

# Integrative Structure Validation Report ?

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*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*

PDB ID	9A71
PDB-Dev ID	PDBDEV_00000330
Structure Title	Integrative model of BUK-SYGB 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)*

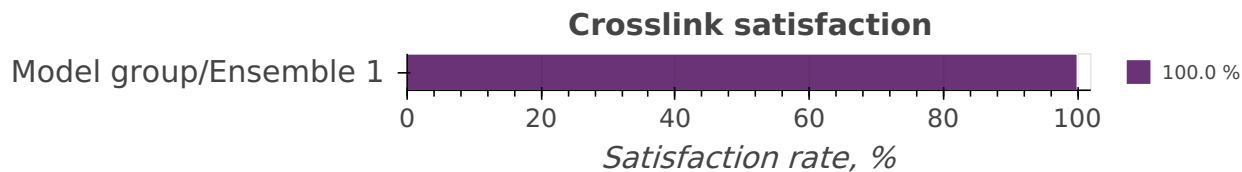
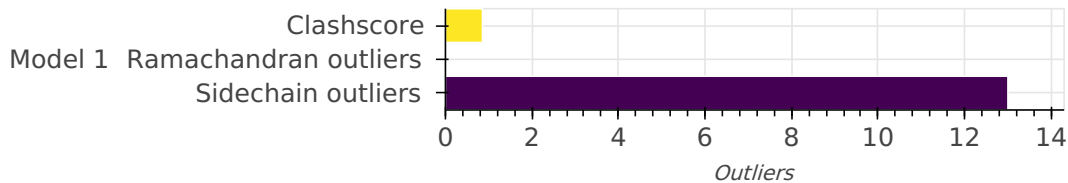
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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	BUK_BACSU	A	363	-	1-363	100.00 / 0.00	Atomic
		2	SYGB_BACSU	B	679	-	1-679	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	PXD035508

## 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 is not available in the [PRIDE Crosslinking](#) database.

## 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 38 bond angle outliers in this entry (0.34% of 11222 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	164	GLN	OE1-CD-NE2	5.70	116.90	122.60	1	1
B	282	GLN	OE1-CD-NE2	5.54	117.06	122.60	1	1
B	316	ASN	OD1-CG-ND2	5.51	117.09	122.60	1	1
B	281	HIS	CB-CG-CD2	4.72	125.07	131.20	1	1
A	44	GLN	OE1-CD-NE2	4.70	117.90	122.60	1	1
B	377	GLN	OE1-CD-NE2	4.64	117.96	122.60	1	1
B	531	GLN	OE1-CD-NE2	4.64	117.96	122.60	1	1
B	119	GLN	OE1-CD-NE2	4.61	117.99	122.60	1	1
B	98	GLN	OE1-CD-NE2	4.58	118.02	122.60	1	1
B	409	GLN	OE1-CD-NE2	4.57	118.03	122.60	1	1
B	188	HIS	CB-CG-CD2	4.54	125.29	131.20	1	1
B	672	ASN	OD1-CG-ND2	4.53	118.07	122.60	1	1
B	226	GLN	OE1-CD-NE2	4.51	118.09	122.60	1	1
B	125	GLN	OE1-CD-NE2	4.49	118.11	122.60	1	1
B	321	ARG	CD-NE-CZ	4.48	130.67	124.40	1	1
B	611	GLN	OE1-CD-NE2	4.47	118.13	122.60	1	1
B	560	GLN	OE1-CD-NE2	4.46	118.14	122.60	1	1
B	590	GLN	OE1-CD-NE2	4.42	118.18	122.60	1	1
B	475	GLN	OE1-CD-NE2	4.41	118.19	122.60	1	1
B	49	ASN	CA-CB-CG	4.38	116.98	112.60	1	1
B	483	GLN	OE1-CD-NE2	4.35	118.25	122.60	1	1
A	352	GLN	OE1-CD-NE2	4.35	118.25	122.60	1	1
B	206	GLN	OE1-CD-NE2	4.33	118.27	122.60	1	1
B	352	HIS	CB-CG-CD2	4.31	125.60	131.20	1	1
A	286	GLN	OE1-CD-NE2	4.31	118.29	122.60	1	1
A	38	HIS	CB-CG-CD2	4.29	125.62	131.20	1	1
B	508	GLN	OE1-CD-NE2	4.28	118.32	122.60	1	1
A	356	GLN	OE1-CD-NE2	4.28	118.32	122.60	1	1
B	614	GLN	OE1-CD-NE2	4.26	118.34	122.60	1	1
B	67	ASP	CA-CB-CG	4.25	116.85	112.60	1	1
A	127	ASN	OD1-CG-ND2	4.24	118.36	122.60	1	1
A	267	GLN	OE1-CD-NE2	4.22	118.38	122.60	1	1
B	131	LEU	CA-C-N	4.22	123.23	116.90	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	270	GLN	OE1-CD-NE2	4.21	118.39	122.60	1	1
A	67	GLN	OE1-CD-NE2	4.19	118.41	122.60	1	1
B	528	ASN	OD1-CG-ND2	4.08	118.52	122.60	1	1
B	122	GLN	OE1-CD-NE2	4.06	118.54	122.60	1	1
B	50	THR	CA-CB-CG2	4.00	117.31	110.50	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	0.86	14

