Integrative Structure Validation Report

July 22, 2024 - 05:13 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	9A35
PDB-Dev ID	PDBDEV_00000190
Structure Title	Model of E. coli GlpD 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

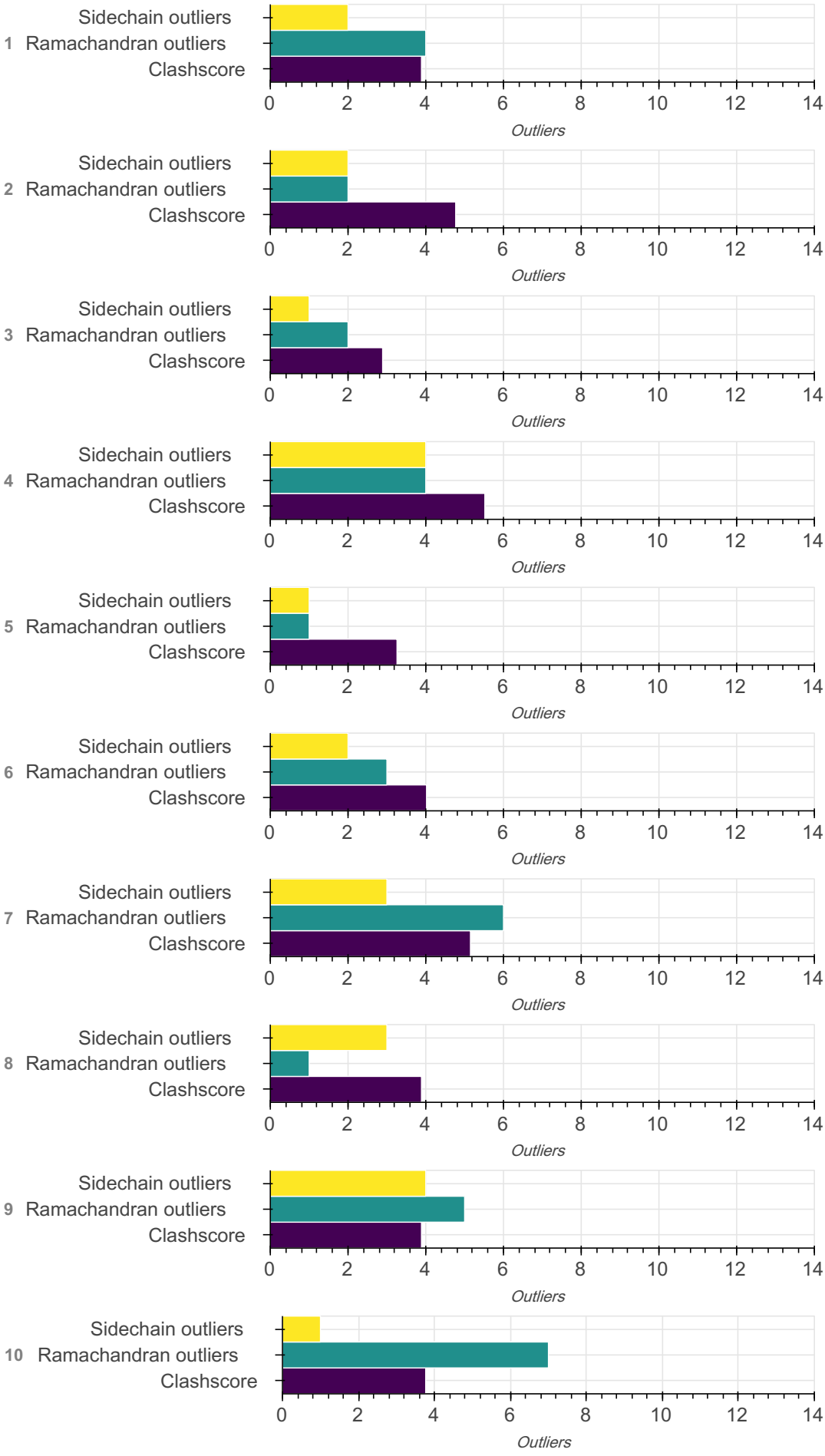
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	P13035	A	A	501
2	1	1	P13035	A	A	501
3	1	1	P13035	A	A	501
4	1	1	P13035	A	A	501
5	1	1	P13035	A	A	501
6	1	1	P13035	A	A	501
7	1	1	P13035	A	A	501
8	1	1	P13035	A	A	501
9	1	1	P13035	A	A	501
10	1	1	P13035	A	A	501

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	-	1-501

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 39610 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	4600
CD1--HD11	1.09	0.97	790
CB--HB3	1.09	0.97	3790
CG2--HG21	1.09	0.97	810
CD1--HD13	1.09	0.97	790
CB--HB2	1.09	0.97	3790
CD--HD3	1.09	0.97	840
CB--HB	1.09	0.97	810
CG--HG2	1.09	0.97	1430
CG--HG3	1.09	0.97	1430
CA--HA3	1.09	0.97	410
CA--HA2	1.09	0.97	410
CD--HD2	1.09	0.97	840
CD1--HD12	1.09	0.97	790
CG2--HG23	1.09	0.97	810
NZ--HZ1	1.01	0.89	250
CB--HB1	1.09	0.97	410
NZ--HZ3	1.01	0.89	250
CD2--HD21	1.09	0.97	530
CG1--HG13	1.09	0.97	560
OG--HG	0.96	0.84	300
NZ--HZ2	1.01	0.89	250

