

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	9A2Z
PDB-Dev ID	PDBDEV_00000184
Structure Title	Model of E. coli FepA 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

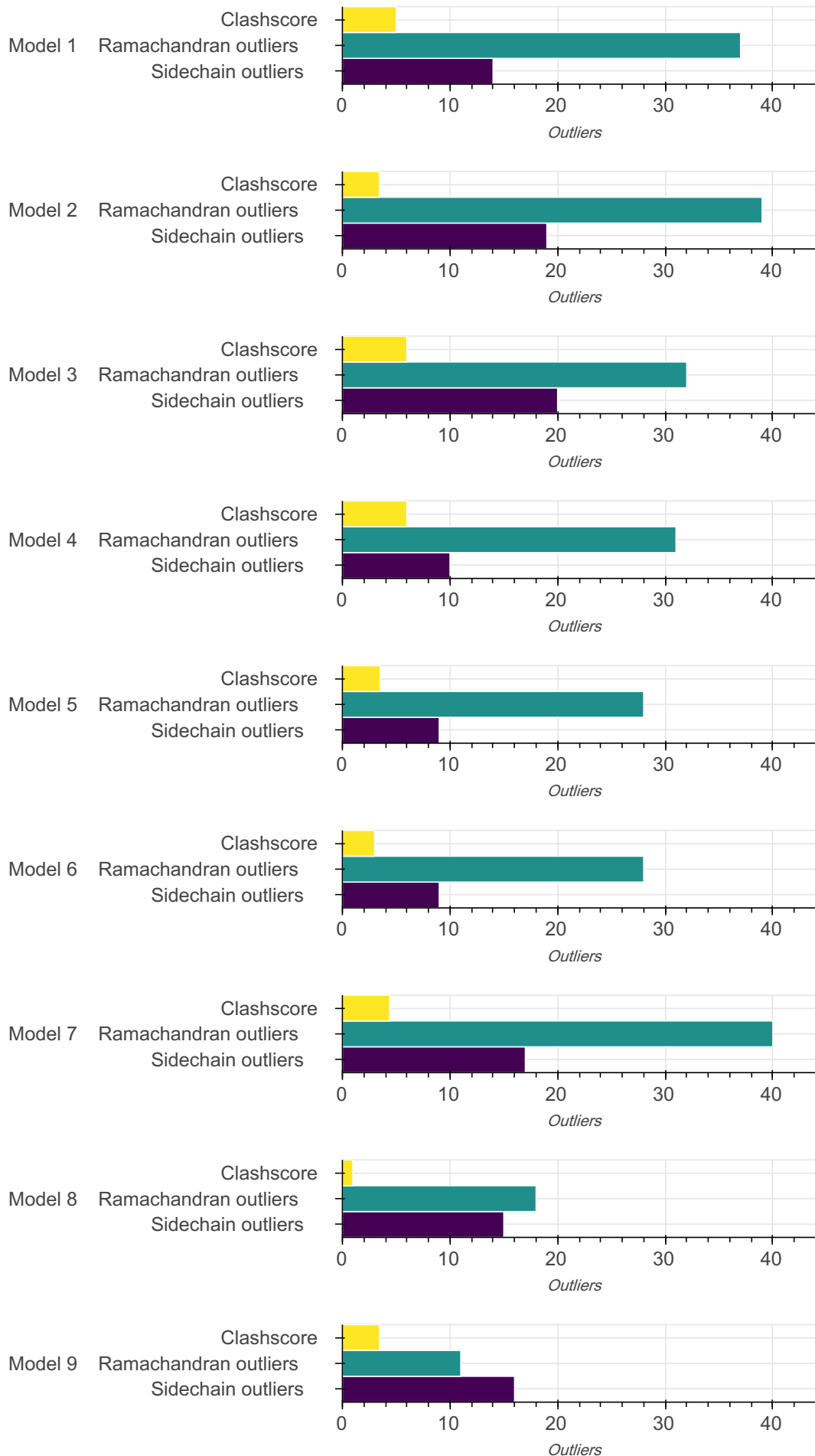
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

