

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	9A2P
PDB-Dev ID	PDBDEV_00000174
Structure Title	Model of E. coli FtsH 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

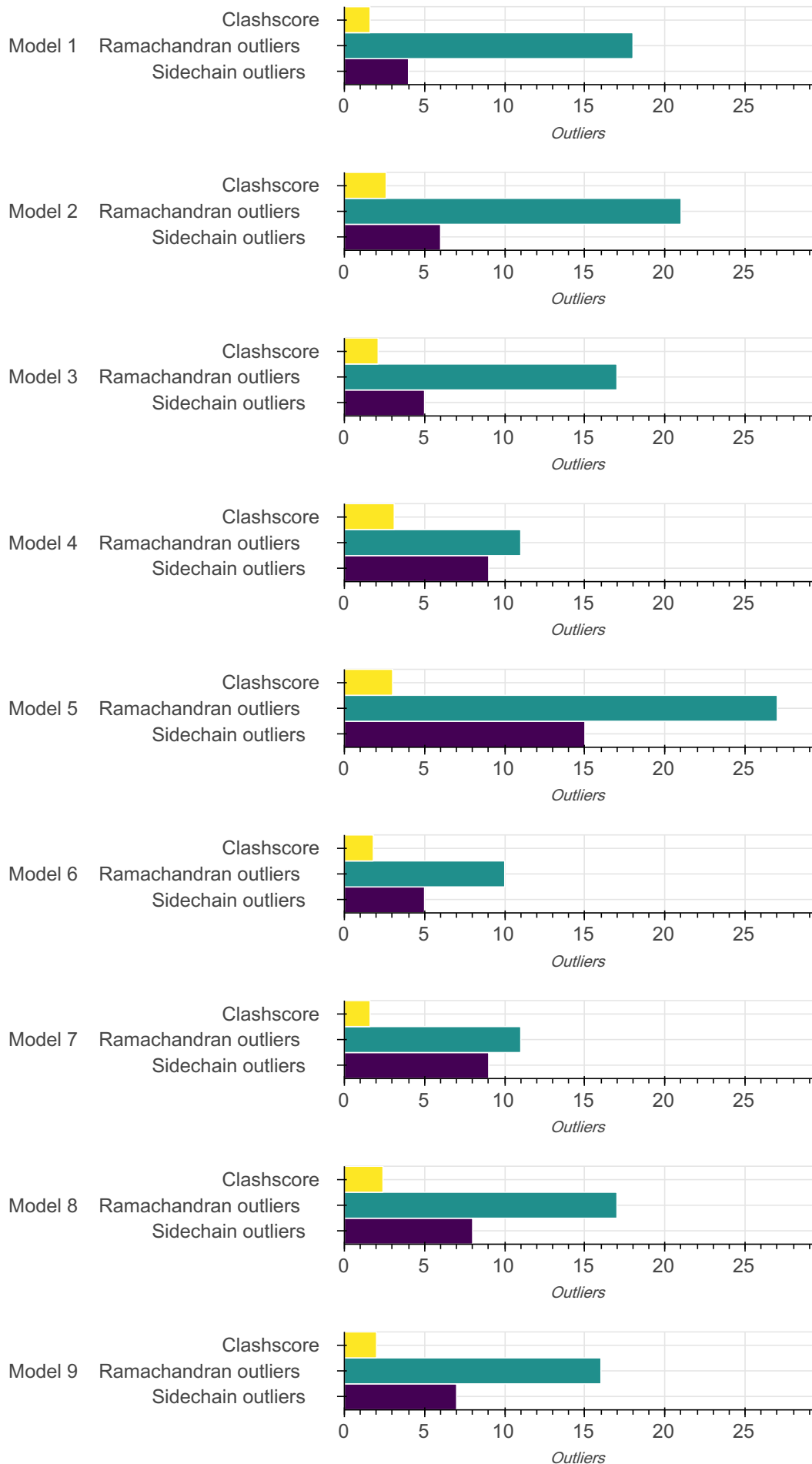
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

