

# 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	9A2W
PDB-Dev ID	PDBDEV_00000181
Structure Title	Model of E. coli MtlA 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)*

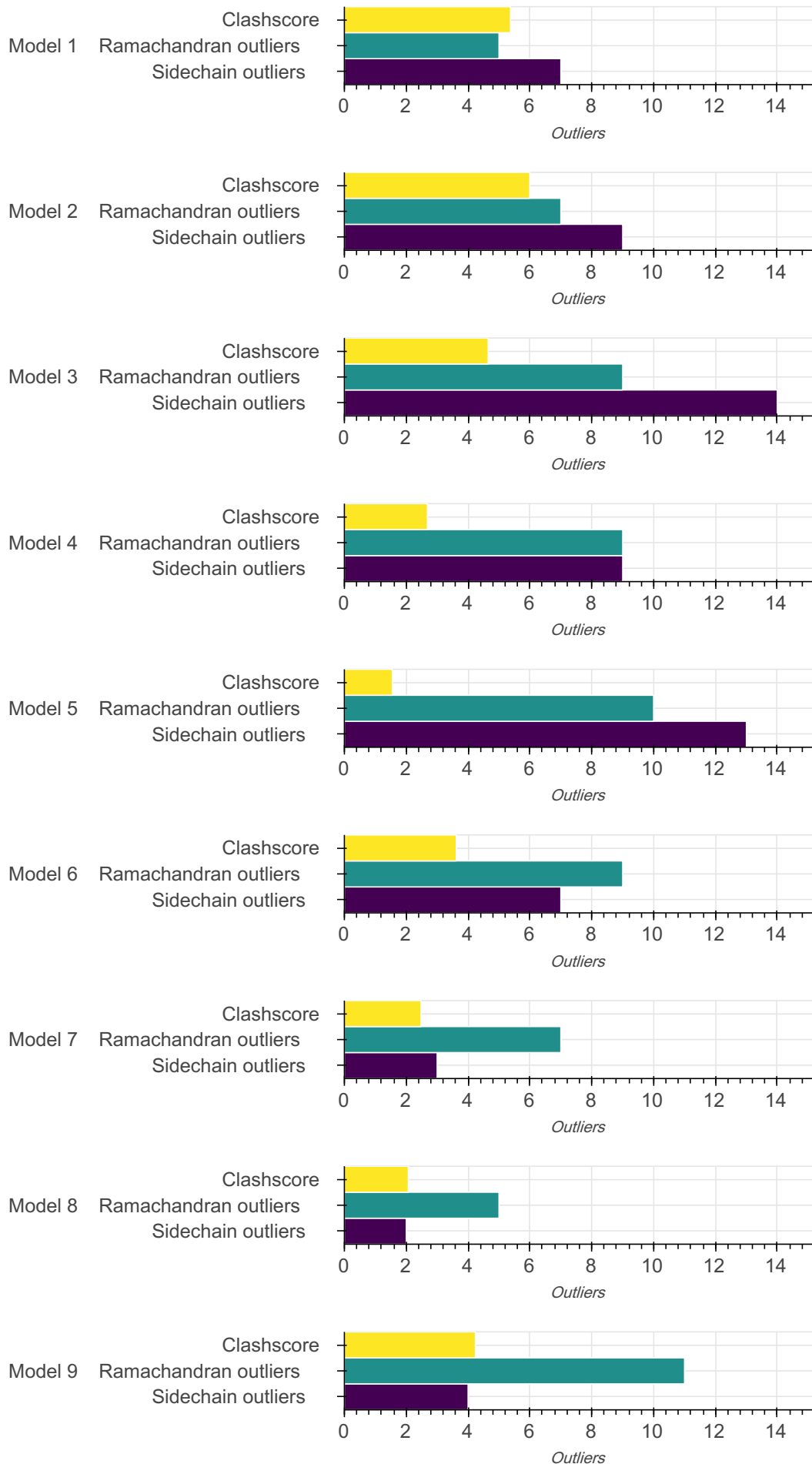
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

