Integrative Structure Validation Report

July 22, 2024 - 05:12 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	9A33
PDB-Dev ID	PDBDEV_00000188
Structure Title	Model of E. coli Icd 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

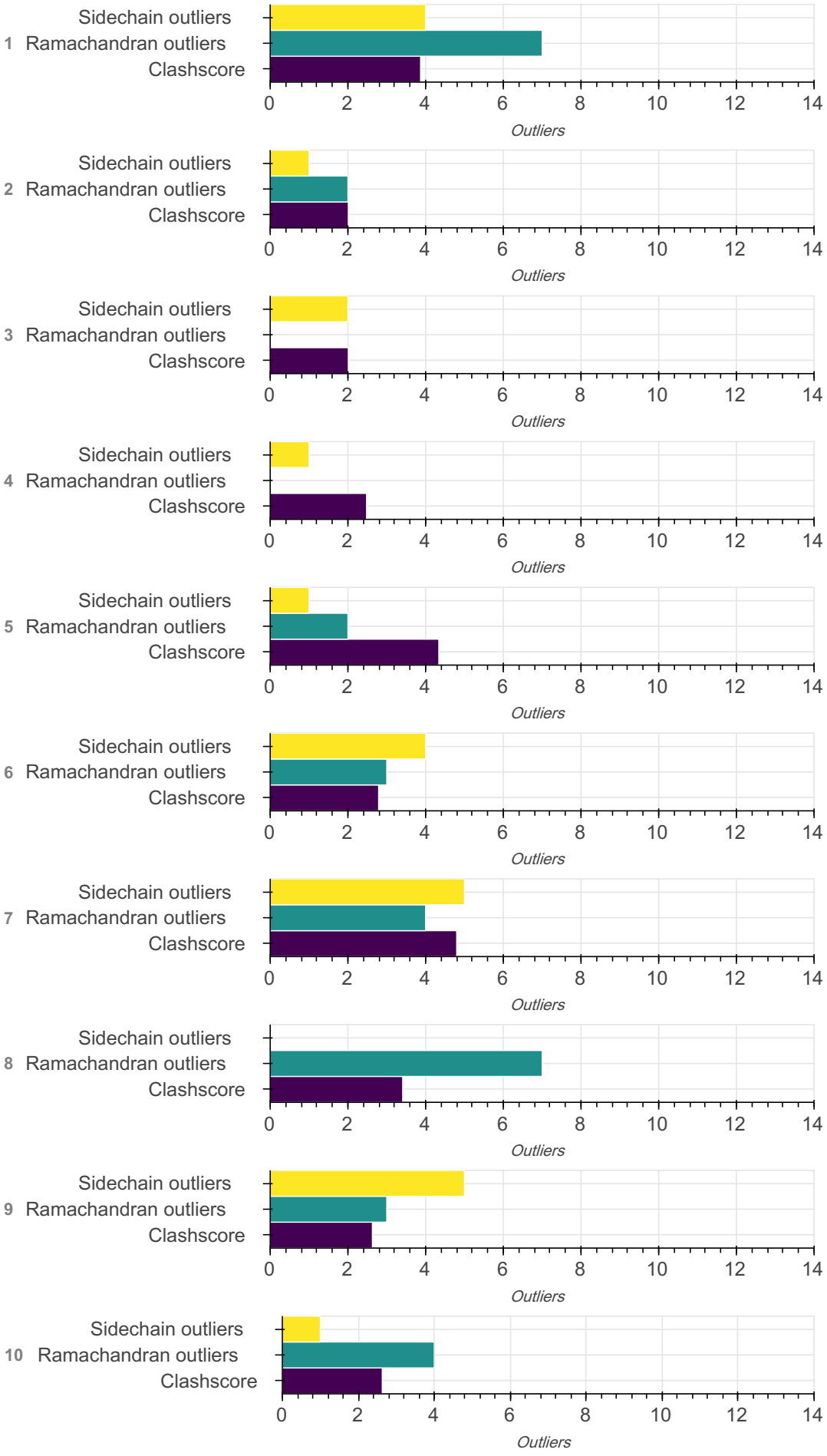
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


1
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
6
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
7
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14
Outliers

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	P08200	A	A	416
2	1	1	P08200	A	A	416
3	1	1	P08200	A	A	416
4	1	1	P08200	A	A	416
5	1	1	P08200	A	A	416
6	1	1	P08200	A	A	416
7	1	1	P08200	A	A	416
8	1	1	P08200	A	A	416
9	1	1	P08200	A	A	416
10	1	1	P08200	A	A	416

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	-	1-416

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	AlphaLink	1.0	model building	https://github.com/lhatsk/AlphaLink

Data quality

Crosslinking-MS

Validation for this section is under development.

