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	9A2K
PDB-Dev ID	PDBDEV_00000169
Structure Title	Model of E. coli AceA 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

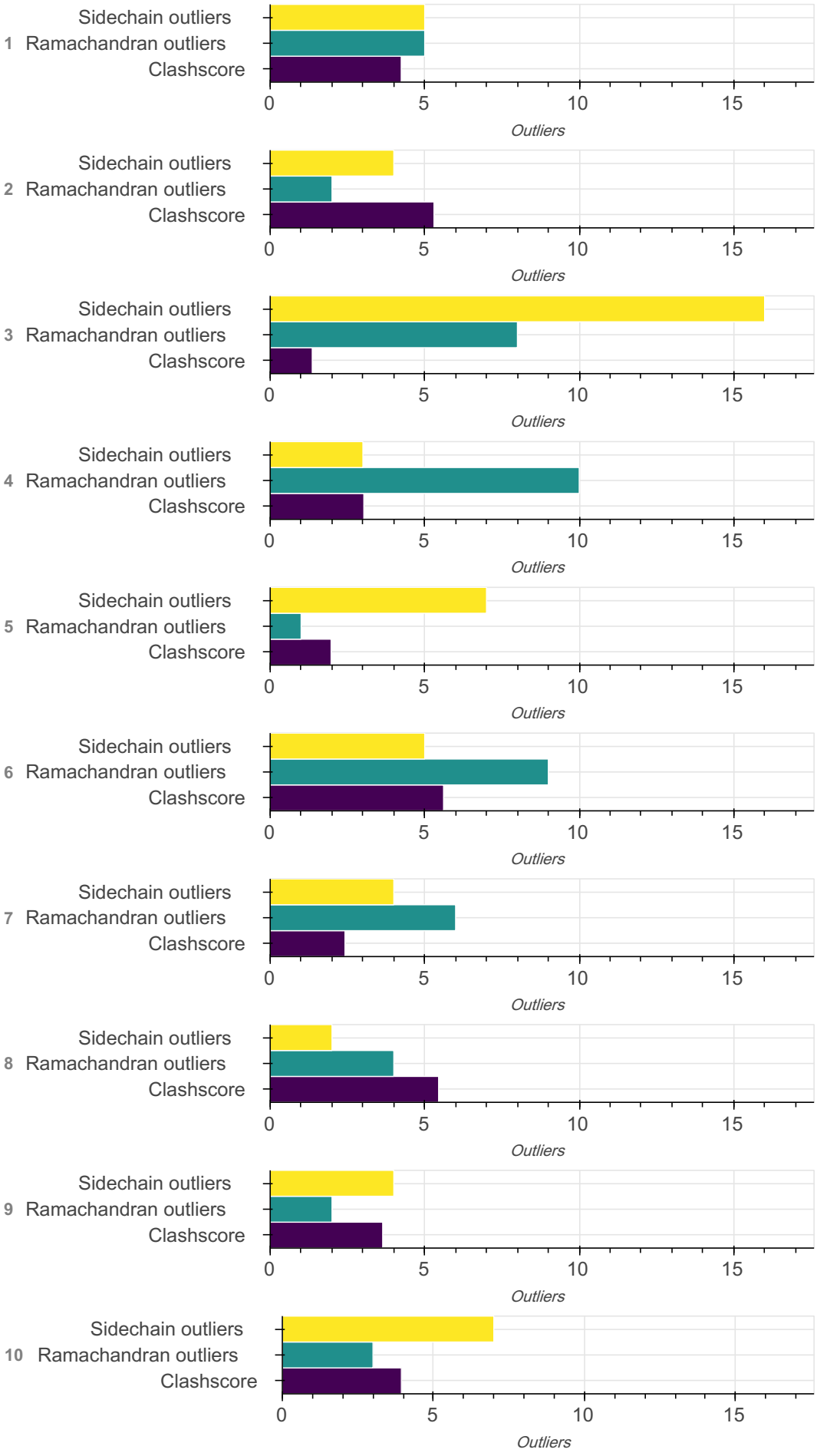
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
5
10
15
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	P0A9G6	A	A	434
2	1	1	P0A9G6	A	A	434
3	1	1	P0A9G6	A	A	434
4	1	1	P0A9G6	A	A	434
5	1	1	P0A9G6	A	A	434
6	1	1	P0A9G6	A	A	434
7	1	1	P0A9G6	A	A	434
8	1	1	P0A9G6	A	A	434
9	1	1	P0A9G6	A	A	434
10	1	1	P0A9G6	A	A	434

