

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	9A30
PDB-Dev ID	PDBDEV_00000185
Structure Title	Model of E. coli btuB 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

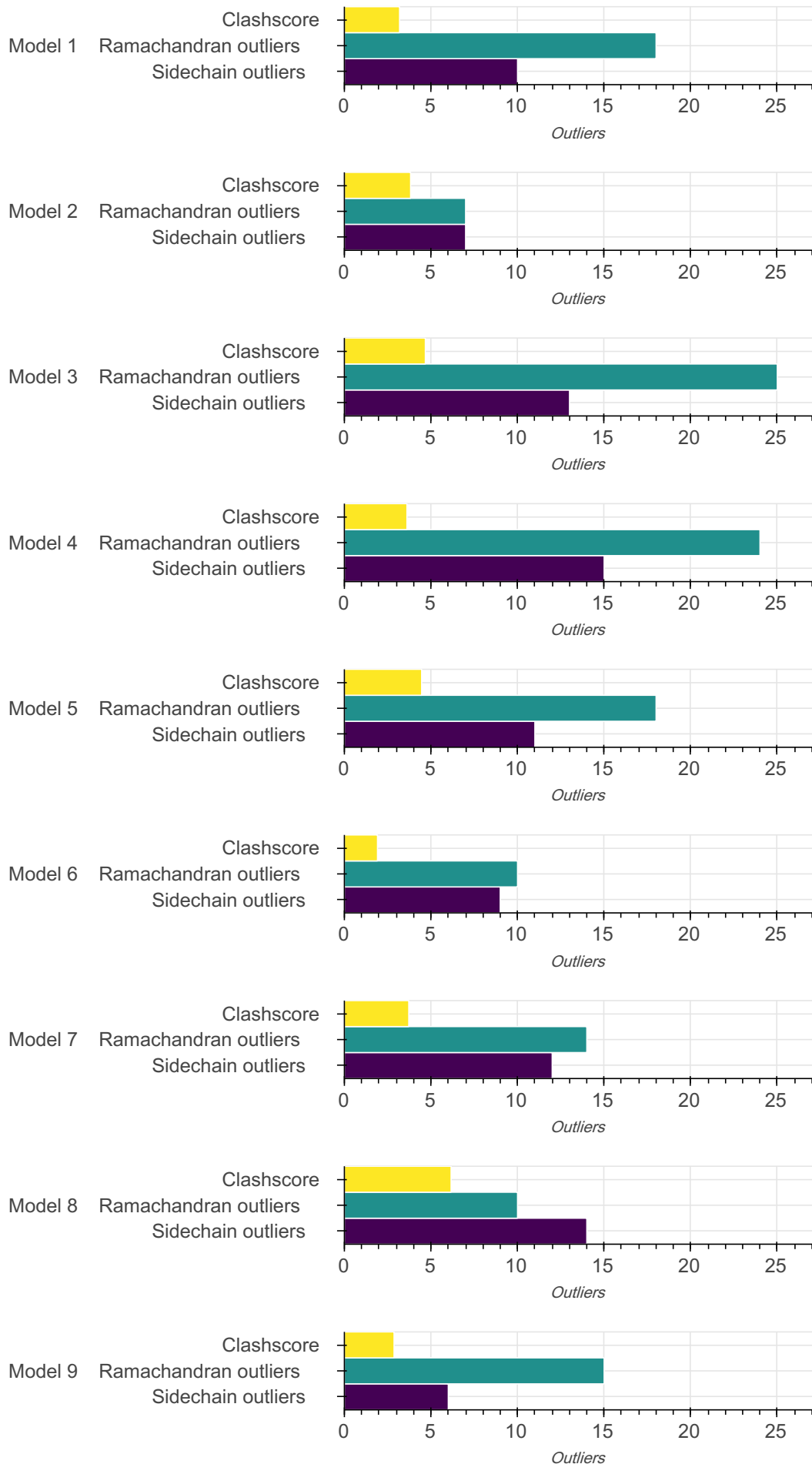
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