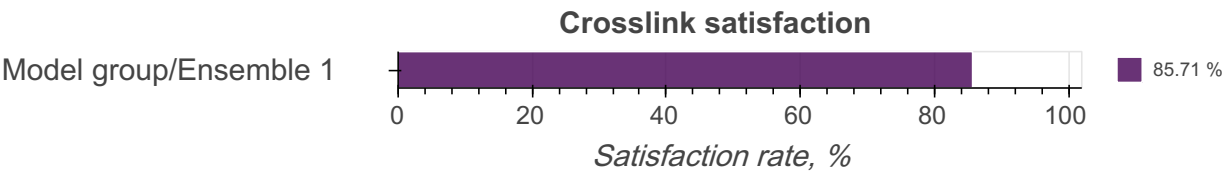
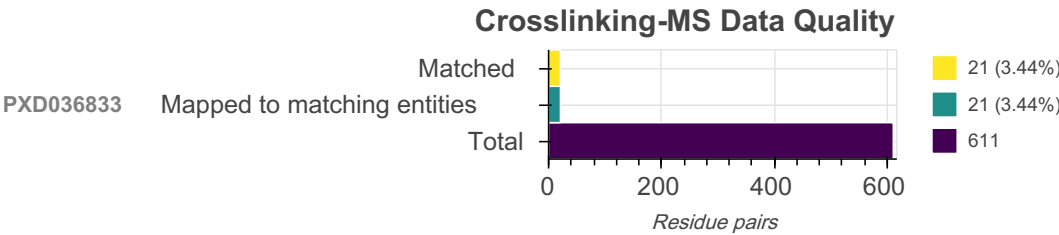
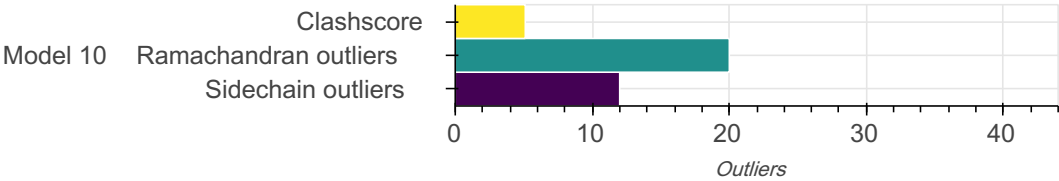
List of references used to build this report is available [here](#).

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	P05825	A	746	-	1-746	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	P05825	dbseq_P05825_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2Z	21	21 (100.00%)	21 (100.00%)
PXD036833	611	21 (3.44%)	21 (3.44%)

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 14 bond length outliers in this entry (0.02% of 59207 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	176	HIS	CE1-NE2	122.95	2.55	1.32	9	1
A	176	HIS	ND1-CE1	82.51	2.15	1.32	9	1
A	505	LYS	CA-CB	76.15	3.05	1.53	9	1
A	176	HIS	CD2-NE2	68.70	2.13	1.37	9	1
A	123	TRP	CD2-CE3	21.56	1.74	1.40	9	1
A	123	TRP	CD2-CE2	19.58	1.74	1.41	9	1
A	123	TRP	CZ2-CH2	19.07	1.73	1.37	9	1
A	123	TRP	CE2-CZ2	15.78	1.73	1.39	9	1
A	123	TRP	CZ3-CH2	13.41	1.74	1.40	9	1
A	123	TRP	CE3-CZ3	11.87	1.74	1.38	9	1
A	39	THR	CA-C	4.74	1.62	1.52	2	1
A	39	THR	CB-OG1	4.73	1.36	1.43	2	1
A	704	ARG	CZ-NH2	4.41	1.27	1.33	6	1
A	186	PRO	N-CD	4.05	1.42	1.47	3	1

Standard geometry: angle outliers ?

