

# 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	9A2O
PDB-Dev ID	PDBDEV_00000173
Structure Title	Model of E. coli BamA 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](mailto:helpdesk@pdb-ihm.org)*

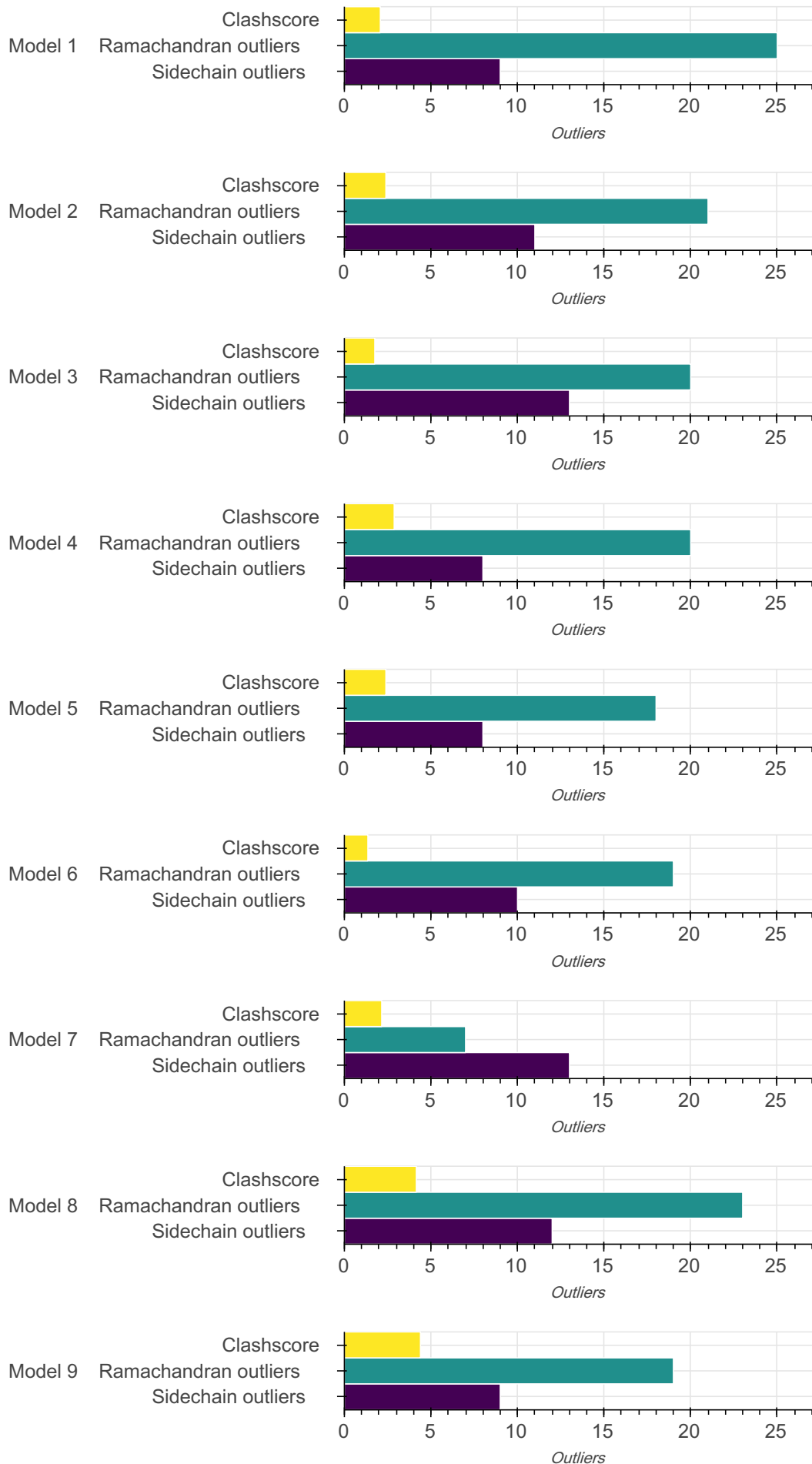
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

