

# 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	9A2Q
PDB-Dev ID	PDBDEV_00000175
Structure Title	Model of E. coli AtpF 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)*

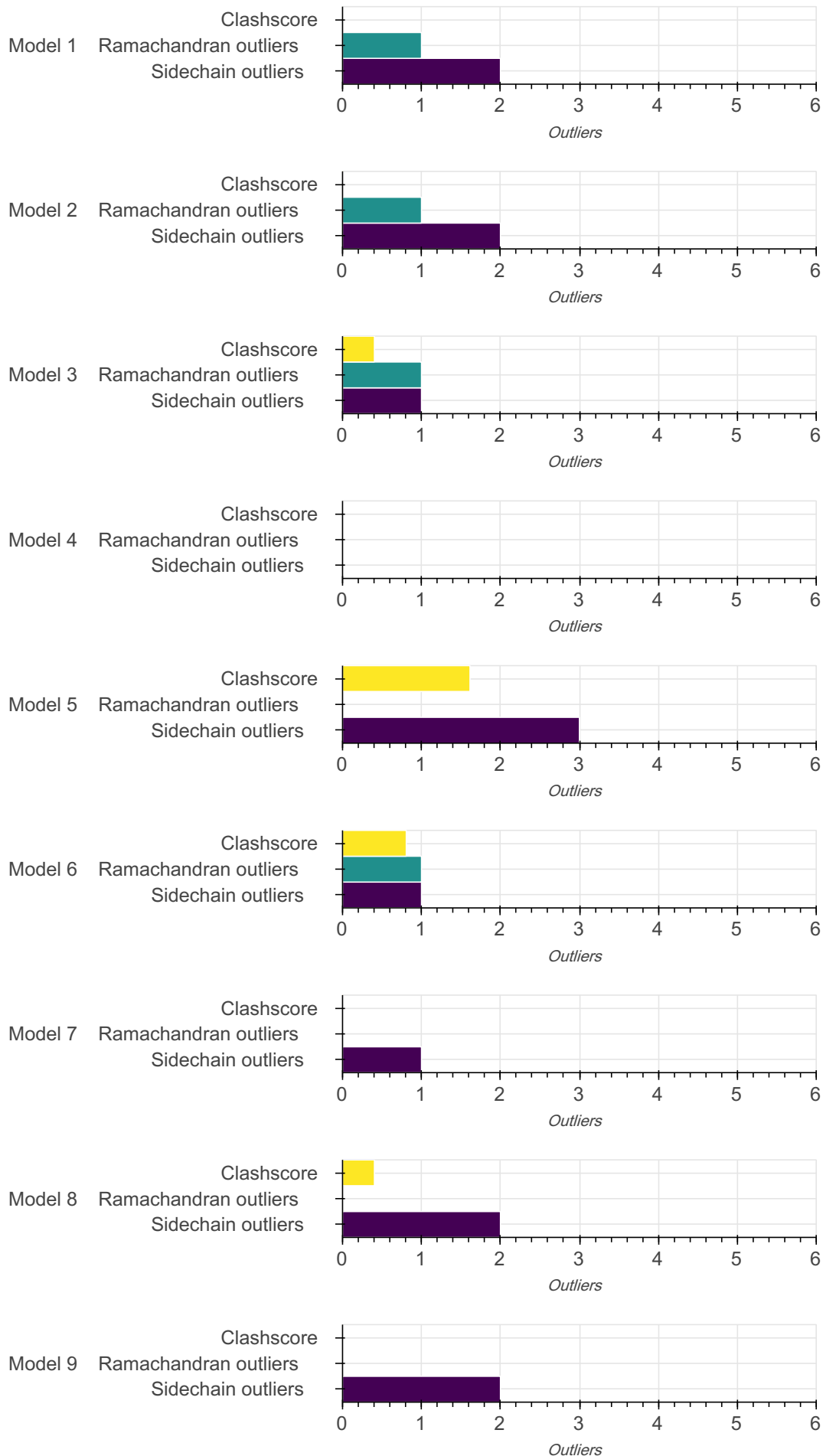
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