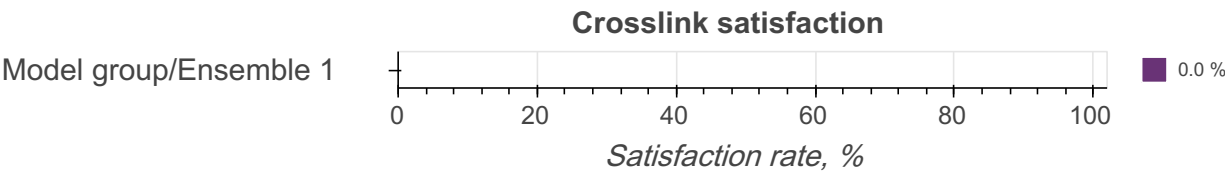
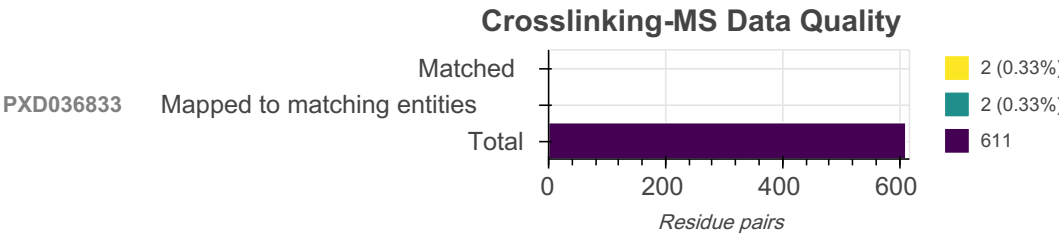
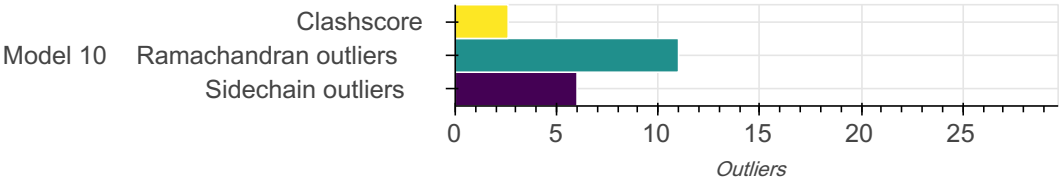
List of references used to build this report is available [here](#).

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	P0AAI3	A	644	-	1-644	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	AlphaLink	1.00	model building	https://github.com/lhatsk/AlphaLink

