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	9A2M
PDB-Dev ID	PDBDEV_00000171
Structure Title	Model of E. coli OmpA 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

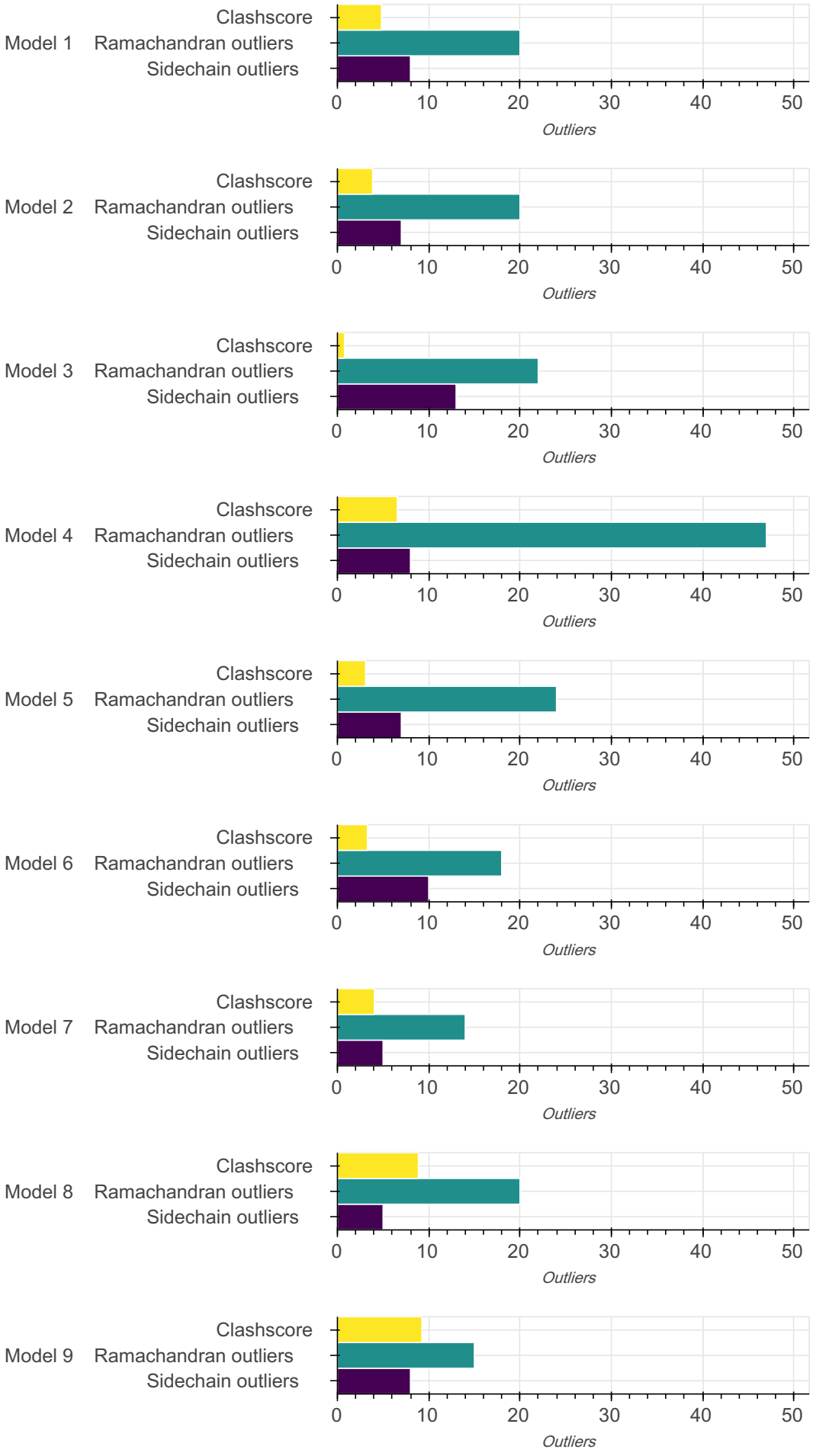
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

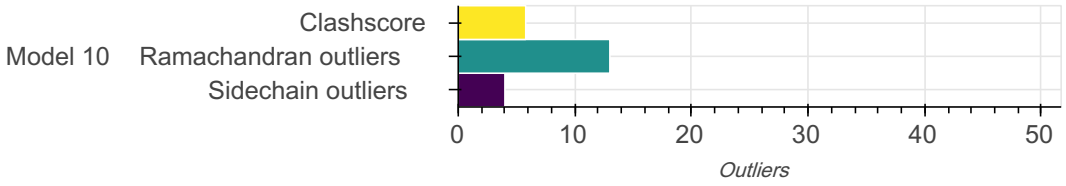
List of references used to build this report is available here.