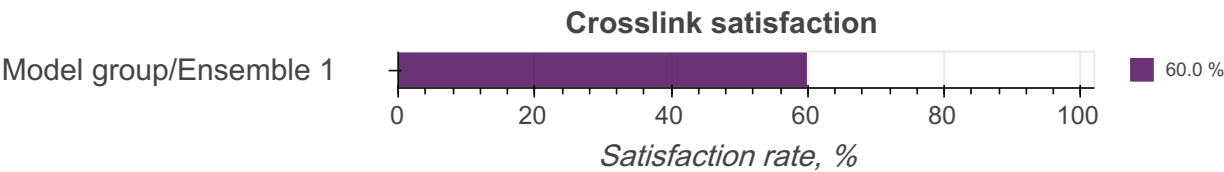
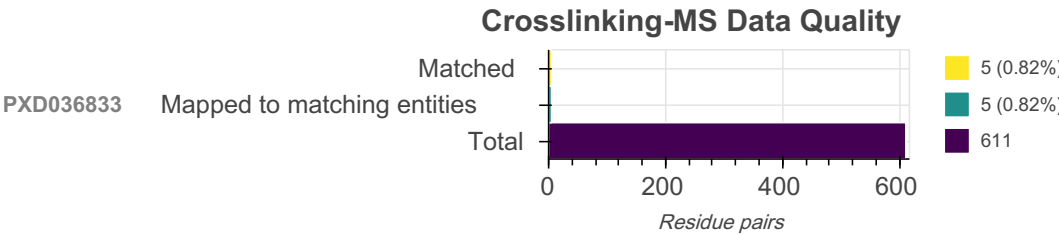
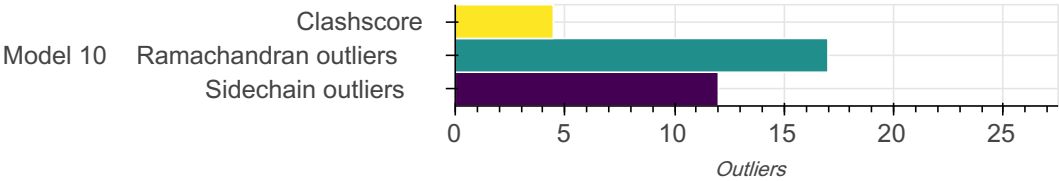
*List of references used to build this report is available [here](#).*

## 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	P0A940	A	810	-	1-810	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	<a href="#">AlphaLink</a>	1.00	model building	<a href="https://github.com/lhatsk/AlphaLink">https://github.com/lhatsk/AlphaLink</a>

## 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	P0A940	dbseq_P0A940_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A2O	5	5 (100.00%)	5 (100.00%)
PXD036833	611	5 (0.82%)	5 (0.82% )

