

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	9A32
PDB-Dev ID	PDBDEV_00000187
Structure Title	Model of E. coli OmpC 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

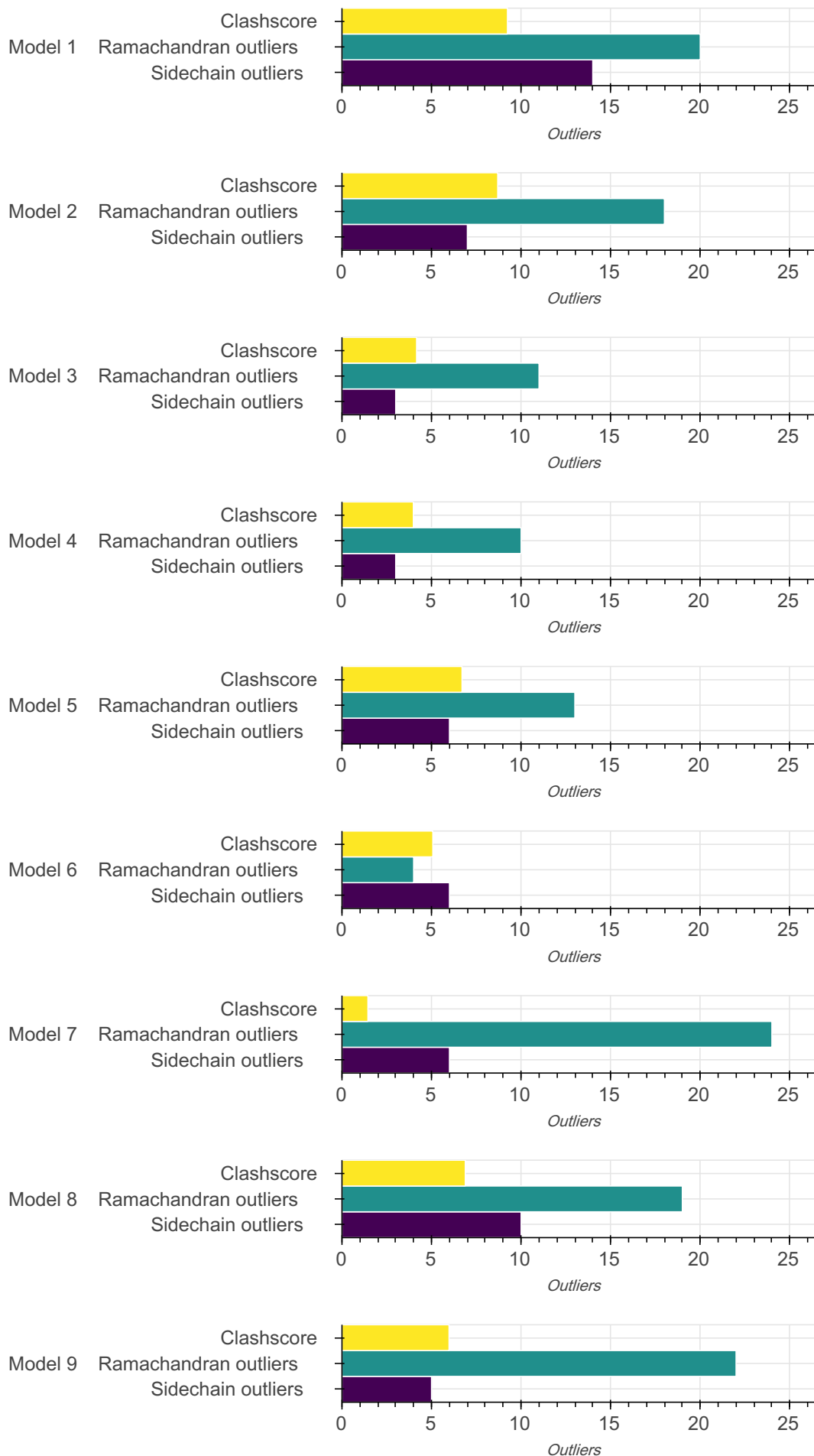
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