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	P0AAI3	dbseq_P0AAI3_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2P	3	3 (100.00%)	2 (66.67%)
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 249 bond angle outliers in this entry (0.36% of 68230 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	639	GLU	C-N-CA	10.60	140.78	121.70	2	4
A	429	ASP	CA-CB-CG	8.87	121.47	112.60	8	1
A	525	VAL	C-N-CA	8.35	136.72	121.70	5	1
A	146	GLN	OE1-CD-NE2	6.97	115.63	122.60	6	10
A	635	ASN	C-N-CA	6.47	133.34	121.70	2	2
A	615	ASP	C-N-CA	6.44	133.29	121.70	1	2
A	134	PHE	CA-CB-CG	6.13	119.93	113.80	3	1
A	626	ASP	C-N-CA	6.11	132.70	121.70	7	2
A	277	GLN	OE1-CD-NE2	6.10	116.50	122.60	1	10
A	643	ASP	C-N-CA	5.99	132.48	121.70	4	2
A	258	ARG	C-N-CA	5.90	132.32	121.70	8	1
A	460	GLN	OE1-CD-NE2	5.84	116.76	122.60	4	8
A	588	GLN	OE1-CD-NE2	5.78	116.82	122.60	8	7
A	178	GLN	OE1-CD-NE2	5.74	116.86	122.60	7	7
A	526	PHE	N-CA-C	5.60	126.68	111.00	5	1
A	129	LYS	O-C-N	5.37	114.40	123.00	6	1
A	642	GLY	C-N-CA	5.34	131.31	121.70	7	3
A	636	THR	C-N-CA	5.29	131.23	121.70	2	3
A	316	GLN	OE1-CD-NE2	5.22	117.38	122.60	10	4
A	629	ARG	C-N-CA	5.14	130.96	121.70	5	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	438	PRO	C-CA-CB	5.14	119.87	110.10	4	1
A	439	ARG	NE-CZ-NH2	5.13	123.82	119.20	9	1
A	442	ALA	C-N-CA	5.09	130.86	121.70	5	1
A	268	HIS	CB-CG-CD2	5.03	124.66	131.20	7	4
A	637	MET	C-N-CA	4.98	130.67	121.70	4	2
A	506	GLN	OE1-CD-NE2	4.96	117.64	122.60	9	6
A	261	GLY	C-N-CA	4.96	130.63	121.70	6	2
A	639	GLU	O-C-N	4.90	115.15	123.00	2	1
A	473	ARG	CD-NE-CZ	4.86	131.20	124.40	4	1
A	617	GLY	C-N-CA	4.82	130.37	121.70	4	2
A	521	GLU	C-N-CA	4.78	130.30	121.70	7	1
A	640	GLN	OE1-CD-NE2	4.77	117.83	122.60	2	7
A	185	PRO	N-CA-CB	4.76	108.24	103.00	5	1
A	437	ILE	CA-CB-CG2	4.73	118.55	110.50	8	1
A	547	GLN	OE1-CD-NE2	4.73	117.87	122.60	5	6
A	624	PRO	C-N-CA	4.71	130.18	121.70	7	3
A	122	GLN	OE1-CD-NE2	4.67	117.93	122.60	2	10
A	329	GLN	OE1-CD-NE2	4.64	117.96	122.60	3	6
A	96	PRO	N-CA-C	4.62	100.55	112.10	3	1
A	298	ASN	OD1-CG-ND2	4.61	117.99	122.60	5	6
A	220	ASP	CA-CB-CG	4.58	117.18	112.60	1	1
A	638	SER	C-N-CA	4.58	129.94	121.70	5	3
A	634	GLY	C-N-CA	4.56	129.90	121.70	2	3
A	73	GLN	OE1-CD-NE2	4.52	118.08	122.60	3	10
A	615	ASP	CA-CB-CG	4.49	117.09	112.60	1	1
