

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	9A2Y
PDB-Dev ID	PDBDEV_00000183
Structure Title	Model of E. coli OmpF 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

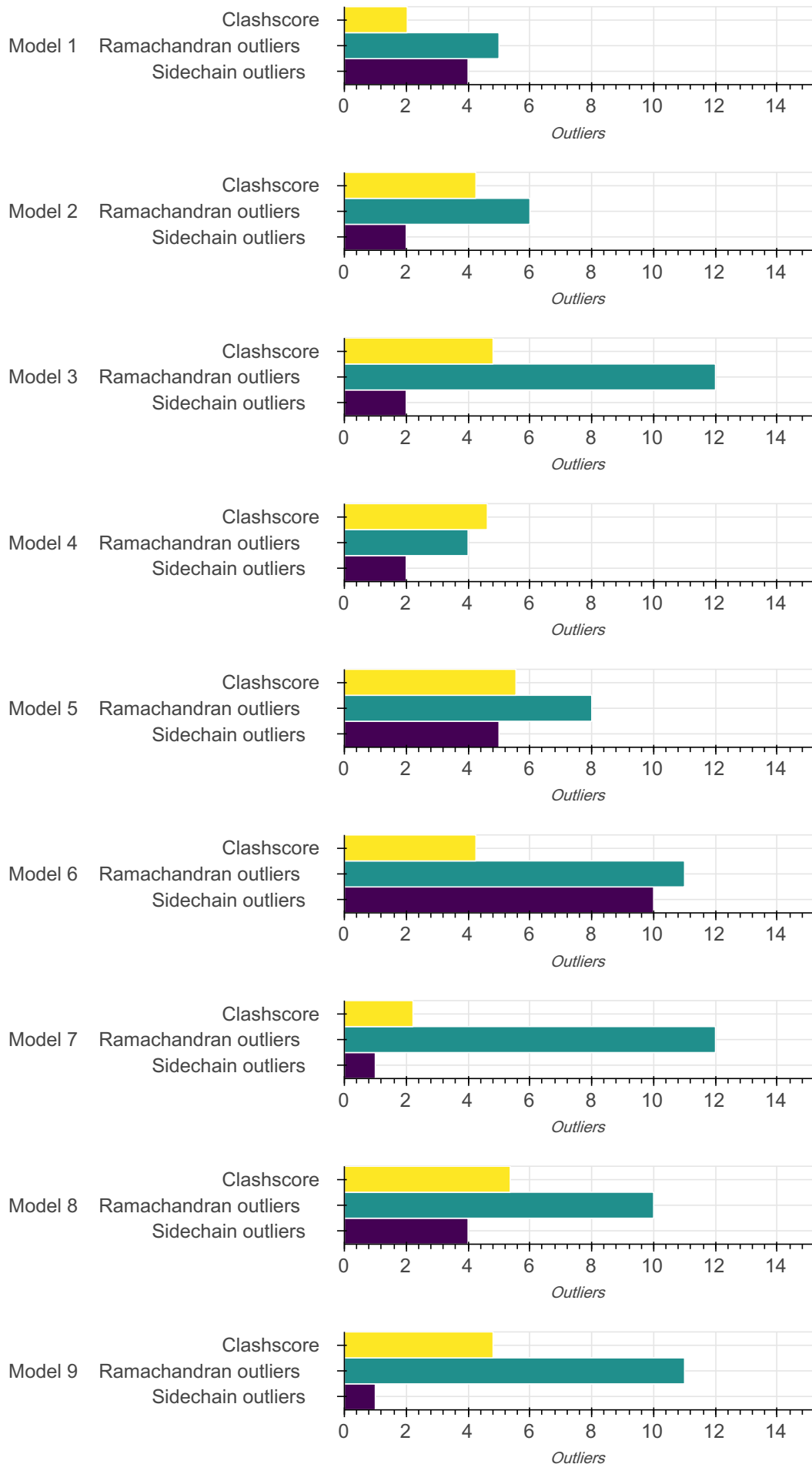
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

