

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	9A31
PDB-Dev ID	PDBDEV_00000186
Structure Title	Model of E. coli fhuA 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

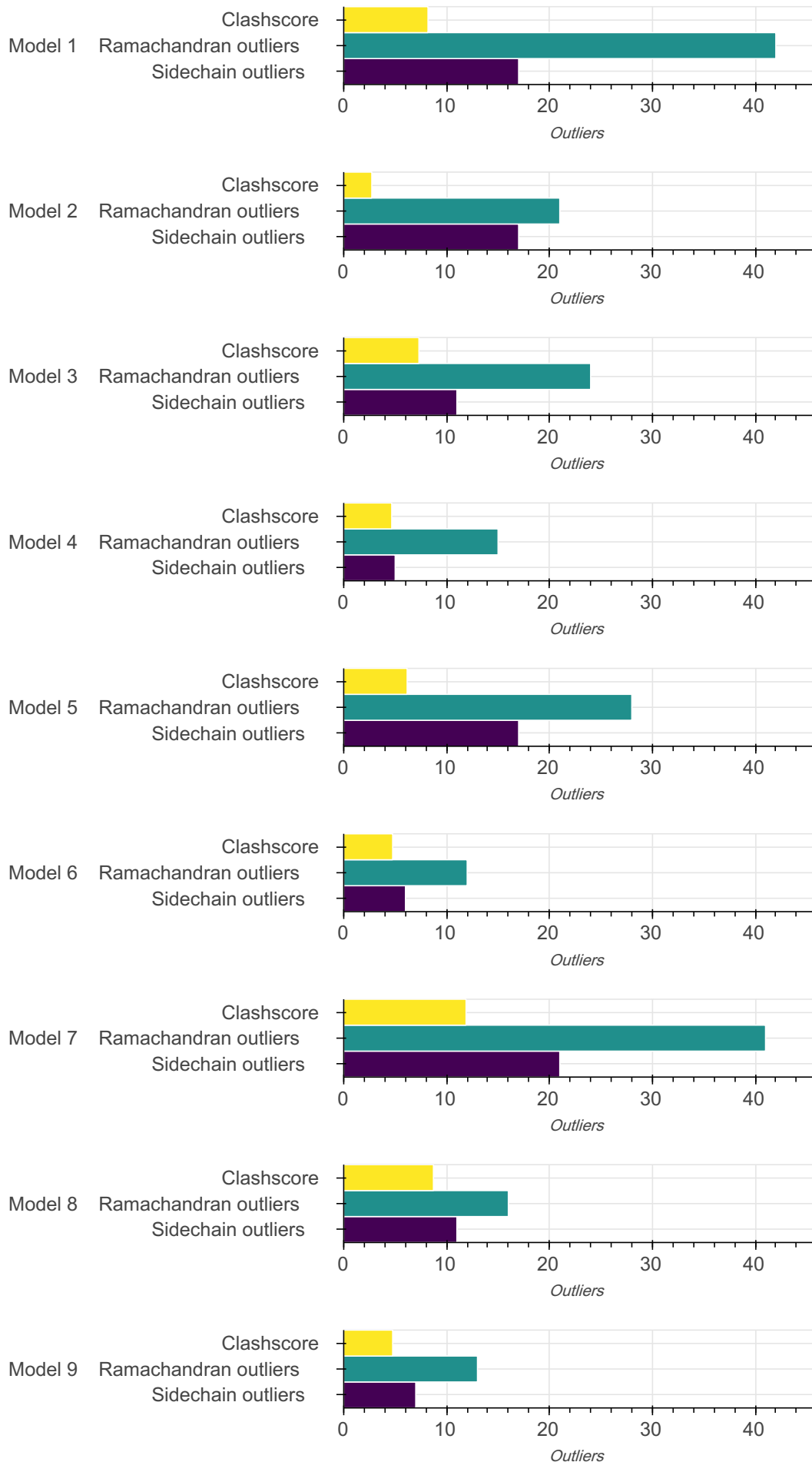
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