A	546	ASP	CA-CB-CG	4.48	117.08	112.60	5	1
A	612	ASN	OD1-CG-ND2	4.45	118.15	122.60	5	3
A	465	GLN	OE1-CD-NE2	4.43	118.17	122.60	8	5
A	265	GLY	C-N-CA	4.41	129.64	121.70	8	2
A	643	ASP	N-CA-C	4.40	123.33	111.00	7	1
A	124	GLN	OE1-CD-NE2	4.40	118.20	122.60	4	6
A	428	HIS	CB-CG-CD2	4.40	125.48	131.20	10	3
A	440	GLY	C-N-CA	4.39	129.60	121.70	8	2
A	20	GLN	OE1-CD-NE2	4.36	118.24	122.60	6	7
A	411	THR	CA-C-N	4.34	124.88	116.20	5	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	184	ILE	CA-CB-CG1	4.33	103.04	110.40	4	1
A	407	GLN	OE1-CD-NE2	4.33	118.27	122.60	8	4
A	414	HIS	C-N-CA	4.33	129.49	121.70	5	1
A	128	GLY	C-N-CA	4.32	129.48	121.70	7	2
A	638	SER	N-CA-C	4.32	123.09	111.00	2	1
A	614	GLY	C-N-CA	4.31	129.46	121.70	1	2
A	39	GLN	OE1-CD-NE2	4.29	118.31	122.60	3	10
A	567	ASN	OD1-CG-ND2	4.29	118.31	122.60	5	1
A	611	ASN	OD1-CG-ND2	4.28	118.32	122.60	6	2
A	273	GLN	OE1-CD-NE2	4.27	118.33	122.60	8	6
A	235	ASP	CA-CB-CG	4.26	116.86	112.60	3	1
A	484	HIS	CB-CG-CD2	4.26	125.67	131.20	10	2
A	418	HIS	CB-CG-CD2	4.25	125.67	131.20	4	2
A	616	ASN	OD1-CG-ND2	4.25	118.35	122.60	5	1
A	599	ARG	CD-NE-CZ	4.25	130.35	124.40	2	1
A	640	GLN	C-N-CA	4.24	129.33	121.70	9	1
A	199	THR	CA-CB-OG1	4.24	115.96	109.60	5	1
A	610	SER	C-N-CA	4.22	129.30	121.70	7	1
A	591	ASP	CA-CB-CG	4.20	108.40	112.60	10	1
A	627	GLU	N-CA-CB	4.19	103.37	110.50	7	1
A	491	ASN	CA-CB-CG	4.18	108.42	112.60	8	1
A	635	ASN	OD1-CG-ND2	4.17	118.43	122.60	9	3
A	45	GLN	OE1-CD-NE2	4.16	118.44	122.60	2	4
A	601	PRO	N-CA-CB	4.13	107.55	103.00	10	1
A	432	HIS	CB-CG-CD2	4.11	125.85	131.20	10	1
A	258	ARG	N-CA-C	4.11	122.52	111.00	4	1
A	261	GLY	O-C-N	4.11	116.42	123.00	7	1
A	264	LEU	C-N-CA	4.09	129.06	121.70	2	1
A	129	LYS	N-CA-C	4.08	122.43	111.00	4	1
A	615	ASP	N-CA-CB	4.08	103.57	110.50	1	1
A	232	ARG	CD-NE-CZ	4.07	130.09	124.40	3	1
A	283	ASP	CA-CB-CG	4.06	116.66	112.60	5	1
A	327	ARG	NE-CZ-NH1	4.06	125.56	121.50	5	1
A	632	ASN	OD1-CG-ND2	4.03	118.57	122.60	5	1
A	288	ASN	OD1-CG-ND2	4.03	118.57	122.60	5	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	635	ASN	N-CA-C	4.02	122.27	111.00	2	1
A	259	GLN	OE1-CD-NE2	4.01	118.59	122.60	4	1
A	428	HIS	C-N-CA	4.01	128.92	121.70	5	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	1.60	16
2	2.61	26
3	2.11	21
4	3.11	31
5	3.01	30
6	1.81	18
7	1.60	16
8	2.41	24
9	2.01	20
10	2.61	26

