

# 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	9A3B
PDB-Dev ID	PDBDEV_00000196
Structure Title	Model of E. coli PtsG 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)*

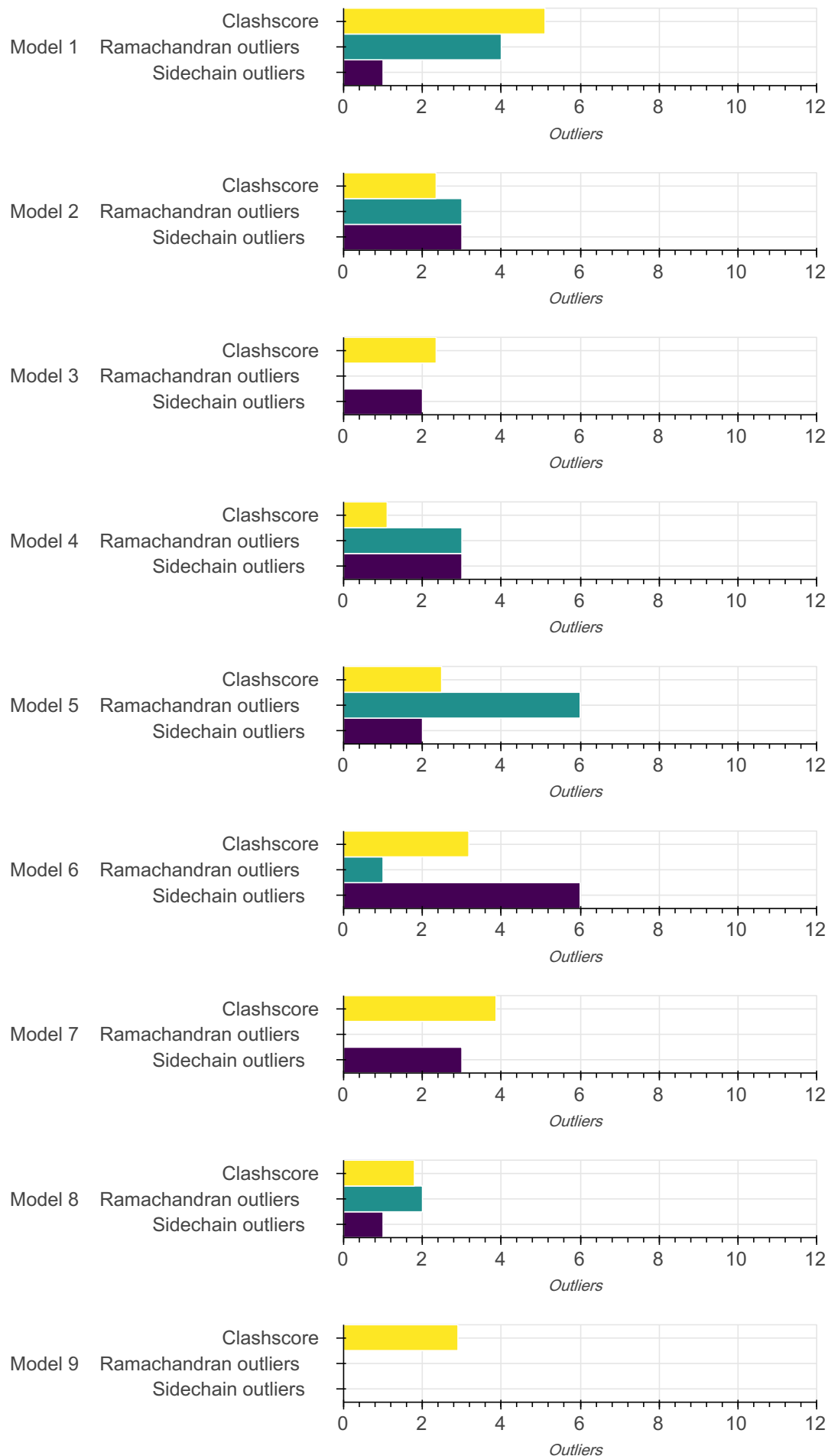
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

