

# Integrative Structure Validation Report ?

February 18, 2025 - 08:37 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	9A3C
PDB-Dev ID	PDBDEV_00000197
Structure Title	Model of E. coli Fiu 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)*

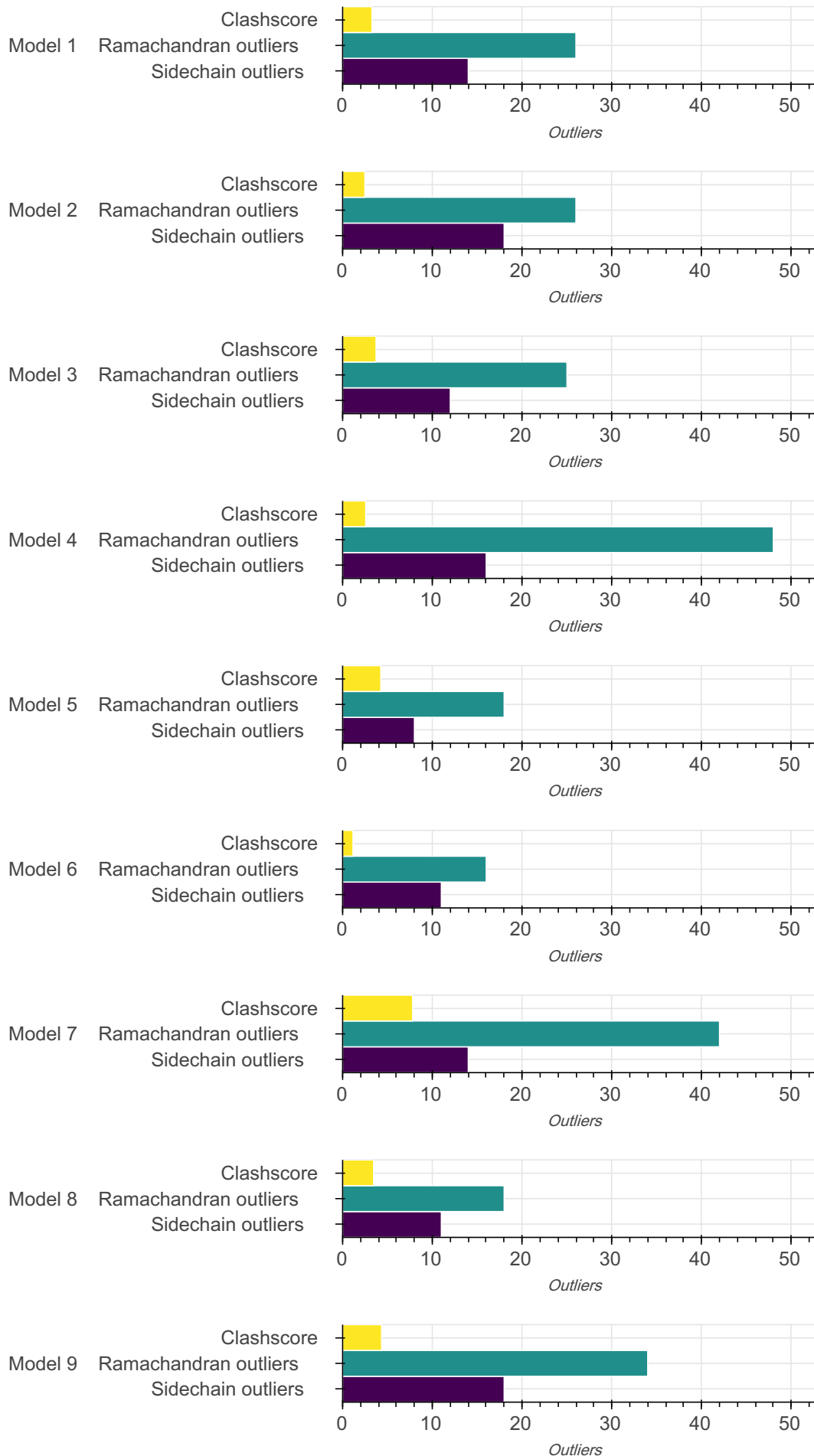
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