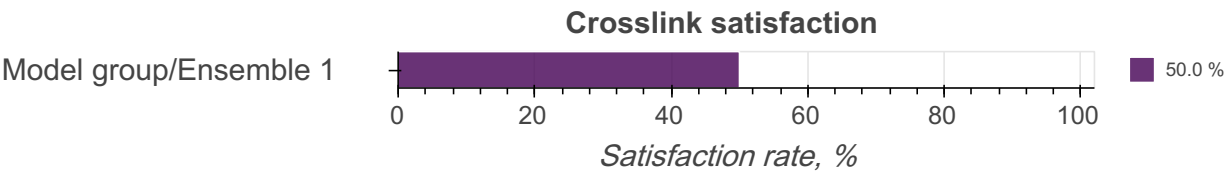
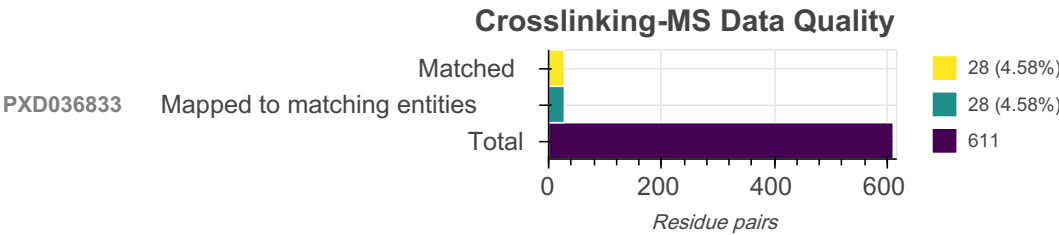
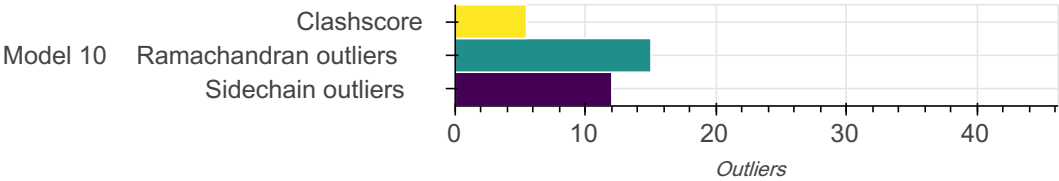
List of references used to build this report is available [here](#).

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	P06971	A	747	-	1-747	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	P06971	dbseq_P06971_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A31	28	28 (100.00%)	28 (100.00%)
PXD036833	611	28 (4.58%)	28 (4.58%)

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 59458 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	310	ARG	CZ-NH2	4.69	1.27	1.33	8	1
A	106	THR	CB-OG1	4.43	1.36	1.43	8	1
A	512	ARG	CZ-NH2	4.02	1.28	1.33	1	1

Standard geometry: angle outliers ?

