

# Integrative Structure Validation Report

February 18, 2025 - 08:44 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	9A7M
PDB-Dev ID	PDBDEV_00000351
Structure Title	Integrative model of MDH-PTAS by crosslinking MS and deep learning
Structure Authors	Kolja Stahl; Oliver Brock; Juri Rappsilber
Deposited on	2024-01-23

*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)*

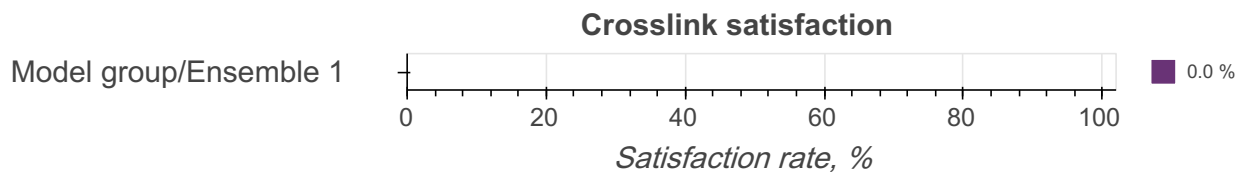
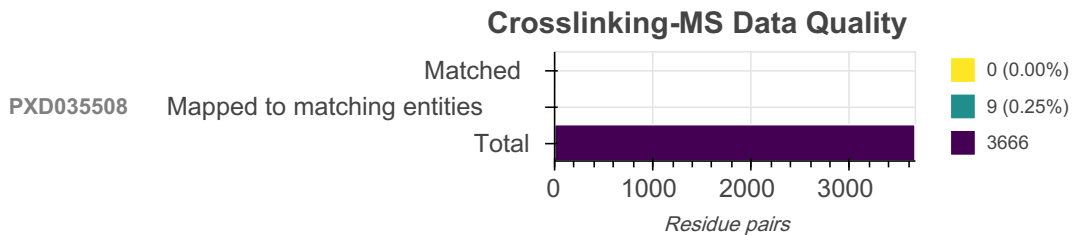
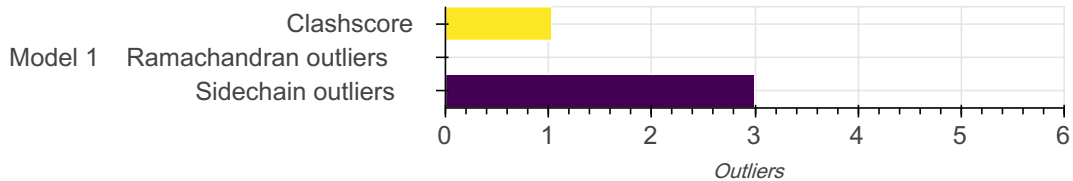
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 1 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	1	MDH_BACSU	A	312	-	1-312	100.00 / 0.00	Atomic
		2	PTAS_BACSU	B	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	PRIDE	<a href="#">PXD035508</a>

## 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	AlphaLink2	AlphaLink2	None	1	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	<a href="#">AlphaLink2</a>	1.00	model building	<a href="https://github.com/Rappsilber-Laboratory/AlphaLink2">https://github.com/Rappsilber-Laboratory/AlphaLink2</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 ( <a href="#">PRIDE ID</a> )	<a href="#">PXD035508</a>
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Number of entities in the crosslinking-MS dataset:	810
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Number of entities in the entry:	2
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Matching entities:	
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Entity ID	Molecule name	Crosslinking-MS Entity ID	E-value	Exact match
1	MDH_BACSU	dbseq_P49814_target	0.00	True
2	PTAS_BACSU	dbseq_P39646_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A7M	1	1 (100.00%)	0 (0.00%)
PXD035508	3666	9 (0.25%)	0 (0.00%)

## 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 9 bond angle outliers in this entry (0.14% of 6597 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	177	ASP	CA-CB-CG	5.37	117.97	112.60	1	1
A	58	GLN	OE1-CD-NE2	4.74	117.86	122.60	1	1
B	138	GLN	OE1-CD-NE2	4.43	118.17	122.60	1	1
A	39	GLN	OE1-CD-NE2	4.39	118.21	122.60	1	1
B	161	GLN	OE1-CD-NE2	4.32	118.28	122.60	1	1
B	9	GLN	OE1-CD-NE2	4.27	118.33	122.60	1	1
A	180	HIS	CD2-NE2-CE1	4.18	104.82	109.00	1	1
A	100	ASN	OD1-CG-ND2	4.14	118.46	122.60	1	1
B	165	ALA	O-C-N	4.07	116.48	123.00	1	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	1.03	10

