Integrative Structure Validation Report

July 22, 2024 - 05:09 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	9A2Y
PDB-Dev ID	PDBDEV_00000183
Structure Title	Model of E. coli OmpF 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

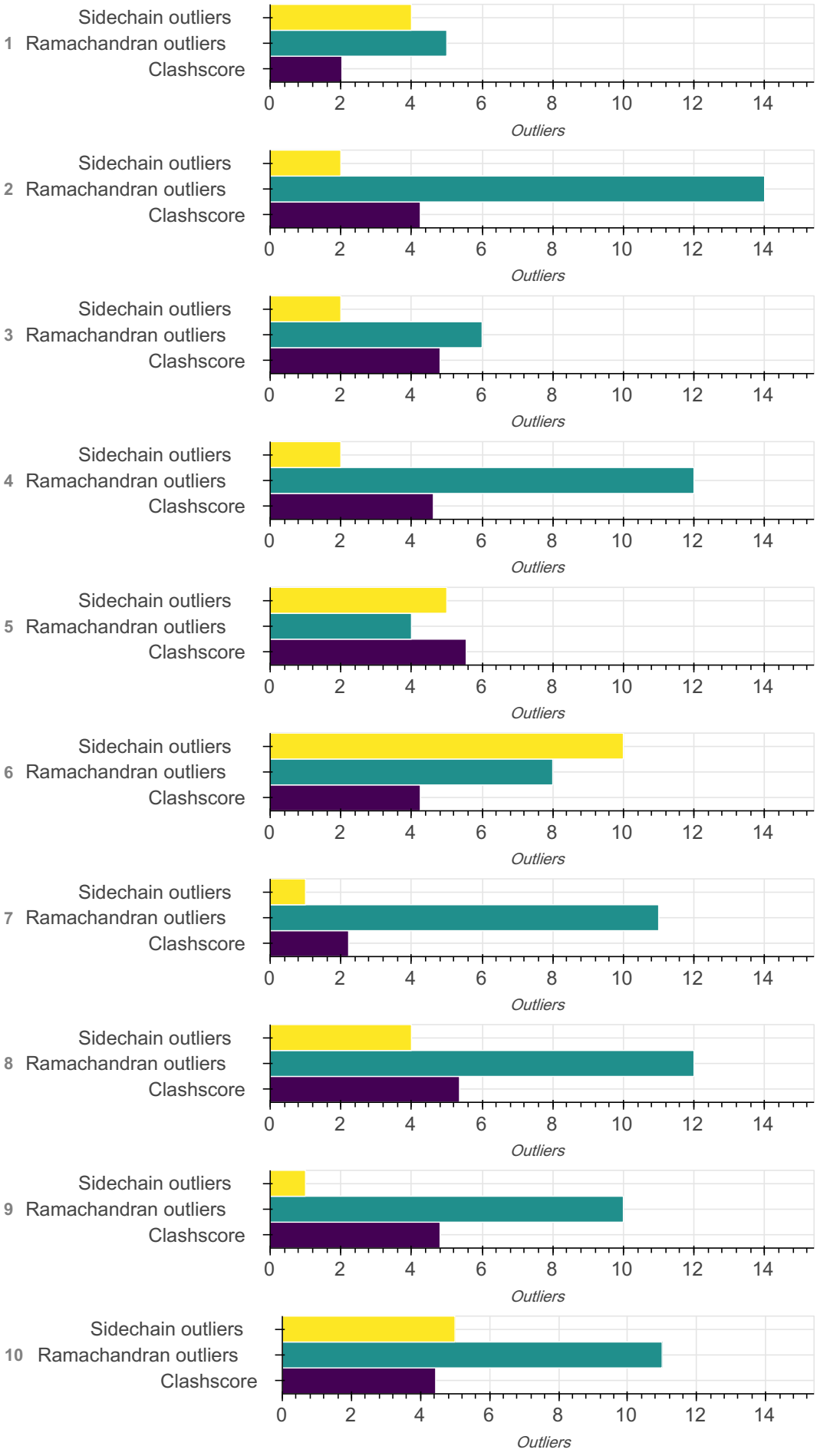
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	P02931	A	A	362
2	1	1	P02931	A	A	362
3	1	1	P02931	A	A	362
4	1	1	P02931	A	A	362
5	1	1	P02931	A	A	362
6	1	1	P02931	A	A	362
7	1	1	P02931	A	A	362
8	1	1	P02931	A	A	362
9	1	1	P02931	A	A	362
10	1	1	P02931	A	A	362

