

# 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	9A2L
PDB-Dev ID	PDBDEV_00000170
Structure Title	Model of E. coli TolB 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)*

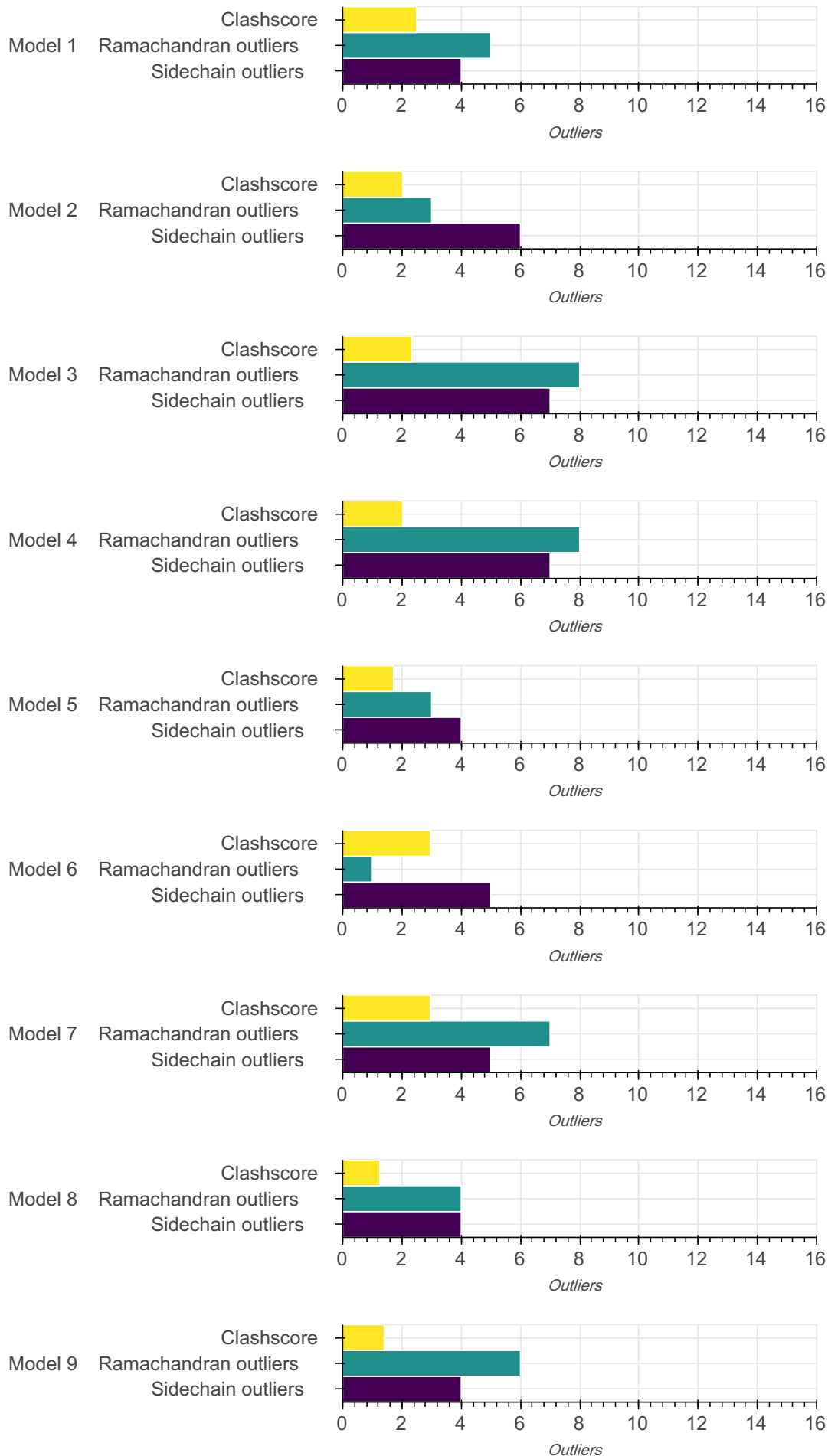
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