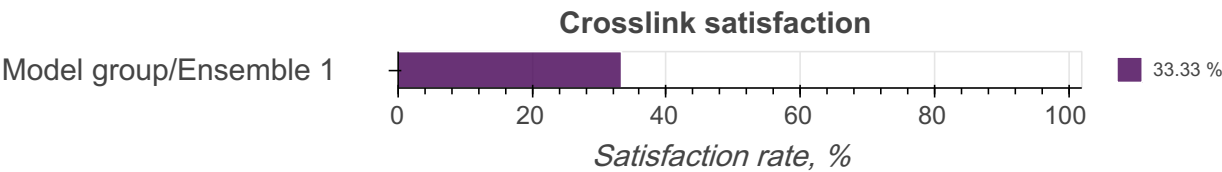
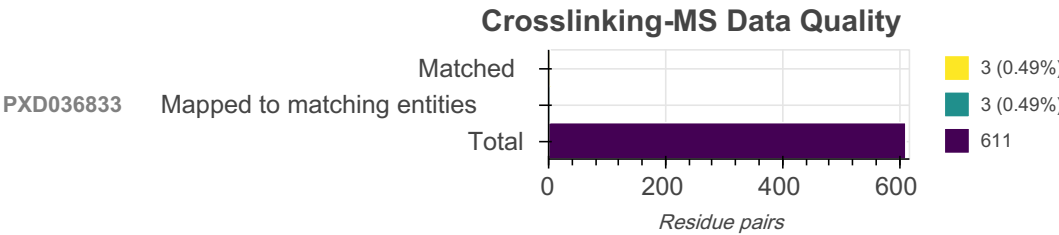
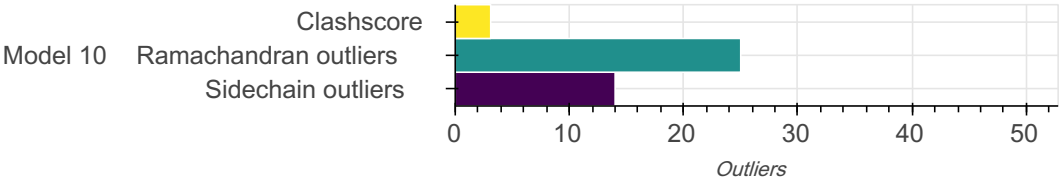
*List of references used to build this report is available [here](#).*

## 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	P75780	A	760	-	1-760	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	P75780	dbseq_P75780_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A3C	3	3 (100.00%)	3 (100.00%)
PXD036833	611	3 (0.49%)	3 (0.49%)

### 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 1 bond length outliers in this entry (0.00% of 59030 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	558	ARG	CZ-NH2	4.09	1.28	1.33	3	1