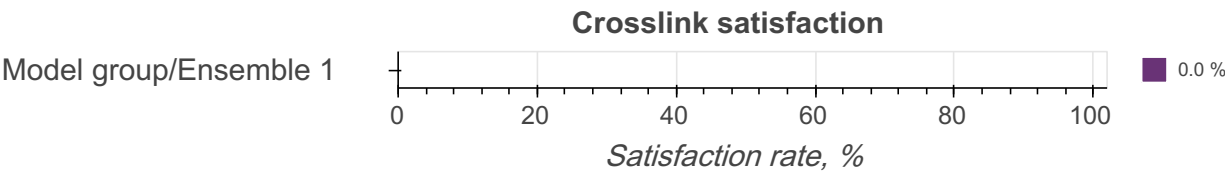
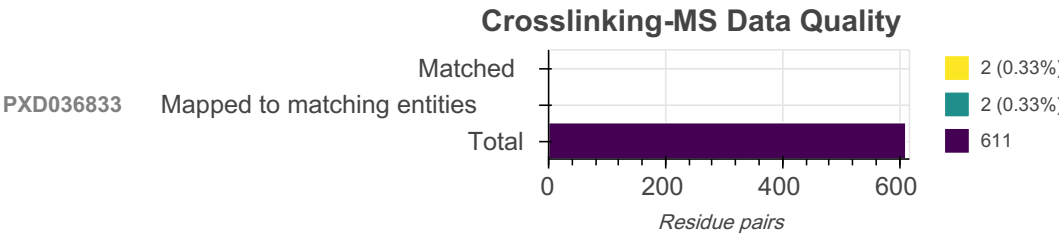
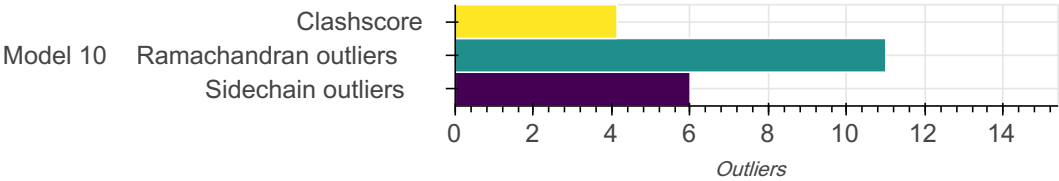
*List of references used to build this report is available [here](#).*

## 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	P00550	A	637	-	1-637	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	P00550	dbseq_P00550_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2W	2	2 (100.00%)	2 (100.00%)
PXD036833	611	2 (0.33%)	2 (0.33%)

