

# 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	9A39
PDB-Dev ID	PDBDEV_00000194
Structure Title	Model of E. coli LptD 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)*

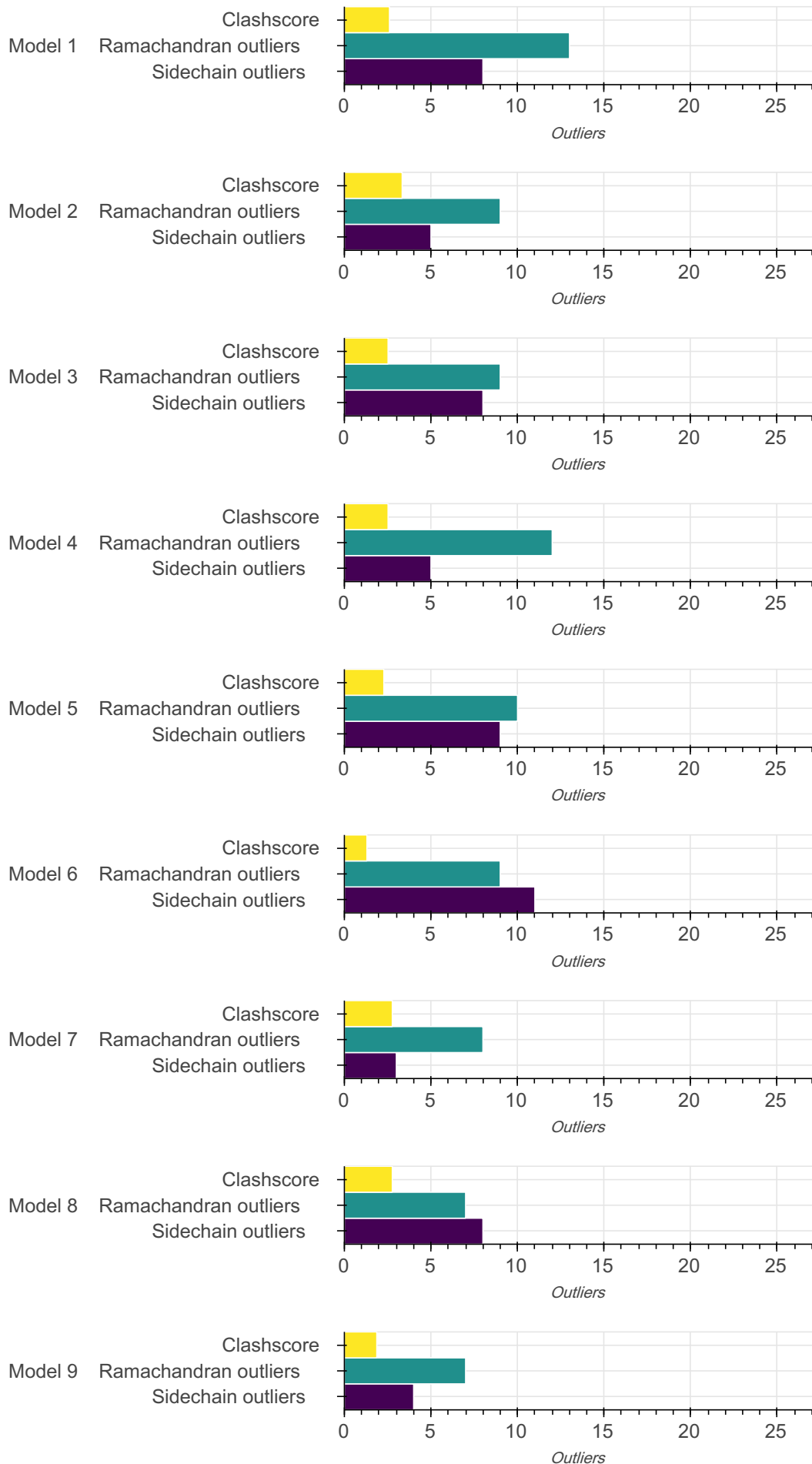
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

