Integrative Structure Validation Report

July 22, 2024 - 05:05 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	9A2S
PDB-Dev ID	PDBDEV_00000177
Structure Title	Model of E. coli AtpD 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

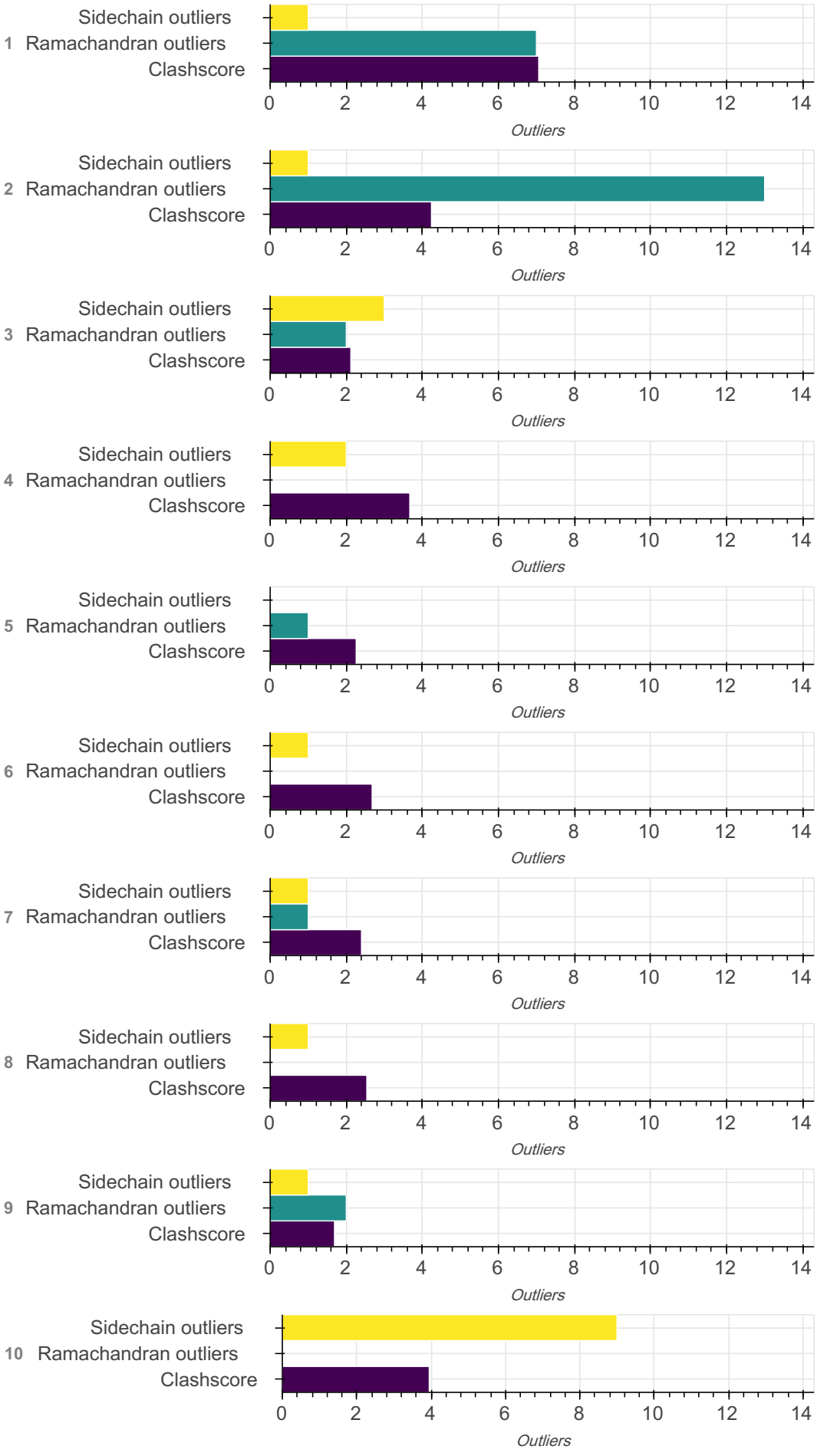
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
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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
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7
Sidechain outliers
Ramachandran outliers
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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	P0ABB4	A	A	460
2	1	1	P0ABB4	A	A	460
3	1	1	P0ABB4	A	A	460
4	1	1	P0ABB4	A	A	460
5	1	1	P0ABB4	A	A	460
6	1	1	P0ABB4	A	A	460
7	1	1	P0ABB4	A	A	460
8	1	1	P0ABB4	A	A	460
9	1	1	P0ABB4	A	A	460
10	1	1	P0ABB4	A	A	460