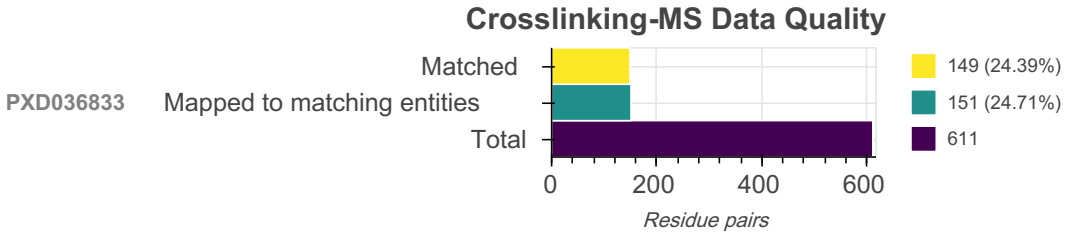
Overall quality

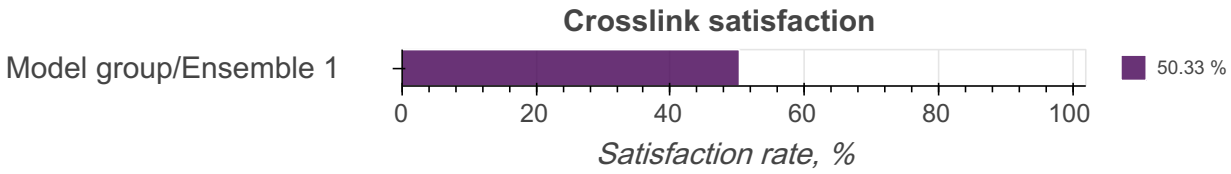
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis


Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Clashscore
Ramachandran outliers
Sidechain outliers
0
10
20
30
40
50
Outliers







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	P0A910	A	346	-	1-346	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	P0A910	dbseq_P0A910_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2M	151	151 (100.00%)	149 (98.68%)
PXD036833	611	151 (24.71%)	149 (24.39%)

