

# Integrative Structure Validation Report ?

February 18, 2025 - 08:36 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	9A2X
PDB-Dev ID	PDBDEV_00000182
Structure Title	Model of E. coli TolC 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)*

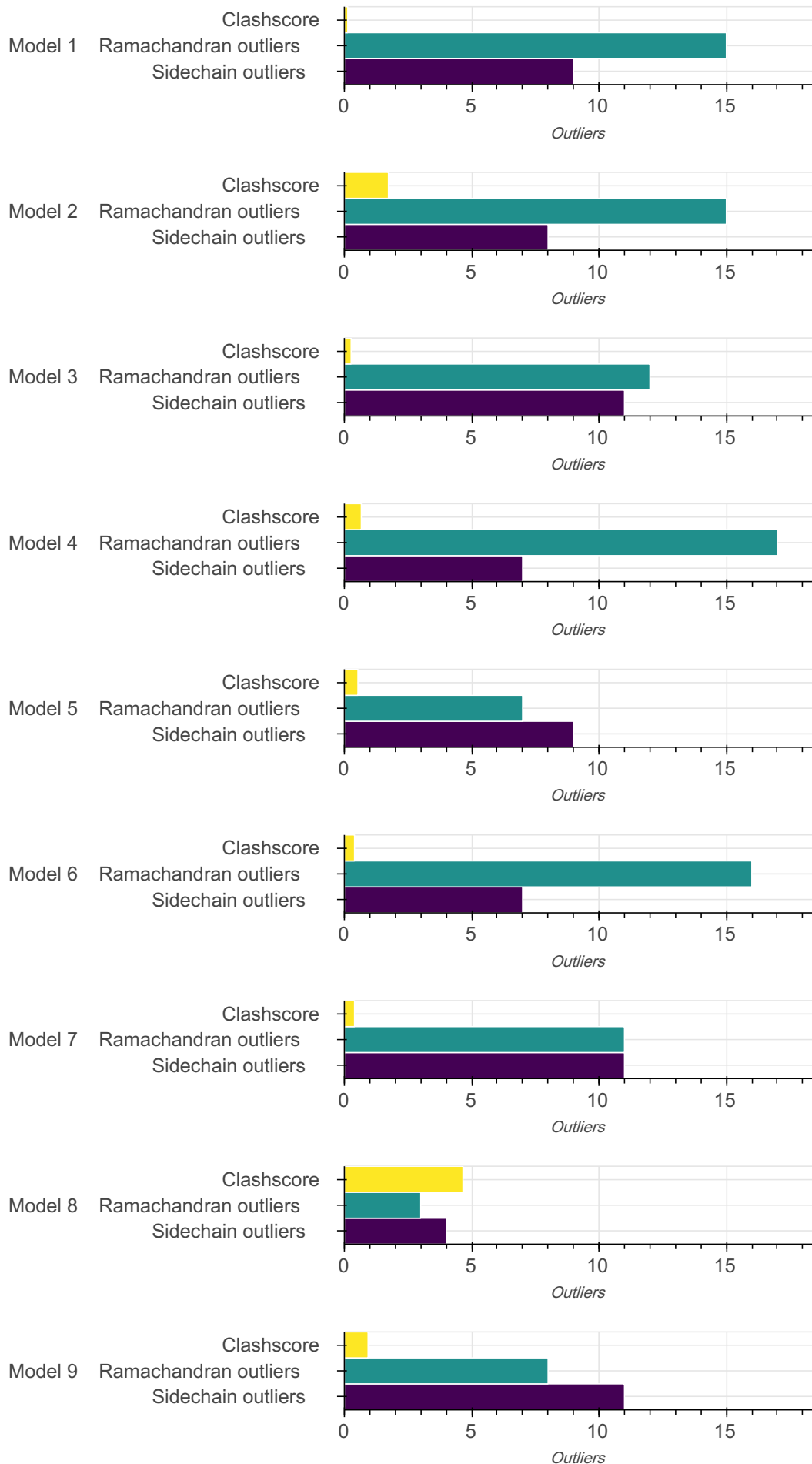
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