There are 544 bond angle outliers in this entry (0.68% of 80544 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	176	HIS	ND1-CE1-NE2	24.25	84.15	108.40	9	1
A	176	HIS	CD2-NE2-CE1	21.55	87.45	109.00	9	1
A	176	HIS	CG-CD2-NE2	21.50	128.70	107.20	9	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	176	HIS	CG-ND1-CE1	12.65	130.81	109.30	9	1
A	39	THR	CA-CB-OG1	10.51	125.36	109.60	2	1
A	505	LYS	C-CA-CB	9.39	127.95	110.10	9	1
A	39	THR	C-N-CA	8.96	137.82	121.70	2	2
A	404	GLN	C-N-CA	8.87	137.67	121.70	7	1
A	505	LYS	N-CA-CB	8.79	125.45	110.50	9	1
A	518	LEU	C-N-CA	8.53	137.06	121.70	7	1
A	8	LEU	C-N-CA	8.51	137.01	121.70	4	1
A	38	VAL	CA-CB-CG1	8.08	124.13	110.40	2	1
A	505	LYS	CA-CB-CG	8.00	130.09	114.10	9	1
A	393	GLN	OE1-CD-NE2	7.67	114.93	122.60	4	9
A	593	ASN	OD1-CG-ND2	7.58	115.02	122.60	2	1
A	6	HIS	C-N-CA	7.55	135.29	121.70	9	4
A	143	ARG	NE-CZ-NH1	7.36	128.86	121.50	4	2
A	46	GLN	C-N-CA	7.29	134.82	121.70	7	1
A	591	SER	C-N-CA	7.28	134.81	121.70	2	1
A	723	ILE	CB-CG1-CD1	7.22	128.95	113.80	4	1
A	366	ASP	C-N-CA	7.13	134.54	121.70	7	1
A	40	ALA	N-CA-CB	7.12	99.71	110.40	2	1
A	122	GLY	C-N-CA	7.08	134.45	121.70	1	1
A	245	ALA	N-CA-CB	7.07	99.79	110.40	4	1
A	4	LYS	C-N-CA	6.95	134.22	121.70	9	3
A	333	HIS	CA-CB-CG	6.94	120.74	113.80	3	1
A	591	SER	C-CA-CB	6.71	122.84	110.10	2	1
A	40	ALA	C-CA-CB	6.67	120.51	110.50	4	2
A	729	TYR	C-N-CA	6.65	133.67	121.70	3	1
A	320	ASP	CA-CB-CG	6.53	119.13	112.60	3	1
A	186	PRO	CA-N-CD	6.46	102.95	112.00	3	1
A	39	THR	C-CA-CB	6.38	123.15	109.10	2	1
A	221	GLN	OE1-CD-NE2	6.21	116.39	122.60	3	8
A	244	PRO	C-N-CA	6.21	132.88	121.70	4	1
A	93	GLN	OE1-CD-NE2	6.19	116.41	122.60	10	9
A	25	PRO	C-N-CA	6.17	132.80	121.70	7	1
A	87	GLN	OE1-CD-NE2	6.14	116.46	122.60	2	4
A	95	ASP	CA-CB-CG	6.07	118.67	112.60	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	264	ALA	CA-C-N	6.03	125.94	116.90	5	1
A	505	LYS	N-CA-C	5.97	94.27	111.00	9	1
A	335	ARG	C-N-CA	5.96	132.42	121.70	2	1
A	3	LYS	C-N-CA	5.93	132.38	121.70	6	5
A	730	THR	C-N-CA	5.89	132.30	121.70	7	1
A	704	ARG	NE-CZ-NH1	5.87	127.37	121.50	6	1
A	44	ASN	CA-CB-CG	5.87	118.47	112.60	2	1
A	2	ASN	C-N-CA	5.85	132.23	121.70	8	4
A	297	SER	C-N-CA	5.76	132.07	121.70	5	2
A	218	ASP	CA-CB-CG	5.75	118.35	112.60	2	1
A	278	GLN	OE1-CD-NE2	5.74	116.86	122.60	8	6
