

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	9A37
PDB-Dev ID	PDBDEV_00000192
Structure Title	Model of E. coli OppA 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

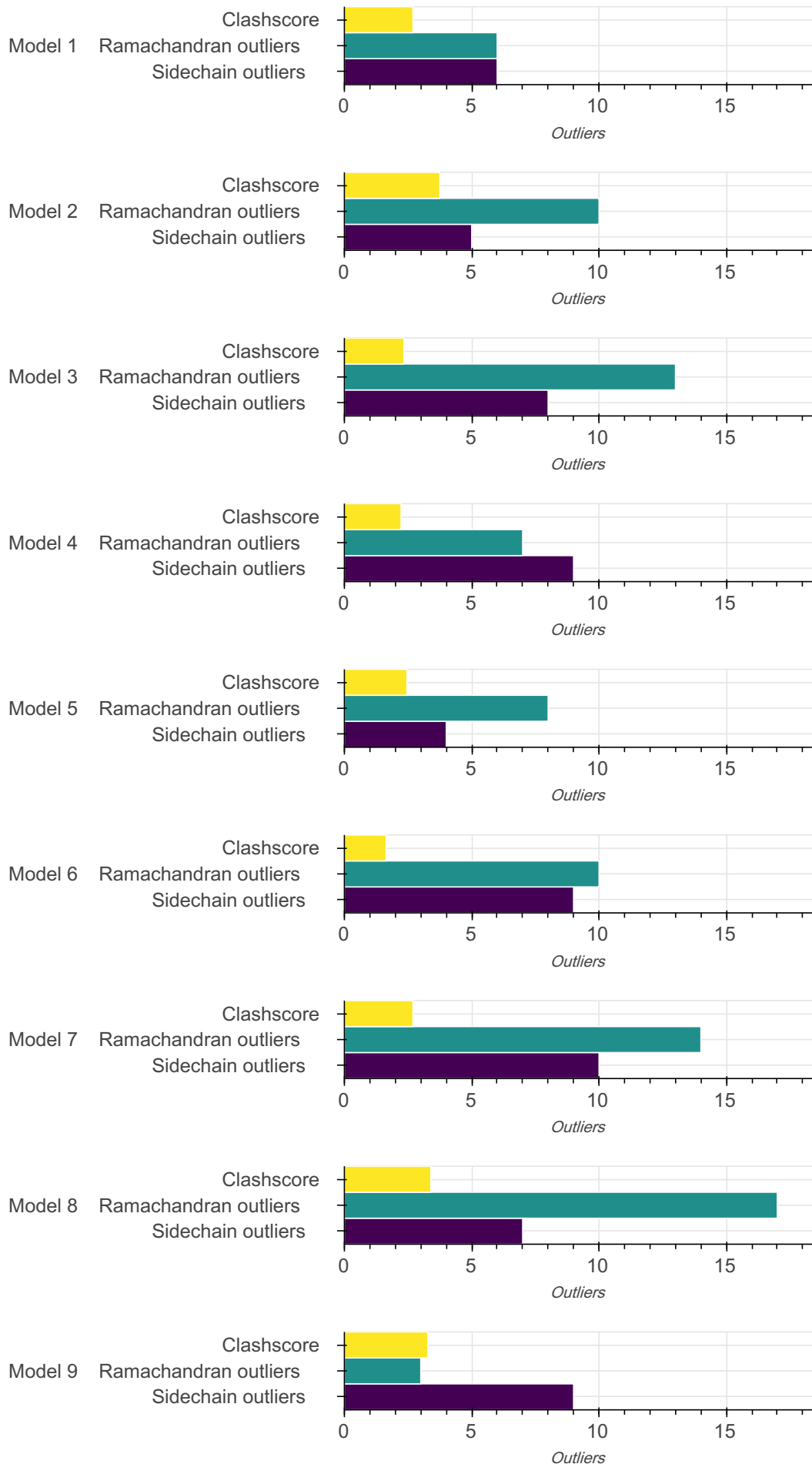
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