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	-	1-460

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 35480 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
CG--HG2	1.09	0.97	1400
CA--HA	1.09	0.97	4150
CG2--HG21	1.09	0.97	980
CD1--HD11	1.09	0.97	690
CE--HE3	1.09	0.97	350
CD1--HD12	1.09	0.97	690
OG1--HG1	0.96	0.84	240
CD--HD3	1.09	0.97	660
CG--HG3	1.09	0.97	1400
CB--HB3	1.09	0.97	3170
CE--HE2	1.09	0.97	350
CD1--HD13	1.09	0.97	690
CG1--HG11	1.09	0.97	470
CB--HB2	1.09	0.97	3170
CG2--HG22	1.09	0.97	980
CD2--HD23	1.09	0.97	420
CG1--HG13	1.09	0.97	740
CG1--HG12	1.09	0.97	740
CB--HB1	1.09	0.97	340
OG--HG	0.96	0.84	250
CD2--HD21	1.09	0.97	420
CB--HB	1.09	0.97	980

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ3	1.01	0.89	200
CA--HA3	1.09	0.97	450
CD--HD2	1.09	0.97	660
CG2--HG23	1.09	0.97	980
CD2--HD22	1.09	0.97	420
CE--HE1	1.09	0.97	150
CG--HG	1.09	0.97	420
OH--HH	0.96	0.84	150
NZ--HZ2	1.01	0.89	200
CA--HA2	1.09	0.97	450
NZ--HZ1	1.01	0.89	200
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	1
SG--HG	1.34	1.20	9
N--H	1.01	0.86	4390
CD2--HD2	1.08	0.93	360
CZ--HZ	1.08	0.93	140
NE2--HE22	1.01	0.86	200
CE2--HE2	1.08	0.93	290
NH2--HH21	1.01	0.86	260
ND2--HD22	1.01	0.86	110

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.01	0.86	260
CD1--HD1	1.08	0.93	300
NE--HE	1.01	0.86	260
CE1--HE1	1.08	0.93	360
NH1--HH11	1.01	0.86	260
NE2--HE2	1.01	0.86	25
NH1--HH12	1.01	0.86	260
ND1--HD1	1.01	0.86	45
ND2--HD21	1.01	0.86	110
CH2--HH2	1.08	0.93	10
NE2--HE21	1.01	0.86	200
CZ3--HZ3	1.08	0.93	10
NE1--HE1	1.01	0.86	10
CZ2--HZ2	1.08	0.93	10
CE3--HE3	1.08	0.93	10