A	556	ASN	CA-CB-CG	5.72	118.32	112.60	9	1
A	40	ALA	C-N-CA	5.70	131.95	121.70	2	1
A	126	GLU	C-N-CA	5.69	131.94	121.70	4	2
A	143	ARG	NE-CZ-NH2	5.66	114.10	119.20	4	1
A	1	MET	C-N-CA	5.66	131.88	121.70	4	3
A	228	ASN	OD1-CG-ND2	5.65	116.95	122.60	5	2
A	362	ILE	C-N-CA	5.64	131.84	121.70	7	1
A	232	GLN	OE1-CD-NE2	5.63	116.97	122.60	6	8
A	46	GLN	OE1-CD-NE2	5.63	116.97	122.60	7	3
A	507	GLN	OE1-CD-NE2	5.61	116.99	122.60	5	6
A	708	ALA	C-N-CA	5.61	131.79	121.70	2	1
A	188	HIS	CB-CG-CD2	5.56	123.97	131.20	6	4
A	212	ARG	NE-CZ-NH2	5.55	124.20	119.20	1	3
A	12	VAL	C-N-CA	5.53	131.65	121.70	2	2
A	89	GLY	C-N-CA	5.49	131.58	121.70	3	2
A	336	ASN	OD1-CG-ND2	5.46	117.14	122.60	4	3
A	592	LEU	N-CA-CB	5.44	119.75	110.50	2	1
A	19	VAL	C-N-CA	5.41	131.44	121.70	2	1
A	366	ASP	CA-CB-CG	5.40	118.00	112.60	8	2
A	722	TYR	C-N-CA	5.37	131.36	121.70	6	2
A	382	ASN	CA-CB-CG	5.36	117.96	112.60	9	2
A	357	GLN	OE1-CD-NE2	5.35	117.25	122.60	7	9
A	477	ASP	CA-CB-CG	5.34	117.94	112.60	8	9
A	45	LEU	C-N-CA	5.33	131.29	121.70	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	366	ASP	N-CA-C	5.33	125.92	111.00	7	1
A	511	ALA	C-N-CA	5.32	131.27	121.70	1	3
A	654	GLN	OE1-CD-NE2	5.27	117.33	122.60	5	4
A	128	ASP	C-N-CA	5.26	131.16	121.70	7	1
A	344	ALA	C-N-CA	5.25	131.15	121.70	4	2
A	568	ASN	OD1-CG-ND2	5.23	117.37	122.60	6	2
A	723	ILE	CG1-CB-CG2	5.21	126.34	110.70	4	1
A	716	ASP	C-N-CA	5.20	131.07	121.70	4	1
A	671	LYS	CA-CB-CG	5.19	124.48	114.10	4	1
A	16	ILE	C-N-CA	5.19	131.04	121.70	2	3
A	21	GLN	OE1-CD-NE2	5.18	117.42	122.60	3	9
A	502	LEU	CD1-CG-CD2	5.14	99.49	110.80	7	1
A	288	ASN	C-N-CA	5.13	130.94	121.70	2	3
A	88	ARG	CD-NE-CZ	5.13	131.59	124.40	2	1
A	39	THR	N-CA-CB	5.13	102.78	111.50	2	1
A	298	LYS	CA-C-N	5.12	126.44	116.20	7	1
A	9	ALA	C-N-CA	5.11	130.90	121.70	6	2
A	537	GLU	CB-CG-CD	5.10	103.93	112.60	2	1
A	295	THR	C-N-CA	5.10	130.87	121.70	3	1
A	365	ASP	CA-CB-CG	5.09	117.69	112.60	9	1
A	267	GLN	OE1-CD-NE2	5.07	117.53	122.60	2	5
A	712	GLN	OE1-CD-NE2	5.06	117.54	122.60	7	6
A	130	ARG	C-N-CA	5.05	130.79	121.70	10	1
A	636	GLN	OE1-CD-NE2	5.03	117.57	122.60	10	9
A	290	ASN	C-N-CA	5.03	130.76	121.70	5	2
A	368	MET	C-N-CA	5.02	130.74	121.70	7	1
A	308	ARG	CD-NE-CZ	5.01	131.41	124.40	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	5.02	57
2	3.44	39
3	5.99	68