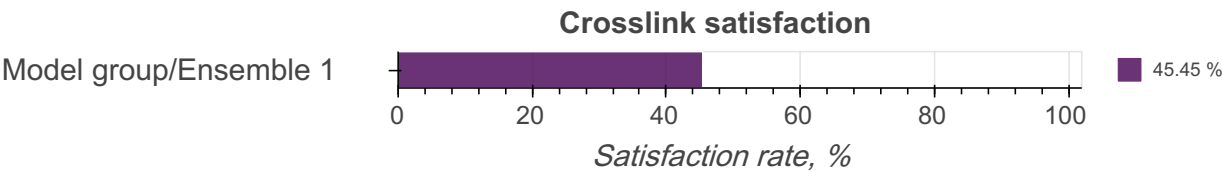
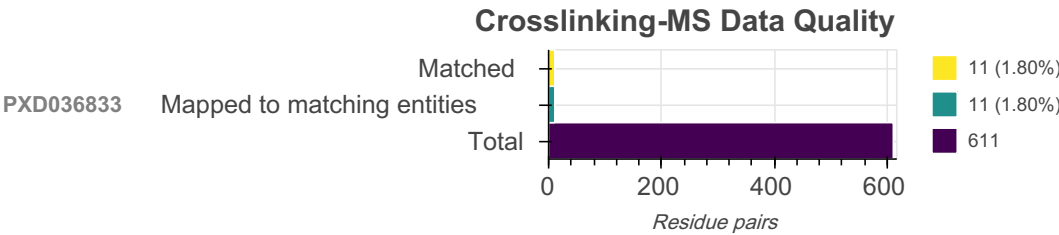
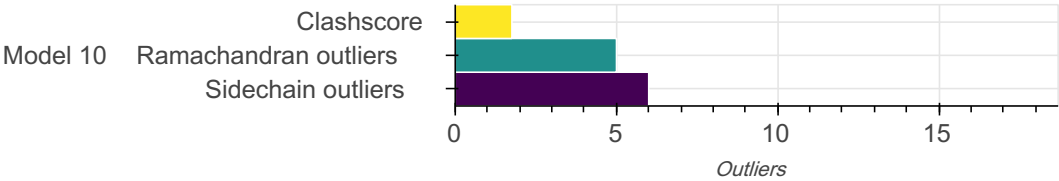
List of references used to build this report is available [here](#).

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	P23843	A	543	-	1-543	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	P23843	dbseq_P23843_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A37	11	11 (100.00%)	11 (100.00%)
PXD036833	611	11 (1.80%)	11 (1.80%)

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 44090 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	55	HIS	CE1-NE2	123.63	2.56	1.32	4	1
A	55	HIS	ND1-CE1	81.75	2.14	1.32	4	1
A	55	HIS	CD2-NE2	68.91	2.13	1.37	4	1

Standard geometry: angle outliers ?