### 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 272 bond angle outliers in this entry (0.41% of 65770 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	251	PHE	CA-CB-CG	12.40	126.20	113.80	10	1
A	486	PHE	C-N-CA	9.31	138.45	121.70	10	3
A	198	PHE	C-N-CA	8.93	137.77	121.70	5	1
A	220	ASN	CA-CB-CG	8.59	121.19	112.60	10	1
A	190	ASN	OD1-CG-ND2	7.26	115.34	122.60	4	2
A	40	THR	CA-CB-CG2	6.80	122.07	110.50	2	1
A	260	PHE	CA-CB-CG	6.77	107.03	113.80	4	3
A	343	ASP	CA-CB-CG	6.63	119.23	112.60	8	6
A	184	ALA	C-N-CA	6.59	133.57	121.70	2	1
A	315	ASN	OD1-CG-ND2	6.55	116.05	122.60	4	4
A	488	ASP	C-N-CA	6.43	133.27	121.70	5	2
A	71	LEU	C-N-CA	6.40	133.22	121.70	3	2
A	95	PRO	CA-N-CD	6.33	103.14	112.00	6	1
A	487	ASP	C-N-CA	6.27	132.99	121.70	10	3
A	198	PHE	CA-CB-CG	6.15	119.95	113.80	10	2
A	353	GLN	C-N-CA	6.00	132.51	121.70	8	2
A	198	PHE	O-C-N	6.00	113.40	123.00	5	1
A	180	PHE	CA-CB-CG	5.93	107.87	113.80	2	1
A	601	ILE	CA-CB-CG2	5.83	120.40	110.50	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	123	LYS	C-N-CA	5.82	132.18	121.70	3	1
A	198	PHE	CA-C-N	5.81	127.82	116.20	5	1
A	484	ASP	C-N-CA	5.73	132.01	121.70	10	7
A	385	ASP	C-N-CA	5.70	131.97	121.70	5	1
A	485	SER	C-N-CA	5.66	131.89	121.70	6	5
A	76	ARG	NE-CZ-NH2	5.60	124.24	119.20	7	4
A	362	ALA	C-N-CA	5.58	131.75	121.70	6	3
A	357	ALA	C-CA-CB	5.58	118.87	110.50	9	1
A	219	ALA	C-N-CA	5.54	131.67	121.70	9	1
A	354	ASP	CA-CB-CG	5.53	118.13	112.60	8	1
A	218	GLU	C-CA-CB	5.46	120.47	110.10	10	1
A	443	GLN	OE1-CD-NE2	5.38	117.22	122.60	6	10
A	353	GLN	OE1-CD-NE2	5.33	117.27	122.60	3	10
A	20	VAL	CA-CB-CG1	5.31	119.43	110.40	5	1
A	489	SER	C-N-CA	5.29	131.23	121.70	10	1
A	10	GLN	OE1-CD-NE2	5.29	117.31	122.60	8	10
A	520	GLN	OE1-CD-NE2	5.27	117.33	122.60	7	2
A	70	LYS	C-N-CA	5.26	131.18	121.70	3	1
A	403	GLN	OE1-CD-NE2	5.14	117.46	122.60	3	10
A	195	HIS	CB-CG-CD2	5.14	124.52	131.20	9	2
A	198	PHE	N-CA-CB	5.13	101.78	110.50	10	1
A	487	ASP	N-CA-C	5.13	125.36	111.00	6	1
A	21	MET	CA-C-N	5.13	124.59	116.90	6	2
A	260	PHE	CA-C-N	5.13	124.59	116.90	9	1
A	21	MET	O-C-N	5.05	114.91	123.00	6	1
A	368	GLY	C-N-CA	5.01	130.72	121.70	1	2
A	533	GLN	OE1-CD-NE2	4.93	117.67	122.60	3	3
A	486	PHE	O-C-N	4.92	115.13	123.00	10	1
A	113	HIS	CB-CG-CD2	4.81	124.94	131.20	5	8
A	486	PHE	CA-C-N	4.81	125.82	116.20	10	1
A	489	SER	N-CA-C	4.79	124.43	111.00	10	1
A	483	LYS	C-N-CA	4.78	130.31	121.70	9	2