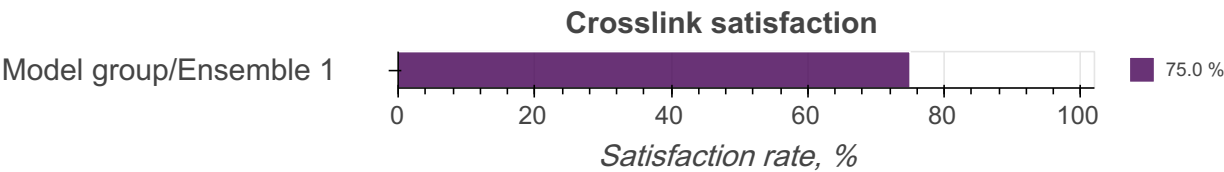
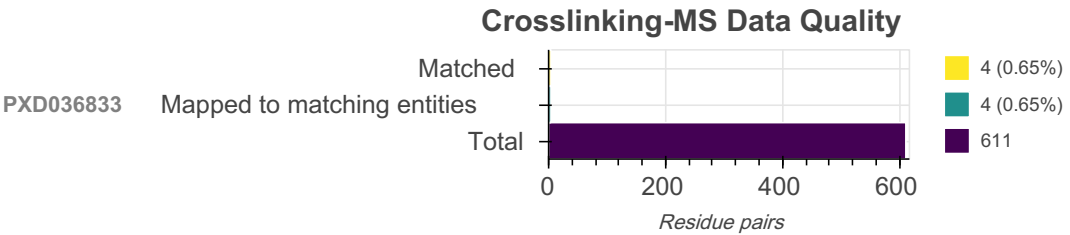
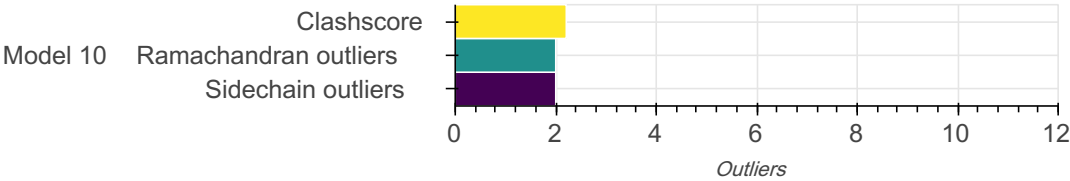
*List of references used to build this report is available [here](#).*

## 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	P69786	A	477	-	1-477	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	P69786	dbseq_P69786_target	0.00	True

Residue pairs stats:

Source	Total	In matched entities	Total matched
9A3B	4	4 (100.00%)	4 (100.00%)
PXD036833	611	4 (0.65%)	4 (0.65%)

### 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 96 bond angle outliers in this entry (0.19% of 49870 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	446	ALA	C-CA-CB	7.79	122.19	110.50	1	1
A	333	ASP	CA-CB-CG	7.67	120.27	112.60	7	1
A	234	HIS	CA-CB-CG	7.51	121.31	113.80	1	1
A	396	THR	C-N-CA	7.07	134.42	121.70	4	1
A	236	ASP	CA-CB-CG	6.81	119.41	112.60	1	1
A	373	ARG	NE-CZ-NH2	6.47	125.03	119.20	10	6
A	302	PHE	CA-CB-CG	6.37	120.17	113.80	10	1
A	219	GLN	OE1-CD-NE2	6.31	116.29	122.60	4	8
A	315	HIS	CB-CG-CD2	5.93	123.49	131.20	9	9
A	425	LEU	C-CA-CB	5.71	120.96	110.10	7	1
A	222	ILE	C-N-CA	5.37	131.36	121.70	1	1
A	112	HIS	CB-CG-CD2	5.11	124.56	131.20	1	2
A	221	GLN	OE1-CD-NE2	5.11	117.49	122.60	5	4
A	391	GLU	C-N-CA	4.99	130.68	121.70	7	1
A	10	GLN	OE1-CD-NE2	4.95	117.65	122.60	9	3
A	424	ARG	C-N-CA	4.91	130.54	121.70	7	1
A	231	GLN	OE1-CD-NE2	4.89	117.71	122.60	6	1
A	211	HIS	CB-CG-CD2	4.86	124.88	131.20	6	10
A	184	GLN	OE1-CD-NE2	4.79	117.81	122.60	4	1
A	227	ASN	N-CA-CB	4.78	102.37	110.50	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	239	ARG	NE-CZ-NH2	4.77	123.49	119.20	1	1
A	335	THR	CA-CB-CG2	4.69	118.47	110.50	5	1
A	238	PRO	CA-N-CD	4.68	105.45	112.00	5	1
A	339	HIS	CB-CG-CD2	4.67	125.12	131.20	9	7
A	215	ASN	OD1-CG-ND2	4.55	118.05	122.60	2	2
A	97	ALA	CA-C-N	4.47	123.60	116.90	4	1
A	180	GLN	OE1-CD-NE2	4.46	118.14	122.60	1	2
A	456	GLN	OE1-CD-NE2	4.44	118.16	122.60	8	4
A	239	ARG	C-N-CA	4.42	129.66	121.70	5	1
A	234	HIS	CB-CG-CD2	4.41	125.47	131.20	7	5
A	18	LEU	C-CA-CB	4.26	118.20	110.10	9	1
A	189	GLN	OE1-CD-NE2	4.26	118.34	122.60	1	3
A	390	THR	C-N-CA	4.23	129.31	121.70	5	1
A	388	ASP	C-CA-CB	4.21	118.10	110.10	10	2
A	335	THR	C-CA-CB	4.20	118.34	109.10	5	1
A	334	GLY	C-N-CA	4.20	129.25	121.70	5	1
A	339	HIS	CA-CB-CG	4.12	117.92	113.80	4	1
A	394	LYS	N-CA-C	4.12	122.53	111.00	1	1
A	395	ALA	C-N-CA	4.10	129.08	121.70	2	1
A	388	ASP	CA-CB-CG	4.09	108.51	112.60	10	1
A	350	ASN	OD1-CG-ND2	4.07	118.53	122.60	1	1
A	212	HIS	CB-CG-CD2	4.06	125.93	131.20	8	1
A	239	ARG	NH1-CZ-NH2	4.04	114.05	119.30	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	5.11	37
2	2.35	17
3	2.35	17
4	1.10	8
5	2.49	18
6	3.18	23
7	3.87	28

