

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	9A3A
PDB-Dev ID	PDBDEV_00000195
Structure Title	Model of E. coli MlaD 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

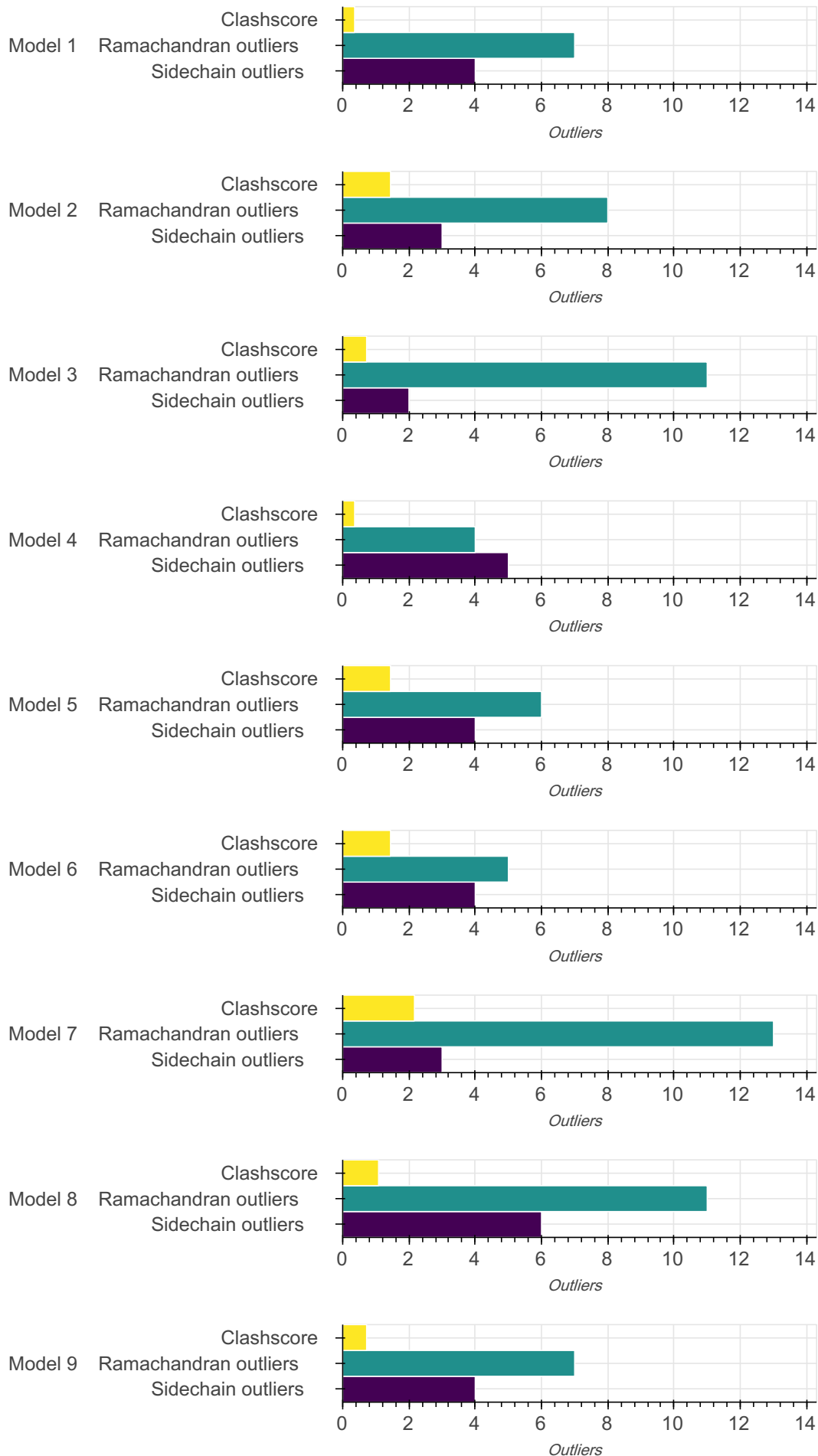
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