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD2--HD23	1.09	0.97	530
OH--HH	0.96	0.84	220
CG2--HG22	1.09	0.97	810
CE--HE2	1.09	0.97	350
CG1--HG12	1.09	0.97	560
CD2--HD22	1.09	0.97	530
CG--HG	1.09	0.97	530
CE--HE3	1.09	0.97	350
CE--HE1	1.09	0.97	100
CG1--HG11	1.09	0.97	300
OG1--HG1	0.96	0.84	250
N--H1	1.01	0.89	10
N--H3	1.01	0.89	10
N--H2	1.01	0.89	10
SG--HG	1.33	1.20	7
SG--HG	1.34	1.20	23
N--H	1.01	0.86	4800
CD2--HD2	1.08	0.93	520
NE--HE	1.01	0.86	390
ND2--HD22	1.01	0.86	130
CE3--HE3	1.08	0.93	120
NH2--HH21	1.01	0.86	390
CE1--HE1	1.08	0.93	520

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD1	1.08	0.93	490
NH1--HH11	1.01	0.86	390
CH2--HH2	1.08	0.93	120
NH2--HH22	1.01	0.86	390
CE2--HE2	1.08	0.93	370
CZ--HZ	1.08	0.93	150
NH1--HH12	1.01	0.86	390
CZ3--HZ3	1.08	0.93	120
ND2--HD21	1.01	0.86	130
CZ2--HZ2	1.08	0.93	120
NE2--HE21	1.01	0.86	160
NE1--HE1	1.01	0.86	120
ND1--HD1	1.01	0.86	130
NE2--HE22	1.01	0.86	160
NE2--HE2	1.01	0.86	20