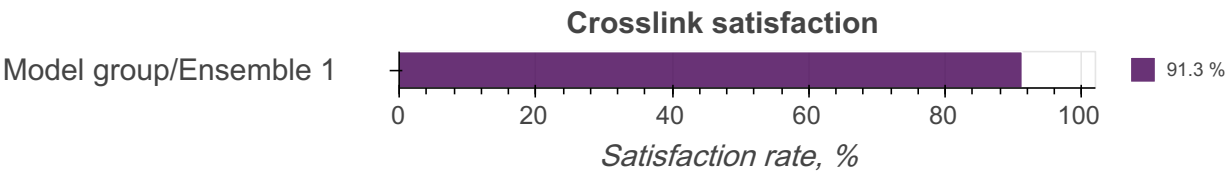
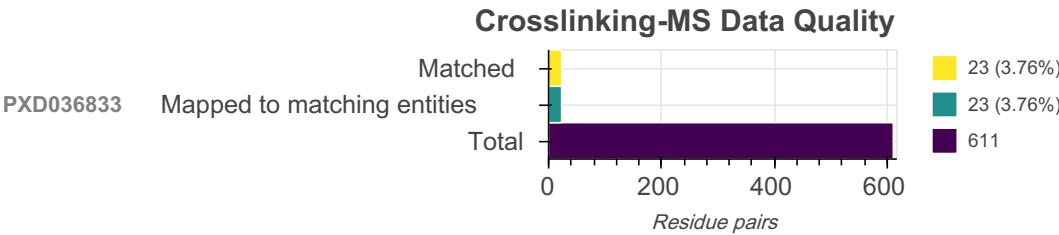
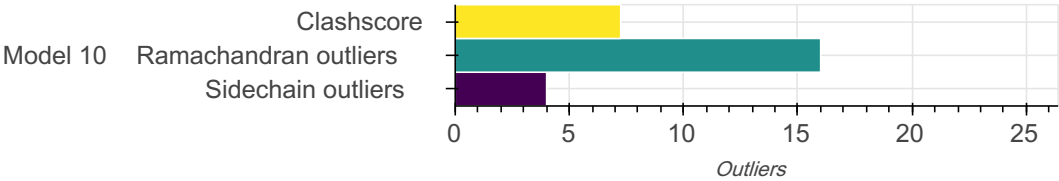
List of references used to build this report is available [here](#).

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	P06996	A	367	-	1-367	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	P06996	dbseq_P06996_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A32	23	23 (100.00%)	23 (100.00%)
PXD036833	611	23 (3.76%)	23 (3.76%)

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 3 bond length outliers in this entry (0.01% of 29180 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	347	PHE	CA-CB	4.27	1.62	1.53	2	1
A	95	ARG	CZ-NH2	4.09	1.28	1.33	4	1
A	191	ARG	CZ-NH2	4.02	1.28	1.33	10	1

Standard geometry: angle outliers ?