#### Standard geometry: angle outliers ?

There are 488 bond angle outliers in this entry (0.61% of 80420 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	746	PRO	CA-N-CD	8.59	99.98	112.00	7	1
A	25	ILE	C-N-CA	7.33	134.90	121.70	6	3
A	108	GLU	C-N-CA	6.76	133.86	121.70	10	2
A	38	THR	C-N-CA	6.71	133.79	121.70	9	1
A	555	SER	C-N-CA	6.62	133.62	121.70	2	1
A	607	GLN	OE1-CD-NE2	6.52	116.08	122.60	7	4
A	692	ASP	CA-CB-CG	6.51	119.11	112.60	1	2
A	125	THR	CA-CB-OG1	6.50	119.35	109.60	10	1
A	149	GLN	OE1-CD-NE2	6.46	116.14	122.60	9	10
A	294	ASN	OD1-CG-ND2	6.46	116.14	122.60	9	4
A	16	THR	C-N-CA	6.30	133.05	121.70	9	5
A	107	GLY	C-N-CA	6.30	133.04	121.70	7	1
A	3	ASN	C-N-CA	6.25	132.94	121.70	1	2
A	600	ASN	OD1-CG-ND2	6.24	116.36	122.60	3	6
A	93	ASP	CA-CB-CG	6.19	118.79	112.60	2	7
A	282	ALA	C-CA-CB	6.11	119.67	110.50	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	17	PHE	C-N-CA	6.06	132.61	121.70	5	2
A	178	ARG	NE-CZ-NH2	6.05	124.65	119.20	10	1
A	378	GLN	OE1-CD-NE2	6.03	116.57	122.60	2	5
A	110	GLY	C-N-CA	5.93	132.37	121.70	6	1
A	303	ASP	CA-CB-CG	5.90	118.50	112.60	3	1
A	86	GLN	OE1-CD-NE2	5.90	116.70	122.60	5	8
A	405	GLN	OE1-CD-NE2	5.86	116.74	122.60	8	8
A	111	ASN	C-N-CA	5.84	132.22	121.70	7	1
A	549	GLN	OE1-CD-NE2	5.81	116.79	122.60	10	5
A	600	ASN	CA-CB-CG	5.80	118.40	112.60	1	1
A	225	ARG	NE-CZ-NH2	5.72	124.34	119.20	4	1
A	743	ARG	C-N-CA	5.69	131.94	121.70	4	1
A	301	ASP	CA-CB-CG	5.68	118.28	112.60	6	1
A	27	PRO	CA-N-CD	5.64	104.10	112.00	8	1
A	58	GLN	OE1-CD-NE2	5.64	116.96	122.60	5	9
A	225	ARG	C-N-CA	5.62	131.82	121.70	10	1
A	15	LEU	C-N-CA	5.60	131.77	121.70	9	2
A	230	ASN	OD1-CG-ND2	5.58	117.02	122.60	3	2
A	732	ASP	CA-CB-CG	5.56	118.16	112.60	4	1
A	636	GLN	OE1-CD-NE2	5.56	117.04	122.60	5	10
A	576	GLN	OE1-CD-NE2	5.54	117.06	122.60	10	5
A	538	GLN	OE1-CD-NE2	5.50	117.10	122.60	5	7
A	602	ASP	CA-CB-CG	5.50	107.10	112.60	1	1
A	348	ASN	OD1-CG-ND2	5.45	117.15	122.60	5	2
A	140	VAL	CA-CB-CG1	5.43	119.63	110.40	9	1
A	34	ALA	C-N-CA	5.42	131.46	121.70	7	3
A	542	GLY	C-N-CA	5.40	131.41	121.70	3	2
A	57	GLN	OE1-CD-NE2	5.37	117.23	122.60	1	5
A	369	ASP	CA-CB-CG	5.36	117.96	112.60	6	3
A	106	ALA	C-CA-CB	5.33	118.50	110.50	5	1
A	745	HIS	CB-CG-CD2	5.33	124.27	131.20	6	3
A	649	GLN	OE1-CD-NE2	5.33	117.27	122.60	3	8
A	603	GLY	C-N-CA	5.31	131.26	121.70	9	1