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 320 bond angle outliers in this entry (0.88% of 36512 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	336	GLY	C-N-CA	8.54	137.06	121.70	3	2
A	338	LYS	C-N-CA	8.43	136.87	121.70	8	5
A	322	ASP	C-N-CA	8.00	136.09	121.70	1	1
A	339	ASP	O-C-N	7.92	110.33	123.00	4	2
A	218	LYS	C-N-CA	7.64	135.45	121.70	6	1
A	317	ARG	C-N-CA	7.56	135.31	121.70	6	2
A	339	ASP	C-N-CA	7.48	135.17	121.70	10	2
A	321	ILE	C-N-CA	7.23	108.69	121.70	1	2
A	169	GLY	C-N-CA	6.96	134.23	121.70	7	2
A	3	LYS	C-N-CA	6.96	134.23	121.70	9	3
A	325	ALA	CA-C-N	6.94	127.30	116.90	6	1
A	2	LYS	C-N-CA	6.91	134.14	121.70	5	3
A	339	ASP	C-CA-CB	6.74	122.90	110.10	4	1
A	26	ASN	OD1-CG-ND2	6.71	115.89	122.60	10	4
A	316	GLN	C-N-CA	6.65	133.67	121.70	1	5
A	342	THR	C-N-CA	6.56	133.51	121.70	4	2
A	206	PRO	C-CA-CB	6.33	122.12	110.10	6	1
A	77	ASP	CA-CB-CG	6.30	118.90	112.60	4	2
A	212	THR	C-N-CA	6.26	132.96	121.70	7	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	45	ILE	C-N-CA	6.21	132.88	121.70	3	2
A	220	ASP	CA-CB-CG	6.21	118.81	112.60	7	1
A	126	ASP	CA-CB-CG	6.12	118.72	112.60	10	1
A	343	GLN	C-CA-CB	6.11	121.72	110.10	8	1
A	99	GLN	OE1-CD-NE2	6.01	116.59	122.60	8	9
A	343	GLN	CA-C-N	6.00	125.90	116.90	8	1
A	329	ARG	C-N-CA	5.96	132.42	121.70	8	1
A	341	VAL	C-N-CA	5.92	132.35	121.70	4	1
A	322	ASP	C-CA-CB	5.91	121.34	110.10	1	1
A	308	GLY	C-N-CA	5.85	132.22	121.70	1	4
A	55	GLN	OE1-CD-NE2	5.84	116.76	122.60	1	2
A	323	CYS	C-N-CA	5.82	132.18	121.70	8	2
A	217	LEU	C-N-CA	5.82	132.18	121.70	6	1
A	235	GLN	OE1-CD-NE2	5.76	116.84	122.60	9	10
A	208	PRO	C-N-CA	5.75	132.04	121.70	1	2
A	202	PRO	C-N-CA	5.71	131.98	121.70	6	1
A	193	GLN	OE1-CD-NE2	5.69	116.91	122.60	7	6
A	324	LEU	CA-CB-CG	5.62	135.98	116.30	1	1
A	1	MET	C-N-CA	5.62	131.81	121.70	1	3
A	309	ASN	C-N-CA	5.62	131.81	121.70	8	4
A	20	GLN	OE1-CD-NE2	5.58	117.02	122.60	5	5
A	193	GLN	C-N-CA	5.50	131.60	121.70	5	1
A	263	ARG	C-N-CA	5.50	131.60	121.70	6	2
A	340	VAL	CA-CB-CG1	5.50	119.75	110.40	10	1
A	317	ARG	N-CA-C	5.50	126.39	111.00	1	1
A	319	ALA	C-N-CA	5.49	131.59	121.70	7	1
A	345	GLN	OE1-CD-NE2	5.44	117.16	122.60	3	9
A	50	PRO	N-CA-CB	5.44	108.98	103.00	10	1
A	180	ASN	OD1-CG-ND2	5.40	117.20	122.60	4	1
A	38	GLN	OE1-CD-NE2	5.39	117.21	122.60	2	8
A	315	LYS	C-N-CA	5.30	131.24	121.70	5	2
A	337	ILE	C-N-CA	5.28	131.21	121.70	6	1
