Integrative Structure Validation Report

July 22, 2024 - 05:04 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	9A2P
PDB-Dev ID	PDBDEV_00000174
Structure Title	Model of E. coli FtsH 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

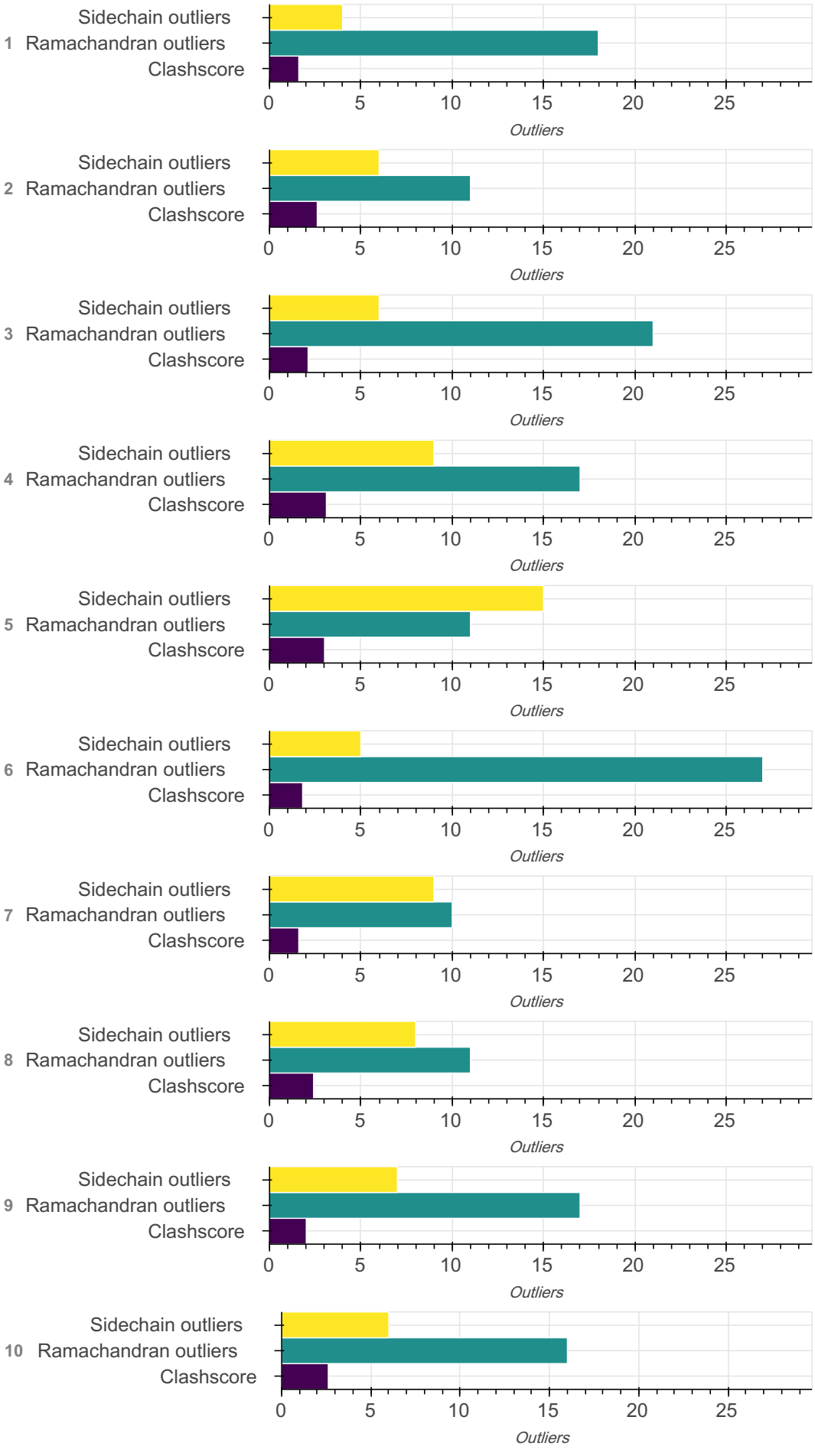
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 5 10 15 20 25
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0 5 10 15 20 25
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	P0AAI3	A	A	644
2	1	1	P0AAI3	A	A	644
3	1	1	P0AAI3	A	A	644
4	1	1	P0AAI3	A	A	644
5	1	1	P0AAI3	A	A	644
6	1	1	P0AAI3	A	A	644
7	1	1	P0AAI3	A	A	644
8	1	1	P0AAI3	A	A	644
9	1	1	P0AAI3	A	A	644
10	1	1	P0AAI3	A	A	644