A	1	MET	C-N-CA	5.30	131.24	121.70	1	6
A	160	ASP	CA-CB-CG	5.28	107.32	112.60	7	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	52	SER	C-N-CA	5.28	131.20	121.70	7	2
A	670	GLN	OE1-CD-NE2	5.27	117.33	122.60	3	10
A	561	PHE	CA-CB-CG	5.25	119.05	113.80	6	1
A	35	GLU	O-C-N	5.23	114.62	123.00	9	2
A	63	LYS	C-N-CA	5.23	131.11	121.70	9	1
A	135	ARG	NE-CZ-NH2	5.22	123.89	119.20	9	2
A	25	ILE	CA-C-N	5.18	126.55	116.20	6	1
A	411	ASN	OD1-CG-ND2	5.15	117.45	122.60	3	3
A	53	LEU	N-CA-CB	5.14	101.77	110.50	7	1
A	738	ASN	C-N-CA	5.13	130.93	121.70	9	1
A	434	ARG	CD-NE-CZ	5.12	131.56	124.40	9	1
A	722	GLN	OE1-CD-NE2	5.09	117.51	122.60	8	2
A	136	ASP	CA-CB-CG	5.07	107.53	112.60	3	1
A	350	THR	C-N-CA	5.04	130.77	121.70	6	1
A	599	GLN	OE1-CD-NE2	5.02	117.58	122.60	3	7
A	293	HIS	CB-CG-CD2	5.01	124.68	131.20	9	3
A	12	PHE	C-N-CA	5.00	130.69	121.70	9	1
A	20	GLY	C-N-CA	4.99	130.68	121.70	8	3
A	42	ASP	C-N-CA	4.98	130.67	121.70	7	1
A	649	GLN	N-CA-C	4.95	124.85	111.00	9	1
A	402	ARG	CD-NE-CZ	4.94	131.32	124.40	9	6
A	41	ASP	C-N-CA	4.94	130.59	121.70	2	2
A	544	ASN	OD1-CG-ND2	4.94	117.66	122.60	10	2
A	598	GLU	CA-CB-CG	4.93	123.96	114.10	3	1
A	44	LEU	C-N-CA	4.91	130.55	121.70	10	2
A	649	GLN	CA-C-N	4.91	126.02	116.20	9	1
A	600	ASN	C-N-CA	4.90	130.53	121.70	1	1
A	455	GLN	OE1-CD-NE2	4.90	117.70	122.60	9	5
A	554	ASN	OD1-CG-ND2	4.90	117.70	122.60	7	2
A	142	ARG	NE-CZ-NH2	4.89	123.60	119.20	2	2
A	353	THR	C-N-CA	4.88	130.48	121.70	7	1
A	746	PRO	C-N-CA	4.87	112.94	121.70	7	1
A	37	GLN	OE1-CD-NE2	4.85	117.75	122.60	1	10
A	537	GLN	OE1-CD-NE2	4.84	117.76	122.60	6	10
A	442	GLN	OE1-CD-NE2	4.83	117.77	122.60	9	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	40	ALA	C-N-CA	4.83	130.39	121.70	2	1
A	111	ASN	CA-CB-CG	4.80	117.40	112.60	1	3
A	558	ARG	C-N-CA	4.78	130.30	121.70	8	1
A	514	ASN	OD1-CG-ND2	4.78	117.82	122.60	7	5
A	27	PRO	C-N-CA	4.77	130.29	121.70	2	2
A	668	GLN	OE1-CD-NE2	4.77	117.83	122.60	5	4
A	595	ASN	CA-CB-CG	4.75	117.35	112.60	5	3
A	601	ASP	C-CA-CB	4.75	119.12	110.10	1	1
A	176	GLN	OE1-CD-NE2	4.74	117.86	122.60	5	6
A	564	GLN	OE1-CD-NE2	4.71	117.89	122.60	9	2
A	123	ALA	C-CA-CB	4.71	117.56	110.50	7	2
A	623	ASN	CA-CB-CG	4.70	117.30	112.60	2	2
A	336	ASP	CA-CB-CG	4.70	117.30	112.60	8	1
A	258	GLN	OE1-CD-NE2	4.69	117.91	122.60	4	8

