Integrative Structure Validation Report

July 22, 2024 - 05:01 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	9A2L
PDB-Dev ID	PDBDEV_00000170
Structure Title	Model of E. coli TolB 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

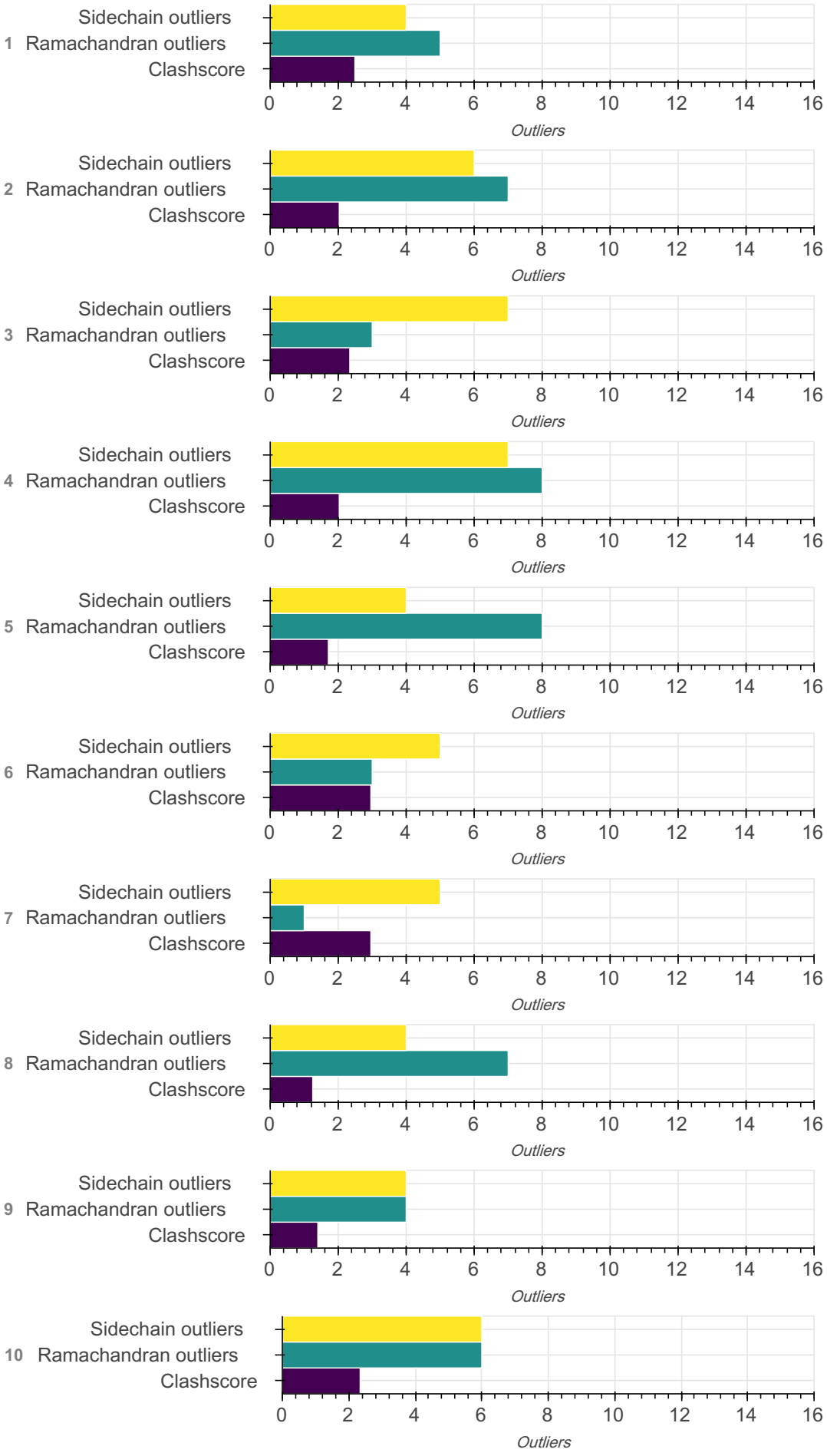
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 16
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
6
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
7
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0 2 4 6 8 10 12 14 16
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	P0A855	A	A	430
2	1	1	P0A855	A	A	430
3	1	1	P0A855	A	A	430
4	1	1	P0A855	A	A	430
5	1	1	P0A855	A	A	430
6	1	1	P0A855	A	A	430
7	1	1	P0A855	A	A	430
8	1	1	P0A855	A	A	430
9	1	1	P0A855	A	A	430
10	1	1	P0A855	A	A	430