There are 14 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:433:HIS:CE1	B:434:TYR:CE2	0.52	1	1
B:11:GLY:HA3	B:162:TRP:CD2	0.51	1	1
A:179:TYR:CE2	A:201:GLY:HA2	0.50	1	1
B:64:LYS:HE2	B:124:GLY:O	0.49	1	1
A:159:PHE:HA	A:194:THR:HG21	0.49	1	1
B:11:GLY:HA3	B:162:TRP:CE2	0.47	1	1
A:187:THR:HG23	A:195:ILE:HG13	0.47	1	1
B:193:HIS:CE1	B:210:GLN:HE22	0.47	1	1
B:184:THR:HG21	B:194:GLU:OE2	0.44	1	1
B:262:PHE:CZ	B:296:PRO:HA	0.43	1	1
B:445:SER:C	B:494:ARG:HH22	0.43	1	1
B:282:GLN:HB3	B:284:TYR:CZ	0.43	1	1
A:29:ARG:CZ	B:322:ALA:HB1	0.42	1	1
B:244:LEU:HD22	B:279:LYS: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	1038	1018	20	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	872	841	18	13

There are 13 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	4	LEU	1
A	50	ILE	1
A	144	LEU	1
A	232	LEU	1
A	243	ILE	1
A	248	VAL	1
B	41	THR	1
B	102	VAL	1
B	246	ASP	1
B	358	LEU	1
B	372	LEU	1
B	407	GLU	1
B	678	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.

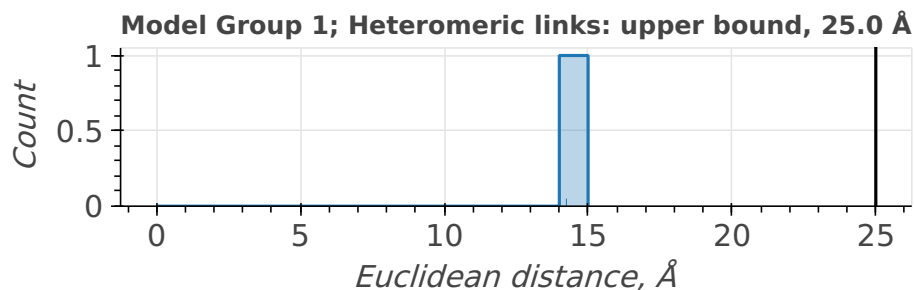
There are 1 crosslinking restraints combined in 1 restraint groups.

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.



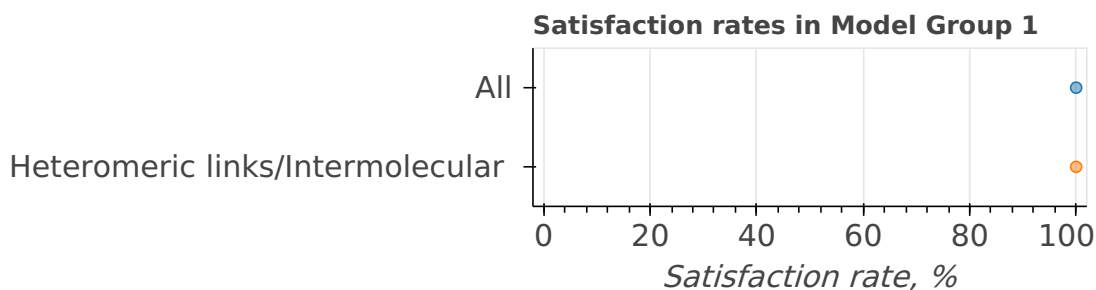
### Satisfaction of restraints

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	100.00	0.00	1
				Heteromeric links/Intermolecular	100.00	0.00	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

*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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