

# Integrative Structure Validation Report ?

February 18, 2025 - 08:34 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	9A2J
PDB-Dev ID	PDBDEV_00000168
Structure Title	Model of E. coli RplJ 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)*

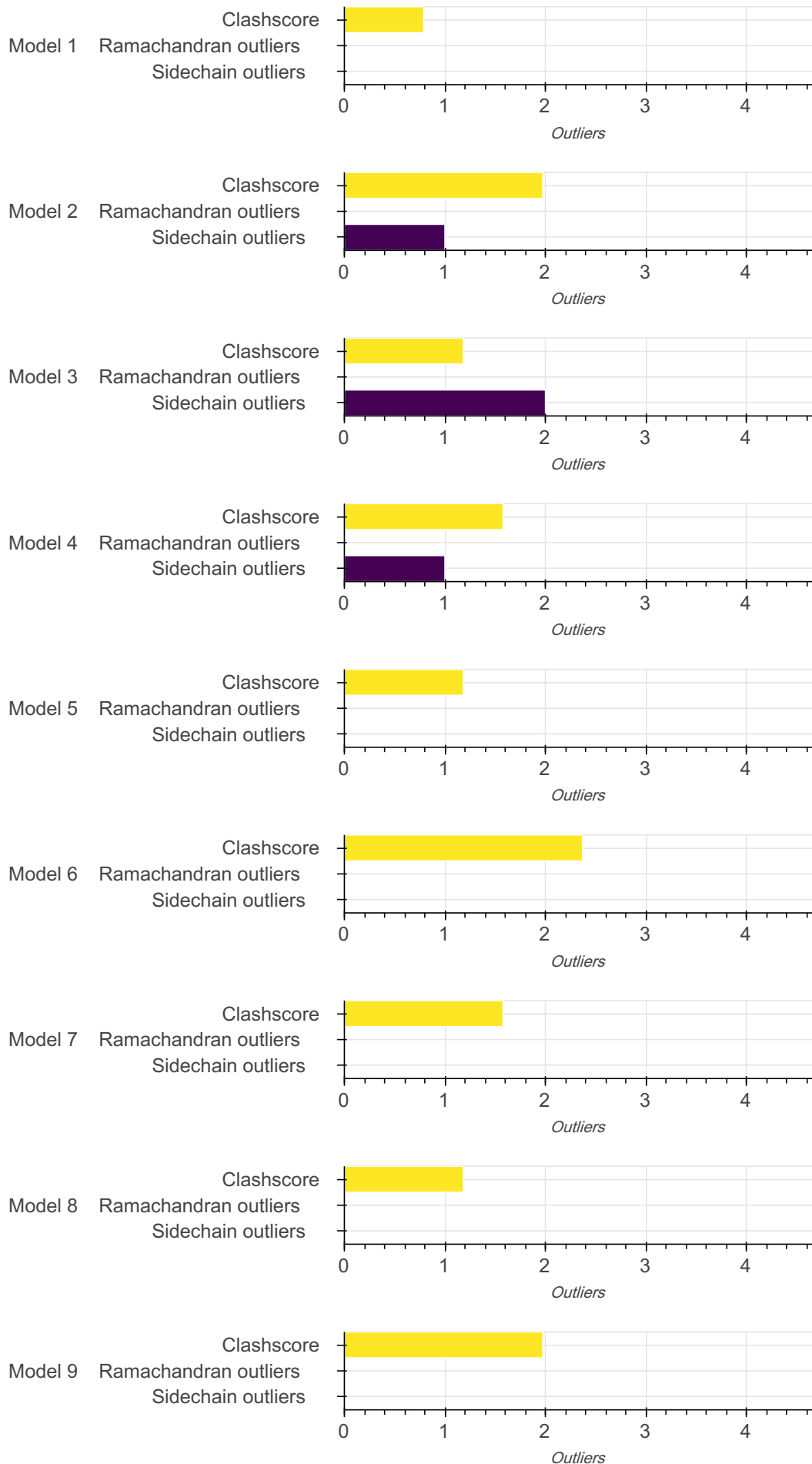
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