A	25	ASP	C-N-CA	5.27	131.19	121.70	4	1
A	213	LYS	C-N-CA	5.26	131.16	121.70	5	2
A	65	GLN	OE1-CD-NE2	5.21	117.39	122.60	5	9

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	320	LEU	C-N-CA	5.21	131.08	121.70	1	1
A	170	ASP	CA-CB-CG	5.20	117.80	112.60	5	1
A	166	ASN	OD1-CG-ND2	5.18	117.42	122.60	5	4
A	328	ARG	C-N-CA	5.16	130.99	121.70	5	3
A	254	SER	C-N-CA	5.15	130.97	121.70	5	1
A	255	VAL	C-N-CA	5.14	130.96	121.70	10	1
A	96	GLN	OE1-CD-NE2	5.11	117.49	122.60	5	10
A	211	GLN	OE1-CD-NE2	5.09	117.51	122.60	4	2
A	344	PRO	C-N-CA	5.05	130.78	121.70	2	1
A	316	GLN	OE1-CD-NE2	5.02	117.58	122.60	4	5
A	240	GLN	OE1-CD-NE2	5.02	117.58	122.60	8	9
A	334	VAL	C-N-CA	5.02	130.73	121.70	5	1
A	197	ALA	CA-C-O	5.01	112.29	120.80	8	1
A	282	VAL	CA-CB-CG1	4.99	118.89	110.40	10	1
A	195	GLU	C-N-CA	4.98	130.67	121.70	7	1
A	170	ASP	C-N-CA	4.98	130.66	121.70	5	1
A	328	ARG	NE-CZ-NH2	4.97	123.68	119.20	6	1
A	216	THR	CA-CB-CG2	4.94	118.90	110.50	9	1
A	286	ILE	CA-CB-CG2	4.94	118.89	110.50	10	1
A	218	LYS	CA-C-N	4.92	126.04	116.20	6	2
A	318	ALA	C-N-CA	4.91	130.55	121.70	8	2
A	113	ASP	CA-CB-CG	4.90	117.50	112.60	3	1
A	343	GLN	OE1-CD-NE2	4.87	117.73	122.60	6	6
A	319	ALA	N-CA-CB	4.87	103.10	110.40	1	1
A	135	ASN	C-N-CA	4.82	130.37	121.70	4	1
A	82	MET	CA-CB-CG	4.81	104.48	114.10	8	1
A	244	GLN	OE1-CD-NE2	4.80	117.80	122.60	4	10
A	313	ASN	OD1-CG-ND2	4.80	117.80	122.60	10	1
A	153	THR	CA-C-N	4.80	124.09	116.90	3	1
A	324	LEU	C-N-CA	4.75	130.25	121.70	1	1
A	67	ASN	OD1-CG-ND2	4.74	117.86	122.60	4	1
A	199	VAL	N-CA-C	4.72	97.79	111.00	8	1
A	13	ALA	C-N-CA	4.71	130.18	121.70	5	1
A	323	CYS	CA-C-N	4.70	125.61	116.20	1	1
A	37	SER	C-CA-CB	4.68	118.99	110.10	4	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	262	ASP	CA-CB-CG	4.66	117.26	112.60	4	1
A	46	ASN	OD1-CG-ND2	4.65	117.95	122.60	2	1
A	163	GLN	OE1-CD-NE2	4.65	117.95	122.60	6	7
A	253	GLY	C-N-CA	4.63	130.04	121.70	10	3
A	319	ALA	N-CA-C	4.62	123.93	111.00	6	2
A	345	GLN	C-N-CA	4.60	129.98	121.70	5	2
A	46	ASN	C-N-CA	4.59	129.96	121.70	3	2
A	159	ARG	NE-CZ-NH2	4.58	123.32	119.20	10	2
A	338	LYS	CA-C-N	4.58	125.35	116.20	8	1
A	172	HIS	CB-CG-CD2	4.57	125.26	131.20	8	4
A	167	ASN	CA-CB-CG	4.56	117.16	112.60	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	4.82	25
2	3.86	20
3	0.77	4
4	6.56	34
5	3.09	16
6	3.28	17
7	4.05	21
8	8.87	46
9	9.26	48
10	5.78	30

