

Integrative Structure Validation Report ?

February 18, 2025 - 08:35 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	9A2T
PDB-Dev ID	PDBDEV_00000178
Structure Title	Model of E. coli CysK 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

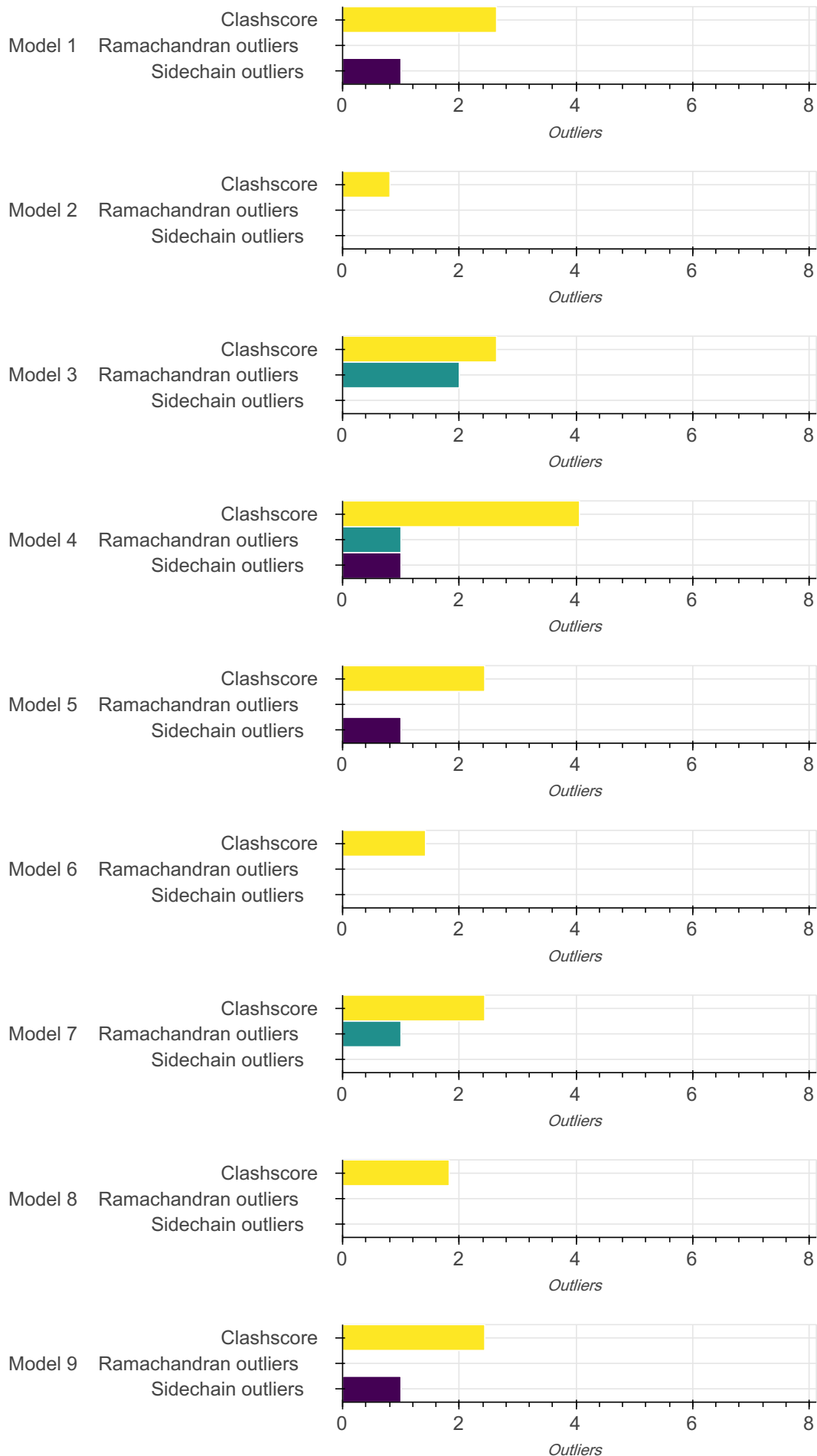
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