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	-	1-434

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 32510 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	3260
CB--HB2	1.09	0.97	3260
OH--HH	0.96	0.84	170
CG1--HG11	1.09	0.97	260
CE--HE2	1.09	0.97	310
CD2--HD22	1.09	0.97	330
CG--HG3	1.09	0.97	1200
CA--HA	1.09	0.97	3990
CG1--HG13	1.09	0.97	460
CB--HB1	1.09	0.97	560
CA--HA2	1.09	0.97	350
CD1--HD11	1.09	0.97	530
N--H3	1.01	0.89	10
CG2--HG22	1.09	0.97	730
NZ--HZ2	1.01	0.89	210
CD--HD3	1.09	0.97	540
CG1--HG12	1.09	0.97	460
CG--HG2	1.09	0.97	1200
CG2--HG23	1.09	0.97	730
CG--HG	1.09	0.97	330
CD--HD2	1.09	0.97	540
CB--HB	1.09	0.97	730

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ1	1.01	0.89	210
CG2--HG21	1.09	0.97	730
CA--HA3	1.09	0.97	350
CD2--HD21	1.09	0.97	330
CD2--HD23	1.09	0.97	330
OG1--HG1	0.96	0.84	270
CD1--HD13	1.09	0.97	530
CE--HE3	1.09	0.97	310
NZ--HZ3	1.01	0.89	210
OG--HG	0.96	0.84	250
CD1--HD12	1.09	0.97	530
CE--HE1	1.09	0.97	100
N--H1	1.01	0.89	10
N--H2	1.01	0.89	10
SG--HG	1.33	1.20	11
SG--HG	1.34	1.20	39
NE2--HE22	1.01	0.86	290
N--H	1.01	0.86	4160
CD2--HD2	1.08	0.93	440
NH2--HH21	1.01	0.86	160
CZ--HZ	1.08	0.93	190
CD1--HD1	1.08	0.93	440
CH2--HH2	1.08	0.93	80

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE2--HE2	1.08	0.93	360
NE1--HE1	1.01	0.86	80
CZ2--HZ2	1.08	0.93	80
CE1--HE1	1.08	0.93	440
CZ3--HZ3	1.08	0.93	80
ND2--HD21	1.01	0.86	120
NH1--HH12	1.01	0.86	160
NH1--HH11	1.01	0.86	160
ND1--HD1	1.01	0.86	62
CE3--HE3	1.08	0.93	80
NH2--HH22	1.01	0.86	160
NE2--HE21	1.01	0.86	290
NE--HE	1.01	0.86	160
ND2--HD22	1.01	0.86	120
NE2--HE2	1.01	0.86	18