### 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	3.28	37
2	2.48	28
3	3.72	42
4	2.57	29
5	4.26	48
6	1.15	13
7	7.80	88
8	3.46	39
9	4.35	49
10	3.10	35

There are 408 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:611:LYS:HE3	A:655:LEU:HD11	0.90	8	1
A:512:LEU:HD11	A:539:PRO:HD3	0.90	7	1
A:123:ALA:HB2	A:167:THR:HG21	0.87	9	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:701:THR:HG21	A:745:HIS:CE1	0.86	4	1
A:68:VAL:HG22	A:75:MET:HE3	0.80	5	1
A:140:VAL:HG12	A:333:VAL:HG11	0.79	10	1
A:156:PRO:HG3	A:534:ALA:HB3	0.78	1	1
A:225:ARG:CZ	A:737:ILE:HG23	0.78	2	1
A:156:PRO:CG	A:534:ALA:HB3	0.77	1	3
A:140:VAL:HG22	A:333:VAL:CG2	0.77	9	1
A:140:VAL:HG22	A:333:VAL:HG23	0.76	9	1
A:137:ILE:HD12	A:333:VAL:HG23	0.75	1	1
A:140:VAL:CG1	A:333:VAL:HG11	0.75	10	1
A:689:LYS:HE2	A:701:THR:HG22	0.74	4	1
A:145:PHE:CD1	A:216:MET:HE2	0.74	7	1
A:161:TYR:CD1	A:451:PHE:CE1	0.73	7	1
A:54:TYR:CE1	A:631:ILE:HD11	0.73	8	1
A:547:LEU:HD13	A:605:TYR:CZ	0.73	8	1
A:60:ALA:HB1	A:313:ARG:NH1	0.72	10	1
A:54:TYR:HE1	A:631:ILE:HD11	0.72	8	1
A:137:ILE:CD1	A:333:VAL:HG23	0.71	1	1
A:159:THR:HG22	A:451:PHE:CE1	0.71	3	1
A:161:TYR:CE1	A:451:PHE:CD1	0.70	7	1
A:598:GLU:HB3	A:608:TYR:CE1	0.70	3	1
A:489:ILE:HD13	A:503:THR:HG21	0.69	2	1
A:123:ALA:HB3	A:167:THR:CG2	0.69	10	2
A:547:LEU:HD13	A:605:TYR:CE1	0.69	8	1
A:156:PRO:CB	A:534:ALA:HB3	0.68	5	1
A:112:SER:HA	A:140:VAL:HG22	0.67	4	1
A:161:TYR:CD1	A:451:PHE:CZ	0.67	7	1
A:116:ASP:O	A:140:VAL:HG21	0.67	8	1
A:72:THR:HG22	A:520:LEU:HD22	0.67	9	1
A:114:THR:HG21	A:261:THR:HG21	0.67	2	1
A:282:ALA:HB1	A:290:VAL:HG13	0.66	2	1
A:145:PHE:CE1	A:216:MET:HE2	0.66	7	1
A:547:LEU:HD22	A:605:TYR:OH	0.66	8	1
A:131:ILE:HG23	A:659:PRO:HD2	0.66	5	1
A:156:PRO:HB2	A:534:ALA:HB3	0.66	7	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:72:THR:HG21	A:463:ASN:HD21	0.65	10	1
A:269:ILE:HD12	A:361:TRP:CZ3	0.65	8	1
A:156:PRO:HG2	A:534:ALA:HB3	0.65	3	2
A:68:VAL:HG22	A:75:MET:CE	0.65	4	2
A:611:LYS:HE3	A:655:LEU:CD1	0.64	8	1
A:53:LEU:HD21	A:245:THR:HA	0.64	7	1
A:125:THR:HG22	A:167:THR:OG1	0.64	7	1
A:92:THR:HG23	A:103:ALA:HB1	0.64	3	1
A:140:VAL:HG13	A:307:THR:HG23	0.63	9	1
A:512:LEU:CD1	A:539:PRO:HD3	0.63	7	1
A:689:LYS:CE	A:701:THR:HG22	0.63	4	1
A:54:TYR:CE2	A:82:VAL:HG22	0.63	5	1
A:541:GLY:HA2	A:545:PHE:CE1	0.62	7	1
A:512:LEU:HD11	A:539:PRO:CD	0.62	7	1
A:363:ARG:HH11	A:418:VAL:HG11	0.62	5	1
A:598:GLU:CB	A:608:TYR:CE1	0.62	3	1
A:405:GLN:CD	A:549:GLN:HE22	0.61	2	1
A:489:ILE:CD1	A:503:THR:HG21	0.61	2	1
A:159:THR:HG21	A:516:LYS:HD3	0.61	3	1
A:606:SER:HB3	A:608:TYR:CE2	0.61	4	1
A:108:GLU:OE2	A:339:MET:HE1	0.61	7	1
A:166:PRO:CB	A:566:ALA:HB3	0.61	5	1
A:228:VAL:HG22	A:262:PRO:HA	0.61	9	1
A:602:ASP:CG	A:741:GLY:HA3	0.60	1	1
A:602:ASP:OD2	A:741:GLY:HA3	0.60	1	1
A:282:ALA:CB	A:290:VAL:HG13	0.60	2	1
A:706:VAL:HG22	A:733:TYR:CZ	0.60	7	1
A:53:LEU:HD11	A:245:THR:HG22	0.59	7	1
A:363:ARG:HH21	A:415:LEU:HD13	0.59	8	1
A:548:ALA:HB2	A:605:TYR:OH	0.59	7	1
A:439:ALA:HB1	A:546:ALA:HB1	0.59	3	1
A:156:PRO:HB3	A:568:THR:HB	0.58	7	1
A:78:ILE:HD11	A:98:VAL:CG2	0.58	5	2
A:332:ARG:CZ	A:334:LYS:HE3	0.58	7	2
A:439:ALA:CB	A:546:ALA:HB1	0.58	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:606:SER:CB	A:608:TYR:CE2	0.58	4	1
A:123:ALA:HB3	A:167:THR:HG21	0.58	10	2
A:140:VAL:HB	A:333:VAL:HG21	0.58	10	1
A:271:LEU:HD22	A:359:TRP:CZ3	0.58	9	1
A:159:THR:HG21	A:516:LYS:CD	0.57	3	1
A:749:PRO:O	A:751:THR:HG23	0.57	7	1
A:581:ARG:HH22	A:625:THR:CA	0.57	9	1
A:145:PHE:CG	A:216:MET:HE2	0.57	7	1
A:160:ASP:O	A:161:TYR:CD1	0.57	7	1
A:113:THR:HG22	A:368:LYS:HZ2	0.57	7	1
A:133:GLY:HA2	A:161:TYR:CD1	0.57	3	1
A:166:PRO:HB3	A:566:ALA:HB3	0.57	5	1
A:226:ASP:HB2	A:228:VAL:HG23	0.57	9	1
A:641:ILE:HD11	A:655:LEU:HD23	0.57	8	1
A:414:THR:CG2	A:433:THR:HG23	0.57	1	1
A:134:ILE:HB	A:329:ARG:HH11	0.56	3	2
A:342:ILE:HD13	A:361:TRP:CE3	0.56	8	2
A:417:ALA:H	A:431:GLY:HA2	0.56	3	1
A:604:THR:HG21	A:646:ASP:HB2	0.55	1	1
A:414:THR:HG23	A:433:THR:HG23	0.55	1	1
A:548:ALA:HB2	A:561:PHE:HZ	0.55	1	1
A:688:HIS:CD2	A:690:GLY:H	0.55	7	1
A:145:PHE:CD1	A:216:MET:SD	0.55	3	1
A:68:VAL:HG22	A:75:MET:HE2	0.55	4	1
A:54:TYR:CZ	A:82:VAL:HG22	0.55	5	1
A:295:PHE:CE1	A:420:ILE:HG22	0.55	8	1
A:441:GLY:HA3	A:545:PHE:CD1	0.55	8	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	758	676	56	26
2	758	682	50	26
3	758	668	65	25
4	758	666	44	48