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	-	1-644

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 50060 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
CD--HD2	1.09	0.97	1160
CG--HG2	1.09	0.97	2130
CD1--HD13	1.09	0.97	910
CB--HB3	1.09	0.97	4690
CB--HB2	1.09	0.97	4690
NZ--HZ3	1.01	0.89	370
CE--HE2	1.09	0.97	620
CG1--HG12	1.09	0.97	900
OG1--HG1	0.96	0.84	270
CA--HA	1.09	0.97	5860
CD2--HD22	1.09	0.97	510
CD--HD3	1.09	0.97	1160
CE--HE3	1.09	0.97	620
CG--HG3	1.09	0.97	2130
CG2--HG23	1.09	0.97	1170
CG2--HG22	1.09	0.97	1170
NZ--HZ2	1.01	0.89	370
CB--HB1	1.09	0.97	590
CD1--HD12	1.09	0.97	910
OG--HG	0.96	0.84	320
CB--HB	1.09	0.97	1170
CD1--HD11	1.09	0.97	910

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA2	1.09	0.97	580
CG1--HG13	1.09	0.97	900
NZ--HZ1	1.01	0.89	370
CD2--HD23	1.09	0.97	510
CG1--HG11	1.09	0.97	500
CG2--HG21	1.09	0.97	1170
CE--HE1	1.09	0.97	250
CG--HG	1.09	0.97	510
N--H1	1.01	0.89	10
CD2--HD21	1.09	0.97	510
CA--HA3	1.09	0.97	580
OH--HH	0.96	0.84	100
N--H3	1.01	0.89	10
N--H2	1.01	0.89	10
SG--HG	1.33	1.20	3
SG--HG	1.34	1.20	17
N--H	1.01	0.86	6070
CD1--HD1	1.08	0.93	400
ND2--HD22	1.01	0.86	260
NH2--HH21	1.01	0.86	430
NE--HE	1.01	0.86	430
NE2--HE21	1.01	0.86	220
ND1--HD1	1.01	0.86	86

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE2--HE2	1.08	0.93	350
CZ--HZ	1.08	0.93	250
CD2--HD2	1.08	0.93	440
NH1--HH12	1.01	0.86	430
ND2--HD21	1.01	0.86	260
NH2--HH22	1.01	0.86	430
CE1--HE1	1.08	0.93	440
NH1--HH11	1.01	0.86	430
NE2--HE22	1.01	0.86	220
CZ2--HZ2	1.08	0.93	50
NE1--HE1	1.01	0.86	50
CZ3--HZ3	1.08	0.93	50
CE3--HE3	1.08	0.93	50
CH2--HH2	1.08	0.93	50
NE2--HE2	1.01	0.86	4