Model ID	Clash score	Number of clashes
4	5.99	68
5	3.52	40
6	3.00	34
7	4.40	50
8	0.97	11
9	3.44	39
10	5.11	58

There are 464 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:123:TRP:CD2	A:123:TRP:CE3	1.62	9	1
A:123:TRP:CD2	A:123:TRP:CE2	1.45	9	1
A:123:TRP:CZ3	A:505:LYS:HA	1.35	9	1
A:123:TRP:CH2	A:505:LYS:HA	1.29	9	1
A:176:HIS:CD2	A:176:HIS:NE2	1.16	9	1
A:123:TRP:CE2	A:505:LYS:CB	1.14	9	1
A:176:HIS:CE1	A:176:HIS:ND1	1.14	9	1
A:123:TRP:CE3	A:505:LYS:CB	1.14	9	1
A:123:TRP:CZ2	A:505:LYS:CB	1.14	9	1
A:123:TRP:CD2	A:505:LYS:CB	1.13	9	1
A:123:TRP:CZ3	A:505:LYS:CA	1.13	9	1
A:123:TRP:CE2	A:505:LYS:CA	1.12	9	1
A:123:TRP:CE3	A:505:LYS:CA	1.12	9	1
A:123:TRP:CZ3	A:505:LYS:CB	1.12	9	1
A:123:TRP:CH2	A:505:LYS:CA	1.12	9	1
A:123:TRP:CH2	A:505:LYS:CB	1.12	9	1
A:123:TRP:CZ2	A:505:LYS:CA	1.11	9	1
A:123:TRP:CD2	A:505:LYS:CA	1.11	9	1
A:123:TRP:CZ2	A:505:LYS:HB3	0.98	9	1
A:123:TRP:CD2	A:505:LYS:HB2	0.98	9	1
A:518:LEU:HD12	A:574:LEU:HD12	0.93	10	1
A:72:ARG:HE	A:79:LEU:HD12	0.89	7	1
A:306:LEU:HD11	A:333:HIS:CE1	0.83	5	1
A:343:LEU:HD11	A:360:VAL:HG11	0.83	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:123:TRP:CZ3	A:505:LYS:CG	0.82	9	1
A:123:TRP:CZ2	A:505:LYS:C	0.80	9	1
A:72:ARG:NE	A:79:LEU:HD12	0.78	7	1
A:192:GLY:HA2	A:222:ALA:HB2	0.78	1	1
A:671:LYS:H	A:723:ILE:HG12	0.77	4	1
A:123:TRP:CE2	A:505:LYS:HB2	0.76	9	1
A:186:PRO:HD3	A:319:TRP:CH2	0.75	3	1
A:176:HIS:CE1	A:176:HIS:NE2	0.74	9	1
A:79:LEU:HD13	A:92:ARG:HB3	0.73	7	1
A:94:ILE:HD12	A:119:VAL:HG11	0.73	4	1
A:723:ILE:HG22	A:728:ALA:HB3	0.71	7	1
A:172:SER:HG	A:176:HIS:HE2	0.71	9	1
A:99:MET:HE3	A:161:GLY:HA2	0.70	2	5
A:88:ARG:HH12	A:224:ALA:HB2	0.70	7	1
A:39:THR:HG22	A:592:LEU:HB2	0.70	2	1
A:123:TRP:CD2	A:505:LYS:N	0.70	9	1
A:258:VAL:HG22	A:323:VAL:CG2	0.70	7	1
A:123:TRP:CE3	A:505:LYS:N	0.69	9	1
A:671:LYS:CG	A:723:ILE:HD13	0.69	4	1
A:88:ARG:CZ	A:222:ALA:HB3	0.69	1	1
A:676:TYR:CD1	A:705:LEU:HD11	0.69	1	1
A:193:ALA:HA	A:319:TRP:CH2	0.69	3	1
A:119:VAL:HG21	A:278:GLN:CD	0.68	8	1
A:40:ALA:H	A:592:LEU:CA	0.67	2	1
A:40:ALA:H	A:592:LEU:HA	0.67	2	1
A:71:ILE:HG22	A:77:VAL:HG11	0.67	4	8
A:565:VAL:HG21	A:574:LEU:HD12	0.65	3	1