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	-	1-362

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 26240 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
CB--HB3	1.09	0.97	2510
CB--HB2	1.09	0.97	2510
CG--HG3	1.09	0.97	680
CD1--HD11	1.09	0.97	370
CD1--HD12	1.09	0.97	370
CA--HA	1.09	0.97	3130
CB--HB	1.09	0.97	620
NZ--HZ3	1.01	0.89	190
CG2--HG23	1.09	0.97	620
NZ--HZ2	1.01	0.89	190
CG2--HG21	1.09	0.97	620
CD--HD2	1.09	0.97	360
CG--HG	1.09	0.97	230
CB--HB1	1.09	0.97	340
CG--HG2	1.09	0.97	680
CA--HA3	1.09	0.97	490
OH--HH	0.96	0.84	290
CD2--HD22	1.09	0.97	230
CG1--HG11	1.09	0.97	260
CG2--HG22	1.09	0.97	620
CA--HA2	1.09	0.97	490
CE--HE2	1.09	0.97	240

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD13	1.09	0.97	370
CD2--HD21	1.09	0.97	230
CE--HE3	1.09	0.97	240
NZ--HZ1	1.01	0.89	190
CG1--HG13	1.09	0.97	400
CD2--HD23	1.09	0.97	230
OG--HG	0.96	0.84	160
CD--HD3	1.09	0.97	360
CG1--HG12	1.09	0.97	400
OG1--HG1	0.96	0.84	220
CE--HE1	1.09	0.97	50
N--H2	1.01	0.89	10
N--H1	1.01	0.89	10
N--H3	1.01	0.89	10
CE2--HE2	1.08	0.93	480
N--H	1.01	0.86	3560
CD2--HD2	1.08	0.93	490
CD1--HD1	1.08	0.93	500
CE1--HE1	1.08	0.93	490
ND2--HD21	1.01	0.86	320
ND2--HD22	1.01	0.86	320
NH2--HH21	1.01	0.86	120
NH1--HH11	1.01	0.86	120

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE22	1.01	0.86	130
NH2--HH22	1.01	0.86	120
NE--HE	1.01	0.86	120
CZ--HZ	1.08	0.93	190
NE1--HE1	1.01	0.86	20
NH1--HH12	1.01	0.86	120
NE2--HE21	1.01	0.86	130
CH2--HH2	1.08	0.93	20
CZ3--HZ3	1.08	0.93	20
CZ2--HZ2	1.08	0.93	20
CE3--HE3	1.08	0.93	20
ND1--HD1	1.01	0.86	10