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 32400 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
CA--HA	1.09	0.97	3760
CB--HB2	1.09	0.97	2910
CB--HB3	1.09	0.97	2910
CG1--HG13	1.09	0.97	670
CG2--HG21	1.09	0.97	850
CD1--HD11	1.09	0.97	680
CG2--HG23	1.09	0.97	850
CG--HG3	1.09	0.97	1270
NZ--HZ2	1.01	0.89	310
CB--HB	1.09	0.97	850
OH--HH	0.96	0.84	150
CD2--HD22	1.09	0.97	310
CE--HE2	1.09	0.97	440
CE--HE1	1.09	0.97	130
CD--HD3	1.09	0.97	680
CB--HB1	1.09	0.97	380
CD1--HD12	1.09	0.97	680
CD1--HD13	1.09	0.97	680
OG--HG	0.96	0.84	130
CG--HG2	1.09	0.97	1270
CA--HA2	1.09	0.97	400
CG2--HG22	1.09	0.97	850

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG	1.09	0.97	310
CD2--HD23	1.09	0.97	310
CG1--HG12	1.09	0.97	670
CD--HD2	1.09	0.97	680
NZ--HZ1	1.01	0.89	310
CD2--HD21	1.09	0.97	310
CG1--HG11	1.09	0.97	300
CE--HE3	1.09	0.97	440
CA--HA3	1.09	0.97	400
N--H1	1.01	0.89	10
NZ--HZ3	1.01	0.89	310
OG1--HG1	0.96	0.84	180
N--H2	1.01	0.89	10
N--H3	1.01	0.89	10
SG--HG	1.33	1.20	15
SG--HG	1.34	1.20	45
NE--HE	1.01	0.86	170
ND2--HD22	1.01	0.86	150
N--H	1.01	0.86	3950
ND2--HD21	1.01	0.86	150
CE2--HE2	1.08	0.93	250
CE1--HE1	1.08	0.93	300
CD2--HD2	1.08	0.93	300

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD1	1.08	0.93	310
NH1--HH12	1.01	0.86	170
NH1--HH11	1.01	0.86	170
NE2--HE21	1.01	0.86	110
NH2--HH21	1.01	0.86	170
NH2--HH22	1.01	0.86	170
NE1--HE1	1.01	0.86	60
NE2--HE22	1.01	0.86	110
CZ3--HZ3	1.08	0.93	60
CE3--HE3	1.08	0.93	60
ND1--HD1	1.01	0.86	47
CZ2--HZ2	1.08	0.93	60
CZ--HZ	1.08	0.93	100
CH2--HH2	1.08	0.93	60
NE2--HE2	1.01	0.86	3