A:113:VAL:HG21	A:135:TRP:CZ3	0.64	5	1
A:258:VAL:HG22	A:323:VAL:HG21	0.64	7	1
A:671:LYS:CB	A:723:ILE:HD13	0.64	4	1
A:397:LYS:HE2	A:399:LEU:HD21	0.64	6	1
A:123:TRP:CE2	A:505:LYS:C	0.63	9	1
A:515:GLY:O	A:572:THR:HG23	0.63	4	1
A:119:VAL:HG22	A:306:LEU:HD12	0.63	8	1
A:186:PRO:CG	A:319:TRP:CH2	0.62	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:518:LEU:HD12	A:574:LEU:CD1	0.62	10	1
A:40:ALA:CB	A:154:ARG:HH12	0.62	4	1
A:269:LEU:HD11	A:315:TRP:HE1	0.62	5	1
A:88:ARG:NE	A:222:ALA:HB3	0.62	1	1
A:88:ARG:HH22	A:224:ALA:HB2	0.62	7	1
A:119:VAL:HG22	A:129:THR:HG21	0.62	10	1
A:119:VAL:HG22	A:129:THR:CG2	0.61	10	1
A:82:ASN:HD21	A:84:THR:HG23	0.61	3	1
A:72:ARG:HE	A:79:LEU:CD1	0.61	7	1
A:623:ILE:HD12	A:728:ALA:HA	0.61	1	1
A:38:VAL:HG11	A:43:GLN:HE21	0.61	3	1
A:671:LYS:HB2	A:723:ILE:HD13	0.61	4	1
A:63:VAL:HG22	A:644:GLN:HE22	0.60	2	1
A:40:ALA:H	A:592:LEU:N	0.60	2	1
A:39:THR:HA	A:592:LEU:HA	0.60	2	1
A:303:THR:HG21	A:333:HIS:CE1	0.60	7	1
A:635:TRP:CE2	A:643:MET:HB2	0.59	1	5
A:499:ASN:ND2	A:521:ASN:HD21	0.58	5	1
A:140:MET:HE3	A:212:ARG:HD3	0.58	6	1
A:186:PRO:HG3	A:319:TRP:CH2	0.57	3	1
A:502:LEU:HD12	A:517:TYR:CE1	0.57	7	1
A:69:LYS:CE	A:320:ASP:HB3	0.57	3	1
A:671:LYS:HB2	A:723:ILE:CG2	0.57	4	1
A:269:LEU:HD11	A:315:TRP:NE1	0.57	5	1
A:186:PRO:CD	A:319:TRP:CH2	0.57	3	1
A:192:GLY:C	A:319:TRP:CZ2	0.57	3	1
A:99:MET:HE3	A:554:TYR:OH	0.57	10	1
A:364:LEU:CD1	A:494:TYR:CE2	0.57	5	1
A:399:LEU:C	A:403:THR:HG23	0.56	5	1
A:123:TRP:CE3	A:505:LYS:CG	0.56	9	1
A:635:TRP:CH2	A:643:MET:SD	0.56	4	1
A:111:LYS:HE2	A:314:THR:HG21	0.56	6	1
A:186:PRO:HG3	A:319:TRP:CZ3	0.56	3	1
A:231:HIS:CD2	A:245:ALA:HB3	0.56	10	1
A:93:GLN:HE21	A:129:THR:HG21	0.56	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:330:GLN:HA	A:333:HIS:HB2	0.56	3	1
A:333:HIS:ND1	A:562:TYR:CE2	0.56	3	1
A:235:ARG:HD3	A:240:ALA:HA	0.56	4	1
A:517:TYR:CD2	A:574:LEU:CD1	0.56	1	1
A:88:ARG:HH12	A:224:ALA:CB	0.56	7	1
A:112:PRO:HG2	A:368:MET:HE1	0.56	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	744	644	63	37
2	744	618	87	39
3	744	647	65	32
4	744	655	58	31
5	744	644	72	28
6	744	670	46	28
7	744	626	78	40
8	744	636	90	18
9	744	655	78	11
10	744	674	50	20