Standard geometry: angle outliers

There are 201 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
OE1-CD-NE2	122.60	113.94	1
CA-CB-CG	112.60	119.42	1
C-CA-CB	110.50	120.36	1
C-N-CA	121.70	133.36	1
CA-CB-CG	112.60	119.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.54	1
CA-CB-CG	112.60	118.57	1
CD-NE-CZ	124.40	132.73	1
CA-CB-CG	112.60	118.32	1
OE1-CD-NE2	122.60	116.89	1
NE-CZ-NH2	119.20	124.32	1
NE-CZ-NH2	119.20	124.26	1
OE1-CD-NE2	122.60	116.97	1
NE-CZ-NH2	119.20	124.21	1
NE-CZ-NH2	119.20	124.15	1
CB-CG-CD2	131.20	124.22	1
OE1-CD-NE2	122.60	117.23	1
OE1-CD-NE2	122.60	117.25	1
CA-CB-CG	114.10	124.78	1
NE-CZ-NH2	119.20	124.00	1
OE1-CD-NE2	122.60	117.29	1
CA-CB-CG	112.60	117.90	1
OE1-CD-NE2	122.60	117.33	1
CA-CB-CG	112.60	117.82	1
CA-CB-CG	112.60	117.76	2
OE1-CD-NE2	122.60	117.49	1
CB-CG-CD2	131.20	124.58	1
CA-CB-CG	112.60	117.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.56	1
NE-CZ-NH2	119.20	123.73	1
OE1-CD-NE2	122.60	117.60	1
CA-CB-CG	112.60	117.57	1
CA-CB-CG	114.10	104.19	1
CB-CG-CD2	131.20	124.76	1
OE1-CD-NE2	122.60	117.65	1
CA-CB-CG	112.60	117.55	1
OE1-CD-NE2	122.60	117.67	1
OE1-CD-NE2	122.60	117.69	1
N-CA-CB	110.50	118.85	1
OE1-CD-NE2	122.60	117.74	1
CA-CB-CG	112.60	117.46	1
OE1-CD-NE2	122.60	117.75	1
CA-CB-CG	112.60	117.45	1
OE1-CD-NE2	122.60	117.77	1
OE1-CD-NE2	122.60	117.78	1
CB-CG-CD2	131.20	124.93	1
CA-CB-CG	112.60	117.37	2
OE1-CD-NE2	122.60	117.84	1
CA-CB-CG	112.60	117.35	1
CB-CG-CD2	131.20	125.06	1
CA-CB-CG	112.60	117.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.91	2
CA-CB-CG	113.80	109.11	1
CA-CB-CG	112.60	117.28	1
OE1-CD-NE2	122.60	117.92	1
CB-CG-CD2	131.20	125.11	1
OE1-CD-NE2	122.60	117.93	1
NE-CZ-NH1	121.50	126.17	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	1
OE1-CD-NE2	122.60	117.97	2
CB-CG-CD2	131.20	125.19	1
OE1-CD-NE2	122.60	117.98	1
CA-CB-CG	112.60	117.22	1
NE-CZ-NH1	121.50	126.10	1
OE1-CD-NE2	122.60	118.00	1
CB-CG-CD2	131.20	125.23	2
OE1-CD-NE2	122.60	118.01	1
CA-CB-CG	112.60	117.18	1
CB-CG-CD2	131.20	125.25	1
CB-CG-CD2	131.20	125.26	2
CB-CG-CD2	131.20	125.29	1
CB-CG-CD2	131.20	125.31	1
CA-CB-CG	112.60	117.11	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.33	1
CB-CG-CD2	131.20	125.34	1
CB-CG-CD2	131.20	125.36	1
OE1-CD-NE2	122.60	118.12	1
CD-NE-CZ	124.40	130.66	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.15	1
CA-CB-CG	112.60	117.05	1
CB-CG-CD2	131.20	125.43	1
OE1-CD-NE2	122.60	118.16	1
CB-CG-CD2	131.20	125.44	2
OE1-CD-NE2	122.60	118.17	2
OE1-CD-NE2	122.60	118.18	2
NH1-CZ-NH2	119.30	113.55	1
CB-CG-CD2	131.20	125.46	1
OE1-CD-NE2	122.60	118.19	3
CB-CG-CD2	131.20	125.47	1
N-CA-CB	110.40	103.79	1
OE1-CD-NE2	122.60	118.20	4
CA-CB-CG	112.60	117.00	2
OE1-CD-NE2	122.60	118.21	1
CA-CB-CG	112.60	116.99	1
CB-CG-CD2	131.20	125.50	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.22	1
NE-CZ-NH2	119.20	123.14	1
CA-CB-CG	112.60	116.96	1
OE1-CD-NE2	122.60	118.25	2
CB-CG-CD2	131.20	125.55	1
OE1-CD-NE2	122.60	118.27	1
CB-CG-CD2	131.20	125.57	2
OE1-CD-NE2	122.60	118.28	2
NH1-CZ-NH2	119.30	113.69	1
CA-CB-CG	112.60	116.91	2
NH1-CZ-NH2	119.30	113.70	1
CA-CB-CG	113.80	109.49	1
OE1-CD-NE2	122.60	118.30	1
CB-CG-CD2	131.20	125.62	2
OE1-CD-NE2	122.60	118.31	1
CB-CG-CD2	131.20	125.63	1
CB-CG-CD2	131.20	125.64	2
OE1-CD-NE2	122.60	118.33	1
CB-CG-CD2	131.20	125.65	1
NE-CZ-NH2	119.20	123.03	1
CB-CG-CD2	131.20	125.67	1
CA-CB-CG	112.60	116.85	1
OE1-CD-NE2	122.60	118.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	125.74	1
OE1-CD-NE2	122.60	118.37	1
CB-CG-CD2	131.20	125.71	1
OE1-CD-NE2	122.60	118.39	1
C-N-CA	121.70	129.28	1
CA-CB-CG	112.60	116.81	1
OE1-CD-NE2	122.60	118.41	2
CA-CB-CG	113.80	109.61	1
NH1-CZ-NH2	119.30	113.88	1
CB-CG-CD2	131.20	125.78	1
CA-CB-CG	113.80	109.64	1
CA-CB-CG2	110.50	117.57	1
OE1-CD-NE2	122.60	118.45	1
CD2-NE2-CE1	109.00	104.86	1
CB-CG-CD2	131.20	125.83	1
CB-CG-CD2	131.20	125.84	1
NE-CZ-NH2	119.20	122.91	1
OE1-CD-NE2	122.60	118.48	1
NE-CZ-NH1	121.50	125.61	1
CB-CG-CD2	131.20	125.86	1
OE1-CD-NE2	122.60	118.50	1
OE1-CD-NE2	122.60	118.51	2
CA-CB-CG	112.60	116.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.52	2
OE1-CD-NE2	122.60	118.53	3
NH1-CZ-NH2	119.30	114.01	1
CA-CB-CG	112.60	116.67	2
CA-CB-CG	112.60	108.54	1
CA-C-O	120.80	113.89	1
CB-CG-CD2	131.20	125.92	2
CB-CG-CD2	131.20	125.93	1
OE1-CD-NE2	122.60	118.55	1
C-N-CA	121.70	128.98	1
OE1-CD-NE2	122.60	118.56	1
CA-CB-CG	112.60	116.64	1
CB-CG-CD2	131.20	125.95	1
OE1-CD-NE2	122.60	118.57	2
CA-CB-CG	112.60	116.63	1
CB-CG-CD2	131.20	125.97	1
OE1-CD-NE2	122.60	118.58	1
CA-CB-CG	112.60	116.62	1
OE1-CD-NE2	122.60	118.59	1
OE1-CD-NE2	122.60	118.60	1
HH11-NH1-HH12	107.22	120.00	1
HH21-NH2-HH22	106.98	120.00	1
CZ-NH2-HH21	106.97	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HZ2-NZ-HZ3	94.58	109.00	1
HZ2-NZ-HZ3	94.29	109.00	1
CZ-NH1-HH11	102.88	120.00	1
HH21-NH2-HH22	97.89	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	3.89	31
2	4.77	38
3	2.89	23
4	5.52	44
5	3.26	26
6	4.02	32
7	5.15	41
8	3.89	31
9	3.89	31
10	3.77	30