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	-	1-430

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 31680 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
CG1--HG13	1.09	0.97	550
CA--HA	1.09	0.97	3860
OG--HG	0.96	0.84	390
CB--HB3	1.09	0.97	3100
CG--HG	1.09	0.97	310
NZ--HZ1	1.01	0.89	140
CG1--HG12	1.09	0.97	550
CG2--HG23	1.09	0.97	760
CB--HB	1.09	0.97	760
CA--HA3	1.09	0.97	440
OG1--HG1	0.96	0.84	210
CG2--HG22	1.09	0.97	760
CD1--HD11	1.09	0.97	460
CB--HB2	1.09	0.97	3100
CD1--HD13	1.09	0.97	460
OH--HH	0.96	0.84	130
CD1--HD12	1.09	0.97	460
NZ--HZ2	1.01	0.89	140
NZ--HZ3	1.01	0.89	140
CG2--HG21	1.09	0.97	760
CD--HD3	1.09	0.97	620
CD2--HD23	1.09	0.97	310

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD--HD2	1.09	0.97	620
CG1--HG11	1.09	0.97	400
CG--HG2	1.09	0.97	1090
CE--HE2	1.09	0.97	210
CG--HG3	1.09	0.97	1090
CA--HA2	1.09	0.97	440
CD2--HD21	1.09	0.97	310
CE--HE3	1.09	0.97	210
CB--HB1	1.09	0.97	430
CD2--HD22	1.09	0.97	310
N--H2	1.01	0.89	10
CE--HE1	1.09	0.97	70
N--H1	1.01	0.89	10
N--H3	1.01	0.89	10
N--H	1.01	0.86	4010
CZ--HZ	1.08	0.93	180
CD2--HD2	1.08	0.93	360
NH2--HH22	1.01	0.86	200
NH1--HH12	1.01	0.86	200
NH1--HH11	1.01	0.86	200
CD1--HD1	1.08	0.93	390
NH2--HH21	1.01	0.86	200
CZ3--HZ3	1.08	0.93	80

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--HE2	1.01	0.86	11
ND2--HD22	1.01	0.86	200
NE2--HE21	1.01	0.86	300
CE1--HE1	1.08	0.93	360
NE2--HE22	1.01	0.86	300
ND2--HD21	1.01	0.86	200
CZ2--HZ2	1.08	0.93	80
CE2--HE2	1.08	0.93	310
NE--HE	1.01	0.86	200
CH2--HH2	1.08	0.93	80
ND1--HD1	1.01	0.86	39
NE1--HE1	1.01	0.86	80
CE3--HE3	1.08	0.93	80