There are 228 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:216:ILE:HD11	A:236:MET:SD	0.89	4	1
A:443:LEU:HD11	A:488:GLY:C	0.84	9	1
A:228:VAL:HG21	A:232:ARG:HE	0.77	3	1
A:190:MET:SD	A:199:THR:HG23	0.75	5	1
A:398:ARG:NH2	A:437:ILE:HG23	0.74	8	1
A:537:MET:HE3	A:542:ALA:HB2	0.74	2	3
A:478:ILE:HG21	A:568:MET:HE1	0.71	7	2
A:321:LEU:HD21	A:441:ARG:NH1	0.68	2	1
A:241:LYS:HE2	A:285:PHE:CZ	0.66	9	1
A:401:MET:CE	A:438:PRO:HB3	0.65	6	1
A:473:ARG:HH11	A:493:ILE:HD11	0.64	6	3
A:601:PRO:HD2	A:604:TRP:CG	0.63	10	1
A:285:PHE:CE1	A:291:ILE:HD12	0.62	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:170:TYR:CE1	A:184:ILE:HD13	0.62	10	2
A:141:MET:HE2	A:214:PHE:CE2	0.62	2	2
A:393:MET:CE	A:447:PHE:CE1	0.61	9	1
A:191:VAL:HG11	A:316:GLN:HE21	0.61	9	1
A:241:LYS:HE3	A:285:PHE:CZ	0.60	2	2
A:356:PHE:CE1	A:393:MET:HE3	0.60	4	1
A:225:PHE:CD1	A:271:ARG:HA	0.60	4	1
A:401:MET:HE1	A:440:GLY:N	0.60	9	1
A:424:LEU:HD21	A:598:VAL:HG11	0.59	3	1
A:403:MET:HE1	A:411:THR:CG2	0.59	5	1
A:393:MET:HE2	A:402:VAL:HG11	0.58	2	1
A:225:PHE:CD2	A:271:ARG:HG2	0.58	4	1
A:170:TYR:HB2	A:184:ILE:HD13	0.58	4	1
A:601:PRO:HD2	A:604:TRP:CD2	0.58	10	1
A:335:MET:HB3	A:340:LEU:HD11	0.58	1	8
A:116:TRP:CZ3	A:120:MET:HE2	0.57	7	1
A:425:VAL:HG11	A:464:SER:HB2	0.57	1	1
A:412:ALA:O	A:416:ALA:HB3	0.57	5	1
A:228:VAL:CG2	A:232:ARG:HE	0.57	3	1
A:505:THR:HB	A:518:TYR:CZ	0.56	10	1
A:401:MET:SD	A:438:PRO:HB3	0.55	6	1
A:434:VAL:HG23	A:589:ILE:HD11	0.55	8	4
A:415:GLU:CD	A:444:GLY:HA2	0.55	6	1
A:537:MET:HE3	A:542:ALA:CB	0.55	2	3
A:601:PRO:HD2	A:604:TRP:CD1	0.55	10	1
A:134:PHE:CZ	A:216:ILE:HD11	0.54	5	1
A:393:MET:CE	A:447:PHE:CZ	0.54	9	1
A:505:THR:HB	A:518:TYR:CE1	0.54	10	1
A:27:SER:C	A:29:GLY:H	0.54	3	6
A:429:ASP:CG	A:448:PHE:CD1	0.54	8	1
A:429:ASP:HB2	A:448:PHE:CD1	0.54	8	1
A:537:MET:SD	A:545:ILE:HD12	0.54	7	3
A:473:ARG:NE	A:485:VAL:HG11	0.54	3	1
A:413:TYR:CZ	A:575:LYS:HE2	0.54	10	9
A:473:ARG:CD	A:485:VAL:HG11	0.54	4	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:241:LYS:CE	A:285:PHE:CE2	0.53	2	1
A:241:LYS:HA	A:291:ILE:HD11	0.53	6	2
A:473:ARG:HD2	A:485:VAL:HG11	0.53	3	1