A	419	ASN	CA-CB-CG	4.77	117.37	112.60	6	1
A	445	GLN	OE1-CD-NE2	4.76	117.84	122.60	8	2
A	488	ASP	N-CA-CB	4.75	102.42	110.50	10	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	344	ASP	CA-CB-CG	4.74	117.34	112.60	6	3
A	364	PRO	C-N-CA	4.73	130.21	121.70	5	2
A	220	ASN	OD1-CG-ND2	4.70	117.90	122.60	4	2
A	486	PHE	CA-CB-CG	4.66	118.46	113.80	2	1
A	600	HIS	CB-CG-CD2	4.66	125.14	131.20	1	3
A	342	GLU	CA-C-N	4.66	125.52	116.20	6	1
A	446	HIS	CB-CG-CD2	4.64	125.17	131.20	6	10
A	243	ALA	C-CA-CB	4.64	117.46	110.50	10	1
A	210	GLY	C-N-CA	4.63	130.04	121.70	10	1
A	205	GLN	OE1-CD-NE2	4.63	117.97	122.60	9	3
A	365	LEU	C-N-CA	4.63	130.04	121.70	2	2
A	602	GLN	OE1-CD-NE2	4.60	118.00	122.60	10	7
A	219	ALA	C-CA-CB	4.60	117.39	110.50	9	1
A	241	GLN	OE1-CD-NE2	4.57	118.03	122.60	2	5
A	488	ASP	CA-CB-CG	4.56	117.16	112.60	10	2
A	253	GLY	C-N-CA	4.56	129.91	121.70	2	1
A	347	ALA	N-CA-CB	4.56	117.24	110.40	6	1
A	212	SER	C-N-CA	4.54	129.87	121.70	3	1
A	471	HIS	CB-CG-CD2	4.51	125.34	131.20	1	8
A	250	HIS	CB-CG-CD2	4.47	125.38	131.20	3	4
A	295	ALA	C-N-CA	4.46	129.73	121.70	3	1
A	302	ALA	C-CA-CB	4.46	117.18	110.50	5	1
A	191	ASN	OD1-CG-ND2	4.45	118.15	122.60	4	3
A	414	ASN	OD1-CG-ND2	4.43	118.17	122.60	4	3
A	480	ASP	C-N-CA	4.43	129.67	121.70	9	1
A	482	LEU	C-N-CA	4.36	129.55	121.70	3	1
A	409	GLN	OE1-CD-NE2	4.36	118.24	122.60	9	5
A	215	PHE	N-CA-CB	4.33	103.13	110.50	10	1
A	217	ILE	N-CA-CB	4.33	118.86	111.50	1	1
A	572	GLN	OE1-CD-NE2	4.32	118.28	122.60	2	3
A	19	MET	C-N-CA	4.31	129.47	121.70	5	1
A	481	SER	C-N-CA	4.30	129.45	121.70	4	2
A	21	MET	C-N-CD	4.30	107.39	125.00	6	1
A	430	HIS	CB-CG-CD2	4.29	125.62	131.20	10	5
A	440	GLN	OE1-CD-NE2	4.29	118.31	122.60	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	198	PHE	C-CA-CB	4.27	118.21	110.10	10	1
A	350	ARG	N-CA-CB	4.27	117.75	110.50	6	2
A	154	VAL	N-CA-CB	4.25	104.27	111.50	6	1
A	42	TRP	C-N-CA	4.25	129.36	121.70	4	1
A	609	ASN	OD1-CG-ND2	4.25	118.35	122.60	5	5
A	492	ASN	OD1-CG-ND2	4.24	118.36	122.60	10	1
A	214	PHE	CA-CB-CG	4.23	109.57	113.80	10	1
A	76	ARG	NH1-CZ-NH2	4.23	113.80	119.30	7	2
A	220	ASN	N-CA-CB	4.22	103.33	110.50	3	1
A	350	ARG	CA-C-N	4.22	124.64	116.20	8	2
A	343	ASP	N-CA-CB	4.21	117.66	110.50	6	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	5.37	52
2	5.99	58
3	4.65	45
4	2.69	26
5	1.55	15
6	3.62	35
7	2.48	24
8	2.07	20
9	4.24	41
10	4.13	40