Model ID	Clash score	Number of clashes
8	1.80	13
9	2.90	21
10	2.21	16

There are 198 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:401:MET:HE3	A:466:LEU:HD21	1.11	5	2
A:348:SER:HB3	A:354:LEU:HD21	0.91	7	1
A:218:PHE:CE2	A:222:ILE:HD11	0.86	7	2
A:119:LEU:HB2	A:213:ILE:HD11	0.83	5	1
A:279:LYS:HE2	A:446:ALA:HB2	0.81	9	2
A:268:ILE:HD11	A:304:PHE:CE1	0.80	6	1
A:284:MET:HE1	A:304:PHE:CE1	0.78	3	3
A:195:PHE:CE1	A:222:ILE:HD12	0.75	9	1
A:195:PHE:CE1	A:222:ILE:HG22	0.70	6	1
A:241:MET:HE1	A:347:LEU:HD22	0.69	7	2
A:279:LYS:CE	A:446:ALA:HB2	0.69	9	1
A:93:MET:HE1	A:116:THR:HG21	0.67	4	3
A:284:MET:HE1	A:304:PHE:CZ	0.65	3	2
A:401:MET:CE	A:466:LEU:HD21	0.65	5	2
A:305:MET:HE3	A:306:PHE:CE1	0.65	2	1
A:116:THR:HG22	A:172:TRP:NE1	0.63	1	1
A:270:HIS:C	A:373:ARG:HH12	0.63	9	3
A:98:PRO:HD3	A:108:ILE:HD13	0.63	1	1
A:225:TYR:CE2	A:233:PHE:HB2	0.63	9	1
A:12:VAL:HG22	A:71:PHE:HZ	0.62	9	1
A:284:MET:HE1	A:304:PHE:CE2	0.61	1	1
A:93:MET:HE2	A:112:HIS:HD2	0.60	1	1
A:89:MET:HE1	A:120:GLY:CA	0.58	4	1
A:93:MET:HE2	A:112:HIS:CD2	0.58	1	1
A:240:TYR:CE1	A:334:GLY:HA2	0.58	1	1
A:203:ARG:HH22	A:297:THR:CB	0.58	9	1
A:119:LEU:CB	A:213:ILE:HD11	0.58	5	1
A:273:LYS:NZ	A:389:ALA:H	0.58	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:401:MET:HE3	A:466:LEU:CD2	0.57	2	3
A:31:GLY:HA2	A:347:LEU:HD21	0.57	5	1
A:393:ALA:CB	A:442:LYS:HA	0.57	8	1
A:250:LEU:HD12	A:339:HIS:CE1	0.56	6	1
A:195:PHE:CZ	A:222:ILE:HG22	0.56	6	1
A:401:MET:HE2	A:466:LEU:HD22	0.56	10	1
A:119:LEU:HD22	A:213:ILE:HG12	0.56	7	1
A:119:LEU:HD22	A:210:LEU:HD21	0.55	1	1
A:30:LEU:HD21	A:241:MET:HE2	0.55	2	1
A:241:MET:HE1	A:347:LEU:CD2	0.54	8	2
A:31:GLY:HA3	A:346:VAL:HG12	0.54	7	1
A:271:SER:HA	A:373:ARG:HH12	0.54	7	3
A:13:GLY:HA3	A:306:PHE:CZ	0.54	6	1
A:93:MET:HE1	A:116:THR:HG23	0.54	3	2
A:195:PHE:CZ	A:222:ILE:HD12	0.53	9	1
A:101:LEU:HD21	A:173:PRO:CB	0.53	7	2
A:391:GLU:HB3	A:446:ALA:HB3	0.53	1	1
A:105:ALA:HA	A:108:ILE:HD12	0.53	1	1
A:234:HIS:CB	A:236:ASP:HB2	0.52	1	1
A:98:PRO:HA	A:108:ILE:CD1	0.52	6	2
A:218:PHE:HA	A:222:ILE:HD12	0.52	8	1
A:207:PRO:HG3	A:305:MET:SD	0.52	2	2
A:202:GLU:CD	A:203:ARG:HH21	0.51	5	9