Standard geometry: angle outliers

There are 257 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	137.45	1
C-N-CA	121.70	136.97	1
OE1-CD-NE2	122.60	115.34	1
NE-CZ-NH2	119.20	125.72	1
C-N-CA	121.70	133.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	107.24	1
C-N-CA	121.70	133.39	1
OD1-CG-ND2	122.60	116.46	1
OE1-CD-NE2	122.60	116.46	2
OE1-CD-NE2	122.60	116.58	1
N-CA-CB	111.50	121.73	1
CA-CB-CG2	110.50	120.24	1
OE1-CD-NE2	122.60	117.07	1
OE1-CD-NE2	122.60	117.10	1
CA-CB-CG	113.80	108.30	1
OE1-CD-NE2	122.60	117.12	1
N-CA-CB	110.40	102.22	1
OE1-CD-NE2	122.60	117.17	1
OD1-CG-ND2	122.60	117.19	1
OE1-CD-NE2	122.60	117.22	1
OE1-CD-NE2	122.60	117.23	1
C-N-CA	121.70	131.35	1
OE1-CD-NE2	122.60	117.34	1
CA-C-N	116.90	124.79	1
CA-CB-CG	113.80	108.55	1
C-N-CA	121.70	131.13	1
OE1-CD-NE2	122.60	117.37	1
CA-CB-CG	113.80	108.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	124.43	1
OE1-CD-NE2	122.60	117.40	1
OD1-CG-ND2	122.60	117.40	1
CA-C-N	116.90	124.69	1
CD-NE-CZ	124.40	131.62	1
CA-C-N	116.20	126.46	1
OD1-CG-ND2	122.60	117.48	1
CA-C-N	116.20	126.39	1
OE1-CD-NE2	122.60	117.51	1
OE1-CD-NE2	122.60	117.52	1
CB-CG-CD2	131.20	124.63	1
OE1-CD-NE2	122.60	117.55	1
CE2-CD2-CE3	118.80	113.77	1
OE1-CD-NE2	122.60	117.64	1
OE1-CD-NE2	122.60	117.65	1
OE1-CD-NE2	122.60	117.66	1
C-N-CA	121.70	130.53	1
CA-N-CD	112.00	105.14	1
CB-CG-CD2	131.20	124.84	1
CA-CB-CG	112.60	117.48	1
OE1-CD-NE2	122.60	117.72	2
OE1-CD-NE2	122.60	117.73	1
NE-CZ-NH2	119.20	123.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.46	1
OE1-CD-NE2	122.60	117.75	1
OE1-CD-NE2	122.60	117.77	1
OE1-CD-NE2	122.60	117.79	3
N-CA-CB	110.40	103.20	1
OE1-CD-NE2	122.60	117.80	3
NE-CZ-NH2	119.20	123.51	1
OE1-CD-NE2	122.60	117.82	2
CA-C-O	120.80	112.69	1
C-CA-CB	110.50	117.64	1
OE1-CD-NE2	122.60	117.84	2
OE1-CD-NE2	122.60	117.85	3
CA-CB-CG	112.60	117.33	1
NH1-CZ-NH2	119.30	113.15	1
OE1-CD-NE2	122.60	117.87	1
OE1-CD-NE2	122.60	117.88	1
OE1-CD-NE2	122.60	117.89	1
OE1-CD-NE2	122.60	117.90	1
CA-CB-CG	112.60	117.28	1
OE1-CD-NE2	122.60	117.92	1
OE1-CD-NE2	122.60	117.93	2
OE1-CD-NE2	122.60	117.94	2
OE1-CD-NE2	122.60	117.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.96	2
C-N-CA	121.70	130.04	1
OE1-CD-NE2	122.60	117.97	3
OE1-CD-NE2	122.60	117.98	2
OE1-CD-NE2	122.60	118.00	1
OE1-CD-NE2	122.60	118.01	1
CB-CG-CD2	131.20	125.25	1
OE1-CD-NE2	122.60	118.02	1
CA-N-CD	112.00	105.59	1
OE1-CD-NE2	122.60	118.03	1
CA-CB-CG2	110.40	118.16	1
NE-CZ-NH2	119.20	123.31	1
OE1-CD-NE2	122.60	118.05	1
C-N-CA	121.70	129.89	1
OE1-CD-NE2	122.60	118.06	2
OD1-CG-ND2	122.60	118.06	1
NE-CZ-NH1	121.50	116.96	1
OE1-CD-NE2	122.60	118.07	1
OE1-CD-NE2	122.60	118.08	1
NE-CZ-NH2	119.20	123.27	1
OE1-CD-NE2	122.60	118.09	3
OE1-CD-NE2	122.60	118.10	2
OD1-CG-ND2	122.60	118.10	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.11	2
OE1-CD-NE2	122.60	118.12	1