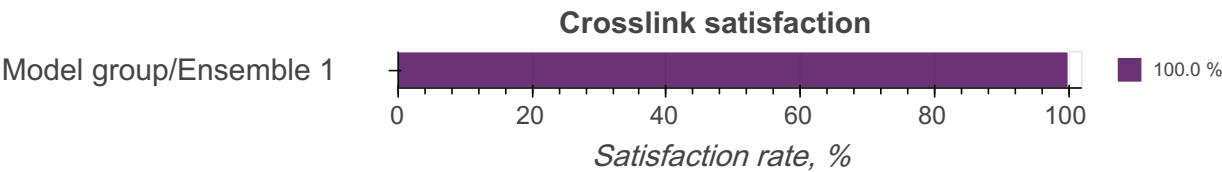
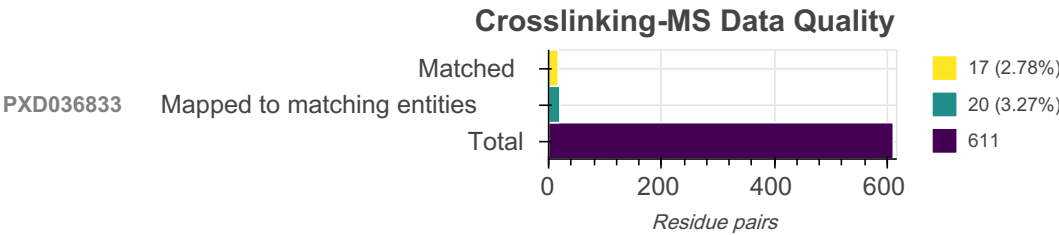
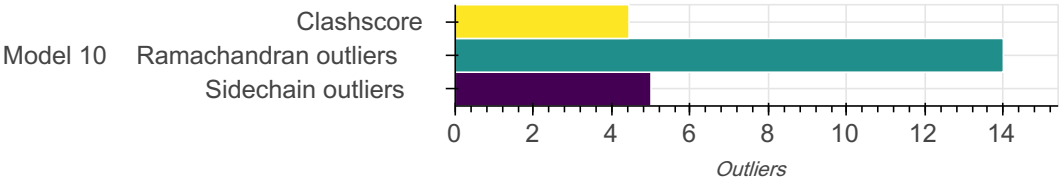
List of references used to build this report is available [here](#).

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	P02931	A	362	-	1-362	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	P02931	dbseq_P02931_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2Y	18	18 (100.00%)	17 (94.44%)
PXD036833	611	20 (3.27%)	17 (2.78%)