### 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 366 bond angle outliers in this entry (0.41% of 88748 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	645	GLU	C-N-CA	7.92	135.96	121.70	10	2
A	656	GLY	C-N-CA	7.84	135.81	121.70	9	1
A	495	GLN	OE1-CD-NE2	7.55	115.05	122.60	9	8
A	748	ASN	C-N-CA	7.53	135.25	121.70	5	1
A	2	ALA	C-N-CA	7.23	134.71	121.70	1	3
A	448	ASN	OD1-CG-ND2	6.92	115.68	122.60	10	2
A	569	ASP	CA-CB-CG	6.75	119.35	112.60	4	7
A	661	ARG	NE-CZ-NH2	6.69	125.22	119.20	4	3
A	556	PRO	N-CA-CB	6.63	110.30	103.00	10	4
A	691	ALA	C-N-CA	6.62	133.62	121.70	3	2
A	587	PRO	C-CA-CB	6.54	122.53	110.10	6	1
A	677	HIS	C-N-CA	6.46	133.33	121.70	6	2
A	126	ASP	CA-CB-CG	6.38	118.98	112.60	8	2
A	547	ARG	CD-NE-CZ	6.37	133.32	124.40	1	2
A	556	PRO	CA-N-CD	6.11	103.45	112.00	4	1
A	448	ASN	C-N-CA	6.07	132.62	121.70	7	1
A	705	ALA	C-CA-CB	5.97	119.46	110.50	1	1
A	211	ASP	C-N-CA	5.95	132.42	121.70	3	3
A	500	ASP	CA-CB-CG	5.85	118.45	112.60	5	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	542	GLN	C-N-CA	5.82	132.18	121.70	8	1
A	775	GLN	OE1-CD-NE2	5.73	116.87	122.60	7	5
A	211	ASP	CA-CB-CG	5.72	118.32	112.60	7	3
A	479	THR	C-N-CA	5.69	131.95	121.70	1	1
A	392	LEU	N-CA-CB	5.69	100.82	110.50	10	1
A	749	TRP	N-CA-CB	5.60	120.02	110.50	5	1
A	286	GLN	OE1-CD-NE2	5.53	117.07	122.60	8	8
A	705	ALA	N-CA-CB	5.53	102.11	110.40	1	1
A	204	PRO	C-N-CA	5.50	131.60	121.70	2	3
A	675	PHE	CA-C-N	5.45	125.08	116.90	8	1
A	488	ARG	CD-NE-CZ	5.43	132.00	124.40	3	1
A	201	ASP	CA-CB-CG	5.29	117.89	112.60	7	1
A	411	GLN	OE1-CD-NE2	5.26	117.34	122.60	7	1
A	477	TYR	C-N-CA	5.24	131.14	121.70	9	2
A	212	ARG	C-N-CA	5.24	131.13	121.70	8	1
A	803	GLN	OE1-CD-NE2	5.23	117.37	122.60	7	4
A	179	GLN	OE1-CD-NE2	5.23	117.37	122.60	8	10
A	659	THR	C-N-CA	5.23	131.11	121.70	9	1
A	206	TRP	CA-CB-CG	5.22	123.52	113.60	8	1
A	542	GLN	OE1-CD-NE2	5.22	117.38	122.60	2	6
A	748	ASN	OD1-CG-ND2	5.21	117.39	122.60	4	2
A	664	GLN	OE1-CD-NE2	5.20	117.40	122.60	8	6
A	561	GLN	OE1-CD-NE2	5.17	117.43	122.60	5	9
A	679	ALA	C-CA-CB	5.14	118.20	110.50	8	1
A	749	TRP	C-N-CA	5.13	130.94	121.70	5	1
A	686	TYR	C-N-CA	5.08	130.85	121.70	8	1
A	561	GLN	N-CA-C	5.05	125.14	111.00	6	1
A	497	ASP	CA-CB-CG	5.05	117.65	112.60	7	3
A	680	SER	C-N-CA	5.03	130.76	121.70	8	1
A	422	ASN	OD1-CG-ND2	5.02	117.58	122.60	10	2
A	758	PRO	N-CA-CB	4.97	108.47	103.00	1	1