A:403:MET:HE1	A:411:THR:HG21	0.53	5	1
A:167:LEU:HD13	A:294:ILE:HD11	0.53	5	1
A:503:MET:CE	A:552:LEU:HD13	0.52	7	1
A:19:PHE:O	A:23:GLY:HA3	0.52	10	1
A:237:PHE:CD2	A:281:GLU:HB3	0.52	1	2
A:221:PHE:HB3	A:274:THR:HG21	0.52	9	4
A:401:MET:HE3	A:403:MET:SD	0.52	4	1
A:122:GLN:C	A:125:GLY:H	0.52	6	1
A:40:GLU:OE1	A:60:LYS:HE2	0.51	4	1
A:139:ALA:HB2	A:216:ILE:HD12	0.51	6	1
A:474:LEU:HD21	A:557:TYR:CZ	0.51	7	2
A:222:VAL:HA	A:225:PHE:CD2	0.51	4	1
A:241:LYS:HE3	A:285:PHE:CE2	0.50	2	1
A:397:GLU:CD	A:438:PRO:HB2	0.50	4	1
A:116:TRP:CH2	A:120:MET:HE2	0.50	7	1
A:601:PRO:HD2	A:604:TRP:CE2	0.50	10	1
A:335:MET:HE2	A:385:PHE:CZ	0.49	2	3
A:412:ALA:HA	A:436:ILE:HG21	0.49	4	2
A:134:PHE:CE1	A:216:ILE:HD11	0.49	5	1
A:191:VAL:HG21	A:316:GLN:HE21	0.49	10	1
A:443:LEU:HD22	A:491:ASN:CG	0.49	8	1
A:224:MET:HE3	A:232:ARG:HH12	0.49	7	1
A:421:ILE:O	A:425:VAL:HG22	0.49	8	2
A:216:ILE:HD11	A:236:MET:CE	0.49	4	1
A:222:VAL:CG2	A:256:VAL:HG13	0.49	6	1
A:195:GLY:H	A:199:THR:HG21	0.48	5	1
A:221:PHE:CE1	A:250:ILE:HG23	0.48	4	1
A:241:LYS:HE2	A:285:PHE:CE2	0.48	2	1
A:194:PRO:HD2	A:441:ARG:HH21	0.48	2	1
A:433:LYS:HE3	A:441:ARG:HD3	0.48	4	1
A:526:PHE:CZ	A:528:GLY:HA2	0.48	10	1
A:141:MET:HE2	A:214:PHE:CZ	0.48	2	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:256:VAL:HG11	A:275:LEU:HG	0.48	6	1
A:505:THR:HG22	A:545:ILE:HD13	0.48	7	1
A:237:PHE:CD2	A:285:PHE:CZ	0.48	1	2
A:351:ARG:O	A:583:THR:HG21	0.48	5	1
A:419:ALA:HB2	A:434:VAL:HG21	0.47	8	2
A:431:VAL:HG22	A:448:PHE:CE1	0.47	1	1
A:225:PHE:CE1	A:274:THR:HB	0.47	4	1
A:443:LEU:HD22	A:491:ASN:ND2	0.47	8	1
A:134:PHE:HZ	A:214:PHE:CD1	0.47	3	1
A:612:ASN:C	A:614:GLY:H	0.47	2	1
A:401:MET:CE	A:438:PRO:CB	0.47	6	1
A:586:ALA:HB3	A:587:PRO:HD3	0.47	8	2
A:414:HIS:NE2	A:443:LEU:HD13	0.47	9	1
A:134:PHE:CZ	A:214:PHE:CD1	0.46	3	1
A:198:LYS:HD2	A:296:ALA:HB1	0.46	5	1
A:279:LEU:HD22	A:312:ARG:HD3	0.46	4	2
A:389:LYS:HG2	A:393:MET:HE2	0.46	10	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	642	592	32	18
2	642	580	41	21
3	642	586	39	17
4	642	587	44	11
5	642	567	48	27
6	642	594	38	10
7	642	592	39	11
8	642	576	49	17
9	642	594	32	16
10	642	595	36	11