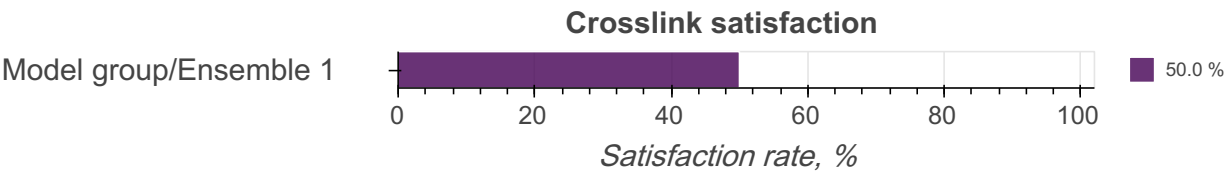
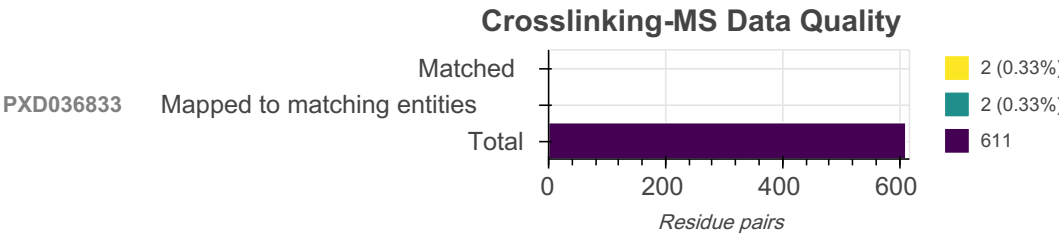
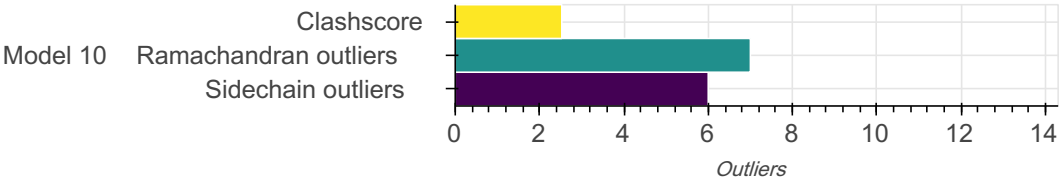
List of references used to build this report is available [here](#).

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	P64604	A	183	-	1-183	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	P64604	dbseq_P64604_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A3A	2	2 (100.00%)	2 (100.00%)
PXD036833	611	2 (0.33%)	2 (0.33%)

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 1 bond length outliers in this entry (0.01% of 14000 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	89	ARG	CZ-NH2	4.04	1.28	1.33	2	1

Standard geometry: angle outliers ?