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 184 bond angle outliers in this entry (0.48% of 38440 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	318	GLU	C-N-CA	9.54	138.88	121.70	8	1
A	235	GLN	CA-CB-CG	8.15	130.39	114.10	10	1
A	309	GLY	C-N-CA	7.42	135.06	121.70	8	2
A	17	ALA	N-CA-CB	7.06	99.82	110.40	3	1
A	148	ASP	CA-CB-CG	6.82	119.42	112.60	5	1
A	326	ASN	OD1-CG-ND2	6.78	115.82	122.60	8	1
A	298	THR	CA-CB-OG1	6.64	99.64	109.60	5	1
A	145	ALA	C-N-CA	6.58	133.54	121.70	8	1
A	147	SER	N-CA-CB	6.58	121.68	110.50	6	1
A	72	GLN	OE1-CD-NE2	6.55	116.05	122.60	6	8
A	54	TYR	C-N-CA	6.19	132.84	121.70	4	1
A	155	VAL	CA-CB-CG2	6.07	120.72	110.40	2	1
A	317	PHE	C-N-CA	6.05	132.58	121.70	8	1
A	277	GLN	OE1-CD-NE2	5.98	116.62	122.60	10	8
A	16	VAL	C-N-CA	5.95	132.42	121.70	3	1
A	326	ASN	C-CA-CB	5.67	120.87	110.10	6	1
A	127	VAL	C-N-CA	5.67	131.91	121.70	6	1
A	235	GLN	OE1-CD-NE2	5.67	116.93	122.60	10	1
A	338	ASN	OD1-CG-ND2	5.62	116.98	122.60	5	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	2	MET	C-N-CA	5.55	131.69	121.70	7	1
A	132	GLY	C-N-CA	5.52	131.64	121.70	10	1
A	165	ASN	CA-CB-CG	5.52	118.12	112.60	10	1
A	82	GLN	OE1-CD-NE2	5.49	117.11	122.60	9	9
A	119	ASP	CA-CB-CG	5.46	118.06	112.60	7	1
A	136	MET	C-N-CA	5.33	131.30	121.70	8	1
A	135	ASP	CA-CB-CG	5.32	117.92	112.60	5	2
A	129	ASP	CA-CB-CG	5.31	117.91	112.60	10	3
A	101	ASN	CA-CB-CG	5.31	117.91	112.60	2	1
A	166	PHE	N-CA-CB	5.24	101.59	110.50	5	1
A	212	ALA	C-CA-CB	5.24	118.36	110.50	10	1
A	326	ASN	CA-CB-CG	5.23	117.83	112.60	6	2
A	339	GLN	OE1-CD-NE2	5.22	117.38	122.60	10	3
A	256	THR	CA-CB-CG2	5.22	119.38	110.50	10	1
A	344	ASN	CA-CB-CG	5.14	117.74	112.60	1	1
A	94	GLY	C-N-CA	5.10	130.88	121.70	3	3
A	128	TYR	C-N-CA	5.08	130.85	121.70	10	1
A	148	ASP	CA-C-N	5.07	126.35	116.20	3	1
A	344	ASN	C-N-CA	5.06	130.81	121.70	2	1
A	192	ASN	CA-CB-CG	5.02	107.58	112.60	4	1
A	104	ARG	CD-NE-CZ	5.00	131.40	124.40	9	1
A	90	ASN	CA-CB-CG	4.98	107.62	112.60	5	1
A	316	TYR	C-N-CA	4.93	130.58	121.70	8	1
A	286	GLN	OE1-CD-NE2	4.91	117.69	122.60	5	7
A	98	GLN	OE1-CD-NE2	4.89	117.71	122.60	8	9
A	310	ASP	N-CA-C	4.87	124.64	111.00	8	1
A	140	PHE	C-N-CA	4.86	130.46	121.70	9	2
A	148	ASP	O-C-N	4.86	115.22	123.00	3	1
A	183	ASN	OD1-CG-ND2	4.86	117.74	122.60	10	3
A	1	MET	C-N-CA	4.84	130.41	121.70	9	2
A	163	ASN	OD1-CG-ND2	4.82	117.78	122.60	1	1
A	252	ASN	OD1-CG-ND2	4.79	117.81	122.60	9	3