There are 297 bond angle outliers in this entry (0.75% of 39530 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	347	PHE	CA-CB-CG	15.82	129.62	113.80	2	1
A	347	PHE	C-CA-CB	11.51	131.96	110.10	2	1
A	350	ASP	CA-CB-CG	11.01	123.61	112.60	2	2
A	349	ARG	C-N-CA	9.89	139.50	121.70	2	1
A	135	THR	C-N-CA	9.06	138.00	121.70	5	1
A	305	ASN	CA-CB-CG	8.95	121.55	112.60	3	3
A	171	GLN	OE1-CD-NE2	8.18	114.42	122.60	7	7
A	345	ASN	C-N-CA	7.95	136.02	121.70	2	2
A	345	ASN	O-C-N	7.89	110.38	123.00	2	1
A	340	ASN	OD1-CG-ND2	7.50	115.10	122.60	3	1
A	347	PHE	O-C-N	7.34	111.25	123.00	2	1
A	261	GLN	OE1-CD-NE2	7.30	115.30	122.60	3	9
A	354	ASN	OD1-CG-ND2	7.26	115.34	122.60	8	4
A	197	ASN	OD1-CG-ND2	7.07	115.53	122.60	6	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	344	ASP	C-N-CA	6.92	134.15	121.70	2	1
A	53	ASP	CA-CB-CG	6.75	119.35	112.60	9	5
A	347	PHE	C-N-CA	6.68	133.73	121.70	2	1
A	139	ASP	CA-CB-CG	6.38	118.98	112.60	1	1
A	143	GLN	OE1-CD-NE2	6.31	116.29	122.60	10	6
A	278	GLN	OE1-CD-NE2	6.20	116.40	122.60	8	10
A	139	ASP	C-N-CA	6.03	132.55	121.70	2	2
A	54	GLN	OE1-CD-NE2	6.01	116.59	122.60	3	5
A	154	ASN	CA-CB-CG	6.00	106.60	112.60	5	3
A	175	GLY	C-N-CA	5.98	132.46	121.70	9	1
A	88	ASN	CA-CB-CG	5.94	118.54	112.60	8	1
A	287	GLN	OE1-CD-NE2	5.88	116.72	122.60	6	8
A	347	PHE	CD1-CG-CD2	5.88	109.78	118.60	2	1
A	228	ASN	OD1-CG-ND2	5.86	116.74	122.60	1	1
A	138	SER	C-N-CA	5.83	132.20	121.70	8	2
A	141	PHE	C-N-CA	5.83	132.20	121.70	7	1
A	114	ASN	OD1-CG-ND2	5.82	116.78	122.60	5	2
A	312	ASP	CA-CB-CG	5.78	118.38	112.60	7	5
A	230	ALA	C-N-CA	5.75	132.06	121.70	9	1
A	33	ASP	CA-CB-CG	5.66	118.26	112.60	6	3
A	354	ASN	N-CA-CB	5.65	120.11	110.50	5	1
A	129	PRO	C-CA-CB	5.63	120.80	110.10	5	1
A	50	VAL	C-N-CA	5.50	131.60	121.70	8	1
A	21	ALA	N-CA-CB	5.46	102.21	110.40	2	1
A	174	ASN	OD1-CG-ND2	5.42	117.18	122.60	1	2
A	145	ARG	NH1-CZ-NH2	5.42	112.26	119.30	9	1
A	366	GLN	OE1-CD-NE2	5.40	117.20	122.60	6	3
A	66	GLN	OE1-CD-NE2	5.38	117.22	122.60	9	5
A	320	ASP	CA-CB-CG	5.37	117.97	112.60	1	2
A	182	PHE	C-N-CA	5.37	131.36	121.70	6	1
A	227	GLN	OE1-CD-NE2	5.34	117.26	122.60	8	1
A	349	ARG	C-CA-CB	5.33	120.22	110.10	2	1
A	355	THR	OG1-CB-CG2	5.30	98.69	109.30	8	1
A	347	PHE	CA-C-N	5.29	126.78	116.20	2	1
A	49	ASP	C-N-CA	5.29	131.22	121.70	10	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	80	GLN	OE1-CD-NE2	5.29	117.31	122.60	4	5