Standard geometry: angle outliers

There are 195 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	138.88	1
CA-CB-CG	114.10	130.39	1
C-N-CA	121.70	135.06	1
N-CA-CB	110.40	99.82	1
CA-CB-CG	112.60	119.42	1
OD1-CG-ND2	122.60	115.82	1
CA-CB-OG1	109.60	99.64	1
C-N-CA	121.70	133.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	121.68	1
OE1-CD-NE2	122.60	116.05	1
C-N-CA	121.70	132.84	1
CA-CB-CG2	110.40	120.72	1
C-N-CA	121.70	132.58	1
OE1-CD-NE2	122.60	116.62	1
C-N-CA	121.70	132.42	1
OE1-CD-NE2	122.60	116.75	1
OE1-CD-NE2	122.60	116.82	1
C-CA-CB	110.10	120.87	1
C-N-CA	121.70	131.91	1
OE1-CD-NE2	122.60	116.93	1
OD1-CG-ND2	122.60	116.98	1
C-N-CA	121.70	131.69	1
C-N-CA	121.70	131.64	1
CA-CB-CG	112.60	118.12	1
OE1-CD-NE2	122.60	117.11	1
CA-CB-CG	112.60	118.06	1
OE1-CD-NE2	122.60	117.21	1
C-N-CA	121.70	131.30	1
CA-CB-CG	112.60	117.92	1
CA-CB-CG	112.60	117.91	2
OE1-CD-NE2	122.60	117.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	101.59	1
C-CA-CB	110.50	118.36	1
CA-CB-CG	112.60	117.83	1
OE1-CD-NE2	122.60	117.38	1
CA-CB-CG2	110.50	119.38	1
OE1-CD-NE2	122.60	117.41	1
OE1-CD-NE2	122.60	117.45	1
CA-CB-CG	112.60	117.74	1
OE1-CD-NE2	122.60	117.47	1
C-N-CA	121.70	130.88	1
C-N-CA	121.70	130.85	1
OE1-CD-NE2	122.60	117.52	1
CA-C-N	116.20	126.35	1
C-N-CA	121.70	130.81	1
OE1-CD-NE2	122.60	117.54	1
C-N-CA	121.70	130.75	1
CA-CB-CG	112.60	107.58	1
OE1-CD-NE2	122.60	117.59	1
CD-NE-CZ	124.40	131.40	1
CA-CB-CG	112.60	107.62	1
C-N-CA	121.70	130.58	1
OE1-CD-NE2	122.60	117.68	2
OE1-CD-NE2	122.60	117.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.71	3
OE1-CD-NE2	122.60	117.73	1
N-CA-C	111.00	124.64	1
C-N-CA	121.70	130.46	1
O-C-N	123.00	115.22	1
OD1-CG-ND2	122.60	117.74	1
C-N-CA	121.70	130.41	1
OE1-CD-NE2	122.60	117.76	1
OE1-CD-NE2	122.60	117.77	1
OD1-CG-ND2	122.60	117.78	1
CA-CB-CG	112.60	117.41	1
CA-CB-CG	112.60	117.39	1
OE1-CD-NE2	122.60	117.81	1
OD1-CG-ND2	122.60	117.81	1
NE-CZ-NH2	119.20	123.50	1
OE1-CD-NE2	122.60	117.82	1
C-N-CA	121.70	130.29	1
C-CA-CB	110.50	117.64	1
CA-CB-CG	112.60	117.36	2
C-N-CA	121.70	130.25	1
NE-CZ-NH2	119.20	123.46	1
OD1-CG-ND2	122.60	117.87	1
C-N-CA	121.70	130.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	124.17	1
OE1-CD-NE2	122.60	117.90	1
OE1-CD-NE2	122.60	117.91	1
NE-CZ-NH2	119.20	123.41	1
OE1-CD-NE2	122.60	117.94	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	1
OD1-CG-ND2	122.60	117.99	1
OE1-CD-NE2	122.60	117.99	1
OD1-CG-ND2	122.60	118.00	1
C-N-CA	121.70	129.97	2
OD1-CG-ND2	122.60	118.01	1
NE-CZ-NH2	119.20	123.33	1
N-CA-CB	110.50	102.70	1
OE1-CD-NE2	122.60	118.03	1
OD1-CG-ND2	122.60	118.03	1
NE-CZ-NH2	119.20	123.30	1
CA-CB-CG2	110.50	118.23	1
CA-CB-CG	112.60	117.13	1
C-N-CA	121.70	129.86	1
OD1-CG-ND2	122.60	118.08	1
C-N-CA	121.70	129.82	1
CA-C-N	116.20	125.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.81	1
OE1-CD-NE2	122.60	118.13	1
CA-CB-CG	112.60	108.14	1
OE1-CD-NE2	122.60	118.16	1
CA-CB-CG	112.60	117.03	1
C-CA-CB	110.10	101.69	1
OE1-CD-NE2	122.60	118.18	1
OD1-CG-ND2	122.60	118.18	1
CA-CB-CG	112.60	117.01	2
CG-CD-CE	111.30	101.16	1
OE1-CD-NE2	122.60	118.22	2
CA-CB-CG	112.60	108.23	1
OE1-CD-NE2	122.60	118.23	1
OE1-CD-NE2	122.60	118.24	1
OE1-CD-NE2	122.60	118.25	1
C-N-CA	121.70	129.53	1
C-N-CA	121.70	129.52	1
OE1-CD-NE2	122.60	118.27	1
OD1-CG-ND2	122.60	118.28	1
C-N-CA	121.70	129.46	1
OE1-CD-NE2	122.60	118.29	2
C-N-CA	121.70	129.45	1
NE-CZ-NH1	121.50	125.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.31	1
C-CA-CB	110.10	118.22	1
OE1-CD-NE2	122.60	118.33	1
CA-C-N	116.20	124.72	1
C-N-CA	121.70	129.36	1
OD1-CG-ND2	122.60	118.34	1
CA-CB-CG	113.80	109.55	1
OD1-CG-ND2	122.60	118.36	3
CA-CB-CG1	110.40	117.60	1
OE1-CD-NE2	122.60	118.37	1
C-N-CA	121.70	129.30	1
C-N-CA	121.70	129.28	1
OE1-CD-NE2	122.60	118.40	2
OD1-CG-ND2	122.60	118.40	1
OE1-CD-NE2	122.60	118.41	1
OD1-CG-ND2	122.60	118.41	1
OD1-CG-ND2	122.60	118.42	1
OD1-CG-ND2	122.60	118.43	2
NH1-CZ-NH2	119.30	113.88	1
CA-CB-CG1	110.40	117.49	1
OE1-CD-NE2	122.60	118.44	1
N-CA-C	111.00	122.64	1
OD1-CG-ND2	122.60	118.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.47	1
NE-CZ-NH2	119.20	122.92	1
OD1-CG-ND2	122.60	118.47	2
N-CA-CB	110.40	104.21	1
N-CA-C	111.00	122.53	1
CA-C-N	116.20	124.43	1
OE1-CD-NE2	122.60	118.49	1
OD1-CG-ND2	122.60	118.50	1
NE-CZ-NH2	119.20	122.88	1
OE1-CD-NE2	122.60	118.51	1
OD1-CG-ND2	122.60	118.51	1
OE1-CD-NE2	122.60	118.52	1
NE-CZ-NH2	119.20	122.87	1
OE1-CD-NE2	122.60	118.53	1
OD1-CG-ND2	122.60	118.54	1
OE1-CD-NE2	122.60	118.55	1
OD1-CG-ND2	122.60	118.55	1
OE1-CD-NE2	122.60	118.57	1
OD1-CG-ND2	122.60	118.57	1
NH1-CZ-NH2	119.30	114.07	1
C-N-CA	121.70	128.93	2
OD1-CG-ND2	122.60	118.59	1
OE1-CD-NE2	122.60	118.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CZ-NH1-HH11	107.82	120.00	1
C-N-H	111.78	124.30	1
C-CA-HA	96.28	109.00	1
C-N-H	111.51	124.30	1
C-N-H	111.35	124.30	1
HZ1-NZ-HZ3	95.89	109.00	1
HH21-NH2-HH22	106.11	120.00	1
HH21-NH2-HH22	105.48	120.00	1
C-N-H	109.62	124.30	1
C-N-H	108.43	124.30	1
C-N-H	106.99	124.30	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	2.03	11
2	4.25	23
3	4.81	26
4	4.62	25
5	5.55	30
6	4.25	23
7	2.22	12
8	5.36	29