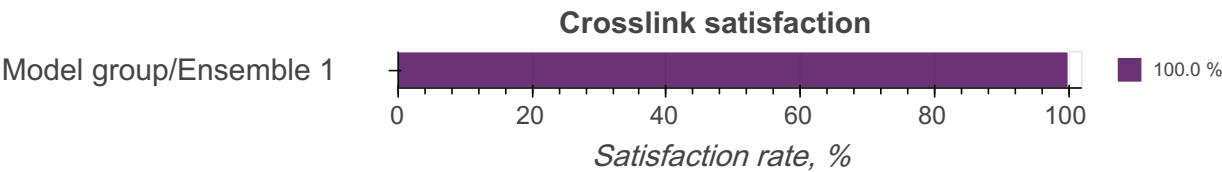
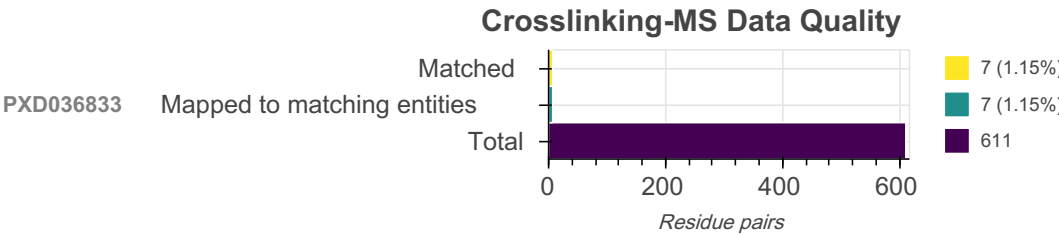
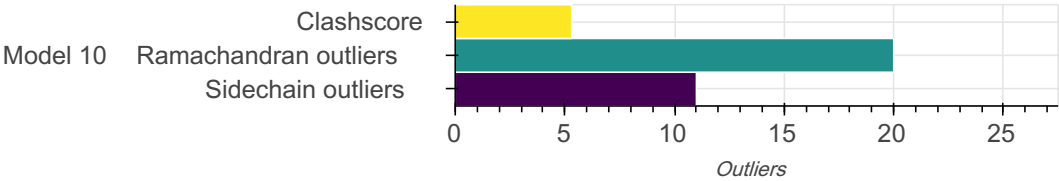
List of references used to build this report is available [here](#).

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	P06129	A	614	-	1-614	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	P06129	dbseq_P06129_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A30	7	7 (100.00%)	7 (100.00%)
PXD036833	611	7 (1.15%)	7 (1.15%)