There are 490 bond angle outliers in this entry (0.61% of 80856 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	43	THR	C-N-CA	10.08	139.85	121.70	7	1
A	137	ASN	CA-CB-CG	9.27	103.33	112.60	7	1
A	181	LEU	C-N-CA	9.07	138.02	121.70	7	2
A	175	LYS	C-N-CA	8.11	136.29	121.70	1	3
A	581	ASN	CA-CB-CG	7.94	104.66	112.60	7	4
A	150	ASN	OD1-CG-ND2	7.73	114.87	122.60	3	4
A	142	LEU	C-CA-CB	7.69	124.70	110.10	2	2
A	55	TRP	C-N-CA	7.58	135.34	121.70	7	1
A	176	SER	C-CA-CB	7.52	95.80	110.10	3	1
A	32	GLN	C-N-CA	7.36	134.96	121.70	4	4
A	135	GLN	C-N-CA	7.34	134.92	121.70	2	1
A	512	ARG	CD-NE-CZ	7.29	114.19	124.40	3	2
A	176	SER	C-N-CA	7.29	134.82	121.70	4	1
A	109	VAL	CA-CB-CG2	7.16	122.57	110.40	8	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	136	ASN	OD1-CG-ND2	7.06	115.54	122.60	7	3
A	48	PRO	C-N-CA	7.05	134.38	121.70	7	1
A	106	THR	CA-CB-CG2	7.01	122.42	110.50	3	2
A	490	ASP	CA-CB-CG	7.01	119.61	112.60	2	2
A	177	SER	C-CA-CB	7.01	123.41	110.10	8	1
A	193	PRO	CA-N-CD	6.88	102.36	112.00	8	1
A	641	GLN	OE1-CD-NE2	6.73	115.87	122.60	6	7
A	133	GLN	OE1-CD-NE2	6.57	116.03	122.60	9	5
A	121	ASP	CA-CB-CG	6.49	119.09	112.60	10	1
A	275	GLY	C-N-CA	6.48	133.36	121.70	1	1
A	440	ASN	N-CA-CB	6.39	99.63	110.50	6	1
A	304	LYS	C-N-CA	6.37	133.17	121.70	1	2
A	114	ARG	NE-CZ-NH2	6.36	124.92	119.20	1	1
A	718	ASP	C-N-CA	6.29	133.01	121.70	4	1
A	7	ALA	C-N-CA	6.22	132.90	121.70	4	3
A	470	GLN	OE1-CD-NE2	6.21	116.39	122.60	5	2
A	491	GLN	OE1-CD-NE2	6.21	116.39	122.60	9	4
A	83	ILE	CA-CB-CG1	6.17	120.88	110.40	1	1
A	183	ASN	CA-CB-CG	6.16	106.44	112.60	10	1
A	190	THR	CA-CB-OG1	6.14	100.38	109.60	8	1
A	1	MET	C-N-CA	6.11	132.71	121.70	3	2
A	419	ASP	CA-CB-CG	6.08	118.68	112.60	9	3
A	206	LEU	N-CA-CB	6.05	100.21	110.50	1	1
A	440	ASN	C-N-CA	6.05	132.58	121.70	1	3
A	721	TYR	C-CA-CB	6.02	121.55	110.10	10	1
A	27	MET	C-N-CA	5.98	132.46	121.70	10	1
A	276	TYR	C-N-CA	5.97	132.45	121.70	9	1
A	133	GLN	C-N-CA	5.96	132.43	121.70	7	1
A	135	GLN	O-C-N	5.96	113.47	123.00	2	1
A	269	GLN	OE1-CD-NE2	5.94	116.66	122.60	1	5
A	178	PRO	C-CA-CB	5.93	98.83	110.10	4	1
A	106	THR	OG1-CB-CG2	5.92	97.46	109.30	8	1
A	157	TYR	C-N-CA	5.90	111.08	121.70	7	2
A	303	ALA	C-N-CA	5.85	132.23	121.70	1	1