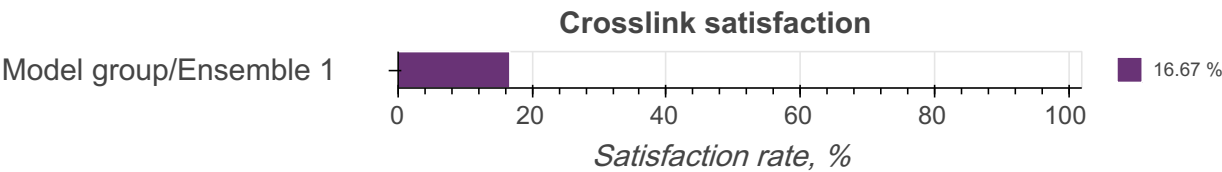
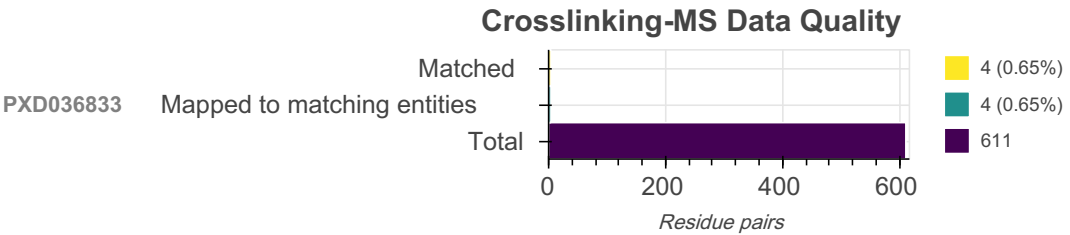
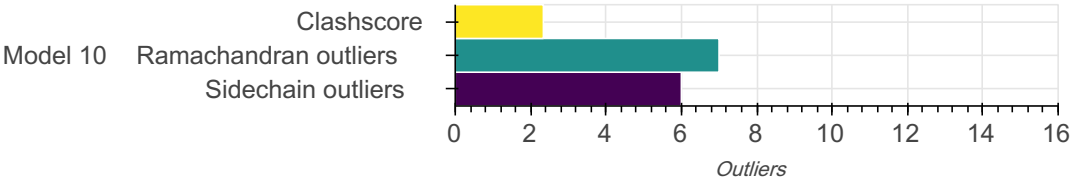
*List of references used to build this report is available [here](#).*

## 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	P0A855	A	430	-	1-430	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	P0A855	dbseq_P0A855_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2L	6	6 (100.00%)	4 (66.67%)
PXD036833	611	4 (0.65%)	4 (0.65%)

### 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 3 bond length outliers in this entry (0.01% of 33260 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	73	ARG	CZ-NH2	4.28	1.27	1.33	4	2
A	409	ARG	CZ-NH2	4.18	1.28	1.33	7	1

#### Standard geometry: angle outliers ?

There are 172 bond angle outliers in this entry (0.38% of 45330 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	12	LEU	C-N-CA	6.74	133.83	121.70	10	2
A	79	GLN	OE1-CD-NE2	6.74	115.86	122.60	10	10
A	308	GLN	OE1-CD-NE2	6.50	116.10	122.60	4	10
A	2	LYS	C-N-CA	6.16	132.80	121.70	3	2
A	31	VAL	C-N-CA	5.69	131.94	121.70	2	1
A	374	THR	CA-CB-CG2	5.45	119.77	110.50	1	1
A	6	ARG	C-N-CA	5.31	131.25	121.70	3	1
A	192	GLN	OE1-CD-NE2	5.12	117.48	122.60	1	6
A	244	ARG	C-N-CA	4.98	130.67	121.70	7	1
A	30	GLY	C-N-CA	4.95	130.61	121.70	7	1
A	246	ASN	OD1-CG-ND2	4.94	117.66	122.60	9	2
A	355	GLN	OE1-CD-NE2	4.93	117.67	122.60	5	8
A	78	GLN	OE1-CD-NE2	4.89	117.71	122.60	4	7
A	420	GLN	OE1-CD-NE2	4.88	117.72	122.60	10	5
A	395	GLN	OE1-CD-NE2	4.87	117.73	122.60	1	2
A	356	GLN	OE1-CD-NE2	4.86	117.74	122.60	4	9