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 348 bond angle outliers in this entry (0.51% of 67720 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	213	ASP	CA-CB-CG	8.22	120.82	112.60	4	2
A	354	ASP	CA-CB-CG	8.17	120.77	112.60	1	7
A	7	LEU	C-N-CA	7.69	135.54	121.70	4	5
A	350	GLU	C-N-CA	7.35	134.92	121.70	3	2
A	33	ASN	CA-CB-CG	6.77	119.37	112.60	5	2
A	118	GLN	OE1-CD-NE2	6.76	115.84	122.60	1	6
A	33	ASN	C-CA-CB	6.71	122.85	110.10	8	1
A	93	ALA	C-N-CA	6.66	133.68	121.70	10	1
A	541	GLN	OE1-CD-NE2	6.62	115.98	122.60	7	8
A	114	ALA	C-N-CA	6.56	133.51	121.70	2	1
A	600	GLN	OE1-CD-NE2	6.46	116.14	122.60	6	9
A	106	ASN	OD1-CG-ND2	6.43	116.17	122.60	2	1
A	423	GLY	C-N-CA	6.21	132.88	121.70	4	1
A	32	ALA	N-CA-CB	6.20	101.11	110.40	6	1
A	134	ARG	NH1-CZ-NH2	6.19	111.25	119.30	10	1
A	338	GLN	OE1-CD-NE2	5.89	116.71	122.60	9	5
A	522	GLN	OE1-CD-NE2	5.88	116.72	122.60	3	7
A	200	VAL	CA-CB-CG2	5.81	120.28	110.40	10	1
A	245	ASN	OD1-CG-ND2	5.79	116.81	122.60	2	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	300	HIS	CA-CB-CG	5.77	119.57	113.80	4	1
A	250	ASP	CA-CB-CG	5.76	118.36	112.60	4	3
A	316	TYR	C-N-CA	5.75	132.05	121.70	4	1
A	37	GLN	OE1-CD-NE2	5.75	116.85	122.60	3	6
A	134	ARG	NE-CZ-NH2	5.74	124.37	119.20	5	1
A	244	ASP	CA-CB-CG	5.73	118.33	112.60	4	2
A	211	GLN	OE1-CD-NE2	5.72	116.88	122.60	7	9
A	77	ASN	CA-CB-CG	5.71	118.31	112.60	9	2
A	33	ASN	OD1-CG-ND2	5.66	116.94	122.60	3	1
A	82	GLN	OE1-CD-NE2	5.65	116.95	122.60	3	3
A	148	ASN	OD1-CG-ND2	5.59	117.01	122.60	10	3
A	33	ASN	C-N-CA	5.59	131.75	121.70	4	1
A	355	GLN	OE1-CD-NE2	5.54	117.06	122.60	2	6
A	600	GLN	C-N-CA	5.46	131.54	121.70	2	1
A	308	ALA	C-N-CA	5.44	131.49	121.70	3	1
A	134	ARG	NE-CZ-NH1	5.43	126.93	121.50	10	1
A	214	ASN	C-N-CA	5.37	131.37	121.70	5	2
A	32	ALA	C-CA-CB	5.37	118.55	110.50	7	1
A	119	PHE	CA-CB-CG	5.35	108.45	113.80	5	3
A	284	GLN	OE1-CD-NE2	5.34	117.26	122.60	9	3
A	34	ARG	NE-CZ-NH2	5.33	124.00	119.20	1	1
A	340	GLN	OE1-CD-NE2	5.32	117.28	122.60	8	3
A	134	ARG	CD-NE-CZ	5.32	131.85	124.40	10	1
A	317	THR	CA-CB-CG2	5.31	119.52	110.50	4	1
A	122	ALA	C-CA-CB	5.29	118.43	110.50	4	1
A	214	ASN	OD1-CG-ND2	5.28	117.32	122.60	9	5
A	317	THR	N-CA-CB	5.24	102.59	111.50	4	1
A	34	ARG	NH1-CZ-NH2	5.23	112.50	119.30	8	1
A	126	ARG	NE-CZ-NH1	5.23	126.73	121.50	5	2
A	170	GLN	OE1-CD-NE2	5.21	117.39	122.60	1	8
A	459	ASP	CA-CB-CG	5.19	117.79	112.60	9	4