Standard geometry: angle outliers

There are 152 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
C-N-CA	121.70	136.68	1
C-N-CA	121.70	136.41	1
C-N-CA	121.70	135.40	1
CA-CB-CG	112.60	119.29	1
CA-CB-CG	112.60	119.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	113.19	1
C-N-CA	121.70	132.59	1
OE1-CD-NE2	122.60	116.57	1
C-N-CA	121.70	132.27	1
OE1-CD-NE2	122.60	116.82	1
NE-CZ-NH2	119.20	124.36	1
OD1-CG-ND2	122.60	116.96	1
CB-CG-CD2	131.20	123.87	1
OE1-CD-NE2	122.60	116.98	1
N-CA-CB	110.50	100.96	1
OD1-CG-ND2	122.60	117.24	1
N-CA-CB	110.40	102.42	1
CA-CB-CG	114.10	124.63	1
NH1-CZ-NH2	119.30	112.46	1
C-N-CA	121.70	131.17	1
OE1-CD-NE2	122.60	117.42	1
OD1-CG-ND2	122.60	117.46	1
CA-C-N	116.20	126.44	1
CB-CG-CD2	131.20	124.55	1
OD1-CG-ND2	122.60	117.50	1
NE-CZ-NH2	119.20	123.77	1
OE1-CD-NE2	122.60	117.58	1
OD1-CG-ND2	122.60	117.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.69	1
CB-CG-CD2	131.20	124.72	1
CA-CB-CG	112.60	117.58	1
NE-CZ-NH2	119.20	123.68	1
OE1-CD-NE2	122.60	117.64	1
OE1-CD-NE2	122.60	117.66	3
C-CA-CB	111.60	121.45	1
OE1-CD-NE2	122.60	117.68	1
CB-CG-CD2	131.20	124.84	1
C-CA-CB	110.10	119.34	1
OE1-CD-NE2	122.60	117.80	1
CD-NE-CZ	124.40	131.10	1
OE1-CD-NE2	122.60	117.82	1
OE1-CD-NE2	122.60	117.83	1
OE1-CD-NE2	122.60	117.85	2
CA-CB-CG	112.60	117.32	1
CA-C-N	116.90	123.93	1
CD-NE-CZ	124.40	130.95	1
OE1-CD-NE2	122.60	117.94	1
NH1-CZ-NH2	119.30	113.26	1
OE1-CD-NE2	122.60	117.95	1
CA-C-N	116.20	125.48	1
NH1-CZ-NH2	119.30	113.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	123.36	1
OE1-CD-NE2	122.60	117.99	2
CB-CG-ND1	122.70	129.61	1
O-C-N	123.00	115.66	1
C-CA-CB	110.10	118.81	1
CB-CG-CD2	131.20	125.25	1
OE1-CD-NE2	122.60	118.04	2
OE1-CD-NE2	122.60	118.06	2
OD1-CG-ND2	122.60	118.09	1
OE1-CD-NE2	122.60	118.12	1
OE1-CD-NE2	122.60	118.14	1
C-N-CA	121.70	129.71	1
C-N-CA	121.70	129.63	1
OE1-CD-NE2	122.60	118.19	1
C-N-CA	121.70	129.62	1
NE-CZ-NH2	119.20	123.15	1
CA-CB-OG1	109.60	116.18	1
C-CA-CB	109.10	118.72	1
CA-N-CD	112.00	105.90	1
OE1-CD-NE2	122.60	118.25	2
OE1-CD-NE2	122.60	118.26	2
NE-CZ-NH2	119.20	123.11	1
CA-CB-CG	112.60	116.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.27	1
NE-CZ-NH2	119.20	123.09	1
OE1-CD-NE2	122.60	118.28	1
NH1-CZ-NH2	119.30	113.69	1
CA-CB-CG	112.60	116.90	1
OE1-CD-NE2	122.60	118.30	2
OD1-CG-ND2	122.60	118.32	2
OE1-CD-NE2	122.60	118.32	1
OE1-CD-NE2	122.60	118.33	1
O-C-N	123.00	116.18	1
CB-CG-CD2	131.20	125.66	1
OE1-CD-NE2	122.60	118.34	1
NH1-CZ-NH2	119.30	113.77	1
OE1-CD-NE2	122.60	118.35	1
OE1-CD-NE2	122.60	118.37	2
NH1-CZ-NH2	119.30	113.81	1
C-N-CA	121.70	129.30	1
NE-CZ-NH2	119.20	123.00	1
CD-NE-CZ	124.40	130.30	1
OE1-CD-NE2	122.60	118.39	1
C-CA-CB	110.50	116.79	1
OE1-CD-NE2	122.60	118.41	1
C-CA-CB	111.60	119.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.42	1
N-CA-CB	103.00	107.57	1
OE1-CD-NE2	122.60	118.46	1
OE1-CD-NE2	122.60	118.47	2
CB-CG-CD2	131.20	125.83	1
CA-C-N	116.90	123.08	1
CA-CB-CG	113.80	117.91	1
OE1-CD-NE2	122.60	118.49	1
C-N-CA	121.70	129.09	1
N-CA-CB	103.00	107.51	1
N-CA-CB	103.00	107.50	1
NE-CZ-NH2	119.20	122.88	1
OE1-CD-NE2	122.60	118.51	2
N-CA-CB	103.00	107.48	1
CB-CG-CD2	131.20	125.91	1
OE1-CD-NE2	122.60	118.53	1
OE1-CD-NE2	122.60	118.54	1
N-CA-CB	103.00	107.46	1
C-N-CA	121.70	129.00	1
NE-CZ-NH2	119.20	122.85	2
N-CA-C	111.00	122.34	1
N-CA-CB	103.00	107.45	1
OE1-CD-NE2	122.60	118.56	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	128.98	1
OD1-CG-ND2	122.60	118.57	1
OE1-CD-NE2	122.60	118.58	1
CA-CB-CG	113.80	117.82	1
N-CA-CB	103.00	107.42	1
CA-CB-CG	112.60	116.62	1
OE1-CD-NE2	122.60	118.59	1
CB-CG-CD2	131.20	125.99	1
OE1-CD-NE2	122.60	118.60	1
HZ1-NZ-HZ2	96.80	109.00	1
HZ2-NZ-HZ3	96.67	109.00	1
CG-ND2-HD22	107.05	120.00	1
C-N-H	110.66	124.30	1
HZ1-NZ-HZ3	95.25	109.00	1
C-N-H	110.46	124.30	1
C-N-H	109.50	124.30	1
HH21-NH2-HH22	93.29	120.00	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	3.87	25
2	2.01	13