All 327 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:218:MET:HE1	A:347:LEU:HD22	0.767
1	A:83:PHE:CE1	A:145:TRP:CE3	0.693
1	A:330:ILE:HG23	A:354:LYS:HE3	0.594

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:223:PRO:HG2	A:224:TYR:CE2	0.572
1	A:317:ARG:NH1	A:319:LEU:HD21	0.570
1	A:348:LEU:HD21	A:365:ALA:HB1	0.562
1	A:322:ASP:CG	A:331:THR:HG21	0.553
1	A:158:MET:HE2	A:387:PRO:HD3	0.539
1	A:360:LYS:HE2	A:364:HIS:CE1	0.522
1	A:380:TRP:CH2	A:384:SER:HB3	0.513
1	A:93:PRO:HG3	A:137:ARG:HH21	0.507
1	A:162:LYS:HE3	A:380:TRP:CZ2	0.497
1	A:311:TRP:CZ2	A:473:GLN:NE2	0.471
1	A:49:ILE:HG22	A:356:THR:HG22	0.469
1	A:49:ILE:CG2	A:356:THR:HG22	0.468
1	A:61:PHE:CE1	A:107:MET:HE1	0.467
1	A:44:ALA:CB	A:315:GLY:HA3	0.466
1	A:311:TRP:CZ2	A:313:TYR:HB3	0.466
1	A:162:LYS:CE	A:380:TRP:CZ2	0.465
1	A:330:ILE:O	A:330:ILE:HG22	0.453
1	A:322:ASP:OD2	A:331:THR:HG21	0.449
1	A:83:PHE:CZ	A:145:TRP:CE3	0.447
1	A:223:PRO:HG2	A:224:TYR:CZ	0.445
1	A:80:HIS:CD2	A:81:ILE:HG23	0.438
1	A:150:ARG:HH12	A:458:GLU:CD	0.436
1	A:468:TRP:O	A:472:LYS:HA	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:224:TYR:OH	A:335:THR:HG21	0.416
1	A:34:ALA:O	A:189:ILE:HD12	0.415
1	A:162:LYS:HE3	A:380:TRP:CE2	0.413
1	A:380:TRP:CH2	A:384:SER:CB	0.402
1	A:114:ARG:HH22	A:142:SER:HB2	0.401
2	A:63:LEU:HD21	A:354:LYS:NZ	0.781
2	A:49:ILE:HD12	A:141:TYR:CG	0.721
2	A:235:VAL:HG11	A:311:TRP:CZ2	0.720
2	A:63:LEU:HD21	A:354:LYS:HZ2	0.624
2	A:63:LEU:HD21	A:354:LYS:HZ1	0.613
2	A:49:ILE:HD12	A:141:TYR:CD1	0.571
2	A:49:ILE:HG13	A:141:TYR:CE2	0.564
2	A:107:MET:HE2	A:111:LEU:HD11	0.557
2	A:332:ARG:O	A:354:LYS:HE3	0.557
2	A:61:PHE:CE1	A:107:MET:HE1	0.548
2	A:83:PHE:CE1	A:145:TRP:CE3	0.527
2	A:158:MET:HE2	A:387:PRO:HD3	0.527
2	A:162:LYS:HE3	A:380:TRP:CE2	0.517
2	A:48:LEU:CD2	A:67:ALA:HB1	0.504
2	A:68:LEU:HD21	A:108:TYR:CD2	0.488
2	A:210:VAL:HG12	A:226:ILE:HD11	0.488
2	A:68:LEU:HD21	A:108:TYR:CE2	0.487
2	A:162:LYS:HE3	A:380:TRP:CZ2	0.487

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:49:ILE:HG12	A:108:TYR:CE2	0.485
2	A:458:GLU:HB3	A:469:ARG:HH12	0.473
2	A:80:HIS:CD2	A:81:ILE:HG23	0.459
2	A:49:ILE:HD12	A:141:TYR:CD2	0.451
2	A:150:ARG:HH12	A:458:GLU:CD	0.450
2	A:210:VAL:CG1	A:226:ILE:HD11	0.447
2	A:87:PHE:HB2	A:141:TYR:CZ	0.441
2	A:49:ILE:HG12	A:108:TYR:CD2	0.440
2	A:73:VAL:HG12	A:77:MET:HE3	0.437
2	A:61:PHE:CD1	A:107:MET:HE1	0.427
2	A:310:VAL:HG23	A:311:TRP:CE3	0.424
2	A:261:TRP:CZ3	A:473:GLN:NE2	0.423
2	A:317:ARG:HH22	A:354:LYS:CG	0.418
2	A:49:ILE:HB	A:141:TYR:CZ	0.417
2	A:49:ILE:CD1	A:141:TYR:CD2	0.414
2	A:90:PRO:HB3	A:135:ILE:HG21	0.414
2	A:271:THR:O	A:272:ASP:CG	0.414
2	A:6:LEU:HD11	A:203:VAL:HG23	0.413
2	A:49:ILE:CD1	A:141:TYR:CG	0.411
2	A:317:ARG:HE	A:319:LEU:HD21	0.403
3	A:83:PHE:CE1	A:145:TRP:CE3	0.551
3	A:158:MET:HE2	A:387:PRO:HD3	0.531
3	A:103:ILE:HG22	A:107:MET:HE2	0.523