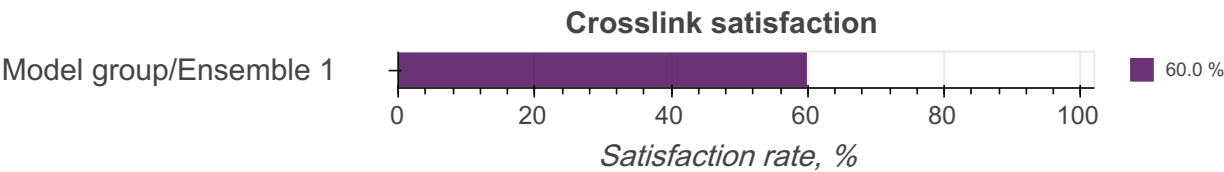
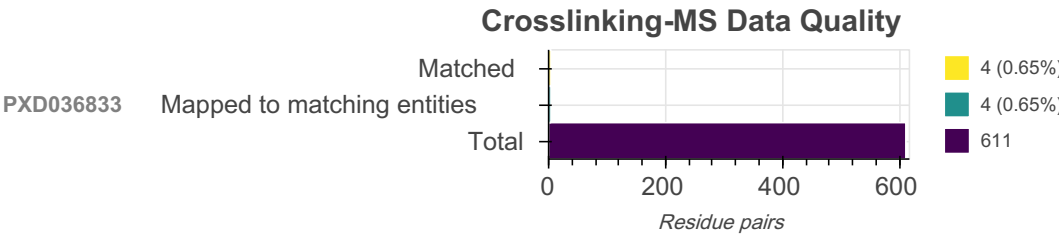
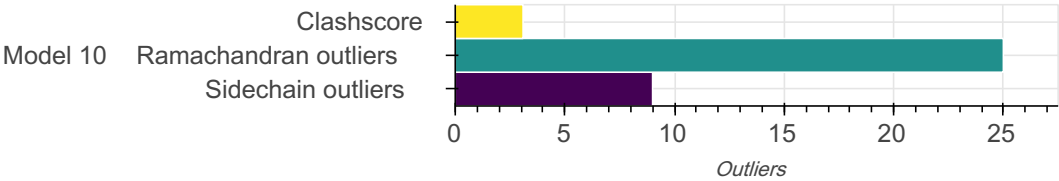
*List of references used to build this report is available [here](#).*

## 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	P31554	A	784	-	1-784	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	P31554	dbseq_P31554_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A39	5	5 (100.00%)	4 (80.00%)
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 no bond length outliers.*