There are 154 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	27	ASP	7
A	4	LYS	6
A	90	ASN	6
A	10	LEU	5
A	731	TYR	5
A	2	ASN	4
A	16	ILE	4
A	19	VAL	4
A	38	VAL	4
A	86	GLY	4
A	88	ARG	4

Chain	Res	Type	Models (Total)
A	123	TRP	4
A	236	ALA	4
A	291	SER	4
A	512	SER	4
A	714	THR	4
A	720	ALA	4
A	726	ALA	4
A	7	SER	3
A	8	LEU	3
A	12	VAL	3
A	32	HIS	3
A	35	THR	3
A	114	SER	3
A	127	ARG	3
A	238	THR	3
A	292	ASP	3
A	293	SER	3
A	296	ARG	3
A	414	ALA	3
A	509	CYS	3
A	704	ARG	3
A	729	TYR	3
A	3	LYS	2
A	5	ILE	2
A	11	LEU	2
A	20	ALA	2
A	22	ALA	2
A	36	ILE	2
A	40	ALA	2
A	47	ALA	2
A	84	THR	2
A	87	GLN	2
A	115	SER	2
A	116	ARG	2
A	118	SER	2

Chain	Res	Type	Models (Total)
A	121	GLN	2
A	122	GLY	2
A	132	ASP	2
A	192	GLY	2
A	226	ASP	2
A	235	ARG	2
A	237	GLY	2
A	239	TYR	2
A	285	ASP	2
A	288	ASN	2
A	301	ASP	2
A	302	GLU	2
A	318	GLY	2
A	345	GLY	2
A	347	THR	2
A	350	LYS	2
A	402	ASN	2
A	408	GLY	2
A	569	ALA	2
A	623	ILE	2
A	708	ALA	2
A	717	LEU	2
A	722	TYR	2
A	728	ALA	2
A	6	HIS	1
A	9	ALA	1
A	13	ASN	1
A	14	LEU	1
A	17	TYR	1
A	23	GLN	1
A	25	PRO	1
A	26	THR	1
A	30	VAL	1
A	33	ASP	1
A	39	THR	1

Chain	Res	Type	Models (Total)
A	41	ALA	1
A	42	GLU	1
A	45	LEU	1
A	46	GLN	1
A	48	PRO	1
A	49	GLY	1
A	63	VAL	1
A	64	ALA	1
A	85	SER	1
A	89	GLY	1
A	119	VAL	1
A	120	ARG	1
A	128	ASP	1
A	231	HIS	1
A	243	LEU	1
A	245	ALA	1
A	265	PRO	1
A	268	SER	1
A	289	THR	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	615	581	20	14
2	615	567	29	19
3	615	568	27	20
4	615	579	26	10
5	615	580	26	9
6	615	590	16	9
7	615	576	22	17
8	615	572	28	15
9	615	563	36	16
10	615	585	18	12

There are 96 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	347	THR	7
A	8	LEU	5
A	10	LEU	5
A	32	HIS	4
A	238	THR	4
A	286	THR	4
A	730	THR	4
A	11	LEU	3
A	38	VAL	3
A	84	THR	3
A	409	THR	3
A	7	SER	2
A	14	LEU	2
A	28	THR	2
A	31	SER	2
A	119	VAL	2
A	123	TRP	2
A	242	THR	2
A	421	THR	2
A	529	SER	2
A	563	VAL	2
A	666	VAL	2
A	12	VAL	1
A	19	VAL	1
A	26	THR	1
A	35	THR	1
A	36	ILE	1
A	39	THR	1
A	44	ASN	1
A	73	THR	1
A	83	SER	1
A	92	ARG	1
A	95	ASP	1
A	108	ILE	1
A	113	VAL	1