A	142	LEU	C-N-CA	5.77	132.09	121.70	2	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	632	THR	C-N-CA	5.76	132.08	121.70	5	1
A	185	VAL	CA-CB-CG1	5.75	120.17	110.40	7	1
A	70	THR	C-N-CA	5.70	131.97	121.70	8	1
A	2	ALA	C-N-CA	5.67	131.91	121.70	10	2
A	586	PRO	N-CA-CB	5.65	109.21	103.00	10	1
A	178	PRO	CA-N-CD	5.64	104.11	112.00	2	1
A	306	ASN	CA-CB-CG	5.59	118.19	112.60	4	2
A	136	ASN	CA-CB-CG	5.58	118.18	112.60	7	1
A	18	VAL	C-N-CA	5.58	131.74	121.70	9	2
A	606	GLU	CB-CG-CD	5.55	103.17	112.60	2	1
A	267	TYR	C-N-CA	5.53	131.65	121.70	8	1
A	269	GLN	C-N-CA	5.51	131.63	121.70	8	1
A	67	ALA	C-N-CA	5.51	131.62	121.70	5	1
A	440	ASN	CA-CB-CG	5.49	107.11	112.60	2	1
A	342	GLN	OE1-CD-NE2	5.47	117.13	122.60	4	6
A	325	ASP	CA-CB-CG	5.45	118.05	112.60	2	1
A	75	PRO	C-CA-CB	5.43	120.41	110.10	3	1
A	122	HIS	CB-CG-CD2	5.38	124.20	131.20	9	4
A	57	PRO	C-N-CA	5.38	131.38	121.70	7	1
A	140	ASN	OD1-CG-ND2	5.37	117.23	122.60	7	1
A	128	PHE	C-N-CA	5.37	131.36	121.70	4	1
A	38	LYS	C-N-CA	5.36	131.35	121.70	5	2
A	189	PRO	C-CA-CB	5.36	120.28	110.10	7	1
A	462	GLN	OE1-CD-NE2	5.35	117.25	122.60	8	5
A	83	ILE	C-N-CA	5.35	131.32	121.70	2	2
A	21	ALA	C-N-CA	5.34	131.32	121.70	5	1
A	51	GLN	OE1-CD-NE2	5.34	117.26	122.60	10	7
A	6	THR	C-N-CA	5.34	131.31	121.70	6	2
A	206	LEU	C-CA-CB	5.34	120.24	110.10	1	1
A	191	THR	C-CA-CB	5.29	120.74	109.10	8	1
A	31	ALA	C-N-CA	5.24	131.14	121.70	3	4
A	310	ARG	NH1-CZ-NH2	5.24	112.49	119.30	7	1
A	538	GLN	OE1-CD-NE2	5.24	117.36	122.60	8	5
A	291	ASN	CA-CB-CG	5.23	117.83	112.60	4	1
A	77	GLN	C-N-CA	5.22	131.10	121.70	2	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	393	GLN	OE1-CD-NE2	5.22	117.38	122.60	9	6
A	175	LYS	CA-C-N	5.18	126.56	116.20	1	1
A	85	VAL	CA-CB-CG2	5.18	119.20	110.40	2	1
A	237	GLN	OE1-CD-NE2	5.14	117.46	122.60	6	5
A	74	THR	CA-C-N	5.14	124.61	116.90	5	1
A	180	GLY	C-N-CA	5.13	130.93	121.70	1	1
A	171	VAL	CA-CB-CG2	5.12	119.10	110.40	1	3
A	306	ASN	OD1-CG-ND2	5.11	117.49	122.60	2	4
A	149	TYR	N-CA-CB	5.10	101.84	110.50	2	1
A	386	GLN	OE1-CD-NE2	5.09	117.51	122.60	2	9
A	126	ARG	CD-NE-CZ	5.09	131.52	124.40	2	1
A	110	SER	C-N-CA	5.08	130.85	121.70	2	1
A	553	GLN	OE1-CD-NE2	5.08	117.52	122.60	7	3
A	130	ALA	N-CA-CB	5.07	102.79	110.40	8	1
A	122	HIS	CA-CB-CG	5.07	108.73	113.80	9	1
A	270	ASN	OD1-CG-ND2	5.07	117.53	122.60	3	2