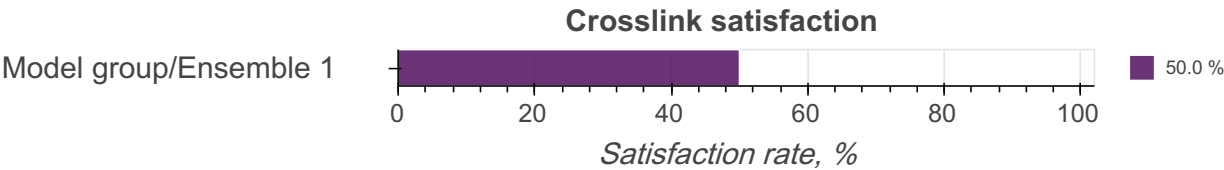
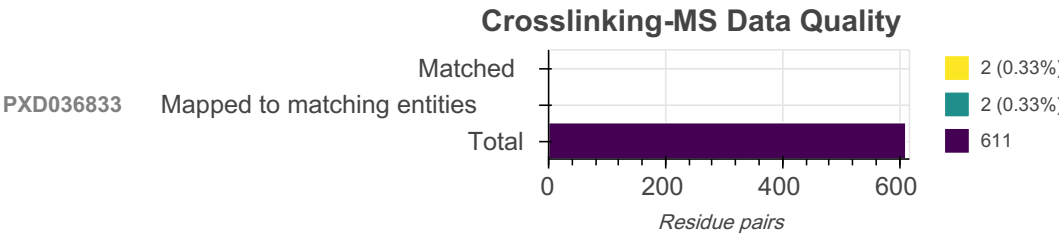
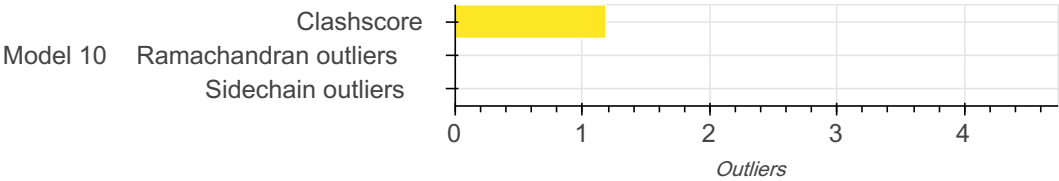
*List of references used to build this report is available [here](#).*

## 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	P0A7J3	A	165	-	1-165	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	P0A7J3	dbseq_P0A7J3_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2J	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 no bond length outliers.*

#### Standard geometry: angle outliers ?

*There are 48 bond angle outliers in this entry (0.28% of 16910 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	53	ARG	NE-CZ-NH2	5.31	123.98	119.20	4	1
A	7	ASP	CA-CB-CG	4.83	117.43	112.60	4	8
A	88	HIS	CB-CG-CD2	4.72	125.06	131.20	1	6
A	9	GLN	OE1-CD-NE2	4.50	118.10	122.60	6	10
A	109	LYS	CG-CD-CE	4.37	101.24	111.30	6	1
A	94	ARG	NH1-CZ-NH2	4.30	113.71	119.30	7	1
A	6	GLN	OE1-CD-NE2	4.29	118.31	122.60	7	9
A	122	GLN	OE1-CD-NE2	4.21	118.39	122.60	7	9
A	94	ARG	NE-CZ-NH2	4.15	122.93	119.20	1	1
A	76	PHE	CA-CB-CG	4.11	117.91	113.80	8	1
A	57	ASN	OD1-CG-ND2	4.03	118.57	122.60	6	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	0.79	2
2	1.97	5
3	1.18	3
4	1.58	4

Model ID	Clash score	Number of clashes
5	1.18	3
6	2.37	6
7	1.58	4
8	1.18	3
9	1.97	5
10	1.18	3