OE1-CD-NE2	122.60	118.14	2
OD1-CG-ND2	122.60	118.15	1
OE1-CD-NE2	122.60	118.15	1
CB-CG-CD2	131.20	125.42	1
OE1-CD-NE2	122.60	118.16	2
N-CA-C	111.00	123.43	1
OE1-CD-NE2	122.60	118.17	3
O-C-N	123.00	115.91	1
OE1-CD-NE2	122.60	118.18	1
OE1-CD-NE2	122.60	118.19	2
CA-CB-CG2	110.50	117.98	1
OE1-CD-NE2	122.60	118.21	3
OE1-CD-NE2	122.60	118.22	2
CB-CG-CD2	131.20	125.52	1
OE1-CD-NE2	122.60	118.24	3
CB-CG-CD2	131.20	125.55	1
OE1-CD-NE2	122.60	118.26	3
OD1-CG-ND2	122.60	118.27	2
OE1-CD-NE2	122.60	118.27	2
OE1-CD-NE2	122.60	118.28	4
OD1-CG-ND2	122.60	118.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.30	1
OE1-CD-NE2	122.60	118.31	2
CA-C-N	116.20	124.76	1
OE1-CD-NE2	122.60	118.32	2
NE-CZ-NH2	119.20	123.05	1
OE1-CD-NE2	122.60	118.33	1
OE1-CD-NE2	122.60	118.34	2
OE1-CD-NE2	122.60	118.35	3
CB-CG-CD2	131.20	125.68	1
CA-CB-CG2	110.40	117.62	1
OE1-CD-NE2	122.60	118.36	2
OE1-CD-NE2	122.60	118.37	2
C-CA-CB	110.50	116.83	1
OE1-CD-NE2	122.60	118.39	2
C-N-CA	121.70	129.28	1
OE1-CD-NE2	122.60	118.40	1
OE1-CD-NE2	122.60	118.41	1
CA-CB-CG	112.60	116.78	1
OD1-CG-ND2	122.60	118.42	1
CB-CG-CD2	131.20	125.78	1
C-CA-CB	110.10	118.03	1
ND1-CG-CD2	106.10	110.27	1
OE1-CD-NE2	122.60	118.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.44	4
CA-CB-CG	112.60	108.44	1
OE1-CD-NE2	122.60	118.45	2
CB-CG-CD2	131.20	125.80	2
C-N-CA	121.70	129.17	1
CA-CB-CG	112.60	116.73	1
OE1-CD-NE2	122.60	118.47	4
OE1-CD-NE2	122.60	118.48	2
OE1-CD-NE2	122.60	118.49	1
CA-CB-CG	112.60	108.49	1
N-CA-CB	103.00	107.52	1
CA-CB-CG	113.80	117.90	1
OE1-CD-NE2	122.60	118.50	2
NE-CZ-NH1	121.50	125.59	1
NE-CZ-NH2	119.20	115.52	1
OE1-CD-NE2	122.60	118.52	2
OD1-CG-ND2	122.60	118.52	1
CA-CB-CG	112.60	116.67	1
OE1-CD-NE2	122.60	118.53	2
OE1-CD-NE2	122.60	118.54	1
CB-CG-CD2	131.20	125.93	2
OE1-CD-NE2	122.60	118.56	3
OD1-CG-ND2	122.60	118.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NH1-CZ-NH2	119.30	114.05	1
OE1-CD-NE2	122.60	118.57	1
OD1-CG-ND2	122.60	118.57	1
CB-CG-CD2	131.20	125.96	1
CA-CB-CG2	110.50	103.66	1
CB-CG-CD2	131.20	125.97	1
OE1-CD-NE2	122.60	118.58	1
OE1-CD-NE2	122.60	118.59	2
CA-CB-CG2	110.50	117.31	1
CB-CG-CD2	131.20	125.99	1
OE1-CD-NE2	122.60	118.60	1
OD1-CG-ND2	122.60	118.60	1
HZ2-NZ-HZ3	96.97	109.00	1
HZ1-NZ-HZ2	96.90	109.00	1
HZ2-NZ-HZ3	96.67	109.00	1
HZ1-NZ-HZ3	96.56	109.00	1
CD-NE2-HE21	107.51	120.00	1
C-N-H	111.55	124.30	1
CZ-NH1-HH12	107.21	120.00	1
HZ1-NZ-HZ3	95.82	109.00	1
CZ-NH2-HH21	106.05	120.00	1
C-N-H	110.30	124.30	1
HH11-NH1-HH12	105.99	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	109.16	124.30	1
HH11-NH1-HH12	103.55	120.00	1
HH11-NH1-HH12	103.34	120.00	1
HH11-NH1-HH12	103.27	120.00	1
HH11-NH1-HH12	102.69	120.00	1
HH21-NH2-HH22	97.00	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	4.24	28
2	5.30	35
3	1.36	9
4	3.03	20
5	1.97	13
6	5.61	37
7	2.42	16
8	5.45	36
9	3.64	24
10	3.94	26