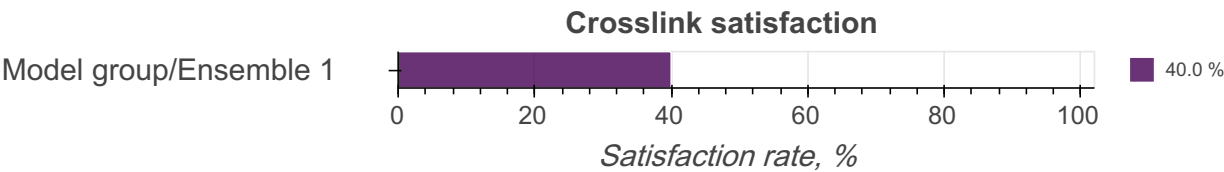
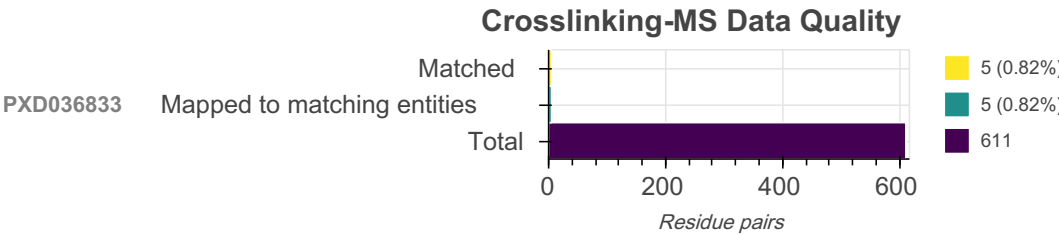
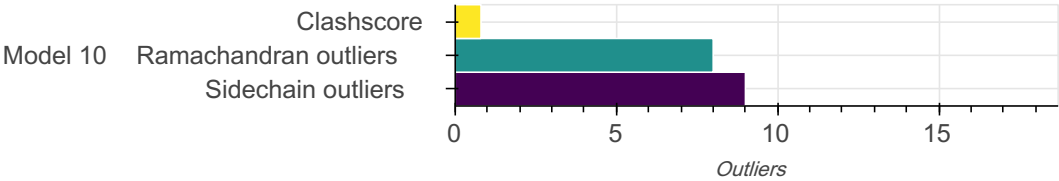
*List of references used to build this report is available [here](#).*

## 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	P02930	A	493	-	1-493	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	P02930	dbseq_P02930_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2X	5	5 (100.00%)	5 (100.00%)
PXD036833	611	5 (0.82%)	5 (0.82%)

### 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 7 bond length outliers in this entry (0.02% of 38350 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	492	ARG	CA-CB	76.91	3.07	1.53	8	1
A	490	PRO	N-CD	32.64	1.93	1.47	8	1
A	490	PRO	N-CA	31.72	1.94	1.47	8	1
A	490	PRO	CA-CB	26.83	2.07	1.53	8	1
A	490	PRO	CG-CD	16.26	2.06	1.50	8	1
A	490	PRO	CB-CG	11.86	2.08	1.49	8	1
A	492	ARG	N-CA	4.13	1.54	1.46	8	1