Model ID	Clash score	Number of clashes
3	2.01	13
4	2.48	16
5	4.34	28
6	2.79	18
7	4.80	31
8	3.41	22
9	2.63	17
10	2.63	17

All 200 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:149:MET:HE1	A:289:ILE:HD11	1.005
1	A:341:THR:HG21	A:351:VAL:HG13	0.908
1	A:149:MET:HE2	A:296:TYR:HB2	0.686
1	A:129:ARG:HH12	A:338:THR:HG21	0.637
1	A:37:ILE:HD12	A:102:PRO:CG	0.588
1	A:341:THR:CG2	A:351:VAL:HG13	0.581
1	A:129:ARG:NH1	A:338:THR:HG21	0.551
1	A:323:ALA:HB3	A:339:HIS:CE1	0.509
1	A:344:LYS:HE3	A:345:TYR:CE2	0.492
1	A:320:ILE:HA	A:393:PHE:CE1	0.480
1	A:150:VAL:HG11	A:216:TYR:CE1	0.478
1	A:106:PRO:HD2	A:111:ILE:HD11	0.476
1	A:289:ILE:HD12	A:293:PRO:HA	0.470

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:322:ILE:HG23	A:355:SER:CB	0.469
1	A:129:ARG:HH22	A:338:THR:HG21	0.461
1	A:358:LEU:HD21	A:380:MET:HE1	0.447
1	A:129:ARG:NH2	A:338:THR:HG21	0.435
1	A:318:GLY:C	A:320:ILE:H	0.434
1	A:322:ILE:HG23	A:355:SER:HB2	0.434
1	A:68:ILE:HD12	A:88:THR:HG23	0.430
1	A:70:THR:CG2	A:88:THR:HG21	0.423
1	A:322:ILE:CG2	A:355:SER:HA	0.419
1	A:296:TYR:HB3	A:299:ILE:HD11	0.410
1	A:37:ILE:HD12	A:102:PRO:HG2	0.405
1	A:128:LEU:HD21	A:152:PHE:CE1	0.401
2	A:149:MET:HE1	A:289:ILE:HD11	0.995
2	A:233:ILE:HD11	A:304:LEU:HD23	0.791
2	A:149:MET:CE	A:289:ILE:HD11	0.699
2	A:147:THR:HG23	A:149:MET:HE3	0.683
2	A:318:GLY:O	A:322:ILE:HD11	0.580
2	A:105:THR:HG23	A:112:ARG:O	0.536
2	A:163:ILE:HG13	A:195:GLY:HA3	0.535
2	A:344:LYS:HE3	A:345:TYR:CE2	0.521
2	A:163:ILE:CG1	A:195:GLY:HA3	0.499
2	A:147:THR:HG21	A:317:VAL:HG11	0.473
2	A:134:TYR:CD2	A:322:ILE:HD12	0.467