A	388	HIS	CB-CG-CD2	5.18	124.47	131.20	8	2
A	114	ALA	C-CA-CB	5.17	118.25	110.50	2	1
A	300	HIS	CB-CG-CD2	5.16	124.50	131.20	4	1
A	11	CYS	C-N-CA	5.15	130.98	121.70	4	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	253	TYR	C-N-CA	5.14	130.95	121.70	4	1
A	300	HIS	N-CA-CB	5.13	119.22	110.50	4	1
A	264	LYS	CG-CD-CE	5.12	99.52	111.30	9	1
A	21	GLN	OE1-CD-NE2	5.09	117.51	122.60	2	7
A	2	ILE	C-N-CA	5.07	130.82	121.70	3	2
A	317	THR	CA-C-N	5.05	126.30	116.20	4	1
A	76	GLN	OE1-CD-NE2	5.04	117.56	122.60	7	8
A	3	LYS	C-N-CA	5.04	130.78	121.70	9	3
A	95	HIS	CB-CG-CD2	5.04	124.65	131.20	3	4
A	209	GLN	OE1-CD-NE2	5.02	117.58	122.60	6	8
A	319	GLN	OE1-CD-NE2	4.99	117.61	122.60	1	5
A	213	ASP	C-CA-CB	4.98	119.57	110.10	4	3
A	77	ASN	C-N-CA	4.94	130.60	121.70	4	1
A	420	GLN	OE1-CD-NE2	4.94	117.66	122.60	2	4
A	268	GLN	OE1-CD-NE2	4.93	117.67	122.60	3	9
A	546	ARG	NE-CZ-NH1	4.92	126.42	121.50	4	1
A	16	PHE	C-N-CA	4.91	130.54	121.70	3	1
A	108	ALA	C-CA-CB	4.90	117.85	110.50	7	1
A	337	TRP	C-CA-CB	4.89	119.39	110.10	5	1
A	166	SER	C-N-CA	4.84	130.41	121.70	7	1
A	24	SER	CA-C-N	4.83	124.15	116.90	10	1
A	125	GLN	OE1-CD-NE2	4.80	117.80	122.60	4	6
A	18	ALA	C-N-CA	4.80	130.35	121.70	1	2
A	1	MET	C-N-CA	4.80	130.34	121.70	1	4
A	437	GLN	OE1-CD-NE2	4.78	117.82	122.60	10	2
A	264	LYS	C-N-CA	4.74	130.23	121.70	10	1
A	199	ASP	CA-CB-CG	4.71	117.31	112.60	9	2
A	208	THR	C-N-CA	4.71	130.18	121.70	6	1
A	251	ALA	C-N-CA	4.71	130.18	121.70	1	2
A	316	TYR	N-CA-CB	4.70	102.52	110.50	4	1
A	311	ASP	CA-CB-CG	4.66	117.26	112.60	2	2
A	317	THR	O-C-N	4.66	115.55	123.00	4	1
A	468	ASP	CA-CB-CG	4.66	117.26	112.60	2	1
A	15	ALA	N-CA-C	4.65	124.03	111.00	8	1
A	215	ASP	CA-CB-CG	4.65	117.25	112.60	4	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	521	GLN	OE1-CD-NE2	4.63	117.97	122.60	2	9
A	43	LEU	C-N-CA	4.57	129.93	121.70	7	1
A	291	HIS	CB-CG-CD2	4.57	125.26	131.20	4	1
A	526	GLN	OE1-CD-NE2	4.56	118.04	122.60	7	2
A	349	VAL	C-N-CA	4.53	129.86	121.70	5	2
A	20	ALA	C-N-CA	4.52	113.56	121.70	9	1
A	133	PRO	CA-N-CD	4.52	105.67	112.00	4	1
A	151	THR	C-N-CA	4.51	129.82	121.70	5	1
A	167	ASN	OD1-CG-ND2	4.50	118.10	122.60	1	1
A	315	GLN	OE1-CD-NE2	4.50	118.10	122.60	4	2
A	16	PHE	N-CA-C	4.48	123.55	111.00	3	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	3.19	30
2	3.82	36
3	4.67	44
4	3.61	34
5	4.46	42
6	1.91	18
7	3.72	35
8	6.16	58
9	2.87	27
10	5.31	50