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:48:LEU:HD11	A:259:ILE:HD11	0.476
3	A:169:ARG:CZ	A:189:ILE:HD11	0.459
3	A:207:GLY:O	A:210:VAL:HG23	0.452
3	A:6:LEU:HD11	A:203:VAL:HG23	0.447
3	A:463:ALA:HB2	A:486:SER:HA	0.447
3	A:153:LEU:HD11	A:470:ARG:NH1	0.445
3	A:363:GLU:CD	A:382:LYS:HZ1	0.439
3	A:24:GLY:HA3	A:380:TRP:CE2	0.436
3	A:442:PHE:CE2	A:451:LEU:HD12	0.427
3	A:13:ILE:HG12	A:355:LEU:HD23	0.425
3	A:46:SER:HB2	A:259:ILE:CD1	0.425
3	A:286:GLU:CD	A:306:ARG:HH22	0.424
3	A:212:GLN:HA	A:219:HIS:CD2	0.415
3	A:80:HIS:CD2	A:81:ILE:HG23	0.411
3	A:398:TYR:CD2	A:401:ARG:NH2	0.411
3	A:451:LEU:HB3	A:488:TRP:CZ3	0.411
3	A:46:SER:HB2	A:259:ILE:HD13	0.407
3	A:162:LYS:HE3	A:380:TRP:CH2	0.406
3	A:48:LEU:HD11	A:259:ILE:CD1	0.405
3	A:55:TYR:HE1	A:354:LYS:HZ2	0.400
4	A:71:ARG:HH22	A:356:THR:HG22	0.767
4	A:468:TRP:CZ2	A:472:LYS:HE3	0.651
4	A:49:ILE:HG12	A:141:TYR:CE2	0.642

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:71:ARG:HH12	A:356:THR:HB	0.628
4	A:158:MET:HE2	A:387:PRO:HD3	0.627
4	A:145:TRP:CZ2	A:261:TRP:CZ3	0.599
4	A:48:LEU:HD23	A:108:TYR:CE2	0.595
4	A:317:ARG:HE	A:319:LEU:HD21	0.585
4	A:61:PHE:CD1	A:107:MET:HE1	0.573
4	A:6:LEU:HD11	A:203:VAL:HG23	0.561
4	A:83:PHE:CE1	A:145:TRP:CE3	0.550
4	A:61:PHE:CE1	A:107:MET:HE1	0.544
4	A:77:MET:HE3	A:384:SER:O	0.542
4	A:470:ARG:CB	A:475:MET:HE2	0.542
4	A:114:ARG:HH21	A:117:LEU:HB3	0.526
4	A:470:ARG:HB3	A:475:MET:HE2	0.511
4	A:468:TRP:CE2	A:472:LYS:HE3	0.505
4	A:44:ALA:HB1	A:145:TRP:HE1	0.499
4	A:68:LEU:HD22	A:114:ARG:HD2	0.497
4	A:48:LEU:HD21	A:68:LEU:HG	0.496
4	A:227:ARG:CZ	A:330:ILE:HD11	0.481
4	A:114:ARG:HH21	A:117:LEU:CB	0.480
4	A:54:ARG:NH1	A:332:ARG:HH21	0.476
4	A:145:TRP:CZ2	A:261:TRP:CH2	0.473
4	A:49:ILE:HG21	A:141:TYR:OH	0.466
4	A:87:PHE:HB2	A:141:TYR:CE2	0.465

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:229:ILE:HD12	A:327:PRO:HB3	0.465
4	A:380:TRP:CZ2	A:384:SER:CB	0.456
4	A:56:LEU:HD13	A:104:GLY:CA	0.451
4	A:210:VAL:HG12	A:226:ILE:HD11	0.447
4	A:87:PHE:HB2	A:141:TYR:CZ	0.446
4	A:56:LEU:HD13	A:104:GLY:HA2	0.445
4	A:49:ILE:HG21	A:141:TYR:CZ	0.443
4	A:107:MET:HE2	A:111:LEU:HD11	0.440
4	A:238:ARG:NH1	A:263:ASP:HA	0.439
4	A:235:VAL:HG11	A:311:TRP:CZ2	0.437
4	A:71:ARG:HH22	A:356:THR:CG2	0.434
4	A:332:ARG:O	A:354:LYS:HE3	0.433
4	A:71:ARG:HG3	A:144:CYS:SG	0.428
4	A:71:ARG:HH12	A:356:THR:CB	0.425
4	A:470:ARG:HB2	A:475:MET:HE2	0.410
4	A:210:VAL:HG12	A:226:ILE:CD1	0.402
4	A:50:HIS:CD2	A:255:ILE:HB	0.402
4	A:463:ALA:HB2	A:486:SER:HA	0.402
5	A:49:ILE:HG23	A:356:THR:HG22	0.906
5	A:262:MET:HE1	A:472:LYS:CB	0.702
5	A:153:LEU:HD21	A:470:ARG:CZ	0.670
5	A:262:MET:HE1	A:472:LYS:HB2	0.661
5	A:48:LEU:HD13	A:87:PHE:CE1	0.628