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:112:ARG:HB2	A:164:GLU:HA	0.458
2	A:296:TYR:HB3	A:299:ILE:HD11	0.428
3	A:344:LYS:HE3	A:345:TYR:CZ	0.640
3	A:199:LYS:HZ2	A:304:LEU:HB3	0.525
3	A:153:ARG:NH2	A:160:TYR:CE2	0.504
3	A:341:THR:HG21	A:352:ASN:H	0.501
3	A:33:GLU:HA	A:42:THR:HG21	0.466
3	A:338:THR:HG22	A:339:HIS:CE1	0.463
3	A:230:LYS:HG2	A:281:ILE:HG22	0.459
3	A:68:ILE:HD12	A:88:THR:HG23	0.456
3	A:137:THR:HG22	A:318:GLY:HA3	0.450
3	A:203:GLU:HA	A:244:TRP:CE3	0.427
3	A:125:TYR:OH	A:205:GLY:HA3	0.418
3	A:228:VAL:HG11	A:309:ILE:HD11	0.413
3	A:391:TYR:CZ	A:395:ARG:HD2	0.408
4	A:149:MET:HE1	A:289:ILE:HD11	0.919
4	A:147:THR:HG23	A:149:MET:HE3	0.746
4	A:165:TRP:CH2	A:175:VAL:HG21	0.737
4	A:149:MET:CE	A:289:ILE:HD11	0.695
4	A:344:LYS:HE3	A:345:TYR:CZ	0.577
4	A:119:ARG:HH21	A:336:GLU:CD	0.549
4	A:119:ARG:NH1	A:153:ARG:HH22	0.528
4	A:150:VAL:HG11	A:216:TYR:CE1	0.499

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:185:VAL:HG11	A:188:ILE:HD12	0.497
4	A:109:GLY:C	A:111:ILE:H	0.487
4	A:228:VAL:HG11	A:309:ILE:HD11	0.453
4	A:70:THR:HG22	A:114:LEU:HD21	0.433
4	A:66:MET:HE1	A:95:TYR:CE2	0.424
4	A:391:TYR:CZ	A:395:ARG:CZ	0.420
4	A:66:MET:HE1	A:95:TYR:CD2	0.410
4	A:129:ARG:CZ	A:338:THR:HG21	0.406
5	A:285:PHE:CZ	A:289:ILE:HD11	0.751
5	A:147:THR:HG23	A:149:MET:HE3	0.618
5	A:322:ILE:CG2	A:355:SER:HB2	0.614
5	A:285:PHE:CE2	A:289:ILE:HD11	0.588
5	A:344:LYS:HE3	A:345:TYR:CE2	0.585
5	A:37:ILE:HG22	A:342:ALA:HB1	0.550
5	A:352:ASN:ND2	A:393:PHE:CZ	0.531
5	A:37:ILE:HD13	A:102:PRO:HG2	0.525
5	A:289:ILE:HD13	A:313:LEU:HD21	0.515
5	A:339:HIS:CD2	A:342:ALA:HB2	0.514
5	A:285:PHE:CE1	A:289:ILE:HD11	0.506
5	A:199:LYS:HZ2	A:304:LEU:HD22	0.495
5	A:38:GLY:C	A:40:ASP:H	0.493
5	A:234:MET:HE3	A:238:GLU:HG3	0.493
5	A:105:THR:HG21	A:112:ARG:C	0.474

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:352:ASN:ND2	A:393:PHE:CE2	0.472
5	A:105:THR:HG21	A:112:ARG:O	0.456
5	A:37:ILE:HG22	A:342:ALA:CB	0.455
5	A:318:GLY:C	A:320:ILE:H	0.452
5	A:199:LYS:NZ	A:304:LEU:HD22	0.445
5	A:150:VAL:HG11	A:216:TYR:CE1	0.444
5	A:322:ILE:CG2	A:355:SER:CB	0.430
5	A:234:MET:HE3	A:238:GLU:OE1	0.428
5	A:125:TYR:CD2	A:126:ILE:HG13	0.425
5	A:320:ILE:HB	A:393:PHE:CZ	0.421
5	A:128:LEU:HD21	A:152:PHE:CE1	0.419
5	A:40:ASP:CB	A:43:PRO:HD2	0.408
5	A:389:VAL:HB	A:393:PHE:HB2	0.405
6	A:199:LYS:NZ	A:304:LEU:HD22	0.695
6	A:37:ILE:HG22	A:351:VAL:HG21	0.663
6	A:341:THR:HG21	A:351:VAL:HG13	0.647
6	A:238:GLU:HG2	A:302:MET:HE1	0.628
6	A:37:ILE:HG22	A:351:VAL:CG2	0.625
6	A:37:ILE:HG23	A:346:ALA:HA	0.570
6	A:37:ILE:HD12	A:341:THR:OG1	0.535
6	A:344:LYS:HE3	A:345:TYR:CZ	0.531
6	A:199:LYS:HZ3	A:304:LEU:HD22	0.512
6	A:36:GLY:C	A:37:ILE:HG13	0.506