Model ID	Clash score	Number of clashes
9	4.81	26
10	4.44	24

All 229 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:42:LEU:HD23	A:332:TYR:OH	0.705
1	A:166:PHE:CE1	A:167:PHE:CZ	0.582
1	A:163:ASN:HD22	A:172:GLY:HA3	0.518
1	A:150:PHE:CZ	A:233:ALA:HB3	0.479
1	A:136:MET:HG3	A:248:TYR:CZ	0.466
1	A:342:SER:HA	A:349:GLY:CA	0.436
1	A:67:PHE:CE1	A:83:TRP:CE3	0.431
1	A:130:ALA:HA	A:210:VAL:HG11	0.428
1	A:38:LYS:HE2	A:40:VAL:CG2	0.421
1	A:140:PHE:CE1	A:334:ASP:HB2	0.405
1	A:236:TRP:CH2	A:253:TYR:CE1	0.400
2	A:151:PHE:O	A:155:VAL:HG22	0.651
2	A:21:ASN:HD21	A:327:LYS:HE3	0.644
2	A:134:THR:HG22	A:250:ALA:HB1	0.587
2	A:21:ASN:HD21	A:327:LYS:CE	0.542
2	A:42:LEU:HD11	A:355:ALA:HB1	0.530
2	A:85:TYR:CE1	A:101:ASN:HB3	0.528
2	A:105:LEU:HD11	A:124:TYR:CZ	0.528
2	A:125:GLY:HA2	A:178:GLN:HE22	0.525