There are 253 bond angle outliers in this entry (0.42% of 60140 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	55	HIS	ND1-CE1-NE2	23.39	85.01	108.40	4	1
A	55	HIS	CD2-NE2-CE1	22.30	86.70	109.00	4	1
A	55	HIS	CG-CD2-NE2	21.99	129.19	107.20	4	1
A	55	HIS	CG-ND1-CE1	12.17	129.99	109.30	4	1
A	4	ILE	C-N-CA	9.73	139.22	121.70	8	3
A	2	THR	C-N-CA	8.37	136.76	121.70	4	6
A	3	ASN	C-N-CA	7.69	135.55	121.70	4	3
A	6	LYS	C-N-CA	7.59	135.35	121.70	2	1
A	337	ASN	OD1-CG-ND2	6.85	115.75	122.60	9	8
A	293	ASP	CA-CB-CG	6.79	119.39	112.60	7	5
A	445	ASP	CA-CB-CG	6.71	119.31	112.60	1	1
A	532	ASN	OD1-CG-ND2	6.52	116.08	122.60	1	5
A	332	VAL	C-N-CA	6.51	133.42	121.70	5	2
A	350	GLY	C-N-CA	6.43	133.28	121.70	6	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	439	ARG	NE-CZ-NH2	6.30	124.87	119.20	5	1
A	140	GLN	OE1-CD-NE2	6.28	116.32	122.60	6	4
A	9	LEU	C-N-CA	6.23	132.91	121.70	4	2
A	1	MET	C-N-CA	6.12	132.72	121.70	2	4
A	531	ASP	C-N-CA	5.82	132.18	121.70	10	1
A	306	GLN	OE1-CD-NE2	5.76	116.84	122.60	1	5
A	35	LEU	C-N-CA	5.76	132.06	121.70	8	1
A	459	ASN	CA-CB-CG	5.74	106.86	112.60	7	1
A	294	PRO	C-N-CA	5.71	131.98	121.70	10	1
A	335	GLN	OE1-CD-NE2	5.66	116.94	122.60	4	3
A	500	ASP	CA-CB-CG	5.65	106.95	112.60	3	3
A	44	ASN	OD1-CG-ND2	5.46	117.14	122.60	6	10
A	10	VAL	C-N-CA	5.42	131.45	121.70	4	2
A	334	ALA	C-N-CA	5.38	131.38	121.70	1	3
A	344	THR	CA-CB-OG1	5.33	101.60	109.60	1	1
A	528	ASP	CA-CB-CG	5.31	107.29	112.60	1	1
A	34	THR	C-N-CA	5.21	131.08	121.70	8	1
A	498	GLN	OE1-CD-NE2	5.20	117.40	122.60	8	7
A	531	ASP	C-CA-CB	5.18	119.94	110.10	7	1
A	421	GLN	OE1-CD-NE2	5.15	117.45	122.60	1	10
A	245	ASN	OD1-CG-ND2	5.12	117.48	122.60	10	2
A	92	ASN	OD1-CG-ND2	5.08	117.52	122.60	9	1
A	4	ILE	O-C-N	5.07	114.88	123.00	8	2
A	502	ASP	CA-CB-CG	5.05	117.65	112.60	8	1
A	392	ASN	OD1-CG-ND2	5.05	117.55	122.60	4	4
A	5	THR	C-N-CA	5.01	130.72	121.70	6	4
A	3	ASN	CA-C-N	4.96	126.11	116.20	4	1
A	8	SER	C-N-CA	4.95	130.62	121.70	4	3
A	532	ASN	CA-CB-CG	4.95	117.55	112.60	1	2
A	334	ALA	C-CA-CB	4.88	117.83	110.50	5	1
A	11	ALA	C-N-CA	4.87	130.46	121.70	2	2
A	39	GLN	OE1-CD-NE2	4.79	117.81	122.60	6	6
A	294	PRO	N-CA-CB	4.77	108.25	103.00	7	2
A	497	GLN	OE1-CD-NE2	4.75	117.85	122.60	7	9
A	4	ILE	CA-C-N	4.73	125.65	116.20	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	101	HIS	CB-CG-CD2	4.72	125.06	131.20	4	9