Standard geometry: angle outliers

There are 184 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	138.78	1
OE1-CD-NE2	122.60	115.77	1
O-C-N	123.00	112.69	1
C-N-CA	121.70	133.29	1
OE1-CD-NE2	122.60	116.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.35	1
C-N-CA	121.70	132.82	1
OE1-CD-NE2	122.60	116.47	1
OE1-CD-NE2	122.60	116.57	1
OE1-CD-NE2	122.60	116.59	1
OE1-CD-NE2	122.60	116.61	1
O-C-N	123.00	113.79	1
OE1-CD-NE2	122.60	116.93	1
CA-CB-CG	112.60	118.20	1
CA-CB-CG	113.80	119.34	1
OE1-CD-NE2	122.60	117.15	1
CA-C-N	116.90	125.04	1
OE1-CD-NE2	122.60	117.19	1
CA-C-N	116.20	127.01	1
OE1-CD-NE2	122.60	117.23	1
OE1-CD-NE2	122.60	117.24	1
OE1-CD-NE2	122.60	117.27	1
OE1-CD-NE2	122.60	117.28	2
OE1-CD-NE2	122.60	117.34	1
OE1-CD-NE2	122.60	117.37	1
C-N-CA	121.70	130.93	1
OE1-CD-NE2	122.60	117.51	3
C-N-CA	121.70	112.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.52	1
OE1-CD-NE2	122.60	117.53	1
OE1-CD-NE2	122.60	117.54	2
OE1-CD-NE2	122.60	117.55	2
OE1-CD-NE2	122.60	117.57	1
CA-CB-CG	112.60	117.62	1
OE1-CD-NE2	122.60	117.63	1
OE1-CD-NE2	122.60	117.67	1
CA-C-N	116.20	126.00	1
C-N-CA	121.70	130.46	1
CA-C-N	116.90	124.18	1
N-CA-CB	103.00	108.34	1
OE1-CD-NE2	122.60	117.81	1
OE1-CD-NE2	122.60	117.83	1
OE1-CD-NE2	122.60	117.85	1
OE1-CD-NE2	122.60	117.86	1
OE1-CD-NE2	122.60	117.88	1
OE1-CD-NE2	122.60	117.90	1
CB-CG-CD2	131.20	125.12	1
OE1-CD-NE2	122.60	117.94	2
OE1-CD-NE2	122.60	117.96	1
OE1-CD-NE2	122.60	117.99	1
N-CA-CB	110.40	103.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.96	1
N-CA-CB	110.40	103.52	1
OE1-CD-NE2	122.60	118.02	1
NE-CZ-NH2	119.20	123.32	1
OE1-CD-NE2	122.60	118.04	2
CA-CB-CG	114.10	104.99	1
OE1-CD-NE2	122.60	118.05	1
OE1-CD-NE2	122.60	118.07	1
OE1-CD-NE2	122.60	118.08	1
CA-CB-CG1	110.40	118.07	1
OD1-CG-ND2	122.60	118.10	1
OE1-CD-NE2	122.60	118.11	1
NE-CZ-NH1	121.50	125.98	1
OE1-CD-NE2	122.60	118.12	1
C-N-CA	121.70	129.74	1
CA-CB-CG	113.80	118.26	1
C-CA-CB	110.50	103.81	1
OE1-CD-NE2	122.60	118.15	1
CB-CG-CD2	131.20	125.44	1
OE1-CD-NE2	122.60	118.18	1
N-CA-CB	103.00	107.84	1
OE1-CD-NE2	122.60	118.20	1
C-N-CA	121.70	129.61	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	125.87	1
CB-CG-CD2	131.20	125.53	1
OE1-CD-NE2	122.60	118.25	2
NE-CZ-NH1	121.50	125.84	1
CA-CB-CG	114.10	105.41	1