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:35:LEU:HD11	A:65:LEU:HD11	0.507
2	A:21:ASN:ND2	A:328:ASN:HD21	0.499
2	A:311:VAL:HG11	A:346:LEU:HB2	0.494
2	A:35:LEU:HD13	A:67:PHE:CE1	0.493
2	A:77:LEU:HD13	A:112:TYR:CZ	0.488
2	A:134:THR:HG23	A:252:ASN:ND2	0.487
2	A:134:THR:HG22	A:250:ALA:CB	0.466
2	A:150:PHE:CZ	A:154:ARG:NH1	0.459
2	A:191:SER:HB3	A:219:THR:HG21	0.450
2	A:68:LYS:HE3	A:167:PHE:CZ	0.440
2	A:42:LEU:HD13	A:332:TYR:OH	0.435
2	A:21:ASN:O	A:22:ALA:C	0.434
2	A:35:LEU:HD12	A:66:GLY:O	0.427
2	A:68:LYS:HE3	A:167:PHE:CE2	0.405
2	A:139:GLU:HG2	A:332:TYR:CG	0.402
3	A:162:ARG:HH12	A:176:ALA:HB2	0.802
3	A:137:LEU:HD11	A:296:ALA:CB	0.714
3	A:227:LEU:HD12	A:271:GLY:HA3	0.685
3	A:140:PHE:CE2	A:355:ALA:HB2	0.575
3	A:137:LEU:HD11	A:296:ALA:HB3	0.570
3	A:107:PHE:CE2	A:167:PHE:CE1	0.543
3	A:60:MET:HE1	A:144:THR:HA	0.533
3	A:150:PHE:CE2	A:261:PRO:HD2	0.508

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:162:ARG:NH1	A:176:ALA:HB2	0.493
3	A:311:VAL:HG11	A:346:LEU:HD11	0.493
3	A:107:PHE:CZ	A:167:PHE:CZ	0.491
3	A:227:LEU:HD12	A:271:GLY:CA	0.491
3	A:137:LEU:HD11	A:296:ALA:HB2	0.489
3	A:262:ILE:HD11	A:273:ALA:HB2	0.487
3	A:137:LEU:HD13	A:318:GLU:CD	0.485
3	A:126:VAL:HG21	A:198:GLY:C	0.484
3	A:233:ALA:HB1	A:259:ALA:HB2	0.476
3	A:17:ALA:HB1	A:361:GLN:HE22	0.472
3	A:42:LEU:HD11	A:355:ALA:HB1	0.463
3	A:260:THR:HB	A:273:ALA:HB3	0.463
3	A:155:VAL:CG2	A:160:THR:HG22	0.449
3	A:150:PHE:CZ	A:260:THR:HG23	0.437
3	A:138:PRO:HB2	A:332:TYR:CD2	0.414
3	A:145:ALA:O	A:149:ASP:HB2	0.410
3	A:148:ASP:O	A:152:VAL:N	0.405
3	A:35:LEU:HD12	A:66:GLY:O	0.403
4	A:155:VAL:HG22	A:189:ARG:CZ	0.822
4	A:154:ARG:HH12	A:256:THR:HG21	0.727
4	A:131:LEU:HD21	A:155:VAL:HG21	0.692
4	A:131:LEU:CD2	A:155:VAL:HG21	0.630
4	A:155:VAL:HG22	A:189:ARG:NE	0.588