There are 10 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)
B:152:VAL:HG12	B:165:ALA:HB2	0.75	1	1
B:114:TYR:HA	B:297:MET:HE1	0.64	1	1
B:1:MET:HE2	B:286:GLU:OE2	0.56	1	1
A:5:ARG:HH22	A:61:ASP:HB3	0.55	1	1
B:152:VAL:HG13	B:293:GLN:NE2	0.55	1	1
A:186:PRO:HG3	A:211:VAL:HG13	0.49	1	1
B:41:VAL:HG11	B:316:LEU:HD21	0.47	1	1
A:184:MET:HE3	A:215:ARG:HA	0.46	1	1
A:188:VAL:HG11	A:207:ILE:HG21	0.41	1	1
B:191:MET:HE1	B:321:GLN:HG2	0.40	1	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	631	621	10	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	514	505	6	3

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

Chain	Res	Type	Models (Total)
A	175	PHE	1
B	63	THR	1
B	276	TYR	1

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

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

### Restraint types

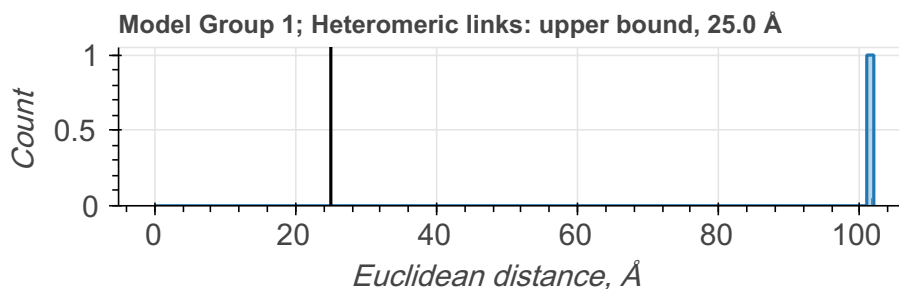
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 1 crosslinking restraints combined in 1 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
SDA	LYS	CA	LYS	CA	upper bound	25.0	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.



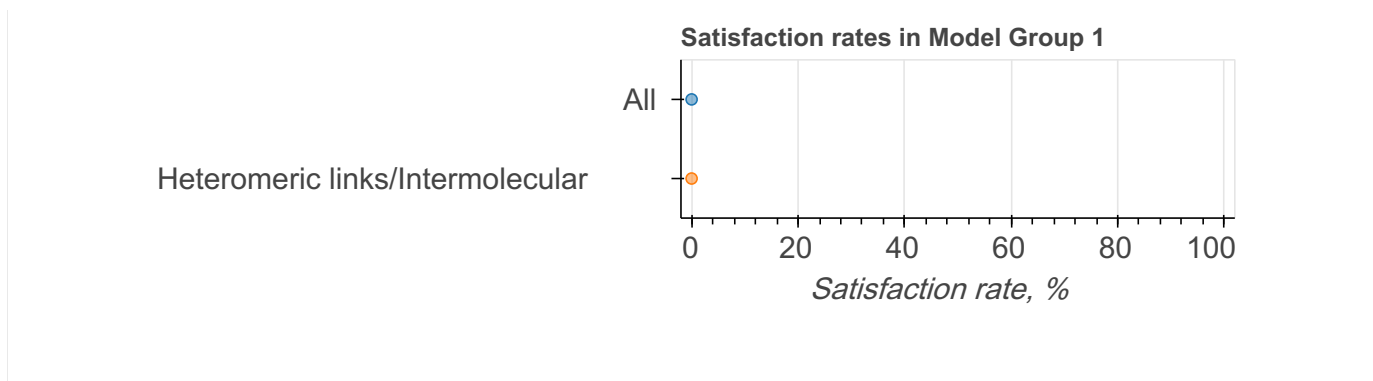
### Satisfaction of restraints

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=1)
1	1	1	1/1	All	0.00	100.00	1
				Heteromeric links/ Intermolecular	0.00	100.00	1

### 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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