There are 261 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:230:LEU:HD22	A:284:TYR:CE2	0.90	9	2
A:230:LEU:HD13	A:284:TYR:CD1	0.86	10	1
A:322:ASP:C	A:324:LEU:HB2	0.86	1	1
A:286:ILE:HD13	A:295:ILE:HD13	0.82	10	2
A:217:LEU:HA	A:345:GLN:HA	0.82	9	1
A:238:LEU:HB3	A:285:LEU:HD21	0.77	8	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:258:LEU:CD2	A:330:VAL:H	0.77	8	2
A:261:THR:HG22	A:273:LEU:CD2	0.76	8	1
A:241:LEU:HD22	A:340:VAL:HG21	0.70	4	1
A:238:LEU:CB	A:285:LEU:HD21	0.68	8	1
A:258:LEU:HD22	A:329:ARG:HA	0.67	9	3
A:123:TRP:CZ2	A:169:GLY:HA2	0.67	9	1
A:101:THR:HG22	A:119:GLY:HA3	0.66	5	1
A:322:ASP:O	A:324:LEU:HB2	0.65	1	1
A:278:ALA:HB1	A:297:ALA:HB1	0.65	1	4
A:165:THR:HB	A:168:ILE:HD11	0.64	9	2
A:94:LYS:HE3	A:126:ASP:HB2	0.64	10	1
A:230:LEU:HD13	A:284:TYR:CG	0.64	10	1
A:258:LEU:CD2	A:300:MET:HE2	0.64	4	1
A:209:GLU:HB3	A:217:LEU:HD13	0.64	8	1
A:261:THR:HG22	A:273:LEU:HD23	0.64	8	1
A:333:GLU:O	A:334:VAL:HG23	0.64	5	1
A:211:GLN:O	A:212:THR:HG23	0.63	5	1
A:302:GLU:CD	A:320:LEU:HD11	0.63	5	1
A:39:TYR:CE1	A:82:MET:HE2	0.63	9	1
A:209:GLU:CB	A:217:LEU:HB3	0.62	2	1
A:323:CYS:N	A:324:LEU:HB2	0.62	1	1
A:210:VAL:O	A:217:LEU:HD12	0.61	8	1
A:43:GLY:CA	A:176:THR:HG21	0.60	6	2
A:200:VAL:HG13	A:269:TYR:CE1	0.60	9	1
A:248:LEU:HD11	A:339:ASP:HB2	0.60	4	1
A:42:THR:HG21	A:82:MET:HE1	0.59	10	1
A:123:TRP:CZ2	A:169:GLY:CA	0.59	9	1
A:230:LEU:HD11	A:284:TYR:CZ	0.59	7	1
A:24:LYS:H	A:193:GLN:NE2	0.58	5	1
A:215:PHE:CE2	A:217:LEU:HD11	0.58	8	1
A:230:LEU:HD22	A:284:TYR:CD2	0.58	10	2
A:286:ILE:HG12	A:295:ILE:HD12	0.57	4	1
A:111:ASP:CG	A:143:VAL:HG13	0.57	4	1
A:230:LEU:HD13	A:284:TYR:CE1	0.57	10	1
A:258:LEU:HD22	A:330:VAL:H	0.57	8	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:39:TYR:CD1	A:82:MET:HE1	0.56	8	1
A:123:TRP:HZ3	A:125:ALA:HB2	0.56	9	1
A:144:PHE:HB2	A:164:TRP:CD1	0.56	5	1
A:33:LYS:C	A:35:GLY:H	0.56	4	1
A:341:VAL:O	A:342:THR:HG23	0.56	10	1
A:19:ALA:HA	A:191:PHE:CZ	0.56	7	2
A:39:TYR:CE1	A:53:GLU:HB2	0.56	5	1
A:39:TYR:CZ	A:178:PRO:CG	0.56	1	1
A:287:SER:C	A:346:ALA:HB3	0.55	4	1
A:230:LEU:HB3	A:284:TYR:CE1	0.55	9	1
A:124:ARG:HH21	A:136:HIS:CE1	0.55	9	1
A:217:LEU:HD23	A:345:GLN:HA	0.55	9	1
A:306:VAL:O	A:307:THR:HG23	0.55	2	2
A:199:VAL:C	A:201:ALA:H	0.55	8	1
A:282:VAL:HG13	A:295:ILE:HG21	0.55	4	3
A:43:GLY:HA3	A:176:THR:HG21	0.55	2	1
A:218:LYS:C	A:346:ALA:HA	0.55	9	1
A:197:ALA:O	A:198:PRO:C	0.55	8	3
A:290:ILE:HG21	A:295:ILE:HD11	0.54	4	1
A:39:TYR:CZ	A:178:PRO:HG3	0.54	1	1
A:123:TRP:CH2	A:169:GLY:HA3	0.54	9	1
A:43:GLY:HA2	A:176:THR:HG21	0.54	6	1
A:250:PRO:HG2	A:338:LYS:HE3	0.54	1	1
A:282:VAL:HG22	A:295:ILE:CG2	0.54	9	2
A:215:PHE:HE2	A:217:LEU:HD11	0.53	8	1
A:121:MET:HE2	A:123:TRP:HB3	0.53	7	1
A:230:LEU:HB2	A:284:TYR:CZ	0.53	10	1
A:209:GLU:HB3	A:217:LEU:HB3	0.53	2	1
A:155:GLU:CG	A:194:GLY:HA3	0.53	9	1
A:217:LEU:HA	A:345:GLN:CA	0.53	9	1
A:258:LEU:HD22	A:300:MET:HE2	0.52	4	1
A:321:ILE:HG23	A:323:CYS:SG	0.52	1	1
A:19:ALA:HA	A:28:TRP:CD1	0.52	10	1
A:230:LEU:HD12	A:284:TYR:CG	0.52	4	1
A:286:ILE:CG1	A:295:ILE:HD12	0.52	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:122:VAL:HG23	A:143:VAL:CG2	0.51	5	1
A:39:TYR:CD1	A:82:MET:SD	0.51	8	1
A:256:VAL:HA	A:331:GLU:HA	0.51	8	1
A:39:TYR:CD1	A:82:MET:CE	0.51	8	1
A:216:THR:HB	A:345:GLN:CD	0.51	9	1
A:319:ALA:C	A:321:ILE:H	0.51	1	1
A:199:VAL:C	A:201:ALA:N	0.51	8	1
A:213:LYS:O	A:214:HIS:CD2	0.51	9	1
A:3:LYS:O	A:4:THR:HG23	0.50	2	1
A:209:GLU:CD	A:217:LEU:HD22	0.50	2	1
A:153:THR:HB	A:154:PRO:HD2	0.50	5	1
A:230:LEU:CB	A:284:TYR:CZ	0.50	10	1
A:333:GLU:OE2	A:335:LYS:HE3	0.50	2	1
A:19:ALA:HA	A:191:PHE:CE1	0.50	7	1
A:261:THR:HG22	A:273:LEU:HD22	0.50	8	1
A:202:PRO:HA	A:338:LYS:HE3	0.50	4	1
A:217:LEU:HD23	A:345:GLN:H	0.50	9	1
A:309:ASN:O	A:310:THR:HG23	0.50	4	1
A:217:LEU:HD23	A:345:GLN:N	0.50	9	1
A:238:LEU:HD13	A:285:LEU:CD2	0.50	10	1
A:15:PHE:CE2	A:30:THR:HG23	0.50	7	1
A:255:VAL:HG21	A:337:ILE:CD1	0.49	2	1
A:168:ILE:HD12	A:180:ASN:HB2	0.49	9	1
A:274:SER:HB3	A:299:GLY:CA	0.49	9	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	344	288	36	20
2	344	298	26	20
3	344	243	79	22
4	344	236	61	47
5	344	281	39	24
6	344	296	30	18
7	344	304	26	14

