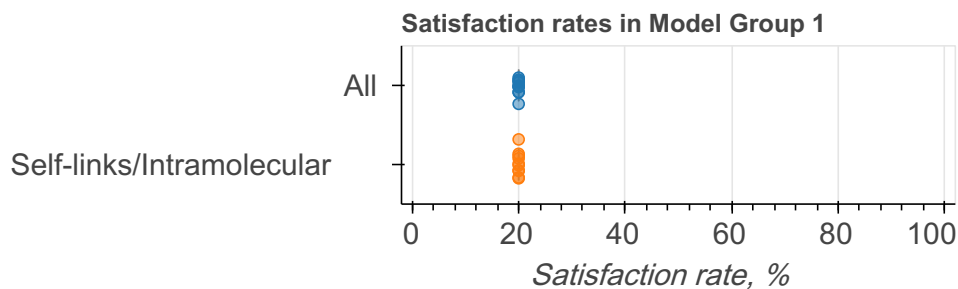
### Satisfaction of restraints

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=5)
1	1	1	10/10	All	20.00	80.00	5
				Self-links/ Intramolecular	20.00	80.00	5

### 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

*The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.*

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