#### Standard geometry: angle outliers ?

There are 371 bond angle outliers in this entry (0.71% of 52160 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	492	ARG	CA-CB-CG	10.65	135.41	114.10	8	1
A	492	ARG	C-CA-CB	9.74	128.61	110.10	8	1
A	4	LEU	C-N-CA	9.51	138.81	121.70	2	3
A	492	ARG	N-CA-CB	9.08	125.93	110.50	8	1
A	491	PHE	C-N-CA	8.44	136.89	121.70	9	5
A	482	THR	C-N-CA	8.31	136.65	121.70	7	3
A	2	LYS	C-N-CA	7.90	135.92	121.70	7	5
A	486	ASN	C-N-CA	7.88	135.89	121.70	5	5
A	475	VAL	C-N-CA	6.78	133.90	121.70	4	3
A	492	ARG	N-CA-C	6.59	92.55	111.00	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	488	HIS	C-N-CA	6.49	133.38	121.70	4	1
A	480	ALA	C-N-CA	6.44	133.28	121.70	3	2
A	468	PRO	C-N-CA	6.21	132.88	121.70	6	5
A	492	ARG	C-N-CA	6.15	132.78	121.70	5	4
A	471	PRO	C-N-CA	6.04	132.58	121.70	2	3
A	485	SER	C-N-CA	5.99	132.49	121.70	3	6
A	477	GLN	C-N-CA	5.96	132.43	121.70	3	2
A	471	PRO	CA-N-CD	5.87	103.78	112.00	2	1
A	483	THR	C-N-CA	5.87	132.26	121.70	3	5
A	3	LYS	C-N-CA	5.77	132.08	121.70	2	2
A	4	LEU	CA-C-N	5.62	127.43	116.20	2	2
A	473	PRO	CA-N-CD	5.55	104.24	112.00	1	2
A	116	GLN	OE1-CD-NE2	5.52	117.08	122.60	4	7
A	316	GLN	OE1-CD-NE2	5.48	117.12	122.60	4	10
A	487	GLY	C-N-CA	5.41	131.43	121.70	4	2
A	288	THR	C-N-CA	5.34	131.31	121.70	2	4
A	419	GLN	OE1-CD-NE2	5.28	117.32	122.60	4	8
A	489	ASN	N-CA-CB	5.18	101.70	110.50	4	1
A	4	LEU	O-C-N	5.15	114.76	123.00	2	2
A	291	ALA	C-N-CA	5.11	130.90	121.70	2	2
A	21	GLN	C-N-CA	5.11	130.89	121.70	8	1
A	303	GLN	OE1-CD-NE2	5.09	117.51	122.60	5	4
A	481	ARG	N-CA-CB	5.05	101.91	110.50	3	2
A	292	ALA	C-N-CA	5.05	130.79	121.70	2	1
A	472	ALA	N-CA-CB	5.05	102.83	110.40	2	1
A	295	GLN	N-CA-CB	5.02	101.97	110.50	7	1
A	182	GLN	OE1-CD-NE2	5.00	117.60	122.60	10	9
A	455	GLN	C-N-CA	4.99	130.69	121.70	2	1
A	11	LEU	C-N-CA	4.89	130.51	121.70	9	3
A	490	PRO	C-N-CA	4.87	130.46	121.70	8	1
A	124	GLN	OE1-CD-NE2	4.86	117.74	122.60	8	10
A	486	ASN	O-C-N	4.81	115.30	123.00	5	3
A	469	ASP	C-N-CA	4.81	130.35	121.70	2	1
A	27	GLN	OE1-CD-NE2	4.79	117.81	122.60	8	3
A	31	GLN	OE1-CD-NE2	4.79	117.81	122.60	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	455	GLN	OE1-CD-NE2	4.78	117.82	122.60	8	10
A	121	GLN	OE1-CD-NE2	4.77	117.83	122.60	5	10
A	104	ARG	NE-CZ-NH2	4.75	123.47	119.20	6	2
A	263	GLN	OE1-CD-NE2	4.72	117.88	122.60	1	10
A	1	MET	C-N-CA	4.72	130.19	121.70	6	2
A	486	ASN	CA-C-N	4.71	125.61	116.20	5	3
A	109	GLN	OE1-CD-NE2	4.69	117.91	122.60	8	10
A	104	ARG	CD-NE-CZ	4.68	130.95	124.40	2	1
A	473	PRO	C-N-CA	4.67	130.11	121.70	6	3
A	484	THR	C-N-CA	4.66	130.09	121.70	2	3
A	483	THR	N-CA-CB	4.65	103.60	111.50	7	1
A	161	GLN	OE1-CD-NE2	4.64	117.96	122.60	9	9
A	21	GLN	OE1-CD-NE2	4.64	117.96	122.60	6	10
A	490	PRO	CA-C-N	4.59	125.39	116.20	8	1
A	468	PRO	CA-N-CD	4.57	105.60	112.00	2	1
A	474	VAL	C-N-CA	4.56	129.90	121.70	6	1
A	328	GLN	OE1-CD-NE2	4.55	118.05	122.60	6	10
A	252	GLN	OE1-CD-NE2	4.54	118.06	122.60	8	3
A	203	GLN	OE1-CD-NE2	4.53	118.07	122.60	10	9
A	451	ASN	OD1-CG-ND2	4.53	118.07	122.60	2	6
A	92	GLN	OE1-CD-NE2	4.51	118.09	122.60	9	8
A	459	GLN	OE1-CD-NE2	4.51	118.09	122.60	7	6
A	24	ASN	C-CA-CB	4.51	118.66	110.10	10	2
A	125	GLN	OE1-CD-NE2	4.50	118.10	122.60	6	3
A	481	ARG	C-N-CA	4.48	129.76	121.70	2	1
A	296	TYR	C-N-CA	4.48	129.76	121.70	7	1
A	10	GLY	C-N-CA	4.48	129.76	121.70	6	1
A	368	GLN	OE1-CD-NE2	4.47	118.13	122.60	4	1
A	195	ASN	OD1-CG-ND2	4.46	118.14	122.60	9	2
A	290	GLY	C-N-CA	4.45	129.71	121.70	9	1
A	486	ASN	N-CA-C	4.45	123.46	111.00	4	1
A	476	GLN	C-N-CA	4.44	129.70	121.70	1	1
A	151	GLN	OE1-CD-NE2	4.44	118.16	122.60	8	9
A	476	GLN	OE1-CD-NE2	4.43	118.17	122.60	3	9
A	177	GLN	OE1-CD-NE2	4.43	118.17	122.60	5	9