Model ID	Analysed	Favored	Allowed	Outliers
5	758	681	59	18
6	758	694	48	16
7	758	662	54	42
8	758	696	44	18
9	758	649	75	34
10	758	669	64	25

There are 147 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	17	PHE	7
A	44	LEU	6
A	553	GLY	6
A	14	SER	5
A	21	LEU	5
A	41	ASP	5
A	22	CYS	4
A	33	ALA	4
A	35	GLU	4
A	37	GLN	4
A	38	THR	4
A	42	ASP	4
A	108	GLU	4
A	265	GLY	4
A	346	ALA	4
A	2	GLU	3
A	16	THR	3
A	23	ILE	3
A	25	ILE	3
A	27	PRO	3
A	32	LEU	3
A	34	ALA	3
A	45	VAL	3
A	46	VAL	3
A	49	SER	3
A	56	PRO	3

Chain	Res	Type	Models (Total)
A	109	ASN	3
A	351	GLN	3
A	432	LEU	3
A	434	ARG	3
A	557	ASN	3
A	695	VAL	3
A	748	GLU	3
A	9	ALA	2
A	12	PHE	2
A	15	LEU	2
A	18	PHE	2
A	20	GLY	2
A	24	GLY	2
A	28	VAL	2
A	31	ALA	2
A	36	GLY	2
A	43	THR	2
A	48	ALA	2
A	50	THR	2
A	52	SER	2
A	53	LEU	2
A	57	GLN	2
A	72	THR	2
A	107	GLY	2
A	112	SER	2
A	138	GLY	2
A	164	SER	2
A	282	ALA	2
A	283	ALA	2
A	287	SER	2
A	296	TYR	2
A	349	ILE	2
A	354	SER	2
A	367	THR	2
A	429	PRO	2

Chain	Res	Type	Models (Total)
A	543	ASN	2
A	544	ASN	2
A	552	SER	2
A	554	ASN	2
A	555	SER	2
A	604	THR	2
A	609	GLY	2
A	648	ALA	2
A	649	GLN	2
A	657	TYR	2
A	693	GLY	2
A	743	ARG	2
A	4	ASN	1
A	5	ARG	1
A	8	PRO	1
A	11	GLN	1
A	13	HIS	1
A	26	THR	1
A	30	GLN	1
A	47	GLU	1
A	55	ALA	1
A	58	GLN	1
A	60	ALA	1
A	63	LYS	1
A	65	SER	1
A	68	VAL	1
A	105	PHE	1
A	106	ALA	1
A	110	GLY	1
A	111	ASN	1
A	115	GLY	1
A	116	ASP	1
A	127	ASN	1
A	139	SER	1
A	142	ARG	1