#### Standard geometry: angle outliers ?

*There are 388 bond angle outliers in this entry (0.44% of 88470 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	423	ASP	CA-CB-CG	8.84	121.44	112.60	9	3
A	342	ASP	CA-CB-CG	7.81	120.41	112.60	5	1
A	545	THR	C-N-CA	7.52	135.23	121.70	1	1
A	267	ARG	CD-NE-CZ	7.50	134.90	124.40	1	1
A	581	GLN	OE1-CD-NE2	6.58	116.02	122.60	10	7
A	393	GLN	OE1-CD-NE2	6.57	116.03	122.60	1	7
A	552	ILE	C-N-CA	6.36	133.15	121.70	10	2
A	352	ASP	CA-CB-CG	6.35	118.95	112.60	2	1
A	413	GLN	OE1-CD-NE2	6.32	116.28	122.60	1	2
A	553	ALA	C-CA-CB	6.30	119.95	110.50	8	1
A	544	ARG	C-N-CA	6.30	133.04	121.70	1	1
A	548	GLY	C-N-CA	6.29	133.02	121.70	1	1
A	781	GLN	OE1-CD-NE2	6.19	116.41	122.60	7	7
A	350	SER	C-N-CA	6.16	132.79	121.70	1	1
A	764	ASN	C-N-CA	6.15	132.78	121.70	7	1
A	116	GLN	OE1-CD-NE2	6.08	116.52	122.60	2	6
A	712	GLN	OE1-CD-NE2	6.04	116.56	122.60	8	1
A	115	ASN	OD1-CG-ND2	6.03	116.57	122.60	3	5
A	41	PRO	C-N-CA	5.96	132.43	121.70	5	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	39	ASP	C-N-CA	5.84	132.22	121.70	5	1
A	460	GLN	OE1-CD-NE2	5.84	116.76	122.60	9	5
A	336	ASP	CA-CB-CG	5.78	106.82	112.60	7	2
A	384	ASN	OD1-CG-ND2	5.75	116.85	122.60	4	1
A	346	LYS	C-N-CA	5.73	132.02	121.70	4	1
A	550	ASP	CA-CB-CG	5.72	118.32	112.60	1	2
A	376	GLN	OE1-CD-NE2	5.72	116.88	122.60	6	9
A	38	TYR	C-N-CA	5.71	131.98	121.70	5	1
A	348	GLY	C-N-CA	5.68	131.92	121.70	10	1
A	367	ASN	OD1-CG-ND2	5.67	116.93	122.60	9	8
A	600	ASP	C-N-CA	5.64	131.86	121.70	3	1
A	764	ASN	OD1-CG-ND2	5.63	116.97	122.60	8	1
A	529	ASP	CA-CB-CG	5.57	118.17	112.60	5	3
A	232	ASN	OD1-CG-ND2	5.56	117.04	122.60	1	1
A	513	GLN	OE1-CD-NE2	5.54	117.06	122.60	8	1
A	770	GLN	OE1-CD-NE2	5.54	117.06	122.60	8	4
A	419	ASN	OD1-CG-ND2	5.49	117.11	122.60	6	2
A	344	ASP	CA-CB-CG	5.42	118.02	112.60	4	4
A	677	GLN	OE1-CD-NE2	5.38	117.22	122.60	4	2
A	764	ASN	CA-CB-CG	5.29	107.31	112.60	8	1
A	475	ASP	CA-CB-CG	5.28	117.88	112.60	8	1
A	44	GLN	OE1-CD-NE2	5.27	117.33	122.60	5	10
A	250	ASN	OD1-CG-ND2	5.26	117.34	122.60	2	4
A	6	PRO	CA-N-CD	5.24	104.66	112.00	5	1
A	459	GLN	OE1-CD-NE2	5.22	117.38	122.60	6	3
A	429	ARG	NE-CZ-NH2	5.15	123.83	119.20	8	2
A	39	ASP	N-CA-CB	5.14	101.76	110.50	5	1
A	256	ASP	CA-CB-CG	5.14	117.74	112.60	3	6
A	156	GLN	OE1-CD-NE2	5.09	117.51	122.60	1	5
A	267	ARG	NH1-CZ-NH2	5.08	112.69	119.30	7	1