Standard geometry: angle outliers

There are 181 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	133.83	1
OE1-CD-NE2	122.60	115.86	1
OE1-CD-NE2	122.60	116.10	1
OE1-CD-NE2	122.60	116.37	1
C-N-CA	121.70	132.80	1
OE1-CD-NE2	122.60	116.47	1
OE1-CD-NE2	122.60	116.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.84	1
C-N-CA	121.70	131.94	1
OE1-CD-NE2	122.60	116.92	1
OE1-CD-NE2	122.60	117.08	1
OE1-CD-NE2	122.60	117.11	1
CA-CB-CG2	110.50	119.77	1
OE1-CD-NE2	122.60	117.18	1
C-N-CA	121.70	131.25	1
OE1-CD-NE2	122.60	117.43	1
OE1-CD-NE2	122.60	117.48	1
OE1-CD-NE2	122.60	117.52	2
OE1-CD-NE2	122.60	117.53	1
C-N-CA	121.70	130.67	1
C-N-CA	121.70	130.61	1
OD1-CG-ND2	122.60	117.66	2
OE1-CD-NE2	122.60	117.67	1
OE1-CD-NE2	122.60	117.71	1
OE1-CD-NE2	122.60	117.72	1
OE1-CD-NE2	122.60	117.73	1
OE1-CD-NE2	122.60	117.74	1
CD-NE-CZ	124.40	131.20	1
OE1-CD-NE2	122.60	117.78	1
OE1-CD-NE2	122.60	117.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.82	1
OE1-CD-NE2	122.60	117.83	2
OE1-CD-NE2	122.60	117.84	1
OE1-CD-NE2	122.60	117.89	1
OE1-CD-NE2	122.60	117.91	1
N-CA-CB	111.50	103.53	1
OE1-CD-NE2	122.60	117.93	4
C-N-CA	121.70	130.10	1
OE1-CD-NE2	122.60	117.94	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
N-CA-CB	110.50	102.71	1
OE1-CD-NE2	122.60	118.02	1
OE1-CD-NE2	122.60	118.03	1
OE1-CD-NE2	122.60	118.04	1
CB-CG-CD2	131.20	125.28	1
OE1-CD-NE2	122.60	118.06	1
OE1-CD-NE2	122.60	118.08	2
OE1-CD-NE2	122.60	118.09	3
OE1-CD-NE2	122.60	118.12	1
OE1-CD-NE2	122.60	118.14	1
OE1-CD-NE2	122.60	118.15	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.16	2
OE1-CD-NE2	122.60	118.17	2
CD-NE-CZ	124.40	130.59	1
OD1-CG-ND2	122.60	118.19	1
OE1-CD-NE2	122.60	118.19	1
OE1-CD-NE2	122.60	118.20	1
OE1-CD-NE2	122.60	118.21	1
OE1-CD-NE2	122.60	118.22	3
OE1-CD-NE2	122.60	118.23	1
OE1-CD-NE2	122.60	118.24	1
OE1-CD-NE2	122.60	118.25	2
OD1-CG-ND2	122.60	118.26	3
OE1-CD-NE2	122.60	118.26	4
OE1-CD-NE2	122.60	118.27	3
OD1-CG-ND2	122.60	118.27	1
OE1-CD-NE2	122.60	118.28	4
OE1-CD-NE2	122.60	118.29	3
OE1-CD-NE2	122.60	118.30	2
N-CA-CB	103.00	107.73	1
CB-CG-CD2	131.20	125.62	1
OE1-CD-NE2	122.60	118.31	1
OE1-CD-NE2	122.60	118.32	3
OE1-CD-NE2	122.60	118.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.34	1
NH1-CZ-NH2	119.30	113.78	1
OD1-CG-ND2	122.60	118.36	1
OE1-CD-NE2	122.60	118.36	1
OE1-CD-NE2	122.60	118.37	6
OD1-CG-ND2	122.60	118.37	1
OD1-CG-ND2	122.60	118.38	1
OE1-CD-NE2	122.60	118.38	1
OE1-CD-NE2	122.60	118.39	1
NH1-CZ-NH2	119.30	113.83	1
OE1-CD-NE2	122.60	118.40	3
OD1-CG-ND2	122.60	118.40	1
NH1-CZ-NH2	119.30	113.85	1
CB-CG-CD2	131.20	125.75	1
OE1-CD-NE2	122.60	118.41	2
C-N-CA	121.70	129.23	1
CA-CB-OG1	109.60	103.33	1
CA-CB-CG	112.60	116.78	1
OE1-CD-NE2	122.60	118.42	1
C-N-CA	121.70	129.20	1
OE1-CD-NE2	122.60	118.43	2
OE1-CD-NE2	122.60	118.44	3
OE1-CD-NE2	122.60	118.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.46	2
CB-CG-CD2	131.20	125.81	1
CB-CG-CD2	131.20	125.83	1
OE1-CD-NE2	122.60	118.47	1
OD1-CG-ND2	122.60	118.48	1
OE1-CD-NE2	122.60	118.49	2
CB-CG-CD2	131.20	125.86	1
OE1-CD-NE2	122.60	118.52	1
OE1-CD-NE2	122.60	118.53	2
OE1-CD-NE2	122.60	118.54	2
CB-CG-CD2	131.20	125.93	1
OD1-CG-ND2	122.60	118.55	1
NH1-CZ-NH2	119.30	114.03	1
OE1-CD-NE2	122.60	118.55	5
OE1-CD-NE2	122.60	118.56	1
C-N-CA	121.70	128.96	1
N-CA-CB	103.00	107.43	1
OE1-CD-NE2	122.60	118.57	2
OE1-CD-NE2	122.60	118.58	3
OE1-CD-NE2	122.60	118.59	2
CZ-NH2-HH22	107.22	120.00	1
C-N-H	108.27	124.30	1
HH21-NH2-HH22	100.24	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HH21-NH2-HH22	97.93	120.00	1
HH21-NH2-HH22	97.14	120.00	1
HH21-NH2-HH22	96.93	120.00	1
HH21-NH2-HH22	96.92	120.00	1
HH21-NH2-HH22	94.53	120.00	1
HH21-NH2-HH22	94.44	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	2.49	16
2	2.03	13
3	2.34	15
4	2.03	13
5	1.71	11
6	2.96	19
7	2.96	19
8	1.25	8
9	1.40	9
10	2.34	15