A:119:LEU:HD22	A:213:ILE:HD11	0.51	3	1
A:218:PHE:CZ	A:222:ILE:HD11	0.51	7	1
A:14:LYS:HZ3	A:421:CYS:HA	0.50	1	1
A:271:SER:HA	A:373:ARG:NH1	0.50	7	2
A:77:VAL:HG22	A:151:ARG:NH1	0.50	8	1
A:31:GLY:CA	A:347:LEU:HD21	0.50	5	1
A:344:PHE:CZ	A:354:LEU:HD22	0.50	7	1
A:305:MET:HE1	A:315:HIS:CB	0.50	1	1
A:11:LYS:HE2	A:71:PHE:HA	0.49	7	1
A:13:GLY:HA3	A:306:PHE:CE2	0.49	10	1
A:280:VAL:HG21	A:385:GLY:HA3	0.49	10	3
A:284:MET:HE2	A:284:MET:N	0.49	3	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:198:TYR:HA	A:214:TRP:CH2	0.49	10	1
A:207:PRO:HB3	A:306:PHE:CZ	0.48	5	1
A:253:GLY:HA2	A:256:PHE:CE2	0.48	2	5
A:241:MET:HE1	A:347:LEU:HD21	0.48	8	1
A:348:SER:CB	A:354:LEU:HD21	0.48	7	1
A:305:MET:HE1	A:315:HIS:CG	0.48	1	1
A:364:TYR:CE2	A:368:TYR:CE1	0.48	1	1
A:391:GLU:OE1	A:458:ILE:HD12	0.48	1	1
A:273:LYS:HZ2	A:389:ALA:H	0.48	1	1
A:351:SER:HB2	A:354:LEU:HD21	0.47	6	3
A:172:TRP:CZ3	A:213:ILE:HD13	0.47	1	1
A:284:MET:CE	A:304:PHE:CZ	0.47	3	1
A:257:LYS:HG2	A:297:THR:HG21	0.47	6	1
A:401:MET:HE2	A:466:LEU:CD2	0.47	10	1
A:240:TYR:CE1	A:334:GLY:CA	0.47	1	1
A:23:LEU:HD13	A:337:PHE:CE2	0.47	2	1
A:401:MET:CE	A:466:LEU:CD2	0.47	8	1
A:336:SER:HA	A:347:LEU:HD11	0.46	1	1
A:93:MET:HB3	A:112:HIS:CD2	0.46	1	1
A:276:ASN:HD21	A:392:ASP:CG	0.46	4	1
A:240:TYR:CD2	A:334:GLY:HA3	0.46	8	1
A:292:PHE:CE2	A:341:LEU:HD22	0.46	7	3
A:116:THR:HG22	A:172:TRP:CD1	0.45	1	1
A:56:PHE:CZ	A:337:PHE:CZ	0.45	6	1
A:268:ILE:HD11	A:304:PHE:HE1	0.45	6	1
A:191:PRO:CB	A:249:LYS:HE2	0.45	8	1
A:234:HIS:CG	A:236:ASP:HB2	0.45	1	1
A:179:ILE:HG22	A:217:PRO:HG2	0.45	5	2
A:405:LEU:CD1	A:466:LEU:HD22	0.45	5	1
A:35:ALA:HB3	A:37:PHE:CE2	0.45	4	1
A:101:LEU:HD21	A:173:PRO:HB2	0.45	7	1
A:279:LYS:HZ3	A:446:ALA:HA	0.45	7	1
A:207:PRO:CG	A:305:MET:SD	0.44	2	1
A:373:ARG:CZ	A:377:LYS:HE3	0.44	6	2
A:8:ASN:O	A:12:VAL:HG23	0.44	9	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:279:LYS:HE3	A:461:THR:HG23	0.44	1	1
A:401:MET:HE2	A:466:LEU:HD21	0.44	3	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	475	460	11	4
2	475	466	6	3
3	475	470	5	0
4	475	465	7	3
5	475	455	14	6
6	475	463	11	1
7	475	462	13	0
8	475	465	8	2
9	475	469	6	0
10	475	468	5	2