A	217	GLN	OE1-CD-NE2	5.04	117.56	122.60	2	2
A	779	PRO	N-CA-CB	5.03	108.53	103.00	10	1
A	194	GLN	OE1-CD-NE2	4.95	117.65	122.60	7	6
A	400	GLN	OE1-CD-NE2	4.93	117.67	122.60	5	3
A	91	GLN	OE1-CD-NE2	4.93	117.67	122.60	10	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	601	ASP	CA-CB-CG	4.93	117.53	112.60	7	2
A	300	ASP	CA-CB-CG	4.92	117.52	112.60	4	3
A	111	HIS	CB-CG-CD2	4.90	124.83	131.20	5	1
A	500	LEU	C-N-CA	4.89	130.49	121.70	1	1
A	597	TRP	C-N-CA	4.88	130.49	121.70	1	1
A	549	LEU	C-N-CA	4.88	130.48	121.70	1	1
A	710	ASN	OD1-CG-ND2	4.87	117.73	122.60	2	8
A	484	GLN	OE1-CD-NE2	4.84	117.76	122.60	8	4
A	506	GLN	OE1-CD-NE2	4.82	117.78	122.60	8	4
A	586	THR	C-N-CA	4.82	130.37	121.70	8	1
A	146	GLN	OE1-CD-NE2	4.80	117.80	122.60	6	7
A	145	ARG	C-N-CA	4.78	130.31	121.70	1	1
A	189	HIS	CB-CG-CD2	4.76	125.01	131.20	3	2
A	557	GLN	OE1-CD-NE2	4.76	117.84	122.60	1	5
A	720	GLN	OE1-CD-NE2	4.70	117.90	122.60	6	3
A	97	GLN	OE1-CD-NE2	4.70	117.90	122.60	7	10
A	166	ASP	CA-CB-CG	4.69	117.29	112.60	4	8
A	88	GLN	OE1-CD-NE2	4.69	117.91	122.60	5	7
A	141	GLN	OE1-CD-NE2	4.63	117.97	122.60	10	2
A	267	ARG	NE-CZ-NH2	4.60	123.34	119.20	9	1
A	384	ASN	CA-CB-CG	4.60	117.20	112.60	4	1
A	20	GLN	OE1-CD-NE2	4.58	118.02	122.60	7	6
A	383	GLN	OE1-CD-NE2	4.57	118.03	122.60	9	8
A	267	ARG	NE-CZ-NH1	4.57	126.07	121.50	3	2
A	39	ASP	CA-CB-CG	4.56	117.16	112.60	5	1
A	281	GLN	OE1-CD-NE2	4.56	118.04	122.60	9	7
A	419	ASN	CA-CB-CG	4.55	108.05	112.60	5	1
A	40	ARG	NE-CZ-NH1	4.55	126.05	121.50	4	1
A	653	GLN	OE1-CD-NE2	4.54	118.06	122.60	8	2
A	148	ARG	NE-CZ-NH2	4.53	123.27	119.20	5	1
A	347	TYR	C-N-CA	4.52	129.83	121.70	5	1
A	349	SER	N-CA-C	4.51	123.62	111.00	10	1
A	115	ASN	CA-CB-CG	4.49	117.09	112.60	3	1
A	646	ARG	C-N-CA	4.48	129.77	121.70	8	3
A	627	GLN	OE1-CD-NE2	4.48	118.12	122.60	2	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	778	LEU	CA-C-N	4.47	123.61	116.90	10	1
A	518	PRO	C-N-CA	4.47	129.74	121.70	10	1
A	781	GLN	C-N-CA	4.46	129.73	121.70	6	1
A	437	ASN	OD1-CG-ND2	4.46	118.14	122.60	6	1
A	534	GLN	OE1-CD-NE2	4.45	118.15	122.60	1	1
A	37	SER	C-N-CA	4.44	129.70	121.70	5	1
A	366	GLN	C-N-CA	4.43	129.68	121.70	3	1
A	598	GLU	C-N-CA	4.43	129.68	121.70	1	1
A	366	GLN	OE1-CD-NE2	4.43	118.17	122.60	3	3
A	576	ASN	OD1-CG-ND2	4.43	118.17	122.60	5	4
A	665	GLN	OE1-CD-NE2	4.43	118.17	122.60	10	5