Standard geometry: angle outliers

There are 279 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	140.78	1
CA-CB-CG	112.60	121.47	1
C-N-CA	121.70	136.72	1
OE1-CD-NE2	122.60	115.63	1
C-N-CA	121.70	133.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	133.29	1
CA-CB-CG	113.80	119.93	1
C-N-CA	121.70	132.70	1
OE1-CD-NE2	122.60	116.50	1
C-N-CA	121.70	132.48	1
C-N-CA	121.70	132.37	1
C-N-CA	121.70	132.32	1
OE1-CD-NE2	122.60	116.76	1
OE1-CD-NE2	122.60	116.82	1
OE1-CD-NE2	122.60	116.86	1
OE1-CD-NE2	122.60	116.87	1
OE1-CD-NE2	122.60	116.88	1
OE1-CD-NE2	122.60	116.92	1
OE1-CD-NE2	122.60	116.99	2
N-CA-C	111.00	126.68	1
OE1-CD-NE2	122.60	117.03	1
OE1-CD-NE2	122.60	117.06	1
O-C-N	123.00	114.40	1
C-N-CA	121.70	131.31	1
C-N-CA	121.70	131.30	1
OE1-CD-NE2	122.60	117.28	1
C-N-CA	121.70	131.23	1
OE1-CD-NE2	122.60	117.32	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.19	1
OE1-CD-NE2	122.60	117.33	1
OE1-CD-NE2	122.60	117.38	1
C-N-CA	121.70	130.96	1
C-CA-CB	110.10	119.87	1
NE-CZ-NH2	119.20	123.82	1
C-N-CA	121.70	130.86	1
OE1-CD-NE2	122.60	117.51	1
C-N-CA	121.70	130.85	1
OE1-CD-NE2	122.60	117.55	1
CB-CG-CD2	131.20	124.66	1
C-N-CA	121.70	130.67	1
OE1-CD-NE2	122.60	117.64	2
C-N-CA	121.70	130.63	1
OE1-CD-NE2	122.60	117.65	1
C-N-CA	121.70	130.62	1
O-C-N	123.00	115.15	1
CD-NE-CZ	124.40	131.20	1
C-N-CA	121.70	130.37	1
OE1-CD-NE2	122.60	117.80	1
C-N-CA	121.70	130.30	1
OE1-CD-NE2	122.60	117.83	1
C-N-CA	121.70	130.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	108.24	1
C-N-CA	121.70	130.25	1
C-N-CA	121.70	130.24	1
OE1-CD-NE2	122.60	117.86	1
CA-CB-CG2	110.50	118.55	1
C-N-CA	121.70	130.21	1
OE1-CD-NE2	122.60	117.87	1
C-N-CA	121.70	130.18	1
C-N-CA	121.70	130.16	1
CB-CG-CD2	131.20	125.09	1
OE1-CD-NE2	122.60	117.91	2
OE1-CD-NE2	122.60	117.93	2
OE1-CD-NE2	122.60	117.94	1
C-N-CA	121.70	130.06	1
OE1-CD-NE2	122.60	117.96	1
OE1-CD-NE2	122.60	117.97	1
OE1-CD-NE2	122.60	117.98	2
N-CA-C	112.10	100.55	1
OD1-CG-ND2	122.60	117.99	1
CA-CB-CG	112.60	117.18	1
C-N-CA	121.70	129.94	1
OE1-CD-NE2	122.60	118.04	2
C-N-CA	121.70	129.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.08	3
OE1-CD-NE2	122.60	118.09	2
OE1-CD-NE2	122.60	118.10	2
C-N-CA	121.70	129.79	1
CA-CB-CG	112.60	117.09	1
CA-CB-CG	112.60	117.08	1
OE1-CD-NE2	122.60	118.12	2
C-N-CA	121.70	129.77	1
OE1-CD-NE2	122.60	118.13	1
OD1-CG-ND2	122.60	118.15	1
OE1-CD-NE2	122.60	118.15	1
OE1-CD-NE2	122.60	118.16	3
OE1-CD-NE2	122.60	118.17	1
OE1-CD-NE2	122.60	118.18	3
C-N-CA	121.70	129.64	1
OE1-CD-NE2	122.60	118.19	1
N-CA-C	111.00	123.33	1
OE1-CD-NE2	122.60	118.20	1
CB-CG-CD2	131.20	125.48	1
OE1-CD-NE2	122.60	118.21	3
C-N-CA	121.70	129.60	1
C-N-CA	121.70	129.59	1
OE1-CD-NE2	122.60	118.22	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.23	2
OE1-CD-NE2	122.60	118.24	3
C-N-CA	121.70	129.54	1
OE1-CD-NE2	122.60	118.25	3
CA-C-N	116.20	124.88	1
OE1-CD-NE2	122.60	118.26	1
CA-CB-CG1	110.40	103.04	1
OE1-CD-NE2	122.60	118.27	1
C-N-CA	121.70	129.49	2
C-N-CA	121.70	129.48	1
N-CA-C	111.00	123.09	1
OE1-CD-NE2	122.60	118.28	2
OE1-CD-NE2	122.60	118.29	1
C-N-CA	121.70	129.46	2
OE1-CD-NE2	122.60	118.30	3
OE1-CD-NE2	122.60	118.31	2
OD1-CG-ND2	122.60	118.31	1
OD1-CG-ND2	122.60	118.32	1
OE1-CD-NE2	122.60	118.32	1
OE1-CD-NE2	122.60	118.33	2
OE1-CD-NE2	122.60	118.34	2
CA-CB-CG	112.60	116.86	1