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:83:PHE:CE1	A:145:TRP:CE3	0.589
5	A:169:ARG:HD2	A:189:ILE:HD11	0.558
5	A:151:LEU:HD23	A:355:LEU:HD11	0.541
5	A:48:LEU:HD13	A:87:PHE:CZ	0.514
5	A:49:ILE:HD11	A:146:VAL:HG21	0.479
5	A:158:MET:HE2	A:387:PRO:HD3	0.466
5	A:83:PHE:CE1	A:395:ARG:NH1	0.463
5	A:262:MET:CE	A:472:LYS:HD3	0.463
5	A:73:VAL:HG12	A:77:MET:SD	0.448
5	A:46:SER:HB2	A:145:TRP:CE2	0.447
5	A:317:ARG:NH1	A:319:LEU:HD21	0.444
5	A:177:ARG:HH12	A:339:HIS:CE1	0.442
5	A:87:PHE:CE1	A:245:ALA:HB3	0.439
5	A:48:LEU:HD22	A:87:PHE:HZ	0.429
5	A:97:PRO:HD2	A:100:MET:HE2	0.425
5	A:442:PHE:CE2	A:451:LEU:HD12	0.425
5	A:46:SER:HB3	A:145:TRP:CZ2	0.420
5	A:73:VAL:CG1	A:77:MET:SD	0.411
5	A:361:LEU:C	A:361:LEU:HD23	0.411
5	A:262:MET:SD	A:475:MET:CE	0.405
5	A:106:PHE:CZ	A:110:HIS:CE1	0.404
6	A:49:ILE:HD12	A:146:VAL:HG21	0.745
6	A:151:LEU:HD23	A:355:LEU:HD11	0.686

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:49:ILE:HG23	A:356:THR:HG22	0.638
6	A:45:SER:HA	A:233:HIS:CE1	0.637
6	A:6:LEU:HD11	A:203:VAL:HG23	0.611
6	A:227:ARG:NH1	A:330:ILE:HD11	0.589
6	A:150:ARG:HH21	A:420:THR:CG2	0.586
6	A:467:LEU:HD21	A:477:LEU:HD12	0.569
6	A:68:LEU:HD21	A:108:TYR:CZ	0.557
6	A:77:MET:HE3	A:384:SER:O	0.527
6	A:240:HIS:NE2	A:258:VAL:HG12	0.519
6	A:63:LEU:HD21	A:354:LYS:NZ	0.510
6	A:177:ARG:HH12	A:339:HIS:CE1	0.493
6	A:158:MET:HE2	A:387:PRO:HD3	0.489
6	A:460:VAL:HG23	A:469:ARG:NH1	0.482
6	A:89:LEU:HD11	A:141:TYR:CE1	0.479
6	A:13:ILE:HG12	A:355:LEU:HD12	0.465
6	A:83:PHE:CE1	A:145:TRP:CE3	0.463
6	A:262:MET:HE1	A:471:THR:HA	0.458
6	A:89:LEU:HD11	A:141:TYR:CD1	0.452
6	A:49:ILE:HD12	A:146:VAL:CG2	0.443
6	A:476:TRP:O	A:477:LEU:HD23	0.430
6	A:313:TYR:CE1	A:473:GLN:NE2	0.427
6	A:41:THR:C	A:43:SER:H	0.426
6	A:332:ARG:O	A:354:LYS:HE3	0.421

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:63:LEU:HD21	A:354:LYS:HZ2	0.419
6	A:262:MET:HE1	A:471:THR:CA	0.412
6	A:43:SER:C	A:45:SER:N	0.410
6	A:227:ARG:CZ	A:330:ILE:HD11	0.410
6	A:242:GLN:HB2	A:244:GLN:OE1	0.409
6	A:233:HIS:CD2	A:269:GLY:HA3	0.402
6	A:73:VAL:CG1	A:77:MET:SD	0.400
7	A:210:VAL:CG1	A:226:ILE:HD11	0.784
7	A:210:VAL:HG12	A:226:ILE:HD11	0.780
7	A:61:PHE:CD1	A:107:MET:HE1	0.731
7	A:92:ARG:HH22	A:298:THR:HG22	0.650
7	A:210:VAL:HG12	A:226:ILE:CD1	0.626
7	A:6:LEU:HD11	A:203:VAL:HG23	0.622
7	A:83:PHE:CE1	A:145:TRP:CE3	0.609
7	A:261:TRP:CZ3	A:262:MET:HE2	0.597
7	A:56:LEU:HD13	A:104:GLY:CA	0.561
7	A:61:PHE:CE1	A:107:MET:HE1	0.556
7	A:158:MET:HE2	A:387:PRO:HD3	0.556
7	A:54:ARG:HH22	A:328:GLN:HA	0.545
7	A:56:LEU:HD13	A:104:GLY:HA3	0.533
7	A:68:LEU:HD21	A:108:TYR:CE2	0.531
7	A:48:LEU:HD22	A:87:PHE:CZ	0.526
7	A:210:VAL:HG11	A:226:ILE:HD11	0.515