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:341:THR:HG21	A:351:VAL:CG1	0.498
6	A:36:GLY:C	A:37:ILE:CG1	0.495
6	A:105:THR:HG21	A:114:LEU:H	0.464
6	A:37:ILE:HG23	A:346:ALA:CA	0.459
6	A:125:TYR:CE2	A:126:ILE:HG13	0.439
6	A:391:TYR:CZ	A:395:ARG:HD2	0.431
6	A:119:ARG:HH21	A:336:GLU:CD	0.422
6	A:37:ILE:CD1	A:341:THR:C	0.413
7	A:69:TYR:CE1	A:114:LEU:HD22	0.720
7	A:103:LEU:HD12	A:115:ASN:CG	0.668
7	A:228:VAL:HG13	A:282:ALA:HB3	0.663
7	A:162:GLY:N	A:199:LYS:HB2	0.645
7	A:231:GLY:H	A:304:LEU:HD22	0.588
7	A:230:LYS:HG3	A:304:LEU:HD13	0.578
7	A:228:VAL:CG1	A:282:ALA:HB3	0.576
7	A:37:ILE:HD12	A:351:VAL:HG11	0.544
7	A:103:LEU:HD12	A:115:ASN:ND2	0.526
7	A:35:ASP:H	A:103:LEU:HD23	0.520
7	A:285:PHE:CD1	A:309:ILE:HD11	0.519
7	A:66:MET:HE1	A:95:TYR:CE2	0.514
7	A:100:LYS:CE	A:103:LEU:HD11	0.512
7	A:324:PRO:HB3	A:362:MET:HE1	0.505
7	A:103:LEU:CD1	A:115:ASN:CG	0.488

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:162:GLY:CA	A:199:LYS:HB2	0.473
7	A:344:LYS:HE3	A:345:TYR:CZ	0.469
7	A:285:PHE:HB2	A:305:ASN:CG	0.451
7	A:69:TYR:CE1	A:71:GLY:HA2	0.440
7	A:391:TYR:CZ	A:395:ARG:CZ	0.435
7	A:165:TRP:CH2	A:198:ILE:HD12	0.433
7	A:162:GLY:C	A:199:LYS:O	0.432
7	A:230:LYS:HE3	A:304:LEU:CD1	0.429
7	A:226:THR:CG2	A:280:VAL:HG22	0.421
7	A:285:PHE:HE1	A:289:ILE:HD11	0.414
7	A:157:GLU:HB3	A:160:TYR:CD2	0.412
7	A:344:LYS:HE3	A:345:TYR:CE2	0.411
7	A:162:GLY:N	A:201:CYS:SG	0.411
7	A:149:MET:HA	A:297:ASP:O	0.406
7	A:161:ALA:C	A:201:CYS:SG	0.405
7	A:328:ILE:HB	A:332:CYS:SG	0.400
8	A:176:ILE:HG13	A:196:ILE:HD11	0.719
8	A:104:THR:HG22	A:341:THR:HB	0.676
8	A:338:THR:HG22	A:339:HIS:CD2	0.671
8	A:104:THR:CG2	A:341:THR:HB	0.608
8	A:317:VAL:O	A:322:ILE:HD11	0.596
8	A:165:TRP:CH2	A:175:VAL:HG21	0.586
8	A:344:LYS:HE3	A:345:TYR:CE2	0.571