There are 374 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:249:TYR:CE2	A:251:ALA:HB2	0.81	10	1
A:138:TYR:CD2	A:146:VAL:HG21	0.80	4	3
A:529:TRP:CZ2	A:531:LEU:HD13	0.77	5	1
A:44:ALA:HA	A:134:ARG:HH11	0.77	10	1
A:151:THR:HG21	A:189:LEU:HD11	0.76	4	1
A:91:THR:HG21	A:144:GLY:HA2	0.74	10	5

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:130:ILE:HG21	A:134:ARG:HD2	0.73	4	1
A:198:TYR:CE2	A:602:ALA:HB2	0.73	5	1
A:130:ILE:HG21	A:134:ARG:CD	0.73	4	1
A:42:VAL:HG13	A:134:ARG:NH1	0.73	6	1
A:32:ALA:HB1	A:137:VAL:CG1	0.72	7	1
A:32:ALA:CB	A:137:VAL:HG11	0.72	6	1
A:23:THR:HG22	A:126:ARG:HH12	0.71	8	1
A:57:TRP:CD1	A:526:GLN:HE22	0.71	5	4
A:495:LEU:HD11	A:527:LEU:HD11	0.70	2	1
A:545:THR:HG21	A:560:LYS:CE	0.69	3	4
A:545:THR:HG21	A:560:LYS:HE2	0.69	3	1
A:83:LEU:HD11	A:198:TYR:CZ	0.68	3	1
A:566:LEU:HD21	A:593:TYR:CD1	0.67	7	1
A:355:GLN:HE21	A:382:ASN:HD21	0.67	2	1
A:42:VAL:HG13	A:134:ARG:CZ	0.66	5	2
A:85:SER:HA	A:93:ALA:HB2	0.66	8	1
A:107:LEU:HD13	A:198:TYR:OH	0.64	3	1
A:309:THR:HG21	A:346:THR:HG23	0.64	8	1
A:103:VAL:HB	A:239:ARG:HH22	0.63	7	1
A:43:LEU:HD21	A:372:THR:HB	0.63	4	1
A:198:TYR:CD2	A:213:ASP:HB3	0.63	10	1
A:32:ALA:HB2	A:137:VAL:O	0.62	5	1
A:355:GLN:NE2	A:382:ASN:HD21	0.62	2	3
A:301:TYR:HB3	A:304:TYR:CE1	0.62	5	1
A:37:GLN:HE21	A:42:VAL:HG22	0.62	8	1
A:299:PRO:HA	A:316:TYR:O	0.62	4	1
A:120:PRO:HG3	A:221:THR:HG21	0.61	9	1
A:34:ARG:HH22	A:319:GLN:NE2	0.61	9	1
A:243:TYR:CZ	A:245:ASN:HB2	0.60	1	2
A:348:TYR:CE2	A:423:GLY:HA2	0.60	10	1
A:32:ALA:HB1	A:137:VAL:HG11	0.60	6	2
A:66:LEU:CB	A:74:ILE:HD11	0.59	3	2
A:30:VAL:HG21	A:42:VAL:HG21	0.59	10	2
A:195:THR:HG22	A:217:PHE:CD1	0.59	6	2
A:566:LEU:HD11	A:596:VAL:HG11	0.59	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:120:PRO:HG3	A:173:ASP:CG	0.59	1	1
A:81:GLY:O	A:195:THR:HG21	0.59	1	1
A:83:LEU:HD21	A:263:ARG:HH12	0.59	6	1
A:564:VAL:HG11	A:596:VAL:HG22	0.58	3	1
A:79:GLY:HA3	A:198:TYR:CZ	0.58	6	1
A:98:VAL:HG12	A:105:LEU:HD12	0.58	1	1
A:123:LEU:HD22	A:175:SER:HB3	0.58	4	1
A:309:THR:CG2	A:346:THR:HG23	0.58	8	1
A:107:LEU:CD2	A:114:ALA:HB2	0.58	1	1
A:66:LEU:HB2	A:74:ILE:HD11	0.58	3	3
A:123:LEU:HG	A:189:LEU:HD13	0.57	2	3
A:103:VAL:HG22	A:189:LEU:HD21	0.57	3	1
A:120:PRO:CD	A:189:LEU:HD11	0.57	7	1
A:123:LEU:CD2	A:189:LEU:HD22	0.56	8	1
A:541:GLN:HE21	A:543:LEU:HD21	0.56	7	4
A:32:ALA:HB2	A:138:TYR:CE2	0.56	3	1
A:30:VAL:HG21	A:42:VAL:CG2	0.56	5	1
A:57:TRP:NE1	A:526:GLN:HE22	0.56	9	1
A:175:SER:HB3	A:189:LEU:HD12	0.56	2	2
A:250:ASP:OD1	A:260:LEU:HD23	0.56	8	1
A:304:TYR:CE2	A:344:PRO:HD2	0.56	5	1
A:75:THR:HG21	A:599:TYR:CE1	0.56	3	1
A:32:ALA:HB2	A:137:VAL:HG11	0.56	6	1
A:301:TYR:CB	A:304:TYR:CE1	0.55	5	1
A:30:VAL:HG22	A:134:ARG:HH22	0.55	8	1
A:201:VAL:HG13	A:210:ALA:HA	0.55	8	1
A:29:VAL:HG23	A:126:ARG:HH21	0.55	8	1
A:218:LEU:HD21	A:220:LYS:HE3	0.55	9	3
A:310:LEU:HD11	A:337:TRP:N	0.55	5	1
A:58:GLN:HE21	A:535:ASP:HB3	0.55	1	1
A:522:GLN:NE2	A:524:LYS:HE3	0.55	3	1
A:169:TYR:HA	A:195:THR:HG22	0.55	10	1
A:97:LEU:HB3	A:146:VAL:HG22	0.55	4	1
A:123:LEU:HD23	A:189:LEU:HD13	0.54	9	2
A:325:ILE:HG23	A:366:GLN:HE22	0.54	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:130:ILE:HG21	A:134:ARG:HD3	0.54	4	1
A:561:MET:HE3	A:596:VAL:CB	0.54	8	1
A:344:PRO:HD3	A:353:TYR:CE1	0.54	7	1
A:100:ILE:HD12	A:105:LEU:HD13	0.54	8	1
A:293:LYS:HE2	A:312:GLU:CD	0.54	10	1
A:32:ALA:HB2	A:138:TYR:CZ	0.54	3	1
A:22:ASP:C	A:24:SER:H	0.53	9	1
A:545:THR:HG21	A:560:LYS:HE3	0.53	1	8
A:57:TRP:CD1	A:526:GLN:NE2	0.53	2	2
A:325:ILE:HG23	A:366:GLN:NE2	0.53	5	1
A:284:GLN:HE21	A:321:ALA:HB3	0.53	8	1
A:58:GLN:HE22	A:582:ARG:HG2	0.53	10	1
A:44:ALA:HB1	A:45:PRO:HD2	0.53	7	1
A:88:ILE:HD12	A:96:VAL:HG22	0.53	8	5
A:545:THR:HG23	A:560:LYS:HE3	0.53	7	1
A:29:VAL:HG22	A:36:GLU:HG2	0.53	3	1
A:249:TYR:HE1	A:251:ALA:HB2	0.53	9	1
A:129:TYR:CZ	A:131:ARG:HD3	0.52	1	1
A:566:LEU:HD21	A:596:VAL:HG21	0.52	3	1
A:57:TRP:HE1	A:526:GLN:NE2	0.52	8	1
A:43:LEU:HD11	A:372:THR:C	0.52	4	1
A:134:ARG:O	A:137:VAL:HG22	0.52	9	1
A:92:ASN:CG	A:515:LEU:HD13	0.52	10	1
A:123:LEU:HD22	A:175:SER:CB	0.52	4	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	612	572	22	18
2	612	570	35	7
3	612	558	29	25
4	612	533	55	24
5	612	564	30	18
6	612	572	30	10
7	612	569	29	14