All 244 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:95:VAL:HG21	A:117:VAL:HG22	0.901

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:203:LEU:HD13	A:275:ARG:HH22	0.695
1	A:356:HIS:CD2	A:382:VAL:HG11	0.677
1	A:203:LEU:HD13	A:275:ARG:NH2	0.623
1	A:110:SER:HB2	A:162:PHE:CZ	0.614
1	A:320:PRO:HD3	A:350:ILE:HG23	0.586
1	A:105:MET:HB2	A:408:PHE:CZ	0.545
1	A:328:LEU:HD22	A:332:THR:HG21	0.530
1	A:324:TRP:CZ3	A:375:MET:HG3	0.525
1	A:165:VAL:HG13	A:215:ALA:HB2	0.513
1	A:296:GLU:CD	A:299:ARG:HH12	0.510
1	A:245:CYS:CB	A:253:ILE:HD11	0.504
1	A:203:LEU:HD11	A:238:ALA:CB	0.491
1	A:325:GLN:HB2	A:379:VAL:HG11	0.487
1	A:105:MET:SD	A:408:PHE:CE2	0.460
1	A:95:VAL:HG12	A:112:TYR:CG	0.447
1	A:245:CYS:HB3	A:253:ILE:HD11	0.445
1	A:188:GLN:HE22	A:194:LYS:HE3	0.437
1	A:203:LEU:HD11	A:238:ALA:HB1	0.435
1	A:350:ILE:CD1	A:375:MET:SD	0.431
1	A:102:ALA:C	A:104:SER:H	0.428
1	A:117:VAL:HB	A:175:MET:HE1	0.427
1	A:328:LEU:HD22	A:332:THR:CG2	0.427
1	A:117:VAL:CB	A:175:MET:HE1	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:269:ILE:HD12	A:297:LEU:HG	0.414
1	A:83:ALA:HB1	A:367:ASN:HA	0.411
1	A:203:LEU:HD11	A:238:ALA:HB3	0.405
1	A:96:ALA:HA	A:112:TYR:CE1	0.404
2	A:53:MET:HE1	A:347:PHE:CE2	0.855
2	A:196:GLY:HA2	A:201:LYS:HE3	0.662
2	A:53:MET:HE1	A:347:PHE:CD2	0.660
2	A:333:ILE:HG21	A:375:MET:HB2	0.644
2	A:333:ILE:HG21	A:375:MET:CB	0.629
2	A:320:PRO:CB	A:378:TYR:CE1	0.624
2	A:387:PHE:CD1	A:395:THR:HG21	0.602
2	A:320:PRO:HB2	A:378:TYR:CE1	0.591
2	A:352:LEU:HD21	A:365:LEU:HD21	0.538
2	A:105:MET:HE2	A:109:GLN:O	0.536
2	A:355:ILE:HG23	A:411:VAL:CG2	0.531
2	A:159:GLU:OE1	A:193:LYS:HE2	0.523
2	A:14:GLU:CD	A:19:ARG:HH21	0.494
2	A:196:GLY:HA2	A:201:LYS:CE	0.486
2	A:355:ILE:HG23	A:411:VAL:HG22	0.482
2	A:350:ILE:HD13	A:369:TYR:CE1	0.465
2	A:353:ALA:C	A:355:ILE:H	0.465
2	A:117:VAL:HB	A:175:MET:HE1	0.458
2	A:189:LEU:HD23	A:192:VAL:HG22	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:293:PRO:HD3	A:322:PHE:HB3	0.453
2	A:189:LEU:HD22	A:242:THR:CG2	0.451
2	A:319:SER:O	A:322:PHE:CD2	0.451
2	A:189:LEU:HD22	A:242:THR:HG21	0.442
2	A:358:MET:CG	A:420:SER:HA	0.438
2	A:320:PRO:HB3	A:378:TYR:CE1	0.426
2	A:157:ASP:CG	A:184:HIS:NE2	0.424
2	A:350:ILE:HG21	A:369:TYR:CZ	0.416
2	A:378:TYR:C	A:378:TYR:CD1	0.414
2	A:76:GLN:HG3	A:359:TRP:CE3	0.410
2	A:76:GLN:HG3	A:359:TRP:CZ3	0.408
2	A:155:VAL:HG21	A:347:PHE:CZ	0.407
2	A:20:TRP:CD2	A:25:ARG:NH2	0.406
2	A:189:LEU:HD23	A:192:VAL:CG2	0.405
2	A:157:ASP:CG	A:184:HIS:HE2	0.403
2	A:187:ASP:OD2	A:275:ARG:NH1	0.403
3	A:293:PRO:HD2	A:322:PHE:CZ	0.638
3	A:324:TRP:CD1	A:328:LEU:HD12	0.606
3	A:293:PRO:HD2	A:322:PHE:CE2	0.600
3	A:245:CYS:SG	A:253:ILE:HD13	0.499
3	A:293:PRO:HD2	A:322:PHE:CE1	0.487
3	A:376:LYS:HE2	A:380:GLU:OE1	0.471
3	A:293:PRO:CD	A:322:PHE:CE2	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:292:THR:HA	A:322:PHE:CZ	0.414
3	A:245:CYS:SG	A:263:PHE:CE2	0.412
4	A:240:LEU:HD11	A:425:LEU:HD21	0.778
4	A:105:MET:HE1	A:403:VAL:O	0.668
4	A:245:CYS:SG	A:253:ILE:HD13	0.603
4	A:293:PRO:HD3	A:322:PHE:HB3	0.586
4	A:109:GLN:HB2	A:160:ALA:HB1	0.517
4	A:117:VAL:HB	A:175:MET:HE1	0.499
4	A:100:ASN:OD1	A:105:MET:HG2	0.483
4	A:390:ALA:HB2	A:395:THR:CG2	0.472
4	A:93:TRP:NE1	A:193:LYS:HE2	0.468
4	A:232:ARG:HD2	A:287:TRP:CH2	0.467
4	A:336:PHE:CE1	A:340:LEU:HD11	0.453
4	A:186:GLU:OE1	A:193:LYS:HE3	0.442
4	A:93:TRP:HE1	A:193:LYS:HE2	0.438
4	A:355:ILE:HD11	A:399:HIS:CD2	0.437
4	A:232:ARG:HD2	A:287:TRP:CZ3	0.431
4	A:390:ALA:HA	A:395:THR:HG23	0.427
4	A:90:LEU:HD12	A:121:VAL:HG22	0.425
4	A:376:LYS:HE2	A:380:GLU:OE1	0.421
4	A:19:ARG:HH12	A:54:TRP:HB2	0.414
4	A:72:LEU:HD11	A:94:GLN:HG2	0.414
5	A:72:LEU:HD21	A:94:GLN:C	0.640