A	218	ARG	NE-CZ-NH2	4.78	123.50	119.20	1	5
A	88	GLN	OE1-CD-NE2	4.78	117.82	122.60	9	6
A	233	ALA	C-CA-CB	4.76	117.64	110.50	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	149	ASP	CA-CB-CG	4.76	117.36	112.60	8	2
A	91	ASN	OD1-CG-ND2	4.73	117.87	122.60	1	1
A	95	ALA	N-CA-C	4.70	124.17	111.00	9	3
A	122	ARG	NE-CZ-NH2	4.68	123.41	119.20	4	1
A	18	GLY	C-N-CA	4.60	129.97	121.70	5	1
A	151	PHE	C-N-CA	4.59	129.97	121.70	3	1
A	129	ASP	N-CA-CB	4.59	102.70	110.50	10	1
A	284	GLN	OE1-CD-NE2	4.57	118.03	122.60	8	1
A	192	ASN	OD1-CG-ND2	4.57	118.03	122.60	5	5
A	298	THR	CA-CB-CG2	4.55	118.23	110.50	5	1
A	90	ASN	C-N-CA	4.53	129.86	121.70	2	1
A	315	ASN	OD1-CG-ND2	4.52	118.08	122.60	5	6
A	311	VAL	C-N-CA	4.51	129.82	121.70	8	1
A	315	ASN	CA-C-N	4.50	125.20	116.20	8	1
A	318	GLU	O-C-N	4.49	115.81	123.00	8	1
A	274	ASN	CA-CB-CG	4.46	108.14	112.60	6	1
A	361	GLN	OE1-CD-NE2	4.44	118.16	122.60	5	1
A	96	ASP	CA-CB-CG	4.43	117.03	112.60	4	1
A	147	SER	C-CA-CB	4.42	101.69	110.10	6	1
A	68	LYS	CG-CD-CE	4.41	101.16	111.30	5	1
A	310	ASP	CA-CB-CG	4.41	117.01	112.60	10	1
A	338	ASN	CA-CB-CG	4.37	108.23	112.60	1	1
A	163	ASN	C-N-CA	4.35	129.53	121.70	1	1
A	91	ASN	C-N-CA	4.34	129.52	121.70	6	1
A	264	ASN	OD1-CG-ND2	4.32	118.28	122.60	9	1
A	20	ALA	C-N-CA	4.31	129.46	121.70	2	1
A	222	GLN	OE1-CD-NE2	4.31	118.29	122.60	9	1
A	110	LEU	C-N-CA	4.31	129.45	121.70	6	1
A	154	ARG	NE-CZ-NH1	4.30	125.80	121.50	9	1
A	27	ASN	C-CA-CB	4.27	118.22	110.10	5	1
A	133	TYR	CA-C-N	4.26	124.72	116.20	10	1
A	257	ARG	C-N-CA	4.26	129.36	121.70	1	1
A	140	PHE	CA-CB-CG	4.25	109.55	113.80	9	1
A	220	ASN	OD1-CG-ND2	4.24	118.36	122.60	6	1
A	314	VAL	CA-CB-CG1	4.24	117.60	110.40	10	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	56	GLY	C-N-CA	4.22	129.30	121.70	9	1
A	101	ASN	OD1-CG-ND2	4.19	118.41	122.60	1	1
A	218	ARG	NH1-CZ-NH2	4.17	113.88	119.30	4	2
A	319	VAL	CA-CB-CG1	4.17	117.49	110.40	8	1
A	344	ASN	OD1-CG-ND2	4.17	118.43	122.60	6	1
A	178	GLN	OE1-CD-NE2	4.16	118.44	122.60	6	2
A	246	ASN	OD1-CG-ND2	4.13	118.47	122.60	4	1
A	212	ALA	N-CA-CB	4.12	104.21	110.40	10	1
A	318	GLU	CA-C-N	4.11	124.43	116.20	8	1
A	57	ASN	OD1-CG-ND2	4.10	118.50	122.60	1	1
A	64	ARG	NE-CZ-NH2	4.09	122.88	119.20	4	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	2.03	11
2	4.25	23
3	4.81	26
4	4.62	25
5	5.55	30
6	4.25	23
7	2.22	12
8	5.36	29
9	4.81	26
10	4.44	24