There are 71 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	28	ASN	9

Chain	Res	Type	Models (Total)
A	266	GLY	7
A	26	GLU	6
A	264	LEU	5
A	536	HIS	5
A	582	GLU	5
A	617	GLY	5
A	634	GLY	5
A	128	GLY	4
A	611	ASN	4
A	614	GLY	4
A	615	ASP	4
A	618	SER	4
A	635	ASN	4
A	640	GLN	4
A	129	LYS	3
A	443	LEU	3
A	520	GLU	3
A	612	ASN	3
A	636	THR	3
A	637	MET	3
A	641	LEU	3
A	25	SER	2
A	261	GLY	2
A	287	GLY	2
A	441	ARG	2
A	516	LEU	2
A	522	GLU	2
A	526	PHE	2
A	527	LEU	2
A	532	ALA	2
A	533	LYS	2
A	535	LYS	2
A	616	ASN	2
A	639	GLU	2
A	642	GLY	2

Chain	Res	Type	Models (Total)
A	27	SER	1
A	94	GLU	1
A	127	GLY	1
A	130	GLY	1
A	136	LYS	1
A	225	PHE	1
A	259	GLN	1
A	260	ARG	1
A	262	ALA	1
A	265	GLY	1
A	288	ASN	1
A	400	SER	1
A	417	GLY	1
A	431	VAL	1
A	433	LYS	1
A	440	GLY	1
A	444	GLY	1
A	452	GLY	1
A	453	ASP	1
A	455	ILE	1
A	482	PRO	1
A	489	ALA	1
A	490	SER	1
A	508	GLY	1
A	517	LEU	1
A	518	TYR	1
A	521	GLU	1
A	525	VAL	1
A	530	SER	1
A	531	VAL	1
A	598	VAL	1
A	619	PRO	1
A	633	PRO	1
A	638	SER	1
A	643	ASP	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	527	508	15	4
2	527	508	13	6
3	527	507	15	5
4	527	500	18	9
5	527	498	14	15
6	527	506	16	5
7	527	498	20	9
8	527	506	13	8
9	527	503	17	7
10	527	511	10	6

There are 42 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	5	LEU	9
A	98	LEU	6
A	112	LEU	5
A	9	LEU	3
A	630	THR	3
A	1	MET	2
A	19	PHE	2
A	103	PHE	2
A	111	LEU	2
A	429	ASP	2
A	445	VAL	2
A	483	GLU	2
A	526	PHE	2
A	530	SER	2
A	636	THR	2
A	641	LEU	2
A	16	MET	1
A	119	PHE	1
A	120	MET	1
A	132	MET	1

Chain	Res	Type	Models (Total)
A	134	PHE	1
A	166	GLU	1
A	228	VAL	1
A	258	ARG	1
A	401	MET	1
A	424	LEU	1
A	425	VAL	1
A	431	VAL	1
A	433	LYS	1
A	453	ASP	1
A	456	SER	1
A	474	LEU	1
A	499	LEU	1
A	509	PHE	1
A	510	SER	1
A	517	LEU	1
A	583	THR	1
A	584	ILE	1
A	592	LEU	1
A	597	ASP	1
A	604	TRP	1
A	613	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.

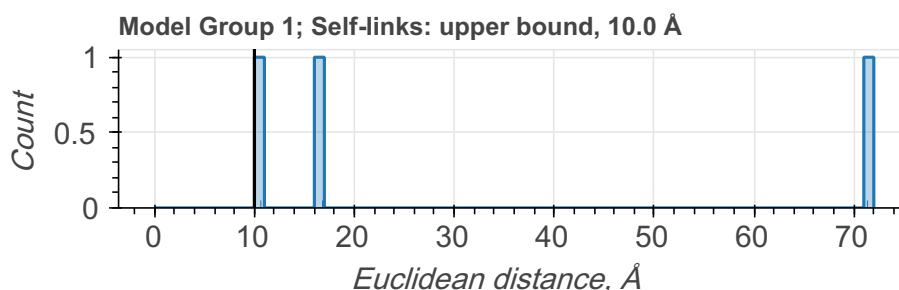
There are 3 crosslinking restraints combined in 3 restraint groups.

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

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	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.



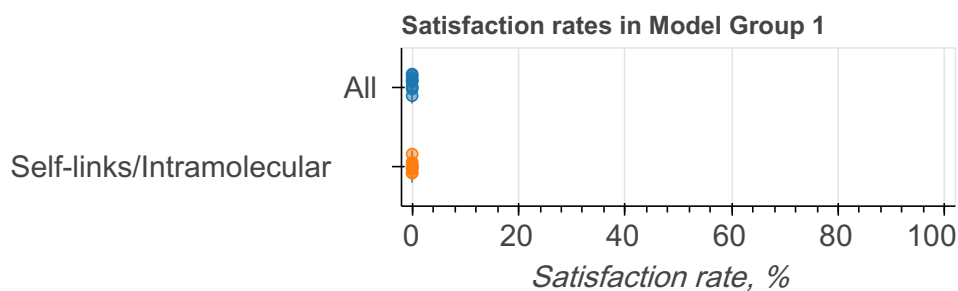
Satisfaction of restraints

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	0.00	100.00	3
				Self-links/ Intramolecular	0.00	100.00	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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