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	453	ALA	N-CA-CB	4.40	103.79	110.40	10	1
A	432	GLN	OE1-CD-NE2	4.38	118.22	122.60	1	9
A	490	PRO	N-CA-CB	4.38	107.81	103.00	8	1
A	477	GLN	OE1-CD-NE2	4.37	118.23	122.60	3	9
A	337	GLN	OE1-CD-NE2	4.33	118.27	122.60	8	8
A	490	PRO	N-CA-C	4.32	122.89	112.10	8	1
A	30	GLN	OE1-CD-NE2	4.32	118.28	122.60	5	3
A	74	ASN	OD1-CG-ND2	4.31	118.29	122.60	1	1
A	323	GLN	OE1-CD-NE2	4.29	118.31	122.60	5	7
A	63	GLN	OE1-CD-NE2	4.28	118.32	122.60	10	1
A	95	GLN	OE1-CD-NE2	4.27	118.33	122.60	9	3
A	477	GLN	O-C-N	4.22	116.25	123.00	3	1
A	78	ASP	CA-CB-CG	4.20	116.80	112.60	5	2
A	460	ASN	OD1-CG-ND2	4.17	118.43	122.60	1	3
A	488	HIS	CB-CG-CD2	4.17	125.78	131.20	9	1
A	462	ILE	CA-CB-CG1	4.15	117.45	110.40	6	1
A	206	GLN	OE1-CD-NE2	4.15	118.45	122.60	10	2
A	258	GLN	OE1-CD-NE2	4.13	118.47	122.60	8	3
A	12	SER	C-N-CA	4.12	129.12	121.70	4	1
A	491	PHE	O-C-N	4.11	116.42	123.00	8	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	0.13	1
2	1.73	13
3	0.27	2
4	0.67	5
5	0.53	4
6	0.40	3
7	0.40	3
8	4.66	35
9	0.93	7
10	0.80	6