There are 94 bond angle outliers in this entry (0.49% of 19060 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	182	THR	C-N-CA	7.78	135.70	121.70	4	7
A	172	ASN	CA-CB-CG	6.87	119.47	112.60	2	6
A	175	THR	C-N-CA	6.61	133.59	121.70	7	4
A	135	GLN	OE1-CD-NE2	6.54	116.06	122.60	7	8
A	158	ASP	CA-CB-CG	5.94	118.54	112.60	6	3
A	172	ASN	C-N-CA	5.94	132.39	121.70	3	1
A	176	THR	C-N-CA	5.75	132.05	121.70	9	3
A	172	ASN	OD1-CG-ND2	5.60	117.00	122.60	2	6
A	110	GLN	OE1-CD-NE2	5.49	117.11	122.60	10	5
A	149	GLN	OE1-CD-NE2	5.24	117.36	122.60	7	9
A	161	ASN	C-N-CA	5.20	131.07	121.70	1	2
A	178	PRO	CA-N-CD	5.20	104.72	112.00	3	2
A	159	ASN	C-N-CA	4.87	130.47	121.70	1	2
A	166	PRO	C-N-CA	4.83	130.39	121.70	9	1
A	182	THR	CA-CB-OG1	4.82	116.83	109.60	8	3
A	89	ARG	CD-NE-CZ	4.78	131.10	124.40	10	2
A	32	THR	CA-CB-CG2	4.70	118.49	110.50	7	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	175	THR	CA-CB-CG2	4.67	118.44	110.50	3	1
A	181	THR	C-N-CA	4.65	130.07	121.70	1	4
A	89	ARG	NE-CZ-NH2	4.64	123.38	119.20	1	1
A	89	ARG	NE-CZ-NH1	4.45	125.95	121.50	4	2
A	159	ASN	OD1-CG-ND2	4.44	118.16	122.60	1	1
A	173	ASN	OD1-CG-ND2	4.40	118.20	122.60	2	4
A	163	GLY	C-N-CA	4.32	129.47	121.70	9	1
A	88	GLN	OE1-CD-NE2	4.31	118.29	122.60	8	6
A	180	GLY	C-N-CA	4.31	129.46	121.70	3	1
A	176	THR	O-C-N	4.28	116.16	123.00	1	1
A	178	PRO	C-N-CA	4.25	129.36	121.70	3	2
A	172	ASN	N-CA-C	4.15	122.63	111.00	3	1
A	158	ASP	C-CA-CB	4.11	117.92	110.10	6	1
A	2	GLN	OE1-CD-NE2	4.02	118.58	122.60	6	1
A	31	VAL	CA-CB-CG2	4.02	117.23	110.40	6	1
A	167	ALA	C-N-CA	4.00	128.90	121.70	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	0.36	1
2	1.44	4
3	0.72	2
4	0.36	1
5	1.44	4
6	1.44	4
7	2.17	6
8	1.08	3
9	0.72	2
10	2.53	7

There are 34 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:27:LYS:O	A:31:VAL:HG23	0.59	10	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:116:VAL:CG1	A:128:LEU:HD21	0.58	10	1
A:93:ILE:HD13	A:114:LEU:HD21	0.57	4	4
A:142:VAL:HG12	A:144:GLU:OE1	0.56	10	1
A:37:GLU:CD	A:89:ARG:HH21	0.55	5	1
A:35:ARG:HH21	A:39:THR:HG21	0.50	3	1
A:28:ALA:HA	A:31:VAL:HG22	0.50	9	1
A:124:GLY:O	A:125:THR:HG23	0.48	10	1
A:35:ARG:HH12	A:85:GLU:CB	0.48	6	1
A:33:SER:HB3	A:67:ARG:HH12	0.47	10	1
A:35:ARG:HH12	A:85:GLU:CD	0.47	9	1
A:35:ARG:HH12	A:85:GLU:HB3	0.46	6	1
A:35:ARG:C	A:37:GLU:H	0.46	2	2
A:141:MET:SD	A:146:LEU:HD21	0.44	3	3
A:42:LEU:HD11	A:128:LEU:HD13	0.44	7	2
A:60:ILE:HD11	A:114:LEU:HD23	0.43	6	1
A:116:VAL:HG13	A:128:LEU:HD11	0.43	7	1
A:125:THR:C	A:127:ILE:H	0.42	7	1
A:119:GLU:HA	A:135:GLN:HE21	0.42	7	1
A:46:PHE:CE2	A:137:THR:HB	0.42	2	2
A:30:ASN:CG	A:55:ARG:HH22	0.41	8	1
A:157:ASP:C	A:159:ASN:H	0.41	8	1
A:46:PHE:CD2	A:137:THR:HB	0.41	7	1
A:52:LEU:HD13	A:103:THR:HG22	0.41	10	1
A:116:VAL:CG1	A:128:LEU:HD11	0.41	2	1
A:107:LEU:CD1	A:143:LEU:HD22	0.40	7	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	181	163	11	7
2	181	156	17	8
3	181	155	15	11
4	181	167	10	4
5	181	163	12	6
6	181	165	11	5

