

# Integrative Structure Validation Report

July 22, 2024 - 05:08 PM PDT

The following software was used in the production of this report:

*Python-IHM Version 1.3*

*MolProbity Version 4.5.2*

*Integrative Modeling Validation Version 1.2*

PDB ID	9A2X
PDB-Dev ID	PDBDEV_00000182
Structure Title	Model of E. coli TolC by in-cell photo-crosslinking MS and deep learning
Structure Authors	Stahl, K.; Graziadei, A.; Dau, T.; Brock, O.; Rappsilber, J.

*This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.*

*We welcome your comments at [pdb-dev@mail.wwpdb.org](mailto:pdb-dev@mail.wwpdb.org)*

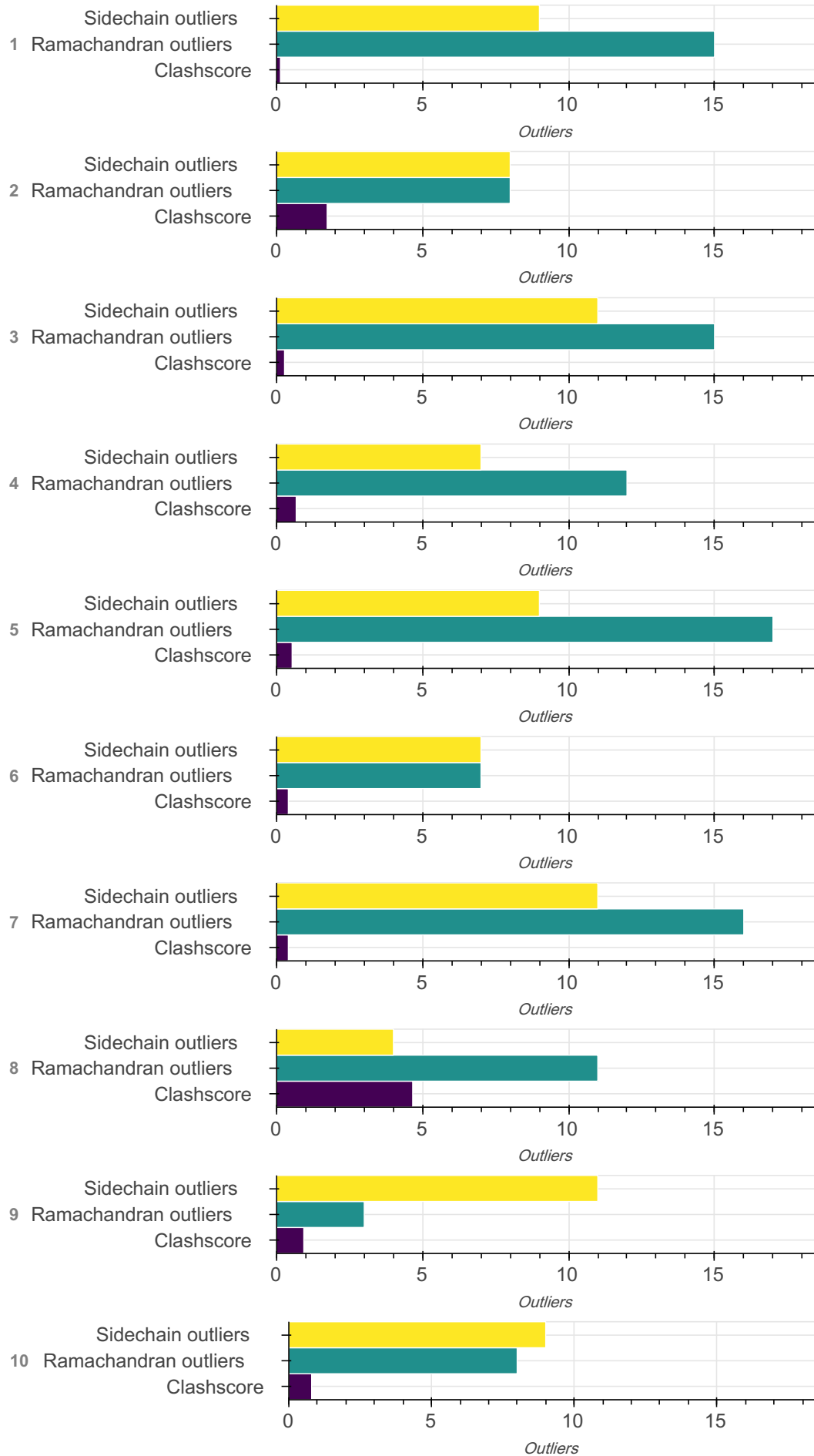
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.*