### 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	2.60	32
2	3.34	41
3	2.52	31
4	2.52	31
5	2.28	28
6	1.30	16
7	2.77	34
8	2.77	34
9	1.87	23
10	3.09	38

There are 308 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:700:VAL:HG21	A:773:LEU:CD1	0.97	4	1
A:461:THR:HG22	A:473:LYS:HE3	0.88	6	1
A:700:VAL:HG21	A:773:LEU:HD11	0.84	4	1
A:584:TYR:CE1	A:606:LEU:HD12	0.83	3	2
A:533:LEU:HD13	A:550:ASP:H	0.82	1	1
A:700:VAL:HG21	A:773:LEU:HD13	0.80	4	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:234:LYS:HE2	A:751:ALA:HB1	0.79	7	5
A:581:GLN:HE21	A:606:LEU:HD22	0.76	10	2
A:27:LEU:HB3	A:696:ARG:HH12	0.75	8	1
A:472:THR:HG21	A:523:SER:HB2	0.69	3	3
A:700:VAL:HG23	A:773:LEU:HD21	0.68	3	2
A:419:ASN:HD22	A:424:MET:HB3	0.67	2	1
A:474:LEU:HD13	A:526:TYR:CE1	0.67	1	1
A:482:MET:HE3	A:517:VAL:HG22	0.67	1	1
A:700:VAL:HG11	A:773:LEU:HD13	0.67	5	1
A:553:ALA:HB2	A:590:THR:HG23	0.66	5	1
A:474:LEU:HD13	A:526:TYR:CE2	0.65	10	1
A:530:SER:HA	A:533:LEU:HD12	0.65	1	1
A:406:PHE:CZ	A:408:THR:HG23	0.64	1	1
A:664:ILE:HG23	A:668:LEU:HD12	0.64	8	2
A:584:TYR:CZ	A:606:LEU:HD12	0.64	3	1
A:375:LYS:HE2	A:377:PHE:CZ	0.64	5	6
A:355:ALA:HB2	A:380:PHE:CE2	0.64	2	1
A:413:GLN:NE2	A:549:LEU:HD12	0.63	4	2
A:195:VAL:HG13	A:225:ARG:CZ	0.63	3	1
A:189:HIS:CD2	A:220:VAL:HG21	0.63	3	2
A:236:THR:HG22	A:751:ALA:HB2	0.62	2	2
A:590:THR:HG21	A:597:TRP:CD1	0.62	8	1
A:688:VAL:HG11	A:777:ILE:HG23	0.62	10	1
A:664:ILE:HG21	A:678:TYR:HB3	0.62	8	1
A:267:ARG:HH22	A:342:ASP:HB3	0.62	5	1
A:465:TRP:CZ2	A:469:ARG:CZ	0.61	9	2
A:75:ILE:HD11	A:87:VAL:HG11	0.61	2	6
A:461:THR:HG22	A:473:LYS:CE	0.61	6	1
A:341:ASN:OD1	A:351:THR:HG22	0.60	1	1
A:466:TYR:CE1	A:474:LEU:HD11	0.60	10	1
A:355:ALA:HB2	A:380:PHE:CZ	0.59	2	1
A:533:LEU:HD22	A:550:ASP:CB	0.58	1	1
A:688:VAL:HG11	A:777:ILE:CG2	0.58	10	1
A:733:GLU:HG2	A:751:ALA:HB3	0.58	7	1
A:326:ARG:NH1	A:364:ALA:HB3	0.57	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:195:VAL:HG11	A:225:ARG:NE	0.57	8	1
A:422:ASP:HA	A:466:TYR:CE1	0.56	6	1
A:298:TYR:CD1	A:310:ARG:HD2	0.56	5	1
A:480:ARG:CZ	A:525:ILE:HD12	0.56	3	1
A:546:TYR:CE2	A:553:ALA:HB2	0.56	4	1
A:352:ASP:HB2	A:354:TYR:CE2	0.56	2	1
A:267:ARG:HH22	A:342:ASP:CB	0.55	5	1