There are 356 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:386:ALA:HB1	A:388:MET:HE2	1.04	1	1
A:180:PHE:CZ	A:197:ILE:HD11	0.95	2	1
A:98:LEU:HD23	A:192:ALA:HB1	0.88	10	1
A:174:LEU:CD1	A:179:ILE:HD11	0.85	2	1
A:259:TYR:CD1	A:273:VAL:HG22	0.81	4	1
A:34:THR:HG23	A:38:ILE:HD12	0.80	2	2



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:198:PHE:HB3	A:214:PHE:CZ	0.80	10	1
A:98:LEU:HD13	A:154:VAL:HG22	0.77	3	1
A:16:LEU:HD22	A:101:MET:HE2	0.77	6	1
A:55:MET:HE1	A:84:THR:HG22	0.74	3	1
A:265:MET:HE1	A:348:ALA:HB2	0.73	9	1
A:57:THR:HA	A:96:MET:HE1	0.73	2	1
A:239:ALA:HA	A:345:ILE:HD11	0.72	7	1
A:33:ILE:HD11	A:140:MET:HA	0.72	3	1
A:161:LEU:HD22	A:214:PHE:CE1	0.71	1	1
A:386:ALA:HB1	A:388:MET:CE	0.71	1	1
A:369:ASP:CG	A:601:ILE:HG23	0.71	6	1
A:242:SER:HB2	A:388:MET:HE2	0.71	10	1
A:20:VAL:HG11	A:260:PHE:CZ	0.70	4	1
A:265:MET:HE1	A:348:ALA:CB	0.69	9	1
A:60:LEU:HD21	A:186:ILE:HG21	0.69	2	1
A:203:ILE:HD11	A:291:LEU:H	0.69	9	1
A:256:HIS:CG	A:273:VAL:HG13	0.69	2	1
A:70:LYS:HE2	A:75:GLU:HA	0.68	1	1
A:161:LEU:HD22	A:214:PHE:CZ	0.68	1	1
A:232:MET:HE2	A:244:GLY:HA2	0.67	1	1
A:19:MET:HE1	A:101:MET:HA	0.67	8	4
A:65:GLY:HA2	A:388:MET:SD	0.67	1	1
A:186:ILE:HD11	A:273:VAL:HG21	0.67	8	1
A:19:MET:HE3	A:68:GLY:HA3	0.66	8	2
A:42:TRP:CZ2	A:234:PHE:CD2	0.66	9	1
A:30:TRP:NE1	A:56:ILE:HD11	0.66	9	1
A:181:VAL:HG12	A:185:LYS:HE3	0.66	3	2
A:30:TRP:HE1	A:56:ILE:HD11	0.65	9	1
A:192:ALA:HA	A:197:ILE:HD12	0.65	2	1
A:370:VAL:HG11	A:374:LEU:HD21	0.65	8	1
A:1:MET:HE3	A:5:ILE:HG22	0.64	7	2
A:88:VAL:HA	A:96:MET:HE3	0.64	1	1
A:337:SER:HB3	A:339:VAL:HG23	0.64	8	1
A:307:THR:HG23	A:315:ASN:HD22	0.63	4	1
A:259:TYR:CE1	A:273:VAL:HG22	0.63	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:198:PHE:CG	A:214:PHE:CE1	0.63	10	1
A:40:THR:CG2	A:193:ILE:HG23	0.63	2	1
A:56:ILE:HG21	A:213:ILE:HG12	0.62	3	1
A:307:THR:CG2	A:315:ASN:HD22	0.62	4	1
A:98:LEU:HD22	A:187:LEU:O	0.62	8	1
A:34:THR:HG23	A:38:ILE:CD1	0.61	2	1
A:478:VAL:HG13	A:482:LEU:HD12	0.61	2	1
A:95:PRO:HD2	A:154:VAL:CG1	0.61	6	1
A:417:ILE:HD11	A:437:ALA:HB2	0.61	6	4