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	326	ARG	CD-NE-CZ	4.85	131.20	124.40	6	2
A	84	GLN	OE1-CD-NE2	4.78	117.82	122.60	10	10
A	333	GLN	OE1-CD-NE2	4.77	117.83	122.60	4	10
A	43	GLN	OE1-CD-NE2	4.76	117.84	122.60	10	1
A	13	ILE	N-CA-CB	4.69	103.53	111.50	10	1
A	229	GLN	OE1-CD-NE2	4.67	117.93	122.60	7	1
A	68	PHE	N-CA-CB	4.58	102.71	110.50	7	1
A	245	HIS	CB-CG-CD2	4.55	125.28	131.20	6	5
A	313	GLN	OE1-CD-NE2	4.54	118.06	122.60	5	4
A	279	GLN	OE1-CD-NE2	4.51	118.09	122.60	4	10
A	301	ASN	OD1-CG-ND2	4.41	118.19	122.60	5	10
A	238	GLN	OE1-CD-NE2	4.38	118.22	122.60	6	10
A	172	GLN	OE1-CD-NE2	4.35	118.25	122.60	6	10
A	3	GLN	OE1-CD-NE2	4.32	118.28	122.60	1	5
A	70	PRO	N-CA-CB	4.30	107.73	103.00	2	2
A	357	HIS	CB-CG-CD2	4.30	125.62	131.20	4	1
A	103	GLN	OE1-CD-NE2	4.28	118.32	122.60	2	4
A	73	ARG	NH1-CZ-NH2	4.24	113.78	119.30	7	1
A	64	ASN	OD1-CG-ND2	4.23	118.37	122.60	8	2
A	300	GLN	OE1-CD-NE2	4.23	118.37	122.60	9	1
A	35	ARG	NH1-CZ-NH2	4.21	113.83	119.30	1	2
A	165	THR	CA-CB-OG1	4.18	103.33	109.60	9	1
A	377	ASP	CA-CB-CG	4.18	116.78	112.60	5	1
A	41	PRO	C-N-CA	4.17	129.20	121.70	10	1
A	87	GLN	OE1-CD-NE2	4.13	118.47	122.60	8	1
A	196	HIS	CB-CG-CD2	4.05	125.93	131.20	7	1
A	326	ARG	NH1-CZ-NH2	4.05	114.03	119.30	7	1
A	335	GLN	OE1-CD-NE2	4.05	118.55	122.60	10	2
A	413	ARG	C-N-CA	4.03	128.96	121.70	3	1
A	131	GLN	OE1-CD-NE2	4.02	118.58	122.60	5	1
A	200	GLN	OE1-CD-NE2	4.01	118.59	122.60	7	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	2.49	16
2	2.03	13
3	2.34	15
4	2.03	13
5	1.71	11
6	2.96	19
7	2.96	19
8	1.25	8
9	1.40	9
10	2.34	15