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	8.19	93
2	2.73	31
3	7.31	83
4	4.67	53
5	6.17	70
6	4.76	54
7	11.89	135
8	8.72	99
9	4.76	54
10	5.46	62

There are 734 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:158:MET:HE3	A:247:ALA:HB3	0.93	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:99:VAL:HG21	A:610:ALA:HB2	0.83	3	2
A:158:MET:HE1	A:247:ALA:HB3	0.82	1	1
A:71:LYS:HZ3	A:265:LEU:HD22	0.82	3	1
A:78:LYS:HA	A:479:LEU:HD21	0.81	1	1
A:157:TYR:CG	A:230:LEU:HD22	0.81	8	1
A:173:TYR:CZ	A:178:PRO:HB3	0.80	4	1
A:60:THR:HB	A:64:ARG:CZ	0.79	7	1
A:158:MET:CE	A:247:ALA:HB3	0.78	3	2
A:173:TYR:CE1	A:178:PRO:HB3	0.78	4	1
A:139:LEU:HD21	A:598:ILE:HD12	0.78	7	1
A:75:PRO:CD	A:171:VAL:HG13	0.78	5	1
A:295:LEU:HD21	A:731:CYS:HB2	0.78	6	1
A:67:ALA:HB2	A:161:ARG:HH21	0.78	10	1
A:110:SER:HB3	A:124:ILE:HD12	0.77	8	1
A:138:TYR:CD1	A:181:LEU:HD22	0.77	7	1
A:103:LEU:HD11	A:164:ILE:HD11	0.76	1	1
A:113:THR:HG21	A:723:ALA:CB	0.74	3	1
A:158:MET:HE3	A:230:LEU:HB3	0.74	1	1
A:244:GLN:H	A:274:THR:HG21	0.74	6	1
A:75:PRO:HD2	A:171:VAL:HG13	0.74	5	1
A:641:GLN:HE21	A:725:CYS:H	0.72	6	1
A:128:PHE:CE1	A:181:LEU:HD13	0.72	1	1
A:113:THR:HG21	A:723:ALA:HB1	0.72	3	1
A:67:ALA:HB2	A:161:ARG:NH2	0.72	10	1
A:157:TYR:CE2	A:230:LEU:HD13	0.72	8	1
A:598:ILE:HD11	A:628:TYR:CE1	0.71	7	1
A:479:LEU:HD23	A:516:ASN:HD22	0.71	1	1
A:68:THR:HG23	A:100:LYS:CE	0.70	8	1
A:58:ALA:HB2	A:746:ARG:NH2	0.70	7	1
A:277:TYR:CE1	A:298:ASP:HA	0.70	8	1
A:459:LEU:HD22	A:496:ARG:HH21	0.69	9	4
A:721:TYR:HB3	A:734:GLY:HA3	0.69	10	1
A:171:VAL:HG21	A:512:ARG:CZ	0.69	8	1
A:157:TYR:CD2	A:230:LEU:HD22	0.69	8	1
A:221:GLY:HA2	A:222:VAL:HG23	0.69	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:171:VAL:HG11	A:512:ARG:NH2	0.69	8	1
A:694:LEU:HD13	A:712:HIS:CE1	0.68	8	4
A:83:ILE:HD13	A:185:VAL:HG21	0.68	7	1
A:138:TYR:CD1	A:180:GLY:HA3	0.68	8	1
A:59:ALA:H	A:194:LEU:HD22	0.67	7	1
A:18:VAL:O	A:19:VAL:HG23	0.67	9	1
A:172:LEU:HB3	A:173:TYR:CE1	0.67	4	1
A:172:LEU:HB3	A:173:TYR:CZ	0.67	4	1
A:191:THR:C	A:193:PRO:HD3	0.67	8	1
A:107:PRO:CG	A:109:VAL:HG22	0.66	8	1
A:641:GLN:HE22	A:724:SER:HA	0.66	7	1
A:120:TYR:CE1	A:726:PHE:CZ	0.66	1	1
A:566:PRO:HG2	A:610:ALA:HB3	0.66	9	4
A:139:LEU:HD12	A:144:LEU:HD11	0.66	1	1
A:124:ILE:HG21	A:642:VAL:HG13	0.66	5	1
A:393:GLN:HE21	A:408:LEU:HD22	0.66	10	1
A:87:THR:HG21	A:121:ASP:CG	0.65	8	1
A:108:GLY:CA	A:184:MET:HE2	0.65	7	1
A:109:VAL:HG22	A:184:MET:HE1	0.65	7	1
A:63:ALA:H	A:226:ARG:HH11	0.65	7	1
A:84:SER:HA	A:166:ARG:CZ	0.65	8	1
A:100:LYS:NZ	A:113:THR:HG23	0.65	9	1
A:119:THR:CG2	A:153:VAL:HG11	0.65	3	1
A:276:TYR:CE2	A:304:LYS:HA	0.65	3	1
A:68:THR:HG23	A:100:LYS:HE3	0.65	8	1
A:79:VAL:HG12	A:81:GLN:H	0.65	7	2
A:71:LYS:HZ3	A:265:LEU:CD2	0.65	3	1
A:326:THR:HG23	A:397:LYS:O	0.65	6	1
A:172:LEU:C	A:408:LEU:HD22	0.64	1	1
A:379:VAL:HG21	A:590:PHE:CZ	0.64	1	1
A:142:LEU:HD23	A:178:PRO:HD3	0.64	2	1
A:100:LYS:HE2	A:113:THR:HG22	0.64	4	1
A:85:VAL:HG11	A:124:ILE:HB	0.64	7	1
A:128:PHE:CD1	A:642:VAL:HG22	0.64	7	1
A:299:PHE:CE1	A:733:TRP:CZ2	0.64	10	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:58:ALA:HB1	A:610:ALA:HB2	0.64	9	1
A:719:ARG:H	A:737:ARG:CZ	0.64	4	1
A:99:VAL:CG2	A:610:ALA:HB2	0.64	3	2
A:129:ALA:HA	A:182:LEU:HD11	0.64	8	1
A:109:VAL:HG21	A:164:ILE:HD13	0.63	9	1
A:74:THR:HG22	A:171:VAL:HA	0.63	5	1
A:280:LEU:HD22	A:348:TYR:OH	0.63	6	1
A:346:TYR:CE2	A:377:LYS:HE3	0.62	8	1
A:94:HIS:HB3	A:105:TYR:CZ	0.62	5	1
A:168:PRO:HB3	A:532:SER:HB3	0.62	9	1
A:312:GLU:CD	A:314:MET:HE3	0.61	1	1
A:108:GLY:HA2	A:184:MET:HE2	0.61	7	1
A:109:VAL:HB	A:162:ALA:HB3	0.61	7	1
A:157:TYR:CE2	A:189:PRO:HA	0.61	8	1
A:172:LEU:HD11	A:472:GLN:CD	0.61	8	1
A:70:THR:HG21	A:79:VAL:HG21	0.61	8	1
A:72:THR:HA	A:173:TYR:CD2	0.61	8	1
A:85:VAL:HG11	A:107:PRO:HD2	0.61	1	1
A:455:PRO:O	A:497:VAL:HG21	0.61	3	2
A:158:MET:SD	A:247:ALA:HB3	0.61	3	2
A:377:LYS:HE2	A:426:TYR:CE2	0.60	7	1
A:103:LEU:HA	A:608:LYS:HZ2	0.60	8	1
A:583:MET:HE2	A:634:TYR:CE2	0.60	3	1
A:276:TYR:CE2	A:277:TYR:CD2	0.60	9	1
A:276:TYR:CZ	A:277:TYR:CE2	0.60	9	1
A:126:ARG:CZ	A:574:TYR:CE1	0.60	1	1
A:719:ARG:H	A:737:ARG:NH1	0.60	4	1
A:141:GLY:HA3	A:165:MET:HE2	0.60	8	1
A:171:VAL:HG22	A:512:ARG:CD	0.60	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	745	638	65	42
2	745	668	56	21