A:26:ALA:CA	A:297:PRO:HG3	0.61	1	1
A:16:LEU:HD21	A:258:ILE:HG21	0.60	2	1
A:37:PHE:CE1	A:48:LEU:HD23	0.60	2	1
A:186:ILE:HD11	A:301:LEU:HB2	0.60	10	1
A:60:LEU:CD2	A:186:ILE:HG21	0.59	2	1
A:42:TRP:CH2	A:234:PHE:CD2	0.59	9	1
A:38:ILE:HD11	A:56:ILE:CD1	0.59	2	1
A:95:PRO:CD	A:154:VAL:CG1	0.59	6	1
A:97:PHE:CE1	A:195:HIS:HB3	0.59	7	1
A:40:THR:HG1	A:42:TRP:CD1	0.59	2	1
A:37:PHE:CD1	A:48:LEU:HD23	0.58	2	1
A:6:LYS:NZ	A:339:VAL:HG22	0.58	8	1
A:219:ALA:HB1	A:296:SER:CB	0.58	5	1
A:86:MET:HE2	A:96:MET:SD	0.58	5	1
A:184:ALA:HB3	A:187:LEU:HD12	0.58	2	1
A:190:ASN:OD1	A:193:ILE:HD12	0.57	9	1
A:16:LEU:HD21	A:258:ILE:CG2	0.57	2	1
A:219:ALA:HB1	A:296:SER:HB2	0.57	5	1
A:343:ASP:O	A:347:ALA:HB3	0.57	1	2
A:28:ILE:HA	A:255:ILE:HD11	0.57	6	1
A:55:MET:HE1	A:246:ALA:HA	0.57	1	1
A:86:MET:O	A:90:VAL:HG23	0.57	4	1
A:357:ALA:HB1	A:362:ALA:O	0.57	9	2
A:95:PRO:CD	A:154:VAL:HG12	0.56	6	1
A:189:LEU:HD11	A:227:VAL:HG21	0.56	2	1
A:59:LEU:HD22	A:255:ILE:HD13	0.56	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:96:MET:SD	A:154:VAL:HG12	0.56	7	1
A:188:PHE:CZ	A:356:LYS:HE3	0.56	7	1
A:150:ILE:HG22	A:154:VAL:HG23	0.56	3	1
A:42:TRP:CH2	A:234:PHE:CE2	0.56	9	1
A:107:GLY:HA2	A:142:LEU:CD1	0.56	4	2
A:219:ALA:HB1	A:296:SER:H	0.55	5	1
A:233:PHE:HB2	A:234:PHE:CD2	0.55	9	1
A:219:ALA:HB1	A:224:GLY:HA3	0.55	10	1
A:40:THR:HG22	A:193:ILE:HG23	0.55	2	1
A:38:ILE:HD11	A:56:ILE:HD13	0.55	2	1
A:111:ILE:HD11	A:135:ALA:HA	0.55	3	1
A:239:ALA:HB2	A:265:MET:HE1	0.55	7	1
A:186:ILE:HD11	A:301:LEU:CB	0.54	10	1
A:64:ILE:HD12	A:97:PHE:CD1	0.54	2	1
A:243:ALA:HB1	A:246:ALA:O	0.54	10	1
A:459:THR:HG21	A:601:ILE:HG21	0.54	1	1
A:185:LYS:HE2	A:194:ASN:ND2	0.54	9	1
A:70:LYS:HE2	A:75:GLU:CA	0.54	1	1
A:71:LEU:HA	A:355:MET:HE1	0.53	2	1
A:87:GLY:HA3	A:96:MET:CE	0.53	10	1
A:14:ARG:HH21	A:264:LEU:HD22	0.53	9	1
A:88:VAL:HG11	A:99:GLY:HA3	0.53	7	3
A:90:VAL:HG23	A:91:GLY:O	0.53	5	1
A:16:LEU:HD23	A:97:PHE:CZ	0.53	3	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	635	610	20	5
2	635	603	25	7
3	635	595	31	9
4	635	603	23	9
5	635	596	29	10
6	635	608	18	9