There are 229 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:15:LEU:HD21	A:68:LYS:HZ3	0.84	5	1
A:10:ILE:HG21	A:292:ARG:HH22	0.83	5	1
A:155:VAL:HG22	A:189:ARG:CZ	0.82	4	1
A:162:ARG:HH12	A:176:ALA:HB2	0.80	3	1
A:15:LEU:HD13	A:167:PHE:HB3	0.77	5	1
A:151:PHE:CE2	A:212:ALA:HB1	0.73	10	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:262:ILE:HD11	A:305:VAL:HG13	0.73	9	1
A:154:ARG:HH12	A:256:THR:HG21	0.73	4	1
A:137:LEU:HD11	A:296:ALA:CB	0.71	3	1
A:42:LEU:HD23	A:332:TYR:OH	0.70	1	1
A:311:VAL:HG11	A:346:LEU:HB2	0.70	9	2
A:131:LEU:HD21	A:155:VAL:HG21	0.69	4	1
A:227:LEU:HD12	A:271:GLY:HA3	0.69	3	1
A:15:LEU:HD21	A:68:LYS:NZ	0.68	5	1
A:291:LEU:HD12	A:361:GLN:O	0.67	8	1
A:136:MET:HE1	A:321:ALA:HB3	0.67	10	1
A:151:PHE:CE1	A:280:LEU:HD11	0.66	7	1
A:151:PHE:O	A:155:VAL:HG22	0.65	2	1
A:191:SER:HB3	A:219:THR:HG21	0.65	9	2
A:21:ASN:HD21	A:327:LYS:HE3	0.64	2	1
A:60:MET:HE3	A:88:GLN:NE2	0.64	9	2
A:128:TYR:CZ	A:147:SER:HB3	0.64	6	1
A:154:ARG:NH1	A:256:THR:HG22	0.64	10	1
A:131:LEU:CD2	A:155:VAL:HG21	0.63	4	1
A:180:LEU:HD21	A:192:ASN:ND2	0.63	9	1
A:68:LYS:HE3	A:167:PHE:CE2	0.62	5	2
A:112:TYR:CE2	A:326:ASN:HB3	0.62	6	1
A:128:TYR:CE1	A:147:SER:HB3	0.61	6	1
A:35:LEU:HD13	A:67:PHE:CE2	0.61	9	3
A:165:ASN:HB3	A:167:PHE:CZ	0.61	10	1
A:136:MET:HE1	A:294:SER:CB	0.61	8	1
A:329:MET:HE1	A:332:TYR:CZ	0.61	10	1
A:42:LEU:HD13	A:62:TYR:CE1	0.60	8	1
A:262:ILE:HD11	A:306:GLU:OE1	0.60	6	1
A:154:ARG:CZ	A:256:THR:HG22	0.59	10	1
A:155:VAL:HG22	A:189:ARG:NE	0.59	4	1
A:134:THR:HG22	A:250:ALA:HB1	0.59	2	1
A:128:TYR:CZ	A:147:SER:CB	0.59	6	1
A:317:PHE:CZ	A:319:VAL:HG21	0.59	6	1
A:128:TYR:CE2	A:147:SER:N	0.58	6	1
A:8:ALA:O	A:9:VAL:HG23	0.58	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:166:PHE:CE2	A:167:PHE:CZ	0.58	1	1
A:140:PHE:CE2	A:355:ALA:HB2	0.57	3	1
A:15:LEU:CD2	A:68:LYS:HZ3	0.57	5	1
A:127:VAL:HG21	A:235:GLN:HG3	0.57	7	1
A:137:LEU:HD11	A:296:ALA:HB3	0.57	3	1
A:140:PHE:CZ	A:280:LEU:CD2	0.57	7	1
A:60:MET:HE1	A:143:ASP:O	0.57	5	1
A:154:ARG:NH1	A:256:THR:HG21	0.56	4	1
A:155:VAL:HG12	A:180:LEU:HD13	0.56	7	1
A:47:LYS:HE3	A:58:GLY:H	0.56	9	1
A:159:ALA:HB3	A:161:TYR:CZ	0.56	10	1
A:42:LEU:HD12	A:62:TYR:CE2	0.55	9	1
A:60:MET:HG2	A:90:ASN:HD21	0.55	9	1
A:151:PHE:HE1	A:280:LEU:HD11	0.55	7	1
A:236:TRP:CH2	A:253:TYR:CE1	0.55	6	3
A:7:LEU:HD13	A:33:VAL:HG21	0.55	6	1
A:107:PHE:CE1	A:167:PHE:CE2	0.54	3	1
A:21:ASN:HD21	A:327:LYS:CE	0.54	2	1
A:10:ILE:HD11	A:286:GLN:HG2	0.54	5	1
A:155:VAL:HA	A:189:ARG:NH2	0.54	4	1
A:60:MET:HE1	A:144:THR:HA	0.53	3	1
A:265:LYS:HZ2	A:348:VAL:HA	0.53	9	1
A:42:LEU:HD11	A:355:ALA:HB1	0.53	2	3
A:150:PHE:CZ	A:233:ALA:HB1	0.53	9	1
A:42:LEU:HD21	A:143:ASP:H	0.53	8	1
A:85:TYR:CE2	A:101:ASN:HB3	0.53	2	1
A:105:LEU:HD11	A:124:TYR:CZ	0.53	2	1
A:326:ASN:HD22	A:359:VAL:HG22	0.53	8	1
A:329:MET:CE	A:359:VAL:HG21	0.53	10	1
A:125:GLY:HA2	A:178:GLN:HE22	0.53	2	1
A:151:PHE:CZ	A:212:ALA:HB1	0.52	10	1
A:126:VAL:HG11	A:128:TYR:CE2	0.52	10	1
A:265:LYS:HE3	A:266:PHE:CZ	0.52	4	1
A:163:ASN:HD22	A:172:GLY:HA3	0.52	1	1
A:326:ASN:HD22	A:359:VAL:CG2	0.52	8	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:154:ARG:CZ	A:235:GLN:HB2	0.52	10	1
A:155:VAL:HG11	A:180:LEU:HD11	0.51	9	1
A:188:ALA:CB	A:221:LEU:HD22	0.51	10	1
A:150:PHE:CE2	A:261:PRO:HD2	0.51	3	1
A:35:LEU:HD11	A:65:LEU:HD11	0.51	2	2
A:274:ASN:ND2	A:313:LEU:HD12	0.51	6	1
A:132:GLY:C	A:134:THR:H	0.51	4	1
A:302:ALA:HB2	A:314:VAL:HG22	0.50	6	1
A:21:ASN:ND2	A:328:ASN:HD21	0.50	2	1
A:338:ASN:ND2	A:350:SER:H	0.50	9	1
A:225:GLN:OE1	A:316:TYR:CD1	0.50	8	1
A:155:VAL:HG13	A:189:ARG:NH2	0.49	4	1
A:154:ARG:NH1	A:235:GLN:HB3	0.49	10	1
A:162:ARG:NH1	A:176:ALA:HB2	0.49	3	1
A:311:VAL:HG11	A:346:LEU:HD11	0.49	3	1
A:53:SER:C	A:55:GLY:H	0.49	4	1
A:311:VAL:HG21	A:346:LEU:HD12	0.49	9	1
A:107:PHE:CZ	A:167:PHE:CZ	0.49	3	1
A:227:LEU:HD12	A:271:GLY:CA	0.49	3	1
A:151:PHE:CE1	A:278:ASP:HB3	0.49	7	1
A:154:ARG:NH2	A:189:ARG:HA	0.49	7	1
A:45:PHE:CZ	A:336:ILE:CD1	0.49	9	1
A:160:THR:HG21	A:162:ARG:NH1	0.49	9	1
A:137:LEU:HD11	A:296:ALA:HB2	0.49	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	360	335	20	5
2	360	322	32	6
3	360	317	31	12
4	360	329	27	4
5	360	327	25	8
6	360	317	32	11