Model ID	Analysed	Favored	Allowed	Outliers
7	181	149	19	13
8	181	156	14	11
9	181	163	11	7
10	181	158	16	7

There are 34 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	34	ILE	6
A	160	LYS	6
A	179	VAL	5
A	91	ASN	4
A	124	GLY	4
A	156	GLY	4
A	178	PRO	4
A	50	GLY	3
A	161	ASN	3
A	171	GLY	3
A	177	GLU	3
A	182	THR	3
A	31	VAL	2
A	32	THR	2
A	33	SER	2
A	36	THR	2
A	116	VAL	2
A	158	ASP	2
A	163	GLY	2
A	164	ASP	2
A	175	THR	2
A	126	ALA	1
A	153	GLY	1
A	154	SER	1
A	157	ASP	1
A	162	SER	1
A	166	PRO	1
A	167	ALA	1

Chain	Res	Type	Models (Total)
A	170	PRO	1
A	172	ASN	1
A	173	ASN	1
A	174	GLU	1
A	176	THR	1
A	180	GLY	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	150	139	7	4
2	150	138	9	3
3	150	145	3	2
4	150	138	7	5
5	150	139	7	4
6	150	138	8	4
7	150	139	8	3
8	150	138	6	6
9	150	140	6	4
10	150	139	5	6

There are 18 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	3	THR	6
A	181	THR	6
A	182	THR	6
A	18	LEU	3
A	31	VAL	3
A	36	THR	3
A	123	LEU	2
A	172	ASN	2
A	1	MET	1
A	14	LEU	1
A	26	LEU	1
A	32	THR	1

Chain	Res	Type	Models (Total)
A	73	LEU	1
A	89	ARG	1
A	118	PHE	1
A	125	THR	1
A	142	VAL	1
A	158	ASP	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

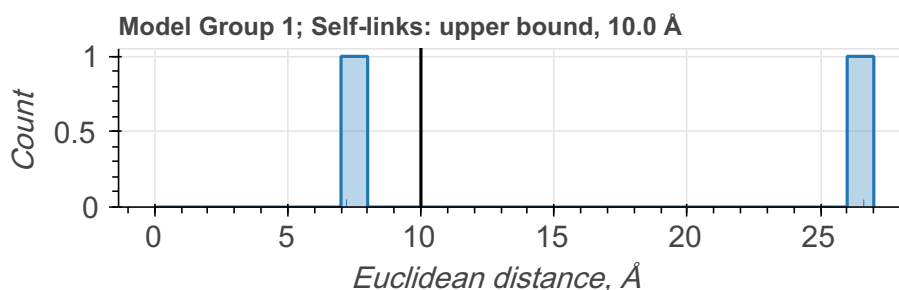
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 2 crosslinking restraints combined in 2 restraint groups.

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

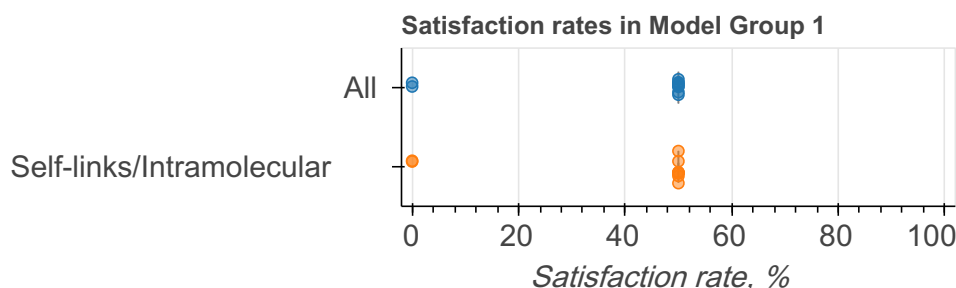
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=2)
1	1	1	10/10	All	50.00	50.00	2
				Self-links/ Intramolecular	50.00	50.00	2

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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