There are 138 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:329:TRP:CH2	A:368:VAL:HG21	0.93	3	1
A:329:TRP:CZ3	A:368:VAL:HG21	0.93	3	1
A:27:ILE:HG21	A:68:PHE:HB3	0.70	7	1
A:78:GLN:HE22	A:86:VAL:HA	0.65	8	1
A:242:PHE:CE1	A:264:LYS:HE2	0.64	8	6
A:35:ARG:HH21	A:97:ASP:CG	0.62	6	6
A:242:PHE:CD2	A:262:LEU:HD13	0.60	8	5
A:226:LEU:HD11	A:249:PRO:HB3	0.60	9	6
A:37:ILE:HD12	A:156:LEU:HD11	0.60	7	1
A:21:ALA:O	A:417:THR:HG21	0.58	1	1
A:242:PHE:H	A:246:ASN:HD21	0.58	6	2
A:23:VAL:HG12	A:414:LEU:HD22	0.58	3	1
A:239:VAL:HG13	A:273:MET:SD	0.57	9	7
A:78:GLN:HE21	A:91:TRP:NE1	0.57	6	7
A:42:PHE:CE1	A:58:VAL:HG11	0.57	10	1
A:37:ILE:HD11	A:100:VAL:HG23	0.56	7	1
A:355:GLN:HB3	A:374:THR:HG21	0.56	5	1
A:291:THR:HG23	A:292:GLU:OE1	0.56	5	1
A:240:ALA:HB1	A:242:PHE:CZ	0.56	7	1
A:25:ILE:HD12	A:59:ALA:HB1	0.55	7	1
A:281:ARG:HH21	A:319:ILE:HD12	0.55	3	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:40:VAL:HG21	A:91:TRP:CZ3	0.55	10	1
A:273:MET:HE2	A:278:GLY:HA2	0.55	2	3
A:42:PHE:CZ	A:100:VAL:HG11	0.54	10	1
A:346:MET:HE2	A:361:GLN:NE2	0.54	2	1
A:401:LEU:HG	A:421:VAL:HG21	0.53	4	1
A:76:LEU:HD22	A:91:TRP:CH2	0.52	10	1
A:78:GLN:HE21	A:91:TRP:CD1	0.52	9	5
A:27:ILE:HD13	A:31:VAL:HG21	0.52	3	1
A:27:ILE:CG2	A:68:PHE:HB3	0.52	7	1
A:76:LEU:HD22	A:91:TRP:CZ3	0.52	10	1
A:242:PHE:CE2	A:264:LYS:HE2	0.52	3	1
A:328:THR:HA	A:329:TRP:CE3	0.51	4	1
A:242:PHE:CE2	A:262:LEU:HD13	0.50	6	2
A:240:ALA:HB1	A:242:PHE:HE2	0.50	4	1
A:53:ASP:CG	A:73:ARG:HH22	0.49	3	4
A:242:PHE:CG	A:262:LEU:HD13	0.49	7	1
A:242:PHE:CG	A:262:LEU:HD11	0.49	9	1
A:9:PHE:HB3	A:11:PHE:CD2	0.49	7	1
A:44:TRP:CE3	A:104:VAL:HG23	0.48	10	1
A:86:VAL:HG13	A:91:TRP:NE1	0.48	7	1
A:306:SER:HB3	A:315:TYR:CD1	0.48	10	9
A:27:ILE:HG21	A:31:VAL:HG23	0.48	6	2
A:64:ASN:HA	A:410:PHE:CE2	0.47	6	1
A:242:PHE:CE1	A:262:LEU:HD13	0.47	3	1
A:331:GLY:HA2	A:352:ASN:OD1	0.46	6	1
A:245:HIS:CE1	A:247:GLY:HA3	0.46	10	1
A:308:GLN:NE2	A:315:TYR:CE2	0.46	5	9
A:78:GLN:HE22	A:87:GLN:H	0.45	2	3
A:242:PHE:CZ	A:262:LEU:HD22	0.45	7	1
A:329:TRP:HE1	A:366:GLY:HA3	0.44	1	1
A:27:ILE:HG21	A:68:PHE:CB	0.44	7	1
A:86:VAL:HG11	A:101:VAL:CG1	0.44	7	1
A:390:ILE:HG23	A:426:TRP:HE1	0.44	9	1
A:329:TRP:CZ3	A:368:VAL:CG2	0.44	3	1
A:78:GLN:HE22	A:87:GLN:N	0.44	6	2



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:86:VAL:HG13	A:91:TRP:HE1	0.43	7	1
A:27:ILE:HG21	A:31:VAL:CG2	0.42	1	1
A:71:LEU:HD11	A:96:ILE:CD1	0.42	1	1
A:71:LEU:HD22	A:76:LEU:HD21	0.42	10	1
A:76:LEU:HD22	A:91:TRP:HH2	0.42	6	1
A:86:VAL:HG11	A:101:VAL:HG11	0.42	7	1
A:326:ARG:HD3	A:329:TRP:CZ3	0.42	6	1
A:262:LEU:HG	A:271:TYR:CE1	0.42	10	1
A:71:LEU:HD11	A:96:ILE:HD11	0.42	1	1
A:25:ILE:CG2	A:412:ALA:HB1	0.41	2	1
A:405:SER:OG	A:411:LYS:HE2	0.41	10	1
A:315:TYR:CE2	A:326:ARG:HB2	0.41	6	1
A:42:PHE:CE1	A:58:VAL:CG1	0.41	10	1
A:35:ARG:HH21	A:97:ASP:HB2	0.40	9	1
A:23:VAL:CG1	A:414:LEU:HB3	0.40	3	1
A:242:PHE:CD2	A:262:LEU:HD22	0.40	4	1
A:410:PHE:CZ	A:412:ALA:HB2	0.40	4	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	428	406	17	5
2	428	408	17	3
3	428	411	9	8
4	428	402	18	8
5	428	400	25	3
6	428	418	9	1
7	428	399	22	7
8	428	408	16	4
9	428	400	22	6
10	428	403	18	7