A	183	THR	C-N-CA	5.25	131.15	121.70	9	2
A	152	TYR	CA-CB-CG	5.24	123.33	113.90	5	1
A	305	ASN	OD1-CG-ND2	5.23	117.37	122.60	3	3
A	134	ASP	CA-CB-CG	5.21	117.81	112.60	5	1
A	346	GLN	OE1-CD-NE2	5.17	117.43	122.60	8	6
A	354	ASN	CA-CB-CG	5.17	117.77	112.60	5	2
A	122	THR	C-N-CA	5.16	130.98	121.70	8	1
A	300	GLN	OE1-CD-NE2	5.15	117.45	122.60	8	9
A	231	ALA	C-N-CA	5.14	130.94	121.70	5	1
A	314	ASP	C-N-CA	5.13	130.94	121.70	10	1
A	258	GLN	OE1-CD-NE2	5.12	117.48	122.60	1	9
A	350	ASP	N-CA-CB	5.08	119.13	110.50	2	1
A	169	GLN	OE1-CD-NE2	5.07	117.53	122.60	7	3
A	197	ASN	CA-CB-CG	5.06	107.54	112.60	2	1
A	285	GLN	OE1-CD-NE2	5.06	117.54	122.60	8	2
A	233	ILE	CA-CB-CG2	5.05	119.08	110.50	10	1
A	47	ASN	C-N-CA	5.05	130.78	121.70	1	2
A	76	GLN	OE1-CD-NE2	5.04	117.56	122.60	1	5
A	196	GLN	OE1-CD-NE2	5.00	117.60	122.60	6	4
A	88	ASN	OD1-CG-ND2	4.99	117.61	122.60	8	1
A	91	ASN	CA-CB-CG	4.96	117.56	112.60	8	1
A	147	ASN	CA-CB-CG	4.94	117.54	112.60	10	2
A	186	VAL	C-N-CA	4.94	130.59	121.70	3	2
A	129	PRO	N-CA-CB	4.88	108.37	103.00	10	1
A	275	ASN	OD1-CG-ND2	4.87	117.73	122.60	8	5
A	190	GLY	C-N-CA	4.87	130.46	121.70	8	1
A	1	MET	CA-C-N	4.87	125.93	116.20	9	1
A	311	ASP	C-N-CA	4.85	130.42	121.70	9	1
A	367	PHE	CA-CB-CG	4.80	109.00	113.80	5	1
A	343	ASP	C-N-CA	4.78	130.31	121.70	1	1
A	354	ASN	C-N-CA	4.77	130.28	121.70	1	1
A	279	ASN	OD1-CG-ND2	4.76	117.84	122.60	9	1
A	144	GLN	OE1-CD-NE2	4.75	117.85	122.60	1	4
A	344	ASP	CA-CB-CG	4.75	117.35	112.60	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	86	ALA	C-N-CA	4.70	130.15	121.70	7	1
A	150	ALA	N-CA-CB	4.70	103.36	110.40	5	1
A	82	GLN	OE1-CD-NE2	4.69	117.91	122.60	8	3
A	224	THR	C-N-CA	4.68	130.12	121.70	1	1
A	128	LEU	C-CA-CB	4.67	118.97	110.10	2	1
A	312	ASP	C-N-CA	4.67	130.10	121.70	5	1
A	84	ASN	OD1-CG-ND2	4.65	117.95	122.60	1	1
A	27	LYS	C-N-CA	4.65	130.07	121.70	7	1
A	266	THR	OG1-CB-CG2	4.63	100.04	109.30	10	1
A	26	ASN	OD1-CG-ND2	4.62	117.98	122.60	8	1
A	357	ASN	OD1-CG-ND2	4.59	118.01	122.60	8	1
A	266	THR	CA-CB-OG1	4.58	116.47	109.60	10	2
A	189	ASN	CA-CB-CG	4.57	117.17	112.60	10	1
A	52	GLY	C-N-CA	4.57	129.92	121.70	8	1
A	191	ARG	NE-CZ-NH1	4.54	126.04	121.50	5	1
A	344	ASP	N-CA-C	4.53	123.68	111.00	1	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	9.24	51
2	8.69	48
3	4.17	23
4	3.98	22
5	6.70	37
6	5.07	28
7	1.45	8
8	6.88	38
9	5.98	33
10	7.25	40