All 138 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:35:ARG:HH21	A:97:ASP:CG	0.624

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:21:ALA:O	A:417:THR:HG21	0.583
1	A:226:LEU:HD11	A:249:PRO:HB3	0.582
1	A:242:PHE:CD2	A:262:LEU:HD13	0.496
1	A:306:SER:HB3	A:315:TYR:CD2	0.454
1	A:78:GLN:HE21	A:91:TRP:NE1	0.446
1	A:329:TRP:HE1	A:366:GLY:HA3	0.443
1	A:242:PHE:CE1	A:264:LYS:HE2	0.440
1	A:308:GLN:NE2	A:315:TYR:CE1	0.440
1	A:239:VAL:HG13	A:273:MET:SD	0.429
1	A:27:ILE:HG21	A:31:VAL:CG2	0.424
1	A:71:LEU:HD11	A:96:ILE:CD1	0.424
1	A:71:LEU:HD11	A:96:ILE:HD11	0.416
1	A:27:ILE:HG21	A:31:VAL:HG23	0.414
1	A:53:ASP:CG	A:73:ARG:HH22	0.409
1	A:78:GLN:HE22	A:87:GLN:H	0.401
2	A:273:MET:HE2	A:278:GLY:HA2	0.545
2	A:346:MET:HE2	A:361:GLN:NE2	0.537
2	A:242:PHE:CE1	A:264:LYS:HE2	0.520
2	A:78:GLN:HE21	A:91:TRP:NE1	0.493
2	A:239:VAL:HG13	A:273:MET:SD	0.465
2	A:308:GLN:NE2	A:315:TYR:CE1	0.454
2	A:78:GLN:HE22	A:87:GLN:H	0.454
2	A:242:PHE:CD2	A:262:LEU:HD13	0.440

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:78:GLN:HE21	A:91:TRP:CD1	0.431
2	A:78:GLN:HE22	A:87:GLN:N	0.421
2	A:306:SER:HB3	A:315:TYR:CD2	0.416
2	A:25:ILE:CG2	A:412:ALA:HB1	0.415
2	A:35:ARG:HH21	A:97:ASP:CG	0.410
3	A:329:TRP:CH2	A:368:VAL:HG21	0.934
3	A:329:TRP:CZ3	A:368:VAL:HG21	0.926
3	A:23:VAL:HG12	A:414:LEU:HD22	0.579
3	A:281:ARG:HH21	A:319:ILE:HD12	0.547
3	A:27:ILE:HD13	A:31:VAL:HG21	0.521
3	A:242:PHE:CE1	A:264:LYS:HE2	0.515
3	A:53:ASP:CG	A:73:ARG:HH22	0.494
3	A:242:PHE:CE2	A:262:LEU:HD13	0.466
3	A:226:LEU:HD11	A:249:PRO:HB3	0.462
3	A:242:PHE:H	A:246:ASN:HD21	0.453
3	A:329:TRP:CZ3	A:368:VAL:CG2	0.439
3	A:35:ARG:HH21	A:97:ASP:CG	0.429
3	A:306:SER:HB3	A:315:TYR:CD2	0.425
3	A:78:GLN:HE21	A:91:TRP:NE1	0.408
3	A:23:VAL:CG1	A:414:LEU:HB3	0.403
4	A:35:ARG:HH21	A:97:ASP:CG	0.563
4	A:401:LEU:HG	A:421:VAL:HG21	0.533
4	A:78:GLN:HE21	A:91:TRP:CD1	0.518