A	466	HIS	CB-CG-CD2	4.69	125.11	131.20	9	6
A	291	HIS	CA-CB-CG	4.66	109.14	113.80	7	1
A	532	ASN	N-CA-CB	4.66	102.58	110.50	10	1
A	353	LEU	C-N-CA	4.65	130.07	121.70	3	1
A	537	ASN	OD1-CG-ND2	4.64	117.96	122.60	1	2
A	436	ASP	CA-CB-CG	4.64	117.24	112.60	4	2
A	7	ARG	C-N-CA	4.63	130.04	121.70	4	2
A	348	THR	OG1-CB-CG2	4.62	100.06	109.30	2	1
A	55	HIS	CB-CG-CD2	4.61	125.21	131.20	9	2
A	543	HIS	CA-CB-CG	4.58	118.38	113.80	2	1
A	207	GLN	OE1-CD-NE2	4.58	118.02	122.60	10	3
A	333	LYS	C-N-CA	4.57	129.92	121.70	7	1
A	363	GLN	OE1-CD-NE2	4.55	118.05	122.60	3	9
A	9	LEU	O-C-N	4.54	115.74	123.00	4	1
A	2	THR	CA-C-N	4.53	125.26	116.20	4	1
A	3	ASN	O-C-N	4.51	115.79	123.00	4	1
A	515	ARG	NE-CZ-NH2	4.51	123.25	119.20	3	1
A	344	THR	C-CA-CB	4.49	118.98	109.10	1	1
A	3	ASN	C-CA-CB	4.47	118.60	110.10	8	2
A	81	HIS	CB-CG-CD2	4.44	125.42	131.20	4	3
A	43	ARG	NE-CZ-NH1	4.44	125.94	121.50	2	1
A	355	GLN	OE1-CD-NE2	4.44	118.16	122.60	7	4
A	343	TYR	C-N-CA	4.44	129.69	121.70	8	1
A	349	ASP	CA-CB-CG	4.43	117.03	112.60	7	1
A	445	ASP	C-N-CA	4.38	129.59	121.70	9	1
A	487	GLN	OE1-CD-NE2	4.37	118.23	122.60	3	9
A	428	ASP	CA-CB-CG	4.35	116.95	112.60	9	2
A	464	THR	CA-CB-OG1	4.35	116.13	109.60	7	1
A	280	GLN	OE1-CD-NE2	4.34	118.26	122.60	2	7
A	397	HIS	CB-CG-CD2	4.33	125.58	131.20	5	2
A	13	GLY	C-N-CA	4.28	129.41	121.70	5	1
A	19	MET	C-N-CA	4.28	129.40	121.70	7	1
A	14	VAL	C-N-CA	4.26	129.37	121.70	5	1
A	77	ASP	CA-CB-CG	4.26	116.86	112.60	5	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	531	ASP	CA-CB-CG	4.26	116.86	112.60	7	2
A	50	GLN	OE1-CD-NE2	4.24	118.36	122.60	9	1
A	454	ASN	OD1-CG-ND2	4.23	118.37	122.60	1	1
A	2	THR	O-C-N	4.23	116.23	123.00	4	1
A	124	GLN	OE1-CD-NE2	4.22	118.38	122.60	4	2
A	18	LEU	C-N-CA	4.22	129.29	121.70	4	1
A	1	MET	CA-C-N	4.20	124.60	116.20	2	1
A	91	ASP	CA-CB-CG	4.16	116.76	112.60	5	1
A	168	HIS	CB-CG-CD2	4.15	125.80	131.20	5	1
A	6	LYS	N-CA-C	4.14	122.60	111.00	1	1
A	543	HIS	CB-CG-CD2	4.12	125.84	131.20	6	1
A	432	GLN	OE1-CD-NE2	4.09	118.51	122.60	6	1
A	12	ALA	C-N-CA	4.09	129.05	121.70	4	1
A	533	THR	CA-C-N	4.07	124.35	116.20	9	1
A	8	SER	N-CA-C	4.07	122.39	111.00	4	1
A	163	LYS	CG-CD-CE	4.06	101.96	111.30	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	2.69	23
2	3.75	32
3	2.34	20
4	2.23	19
5	2.46	21
6	1.64	14
7	2.69	23
8	3.40	29
9	3.28	28
10	1.76	15