There are 328 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:127:VAL:HG11	A:297:ALA:HB2	0.96	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:120:ASP:H	A:151:THR:HG21	0.91	1	1
A:342:LEU:HD12	A:355:THR:HG22	0.88	8	1
A:141:PHE:HB3	A:262:THR:HG21	0.80	6	1
A:348:THR:HG23	A:354:ASN:HD22	0.75	5	1
A:149:PHE:HB2	A:258:GLN:CD	0.73	1	1
A:346:GLN:HA	A:349:ARG:HE	0.70	1	1
A:191:ARG:HA	A:194:LEU:HD12	0.70	8	1
A:98:PHE:CZ	A:127:VAL:HG22	0.70	2	1
A:127:VAL:HG21	A:169:GLN:NE2	0.69	2	1
A:269:GLY:HA2	A:347:PHE:CE1	0.69	9	1
A:150:ALA:HB1	A:283:VAL:HG21	0.69	1	1
A:316:LEU:HD12	A:342:LEU:HG	0.68	9	1
A:316:LEU:HD21	A:319:VAL:HG23	0.67	10	1
A:345:ASN:HA	A:348:THR:HG22	0.66	2	1
A:95:ARG:CZ	A:149:PHE:CE1	0.66	10	1
A:147:ASN:HB2	A:149:PHE:CZ	0.65	10	1
A:299:LEU:HD22	A:318:TYR:CE1	0.65	10	1
A:37:LYS:HE2	A:58:ARG:CZ	0.65	4	1
A:16:ALA:HB1	A:331:MET:SD	0.64	2	1
A:347:PHE:CD1	A:350:ASP:CG	0.64	2	1
A:266:THR:HG23	A:273:TRP:CH2	0.64	9	1
A:34:LEU:HD23	A:367:PHE:CZ	0.63	1	2
A:347:PHE:CE1	A:350:ASP:HB2	0.63	2	1
A:223:ARG:HH22	A:231:ALA:CB	0.63	4	1
A:129:PRO:HB2	A:334:TYR:CG	0.63	5	1
A:124:TRP:HD1	A:135:THR:HG21	0.63	2	1
A:133:GLY:N	A:217:ALA:HB3	0.62	2	1
A:34:LEU:HD11	A:59:LEU:HD11	0.62	4	1
A:128:LEU:HD21	A:338:LYS:HE2	0.62	5	1
A:269:GLY:CA	A:347:PHE:CE1	0.61	9	1
A:125:THR:HG22	A:334:TYR:CG	0.61	1	1
A:19:ALA:HB1	A:367:PHE:CE1	0.61	4	1
A:316:LEU:HD11	A:340:ASN:HD21	0.61	9	1
A:348:THR:HG21	A:355:THR:CG2	0.61	10	1
A:95:ARG:HH21	A:145:ARG:NH2	0.60	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:149:PHE:CZ	A:262:THR:HG23	0.60	5	1
A:316:LEU:HD13	A:342:LEU:HD12	0.60	3	1
A:316:LEU:HD21	A:319:VAL:CG2	0.59	10	1
A:136:TYR:CD1	A:273:TRP:CZ3	0.59	10	1
A:223:ARG:NH1	A:233:ILE:HG22	0.59	2	1
A:124:TRP:CD1	A:135:THR:HG21	0.59	2	1
A:128:LEU:HD12	A:131:PHE:CE2	0.59	4	1
A:267:ARG:HB2	A:273:TRP:CZ2	0.59	2	1
A:146:GLY:HA3	A:149:PHE:CE2	0.59	6	1
A:146:GLY:HA2	A:149:PHE:CZ	0.58	6	1
A:271:LEU:HD22	A:310:TYR:HE2	0.58	10	1
A:347:PHE:CB	A:349:ARG:HA	0.58	2	1
A:342:LEU:CD1	A:355:THR:HG22	0.58	8	1
A:42:HIS:CD2	A:44:PHE:CZ	0.58	10	1
A:306:LEU:HD11	A:314:ASP:CG	0.58	2	1
A:271:LEU:HD13	A:312:ASP:HB2	0.58	8	1
A:347:PHE:CD2	A:349:ARG:C	0.58	2	1
A:347:PHE:CD2	A:349:ARG:CA	0.58	2	1
A:141:PHE:CE1	A:239:ALA:HB1	0.58	9	1
A:52:GLY:HA2	A:86:ALA:HB2	0.57	4	1
A:115:TYR:CE2	A:219:SER:HB3	0.57	1	1
A:268:VAL:HG22	A:277:ALA:HB2	0.57	3	1
A:316:LEU:HD12	A:342:LEU:CG	0.57	9	1
A:348:THR:HG23	A:354:ASN:ND2	0.57	5	1
A:16:ALA:HB2	A:365:TYR:OH	0.57	2	1
A:129:PRO:HA	A:132:GLY:H	0.57	5	1
A:19:ALA:HB1	A:21:ALA:HB2	0.57	9	1
A:348:THR:CG2	A:354:ASN:HB2	0.56	5	1
A:120:ASP:N	A:151:THR:HG21	0.56	1	1
A:131:PHE:CD1	A:338:LYS:HE3	0.56	6	1
A:142:MET:HA	A:171:GLN:CD	0.56	1	1
A:128:LEU:HD11	A:297:ALA:HB3	0.56	4	2
A:117:VAL:HG11	A:245:GLY:N	0.55	1	1
A:136:TYR:CE2	A:267:ARG:CZ	0.55	9	1
A:141:PHE:CE1	A:316:LEU:HD11	0.55	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:144:GLN:HE22	A:241:THR:HG21	0.55	10	1
A:21:ALA:HB1	A:367:PHE:CD1	0.55	2	1
A:128:LEU:HD11	A:297:ALA:CB	0.55	6	3
A:266:THR:HG1	A:273:TRP:CD1	0.55	1	1
A:19:ALA:HA	A:367:PHE:CZ	0.55	5	1
A:37:LYS:HE2	A:39:ASP:OD2	0.55	8	1
A:128:LEU:HD13	A:320:ASP:OD2	0.54	6	1
A:122:THR:HG21	A:144:GLN:OE1	0.54	10	1
A:128:LEU:CD2	A:338:LYS:HE2	0.54	5	1
A:136:TYR:CZ	A:269:GLY:HA3	0.54	3	1
A:128:LEU:HD22	A:334:TYR:CE1	0.54	3	1
A:347:PHE:CD2	A:349:ARG:CB	0.54	2	1
A:34:LEU:HD13	A:61:PHE:CE2	0.54	4	2
A:150:ALA:HA	A:293:ARG:HH22	0.54	2	1
A:189:ASN:HD22	A:191:ARG:HH21	0.54	5	1
A:131:PHE:CE2	A:364:VAL:HG13	0.54	3	1
A:271:LEU:HD13	A:312:ASP:CB	0.54	8	1
A:348:THR:HG21	A:355:THR:HG21	0.54	10	1
A:79:TYR:CD1	A:94:THR:HG22	0.53	1	1
A:133:GLY:CA	A:316:LEU:HD22	0.53	1	1
A:141:PHE:CD2	A:221:SER:CB	0.53	1	1
A:347:PHE:CG	A:350:ASP:N	0.53	2	1
A:42:HIS:CD2	A:44:PHE:CE2	0.53	10	1
A:127:VAL:HG21	A:169:GLN:CD	0.53	2	1
A:303:GLY:N	A:315:ILE:HD12	0.53	9	1
A:141:PHE:CG	A:221:SER:HB2	0.53	1	1
A:34:LEU:HD13	A:61:PHE:CE1	0.53	6	1
A:122:THR:HG23	A:145:ARG:HH12	0.53	8	1
A:150:ALA:CB	A:283:VAL:HG21	0.53	1	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	365	313	32	20
2	365	314	33	18