There are 28 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	19	LEU	5

Chain	Res	Type	Models (Total)
A	17	SER	4
A	20	HIS	4
A	31	VAL	4
A	2	LYS	3
A	3	GLN	3
A	18	VAL	3
A	21	ALA	2
A	22	GLU	2
A	25	ILE	2
A	29	SER	2
A	418	ASP	2
A	7	VAL	1
A	11	PHE	1
A	13	ILE	1
A	14	LEU	1
A	15	TRP	1
A	16	ALA	1
A	23	VAL	1
A	24	ARG	1
A	27	ILE	1
A	28	ASP	1
A	32	ASP	1
A	78	GLN	1
A	80	PRO	1
A	86	VAL	1
A	245	HIS	1
A	396	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	343	334	5	4
2	343	330	7	6
3	343	332	4	7

Model ID	Analysed	Favored	Allowed	Outliers
4	343	333	3	7
5	343	330	9	4
6	343	335	3	5
7	343	331	7	5
8	343	331	8	4
9	343	335	4	4
10	343	331	6	6

There are 20 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	12	LEU	8
A	374	THR	8
A	5	LEU	7
A	14	LEU	4
A	17	SER	4
A	9	PHE	3
A	267	SER	3
A	29	SER	2
A	417	THR	2
A	1	MET	1
A	26	VAL	1
A	31	VAL	1
A	32	ASP	1
A	71	LEU	1
A	111	SER	1
A	246	ASN	1
A	292	GLU	1
A	328	THR	1
A	329	TRP	1
A	421	VAL	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

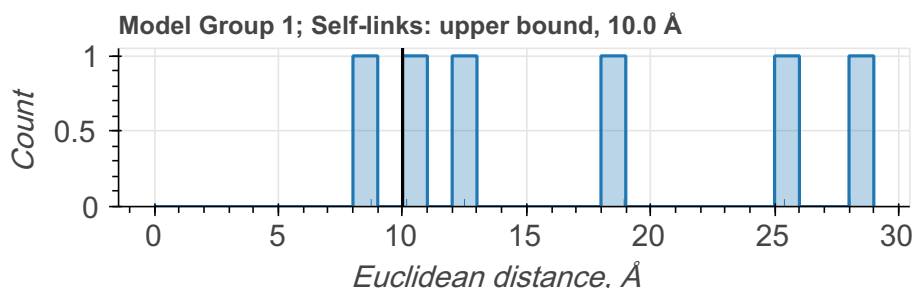
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 6 crosslinking restraints combined in 6 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	LEU	CA	PRO	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	TRP	CA	upper bound	10.0	1
L-Photo-Leucine	GLY	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ALA	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	HIS	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.



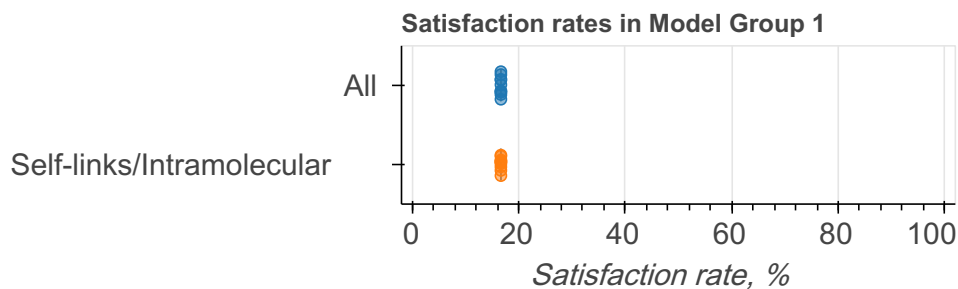
#### Satisfaction of restraints

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=6)
1	1	1	10/10	All	16.67	83.33	6
				Self-links/ Intramolecular	16.67	83.33	6

#### 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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