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:90:LEU:HD21	A:124:ILE:HD12	0.594
5	A:352:LEU:CD1	A:362:MET:HE1	0.526
5	A:232:ARG:HD2	A:287:TRP:CZ3	0.518
5	A:105:MET:CE	A:405:THR:HB	0.486
5	A:352:LEU:HD13	A:362:MET:HE1	0.468
5	A:187:ASP:HB2	A:275:ARG:HH21	0.466
5	A:105:MET:SD	A:405:THR:HA	0.454
5	A:186:GLU:HB3	A:232:ARG:HD3	0.453
5	A:105:MET:HE3	A:405:THR:HB	0.444
5	A:93:TRP:NE1	A:109:GLN:HE22	0.443
5	A:100:ASN:ND2	A:108:ASP:H	0.440
5	A:159:GLU:C	A:186:GLU:HG2	0.425
6	A:72:LEU:HD21	A:94:GLN:HB3	0.701
6	A:328:LEU:HD22	A:332:THR:HG21	0.649
6	A:333:ILE:HG21	A:375:MET:CB	0.639
6	A:333:ILE:HG21	A:375:MET:HB2	0.617
6	A:162:PHE:CE2	A:190:ALA:HB1	0.577
6	A:291:SER:C	A:322:PHE:CE2	0.557
6	A:158:ALA:HB1	A:171:LEU:HD21	0.550
6	A:19:ARG:HA	A:54:TRP:CZ2	0.546
6	A:352:LEU:CD1	A:362:MET:HE1	0.546
6	A:291:SER:HA	A:322:PHE:CE2	0.533
6	A:157:ASP:HA	A:184:HIS:CD2	0.529

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:328:LEU:HD22	A:332:THR:CG2	0.529
6	A:324:TRP:CZ3	A:333:ILE:HG12	0.526
6	A:72:LEU:HD21	A:94:GLN:CB	0.499
6	A:54:TRP:CZ2	A:58:HIS:CE1	0.488
6	A:296:GLU:CD	A:299:ARG:HH12	0.486
6	A:291:SER:O	A:292:THR:HG23	0.475
6	A:369:TYR:CD2	A:374:GLY:HA3	0.470
6	A:399:HIS:CE1	A:403:VAL:HG21	0.469
6	A:161:GLY:HA3	A:188:GLN:O	0.463
6	A:324:TRP:CZ3	A:328:LEU:HD12	0.452
6	A:399:HIS:CE1	A:403:VAL:CG2	0.451
6	A:117:VAL:CG1	A:175:MET:HE1	0.447
6	A:187:ASP:HB2	A:275:ARG:HH21	0.443
6	A:93:TRP:HZ3	A:354:GLY:H	0.443
6	A:72:LEU:HD21	A:94:GLN:C	0.432
6	A:162:PHE:CE2	A:190:ALA:CB	0.432
6	A:158:ALA:HB1	A:171:LEU:CD2	0.430
6	A:291:SER:O	A:322:PHE:CZ	0.430
6	A:244:ASP:HA	A:253:ILE:HD13	0.424
6	A:324:TRP:CZ2	A:375:MET:HE2	0.423
6	A:93:TRP:CZ3	A:353:ALA:HA	0.415
6	A:321:SER:C	A:322:PHE:CD2	0.408
6	A:157:ASP:CG	A:184:HIS:NE2	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:96:ALA:HA	A:112:TYR:CZ	0.403
6	A:352:LEU:HD13	A:362:MET:HE1	0.403
6	A:58:HIS:CE1	A:313:LEU:HD11	0.402
7	A:333:ILE:HD13	A:379:VAL:HG21	0.698
7	A:413:THR:HG23	A:418:GLY:O	0.643
7	A:355:ILE:HD11	A:359:TRP:CZ2	0.590
7	A:97:ALA:HB1	A:408:PHE:CE2	0.552
7	A:70:GLY:C	A:94:GLN:HE22	0.486
7	A:350:ILE:HD11	A:369:TYR:OH	0.479
7	A:194:LYS:O	A:195:CYS:C	0.469
7	A:360:PHE:CE2	A:382:VAL:HG21	0.448
7	A:89:TYR:HE1	A:351:THR:HG22	0.433
7	A:320:PRO:HG2	A:378:TYR:CD1	0.420
7	A:360:PHE:CZ	A:382:VAL:CG2	0.415
7	A:232:ARG:HD2	A:287:TRP:CZ3	0.413
7	A:376:LYS:HE2	A:380:GLU:OE1	0.413
7	A:399:HIS:CE1	A:403:VAL:HG11	0.413
7	A:336:PHE:CE1	A:340:LEU:HD11	0.411
7	A:95:VAL:HG21	A:117:VAL:HG22	0.410
8	A:352:LEU:HD13	A:362:MET:HE1	0.777
8	A:195:CYS:H	A:198:MET:HE2	0.767
8	A:349:PHE:CE1	A:351:THR:HG22	0.735
8	A:161:GLY:HA2	A:190:ALA:HB1	0.698