There are 224 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:55:HIS:CD2	A:55:HIS:NE2	1.16	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:55:HIS:CE1	A:55:HIS:ND1	1.16	4	1
A:36:ALA:HB3	A:540:ILE:HG22	0.91	9	1
A:456:MET:HE1	A:499:LEU:HD22	0.87	8	1
A:343:TYR:CD1	A:505:ILE:HD11	0.86	1	1
A:55:HIS:HE1	A:122:SER:HA	0.82	4	1
A:269:MET:HE1	A:524:TYR:CZ	0.79	3	1
A:276:ILE:HG21	A:333:LYS:C	0.78	5	1
A:535:THR:HA	A:538:MET:HE3	0.78	2	1
A:55:HIS:CE1	A:193:VAL:HG22	0.75	4	1
A:55:HIS:CE1	A:55:HIS:NE2	0.74	4	1
A:55:HIS:CE1	A:122:SER:HA	0.74	4	1
A:55:HIS:CE1	A:122:SER:HB3	0.72	4	1
A:186:VAL:HG21	A:447:ASN:HD22	0.72	1	1
A:55:HIS:CE1	A:122:SER:CA	0.71	4	1
A:462:MET:HA	A:462:MET:HE2	0.70	5	3
A:276:ILE:HD11	A:334:ALA:HB3	0.67	2	1
A:75:VAL:HG21	A:536:ARG:HH12	0.67	9	1
A:247:VAL:HG21	A:535:THR:HG21	0.67	9	1
A:80:GLY:HA2	A:530:LEU:HD12	0.66	9	1
A:55:HIS:CE1	A:122:SER:CB	0.66	4	1
A:522:GLY:HA2	A:534:TYR:CE1	0.65	7	1
A:55:HIS:NE2	A:191:SER:O	0.64	4	1
A:123:TRP:CD1	A:141:TYR:HH	0.64	7	1
A:35:LEU:HD21	A:543:HIS:HB2	0.63	2	1
A:141:TYR:HB2	A:147:ILE:HD12	0.63	7	1
A:276:ILE:HD13	A:334:ALA:O	0.63	7	1
A:247:VAL:HG21	A:539:TYR:OH	0.62	2	1
A:252:ILE:CD1	A:267:ILE:HD11	0.61	9	1
A:450:THR:CG2	A:492:TYR:CZ	0.61	1	1
A:135:TYR:CD2	A:462:MET:HE1	0.61	5	1
A:186:VAL:HG23	A:446:TYR:CZ	0.61	2	1
A:80:GLY:HA2	A:530:LEU:CD1	0.60	9	1
A:340:ALA:HA	A:510:TYR:CE2	0.60	3	1
A:332:VAL:HG11	A:509:TYR:CD2	0.59	3	1
A:456:MET:HE1	A:499:LEU:CD2	0.58	8	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:55:HIS:HE1	A:122:SER:CA	0.58	4	1
A:123:TRP:CG	A:141:TYR:HH	0.57	7	1
A:276:ILE:CD1	A:334:ALA:HB3	0.57	2	2
A:323:MET:SD	A:328:ILE:HD11	0.57	8	1
A:517:VAL:HG21	A:534:TYR:CD2	0.57	7	1
A:217:TYR:CE1	A:539:TYR:CE2	0.56	2	1
A:427:LEU:HD22	A:461:SER:HB2	0.56	8	1
A:299:TYR:CD1	A:439:ARG:NH2	0.56	8	1
A:35:LEU:HD21	A:543:HIS:CG	0.56	2	1
A:67:ARG:CZ	A:188:PRO:HD3	0.55	2	2
A:295:TYR:CZ	A:338:MET:HE2	0.55	10	1
A:163:LYS:HE3	A:165:ILE:HD11	0.55	5	1
A:456:MET:CE	A:499:LEU:HD22	0.54	8	1
A:358:TRP:CH2	A:359:PHE:CE1	0.54	8	1