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:154:ARG:NH1	A:256:THR:HG21	0.562
4	A:155:VAL:HA	A:189:ARG:NH2	0.538
4	A:265:LYS:HE3	A:266:PHE:CZ	0.519
4	A:132:GLY:C	A:134:THR:H	0.505
4	A:155:VAL:HG13	A:189:ARG:NH2	0.495
4	A:53:SER:C	A:55:GLY:H	0.492
4	A:154:ARG:HH12	A:256:THR:CG2	0.481
4	A:158:VAL:HG22	A:300:SER:HB2	0.474
4	A:264:ASN:HB2	A:308:ILE:HD11	0.473
4	A:158:VAL:HG21	A:298:THR:CG2	0.464
4	A:335:TYR:CD2	A:354:VAL:HG22	0.463
4	A:32:LYS:HE2	A:34:ASP:OD1	0.444
4	A:155:VAL:HG13	A:189:ARG:HH22	0.435
4	A:124:TYR:CD1	A:149:ASP:HA	0.423
4	A:131:LEU:HG	A:155:VAL:HB	0.423
4	A:158:VAL:HG13	A:278:ASP:HB3	0.421
4	A:53:SER:HB3	A:134:THR:HG21	0.405
4	A:83:TRP:CH2	A:85:TYR:HB2	0.405
4	A:180:LEU:HG	A:192:ASN:HD21	0.401
4	A:150:PHE:CE1	A:235:GLN:NE2	0.400
5	A:15:LEU:HD21	A:68:LYS:HZ3	0.844
5	A:10:ILE:HG21	A:292:ARG:HH22	0.828
5	A:15:LEU:HD13	A:167:PHE:HB3	0.765

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:15:LEU:HD21	A:68:LYS:NZ	0.680
5	A:68:LYS:HE3	A:167:PHE:CE2	0.620
5	A:8:ALA:O	A:9:VAL:HG23	0.583
5	A:15:LEU:CD2	A:68:LYS:HZ3	0.575
5	A:60:MET:HE1	A:143:ASP:O	0.568
5	A:10:ILE:HD11	A:286:GLN:HG2	0.539
5	A:60:MET:HE1	A:143:ASP:C	0.486
5	A:38:LYS:HE2	A:40:VAL:CG2	0.481
5	A:35:LEU:HD13	A:67:PHE:CE1	0.470
5	A:105:LEU:HD21	A:124:TYR:CE2	0.466
5	A:130:ALA:HA	A:210:VAL:HG11	0.461
5	A:138:PRO:HG2	A:332:TYR:CE2	0.447
5	A:122:ARG:CZ	A:162:ARG:NH2	0.446
5	A:262:ILE:HD11	A:273:ALA:HB2	0.444
5	A:264:ASN:HB2	A:308:ILE:HD11	0.435
5	A:183:ASN:O	A:189:ARG:HG3	0.434
5	A:10:ILE:HD13	A:292:ARG:NH2	0.432
5	A:16:VAL:C	A:18:GLY:H	0.427
5	A:222:GLN:HA	A:272:PHE:CE2	0.427
5	A:9:VAL:HG11	A:169:LEU:HD11	0.424
5	A:148:ASP:HB3	A:152:VAL:CG2	0.424
5	A:15:LEU:HD13	A:167:PHE:CB	0.422
5	A:160:THR:HG21	A:162:ARG:NH2	0.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:225:GLN:HB3	A:271:GLY:HA2	0.415
5	A:218:ARG:HE	A:222:GLN:HB3	0.414
5	A:173:LEU:HD21	A:175:PHE:CZ	0.405
5	A:178:GLN:NE2	A:180:LEU:HD21	0.404
6	A:128:TYR:CZ	A:147:SER:HB3	0.639
6	A:112:TYR:CE2	A:326:ASN:HB3	0.616
6	A:128:TYR:CE2	A:147:SER:HB3	0.615
6	A:262:ILE:HD11	A:306:GLU:OE2	0.604
6	A:128:TYR:CZ	A:147:SER:CB	0.587
6	A:317:PHE:CZ	A:319:VAL:HG21	0.587
6	A:128:TYR:CE1	A:147:SER:N	0.584
6	A:7:LEU:HD13	A:33:VAL:HG21	0.545
6	A:236:TRP:CH2	A:253:TYR:CE1	0.545
6	A:274:ASN:ND2	A:313:LEU:HD12	0.507
6	A:302:ALA:HB2	A:314:VAL:HG22	0.502
6	A:230:GLY:HA2	A:260:THR:HA	0.486
6	A:112:TYR:CD2	A:326:ASN:HB3	0.453
6	A:112:TYR:CD2	A:326:ASN:CG	0.451
6	A:317:PHE:CE1	A:319:VAL:CG2	0.449
6	A:112:TYR:CE2	A:326:ASN:CB	0.447
6	A:173:LEU:HD21	A:175:PHE:CZ	0.429
6	A:274:ASN:ND2	A:313:LEU:CD1	0.428
6	A:236:TRP:CE2	A:255:GLU:HB3	0.427