Model ID	Analysed	Favored	Allowed	Outliers
3	365	335	19	11
4	365	335	20	10
5	365	332	20	13
6	365	343	18	4
7	365	308	33	24
8	365	323	23	19
9	365	323	20	22
10	365	328	21	16

There are 93 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	182	PHE	8
A	184	SER	6
A	136	TYR	5
A	187	THR	5
A	133	GLY	4
A	139	ASP	4
A	233	ILE	4
A	22	ALA	3
A	48	LYS	3
A	50	VAL	3
A	104	GLN	3
A	179	GLY	3
A	185	GLY	3
A	188	ASN	3
A	189	ASN	3
A	231	ALA	3
A	312	ASP	3
A	315	ILE	3
A	3	VAL	2
A	20	ASN	2
A	21	ALA	2
A	128	LEU	2
A	138	SER	2
A	140	ASN	2

Chain	Res	Type	Models (Total)
A	141	PHE	2
A	160	LEU	2
A	181	GLY	2
A	190	GLY	2
A	268	VAL	2
A	313	GLU	2
A	353	ILE	2
A	5	VAL	1
A	6	LEU	1
A	7	SER	1
A	8	LEU	1
A	17	GLY	1
A	19	ALA	1
A	23	GLU	1
A	24	VAL	1
A	25	TYR	1
A	27	LYS	1
A	46	ASP	1
A	47	ASN	1
A	49	ASP	1
A	51	ASP	1
A	52	GLY	1
A	87	GLU	1
A	88	ASN	1
A	91	ASN	1
A	105	ASP	1
A	106	VAL	1
A	114	ASN	1
A	120	ASP	1
A	122	THR	1
A	123	SER	1
A	127	VAL	1
A	129	PRO	1
A	132	GLY	1
A	134	ASP	1