A:536:ARG:HA	A:539:TYR:CD2	0.54	2	1
A:36:ALA:HB3	A:540:ILE:CG2	0.54	9	1
A:49:VAL:HG21	A:65:ILE:HD12	0.54	8	1
A:517:VAL:HG21	A:524:TYR:CE2	0.54	9	1
A:126:SER:HB3	A:141:TYR:CE2	0.53	2	1
A:297:CYS:CB	A:511:TYR:CZ	0.53	2	2
A:64:ASN:ND2	A:271:ASN:HD21	0.53	8	2
A:75:VAL:HB	A:536:ARG:HH22	0.52	10	1
A:135:TYR:HD2	A:462:MET:HE1	0.52	5	1
A:55:HIS:CE1	A:193:VAL:CG2	0.52	4	1
A:339:PRO:HG2	A:341:TYR:CE2	0.52	3	1
A:67:ARG:HD2	A:534:TYR:CE1	0.52	9	1
A:294:PRO:CG	A:531:ASP:HA	0.52	7	1
A:295:TYR:CE1	A:512:VAL:HG13	0.51	6	1
A:299:TYR:CE2	A:439:ARG:NH2	0.51	6	1
A:535:THR:HG22	A:539:TYR:CE1	0.51	2	1
A:296:LEU:HD11	A:444:ALA:O	0.51	10	1
A:517:VAL:HG21	A:534:TYR:HD2	0.51	7	1
A:444:ALA:HB2	A:452:PHE:CE2	0.51	2	1
A:135:TYR:O	A:462:MET:HE3	0.50	5	1
A:444:ALA:HB2	A:452:PHE:HE1	0.50	7	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:276:ILE:HD12	A:335:GLN:HG2	0.50	3	1
A:356:PRO:HD2	A:359:PHE:CE1	0.50	3	1
A:509:TYR:CE2	A:511:TYR:CE1	0.50	8	1
A:343:TYR:CE1	A:505:ILE:CG1	0.50	1	1
A:141:TYR:CD1	A:144:ILE:HD12	0.50	7	1
A:344:THR:HG23	A:493:THR:HG23	0.50	8	1
A:297:CYS:HB2	A:511:TYR:CE1	0.50	1	1
A:69:LEU:HD21	A:230:LEU:HD22	0.50	10	8
A:186:VAL:HG23	A:446:TYR:CE2	0.50	2	1
A:299:TYR:CD2	A:511:TYR:CE1	0.50	5	1
A:371:LYS:HE3	A:411:ASN:O	0.49	10	10
A:125:ARG:HH11	A:193:VAL:HG21	0.49	9	1
A:445:ASP:HB3	A:534:TYR:CE2	0.49	1	1
A:243:VAL:CG2	A:540:ILE:H	0.49	4	1
A:276:ILE:HG21	A:334:ALA:HB1	0.49	1	1
A:186:VAL:CG2	A:446:TYR:CZ	0.49	2	1
A:328:ILE:O	A:332:VAL:HG22	0.49	5	1
A:333:LYS:HE2	A:396:LEU:HD11	0.49	6	1
A:341:TYR:CE1	A:359:PHE:CE1	0.49	8	1
A:297:CYS:HB2	A:511:TYR:CZ	0.48	1	3
A:13:GLY:O	A:14:VAL:HG23	0.48	2	1
A:520:TRP:HB3	A:543:HIS:CD2	0.48	6	1
A:134:PRO:HB3	A:462:MET:HE3	0.48	7	1
A:103:ARG:NH1	A:237:TRP:CE2	0.48	5	1
A:35:LEU:HD21	A:520:TRP:HB2	0.48	10	1
A:344:THR:HG21	A:351:ALA:CB	0.48	1	1
A:243:VAL:CG2	A:539:TYR:HA	0.48	9	1
A:38:LYS:HE2	A:40:THR:O	0.47	9	1
A:517:VAL:HG21	A:524:TYR:CD2	0.47	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	541	502	33	6
2	541	501	30	10