Model ID	Analysed	Favored	Allowed	Outliers
3	745	659	62	24
4	745	693	37	15
5	745	648	69	28
6	745	697	36	12
7	745	632	72	41
8	745	682	47	16
9	745	691	41	13
10	745	679	51	15

There are 143 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	13	LEU	5
A	54	ALA	5
A	2	ALA	4
A	28	SER	4
A	32	GLN	4
A	39	GLU	4
A	52	GLU	4
A	71	LYS	4
A	168	PRO	4
A	9	PRO	3
A	134	SER	3
A	142	LEU	3
A	160	GLU	3
A	169	VAL	3
A	179	GLY	3
A	448	LYS	3
A	5	LYS	2
A	7	ALA	2
A	15	LYS	2
A	19	VAL	2
A	25	SER	2
A	26	GLY	2
A	29	VAL	2
A	34	ALA	2

Chain	Res	Type	Models (Total)
A	42	ILE	2
A	50	PRO	2
A	55	TRP	2
A	58	ALA	2
A	60	THR	2
A	62	ALA	2
A	64	ARG	2
A	68	THR	2
A	73	ASP	2
A	78	LYS	2
A	81	GLN	2
A	114	ARG	2
A	116	ALA	2
A	117	SER	2
A	118	ASN	2
A	123	LEU	2
A	137	ASN	2
A	143	LYS	2
A	148	PHE	2
A	149	TYR	2
A	152	ALA	2
A	154	ILE	2
A	171	VAL	2
A	176	SER	2
A	177	SER	2
A	178	PRO	2
A	180	GLY	2
A	185	VAL	2
A	237	GLN	2
A	304	LYS	2
A	596	GLY	2
A	727	ASN	2
A	736	GLU	2
A	6	THR	1
A	8	GLN	1

Chain	Res	Type	Models (Total)
A	11	HIS	1
A	12	SER	1
A	20	VAL	1
A	23	ALA	1
A	24	VAL	1
A	27	MET	1
A	33	ALA	1
A	40	ASP	1
A	44	VAL	1
A	49	ALA	1
A	51	GLN	1
A	53	SER	1
A	65	GLN	1
A	67	ALA	1
A	69	GLY	1
A	75	PRO	1
A	76	ILE	1
A	80	PRO	1
A	82	SER	1
A	83	ILE	1
A	84	SER	1
A	85	VAL	1
A	86	VAL	1
A	109	VAL	1
A	113	THR	1
A	115	GLY	1
A	122	HIS	1
A	128	PHE	1
A	129	ALA	1
A	130	ALA	1
A	131	GLU	1
A	132	GLY	1
A	133	GLN	1
A	138	TYR	1
A	140	ASN	1

Chain	Res	Type	Models (Total)
A	147	ASN	1
A	153	VAL	1
A	155	ASP	1
A	158	MET	1
A	159	LEU	1
A	161	ARG	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	616	576	23	17
2	616	570	29	17
3	616	591	14	11
4	616	603	8	5
5	616	577	22	17
6	616	594	16	6
7	616	570	25	21
8	616	582	23	11
9	616	598	11	7
10	616	587	17	12