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:352:LEU:CD1	A:362:MET:HE1	0.661
8	A:362:MET:HA	A:362:MET:HE2	0.660
8	A:352:LEU:HD11	A:365:LEU:CD2	0.656
8	A:357:SER:HA	A:362:MET:HE3	0.643
8	A:349:PHE:CZ	A:351:THR:HG22	0.634
8	A:352:LEU:HD11	A:365:LEU:HD22	0.608
8	A:114:ALA:HA	A:162:PHE:CE2	0.571
8	A:320:PRO:HG2	A:375:MET:HE2	0.518
8	A:114:ALA:HA	A:162:PHE:CZ	0.506
8	A:337:GLN:HE22	A:350:ILE:HD11	0.501
8	A:198:MET:SD	A:404:GLY:HA2	0.501
8	A:97:ALA:HB2	A:105:MET:HE3	0.491
8	A:97:ALA:CB	A:105:MET:HE3	0.486
8	A:349:PHE:CE1	A:351:THR:CG2	0.485
8	A:161:GLY:CA	A:190:ALA:HB1	0.482
8	A:324:TRP:CE3	A:328:LEU:CD1	0.480
8	A:296:GLU:CD	A:299:ARG:HH12	0.475
8	A:70:GLY:HA3	A:94:GLN:HE22	0.470
8	A:117:VAL:CG1	A:175:MET:HE1	0.467
8	A:324:TRP:HB3	A:328:LEU:HD11	0.459
8	A:412:THR:HG21	A:421:SER:HB3	0.457
8	A:19:ARG:HH21	A:217:ARG:HH11	0.439
8	A:158:ALA:HB2	A:183:VAL:CG1	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:43:CYS:HB2	A:225:VAL:HG21	0.427
8	A:15:TRP:CZ3	A:226:PRO:HD3	0.420
8	A:352:LEU:HD22	A:378:TYR:CD2	0.413
8	A:365:LEU:HD13	A:378:TYR:HB2	0.412
8	A:195:CYS:N	A:198:MET:HE2	0.410
8	A:316:TYR:HB2	A:345:TYR:CD1	0.410
8	A:352:LEU:HD22	A:378:TYR:CE2	0.407
8	A:95:VAL:HG11	A:117:VAL:HG22	0.402
8	A:93:TRP:CH2	A:107:PRO:HD3	0.400
9	A:291:SER:HB3	A:429:THR:HG23	0.825
9	A:199:GLY:HA2	A:424:ALA:HB2	0.649
9	A:72:LEU:HD21	A:94:GLN:HB3	0.612
9	A:199:GLY:CA	A:424:ALA:HB2	0.600
9	A:291:SER:CB	A:429:THR:HG23	0.557
9	A:394:TYR:HB3	A:396:PHE:CE2	0.508
9	A:357:SER:CB	A:362:MET:HE2	0.494
9	A:357:SER:OG	A:362:MET:HE2	0.484
9	A:120:VAL:HG22	A:123:ARG:HH21	0.481
9	A:359:TRP:CD2	A:396:PHE:CE1	0.461
9	A:89:TYR:CE1	A:351:THR:HG22	0.455
9	A:160:ALA:C	A:162:PHE:H	0.444
9	A:430:GLU:O	A:434:PHE:CD2	0.436
9	A:97:ALA:CB	A:403:VAL:HG12	0.432