There are 79 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:490:PRO:CD	A:490:PRO:CG	1.34	8	1
A:490:PRO:CA	A:490:PRO:CB	1.32	8	1
A:490:PRO:CD	A:490:PRO:N	1.31	8	1
A:490:PRO:CB	A:490:PRO:CG	1.31	8	1
A:490:PRO:CA	A:490:PRO:N	1.29	8	1
A:490:PRO:CA	A:492:ARG:HA	1.27	8	1
A:490:PRO:CB	A:492:ARG:HA	1.18	8	1
A:490:PRO:CG	A:492:ARG:CB	1.11	8	1
A:490:PRO:CB	A:492:ARG:CA	1.11	8	1
A:490:PRO:CD	A:492:ARG:CA	1.10	8	1
A:490:PRO:CB	A:492:ARG:CB	1.09	8	1
A:490:PRO:CA	A:492:ARG:CB	1.08	8	1
A:490:PRO:CA	A:492:ARG:CA	1.07	8	1
A:490:PRO:CG	A:492:ARG:CA	1.07	8	1
A:490:PRO:CD	A:492:ARG:CB	1.07	8	1
A:490:PRO:CD	A:492:ARG:HB2	0.98	8	1
A:490:PRO:N	A:492:ARG:CB	0.96	8	1
A:490:PRO:N	A:492:ARG:CA	0.91	8	1
A:490:PRO:CB	A:492:ARG:HB3	0.86	8	1
A:490:PRO:CG	A:492:ARG:HB3	0.79	8	1
A:490:PRO:HG2	A:492:ARG:C	0.78	8	1
A:490:PRO:C	A:492:ARG:HA	0.76	8	1
A:490:PRO:CG	A:492:ARG:C	0.74	8	1
A:490:PRO:HD3	A:492:ARG:HB2	0.69	8	1
A:380:MET:SD	A:397:ALA:HB2	0.67	5	1
A:490:PRO:HA	A:492:ARG:CG	0.66	8	1
A:490:PRO:HB2	A:492:ARG:HA	0.65	8	1
A:490:PRO:CA	A:492:ARG:CG	0.62	8	1
A:287:LYS:HE3	A:293:GLY:HA2	0.59	2	1
A:490:PRO:HB3	A:492:ARG:HB3	0.59	8	1
A:155:ILE:HD13	A:182:GLN:HG3	0.58	2	1
A:64:LEU:HD11	A:91:LEU:HD11	0.57	5	1
A:490:PRO:N	A:492:ARG:N	0.55	8	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:287:LYS:CE	A:293:GLY:HA2	0.54	2	1
A:477:GLN:HB3	A:478:THR:HG23	0.53	3	1
A:104:ARG:HE	A:264:ASP:CG	0.52	2	1
A:155:ILE:HD12	A:186:VAL:HG21	0.51	2	1
A:26:MET:HE3	A:435:LEU:HG	0.51	10	3
A:490:PRO:HG3	A:492:ARG:CB	0.50	8	1
A:205:ARG:HD3	A:211:TYR:CZ	0.50	10	1
A:149:GLN:NE2	A:453:ALA:HB1	0.50	10	1
A:299:SER:C	A:301:MET:H	0.49	4	1
A:313:PRO:CB	A:316:GLN:HE21	0.49	4	1
A:234:LEU:HD13	A:422:ILE:HD11	0.48	4	9
A:111:LYS:HE3	A:257:GLU:CG	0.47	10	2
A:165:ARG:HH22	A:385:SER:HA	0.47	9	1
A:313:PRO:HB3	A:316:GLN:HE21	0.47	2	2
A:472:ALA:HB1	A:473:PRO:HD2	0.47	2	1
A:22:ALA:HB2	A:444:PRO:HB3	0.46	9	1
A:490:PRO:HD2	A:492:ARG:CA	0.45	8	1
A:155:ILE:CD1	A:186:VAL:HG21	0.45	9	1
A:490:PRO:CD	A:492:ARG:N	0.45	8	1
A:104:ARG:HD2	A:261:GLN:HA	0.44	2	1
A:490:PRO:HG3	A:492:ARG:HB3	0.44	8	1
A:490:PRO:HA	A:492:ARG:HG2	0.44	8	1
A:14:SER:HB3	A:16:PHE:CE2	0.43	10	1
A:472:ALA:HB1	A:473:PRO:CD	0.43	2	1
A:128:ILE:HG23	A:434:LEU:HD12	0.43	7	1
A:104:ARG:CZ	A:260:ARG:HB3	0.43	9	2
A:490:PRO:CG	A:492:ARG:HB2	0.42	8	1
A:461:ALA:C	A:462:ILE:HG13	0.42	9	1
A:111:LYS:HE3	A:257:GLU:HG2	0.42	6	1
A:29:TYR:HA	A:131:THR:HG21	0.41	5	1
A:266:HIS:CD2	A:320:VAL:HG11	0.41	2	1
A:25:LEU:HG	A:434:LEU:CD2	0.41	7	1
A:223:PHE:CE1	A:415:TYR:CD2	0.41	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	491	455	21	15
2	491	450	26	15
3	491	460	19	12
4	491	456	18	17
5	491	453	31	7
6	491	449	26	16
7	491	451	29	11
8	491	464	24	3
9	491	460	23	8
10	491	460	23	8

There are 50 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	13	LEU	7
A	17	SER	7
A	289	ARG	7
A	20	SER	6
A	2	LYS	5
A	3	LYS	4
A	469	ASP	4
A	484	THR	4
A	486	ASN	4
A	492	ARG	4
A	292	ALA	3
A	300	ASN	3
A	447	THR	3
A	462	ILE	3
A	4	LEU	2
A	12	SER	2
A	15	GLY	2
A	446	SER	2
A	459	GLN	2
A	464	ASP	2
A	470	SER	2