CA-CB-CG2	110.40	117.78	1
CA-CB-CG	114.10	105.44	1
CA-CB-CG	112.60	116.93	2
CB-CG-CD2	131.20	125.58	1
OE1-CD-NE2	122.60	118.28	1
OE1-CD-NE2	122.60	118.29	1
NE-CZ-NH2	119.20	123.07	1
OE1-CD-NE2	122.60	118.31	3
O-C-N	123.00	116.13	1
CB-CG-CD2	131.20	125.65	1
OE1-CD-NE2	122.60	118.34	1
O-C-N	123.00	116.18	1
CB-CG-CD2	131.20	125.66	1
CA-CB-CG	113.80	118.05	1
OE1-CD-NE2	122.60	118.35	2
CA-C-N	116.90	123.26	1
OE1-CD-NE2	122.60	118.36	1
CB-CG-CD2	131.20	125.69	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.37	1
CB-CG-CD2	131.20	125.70	1
CB-CG-CD2	131.20	125.71	2
CA-CB-CG	114.10	105.65	1
OE1-CD-NE2	122.60	118.39	1
CB-CG-CD2	131.20	125.73	1
OD1-CG-ND2	122.60	118.40	1
O-C-N	123.00	116.28	1
OE1-CD-NE2	122.60	118.40	1
CG-SD-CE	100.90	91.67	1
CB-CG-CD2	131.20	125.75	1
OE1-CD-NE2	122.60	118.41	1
NE-CZ-NH1	121.50	125.69	1
CA-CB-CG	112.60	116.78	1
CB-CG-CD2	131.20	125.76	1
OE1-CD-NE2	122.60	118.42	2
CB-CG-CD2	131.20	125.77	2
C-N-CA	121.70	129.21	1
OE1-CD-NE2	122.60	118.43	1
CB-CG-CD2	131.20	125.79	1
OE1-CD-NE2	122.60	118.44	2
C-N-CA	121.70	129.17	1
CB-CG-CD2	131.20	125.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.45	1
OD1-CG-ND2	122.60	118.45	1
O-C-N	123.00	116.38	1
CB-CG-CD2	131.20	125.83	2
OE1-CD-NE2	122.60	118.47	1
O-C-N	123.00	116.40	1
OD1-CG-ND2	122.60	118.48	1
OE1-CD-NE2	122.60	118.48	1
N-CA-CB	103.00	107.53	1
CA-N-CD	112.00	106.24	1
CA-CB-OG1	109.60	115.77	1
OE1-CD-NE2	122.60	118.49	1
OD1-CG-ND2	122.60	118.49	1
OE1-CD-NE2	122.60	118.50	2
C-CA-CB	110.50	116.66	1
OD1-CG-ND2	122.60	118.50	1
C-N-CA	121.70	129.06	1
CD-NE-CZ	124.40	130.12	1
OE1-CD-NE2	122.60	118.52	2
CA-CB-CG	112.60	116.68	1
NE-CZ-NH1	121.50	125.57	1
OE1-CD-NE2	122.60	118.54	3
CA-CB-OG	111.10	119.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NH1-CZ-NH2	119.30	114.03	1
NE-CZ-NH1	121.50	125.55	1
C-CA-CB	110.50	116.57	1
CA-CB-CG	114.10	106.01	1
OD1-CG-ND2	122.60	118.55	1
CA-CB-CG	114.10	106.03	1
CB-CG-CD2	131.20	125.96	1
OD1-CG-ND2	122.60	118.57	1
CA-C-N	116.20	124.26	1
OE1-CD-NE2	122.60	118.57	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
CG-CD-CE	111.30	102.08	1
C-N-H	111.83	124.30	1
CD-NE2-HE21	107.16	120.00	1
C-N-H	110.98	124.30	1
HH11-NH1-HH12	105.34	120.00	1
C-N-H	109.51	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