Model ID	Analysed	Favored	Allowed	Outliers
8	344	296	28	20
9	344	286	43	15
10	344	303	28	13

There are 108 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	345	GLN	7
A	174	ILE	6
A	340	VAL	6
A	342	THR	6
A	3	LYS	5
A	200	VAL	5
A	313	ASN	5
A	317	ARG	5
A	2	LYS	4
A	17	THR	4
A	47	ASN	4
A	90	ASN	4
A	211	GLN	4
A	213	LYS	4
A	214	HIS	4
A	264	ILE	4
A	309	ASN	4
A	15	PHE	3
A	46	ASN	3
A	170	ASP	3
A	171	ALA	3
A	199	VAL	3
A	302	GLU	3
A	308	GLY	3
A	315	LYS	3
A	323	CYS	3
A	339	ASP	3
A	344	PRO	3
A	12	LEU	2

Chain	Res	Type	Models (Total)
A	14	GLY	2
A	26	ASN	2
A	45	ILE	2
A	52	HIS	2
A	53	GLU	2
A	172	HIS	2
A	273	LEU	2
A	304	ASN	2
A	305	PRO	2
A	316	GLN	2
A	319	ALA	2
A	324	LEU	2
A	325	ALA	2
A	327	ASP	2
A	329	ARG	2
A	333	GLU	2
A	337	ILE	2
A	343	GLN	2
A	7	ALA	1
A	10	VAL	1
A	13	ALA	1
A	16	ALA	1
A	18	VAL	1
A	22	ALA	1
A	23	PRO	1
A	34	LEU	1
A	36	TRP	1
A	38	GLN	1
A	40	HIS	1
A	41	ASP	1
A	43	GLY	1
A	44	PHE	1
A	48	ASN	1
A	51	THR	1
A	58	ALA	1

Chain	Res	Type	Models (Total)
A	62	GLY	1
A	85	LYS	1
A	130	ASN	1
A	134	LYS	1
A	136	HIS	1
A	137	ASP	1
A	140	VAL	1
A	148	VAL	1
A	153	THR	1
A	168	ILE	1
A	176	THR	1
A	179	ASP	1
A	181	GLY	1
A	193	GLN	1
A	194	GLY	1
A	195	GLU	1
A	202	PRO	1
A	203	ALA	1
A	207	ALA	1
A	209	GLU	1
A	210	VAL	1
A	212	THR	1
A	217	LEU	1
A	219	SER	1
A	228	ALA	1
A	249	ASP	1
A	250	PRO	1
A	252	ASP	1
A	275	GLU	1
A	287	SER	1
A	301	GLY	1
A	306	VAL	1
A	307	THR	1
A	310	THR	1
A	311	CYS	1

Chain	Res	Type	Models (Total)
A	312	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	271	248	15	8
2	271	255	9	7
3	271	249	9	13
4	271	244	19	8
5	271	256	8	7
6	271	252	9	10
7	271	260	6	5
8	271	258	8	5
9	271	259	4	8
10	271	256	11	4

There are 50 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	4	THR	6
A	241	LEU	6
A	173	THR	3
A	222	LEU	3
A	225	PHE	3
A	230	LEU	3
A	51	THR	2
A	164	TRP	2
A	185	LEU	2
A	219	SER	2
A	248	LEU	2
A	307	THR	2
A	314	VAL	2
A	17	THR	1
A	18	VAL	1
A	77	ASP	1
A	84	TYR	1