Chain	Res	Type	Models (Total)
A	158	GLY	1
A	163	ARG	1
A	166	PRO	1
A	223	ALA	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	617	587	16	14
2	617	578	21	18
3	617	587	18	12
4	617	578	23	16
5	617	591	18	8
6	617	581	25	11
7	617	585	18	14
8	617	592	14	11
9	617	583	16	18
10	617	578	25	14

There are 68 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	15	LEU	9
A	21	LEU	8
A	26	THR	8
A	50	THR	6
A	44	LEU	5
A	356	VAL	5
A	503	THR	5
A	697	THR	5
A	17	PHE	4
A	43	THR	4
A	14	SER	3
A	216	MET	3
A	275	SER	3
A	350	THR	3

Chain	Res	Type	Models (Total)
A	360	THR	3
A	664	THR	3
A	16	THR	2
A	28	VAL	2
A	160	ASP	2
A	298	THR	2
A	422	HIS	2
A	433	THR	2
A	695	VAL	2
A	25	ILE	1
A	52	SER	1
A	53	LEU	1
A	54	TYR	1
A	59	SER	1
A	65	SER	1
A	112	SER	1
A	113	THR	1
A	116	ASP	1
A	128	SER	1
A	137	ILE	1
A	140	VAL	1
A	157	SER	1
A	159	THR	1
A	164	SER	1
A	191	SER	1
A	221	HIS	1
A	225	ARG	1
A	269	ILE	1
A	274	TYR	1
A	281	THR	1
A	286	HIS	1
A	292	THR	1
A	300	SER	1
A	333	VAL	1
A	337	TYR	1



Chain	Res	Type	Models (Total)
A	338	LEU	1
A	342	ILE	1
A	440	ASN	1
A	489	ILE	1
A	505	ASP	1
A	506	THR	1
A	539	PRO	1
A	567	ASN	1
A	601	ASP	1
A	658	THR	1
A	688	HIS	1
A	692	ASP	1
A	730	ASP	1
A	731	THR	1
A	736	SER	1
A	740	SER	1
A	744	TYR	1
A	745	HIS	1
A	751	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.

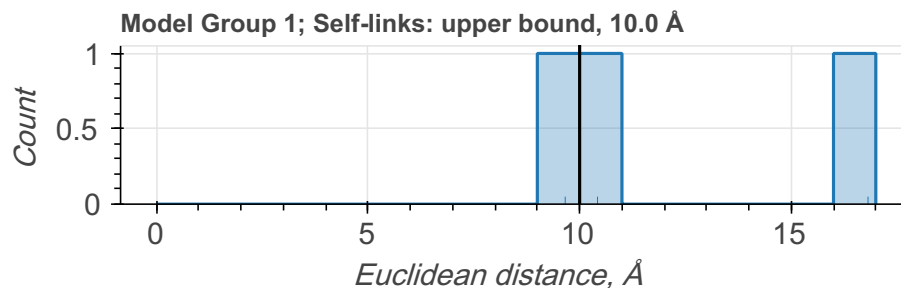
There are 3 crosslinking restraints combined in 3 restraint groups.

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	1
L-Photo-Leucine	ALA	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ASP	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.



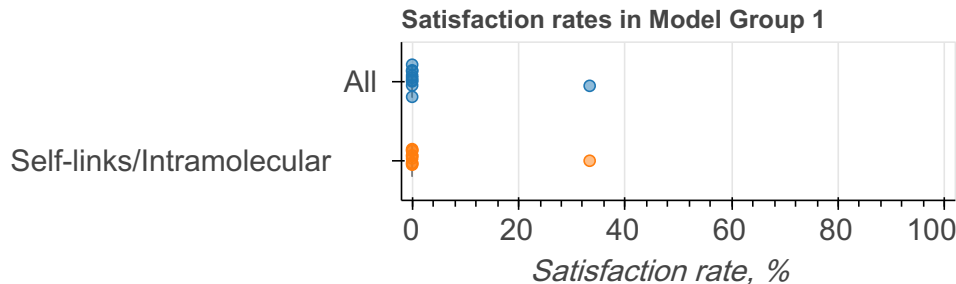
### Satisfaction of restraints

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=3)
1	1	1	10/10	All	33.33	66.67	3
				Self-links/Intramolecular	33.33	66.67	3

### 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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