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:328:THR:HA	A:329:TRP:CE3	0.509
4	A:240:ALA:HB1	A:242:PHE:HE2	0.502
4	A:53:ASP:CG	A:73:ARG:HH22	0.481
4	A:242:PHE:CE1	A:264:LYS:HE2	0.478
4	A:306:SER:HB3	A:315:TYR:CD2	0.468
4	A:78:GLN:HE21	A:91:TRP:NE1	0.457
4	A:226:LEU:HD11	A:249:PRO:HB3	0.436
4	A:308:GLN:NE2	A:315:TYR:CE1	0.408
4	A:242:PHE:CD2	A:262:LEU:HD22	0.403
4	A:410:PHE:CZ	A:412:ALA:HB2	0.402
5	A:355:GLN:HB3	A:374:THR:HG21	0.559
5	A:291:THR:HG23	A:292:GLU:OE2	0.557
5	A:242:PHE:CE1	A:264:LYS:HE2	0.496
5	A:306:SER:HB3	A:315:TYR:CD2	0.464
5	A:53:ASP:CG	A:73:ARG:HH22	0.460
5	A:308:GLN:NE2	A:315:TYR:CE1	0.457
5	A:78:GLN:HE21	A:91:TRP:NE1	0.451
5	A:78:GLN:HE21	A:91:TRP:CD1	0.443
5	A:273:MET:HE2	A:278:GLY:HA2	0.436
5	A:242:PHE:CD2	A:262:LEU:HD13	0.429
5	A:239:VAL:HG13	A:273:MET:SD	0.408
6	A:35:ARG:HH21	A:97:ASP:CG	0.624
6	A:242:PHE:H	A:246:ASN:HD21	0.582

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:78:GLN:HE21	A:91:TRP:NE1	0.567
6	A:226:LEU:HD11	A:249:PRO:HB3	0.562
6	A:242:PHE:CE2	A:262:LEU:HD13	0.504
6	A:281:ARG:HH21	A:319:ILE:HD12	0.482
6	A:27:ILE:HG21	A:31:VAL:HG23	0.477
6	A:64:ASN:HA	A:410:PHE:CE1	0.470
6	A:78:GLN:HE21	A:91:TRP:CD1	0.467
6	A:306:SER:HB3	A:315:TYR:CD2	0.466
6	A:331:GLY:HA2	A:352:ASN:OD1	0.464
6	A:239:VAL:HG13	A:273:MET:SD	0.461
6	A:242:PHE:CE1	A:264:LYS:HE2	0.455
6	A:78:GLN:HE22	A:87:GLN:H	0.447
6	A:78:GLN:HE22	A:87:GLN:N	0.438
6	A:308:GLN:NE2	A:315:TYR:CE1	0.424
6	A:76:LEU:HD22	A:91:TRP:HH2	0.422
6	A:326:ARG:HD3	A:329:TRP:CZ3	0.418
6	A:315:TYR:CE1	A:326:ARG:HB2	0.407
7	A:27:ILE:HG21	A:68:PHE:HB3	0.701
7	A:37:ILE:HD12	A:156:LEU:HD11	0.596
7	A:37:ILE:HD11	A:100:VAL:HG23	0.563
7	A:240:ALA:HB1	A:242:PHE:CZ	0.556
7	A:25:ILE:HD12	A:59:ALA:HB1	0.550
7	A:239:VAL:HG13	A:273:MET:SD	0.527

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:27:ILE:CG2	A:68:PHE:HB3	0.518
7	A:242:PHE:CG	A:262:LEU:HD13	0.491
7	A:9:PHE:HB3	A:11:PHE:CD2	0.488
7	A:86:VAL:HG13	A:91:TRP:NE1	0.483
7	A:242:PHE:CD2	A:262:LEU:HD13	0.472
7	A:306:SER:HB3	A:315:TYR:CD2	0.468
7	A:242:PHE:CZ	A:262:LEU:HD22	0.450
7	A:281:ARG:HH21	A:319:ILE:HD12	0.444
7	A:27:ILE:HG21	A:68:PHE:CB	0.442
7	A:86:VAL:HG11	A:101:VAL:CG1	0.441
7	A:308:GLN:NE2	A:315:TYR:CE1	0.440
7	A:86:VAL:HG13	A:91:TRP:HE1	0.435
7	A:86:VAL:HG11	A:101:VAL:HG11	0.422
8	A:78:GLN:HE22	A:86:VAL:HA	0.645
8	A:242:PHE:CE1	A:264:LYS:HE2	0.635
8	A:242:PHE:CD2	A:262:LEU:HD13	0.601
8	A:226:LEU:HD11	A:249:PRO:HB3	0.572
8	A:35:ARG:HH21	A:97:ASP:CG	0.539
8	A:242:PHE:CE2	A:262:LEU:HD13	0.475
8	A:306:SER:HB3	A:315:TYR:CD2	0.461
8	A:308:GLN:NE2	A:315:TYR:CE1	0.433
9	A:226:LEU:HD11	A:249:PRO:HB3	0.596
9	A:239:VAL:HG13	A:273:MET:SD	0.571