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:137:THR:HG21	A:322:ILE:HD13	0.562
8	A:83:TRP:CZ3	A:105:THR:HG21	0.556
8	A:151:ILE:HD11	A:313:LEU:HD12	0.546
8	A:228:VAL:HG11	A:309:ILE:HD11	0.523
8	A:344:LYS:HE3	A:345:TYR:CZ	0.500
8	A:165:TRP:CZ3	A:175:VAL:HG21	0.462
8	A:338:THR:HG22	A:339:HIS:NE2	0.455
8	A:163:ILE:HG22	A:165:TRP:CZ2	0.448
8	A:83:TRP:CE3	A:105:THR:HG21	0.442
8	A:128:LEU:HD21	A:152:PHE:CE1	0.442
8	A:167:ALA:HB1	A:193:HIS:C	0.436
8	A:163:ILE:HG22	A:165:TRP:CH2	0.432
8	A:104:THR:HG22	A:341:THR:CB	0.430
8	A:155:ASN:O	A:159:ILE:HD11	0.423
8	A:116:VAL:HG13	A:159:ILE:HG21	0.417
9	A:147:THR:HG21	A:317:VAL:HG11	0.892
9	A:199:LYS:NZ	A:304:LEU:HD13	0.734
9	A:149:MET:HE1	A:289:ILE:CD1	0.679
9	A:199:LYS:HZ2	A:304:LEU:HD13	0.671
9	A:238:GLU:HG2	A:302:MET:HE1	0.645
9	A:149:MET:HE1	A:289:ILE:HD11	0.630
9	A:68:ILE:HD12	A:88:THR:HG23	0.482
9	A:165:TRP:CD1	A:172:ALA:HB2	0.482

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:149:MET:CE	A:289:ILE:HD11	0.453
9	A:289:ILE:HG12	A:313:LEU:CD2	0.444
9	A:188:ILE:HG21	A:190:PHE:CE2	0.414
9	A:352:ASN:ND2	A:393:PHE:CE2	0.412
9	A:327:ASN:HD21	A:336:GLU:CD	0.411
9	A:128:LEU:HD21	A:152:PHE:CE1	0.410
9	A:305:ASN:HA	A:308:TYR:CZ	0.409
9	A:125:TYR:HB2	A:208:ARG:CZ	0.408
9	A:137:THR:HG21	A:318:GLY:C	0.405
10	A:231:GLY:HA2	A:234:MET:HE2	0.671
10	A:167:ALA:HB2	A:192:GLU:HA	0.646
10	A:231:GLY:H	A:281:ILE:HG23	0.584
10	A:163:ILE:HD11	A:171:ASP:HB3	0.576
10	A:131:VAL:HG11	A:313:LEU:HB3	0.558
10	A:344:LYS:HE3	A:345:TYR:CE2	0.549
10	A:228:VAL:HG11	A:309:ILE:HD11	0.521
10	A:337:ALA:HB2	A:356:ILE:HB	0.480
10	A:102:PRO:CG	A:339:HIS:CD2	0.465
10	A:199:LYS:HE2	A:304:LEU:H	0.459
10	A:102:PRO:HG3	A:339:HIS:CD2	0.419
10	A:125:TYR:CE2	A:126:ILE:HG13	0.415
10	A:165:TRP:CD1	A:172:ALA:HB2	0.412
10	A:151:ILE:HD11	A:313:LEU:HD12	0.410

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:177:LYS:HE2	A:181:GLU:OE2	0.408
10	A:102:PRO:HG2	A:339:HIS:CD2	0.407
10	A:167:ALA:CB	A:192:GLU:HA	0.401

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	Analyzed	Favored	Allowed	Outliers
1	414	393	14	7
2	414	405	7	2
3	414	402	12	0
4	414	406	8	0
5	414	398	14	2
6	414	387	24	3
7	414	400	10	4
8	414	388	19	7
9	414	397	14	3
10	414	394	16	4

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	338	331	3	4
2	338	331	6	1
3	338	334	2	2

Model ID	Analyzed	Favored	Allowed	Outliers
4	338	333	4	1
5	338	330	7	1
6	338	326	8	4
7	338	324	9	5
8	338	333	5	0
9	338	328	5	5
10	338	331	6	1

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	37	ILE
1	A	141	VAL
1	A	339	HIS
1	A	388	THR
2	A	394	GLU
3	A	157	GLU
3	A	341	THR
4	A	159	ILE
5	A	388	THR
6	A	105	THR
6	A	185	VAL
6	A	232	ASN
6	A	341	THR
7	A	105	THR

Model ID	Chain	Residue ID	Residue type
7	A	107	VAL
7	A	137	THR
7	A	313	LEU
7	A	328	ILE
9	A	156	SER
9	A	202	SER
9	A	283	ASP
9	A	320	ILE
9	A	370	THR
10	A	104	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 labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, 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.