Model ID	Clash score	Number of clashes
1	7.06	50
2	4.24	30
3	2.12	15
4	3.67	26
5	2.26	16
6	2.68	19
7	2.40	17
8	2.54	18
9	1.69	12
10	3.95	28

All 231 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:250:LEU:HD13	A:334:ALA:HB1	0.915
1	A:279:LEU:HD22	A:313:PHE:CZ	0.906
1	A:218:LEU:HD13	A:276:MET:CE	0.820
1	A:338:LEU:HD22	A:366:GLN:HE21	0.718
1	A:132:LYS:HE3	A:419:VAL:HG11	0.689
1	A:218:LEU:HD13	A:276:MET:HE1	0.666
1	A:279:LEU:HD22	A:313:PHE:CE2	0.641
1	A:8:GLN:NE2	A:10:ILE:HD11	0.620
1	A:320:VAL:HG22	A:337:PRO:HB2	0.611
1	A:297:VAL:HG21	A:312:THR:CG2	0.574
1	A:320:VAL:HA	A:337:PRO:HB3	0.555

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:248:TYR:CD1	A:308:SER:HB2	0.547
1	A:297:VAL:HG21	A:312:THR:HG21	0.543
1	A:324:ARG:NH2	A:365:LEU:HD13	0.542
1	A:324:ARG:HH22	A:365:LEU:CD1	0.539
1	A:131:ILE:HG21	A:134:ILE:HD12	0.537
1	A:177:PHE:CE1	A:241:PHE:CD2	0.536
1	A:215:GLY:HA3	A:269:GLN:HE22	0.533
1	A:8:GLN:HE21	A:10:ILE:HD11	0.532
1	A:338:LEU:HD22	A:366:GLN:NE2	0.524
1	A:246:TYR:OH	A:313:PHE:CE2	0.523
1	A:324:ARG:HH22	A:365:LEU:HD13	0.523
1	A:131:ILE:HD13	A:134:ILE:HD12	0.516
1	A:279:LEU:C	A:279:LEU:HD23	0.487
1	A:215:GLY:HA3	A:269:GLN:OE1	0.483
1	A:320:VAL:HG22	A:337:PRO:CB	0.483
1	A:133:VAL:HG13	A:136:LEU:CD1	0.474
1	A:364:ILE:HD12	A:432:MET:HG2	0.466
1	A:145:LYS:H	A:292:THR:HG23	0.463
1	A:405:PHE:HB2	A:408:ALA:HB3	0.461
1	A:133:VAL:O	A:133:VAL:HG12	0.447
1	A:12:ALA:CB	A:213:PRO:HG3	0.445
1	A:279:LEU:O	A:279:LEU:HD23	0.440
1	A:132:LYS:H	A:403:GLN:NE2	0.439

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:215:GLY:HA3	A:269:GLN:NE2	0.434
1	A:164:ILE:HG23	A:177:PHE:CE1	0.430
1	A:149:PHE:CZ	A:163:LEU:CD2	0.429
1	A:132:LYS:HE2	A:424:THR:HA	0.427
1	A:256:SER:CB	A:263:PRO:HA	0.427
1	A:133:VAL:HG13	A:136:LEU:HG	0.420
1	A:320:VAL:HA	A:337:PRO:CB	0.420
1	A:408:ALA:HB1	A:412:THR:HG23	0.415
1	A:406:PHE:HA	A:416:GLY:HA3	0.414
1	A:345:LEU:O	A:355:TYR:CE2	0.413
1	A:279:LEU:CD2	A:313:PHE:CZ	0.410
1	A:144:GLY:HA2	A:293:SER:H	0.409
1	A:276:MET:HA	A:276:MET:HE2	0.407
1	A:279:LEU:HD22	A:313:PHE:CE1	0.403
1	A:322:LEU:C	A:324:ARG:H	0.402
1	A:167:ILE:HG22	A:239:LEU:HD22	0.400
2	A:221:ALA:CB	A:245:ILE:HD11	0.702
2	A:167:ILE:HD12	A:239:LEU:HD22	0.659
2	A:322:LEU:HD23	A:334:ALA:O	0.620
2	A:149:PHE:CE2	A:319:THR:HG23	0.573
2	A:221:ALA:HB2	A:245:ILE:HD11	0.568
2	A:219:ARG:HH12	A:269:GLN:NE2	0.542
2	A:357:THR:HA	A:432:MET:HE1	0.541