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:78:GLN:HE21	A:91:TRP:CD1	0.521
9	A:242:PHE:CG	A:262:LEU:HD11	0.491
9	A:78:GLN:HE21	A:91:TRP:NE1	0.465
9	A:390:ILE:HG23	A:426:TRP:HE1	0.440
9	A:35:ARG:HH21	A:97:ASP:HB2	0.404
9	A:308:GLN:NE2	A:315:TYR:CE1	0.404
9	A:281:ARG:HH21	A:319:ILE:HD12	0.403
10	A:42:PHE:CE2	A:58:VAL:HG11	0.567
10	A:40:VAL:HG21	A:91:TRP:CZ3	0.546
10	A:42:PHE:CZ	A:100:VAL:HG11	0.538
10	A:76:LEU:HD22	A:91:TRP:CH2	0.522
10	A:76:LEU:HD22	A:91:TRP:CZ3	0.516
10	A:239:VAL:HG13	A:273:MET:SD	0.501
10	A:44:TRP:CE3	A:104:VAL:HG23	0.484
10	A:306:SER:HB3	A:315:TYR:CD2	0.480
10	A:273:MET:HE2	A:278:GLY:HA2	0.472
10	A:245:HIS:CE1	A:247:GLY:HA3	0.464
10	A:308:GLN:NE2	A:315:TYR:CE1	0.427
10	A:71:LEU:HD22	A:76:LEU:HD21	0.424
10	A:262:LEU:HG	A:271:TYR:CE2	0.418
10	A:405:SER:OG	A:411:LYS:HE2	0.409
10	A:42:PHE:CE2	A:58:VAL:CG1	0.407

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	428	406	17	5
2	428	403	18	7
3	428	408	17	3
4	428	411	9	8
5	428	402	18	8
6	428	400	25	3
7	428	418	9	1
8	428	399	22	7
9	428	408	16	4
10	428	400	22	6

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	343	334	5	4
2	343	330	7	6
3	343	332	4	7
4	343	333	3	7
5	343	330	9	4
6	343	335	3	5
7	343	331	7	5
8	343	331	8	4
9	343	335	4	4

Model ID	Analyzed	Favored	Allowed	Outliers
10	343	331	6	6

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	9	PHE
1	A	12	LEU
1	A	17	SER
1	A	374	THR
2	A	1	MET
2	A	5	LEU
2	A	14	LEU
2	A	246	ASN
2	A	374	THR
2	A	421	VAL
3	A	5	LEU
3	A	9	PHE
3	A	12	LEU
3	A	14	LEU
3	A	267	SER
3	A	374	THR
3	A	417	THR
4	A	12	LEU
4	A	14	LEU
4	A	17	SER

Model ID	Chain	Residue ID	Residue type
4	A	29	SER
4	A	267	SER
4	A	329	TRP
4	A	374	THR
5	A	5	LEU
5	A	12	LEU
5	A	328	THR
5	A	417	THR
6	A	5	LEU
6	A	9	PHE
6	A	26	VAL
6	A	267	SER
6	A	374	THR
7	A	5	LEU
7	A	12	LEU
7	A	17	SER
7	A	31	VAL
7	A	292	GLU
8	A	12	LEU
8	A	29	SER
8	A	32	ASP
8	A	374	THR
9	A	5	LEU

Model ID	Chain	Residue ID	Residue type
9	A	12	LEU
9	A	111	SER
9	A	374	THR
10	A	5	LEU
10	A	12	LEU
10	A	14	LEU
10	A	17	SER
10	A	71	LEU
10	A	374	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.

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