Model ID	Analysed	Favored	Allowed	Outliers
7	635	611	17	7
8	635	614	16	5
9	635	603	21	11
10	635	595	29	11

*There are 59 unique backbone outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	367	ALA	6
A	485	SER	6
A	44	PRO	3
A	338	LYS	3
A	482	LEU	3
A	483	LYS	3
A	484	ASP	3
A	189	LEU	2
A	365	LEU	2
A	487	ASP	2
A	490	SER	2
A	21	MET	1
A	22	PRO	1
A	23	ASN	1
A	42	TRP	1
A	43	LEU	1
A	45	ASN	1
A	68	GLY	1
A	71	LEU	1
A	72	VAL	1
A	89	ILE	1
A	95	PRO	1
A	124	SER	1
A	185	LYS	1
A	199	SER	1
A	200	PRO	1
A	202	GLY	1
A	210	GLY	1

Chain	Res	Type	Models (Total)
A	213	ILE	1
A	215	PHE	1
A	217	ILE	1
A	218	GLU	1
A	220	ASN	1
A	241	GLN	1
A	253	GLY	1
A	296	SER	1
A	297	PRO	1
A	298	GLY	1
A	337	SER	1
A	339	VAL	1
A	340	LYS	1
A	341	GLU	1
A	343	ASP	1
A	360	LYS	1
A	361	GLY	1
A	362	ALA	1
A	363	SER	1
A	364	PRO	1
A	366	SER	1
A	369	ASP	1
A	370	VAL	1
A	373	ASP	1
A	386	ALA	1
A	389	GLY	1
A	480	ASP	1
A	481	SER	1
A	486	PHE	1
A	489	SER	1
A	492	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	506	488	11	7
2	506	485	12	9
3	506	478	14	14
4	506	490	7	9
5	506	480	13	13
6	506	487	12	7
7	506	494	9	3
8	506	497	7	2
9	506	491	11	4
10	506	492	8	6

There are 49 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	493	LEU	5
A	471	HIS	4
A	62	LEU	3
A	216	LEU	3
A	292	VAL	3
A	1	MET	2
A	24	ILE	2
A	30	TRP	2
A	43	LEU	2
A	48	LEU	2
A	60	LEU	2
A	189	LEU	2
A	198	PHE	2
A	213	ILE	2
A	220	ASN	2
A	343	ASP	2
A	480	ASP	2
A	34	THR	1
A	42	TRP	1
A	51	LEU	1
A	66	TYR	1
A	84	THR	1

Chain	Res	Type	Models (Total)
A	86	MET	1
A	90	VAL	1
A	93	ASP	1
A	94	MET	1
A	117	TRP	1
A	129	LEU	1
A	176	LEU	1
A	182	GLU	1
A	197	ILE	1
A	199	SER	1
A	201	LEU	1
A	207	HIS	1
A	214	PHE	1
A	215	PHE	1
A	252	LEU	1
A	260	PHE	1
A	363	SER	1
A	365	LEU	1
A	366	SER	1
A	370	VAL	1
A	388	MET	1
A	472	THR	1
A	481	SER	1
A	485	SER	1
A	487	ASP	1
A	601	ILE	1
A	608	THR	1

## Fit of model to data used for modeling ?

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

#### Restraint types

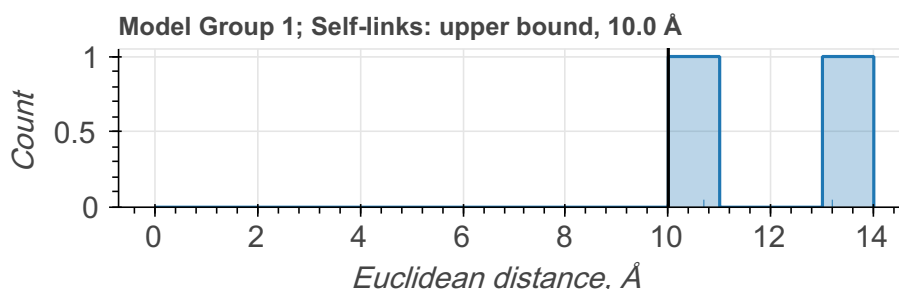
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 2 crosslinking restraints combined in 2 restraint groups.

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

#### 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.



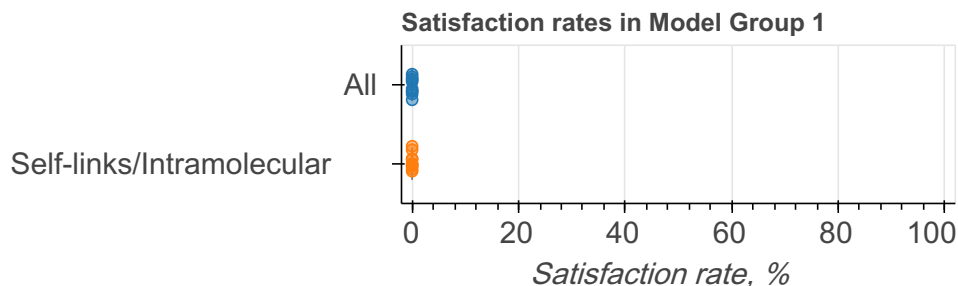
#### Satisfaction of restraints

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=2)
1	1	1	10/10	All	0.00	100.00	2
				Self-links/ Intramolecular	0.00	100.00	2

#### 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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