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:217:ARG:NH1	A:248:TYR:CE1	0.528
2	A:320:VAL:HG13	A:335:VAL:HG22	0.524
2	A:12:ALA:HB2	A:213:PRO:CB	0.522
2	A:12:ALA:HB2	A:213:PRO:HB3	0.504
2	A:239:LEU:HD23	A:241:PHE:CZ	0.504
2	A:177:PHE:HB3	A:205:LEU:HD23	0.501
2	A:8:GLN:NE2	A:10:ILE:HD11	0.490
2	A:239:LEU:CD2	A:241:PHE:CZ	0.485
2	A:179:GLY:O	A:220:VAL:HG11	0.472
2	A:55:ILE:HD13	A:215:GLY:HA3	0.460
2	A:345:LEU:HB2	A:350:VAL:HG13	0.459
2	A:55:ILE:CD1	A:215:GLY:HA3	0.449
2	A:126:LEU:HD11	A:350:VAL:HG12	0.448
2	A:140:PHE:CE1	A:146:VAL:HG11	0.447
2	A:149:PHE:CD2	A:319:THR:HG23	0.443
2	A:161:MET:HG3	A:190:PHE:CE1	0.443
2	A:182:GLU:O	A:183:ARG:C	0.436
2	A:12:ALA:HB2	A:213:PRO:HB2	0.428
2	A:160:MET:HE3	A:241:PHE:CD1	0.422
2	A:136:LEU:HD22	A:428:PHE:CD2	0.419
2	A:137:MET:HE1	A:362:GLN:HG3	0.417
2	A:239:LEU:HD23	A:241:PHE:CE2	0.412
2	A:1:MET:HE2	A:72:LEU:HA	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:333:PRO:HD3	A:405:PHE:CE2	0.607
3	A:127:LEU:HD11	A:167:ILE:CD1	0.597
3	A:127:LEU:HD11	A:167:ILE:HD11	0.581
3	A:126:LEU:HD11	A:350:VAL:HG12	0.541
3	A:333:PRO:CD	A:405:PHE:CE2	0.506
3	A:333:PRO:CD	A:405:PHE:CZ	0.501
3	A:333:PRO:HD3	A:405:PHE:CZ	0.469
3	A:133:VAL:HG11	A:335:VAL:HB	0.465
3	A:8:GLN:NE2	A:10:ILE:HD11	0.440
3	A:323:SER:O	A:334:ALA:HB1	0.439
3	A:145:LYS:HE2	A:284:THR:CG2	0.435
3	A:326:ILE:CD1	A:336:ASP:HA	0.422
3	A:140:PHE:CZ	A:146:VAL:HG11	0.419
3	A:333:PRO:HD2	A:405:PHE:CZ	0.417
3	A:246:TYR:CE1	A:250:LEU:HD11	0.408
4	A:333:PRO:CG	A:402:SER:HB3	0.663
4	A:8:GLN:NE2	A:10:ILE:HD11	0.641
4	A:246:TYR:CD1	A:276:MET:HE1	0.637
4	A:248:TYR:CE1	A:272:LEU:HD23	0.608
4	A:215:GLY:HA3	A:268:TYR:CE1	0.585
4	A:215:GLY:HA3	A:268:TYR:CZ	0.564
4	A:180:VAL:HG23	A:210:MET:CE	0.553
4	A:246:TYR:CE1	A:276:MET:HE1	0.523

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:8:GLN:HE21	A:10:ILE:HD11	0.511
4	A:332:TYR:CZ	A:412:THR:HG22	0.499
4	A:357:THR:HA	A:432:MET:HE1	0.490
4	A:133:VAL:HG21	A:335:VAL:HB	0.489
4	A:248:TYR:CD2	A:308:SER:HB3	0.475
4	A:161:MET:HE2	A:190:PHE:HA	0.471
4	A:180:VAL:HG23	A:210:MET:HE2	0.469
4	A:180:VAL:HG21	A:217:ARG:HD3	0.465
4	A:242:VAL:HG13	A:245:ILE:HD12	0.463
4	A:149:PHE:CE1	A:313:PHE:CE1	0.454
4	A:333:PRO:HG3	A:402:SER:HB3	0.447
4	A:164:ILE:CD1	A:190:PHE:CZ	0.442
4	A:149:PHE:CZ	A:313:PHE:CE1	0.433
4	A:210:MET:HE1	A:244:ASN:ND2	0.427
4	A:180:VAL:HG23	A:210:MET:HE1	0.426
4	A:230:LYS:HE3	A:234:GLU:OE1	0.408
4	A:248:TYR:CD2	A:308:SER:CB	0.406
4	A:333:PRO:CG	A:402:SER:CB	0.404
5	A:137:MET:HE1	A:362:GLN:HG3	0.757
5	A:137:MET:HE1	A:362:GLN:CG	0.587
5	A:8:GLN:NE2	A:10:ILE:HD11	0.586
5	A:149:PHE:CE1	A:313:PHE:CZ	0.534
5	A:308:SER:HB2	A:309:PRO:HD3	0.504