A	573	ASN	OD1-CG-ND2	4.96	117.64	122.60	1	1
A	466	GLN	OE1-CD-NE2	4.94	117.66	122.60	9	6
A	478	PHE	C-N-CA	4.94	130.59	121.70	1	1
A	645	GLU	O-C-N	4.93	115.11	123.00	10	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	478	PHE	N-CA-CB	4.93	102.13	110.50	8	1
A	677	HIS	CA-C-N	4.90	126.00	116.20	6	1
A	202	GLU	C-N-CA	4.89	130.51	121.70	8	1
A	709	ASN	CA-CB-CG	4.87	117.47	112.60	10	1
A	497	ASP	C-CA-CB	4.87	119.36	110.10	10	1
A	540	GLN	OE1-CD-NE2	4.85	117.75	122.60	5	5
A	4	LYS	C-N-CA	4.83	130.40	121.70	10	1
A	679	ALA	C-N-CA	4.82	130.38	121.70	8	1
A	680	SER	N-CA-C	4.80	124.45	111.00	1	1
A	209	VAL	CA-CB-CG2	4.80	118.56	110.40	3	1
A	624	ASP	CA-CB-CG	4.80	117.40	112.60	4	6
A	170	GLN	OE1-CD-NE2	4.79	117.81	122.60	2	10
A	677	HIS	CB-CG-CD2	4.79	124.97	131.20	2	3
A	654	ALA	N-CA-CB	4.79	103.22	110.40	10	1
A	422	ASN	N-CA-CB	4.79	102.36	110.50	10	1
A	659	THR	N-CA-CB	4.77	103.39	111.50	3	1
A	668	ILE	C-CA-CB	4.76	121.12	111.60	5	1
A	441	GLN	OE1-CD-NE2	4.73	117.87	122.60	3	9
A	2	ALA	O-C-N	4.73	115.44	123.00	1	1
A	801	GLN	OE1-CD-NE2	4.72	117.88	122.60	3	8
A	658	SER	C-CA-CB	4.71	119.05	110.10	9	1
A	579	ASN	OD1-CG-ND2	4.70	117.90	122.60	10	2
A	797	ASP	CA-CB-CG	4.70	117.30	112.60	5	6
A	217	GLN	OE1-CD-NE2	4.67	117.93	122.60	8	7
A	634	ARG	CD-NE-CZ	4.66	130.92	124.40	1	1
A	678	GLN	OE1-CD-NE2	4.62	117.98	122.60	9	6
A	445	GLN	OE1-CD-NE2	4.61	117.99	122.60	7	6
A	677	HIS	O-C-N	4.61	115.63	123.00	6	1
A	655	GLY	C-N-CA	4.61	113.40	121.70	5	1
A	805	ASN	OD1-CG-ND2	4.60	118.00	122.60	1	1
A	809	THR	C-N-CA	4.59	129.96	121.70	6	1
A	323	GLN	OE1-CD-NE2	4.58	118.02	122.60	6	7
A	693	GLN	OE1-CD-NE2	4.57	118.03	122.60	3	10
A	666	ASN	N-CA-CB	4.53	102.79	110.50	2	1
A	3	MET	C-N-CA	4.52	129.84	121.70	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	557	SER	C-N-CA	4.51	129.81	121.70	4	2
A	690	CYS	C-N-CA	4.51	129.81	121.70	10	1
A	35	GLN	OE1-CD-NE2	4.50	118.10	122.60	2	8
A	689	GLU	C-N-CA	4.49	129.79	121.70	8	2
A	654	ALA	C-CA-CB	4.49	117.23	110.50	10	1
A	126	ASP	C-CA-CB	4.48	118.62	110.10	8	1
A	215	GLN	OE1-CD-NE2	4.46	118.14	122.60	9	7
A	652	PHE	C-N-CA	4.45	129.70	121.70	9	1
A	585	TYR	C-N-CA	4.43	129.68	121.70	6	1
A	789	GLN	OE1-CD-NE2	4.42	118.18	122.60	9	4
A	11	LEU	C-N-CA	4.41	129.65	121.70	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	2.08	26
2	2.40	30
3	1.76	22
4	2.88	36
5	2.40	30
6	1.36	17
7	2.16	27
8	4.15	52
9	4.39	55
10	4.47	56