Model ID	Analysed	Favored	Allowed	Outliers
3	541	500	28	13
4	541	515	19	7
5	541	509	24	8
6	541	515	16	10
7	541	500	27	14
8	541	485	39	17
9	541	523	15	3
10	541	511	25	5

There are 45 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	22	ASN	7
A	6	LYS	6
A	4	ILE	5
A	9	LEU	5
A	2	THR	4
A	3	ASN	4
A	334	ALA	4
A	10	VAL	3
A	12	ALA	3
A	24	ALA	3
A	26	ALA	3
A	351	ALA	3
A	5	THR	2
A	8	SER	2
A	15	LEU	2
A	17	ALA	2
A	19	MET	2
A	23	VAL	2
A	28	ASP	2
A	295	TYR	2
A	333	LYS	2
A	335	GLN	2
A	11	ALA	1
A	14	VAL	1

Chain	Res	Type	Models (Total)
A	16	ALA	1
A	18	LEU	1
A	20	ALA	1
A	21	GLY	1
A	25	LEU	1
A	33	VAL	1
A	35	LEU	1
A	36	ALA	1
A	338	MET	1
A	340	ALA	1
A	342	GLY	1
A	343	TYR	1
A	344	THR	1
A	354	THR	1
A	393	THR	1
A	447	ASN	1
A	531	ASP	1
A	533	THR	1
A	540	ILE	1
A	541	VAL	1
A	542	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	468	457	5	6
2	468	452	11	5
3	468	451	9	8
4	468	448	11	9
5	468	457	7	4
6	468	451	8	9
7	468	448	10	10
8	468	455	6	7
9	468	454	5	9
10	468	453	9	6

There are 36 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	15	LEU	10
A	2	THR	8
A	5	THR	6
A	35	LEU	4
A	19	MET	3
A	276	ILE	3
A	535	THR	3
A	18	LEU	2
A	23	VAL	2
A	354	THR	2
A	394	SER	2
A	448	GLU	2
A	505	ILE	2
A	531	ASP	2
A	4	ILE	1
A	8	SER	1
A	33	VAL	1
A	44	ASN	1
A	76	SER	1
A	122	SER	1
A	137	SER	1
A	243	VAL	1
A	273	SER	1
A	293	ASP	1
A	295	TYR	1
A	335	GLN	1
A	344	THR	1
A	347	TYR	1
A	349	ASP	1
A	439	ARG	1
A	446	TYR	1
A	449	PRO	1
A	462	MET	1
A	532	ASN	1

Chain	Res	Type	Models (Total)
A	533	THR	1
A	543	HIS	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

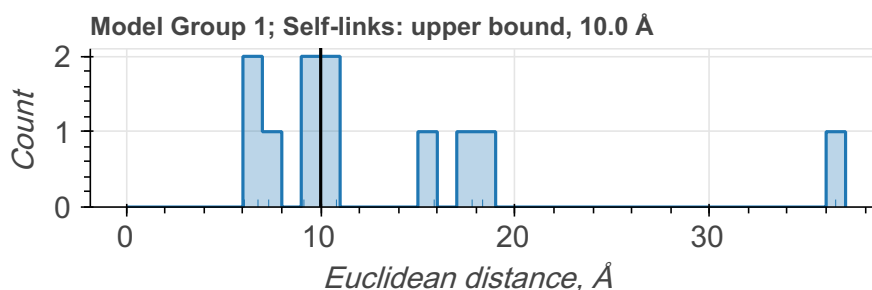
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 11 crosslinking restraints combined in 11 restraint groups.

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

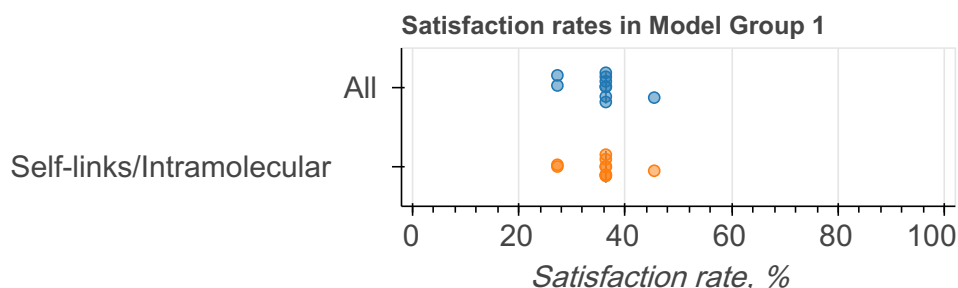
Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=11)
1	1	1	10/10	All	45.45	54.55	11
				Self-links/ Intramolecular	45.45	54.55	11

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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