### Entry composition

*There are 10 unique types of models in this entry. These models are titled None, None, None, None, None, None, None, None, None, None respectively.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	P02930	A	A	493
2	1	1	P02930	A	A	493
3	1	1	P02930	A	A	493
4	1	1	P02930	A	A	493
5	1	1	P02930	A	A	493
6	1	1	P02930	A	A	493
7	1	1	P02930	A	A	493
8	1	1	P02930	A	A	493
9	1	1	P02930	A	A	493
10	1	1	P02930	A	A	493

### 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

### Representation ?

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-493

### 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 with 10 msa subsamples	AlphaLink	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>	1.0	model building	<a href="https://github.com/lhatsk/AlphaLink">https://github.com/lhatsk/AlphaLink</a>

### Data quality ?

#### Crosslinking-MS

Validation for this section is under development.

### Model quality ?

For models with atomic structures, molprobit analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

## Standard geometry: bond outliers?

There are 37300 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG3	1.09	0.97	1270
CD1--HD12	1.09	0.97	740
CD--HD2	1.09	0.97	570
CB--HB3	1.09	0.97	3840
CG2--HG21	1.09	0.97	850
OG--HG	0.96	0.84	440
CB--HB2	1.09	0.97	3840
CA--HA	1.09	0.97	4690
CG1--HG13	1.09	0.97	490
CB--HB1	1.09	0.97	570
CG--HG2	1.09	0.97	1270
CG2--HG23	1.09	0.97	850
CE--HE3	1.09	0.97	240
CD--HD3	1.09	0.97	570
CE--HE2	1.09	0.97	240
OH--HH	0.96	0.84	210
CD2--HD23	1.09	0.97	530
CD2--HD21	1.09	0.97	530
CD1--HD11	1.09	0.97	740
CG1--HG12	1.09	0.97	490
CA--HA2	1.09	0.97	240
CG2--HG22	1.09	0.97	850

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG1--HG1	0.96	0.84	360
CB--HB	1.09	0.97	850
CD1--HD13	1.09	0.97	740
CA--HA3	1.09	0.97	240
CG1--HG11	1.09	0.97	280
NZ--HZ1	1.01	0.89	180
CG--HG	1.09	0.97	530
CD2--HD22	1.09	0.97	530
CE--HE1	1.09	0.97	60
NZ--HZ3	1.01	0.89	180
NZ--HZ2	1.01	0.89	180
N--H1	1.01	0.89	10
N--H2	1.01	0.89	10
N--H3	1.01	0.89	10
NE2--HE21	1.01	0.86	440
N--H	1.01	0.86	4750
ND2--HD22	1.01	0.86	430
NH1--HH11	1.01	0.86	220
NE2--HE22	1.01	0.86	440
NH2--HH21	1.01	0.86	220
CE1--HE1	1.08	0.93	340
ND2--HD21	1.01	0.86	430
NH1--HH12	1.01	0.86	220

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD2	1.08	0.93	340
NE--HE	1.01	0.86	220
CZ--HZ	1.08	0.93	100
CZ2--HZ2	1.08	0.93	10
CD1--HD1	1.08	0.93	320
NH2--HH22	1.01	0.86	220
CE2--HE2	1.08	0.93	310
ND1--HD1	1.01	0.86	30
NE1--HE1	1.01	0.86	10
CZ3--HZ3	1.08	0.93	10
CH2--HH2	1.08	0.93	10
CE3--HE3	1.08	0.93	10