Chain	Res	Type	Models (Total)
A	88	VAL	1
A	113	ASP	1
A	116	THR	1
A	127	THR	1
A	131	VAL	1
A	138	THR	1
A	158	THR	1
A	172	HIS	1
A	206	PRO	1
A	212	THR	1
A	217	LEU	1
A	226	ASN	1
A	238	LEU	1
A	261	THR	1
A	262	ASP	1
A	263	ARG	1
A	267	ASP	1
A	269	TYR	1
A	273	LEU	1
A	274	SER	1
A	275	GLU	1
A	295	ILE	1
A	303	SER	1
A	306	VAL	1
A	310	THR	1
A	311	CYS	1
A	320	LEU	1
A	323	CYS	1
A	327	ASP	1
A	339	ASP	1
A	340	VAL	1
A	341	VAL	1
A	343	GLN	1

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

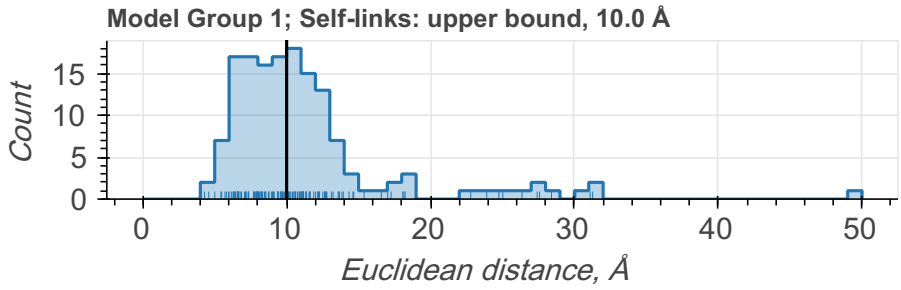
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

There are 151 crosslinking restraints combined in 151 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	11
L-Photo-Leucine	GLU	CA	LEU	CA	upper bound	10.0	11
L-Photo-Leucine	LEU	CA	VAL	CA	upper bound	10.0	17
L-Photo-Leucine	GLY	CA	LEU	CA	upper bound	10.0	15
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	21
L-Photo-Leucine	LEU	CA	THR	CA	upper bound	10.0	8
L-Photo-Leucine	ALA	CA	LEU	CA	upper bound	10.0	20
L-Photo-Leucine	ILE	CA	LEU	CA	upper bound	10.0	9
L-Photo-Leucine	LEU	CA	LYS	CA	upper bound	10.0	3
L-Photo-Leucine	CYS	CA	LEU	CA	upper bound	10.0	3
L-Photo-Leucine	ARG	CA	LEU	CA	upper bound	10.0	3
L-Photo-Leucine	LEU	CA	SER	CA	upper bound	10.0	5
L-Photo-Leucine	LEU	CA	PRO	CA	upper bound	10.0	7
L-Photo-Leucine	LEU	CA	LEU	CA	upper bound	10.0	6
L-Photo-Leucine	GLN	CA	LEU	CA	upper bound	10.0	5
L-Photo-Leucine	HIS	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ASN	CA	LEU	CA	upper bound	10.0	4
L-Photo-Leucine	LEU	CA	MET	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.



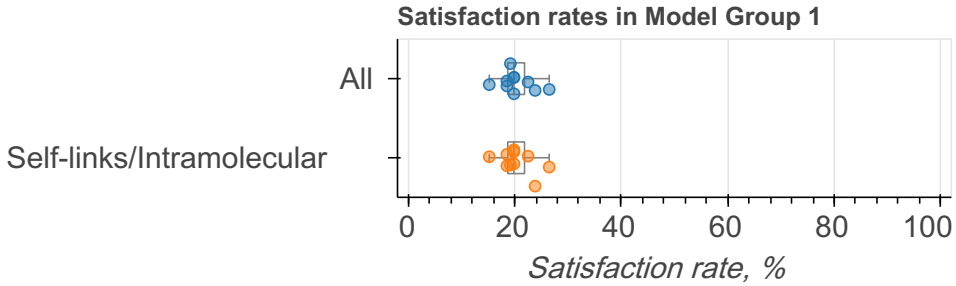
Satisfaction of restraints

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=151)
1	1	1	10/10	All	50.33	49.67	151
				Self-links/ Intramolecular	50.33	49.67	151

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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