Model ID	Analysed	Favored	Allowed	Outliers
8	612	569	33	10
9	612	578	19	15
10	612	555	37	20

There are 83 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	8	LEU	8
A	13	VAL	7
A	2	ILE	6
A	16	PHE	5
A	22	ASP	5
A	4	LYS	4
A	10	ALA	4
A	346	THR	4
A	6	SER	3
A	9	THR	3
A	11	CYS	3
A	12	SER	3
A	18	ALA	3
A	19	TRP	3
A	215	ASP	3
A	254	SER	3
A	260	LEU	3
A	304	TYR	3
A	603	GLY	3
A	14	THR	2
A	15	ALA	2
A	17	SER	2
A	20	ALA	2
A	21	GLN	2
A	23	THR	2
A	26	ASP	2
A	111	SER	2
A	205	ASN	2
A	206	THR	2

Chain	Res	Type	Models (Total)
A	208	THR	2
A	209	GLN	2
A	252	TYR	2
A	297	TYR	2
A	303	ARG	2
A	306	SER	2
A	308	ALA	2
A	311	ASP	2
A	351	ASP	2
A	352	GLY	2
A	424	PHE	2
A	24	SER	1
A	32	ALA	1
A	44	ALA	1
A	45	PRO	1
A	78	GLY	1
A	89	ARG	1
A	91	THR	1
A	94	SER	1
A	108	ALA	1
A	109	GLY	1
A	114	ALA	1
A	133	PRO	1
A	140	SER	1
A	152	THR	1
A	207	GLY	1
A	210	ALA	1
A	212	THR	1
A	251	ALA	1
A	255	PRO	1
A	259	LEU	1
A	261	ASP	1
A	265	LEU	1
A	277	ASN	1
A	282	LYS	1