### Standard geometry: angle outliers

There are 405 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	135.41	1
C-CA-CB	110.10	128.61	1
C-N-CA	121.70	138.81	1
N-CA-CB	110.50	125.93	1
C-N-CA	121.70	136.89	1
C-N-CA	121.70	136.65	1
C-N-CA	121.70	135.95	1
C-N-CA	121.70	135.92	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	135.89	1
C-N-CA	121.70	134.31	1
C-N-CA	121.70	134.09	1
C-N-CA	121.70	133.90	1
N-CA-C	111.00	92.55	1
C-N-CA	121.70	133.40	1
C-N-CA	121.70	133.38	1
C-N-CA	121.70	133.28	1
C-N-CA	121.70	132.88	1
C-N-CA	121.70	132.78	1
C-N-CA	121.70	132.62	1
C-N-CA	121.70	132.60	1
C-N-CA	121.70	132.58	1
C-N-CA	121.70	132.55	1
C-N-CA	121.70	132.49	1
C-N-CA	121.70	132.43	1
CA-N-CD	112.00	103.78	1
C-N-CA	121.70	132.26	1
C-N-CA	121.70	132.08	1
CA-C-N	116.20	127.43	1
CA-N-CD	112.00	104.24	1
OE1-CD-NE2	122.60	117.08	1
OE1-CD-NE2	122.60	117.12	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.49	1
C-N-CA	121.70	131.44	1
C-N-CA	121.70	131.43	2
C-N-CA	121.70	131.37	1
C-N-CA	121.70	131.31	1
OE1-CD-NE2	122.60	117.32	1
C-N-CA	121.70	131.16	1
C-N-CA	121.70	131.07	1
N-CA-CB	110.50	101.70	1
O-C-N	123.00	114.76	1
C-N-CA	121.70	130.90	1
C-N-CA	121.70	130.89	1
C-N-CA	121.70	130.88	1
OE1-CD-NE2	122.60	117.51	3
N-CA-CB	110.50	101.91	1
C-N-CA	121.70	130.79	2
N-CA-CB	110.40	102.83	1
C-N-CA	121.70	130.77	1
N-CA-CB	110.50	101.97	1
OE1-CD-NE2	122.60	117.60	1
C-N-CA	121.70	130.69	1
OE1-CD-NE2	122.60	117.63	1
C-N-CA	121.70	130.63	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.64	1
OE1-CD-NE2	122.60	117.66	1
C-N-CA	121.70	130.55	1
C-N-CA	121.70	130.51	1
C-N-CA	121.70	130.46	1
OE1-CD-NE2	122.60	117.74	3
OE1-CD-NE2	122.60	117.76	1
OE1-CD-NE2	122.60	117.77	2
OE1-CD-NE2	122.60	117.79	1
O-C-N	123.00	115.30	1
C-N-CA	121.70	130.35	1
C-N-CA	121.70	130.34	1
C-N-CA	121.70	130.33	1
OE1-CD-NE2	122.60	117.81	3
OE1-CD-NE2	122.60	117.82	1
OE1-CD-NE2	122.60	117.83	1
C-N-CA	121.70	130.27	1
C-N-CA	121.70	130.26	1
NE-CZ-NH2	119.20	123.47	1
OE1-CD-NE2	122.60	117.86	1
OE1-CD-NE2	122.60	117.88	1
C-N-CA	121.70	130.19	1
C-N-CA	121.70	130.18	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.89	3
CA-C-N	116.20	125.61	1
C-N-CA	121.70	130.16	2
OE1-CD-NE2	122.60	117.91	1
C-N-CA	121.70	130.14	1
OE1-CD-NE2	122.60	117.92	2
CD-NE-CZ	124.40	130.95	1
NE-CZ-NH2	119.20	123.41	1
OE1-CD-NE2	122.60	117.93	2
C-N-CA	121.70	130.11	1
C-N-CA	121.70	130.09	1
OE1-CD-NE2	122.60	117.94	1
OE1-CD-NE2	122.60	117.95	1
C-N-CA	121.70	130.07	1
N-CA-CB	111.50	103.60	1
OE1-CD-NE2	122.60	117.96	6
C-N-CA	121.70	130.05	1
C-N-CA	121.70	130.02	1
OE1-CD-NE2	122.60	117.98	1
OE1-CD-NE2	122.60	117.99	1
OE1-CD-NE2	122.60	118.00	1
OE1-CD-NE2	122.60	118.01	3
CA-C-N	116.20	125.39	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.02	2
CA-N-CD	112.00	105.60	2
OE1-CD-NE2	122.60	118.04	3
O-C-N	123.00	115.71	1
C-N-CA	121.70	129.90	1
OE1-CD-NE2	122.60	118.05	1
OE1-CD-NE2	122.60	118.06	2