There are 38 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:88:HIS:CD2	A:131:THR:HA	0.55	7	2
A:132:TYR:CE2	A:136:ILE:HD11	0.54	5	5
A:143:MET:HA	A:151:LEU:HD11	0.53	9	1
A:143:MET:HG2	A:151:LEU:HD22	0.53	6	2
A:132:TYR:CZ	A:136:ILE:HD11	0.52	2	1
A:29:ASP:HB2	A:109:LYS:HE3	0.51	6	5
A:83:ALA:HB2	A:96:PHE:CZ	0.50	10	9
A:42:ARG:HA	A:52:MET:HE3	0.49	2	2
A:14:GLU:CD	A:53:ARG:HH12	0.49	4	1
A:45:GLY:HA3	A:52:MET:HE2	0.48	6	2
A:55:VAL:HG23	A:60:LEU:HG	0.48	2	1
A:143:MET:HG2	A:151:LEU:CD2	0.46	6	1
A:126:LEU:HD12	A:129:LEU:HD12	0.43	4	1
A:140:MET:SD	A:143:MET:CE	0.42	3	1
A:41:LEU:O	A:52:MET:HE1	0.41	2	1
A:43:LYS:HE2	A:47:GLU:OE2	0.41	8	2
A:42:ARG:HA	A:52:MET:CE	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	163	162	1	0
2	163	162	1	0
3	163	162	1	0
4	163	163	0	0

Model ID	Analysed	Favored	Allowed	Outliers
5	163	162	1	0
6	163	161	2	0
7	163	162	1	0
8	163	163	0	0
9	163	163	0	0
10	163	162	1	0

### 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	123	120	3	0
2	123	119	3	1
3	123	118	3	2
4	123	119	3	1
5	123	120	3	0
6	123	120	3	0
7	123	122	1	0
8	123	121	2	0
9	123	118	5	0
10	123	118	5	0

There are 3 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	154	THR	2
A	5	LEU	1
A	55	VAL	1

### Fit of model to data used for modeling ?

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

#### Restraint types

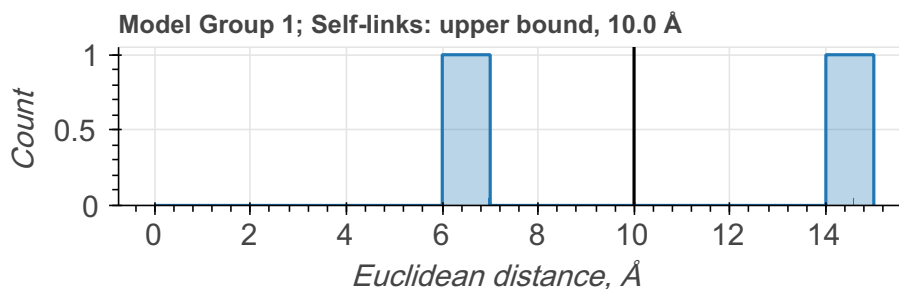
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

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	ALA	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	GLU	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.



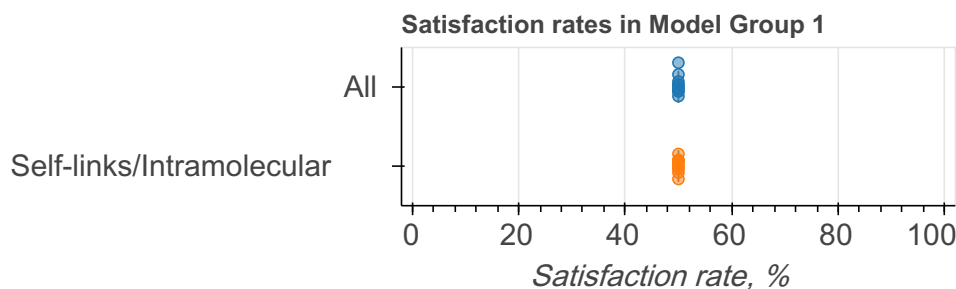
#### Satisfaction of restraints

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

*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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