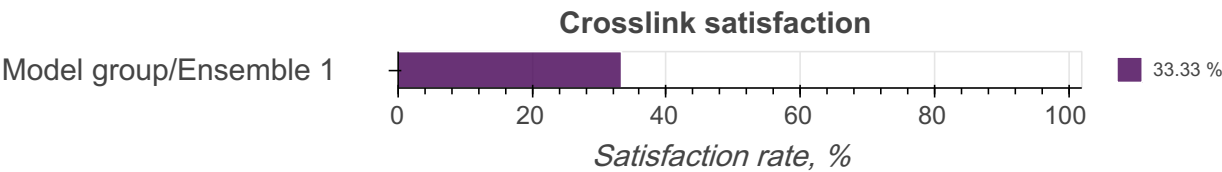
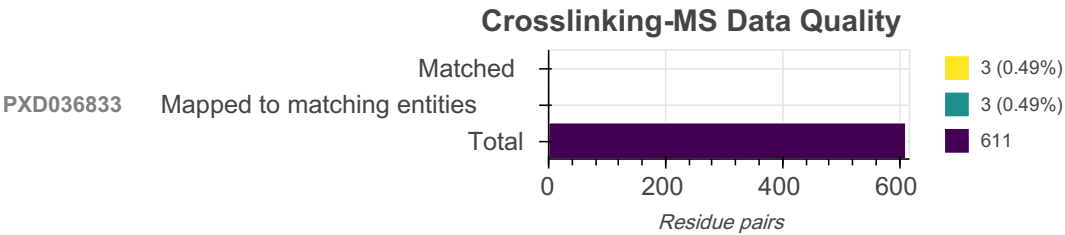
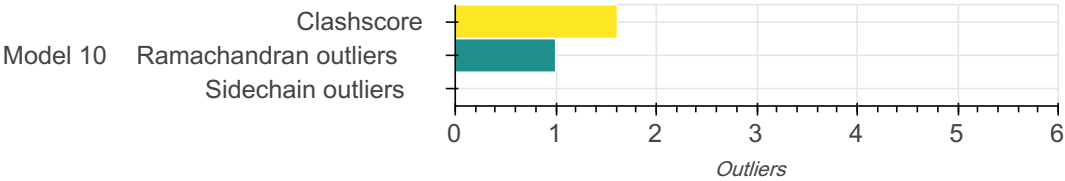
*List of references used to build this report is available [here](#).*

## 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	P0ABA0	A	156	-	1-156	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	P0ABA0	dbseq_P0ABA0_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2Q	3	3 (100.00%)	3 (100.00%)
PXD036833	611	3 (0.49%)	3 (0.49%)

### 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 78 bond angle outliers in this entry (0.48% of 16370 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	104	GLN	OE1-CD-NE2	5.20	117.40	122.60	10	10
A	1	MET	C-N-CA	5.12	130.92	121.70	1	2
A	85	GLN	OE1-CD-NE2	4.84	117.76	122.60	3	10
A	106	GLN	OE1-CD-NE2	4.67	117.93	122.60	5	10
A	142	GLU	C-N-CA	4.62	130.02	121.70	10	1
A	96	GLN	OE1-CD-NE2	4.51	118.09	122.60	3	10
A	143	ALA	N-CA-C	4.41	123.36	111.00	10	1
A	51	HIS	CB-CG-CD2	4.38	125.50	131.20	10	4
A	10	GLN	OE1-CD-NE2	4.31	118.29	122.60	3	10
A	37	GLN	OE1-CD-NE2	4.30	118.30	122.60	6	10
A	78	GLN	OE1-CD-NE2	4.21	118.39	122.60	1	7
A	64	GLN	OE1-CD-NE2	4.11	118.49	122.60	2	3