OE1-CD-NE2	122.60	118.07	1
OD1-CG-ND2	122.60	118.07	1
OE1-CD-NE2	122.60	118.08	1
OE1-CD-NE2	122.60	118.09	2
O-C-N	123.00	115.78	1
C-CA-CB	110.10	118.66	1
OE1-CD-NE2	122.60	118.10	2
C-N-CA	121.70	129.80	1
OE1-CD-NE2	122.60	118.11	3
OD1-CG-ND2	122.60	118.11	1
OE1-CD-NE2	122.60	118.12	2
C-N-CA	121.70	129.76	3
OE1-CD-NE2	122.60	118.13	2
C-N-CA	121.70	129.75	1
CA-C-N	116.20	125.13	1
C-N-CA	121.70	129.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.14	1
C-N-CA	121.70	129.72	1
C-N-CA	121.70	129.71	2
N-CA-C	111.00	123.46	1
OE1-CD-NE2	122.60	118.15	2
OE1-CD-NE2	122.60	118.16	3
C-N-CA	121.70	129.70	1
C-N-CA	121.70	129.69	1
C-N-CA	121.70	129.68	1
OE1-CD-NE2	122.60	118.17	5
OE1-CD-NE2	122.60	118.18	1
OD1-CG-ND2	122.60	118.19	1
N-CA-CB	110.40	103.79	1
OE1-CD-NE2	122.60	118.20	3
C-N-CA	121.70	129.63	1
C-N-CA	121.70	129.62	1
OE1-CD-NE2	122.60	118.21	6
OE1-CD-NE2	122.60	118.22	2
C-N-CA	121.70	129.58	1
N-CA-CB	103.00	107.81	1
OD1-CG-ND2	122.60	118.22	1
OE1-CD-NE2	122.60	118.23	3
N-CA-CB	110.50	103.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.25	3
OE1-CD-NE2	122.60	118.26	4
OD1-CG-ND2	122.60	118.26	1
OE1-CD-NE2	122.60	118.27	4
OE1-CD-NE2	122.60	118.28	3
N-CA-C	112.10	122.89	1
OE1-CD-NE2	122.60	118.29	2
OD1-CG-ND2	122.60	118.29	1
C-N-CA	121.70	129.45	1
OE1-CD-NE2	122.60	118.30	5
OE1-CD-NE2	122.60	118.31	3
OE1-CD-NE2	122.60	118.32	5
C-CA-CB	110.10	118.22	1
OE1-CD-NE2	122.60	118.33	5
CA-C-N	116.20	124.75	1
OE1-CD-NE2	122.60	118.34	4
C-N-CA	121.70	129.37	1
OE1-CD-NE2	122.60	118.35	2
OE1-CD-NE2	122.60	118.36	3
OE1-CD-NE2	122.60	118.37	2
C-N-CA	121.70	129.31	1
O-C-N	123.00	116.25	1
C-N-CA	121.70	129.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.29	1
OE1-CD-NE2	122.60	118.38	3
OE1-CD-NE2	122.60	118.39	2
C-N-CA	121.70	129.28	2
OE1-CD-NE2	122.60	118.40	3
CA-CB-CG	112.60	116.80	1
OE1-CD-NE2	122.60	118.41	6
OE1-CD-NE2	122.60	118.42	3
OE1-CD-NE2	122.60	118.43	8
OD1-CG-ND2	122.60	118.43	1
CB-CG-CD2	131.20	125.78	1
OE1-CD-NE2	122.60	118.44	2
OE1-CD-NE2	122.60	118.45	6
CA-CB-CG1	110.40	117.45	1
OE1-CD-NE2	122.60	118.46	8
OD1-CG-ND2	122.60	118.46	1
OE1-CD-NE2	122.60	118.47	6
C-N-CA	121.70	129.13	1
C-N-CA	121.70	129.12	1
OE1-CD-NE2	122.60	118.48	6
O-C-N	123.00	116.42	1
OE1-CD-NE2	122.60	118.49	4
O-C-N	123.00	116.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	122.89	1
OE1-CD-NE2	122.60	118.50	1
OE1-CD-NE2	122.60	118.51	4
CA-CB-CG	112.60	116.69	1
OE1-CD-NE2	122.60	118.52	2
OE1-CD-NE2	122.60	118.53	3
C-N-CA	121.70	129.03	1
OD1-CG-ND2	122.60	118.53	1
CA-CB-CG	112.60	116.66	1
CA-C-N	116.20	124.32	1
C-N-CA	121.70	129.01	1
OE1-CD-NE2	122.60	118.54	3
OE1-CD-NE2	122.60	118.55	2
OD1-CG-ND2	122.60	118.55	1
O-C-N	123.00	116.52	1
OE1-CD-NE2	122.60	118.56	4
C-CA-CB	110.10	117.76	1
OE1-CD-NE2	122.60	118.57	2
CA-CB-CG	112.60	116.63	1
OE1-CD-NE2	122.60	118.58	2
OD1-CG-ND2	122.60	118.58	1
OE1-CD-NE2	122.60	118.59	9
OD1-CG-ND2	122.60	118.59	1



Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.61	1
C-N-CA	121.70	128.92	1
C-N-CA	121.70	128.91	1
OE1-CD-NE2	122.60	118.60	1
HZ2-NZ-HZ3	96.82	109.00	1
C-N-H	112.08	124.30	1
C-N-H	111.87	124.30	2
N-CA-HA	97.51	110.00	1
C-N-H	111.72	124.30	1
CG-CB-HB3	94.95	108.00	1
C-N-H	111.20	124.30	1
C-N-H	111.03	124.30	1
HH11-NH1-HH12	106.69	120.00	1
C-N-H	110.88	124.30	1
HH11-NH1-HH12	106.57	120.00	1
HH11-NH1-HH12	106.50	120.00	1
C-N-H	110.72	124.30	1
HH11-NH1-HH12	106.28	120.00	1
HH11-NH1-HH12	106.16	120.00	1
HH11-NH1-HH12	105.96	120.00	1
C-N-H	109.75	124.30	1
C-N-H	109.61	124.30	1
HG2-CG-HG3	95.24	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CZ-NH1-HH11	105.23	120.00	1
C-CA-HA	93.96	109.00	1
HH11-NH1-HH12	104.77	120.00	1
C-N-H	108.68	124.30	1
CG-CB-HB2	91.81	108.00	1
C-N-H	108.05	124.30	1
C-N-H	107.84	124.30	1
C-N-H	107.75	124.30	1
C-N-H	107.64	124.30	1
C-N-H	107.59	124.30	1
C-N-H	106.83	124.30	1
C-N-H	106.60	124.30	1
HB2-CB-HB3	90.30	110.00	1
C-CA-HA	88.93	109.00	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 the models in this entry.

Model ID	Clash score	Number of clashes
1	0.13	1
2	1.73	13
3	0.27	2
4	0.67	5
5	0.53	4

Model ID	Clash score	Number of clashes
6	0.40	3
7	0.40	3
8	4.66	35
9	0.93	7
10	0.80	6