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:126:LEU:HD11	A:350:VAL:HG12	0.499
5	A:149:PHE:CE2	A:319:THR:HG23	0.499
5	A:161:MET:HE2	A:190:PHE:HA	0.457
5	A:8:GLN:HE21	A:10:ILE:HD11	0.447
5	A:137:MET:HE2	A:337:PRO:HB2	0.439
5	A:344:GLN:O	A:350:VAL:HG13	0.424
5	A:143:GLY:HA3	A:285:SER:OG	0.421
5	A:230:LYS:HE3	A:234:GLU:OE1	0.419
5	A:149:PHE:CD2	A:319:THR:HG23	0.416
5	A:332:TYR:HA	A:333:PRO:C	0.416
5	A:136:LEU:HD22	A:428:PHE:CD2	0.404
6	A:83:ALA:HB3	A:104:GLU:HG3	0.728
6	A:137:MET:HE1	A:362:GLN:HG3	0.704
6	A:190:PHE:CZ	A:194:MET:HE3	0.643
6	A:137:MET:HE1	A:362:GLN:CG	0.625
6	A:333:PRO:HD3	A:405:PHE:CZ	0.608
6	A:83:ALA:HB3	A:104:GLU:CG	0.569
6	A:160:MET:HE1	A:296:ALA:HB2	0.515
6	A:249:THR:HG23	A:272:LEU:HD21	0.512
6	A:8:GLN:NE2	A:10:ILE:HD11	0.511
6	A:405:PHE:HB2	A:408:ALA:HB3	0.498
6	A:333:PRO:CD	A:405:PHE:CZ	0.497
6	A:160:MET:CE	A:296:ALA:HB2	0.489

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:140:PHE:CZ	A:146:VAL:HG11	0.464
6	A:308:SER:HB2	A:309:PRO:HD3	0.444
6	A:417:LYS:HE2	A:448:GLY:HA3	0.428
6	A:190:PHE:CZ	A:194:MET:CE	0.410
6	A:161:MET:SD	A:193:GLU:HB3	0.408
6	A:244:ASN:ND2	A:298:TYR:H	0.405
6	A:357:THR:HA	A:432:MET:HE1	0.400
7	A:167:ILE:HD12	A:239:LEU:HD11	0.867
7	A:167:ILE:CD1	A:239:LEU:HD11	0.664
7	A:249:THR:HG23	A:272:LEU:HD11	0.558
7	A:157:THR:HG22	A:161:MET:HE3	0.534
7	A:221:ALA:HB2	A:248:TYR:CZ	0.514
7	A:126:LEU:HD11	A:350:VAL:HG12	0.496
7	A:225:LEU:HD22	A:279:LEU:HD12	0.490
7	A:308:SER:HB2	A:309:PRO:HD3	0.484
7	A:357:THR:HA	A:432:MET:HE1	0.476
7	A:368:TYR:CE1	A:372:LYS:HE3	0.470
7	A:149:PHE:CE1	A:313:PHE:CE1	0.467
7	A:132:LYS:HE2	A:403:GLN:HB3	0.432
7	A:149:PHE:CZ	A:313:PHE:CE1	0.432
7	A:219:ARG:HH12	A:275:GLU:CD	0.426
7	A:225:LEU:HD21	A:282:ARG:HB2	0.413
7	A:88:ILE:HG23	A:207:TYR:CD2	0.412

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:137:MET:HE1	A:362:GLN:HB2	0.401
8	A:88:ILE:HG23	A:207:TYR:CE2	0.739
8	A:137:MET:HE2	A:167:ILE:HD11	0.690
8	A:217:ARG:HB3	A:248:TYR:CE1	0.602
8	A:88:ILE:HG23	A:207:TYR:CD2	0.491
8	A:308:SER:HB2	A:309:PRO:HD3	0.480
8	A:164:ILE:CD1	A:190:PHE:CZ	0.476
8	A:12:ALA:HB3	A:213:PRO:HG3	0.475
8	A:246:TYR:CZ	A:308:SER:HA	0.464
8	A:157:THR:HG22	A:161:MET:HE3	0.462
8	A:217:ARG:CB	A:248:TYR:CE1	0.448
8	A:12:ALA:CB	A:213:PRO:HG3	0.444
8	A:149:PHE:CZ	A:313:PHE:CE2	0.436
8	A:12:ALA:HB3	A:213:PRO:CG	0.430
8	A:12:ALA:CB	A:213:PRO:CG	0.418
8	A:20:GLN:HE22	A:49:GLY:C	0.409
8	A:147:GLY:HA3	A:313:PHE:CZ	0.406
8	A:160:MET:HE3	A:190:PHE:CE2	0.404
8	A:187:GLY:HA3	A:207:TYR:CE1	0.400
9	A:253:THR:HG23	A:269:GLN:HE22	0.913
9	A:177:PHE:HB3	A:205:LEU:HD23	0.596
9	A:190:PHE:CE1	A:205:LEU:HD21	0.527
9	A:246:TYR:CE2	A:308:SER:HB2	0.513