#### 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	0.00	0
2	0.00	0
3	0.40	1

Model ID	Clash score	Number of clashes
4	0.00	0
5	1.61	4
6	0.81	2
7	0.00	0
8	0.40	1
9	0.00	0
10	1.61	4

There are 12 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:132:ALA:CB	A:152:LEU:HD23	0.61	10	1
A:132:ALA:HB2	A:152:LEU:HD23	0.47	10	1
A:132:ALA:HB2	A:156:LEU:HD11	0.47	6	1
A:54:LEU:HD21	A:58:LYS:HE3	0.47	5	1
A:136:ILE:HD11	A:152:LEU:CD2	0.45	3	1
A:114:LYS:HE2	A:118:GLU:OE2	0.44	8	2
A:136:ILE:CD1	A:149:VAL:HG22	0.43	10	1
A:125:ALA:HB1	A:156:LEU:HD13	0.43	5	1
A:35:LYS:HE2	A:39:GLU:OE2	0.43	5	2
A:132:ALA:CB	A:156:LEU:HD11	0.42	6	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	154	153	0	1
2	154	153	0	1
3	154	153	0	1
4	154	153	1	0
5	154	153	1	0
6	154	151	2	1
7	154	154	0	0
8	154	153	1	0
9	154	152	2	0
10	154	150	3	1

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

Chain	Res	Type	Models (Total)
A	2	ASN	2
A	143	ALA	2
A	144	ALA	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	122	117	3	2
2	122	120	0	2
3	122	121	0	1
4	122	120	2	0
5	122	118	1	3
6	122	117	4	1
7	122	120	1	1
8	122	119	1	2
9	122	119	1	2
10	122	120	2	0

There are 4 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	152	LEU	7
A	3	LEU	5
A	136	ILE	1
A	147	ASP	1

## Fit of model to data used for modeling ?

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

#### Restraint types

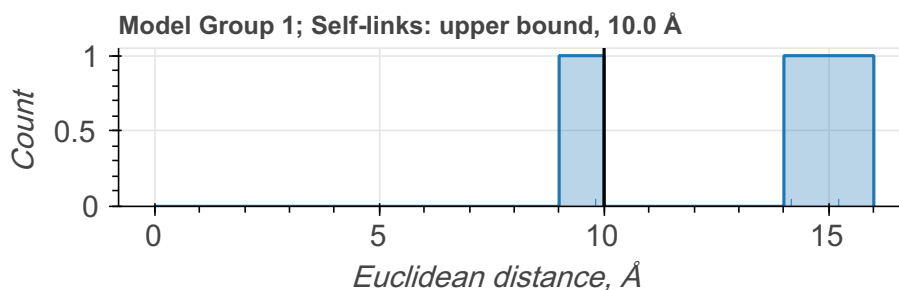
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 3 crosslinking restraints combined in 3 restraint groups.

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



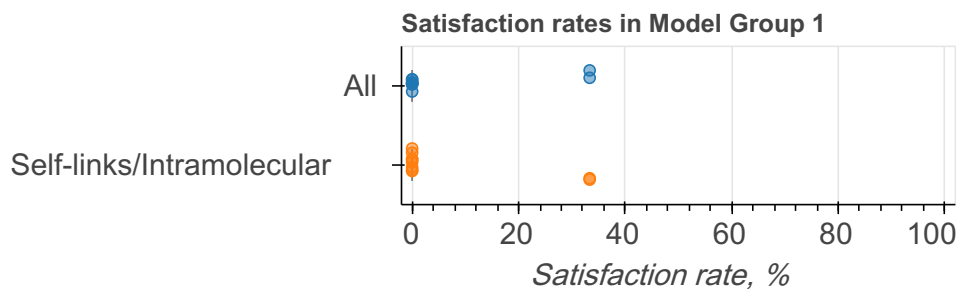
#### Satisfaction of restraints

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=3)
1	1	1	10/10	All	33.33	66.67	3
				Self-links/ Intramolecular	33.33	66.67	3

#### 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.

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### *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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