All 79 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:234:LEU:HD13	A:422:ILE:HD11	0.421
2	A:287:LYS:HE3	A:293:GLY:HA2	0.591
2	A:155:ILE:HD13	A:182:GLN:HG3	0.579
2	A:287:LYS:CE	A:293:GLY:HA2	0.537
2	A:104:ARG:HE	A:264:ASP:CG	0.515
2	A:155:ILE:HD12	A:186:VAL:HG21	0.514
2	A:26:MET:HE3	A:435:LEU:HG	0.490
2	A:313:PRO:HB3	A:316:GLN:HE21	0.471
2	A:472:ALA:HB1	A:473:PRO:HD2	0.471
2	A:234:LEU:HD13	A:422:ILE:HD11	0.448
2	A:104:ARG:HD2	A:261:GLN:HA	0.441
2	A:472:ALA:HB1	A:473:PRO:CD	0.430
2	A:266:HIS:CD2	A:320:VAL:HG11	0.413
2	A:104:ARG:CZ	A:260:ARG:HB3	0.402
3	A:477:GLN:HB3	A:478:THR:HG23	0.529
3	A:234:LEU:HD13	A:422:ILE:HD11	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:299:SER:C	A:301:MET:H	0.488
4	A:313:PRO:CB	A:316:GLN:HE21	0.487
4	A:234:LEU:HD13	A:422:ILE:HD11	0.485
4	A:313:PRO:HB3	A:316:GLN:HE21	0.461
4	A:223:PHE:CE2	A:415:TYR:CD1	0.408
5	A:380:MET:SD	A:397:ALA:HB2	0.672
5	A:64:LEU:HD11	A:91:LEU:HD11	0.567
5	A:234:LEU:HD13	A:422:ILE:HD11	0.476
5	A:29:TYR:HA	A:131:THR:HG21	0.414
6	A:111:LYS:HE3	A:257:GLU:CG	0.459
6	A:234:LEU:HD13	A:422:ILE:HD11	0.426
6	A:111:LYS:HE3	A:257:GLU:HG2	0.418
7	A:234:LEU:HD13	A:422:ILE:HD11	0.436
7	A:128:ILE:HG23	A:434:LEU:HD12	0.430
7	A:25:LEU:HG	A:434:LEU:CD2	0.413
8	A:490:PRO:CD	A:490:PRO:CG	1.341
8	A:490:PRO:CA	A:490:PRO:CB	1.318
8	A:490:PRO:CD	A:490:PRO:N	1.310
8	A:490:PRO:CB	A:490:PRO:CG	1.306
8	A:490:PRO:CA	A:490:PRO:N	1.293
8	A:490:PRO:CA	A:492:ARG:HA	1.271
8	A:490:PRO:CB	A:492:ARG:HA	1.177
8	A:490:PRO:CG	A:492:ARG:CB	1.110

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:490:PRO:CB	A:492:ARG:CA	1.106
8	A:490:PRO:CD	A:492:ARG:CA	1.101
8	A:490:PRO:CB	A:492:ARG:CB	1.089
8	A:490:PRO:CA	A:492:ARG:CB	1.083
8	A:490:PRO:CA	A:492:ARG:CA	1.075
8	A:490:PRO:CG	A:492:ARG:CA	1.069
8	A:490:PRO:CD	A:492:ARG:CB	1.068
8	A:490:PRO:CD	A:492:ARG:HB2	0.979
8	A:490:PRO:N	A:492:ARG:CB	0.964
8	A:490:PRO:N	A:492:ARG:CA	0.913
8	A:490:PRO:CB	A:492:ARG:HB3	0.863
8	A:490:PRO:CG	A:492:ARG:HB3	0.791
8	A:490:PRO:HG2	A:492:ARG:C	0.778
8	A:490:PRO:C	A:492:ARG:HA	0.760
8	A:490:PRO:CG	A:492:ARG:C	0.737
8	A:490:PRO:HD3	A:492:ARG:HB2	0.692
8	A:490:PRO:HA	A:492:ARG:CG	0.664
8	A:490:PRO:HB2	A:492:ARG:HA	0.649
8	A:490:PRO:CA	A:492:ARG:CG	0.620
8	A:490:PRO:HB3	A:492:ARG:HB3	0.586
8	A:490:PRO:N	A:492:ARG:N	0.550
8	A:490:PRO:HG3	A:492:ARG:CB	0.501
8	A:490:PRO:HD2	A:492:ARG:CA	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:490:PRO:CD	A:492:ARG:N	0.450
8	A:490:PRO:HG3	A:492:ARG:HB3	0.439
8	A:490:PRO:HA	A:492:ARG:HG2	0.436
8	A:490:PRO:CG	A:492:ARG:HB2	0.423
9	A:26:MET:HE3	A:435:LEU:HG	0.481
9	A:165:ARG:HH22	A:385:SER:HA	0.472
9	A:22:ALA:HB2	A:444:PRO:HB3	0.458
9	A:234:LEU:HD13	A:422:ILE:HD11	0.455
9	A:155:ILE:CD1	A:186:VAL:HG21	0.452
9	A:104:ARG:CZ	A:260:ARG:HB3	0.426
9	A:461:ALA:C	A:462:ILE:HG13	0.423
10	A:26:MET:HE3	A:435:LEU:HG	0.505
10	A:205:ARG:HD3	A:211:TYR:CZ	0.501
10	A:149:GLN:NE2	A:453:ALA:HB1	0.501
10	A:111:LYS:HE3	A:257:GLU:CG	0.472
10	A:234:LEU:HD13	A:422:ILE:HD11	0.451
10	A:14:SER:HB3	A:16:PHE:CE2	0.431