Chain	Res	Type	Models (Total)
A	115	SER	1
A	121	GLN	1
A	129	THR	1
A	139	GLU	1
A	170	LYS	1
A	191	GLU	1
A	200	SER	1
A	218	ASP	1
A	226	ASP	1
A	266	LEU	1
A	271	LEU	1
A	276	SER	1
A	289	THR	1
A	292	ASP	1
A	295	THR	1
A	301	ASP	1
A	303	THR	1
A	307	TYR	1
A	310	ASN	1
A	314	THR	1
A	315	TRP	1
A	325	THR	1
A	334	THR	1
A	335	ARG	1
A	337	SER	1
A	338	ARG	1
A	365	ASP	1
A	369	LEU	1
A	370	HIS	1
A	373	VAL	1
A	385	LEU	1
A	399	LEU	1
A	402	ASN	1
A	403	THR	1
A	407	THR	1

Chain	Res	Type	Models (Total)
A	410	ASN	1
A	416	ASP	1
A	419	SER	1
A	433	SER	1
A	471	SER	1
A	488	TYR	1
A	496	THR	1
A	501	ILE	1
A	502	LEU	1
A	503	TYR	1
A	504	SER	1
A	532	LYS	1
A	572	THR	1
A	622	SER	1
A	624	ILE	1
A	635	TRP	1
A	646	THR	1
A	705	LEU	1
A	706	TRP	1
A	713	THR	1
A	714	THR	1
A	717	LEU	1
A	723	ILE	1
A	737	THR	1
A	741	SER	1
A	743	ASN	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

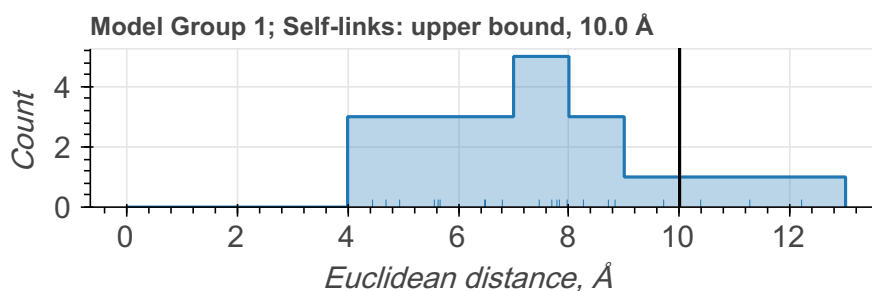
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 21 crosslinking restraints combined in 21 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	LEU	CA	THR	CA	upper bound	10.0	2
L-Photo-Leucine	GLU	CA	LEU	CA	upper bound	10.0	4
L-Photo-Leucine	GLY	CA	LEU	CA	upper bound	10.0	4
L-Photo-Leucine	LEU	CA	TYR	CA	upper bound	10.0	3
L-Photo-Leucine	CYS	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ILE	CA	LEU	CA	upper bound	10.0	2
L-Photo-Leucine	LEU	CA	SER	CA	upper bound	10.0	1
L-Photo-Leucine	GLN	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ALA	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ASP	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

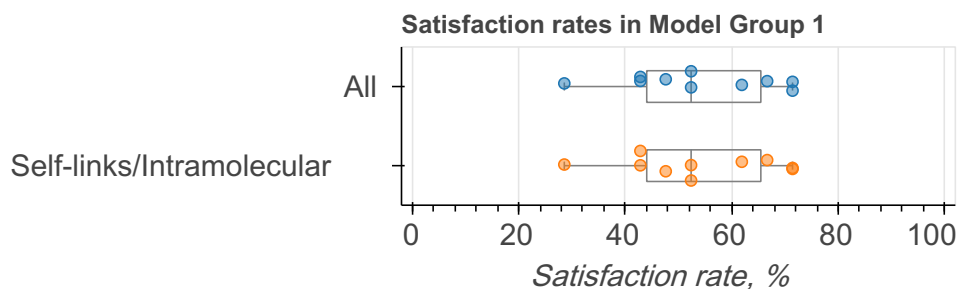
Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=21)
1	1	1	10/10	All	85.71	14.29	21
				Self-links/ Intramolecular	85.71	14.29	21

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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