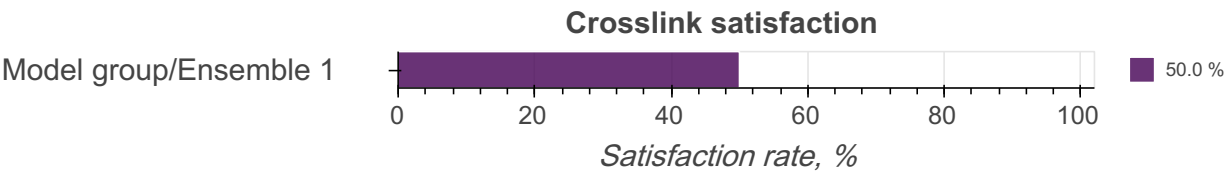
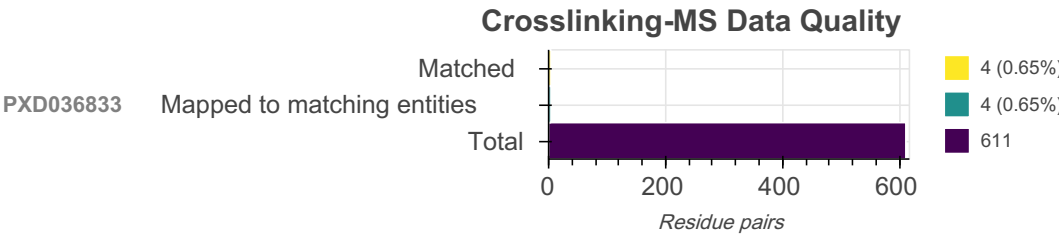
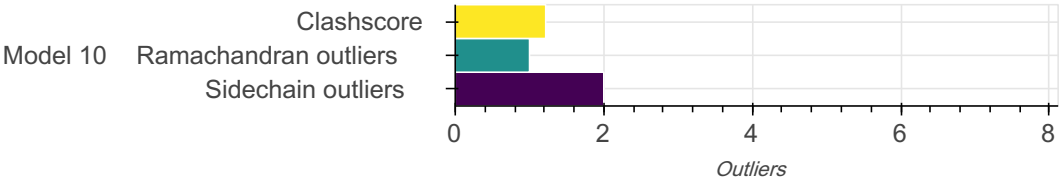
List of references used to build this report is available [here](#).

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 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	P0ABK5	A	323	-	1-323	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	AlphaLink	1.00	model building	https://github.com/lhatsk/AlphaLink

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	P0ABK5	dbseq_P0ABK5_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2T	4	4 (100.00%)	4 (100.00%)
PXD036833	611	4 (0.65%)	4 (0.65%)

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 110 bond angle outliers in this entry (0.33% of 33250 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	36	ASN	CA-CB-CG	6.52	119.12	112.60	10	2
A	176	VAL	CA-CB-CG1	6.24	121.01	110.40	9	1
A	323	GLN	OE1-CD-NE2	6.14	116.46	122.60	2	10
A	8	ASN	OD1-CG-ND2	6.00	116.60	122.60	8	3
A	34	SER	C-N-CA	5.69	131.95	121.70	10	1
A	305	ARG	NE-CZ-NH2	5.69	124.32	119.20	8	3
A	44	ARG	NH1-CZ-NH2	5.53	112.10	119.30	7	1
A	164	ASP	CA-CB-CG	5.24	117.84	112.60	6	9
A	149	ASN	OD1-CG-ND2	5.22	117.38	122.60	10	9
A	41	VAL	CA-CB-CG1	5.04	118.97	110.40	3	1
A	142	GLN	OE1-CD-NE2	5.02	117.58	122.60	1	3
A	305	ARG	NH1-CZ-NH2	4.99	112.81	119.30	2	3
A	7	ASP	CA-CB-CG	4.94	117.54	112.60	7	1
A	143	GLN	OE1-CD-NE2	4.91	117.69	122.60	9	1
A	100	ARG	NE-CZ-NH2	4.78	123.50	119.20	1	1
A	125	GLN	OE1-CD-NE2	4.72	117.88	122.60	9	4
A	44	ARG	NE-CZ-NH1	4.72	126.22	121.50	5	1
A	260	ARG	NE-CZ-NH1	4.69	126.19	121.50	8	1
A	168	GLN	OE1-CD-NE2	4.64	117.96	122.60	4	8
A	213	GLN	OE1-CD-NE2	4.54	118.06	122.60	8	5