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:46:SER:HB3	A:145:TRP:CZ2	0.513
7	A:46:SER:HB3	A:145:TRP:CE2	0.507
7	A:54:ARG:NH2	A:328:GLN:HA	0.504
7	A:48:LEU:HD13	A:87:PHE:CE1	0.498
7	A:107:MET:HE2	A:111:LEU:HD11	0.489
7	A:153:LEU:HD11	A:470:ARG:CD	0.488
7	A:46:SER:CB	A:145:TRP:CE2	0.481
7	A:150:ARG:HH12	A:458:GLU:CD	0.481
7	A:87:PHE:CE1	A:245:ALA:HB3	0.474
7	A:250:ASN:ND2	A:295:VAL:HG22	0.463
7	A:80:HIS:CD2	A:81:ILE:HG23	0.459
7	A:56:LEU:HD13	A:104:GLY:HA2	0.456
7	A:177:ARG:HH12	A:339:HIS:CE1	0.439
7	A:71:ARG:CZ	A:117:LEU:HD12	0.434
7	A:44:ALA:HB3	A:313:TYR:CE1	0.433
7	A:238:ARG:CZ	A:260:PRO:HB3	0.421
7	A:233:HIS:CD2	A:269:GLY:HA3	0.419
7	A:48:LEU:HD22	A:87:PHE:HZ	0.415
7	A:91:HIS:CE1	A:98:ALA:HB2	0.411
7	A:361:LEU:C	A:361:LEU:HD23	0.411
7	A:227:ARG:CZ	A:330:ILE:HD11	0.410
7	A:73:VAL:HG12	A:77:MET:SD	0.408
7	A:96:ARG:NH2	A:249:GLN:HE22	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:209:TRP:CH2	A:280:LYS:CG	0.404
7	A:49:ILE:O	A:49:ILE:HG22	0.401
8	A:227:ARG:NH2	A:330:ILE:HD12	0.706
8	A:227:ARG:HH22	A:330:ILE:HD12	0.667
8	A:6:LEU:HD11	A:203:VAL:HG23	0.645
8	A:60:GLU:CD	A:332:ARG:HH22	0.633
8	A:218:MET:HE1	A:347:LEU:HD22	0.559
8	A:53:LEU:CD2	A:255:ILE:HG21	0.536
8	A:158:MET:HE2	A:387:PRO:HD3	0.534
8	A:68:LEU:HG	A:108:TYR:CE2	0.531
8	A:49:ILE:HD11	A:74:LEU:HD13	0.497
8	A:44:ALA:HB1	A:468:TRP:CH2	0.472
8	A:150:ARG:HH12	A:458:GLU:CD	0.468
8	A:471:THR:HG21	A:475:MET:HB2	0.462
8	A:233:HIS:HB2	A:313:TYR:CZ	0.459
8	A:458:GLU:HB3	A:469:ARG:HH12	0.457
8	A:21:ASP:HA	A:380:TRP:HE1	0.453
8	A:44:ALA:HB1	A:468:TRP:CZ2	0.448
8	A:450:GLU:OE2	A:470:ARG:NH1	0.446
8	A:64:VAL:HG13	A:108:TYR:CD2	0.445
8	A:296:TYR:CD1	A:304:LEU:HD12	0.445
8	A:238:ARG:CZ	A:260:PRO:HB3	0.439
8	A:46:SER:HB2	A:145:TRP:CD1	0.438

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:471:THR:C	A:473:GLN:H	0.433
8	A:61:PHE:CE2	A:107:MET:HE2	0.427
8	A:233:HIS:CD2	A:269:GLY:HA3	0.425
8	A:53:LEU:HD23	A:255:ILE:HD13	0.423
8	A:361:LEU:C	A:361:LEU:HD23	0.422
8	A:458:GLU:HB3	A:469:ARG:NH1	0.422
8	A:68:LEU:HG	A:108:TYR:CD2	0.421
8	A:61:PHE:CZ	A:107:MET:HE2	0.416
8	A:218:MET:HE2	A:220:LEU:HD12	0.412
8	A:106:PHE:CZ	A:123:LEU:HD11	0.402
9	A:467:LEU:HD21	A:477:LEU:HD12	0.663
9	A:83:PHE:CD2	A:145:TRP:CE3	0.651
9	A:317:ARG:HH22	A:354:LYS:HE3	0.646
9	A:83:PHE:CE2	A:145:TRP:CZ3	0.624
9	A:317:ARG:HE	A:319:LEU:HD21	0.621
9	A:56:LEU:HD13	A:104:GLY:HA3	0.560
9	A:158:MET:HE2	A:387:PRO:HD3	0.548
9	A:317:ARG:NH2	A:354:LYS:HE3	0.539
9	A:56:LEU:HD13	A:104:GLY:CA	0.530
9	A:106:PHE:CE2	A:110:HIS:CE1	0.519
9	A:227:ARG:CZ	A:330:ILE:HD11	0.518
9	A:43:SER:C	A:45:SER:H	0.511
9	A:68:LEU:HD21	A:108:TYR:CZ	0.503