Chain	Res	Type	Models (Total)
A	285	LEU	1
A	292	SER	1
A	294	ASP	1
A	295	TYR	1
A	298	ASP	1
A	299	PRO	1
A	301	TYR	1
A	305	ASP	1
A	349	VAL	1
A	350	GLU	1
A	353	TYR	1
A	419	GLY	1
A	423	GLY	1
A	426	GLY	1
A	477	GLY	1
A	517	ARG	1
A	556	TYR	1
A	601	THR	1
A	602	ALA	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	510	486	14	10
2	510	481	22	7
3	510	477	20	13
4	510	471	24	15
5	510	486	13	11
6	510	491	10	9
7	510	484	14	12
8	510	486	10	14
9	510	490	14	6
10	510	487	12	11

There are 60 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	7	LEU	8
A	161	SER	6
A	11	CYS	5
A	14	THR	5
A	8	LEU	4
A	9	THR	4
A	12	SER	4
A	110	VAL	3
A	212	THR	3
A	24	SER	2
A	33	ASN	2
A	173	ASP	2
A	191	ASP	2
A	200	VAL	2
A	241	TYR	2
A	252	TYR	2
A	254	SER	2
A	265	LEU	2
A	280	LEU	2
A	300	HIS	2
A	310	LEU	2
A	317	THR	2
A	435	SER	2
A	601	THR	2
A	2	ILE	1
A	6	SER	1
A	23	THR	1
A	26	ASP	1
A	27	THR	1
A	28	LEU	1
A	30	VAL	1
A	31	THR	1
A	43	LEU	1
A	91	THR	1
A	117	SER	1

Chain	Res	Type	Models (Total)
A	137	VAL	1
A	141	ASP	1
A	189	LEU	1
A	198	TYR	1
A	208	THR	1
A	213	ASP	1
A	215	ASP	1
A	243	TYR	1
A	257	SER	1
A	276	TYR	1
A	298	ASP	1
A	304	TYR	1
A	307	SER	1
A	309	THR	1
A	318	VAL	1
A	341	THR	1
A	342	THR	1
A	343	THR	1
A	348	TYR	1
A	363	THR	1
A	392	GLN	1
A	412	SER	1
A	469	HIS	1
A	559	VAL	1
A	595	THR	1

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

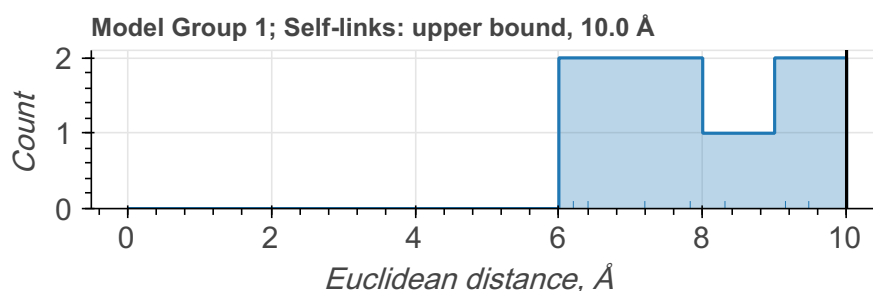
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 7 crosslinking restraints combined in 7 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	2
L-Photo-Leucine	LEU	CA	TYR	CA	upper bound	10.0	2
L-Photo-Leucine	LEU	CA	THR	CA	upper bound	10.0	2
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.



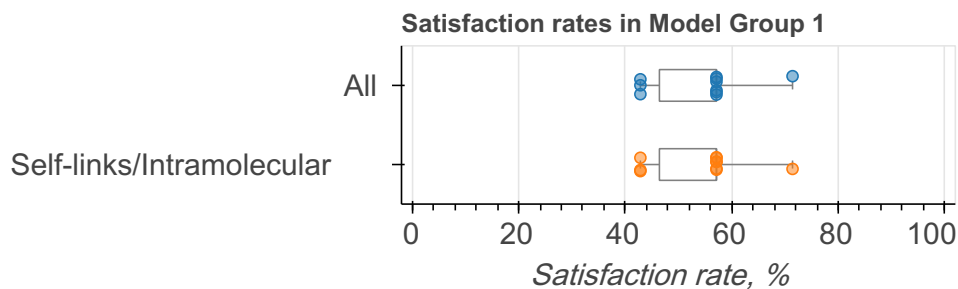
Satisfaction of restraints

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=7)
1	1	1	10/10	All	100.00	0.00	7
				Self-links/ Intramolecular	100.00	0.00	7

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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