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	8	ASN	CA-CB-CG	4.51	117.11	112.60	4	1
A	38	SER	C-N-CA	4.46	129.73	121.70	7	1
A	322	GLN	OE1-CD-NE2	4.40	118.20	122.60	8	10
A	287	ASP	CA-CB-CG	4.37	116.97	112.60	3	7
A	48	ASN	OD1-CG-ND2	4.27	118.33	122.60	3	6
A	225	HIS	CB-CG-CD2	4.20	125.74	131.20	5	5
A	238	ASN	OD1-CG-ND2	4.19	118.41	122.60	4	5
A	35	ARG	N-CA-C	4.15	122.61	111.00	10	1
A	304	GLU	C-N-CA	4.14	129.16	121.70	3	1
A	39	PHE	CA-CB-CG	4.11	117.91	113.80	3	1
A	261	ARG	CD-NE-CZ	4.10	130.15	124.40	8	1
A	12	ILE	C-N-CA	4.08	129.05	121.70	4	1
A	101	ARG	NE-CZ-NH1	4.05	125.55	121.50	4	1
A	260	ARG	NE-CZ-NH2	4.05	115.56	119.20	2	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	2.64	13
2	0.81	4
3	2.64	13
4	4.06	20
5	2.44	12
6	1.42	7
7	2.44	12
8	1.83	9
9	2.44	12
10	1.22	6

There are 108 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:59:LEU:HD21	A:65:LEU:HD21	0.74	8	6
A:43:CYS:HA	A:76:ALA:HB1	0.67	4	4
A:41:VAL:HG13	A:153:HIS:CE1	0.66	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:8:ASN:HB3	A:39:PHE:CE1	0.65	4	1
A:5:PHE:HZ	A:80:VAL:HG22	0.63	4	1
A:176:VAL:HG13	A:230:ILE:O	0.61	9	1
A:41:VAL:HG22	A:153:HIS:HE1	0.60	4	1
A:214:ALA:HB2	A:235:ILE:HD11	0.60	3	3
A:76:ALA:HB2	A:305:ARG:HH12	0.59	9	1
A:41:VAL:HG22	A:153:HIS:CE1	0.58	4	1
A:69:THR:HB	A:143:GLN:HE22	0.56	4	4
A:131:VAL:HG21	A:140:LEU:HB2	0.56	3	7
A:173:ILE:HD11	A:284:LEU:HD12	0.55	4	6
A:8:ASN:HB3	A:39:PHE:CD1	0.55	4	1
A:272:ILE:HD11	A:311:LEU:HD13	0.55	5	1
A:51:TRP:HE1	A:84:ARG:CZ	0.55	3	1
A:176:VAL:HG22	A:211:ILE:CD1	0.55	8	1
A:5:PHE:CZ	A:80:VAL:HG22	0.55	4	1
A:214:ALA:CB	A:235:ILE:HD11	0.54	6	3
A:36:ASN:HB3	A:39:PHE:CD2	0.53	10	1
A:76:ALA:HA	A:305:ARG:HH22	0.53	9	1
A:272:ILE:HD11	A:311:LEU:HD22	0.53	7	1
A:13:GLY:HA2	A:44:ARG:CZ	0.52	9	1
A:176:VAL:HG22	A:211:ILE:HD11	0.52	8	1
A:263:MET:HE1	A:312:PHE:CE2	0.51	5	1
A:140:LEU:HD23	A:142:GLN:HE21	0.51	10	2
A:274:SER:HB3	A:299:LEU:HD22	0.51	4	4
A:76:ALA:O	A:80:VAL:HG23	0.50	4	1
A:176:VAL:HG11	A:239:LEU:HD22	0.50	7	1
A:67:GLU:HG3	A:69:THR:HG22	0.49	4	1
A:272:ILE:CD1	A:311:LEU:HD13	0.49	5	1
A:92:MET:HE1	A:104:LEU:HD13	0.48	6	1
A:37:PRO:HB2	A:79:TYR:CZ	0.48	9	1
A:23:ILE:HD11	A:261:ARG:C	0.47	9	2
A:36:ASN:HB3	A:39:PHE:CE2	0.47	9	1
A:51:TRP:HE1	A:84:ARG:NH2	0.47	3	1
A:5:PHE:CD1	A:11:THR:HG22	0.47	9	1
A:272:ILE:CD1	A:311:LEU:HD22	0.47	7	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:15:THR:HG21	A:33:GLU:HA	0.47	4	2
A:99:GLU:CD	A:99:GLU:H	0.46	5	6
A:260:ARG:HG2	A:315:LEU:HD21	0.46	7	1
A:8:ASN:CB	A:39:PHE:CE1	0.46	4	1
A:310:ALA:HA	A:313:ALA:HB2	0.46	5	1
A:33:GLU:CD	A:300:PRO:HA	0.45	3	1
A:312:PHE:CD1	A:315:LEU:HD12	0.45	7	1
A:41:VAL:HG13	A:153:HIS:HE1	0.44	3	1
A:176:VAL:HG21	A:202:ALA:HB1	0.44	7	1
A:312:PHE:CD1	A:315:LEU:CD1	0.44	7	1
A:100:ARG:HH12	A:228:GLN:NE2	0.44	1	1
A:38:SER:C	A:39:PHE:CD1	0.44	4	1
A:71:GLY:HA3	A:96:MET:HE1	0.43	1	1
A:11:THR:O	A:39:PHE:CE1	0.43	10	1
A:41:VAL:HG23	A:153:HIS:CE1	0.43	5	1
A:69:THR:HG21	A:74:GLY:HA3	0.43	2	1
A:188:TYR:CZ	A:193:LYS:HE2	0.43	5	3
A:37:PRO:CB	A:79:TYR:CZ	0.43	9	1
A:69:THR:CB	A:143:GLN:HE22	0.43	4	1
A:92:MET:HE1	A:111:LEU:HD22	0.43	1	1
A:13:GLY:HA2	A:44:ARG:HH22	0.42	4	1
A:225:HIS:CD2	A:231:GLY:O	0.42	1	1
A:69:THR:HG21	A:74:GLY:CA	0.42	2	1
A:270:ALA:HB1	A:274:SER:CB	0.42	8	1
A:270:ALA:HB1	A:274:SER:HB2	0.41	1	1
A:27:ARG:NH2	A:291:THR:HA	0.41	5	1
A:100:ARG:HH12	A:228:GLN:HE22	0.41	1	1
A:54:GLU:HG3	A:59:LEU:HD12	0.41	9	1
A:13:GLY:CA	A:44:ARG:HH21	0.41	3	1
A:13:GLY:HA2	A:44:ARG:NH2	0.41	4	1
A:72:ASN:HA	A:305:ARG:NH1	0.41	8	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	321	312	9	0
2	321	309	12	0
3	321	309	10	2
4	321	310	10	1
5	321	312	9	0
6	321	312	9	0
7	321	309	11	1
8	321	310	11	0
9	321	306	15	0
10	321	307	13	1