Model ID	Analysed	Favored	Allowed	Outliers
7	360	321	27	12
8	360	319	31	10
9	360	313	36	11
10	360	317	29	14

There are 69 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	54	TYR	6
A	97	ALA	4
A	95	ALA	3
A	141	GLY	3
A	327	LYS	3
A	9	VAL	2
A	12	PRO	2
A	17	ALA	2
A	21	ASN	2
A	29	ASP	2
A	51	GLU	2
A	100	GLY	2
A	133	TYR	2
A	164	SER	2
A	331	THR	2
A	2	MET	1
A	3	LYS	1
A	4	ARG	1
A	5	ASN	1
A	8	ALA	1
A	10	ILE	1
A	13	ALA	1
A	15	LEU	1
A	16	VAL	1
A	18	GLY	1
A	20	ALA	1
A	22	ALA	1
A	24	GLU	1

Chain	Res	Type	Models (Total)
A	55	GLY	1
A	56	GLY	1
A	57	ASN	1
A	59	ASP	1
A	91	ASN	1
A	92	SER	1
A	93	GLU	1
A	94	GLY	1
A	98	GLN	1
A	99	THR	1
A	101	ASN	1
A	115	VAL	1
A	121	GLY	1
A	129	ASP	1
A	131	LEU	1
A	132	GLY	1
A	135	ASP	1
A	136	MET	1
A	137	LEU	1
A	142	GLY	1
A	143	ASP	1
A	145	ALA	1
A	146	TYR	1
A	147	SER	1
A	148	ASP	1
A	149	ASP	1
A	155	VAL	1
A	158	VAL	1
A	161	TYR	1
A	165	ASN	1
A	166	PHE	1
A	168	GLY	1
A	169	LEU	1
A	170	VAL	1
A	229	ASN	1