There are 351 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:536:LEU:HD21	A:670:PRO:HB3	0.93	8	1
A:394:PHE:CE1	A:449:TRP:HA	0.89	10	1
A:502:SER:HB2	A:543:VAL:HG22	0.89	1	1
A:514:THR:HG21	A:526:ARG:HE	0.88	4	1
A:449:TRP:CD1	A:477:TYR:HH	0.86	10	1
A:648:PHE:CE1	A:777:MET:HE3	0.86	6	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:706:VAL:HG13	A:760:TYR:CE1	0.84	6	1
A:783:LEU:HD21	A:785:PHE:CE2	0.83	5	1
A:364:VAL:HG13	A:367:ARG:HH21	0.83	3	1
A:392:LEU:HB3	A:394:PHE:CZ	0.82	10	1
A:547:ARG:HH12	A:679:ALA:HB3	0.79	8	1
A:705:ALA:HB2	A:767:ARG:HH22	0.74	3	1
A:548:TYR:CE1	A:556:PRO:HG3	0.74	10	1
A:547:ARG:NH1	A:679:ALA:HB3	0.71	8	1
A:394:PHE:CZ	A:449:TRP:HA	0.70	10	1
A:501:LEU:HD21	A:678:GLN:HG2	0.70	10	1
A:658:SER:HB2	A:711:MET:HE1	0.70	5	1
A:608:TYR:CE2	A:646:MET:HE3	0.69	6	1
A:360:SER:HA	A:450:LEU:HD11	0.69	8	1
A:706:VAL:HG13	A:760:TYR:CZ	0.69	6	1
A:392:LEU:HD22	A:449:TRP:CE2	0.68	8	1
A:177:ILE:HD11	A:199:LEU:HD22	0.67	4	6
A:586:PHE:CE2	A:777:MET:HE3	0.67	5	1
A:204:PRO:HB2	A:206:TRP:CE3	0.67	8	1
A:586:PHE:CZ	A:719:ILE:HG22	0.67	2	1
A:653:TYR:HB3	A:666:ASN:HD21	0.67	2	1
A:621:ILE:HD11	A:629:VAL:HG23	0.66	9	2
A:392:LEU:HD13	A:394:PHE:CE2	0.66	10	1
A:348:TYR:CZ	A:376:TRP:CZ3	0.66	8	1
A:790:PRO:HG2	A:793:LYS:HE2	0.65	9	1
A:352:ILE:HD11	A:372:MET:HB2	0.65	3	1
A:514:THR:HG21	A:526:ARG:NE	0.65	4	1
A:610:LYS:HE3	A:649:TYR:CE2	0.64	3	1
A:548:TYR:CZ	A:556:PRO:HG3	0.64	10	1
A:610:LYS:CE	A:646:MET:HE1	0.64	9	1
A:504:TYR:CD2	A:652:PHE:CE2	0.64	9	1
A:672:ALA:HB2	A:701:LYS:HE2	0.63	7	1
A:548:TYR:CE1	A:556:PRO:CG	0.63	10	1
A:802:PHE:CE1	A:804:PHE:CE2	0.62	10	1
A:205:TRP:CG	A:254:ILE:HD13	0.62	8	1
A:608:TYR:CD1	A:648:PHE:CZ	0.62	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:652:PHE:CD1	A:767:ARG:HD2	0.62	8	1
A:548:TYR:CE1	A:556:PRO:CD	0.62	4	1
A:369:MET:HE1	A:385:GLY:O	0.61	2	2
A:526:ARG:HH22	A:596:THR:CG2	0.60	5	1
A:369:MET:HE1	A:416:TYR:CE1	0.60	5	1
A:687:ASP:C	A:689:GLU:H	0.60	6	1
A:392:LEU:HD22	A:449:TRP:CD2	0.60	8	1
A:610:LYS:HE3	A:649:TYR:CZ	0.60	3	1
A:465:TYR:CZ	A:657:SER:HB2	0.60	4	1
A:548:TYR:CE1	A:556:PRO:HD2	0.59	4	1
A:488:ARG:HH21	A:526:ARG:NH2	0.59	9	1
A:369:MET:HE1	A:385:GLY:C	0.59	2	1
A:610:LYS:HE3	A:646:MET:HE1	0.59	9	1
A:609:TYR:CE2	A:637:TYR:HB3	0.58	5	1
A:506:ASN:HD21	A:532:VAL:HG13	0.58	9	1
A:652:PHE:CE2	A:719:ILE:HD12	0.58	6	1
A:394:PHE:CZ	A:449:TRP:HB2	0.58	10	1
A:526:ARG:HH22	A:596:THR:HG22	0.58	5	1
A:543:VAL:HG22	A:675:PHE:CZ	0.58	9	1
A:204:PRO:HG2	A:206:TRP:CH2	0.58	8	1
A:394:PHE:CE2	A:449:TRP:HB2	0.57	10	1
A:652:PHE:CD1	A:663:PHE:HB3	0.57	4	1
A:653:TYR:HB3	A:665:SER:HB2	0.56	3	1
A:204:PRO:HB2	A:206:TRP:CZ3	0.56	8	1
A:661:ARG:HH21	A:773:ALA:CB	0.56	4	1
A:506:ASN:HD21	A:532:VAL:CG1	0.56	9	1
A:541:PRO:CB	A:546:TRP:HE1	0.56	7	1
A:592:ARG:HH21	A:594:ASN:ND2	0.55	1	1
A:673:VAL:HG22	A:704:ASP:H	0.55	2	1
A:659:THR:HB	A:663:PHE:CD2	0.55	7	1
A:790:PRO:CG	A:793:LYS:HE2	0.55	9	1
A:494:PHE:CE2	A:496:ALA:HB2	0.55	7	1
A:659:THR:HG21	A:767:ARG:HD3	0.55	9	1
A:548:TYR:CZ	A:556:PRO:CG	0.55	10	1
A:668:ILE:CG2	A:709:ASN:HA	0.55	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:657:SER:C	A:659:THR:H	0.54	6	1
A:367:ARG:CZ	A:449:TRP:CZ2	0.54	10	1
A:177:ILE:HD11	A:214:TYR:CD1	0.54	3	1
A:394:PHE:CZ	A:449:TRP:CA	0.54	10	1
A:586:PHE:HZ	A:719:ILE:HG22	0.54	2	1
A:702:SER:C	A:704:ASP:H	0.53	6	2
A:689:GLU:C	A:691:ALA:H	0.53	10	1
A:783:LEU:HD21	A:785:PHE:CD2	0.53	5	1
A:803:GLN:NE2	A:805:ASN:HD21	0.53	9	1
A:547:ARG:HH22	A:670:PRO:CB	0.53	4	1
A:802:PHE:CE1	A:804:PHE:CZ	0.53	10	1
A:706:VAL:HG21	A:767:ARG:HH12	0.53	8	1
A:348:TYR:CE2	A:411:GLN:HG2	0.52	7	1
A:370:ARG:HH12	A:521:GLU:N	0.52	8	1
A:367:ARG:NH2	A:449:TRP:CE2	0.52	10	1
A:607:GLU:HB3	A:641:LEU:HD12	0.52	8	1
A:488:ARG:HH21	A:526:ARG:CZ	0.52	9	1
A:394:PHE:CD2	A:449:TRP:HB2	0.52	8	1
A:185:ASN:HB3	A:260:ILE:HD11	0.52	9	3
A:543:VAL:HG12	A:547:ARG:HE	0.52	4	1
A:211:ASP:OD2	A:213:LYS:HE3	0.52	9	1
A:610:LYS:HE2	A:646:MET:HE1	0.52	9	1
A:504:TYR:CG	A:652:PHE:CZ	0.52	9	1
A:394:PHE:CD1	A:394:PHE:N	0.52	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	808	751	32	25
2	808	752	35	21
3	808	752	36	20
4	808	749	39	20
5	808	740	50	18
6	808	746	43	19
7	808	768	33	7