There are 5 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	3	LYS	1
A	13	GLY	1
A	37	PRO	1
A	39	PHE	1
A	304	GLU	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	259	252	6	1
2	259	254	5	0
3	259	253	6	0
4	259	253	5	1
5	259	252	6	1
6	259	252	7	0
7	259	250	9	0
8	259	255	4	0
9	259	252	6	1
10	259	252	5	2

There are 6 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	41	VAL	1
A	97	SER	1
A	142	GLN	1
A	298	ILE	1
A	306	TYR	1
A	314	ASP	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

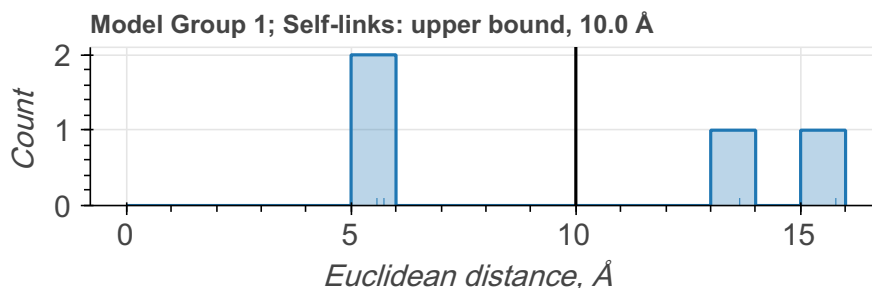
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 4 crosslinking restraints combined in 4 restraint groups.

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

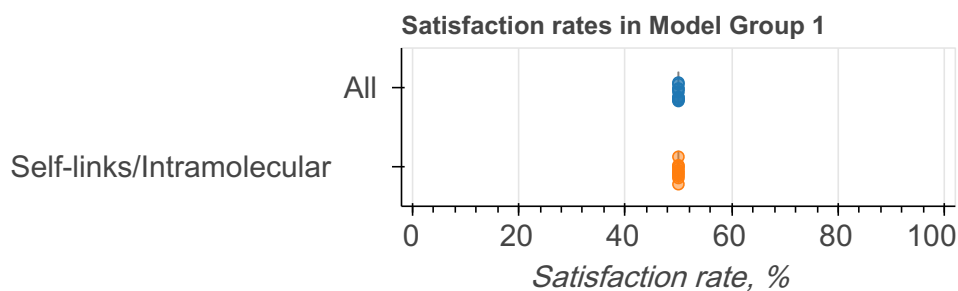
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=4)
1	1	1	10/10	All	50.00	50.00	4
				Self-links/ Intramolecular	50.00	50.00	4

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.

Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.