Chain	Res	Type	Models (Total)
A	135	THR	1
A	137	GLY	1
A	142	MET	1
A	143	GLN	1
A	144	GLN	1
A	146	GLY	1
A	148	GLY	1
A	150	ALA	1
A	151	THR	1
A	155	THR	1
A	156	ASP	1
A	176	ASN	1
A	180	GLU	1
A	183	THR	1
A	186	VAL	1
A	192	ASP	1
A	193	ALA	1
A	194	LEU	1
A	195	ARG	1
A	198	GLY	1
A	225	ASP	1
A	230	ALA	1
A	232	TYR	1
A	251	ASN	1
A	265	ALA	1
A	267	ARG	1
A	269	GLY	1
A	271	LEU	1
A	275	ASN	1
A	314	ASP	1
A	316	LEU	1
A	345	ASN	1
A	346	GLN	1
A	350	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	290	263	13	14
2	290	268	15	7
3	290	278	9	3
4	290	283	4	3
5	290	275	9	6
6	290	278	6	6
7	290	275	9	6
8	290	266	14	10
9	290	280	5	5
10	290	273	13	4

There are 40 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	LEU	4
A	8	LEU	4
A	50	VAL	3
A	122	THR	3
A	136	TYR	3
A	142	MET	3
A	151	THR	3
A	1	MET	2
A	135	THR	2
A	182	PHE	2
A	186	VAL	2
A	268	VAL	2
A	270	SER	2
A	316	LEU	2
A	343	ASP	2
A	7	SER	1
A	13	LEU	1
A	71	LEU	1
A	85	SER	1
A	109	PHE	1

Chain	Res	Type	Models (Total)
A	118	VAL	1
A	121	VAL	1
A	127	VAL	1
A	128	LEU	1
A	130	GLU	1
A	139	ASP	1
A	149	PHE	1
A	157	PHE	1
A	169	GLN	1
A	178	SER	1
A	183	THR	1
A	232	TYR	1
A	233	ILE	1
A	266	THR	1
A	273	TRP	1
A	312	ASP	1
A	320	ASP	1
A	344	ASP	1
A	348	THR	1
A	355	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.

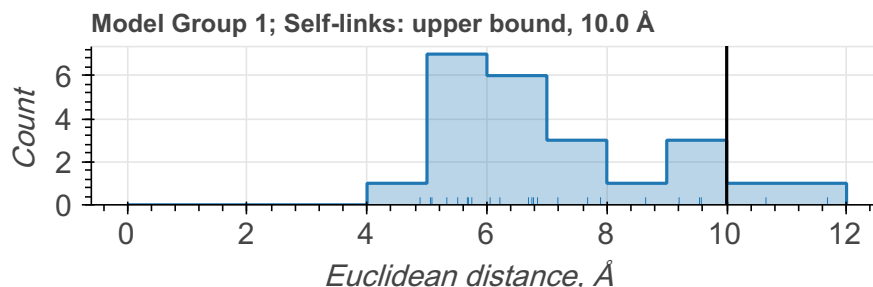
There are 23 crosslinking restraints combined in 23 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	9
L-Photo-Leucine	GLU	CA	LEU	CA	upper bound	10.0	2
L-Photo-Leucine	ILE	CA	LEU	CA	upper bound	10.0	3
L-Photo-Leucine	LEU	CA	PHE	CA	upper bound	10.0	2

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



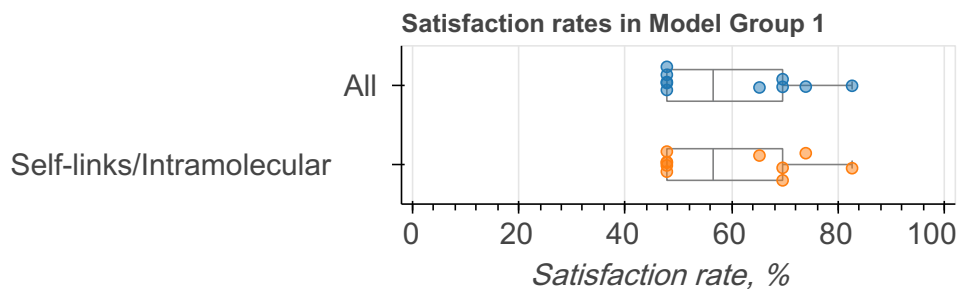
Satisfaction of restraints

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=23)
1	1	1	10/10	All	91.30	8.70	23
				Self-links/ Intramolecular	91.30	8.70	23

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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