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:460:VAL:HG23	A:469:ARG:NH1	0.502
9	A:96:ARG:NH1	A:249:GLN:HE21	0.497
9	A:68:LEU:HD21	A:108:TYR:CE2	0.491
9	A:83:PHE:CD1	A:395:ARG:NH1	0.490
9	A:51:GLY:HA3	A:55:TYR:CD2	0.487
9	A:61:PHE:CD1	A:107:MET:HE1	0.484
9	A:96:ARG:HH11	A:249:GLN:HE21	0.475
9	A:317:ARG:HH22	A:354:LYS:CG	0.462
9	A:80:HIS:CD2	A:81:ILE:HG23	0.451
9	A:51:GLY:CA	A:55:TYR:CE2	0.438
9	A:51:GLY:HA3	A:55:TYR:CE2	0.436
9	A:271:THR:O	A:272:ASP:CG	0.431
9	A:83:PHE:CD2	A:145:TRP:CZ3	0.426
9	A:96:ARG:HH12	A:255:ILE:HD11	0.423
9	A:416:HIS:CD2	A:470:ARG:NH1	0.418
9	A:169:ARG:HB2	A:461:ARG:CZ	0.411
9	A:49:ILE:HD11	A:146:VAL:CG2	0.403
9	A:210:VAL:HG11	A:226:ILE:HD11	0.400
10	A:49:ILE:HG23	A:356:THR:HG22	0.844
10	A:52:GLY:HA3	A:108:TYR:CE2	0.693
10	A:145:TRP:HZ3	A:259:ILE:HG21	0.619
10	A:332:ARG:HB3	A:354:LYS:HE3	0.595
10	A:218:MET:HE1	A:347:LEU:HD22	0.575

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:49:ILE:HD12	A:146:VAL:HG21	0.557
10	A:332:ARG:CB	A:354:LYS:HE3	0.549
10	A:177:ARG:HH12	A:339:HIS:CE1	0.541
10	A:48:LEU:HD11	A:259:ILE:HG12	0.535
10	A:145:TRP:CZ3	A:259:ILE:HG21	0.528
10	A:51:GLY:HA3	A:71:ARG:HH22	0.525
10	A:68:LEU:HD21	A:108:TYR:CZ	0.524
10	A:50:HIS:CD2	A:257:PHE:CZ	0.509
10	A:63:LEU:HD21	A:354:LYS:NZ	0.501
10	A:48:LEU:HD13	A:87:PHE:HE1	0.494
10	A:471:THR:HG22	A:476:TRP:CE3	0.492
10	A:49:ILE:HG23	A:356:THR:CG2	0.481
10	A:83:PHE:CE1	A:395:ARG:NH1	0.477
10	A:83:PHE:CE1	A:145:TRP:CD1	0.469
10	A:80:HIS:CD2	A:81:ILE:HG23	0.466
10	A:73:VAL:HG12	A:77:MET:SD	0.464
10	A:458:GLU:CB	A:469:ARG:HH12	0.460
10	A:468:TRP:CE3	A:473:GLN:HG3	0.437
10	A:52:GLY:CA	A:108:TYR:CE2	0.436
10	A:468:TRP:CZ3	A:473:GLN:HG3	0.431
10	A:458:GLU:HB3	A:469:ARG:NH1	0.429
10	A:49:ILE:O	A:49:ILE:HG22	0.426
10	A:150:ARG:HH12	A:458:GLU:CD	0.413

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:458:GLU:CB	A:469:ARG:NH1	0.404
10	A:317:ARG:CZ	A:319:LEU:HD21	0.403

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	499	479	16	4
2	499	488	9	2
3	499	484	13	2
4	499	478	17	4
5	499	492	6	1
6	499	486	10	3
7	499	477	16	6
8	499	485	13	1
9	499	478	16	5
10	499	481	11	7

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	419	408	9	2
2	419	410	7	2
3	419	414	4	1
4	419	407	8	4

Model ID	Analyzed	Favored	Allowed	Outliers
5	419	412	6	1
6	419	411	6	2
7	419	412	4	3
8	419	405	11	3
9	419	407	8	4
10	419	413	5	1

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	45	SER
1	A	142	SER
2	A	43	SER
2	A	49	ILE
3	A	501	SER
4	A	210	VAL
4	A	355	LEU
4	A	476	TRP
4	A	501	SER
5	A	89	LEU
6	A	324	SER
6	A	473	GLN
7	A	45	SER
7	A	210	VAL
7	A	366	LEU

Model ID	Chain	Residue ID	Residue type
8	A	89	LEU
8	A	116	SER
8	A	324	SER
9	A	50	HIS
9	A	226	ILE
9	A	260	PRO
9	A	355	LEU
10	A	50	HIS

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.