### 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	491	455	21	15
2	491	460	23	8
3	491	450	26	15

Model ID	Analyzed	Favored	Allowed	Outliers
4	491	460	19	12
5	491	456	18	17
6	491	453	31	7
7	491	449	26	16
8	491	451	29	11
9	491	464	24	3
10	491	460	23	8

Detailed list of outliers are tabulated below.

### Torsion angles: Protein sidechains ?

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	412	393	10	9
2	412	395	9	8
3	412	396	5	11
4	412	398	7	7
5	412	398	5	9
6	412	392	13	7
7	412	397	4	11
8	412	397	11	4
9	412	391	10	11
10	412	396	7	9

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	5	LEU

Model ID	Chain	Residue ID	Residue type
1	A	8	LEU
1	A	11	LEU
1	A	14	SER
1	A	78	ASP
1	A	96	SER
1	A	294	THR
1	A	456	THR
1	A	462	ILE
2	A	8	LEU
2	A	11	LEU
2	A	14	SER
2	A	96	SER
2	A	288	THR
2	A	456	THR
2	A	482	THR
2	A	488	HIS
3	A	5	LEU
3	A	8	LEU
3	A	11	LEU
3	A	19	LEU
3	A	96	SER
3	A	288	THR
3	A	294	THR



Model ID	Chain	Residue ID	Residue type
3	A	456	THR
3	A	462	ILE
3	A	478	THR
3	A	482	THR
4	A	8	LEU
4	A	11	LEU
4	A	13	LEU
4	A	96	SER
4	A	288	THR
4	A	446	SER
4	A	462	ILE
5	A	5	LEU
5	A	8	LEU
5	A	11	LEU
5	A	96	SER
5	A	288	THR
5	A	294	THR
5	A	462	ILE
5	A	482	THR
5	A	488	HIS
6	A	5	LEU
6	A	8	LEU
6	A	19	LEU

Model ID	Chain	Residue ID	Residue type
6	A	96	SER
6	A	288	THR
6	A	456	THR
6	A	462	ILE
7	A	5	LEU
7	A	8	LEU
7	A	11	LEU
7	A	13	LEU
7	A	96	SER
7	A	294	THR
7	A	299	SER
7	A	434	LEU
7	A	452	VAL
7	A	482	THR
7	A	488	HIS
8	A	85	ASN
8	A	140	ASN
8	A	438	ASN
8	A	452	VAL
9	A	5	LEU
9	A	8	LEU
9	A	11	LEU
9	A	96	SER

Model ID	Chain	Residue ID	Residue type
9	A	282	SER
9	A	288	THR
9	A	294	THR
9	A	299	SER
9	A	456	THR
9	A	462	ILE
9	A	488	HIS
10	A	8	LEU
10	A	11	LEU
10	A	76	TYR
10	A	78	ASP
10	A	88	SER
10	A	96	SER
10	A	286	SER
10	A	288	THR
10	A	294	THR

### Fit of model to data used for modeling ?

#### Crosslinking-MS

Validation for this section is under development.

### Fit of model to data used for validation ?

Validation for this section is under development.

### *Acknowledgements*

*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 ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*