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:228:GLY:C	A:230:GLY:H	0.422
6	A:128:TYR:CZ	A:147:SER:N	0.418
6	A:317:PHE:CE1	A:319:VAL:HG21	0.413
6	A:128:TYR:CE1	A:144:THR:OG1	0.407
7	A:151:PHE:CE1	A:280:LEU:HD11	0.660
7	A:127:VAL:HG21	A:235:GLN:HG3	0.575
7	A:140:PHE:CZ	A:280:LEU:CD2	0.570
7	A:155:VAL:HG12	A:180:LEU:HD13	0.561
7	A:151:PHE:HE1	A:280:LEU:HD11	0.546
7	A:42:LEU:HD11	A:355:ALA:HB1	0.520
7	A:151:PHE:CE1	A:278:ASP:HB3	0.491
7	A:154:ARG:NH2	A:189:ARG:HA	0.490
7	A:140:PHE:CZ	A:280:LEU:HD23	0.443
7	A:34:ASP:OD2	A:68:LYS:HE3	0.441
7	A:135:ASP:OD1	A:141:GLY:HA2	0.434
7	A:130:ALA:HA	A:210:VAL:HG11	0.401
8	A:291:LEU:HD12	A:361:GLN:O	0.671
8	A:136:MET:HE1	A:294:SER:CB	0.609
8	A:42:LEU:HD13	A:62:TYR:CE2	0.605
8	A:42:LEU:HD21	A:143:ASP:H	0.529
8	A:326:ASN:HD22	A:359:VAL:HG22	0.528
8	A:326:ASN:HD22	A:359:VAL:CG2	0.518
8	A:225:GLN:OE1	A:316:TYR:CD1	0.496

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:41:GLY:HA3	A:327:LYS:HE3	0.478
8	A:326:ASN:ND2	A:359:VAL:HG13	0.476
8	A:329:MET:HE3	A:357:GLY:HA3	0.474
8	A:62:TYR:CD1	A:86:ASN:ND2	0.469
8	A:42:LEU:CD2	A:143:ASP:H	0.464
8	A:60:MET:HE3	A:88:GLN:NE2	0.459
8	A:227:LEU:CD1	A:313:LEU:HD21	0.456
8	A:150:PHE:CE2	A:180:LEU:HB2	0.453
8	A:35:LEU:HD13	A:67:PHE:CE1	0.452
8	A:140:PHE:HB3	A:326:ASN:HA	0.452
8	A:35:LEU:HD11	A:65:LEU:HD11	0.442
8	A:298:THR:HG22	A:325:PHE:CZ	0.440
8	A:299:LYS:HE2	A:301:LYS:HE3	0.440
8	A:180:LEU:HD21	A:192:ASN:HB3	0.438
8	A:315:ASN:O	A:316:TYR:CD1	0.433
8	A:329:MET:SD	A:359:VAL:HG23	0.433
8	A:150:PHE:CD2	A:180:LEU:HB2	0.422
8	A:15:LEU:HD12	A:328:ASN:HD21	0.421
8	A:32:LYS:HE3	A:34:ASP:OD1	0.417
8	A:299:LYS:HE2	A:301:LYS:CE	0.416
8	A:218:ARG:NH2	A:228:GLY:HA3	0.408
8	A:44:TYR:CE2	A:60:MET:SD	0.402
9	A:262:ILE:HD11	A:305:VAL:HG13	0.729