There are 18 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	335	THR	2
A	391	GLU	2
A	397	GLY	2
A	117	GLY	1
A	150	LYS	1
A	223	GLY	1
A	237	ILE	1
A	238	PRO	1
A	239	ARG	1
A	337	PHE	1
A	348	SER	1
A	389	ALA	1
A	390	THR	1
A	392	ASP	1
A	393	ALA	1
A	394	LYS	1

Chain	Res	Type	Models (Total)
A	396	THR	1
A	422	ILE	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	366	358	7	1
2	366	357	6	3
3	366	359	5	2
4	366	358	5	3
5	366	358	6	2
6	366	355	5	6
7	366	359	4	3
8	366	360	5	1
9	366	358	8	0
10	366	359	5	2

*There are 15 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	390	THR	4
A	9	LEU	3
A	1	MET	2
A	364	TYR	2
A	425	LEU	2
A	17	MET	1
A	40	LEU	1
A	225	TYR	1
A	227	ASN	1
A	251	SER	1
A	307	VAL	1
A	336	SER	1
A	343	ASP	1
A	392	ASP	1
A	398	THR	1

## Fit of model to data used for modeling ?

### Fit of model(s) to crosslinking-MS data

#### Restraint types

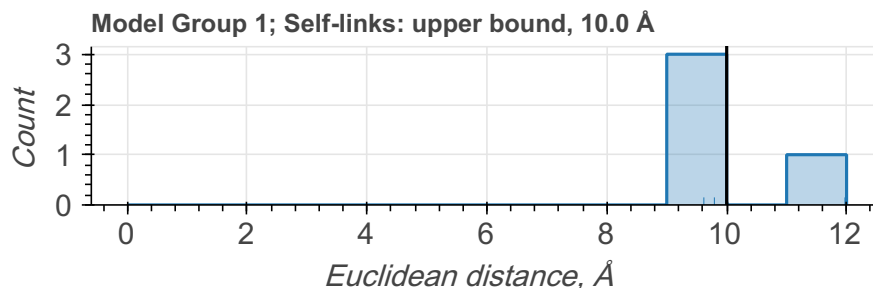
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 4 crosslinking restraints combined in 4 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
L-Photo-Leucine	LEU	CA	PHE	CA	upper bound	10.0	1
L-Photo-Leucine	ASP	CA	LEU	CA	upper bound	10.0	1
L-Photo-Leucine	LEU	CA	LEU	CA	upper bound	10.0	2

#### 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.



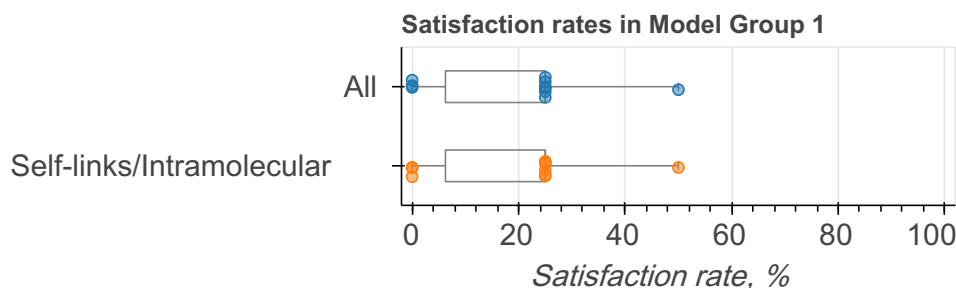
#### Satisfaction of restraints

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=4)
1	1	1	10/10	All	75.00	25.00	4
				Self-links/ Intramolecular	75.00	25.00	4

#### 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

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

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