Chain	Res	Type	Models (Total)
A	472	ALA	2
A	473	PRO	2
A	485	SER	2
A	487	GLY	2
A	490	PRO	2
A	8	LEU	1
A	10	GLY	1
A	11	LEU	1
A	14	SER	1
A	22	ALA	1
A	287	LYS	1
A	288	THR	1
A	290	GLY	1
A	291	ALA	1
A	293	GLY	1
A	298	ASP	1
A	299	SER	1
A	445	VAL	1
A	451	ASN	1
A	457	PRO	1
A	465	GLY	1
A	468	PRO	1
A	471	PRO	1
A	474	VAL	1
A	476	GLN	1
A	481	ARG	1
A	483	THR	1
A	488	HIS	1
A	489	ASN	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	412	394	9	9
2	412	395	9	8

Model ID	Analysed	Favored	Allowed	Outliers
3	412	396	5	11
4	412	398	7	7
5	412	398	5	9
6	412	392	13	7
7	412	397	4	11
8	412	397	11	4
9	412	391	10	11
10	412	396	7	9

There are 26 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	8	LEU	9
A	96	SER	9
A	11	LEU	8
A	288	THR	7
A	5	LEU	6
A	294	THR	6
A	462	ILE	6
A	456	THR	5
A	482	THR	4
A	488	HIS	4
A	13	LEU	2
A	14	SER	2
A	19	LEU	2
A	78	ASP	2
A	299	SER	2
A	452	VAL	2
A	76	TYR	1
A	85	ASN	1
A	88	SER	1
A	140	ASN	1
A	282	SER	1
A	286	SER	1
A	434	LEU	1
A	438	ASN	1

Chain	Res	Type	Models (Total)
A	446	SER	1
A	478	THR	1

## Fit of model to data used for modeling ?

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

#### Restraint types

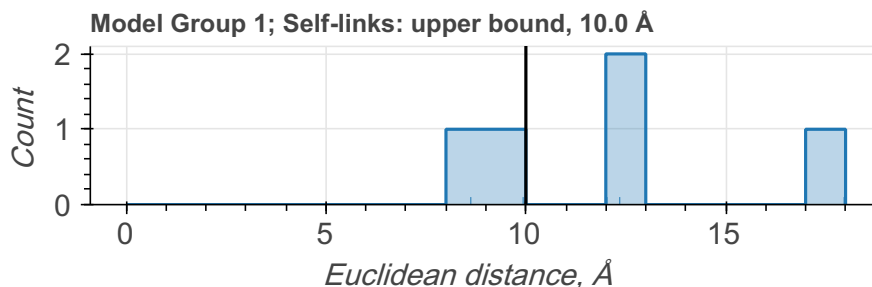
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 5 crosslinking restraints combined in 5 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	LEU	CA	TYR	CA	upper bound	10.0	2
L-Photo-Leucine	ALA	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ASN	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	LYS	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.



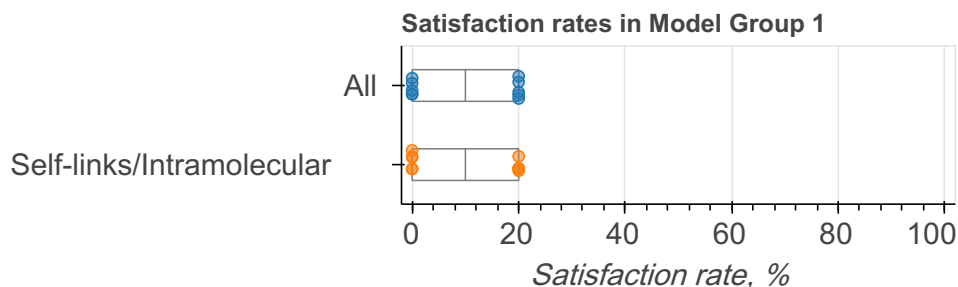
#### Satisfaction of restraints

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=5)
1	1	1	10/10	All	40.00	60.00	5
				Self-links/ Intramolecular	40.00	60.00	5

#### 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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