Model ID	Analysed	Favored	Allowed	Outliers
8	808	754	31	23
9	808	762	27	19
10	808	748	43	17

*There are 88 unique backbone outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	690	CYS	8
A	558	THR	7
A	15	SER	6
A	18	VAL	6
A	212	ARG	6
A	692	THR	5
A	13	PHE	4
A	502	SER	4
A	563	ASN	4
A	667	THR	4
A	689	GLU	4
A	703	ASP	4
A	754	TYR	4
A	2	ALA	3
A	3	MET	3
A	10	SER	3
A	12	LEU	3
A	17	THR	3
A	20	GLY	3
A	209	VAL	3
A	211	ASP	3
A	655	GLY	3
A	657	SER	3
A	678	GLN	3
A	687	ASP	3
A	694	ASP	3
A	4	LYS	2
A	5	LYS	2
A	6	LEU	2

Chain	Res	Type	Models (Total)
A	11	LEU	2
A	201	ASP	2
A	205	TRP	2
A	208	VAL	2
A	553	GLY	2
A	557	SER	2
A	561	GLN	2
A	581	LEU	2
A	583	ARG	2
A	584	GLY	2
A	585	TYR	2
A	651	ASN	2
A	660	VAL	2
A	666	ASN	2
A	677	HIS	2
A	680	SER	2
A	682	TYR	2
A	748	ASN	2
A	749	TRP	2
A	8	ILE	1
A	14	SER	1
A	16	ALA	1
A	21	ALA	1
A	22	GLU	1
A	202	GLU	1
A	210	GLY	1
A	213	LYS	1
A	477	TYR	1
A	478	PHE	1
A	480	VAL	1
A	521	GLU	1
A	543	VAL	1
A	545	MET	1
A	556	PRO	1
A	559	SER	1