A:474:LEU:HD13	A:526:TYR:HE2	0.55	10	1
A:354:TYR:CE1	A:379:VAL:HG13	0.55	4	1
A:415:VAL:HG21	A:429:ARG:HH21	0.55	3	2
A:733:GLU:CG	A:751:ALA:HB3	0.55	7	2
A:42:LEU:HD23	A:115:ASN:HD22	0.54	3	1
A:406:PHE:CE2	A:408:THR:HG23	0.54	1	2
A:27:LEU:CB	A:696:ARG:HH12	0.54	8	1
A:664:ILE:HD12	A:681:GLY:HA2	0.53	3	5
A:142:MET:HE3	A:189:HIS:CG	0.53	9	1
A:581:GLN:HE21	A:606:LEU:CD2	0.53	10	1
A:501:ALA:HB1	A:502:PRO:HD2	0.53	10	1
A:28:ALA:HB1	A:32:MET:HE2	0.53	10	1
A:123:LYS:HE3	A:136:TRP:CG	0.53	10	2
A:352:ASP:CB	A:354:TYR:CE2	0.53	2	1
A:375:LYS:HE2	A:377:PHE:CE2	0.53	4	1
A:379:VAL:HG21	A:387:SER:HB3	0.53	8	1
A:419:ASN:ND2	A:424:MET:HB3	0.53	2	1
A:584:TYR:CD1	A:606:LEU:HD12	0.53	7	2
A:533:LEU:CD1	A:550:ASP:H	0.52	1	1
A:454:LEU:HD13	A:552:ILE:CD1	0.52	3	1
A:711:LYS:HE2	A:739:TRP:CZ3	0.52	2	1
A:653:GLN:HE22	A:781:GLN:NE2	0.52	3	2
A:87:VAL:HG13	A:104:VAL:HG13	0.52	10	1
A:423:ASP:HA	A:465:TRP:CZ3	0.52	7	1
A:454:LEU:HD13	A:552:ILE:HD13	0.51	6	3
A:117:VAL:HG11	A:156:GLN:NE2	0.51	6	2
A:465:TRP:CE2	A:469:ARG:NH2	0.51	10	2
A:423:ASP:HB3	A:465:TRP:CE2	0.51	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:153:LEU:HD21	A:155:LYS:HE3	0.51	2	2
A:142:MET:HE3	A:189:HIS:CE1	0.51	5	1
A:665:GLN:HA	A:673:SER:HB2	0.51	8	1
A:119:LEU:HD11	A:156:GLN:HE21	0.51	10	1
A:224:ARG:HB2	A:248:TYR:CE2	0.51	4	1
A:375:LYS:CE	A:377:PHE:CE2	0.51	4	1
A:376:GLN:HE21	A:391:GLU:CD	0.51	6	2
A:632:LEU:HD22	A:662:GLU:HB2	0.51	5	1
A:700:VAL:CG2	A:773:LEU:HD21	0.50	2	2
A:423:ASP:HB3	A:465:TRP:CZ2	0.50	9	1
A:140:TYR:CE1	A:165:LEU:HD13	0.50	6	8
A:145:ARG:HH22	A:194:GLN:NE2	0.50	2	1
A:251:ILE:HG21	A:255:MET:HE3	0.50	9	1
A:530:SER:HA	A:533:LEU:CD1	0.50	1	1
A:419:ASN:HD22	A:424:MET:CB	0.50	2	1
A:312:LEU:HB2	A:339:TYR:CZ	0.50	4	1
A:700:VAL:CG2	A:773:LEU:HD11	0.50	4	1
A:482:MET:CE	A:552:ILE:HD12	0.50	4	1
A:530:SER:HA	A:533:LEU:HG	0.49	1	1
A:700:VAL:CG2	A:777:ILE:HD11	0.49	1	1
A:230:ILE:HG21	A:756:ILE:O	0.49	9	1
A:350:SER:C	A:352:ASP:H	0.49	10	1
A:43:VAL:HG11	A:50:LEU:HD11	0.49	6	1
A:423:ASP:C	A:465:TRP:CZ2	0.49	2	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	782	737	32	13
2	782	747	26	9
3	782	741	32	9
4	782	741	29	12
5	782	739	33	10
6	782	739	34	9
7	782	738	36	8