Chain	Res	Type	Models (Total)
A	245	ASN	1
A	310	ASP	1
A	314	VAL	1
A	326	ASN	1
A	344	ASN	1
A	345	LYS	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	279	267	8	4
2	279	267	10	2
3	279	271	6	2
4	279	268	9	2
5	279	269	5	5
6	279	257	12	10
7	279	273	5	1
8	279	261	14	4
9	279	272	6	1
10	279	261	13	5

There are 30 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	92	SER	3
A	155	VAL	3
A	144	THR	2
A	269	THR	2
A	2	MET	1
A	11	VAL	1
A	15	LEU	1
A	27	ASN	1
A	77	LEU	1
A	78	THR	1
A	105	LEU	1
A	115	VAL	1

Chain	Res	Type	Models (Total)
A	117	SER	1
A	126	VAL	1
A	134	THR	1
A	136	MET	1
A	151	PHE	1
A	152	VAL	1
A	164	SER	1
A	166	PHE	1
A	170	VAL	1
A	187	THR	1
A	260	THR	1
A	308	ILE	1
A	313	LEU	1
A	319	VAL	1
A	330	SER	1
A	331	THR	1
A	344	ASN	1
A	350	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.

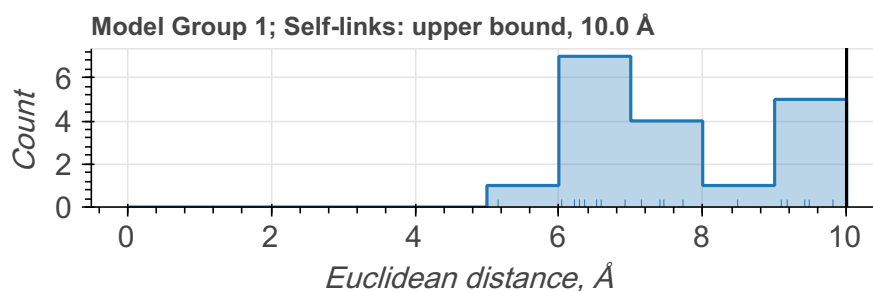
There are 18 crosslinking restraints combined in 18 restraint groups.

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	1
L-Photo-Leucine	LEU	CA	VAL	CA	upper bound	10.0	1
L-Photo-Leucine	GLU	CA	LEU	CA	upper bound	10.0	3
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	4
L-Photo-Leucine	GLN	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ILE	CA	LEU	CA	upper bound	10.0	1

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	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	PRO	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	SER	CA	upper bound	10.0	2
L-Photo-Leucine	LEU	CA	TYR	CA	upper bound	10.0	1
L-Photo-Leucine	ASN	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.



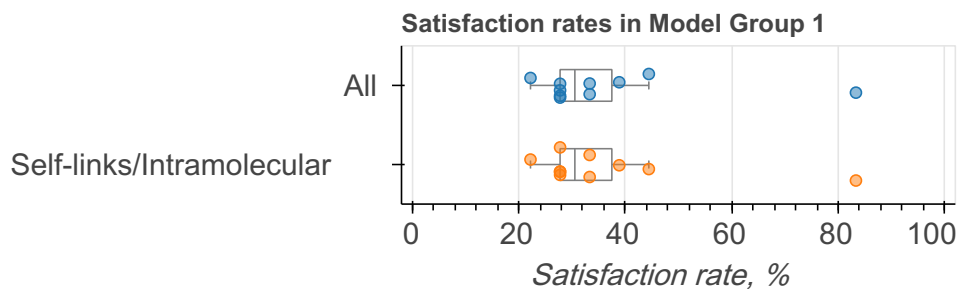
Satisfaction of restraints

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=18)
1	1	1	10/10	All	100.00	0.00	18
				Self-links/ Intramolecular	100.00	0.00	18

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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