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

Chain	Res	Type	Models (Total)
A	6	THR	9
A	41	THR	9
A	22	THR	8
A	45	THR	7
A	169	VAL	4
A	171	VAL	4
A	728	THR	4
A	119	THR	3
A	173	TYR	3
A	177	SER	3
A	414	MET	3
A	60	THR	2

Chain	Res	Type	Models (Total)
A	93	LEU	2
A	113	THR	2
A	123	LEU	2
A	164	ILE	2
A	186	SER	2
A	358	TYR	2
A	433	LEU	2
A	633	THR	2
A	4	SER	1
A	19	VAL	1
A	24	VAL	1
A	28	SER	1
A	43	THR	1
A	44	VAL	1
A	53	SER	1
A	66	SER	1
A	68	THR	1
A	76	ILE	1
A	82	SER	1
A	83	ILE	1
A	85	VAL	1
A	86	VAL	1
A	89	GLU	1
A	109	VAL	1
A	111	VAL	1
A	114	ARG	1
A	122	HIS	1
A	131	GLU	1
A	139	LEU	1
A	142	LEU	1
A	144	LEU	1
A	151	ASP	1
A	153	VAL	1
A	160	GLU	1
A	165	MET	1

Chain	Res	Type	Models (Total)
A	166	ARG	1
A	182	LEU	1
A	203	THR	1
A	206	LEU	1
A	214	SER	1
A	216	SER	1
A	265	LEU	1
A	325	ASP	1
A	328	THR	1
A	344	SER	1
A	351	CYS	1
A	374	LEU	1
A	378	TYR	1
A	435	LEU	1
A	439	VAL	1
A	453	SER	1
A	527	PHE	1
A	582	LEU	1
A	598	ILE	1
A	682	SER	1
A	721	TYR	1
A	737	ARG	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.

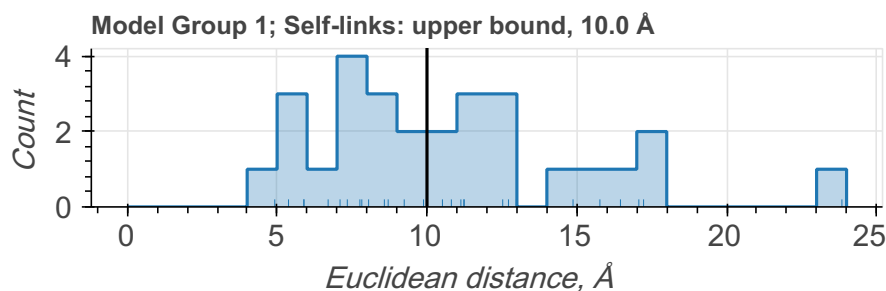
There are 28 crosslinking restraints combined in 28 restraint groups.

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	3
L-Photo-Leucine	ALA	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	GLU	CA	LEU	CA	upper bound	10.0	5
L-Photo-Leucine	ARG	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	3
L-Photo-Leucine	ASN	CA	LEU	CA	upper bound	10.0	4
L-Photo-Leucine	LEU	CA	SER	CA	upper bound	10.0	1
L-Photo-Leucine	ILE	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	GLN	CA	LEU	CA	upper bound	10.0	3
L-Photo-Leucine	LEU	CA	PHE	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	VAL	CA	upper bound	10.0	4
L-Photo-Leucine	GLY	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.



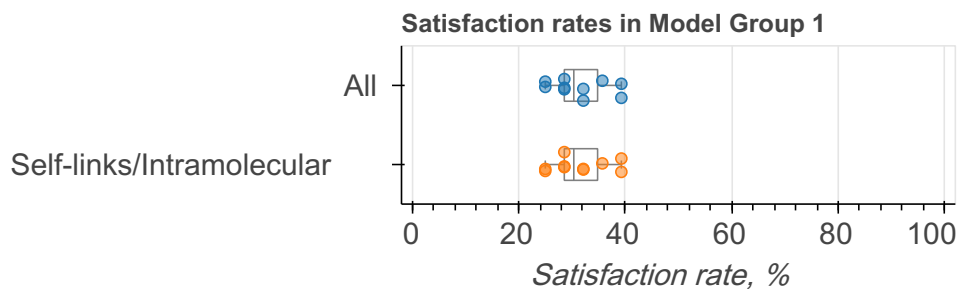
Satisfaction of restraints

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=28)
1	1	1	10/10	All	50.00	50.00	28
				Self-links/ Intramolecular	50.00	50.00	28

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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