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:311:VAL:HG11	A:346:LEU:HB2	0.703
9	A:191:SER:HB3	A:219:THR:HG21	0.649
9	A:60:MET:HE3	A:88:GLN:NE2	0.640
9	A:180:LEU:HD21	A:192:ASN:ND2	0.630
9	A:35:LEU:HD13	A:67:PHE:CE1	0.614
9	A:47:LYS:HE3	A:58:GLY:H	0.561
9	A:42:LEU:HD12	A:62:TYR:CE2	0.554
9	A:60:MET:HG2	A:90:ASN:HD21	0.552
9	A:265:LYS:HZ2	A:348:VAL:HA	0.531
9	A:150:PHE:CZ	A:233:ALA:HB1	0.530
9	A:155:VAL:HG11	A:180:LEU:HD11	0.511
9	A:338:ASN:ND2	A:350:SER:H	0.499
9	A:311:VAL:HG21	A:346:LEU:HD12	0.492
9	A:45:PHE:CZ	A:336:ILE:CD1	0.490
9	A:160:THR:HG21	A:162:ARG:NH1	0.490
9	A:46:SER:HA	A:348:VAL:CG1	0.476
9	A:42:LEU:HD11	A:143:ASP:HB3	0.463
9	A:45:PHE:CZ	A:336:ILE:HD12	0.459
9	A:266:PHE:CE2	A:345:LYS:HA	0.455
9	A:44:TYR:CE2	A:60:MET:SD	0.431
9	A:42:LEU:HD12	A:62:TYR:HE2	0.421
9	A:182:LYS:HE2	A:184:GLU:HG3	0.421
9	A:21:ASN:CG	A:328:ASN:ND2	0.420

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:42:LEU:HD11	A:143:ASP:CB	0.409
9	A:314:VAL:HA	A:340:ILE:HD11	0.404
10	A:151:PHE:CE2	A:212:ALA:HB1	0.734
10	A:136:MET:HE1	A:321:ALA:HB3	0.669
10	A:154:ARG:NH1	A:256:THR:HG22	0.636
10	A:165:ASN:HB3	A:167:PHE:CZ	0.613
10	A:329:MET:HE1	A:332:TYR:CZ	0.608
10	A:154:ARG:CZ	A:256:THR:HG22	0.591
10	A:159:ALA:HB3	A:161:TYR:CZ	0.555
10	A:329:MET:CE	A:359:VAL:HG21	0.528
10	A:151:PHE:CZ	A:212:ALA:HB1	0.522
10	A:126:VAL:HG11	A:128:TYR:CE2	0.520
10	A:154:ARG:CZ	A:235:GLN:HB2	0.516
10	A:188:ALA:CB	A:221:LEU:HD22	0.510
10	A:154:ARG:NH1	A:235:GLN:HB3	0.495
10	A:159:ALA:CB	A:161:TYR:CZ	0.474
10	A:154:ARG:NH1	A:235:GLN:CB	0.466
10	A:188:ALA:HB1	A:221:LEU:HD22	0.462
10	A:149:ASP:CG	A:167:PHE:CZ	0.455
10	A:227:LEU:HD22	A:308:ILE:HD13	0.455
10	A:165:ASN:CB	A:167:PHE:CZ	0.449
10	A:218:ARG:HE	A:222:GLN:HB3	0.447
10	A:313:LEU:HB3	A:316:TYR:CE2	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:236:TRP:CH2	A:253:TYR:CE1	0.420
10	A:329:MET:CE	A:332:TYR:CE2	0.420
10	A:32:LYS:HE3	A:34:ASP:OD1	0.412

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	360	335	20	5
2	360	317	29	14
3	360	322	32	6
4	360	317	31	12
5	360	329	27	4
6	360	327	25	8
7	360	317	32	11
8	360	321	27	12
9	360	319	31	10
10	360	313	36	11

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	279	267	8	4
2	279	267	10	2
3	279	271	6	2

Model ID	Analyzed	Favored	Allowed	Outliers
4	279	268	9	2
5	279	270	4	5
6	279	257	12	10
7	279	273	5	1
8	279	261	14	4
9	279	272	6	1
10	279	261	13	5

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	MET
1	A	166	PHE
1	A	344	ASN
1	A	350	SER
2	A	144	THR
2	A	155	VAL
3	A	92	SER
3	A	155	VAL
4	A	117	SER
4	A	170	VAL
5	A	11	VAL
5	A	15	LEU
5	A	27	ASN
5	A	164	SER

Model ID	Chain	Residue ID	Residue type
5	A	269	THR
6	A	77	LEU
6	A	78	THR
6	A	105	LEU
6	A	115	VAL
6	A	144	THR
6	A	187	THR
6	A	269	THR
6	A	308	ILE
6	A	313	LEU
6	A	330	SER
7	A	92	SER
8	A	152	VAL
8	A	260	THR
8	A	319	VAL
8	A	331	THR
9	A	136	MET
10	A	92	SER
10	A	126	VAL
10	A	134	THR
10	A	151	PHE
10	A	155	VAL

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.

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