Model ID	Analysed	Favored	Allowed	Outliers
8	782	733	42	7
9	782	738	37	7
10	782	716	41	25

*There are 66 unique backbone outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	37	SER	5
A	39	ASP	5
A	42	LEU	4
A	349	SER	4
A	601	ASP	4
A	765	TYR	4
A	591	GLY	3
A	599	ASN	3
A	713	ALA	3
A	767	LEU	3
A	3	LYS	2
A	33	LEU	2
A	146	GLN	2
A	178	ASP	2
A	344	ASP	2
A	345	ASN	2
A	351	THR	2
A	422	ASP	2
A	469	ARG	2
A	549	LEU	2
A	550	ASP	2
A	553	ALA	2
A	554	SER	2
A	597	TRP	2
A	766	GLY	2
A	4	ARG	1
A	6	PRO	1
A	34	GLY	1
A	35	VAL	1

Chain	Res	Type	Models (Total)
A	41	PRO	1
A	45	GLY	1
A	47	THR	1
A	48	ASN	1
A	166	ASP	1
A	240	TYR	1
A	294	SER	1
A	346	LYS	1
A	347	TYR	1
A	348	GLY	1
A	350	SER	1
A	352	ASP	1
A	353	GLY	1
A	366	GLN	1
A	382	GLU	1
A	423	ASP	1
A	473	LYS	1
A	478	VAL	1
A	501	ALA	1
A	519	TYR	1
A	521	ASP	1
A	526	TYR	1
A	531	SER	1
A	537	TYR	1
A	540	LEU	1
A	545	THR	1
A	556	ASN	1
A	590	THR	1
A	593	ASP	1
A	596	THR	1
A	598	GLU	1
A	602	LYS	1
A	603	THR	1
A	764	ASN	1
A	779	PRO	1

Chain	Res	Type	Models (Total)
A	781	GLN	1
A	782	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	681	656	17	8
2	681	655	21	5
3	681	657	16	8
4	681	653	23	5
5	681	652	20	9
6	681	657	13	11
7	681	661	17	3
8	681	657	16	8
9	681	657	20	4
10	681	654	18	9

*There are 43 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	9	LEU	10
A	15	THR	4
A	769	THR	4
A	27	LEU	3
A	148	ARG	3
A	600	ASP	3
A	8	LEU	2
A	38	TYR	2
A	374	THR	2
A	472	THR	2
A	532	LEU	2
A	783	THR	2
A	7	THR	1
A	11	THR	1
A	18	TYR	1
A	33	LEU	1

Chain	Res	Type	Models (Total)
A	237	THR	1
A	240	TYR	1
A	244	TYR	1
A	265	HIS	1
A	294	SER	1
A	385	THR	1
A	387	SER	1
A	408	THR	1
A	453	LEU	1
A	511	ARG	1
A	531	SER	1
A	535	SER	1
A	538	SER	1
A	540	LEU	1
A	545	THR	1
A	550	ASP	1
A	554	SER	1
A	578	SER	1
A	590	THR	1
A	603	THR	1
A	630	THR	1
A	651	LEU	1
A	660	SER	1
A	671	TYR	1
A	700	VAL	1
A	771	GLU	1
A	775	SER	1

## Fit of model to data used for modeling ?

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

#### Restraint types

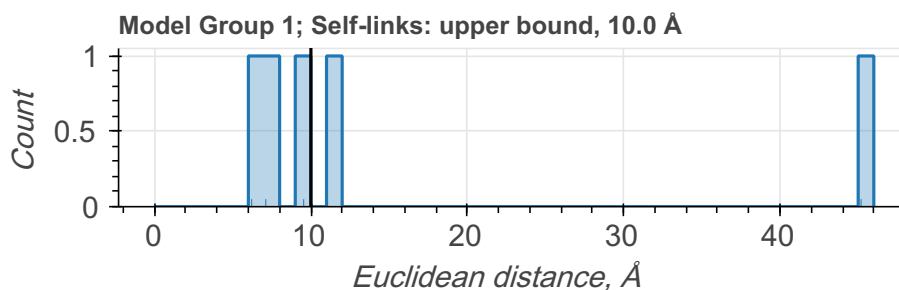
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

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	GLU	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	TYR	CA	upper bound	10.0	2
L-Photo-Leucine	ASP	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

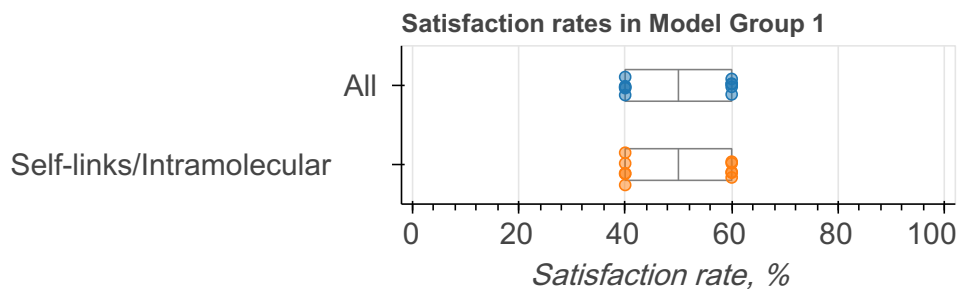
Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=5)
1	1	1	10/10	All	60.00	40.00	5
				Self-links/ Intramolecular	60.00	40.00	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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