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:291:SER:HA	A:433:GLN:HE21	0.432
9	A:157:ASP:CG	A:184:HIS:CE1	0.426
9	A:203:LEU:HG	A:238:ALA:HB3	0.423
9	A:353:ALA:HB1	A:365:LEU:HD21	0.422
9	A:110:SER:N	A:194:LYS:HZ1	0.418
9	A:155:VAL:HG22	A:182:ALA:HB3	0.416
9	A:53:MET:HE1	A:347:PHE:CD2	0.410
9	A:120:VAL:HG22	A:123:ARG:NH2	0.409
9	A:192:VAL:HG11	A:200:GLY:O	0.408
9	A:257:ARG:NH2	A:263:PHE:CZ	0.405
10	A:267:ALA:HB1	A:271:GLN:HB2	0.775
10	A:267:ALA:HB1	A:271:GLN:CB	0.763
10	A:72:LEU:HD21	A:94:GLN:HB3	0.701
10	A:94:GLN:HE21	A:354:GLY:HA2	0.558
10	A:275:ARG:CG	A:275:ARG:HH11	0.556
10	A:72:LEU:HD21	A:94:GLN:CB	0.550
10	A:275:ARG:HB3	A:275:ARG:HH11	0.537
10	A:355:ILE:HG21	A:396:PHE:CE1	0.532
10	A:355:ILE:HG23	A:359:TRP:HE1	0.521
10	A:319:SER:HB3	A:322:PHE:CD2	0.513
10	A:399:HIS:O	A:403:VAL:HG23	0.512
10	A:355:ILE:HG21	A:396:PHE:CD1	0.510
10	A:241:ILE:CD1	A:263:PHE:HB2	0.494

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:275:ARG:CB	A:275:ARG:HH11	0.488
10	A:352:LEU:HD13	A:357:SER:HB3	0.458
10	A:253:ILE:HG22	A:255:GLY:H	0.451
10	A:355:ILE:CG2	A:359:TRP:HE1	0.451
10	A:94:GLN:HE21	A:354:GLY:CA	0.448
10	A:117:VAL:HB	A:175:MET:HE1	0.447
10	A:319:SER:HB3	A:322:PHE:CE2	0.447
10	A:173:LYS:HE2	A:177:GLU:OE1	0.442
10	A:184:HIS:C	A:184:HIS:CD2	0.437
10	A:250:SER:HB3	A:252:PHE:CE1	0.435
10	A:161:GLY:O	A:162:PHE:C	0.432
10	A:241:ILE:HD12	A:263:PHE:HB2	0.409
10	A:390:ALA:HB2	A:397:VAL:HB	0.404

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	432	404	23	5
2	432	413	17	2
3	432	405	19	8
4	432	408	14	10
5	432	421	10	1
6	432	407	16	9
7	432	407	19	6

Model ID	Analyzed	Favored	Allowed	Outliers
8	432	414	14	4
9	432	410	20	2
10	432	406	23	3

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	332	6	5
2	343	335	4	4
3	343	323	4	16
4	343	332	8	3
5	343	331	5	7
6	343	328	10	5
7	343	332	7	4
8	343	333	8	2
9	343	330	9	4
10	343	331	5	7

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	184	HIS
1	A	259	SER
1	A	382	VAL
1	A	422	VAL
1	A	429	THR

Model ID	Chain	Residue ID	Residue type
2	A	73	THR
2	A	184	HIS
2	A	259	SER
2	A	429	THR
3	A	72	LEU
3	A	93	TRP
3	A	104	SER
3	A	159	GLU
3	A	184	HIS
3	A	192	VAL
3	A	234	ASP
3	A	259	SER
3	A	265	THR
3	A	299	ARG
3	A	321	SER
3	A	408	PHE
3	A	413	THR
3	A	419	THR
3	A	420	SER
3	A	429	THR
4	A	259	SER
4	A	419	THR
4	A	420	SER

Model ID	Chain	Residue ID	Residue type
5	A	93	TRP
5	A	165	VAL
5	A	184	HIS
5	A	259	SER
5	A	419	THR
5	A	423	THR
5	A	429	THR
6	A	192	VAL
6	A	287	TRP
6	A	355	ILE
6	A	419	THR
6	A	423	THR
7	A	192	VAL
7	A	259	SER
7	A	324	TRP
7	A	419	THR
8	A	259	SER
8	A	352	LEU
9	A	110	SER
9	A	184	HIS
9	A	259	SER
9	A	428	SER
10	A	197	HIS

Model ID	Chain	Residue ID	Residue type
10	A	259	SER
10	A	266	HIS
10	A	275	ARG
10	A	419	THR
10	A	422	VAL
10	A	423	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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