Chain	Res	Type	Models (Total)
A	560	ASP	1
A	565	PHE	1
A	589	ASP	1
A	646	MET	1
A	647	PRO	1
A	652	PHE	1
A	653	TYR	1
A	656	GLY	1
A	658	SER	1
A	668	ILE	1
A	672	ALA	1
A	675	PHE	1
A	681	ASN	1
A	688	TYR	1
A	697	LYS	1
A	702	SER	1
A	704	ASP	1
A	705	ALA	1
A	706	VAL	1
A	728	LYS	1
A	730	ALA	1
A	750	ASP	1
A	765	ASN	1
A	800	GLU	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	688	658	21	9
2	688	662	15	11
3	688	662	13	13
4	688	662	18	8
5	688	671	9	8
6	688	657	21	10
7	688	661	14	13

Model ID	Analysed	Favored	Allowed	Outliers
8	688	661	15	12
9	688	664	15	9
10	688	660	16	12

*There are 56 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	6	LEU	10
A	7	LEU	9
A	17	THR	6
A	11	LEU	5
A	209	VAL	5
A	10	SER	4
A	247	LEU	4
A	3	MET	3
A	14	SER	3
A	562	ASP	3
A	1	MET	2
A	211	ASP	2
A	581	LEU	2
A	658	SER	2
A	706	VAL	2
A	732	SER	2
A	784	VAL	2
A	15	SER	1
A	93	THR	1
A	129	THR	1
A	173	VAL	1
A	174	SER	1
A	359	THR	1
A	362	ASP	1
A	364	VAL	1
A	392	LEU	1
A	394	PHE	1
A	434	THR	1
A	436	SER	1

Chain	Res	Type	Models (Total)
A	474	THR	1
A	480	VAL	1
A	500	ASP	1
A	505	THR	1
A	542	GLN	1
A	545	MET	1
A	548	TYR	1
A	557	SER	1
A	646	MET	1
A	649	TYR	1
A	659	THR	1
A	660	VAL	1
A	665	SER	1
A	667	THR	1
A	677	HIS	1
A	682	TYR	1
A	688	TYR	1
A	692	THR	1
A	693	GLN	1
A	700	CYS	1
A	711	MET	1
A	722	THR	1
A	726	SER	1
A	727	ASP	1
A	739	TRP	1
A	754	TYR	1
A	772	ILE	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.

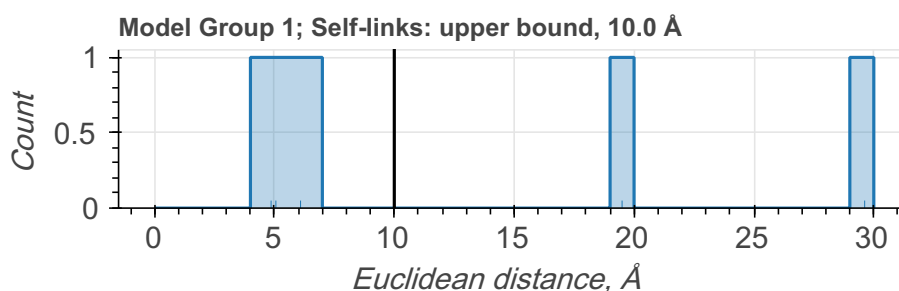


There are 5 crosslinking restraints combined in 5 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	HIS	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	ILE	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	GLU	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	LEU	CA	upper bound	10.0	1
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.



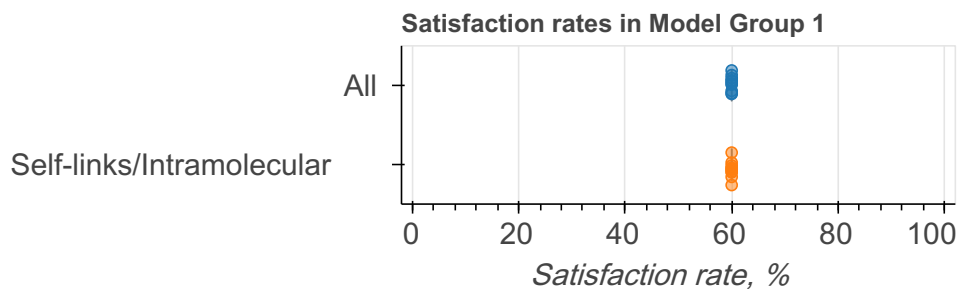
#### Satisfaction of restraints

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=5)
1	1	1	10/10	All	60.00	40.00	5
				Self-links/ Intramolecular	60.00	40.00	5

#### 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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