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:164:ILE:CG1	A:241:PHE:CE2	0.435
9	A:136:LEU:HD22	A:428:PHE:CD2	0.424
9	A:55:ILE:HG23	A:57:MET:CE	0.421
9	A:164:ILE:CD1	A:190:PHE:CZ	0.407
9	A:134:ILE:HA	A:138:CYS:SG	0.405
9	A:164:ILE:HG13	A:241:PHE:CZ	0.405
9	A:243:ASP:HA	A:244:ASN:HA	0.404
9	A:164:ILE:HG12	A:241:PHE:CE2	0.403
10	A:136:LEU:HD22	A:146:VAL:HG13	0.861
10	A:408:ALA:HB1	A:412:THR:OG1	0.753
10	A:118:GLU:OE2	A:287:LYS:HE3	0.603
10	A:328:SER:HA	A:329:LEU:HG	0.597
10	A:160:MET:HE3	A:241:PHE:CD1	0.576
10	A:331:ILE:HG22	A:332:TYR:CG	0.561
10	A:329:LEU:HD23	A:331:ILE:HD11	0.549
10	A:136:LEU:CD2	A:146:VAL:HG13	0.546
10	A:167:ILE:HD12	A:239:LEU:HG	0.546
10	A:408:ALA:HB1	A:412:THR:HG1	0.531
10	A:244:ASN:ND2	A:298:TYR:H	0.510
10	A:134:ILE:H	A:134:ILE:HD12	0.506
10	A:297:VAL:CG2	A:312:THR:HG21	0.503
10	A:249:THR:HA	A:272:LEU:HD11	0.480
10	A:245:ILE:HG21	A:312:THR:HG23	0.472

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:128:GLU:HB3	A:421:LEU:HD22	0.463
10	A:134:ILE:HB	A:137:MET:HB2	0.457
10	A:297:VAL:HG21	A:312:THR:HG21	0.448
10	A:331:ILE:HG22	A:332:TYR:CD1	0.439
10	A:364:ILE:HD12	A:432:MET:HG2	0.439
10	A:118:GLU:CD	A:287:LYS:HE3	0.437
10	A:8:GLN:NE2	A:10:ILE:HD11	0.433
10	A:167:ILE:HD12	A:239:LEU:CG	0.428
10	A:134:ILE:HD13	A:137:MET:HE2	0.423
10	A:1:MET:HG3	A:71:ASP:O	0.415
10	A:132:LYS:HD3	A:403:GLN:HE21	0.411
10	A:317:ASP:C	A:319:THR:N	0.405
10	A:230:LYS:HE3	A:234:GLU:OE1	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	458	430	21	7
2	458	414	31	13
3	458	443	13	2
4	458	447	11	0
5	458	444	13	1
6	458	446	12	0
7	458	450	7	1

Model ID	Analyzed	Favored	Allowed	Outliers
8	458	450	8	0
9	458	436	20	2
10	458	448	10	0

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	381	365	15	1
2	381	376	4	1
3	381	375	3	3
4	381	376	3	2
5	381	376	5	0
6	381	378	2	1
7	381	375	5	1
8	381	373	7	1
9	381	376	4	1
10	381	363	9	9

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	319	THR
2	A	154	VAL
3	A	184	THR
3	A	256	SER
3	A	272	LEU

Model ID	Chain	Residue ID	Residue type
4	A	249	THR
4	A	253	THR
6	A	266	VAL
7	A	311	THR
8	A	182	GLU
9	A	266	VAL
10	A	126	LEU
10	A	137	MET
10	A	138	CYS
10	A	167	ILE
10	A	271	THR
10	A	319	THR
10	A	322	LEU
10	A	329	LEU
10	A	331	ILE

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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