OD1-CG-ND2	122.60	118.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.67	2
OD1-CG-ND2	122.60	118.35	1
OE1-CD-NE2	122.60	118.35	4
CD-NE-CZ	124.40	130.35	1
C-N-CA	121.70	129.33	1
CA-CB-OG1	109.60	115.96	1
OE1-CD-NE2	122.60	118.37	2
OD1-CG-ND2	122.60	118.37	1
C-N-CA	121.70	129.30	2
OE1-CD-NE2	122.60	118.38	3
OE1-CD-NE2	122.60	118.40	3
CA-CB-CG	112.60	108.40	1
OD1-CG-ND2	122.60	118.40	1
OE1-CD-NE2	122.60	118.41	5
N-CA-CB	110.50	103.37	1
C-N-CA	121.70	129.23	1
CA-CB-CG	112.60	108.42	1
C-N-CA	121.70	129.22	1
OE1-CD-NE2	122.60	118.43	2
OD1-CG-ND2	122.60	118.43	1
C-N-CA	121.70	129.20	1
OE1-CD-NE2	122.60	118.44	2
OE1-CD-NE2	122.60	118.45	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.81	1
OE1-CD-NE2	122.60	118.46	2
C-N-CA	121.70	129.16	1
N-CA-CB	103.00	107.55	1
OE1-CD-NE2	122.60	118.47	3
OE1-CD-NE2	122.60	118.48	2
CB-CG-CD2	131.20	125.85	1
N-CA-C	111.00	122.52	1
O-C-N	123.00	116.42	1
OE1-CD-NE2	122.60	118.49	2
CB-CG-CD2	131.20	125.86	2
OE1-CD-NE2	122.60	118.50	1
OD1-CG-ND2	122.60	118.50	2
C-N-CA	121.70	129.06	1
OE1-CD-NE2	122.60	118.51	2
N-CA-C	111.00	122.43	1
OD1-CG-ND2	122.60	118.52	1
N-CA-CB	110.50	103.57	1
OE1-CD-NE2	122.60	118.52	1
OD1-CG-ND2	122.60	118.53	1
CB-CG-CD2	131.20	125.91	1
OE1-CD-NE2	122.60	118.53	1
CD-NE-CZ	124.40	130.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.01	2
CA-CB-CG	112.60	116.66	1
OE1-CD-NE2	122.60	118.54	1
NE-CZ-NH1	121.50	125.56	1
OD1-CG-ND2	122.60	118.55	1
OE1-CD-NE2	122.60	118.56	3
CB-CG-CD2	131.20	125.96	1
OD1-CG-ND2	122.60	118.57	2
OE1-CD-NE2	122.60	118.57	2
C-N-CA	121.70	128.94	1
N-CA-C	111.00	122.27	1
OD1-CG-ND2	122.60	118.58	2
OE1-CD-NE2	122.60	118.58	1
OE1-CD-NE2	122.60	118.59	4
C-N-CA	121.70	128.92	1
CB-CG-CD2	131.20	126.00	1
CZ-OH-HH	122.05	110.00	1
HZ1-NZ-HZ2	96.89	109.00	1
C-N-H	112.17	124.30	1
HH21-NH2-HH22	107.85	120.00	1
C-N-H	112.14	124.30	1
HZ1-NZ-HZ2	96.79	109.00	1
HZ1-NZ-HZ2	96.63	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	111.85	124.30	1
HZ1-NZ-HZ2	96.50	109.00	1
HH21-NH2-HH22	107.48	120.00	1
C-N-H	111.76	124.30	1
C-N-H	111.62	124.30	1
HZ1-NZ-HZ2	96.24	109.00	1
C-N-H	111.54	124.30	1
HZ2-NZ-HZ3	96.19	109.00	1
HZ1-NZ-HZ2	96.14	109.00	1
HZ2-NZ-HZ3	96.12	109.00	1
HZ1-NZ-HZ2	96.08	109.00	1
CD-NE2-HE21	107.08	120.00	1
HZ2-NZ-HZ3	96.01	109.00	1
HZ2-NZ-HZ3	95.98	109.00	1
HZ1-NZ-HZ2	95.83	109.00	1
HZ1-NZ-HZ2	95.76	109.00	1
C-N-H	111.05	124.30	1
HH11-NH1-HH12	105.65	120.00	1
HH11-NH1-HH12	104.72	120.00	1
C-N-H	108.32	124.30	1
C-N-H	108.28	124.30	1
C-N-H	107.45	124.30	1
C-N-H	107.12	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	1.60	16
2	2.61	26
3	2.11	21
4	3.11	31
5	3.01	30
6	1.81	18
7	1.60	16
8	2.41	24
9	2.01	20
10	2.61	26

All 228 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:537:MET:HE3	A:542:ALA:HB2	0.656
1	A:335:MET:HB3	A:340:LEU:HD11	0.581
1	A:425:VAL:HG11	A:464:SER:HB2	0.570
1	A:473:ARG:HH11	A:493:ILE:HD11	0.521
1	A:237:PHE:CD1	A:281:GLU:HB3	0.519
1	A:237:PHE:CD1	A:285:PHE:CZ	0.476
1	A:431:VAL:HG22	A:448:PHE:CE1	0.472
1	A:27:SER:C	A:29:GLY:H	0.470
1	A:166:GLU:CD	A:315:ARG:HH12	0.457

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:473:ARG:HH11	A:493:ILE:CD1	0.457
1	A:237:PHE:HD1	A:285:PHE:CZ	0.450
1	A:425:VAL:CG1	A:464:SER:HB2	0.442
1	A:425:VAL:HG11	A:464:SER:CB	0.435
1	A:413:TYR:CZ	A:575:LYS:HE2	0.423
1	A:445:VAL:HG13	A:447:PHE:CE2	0.421
1	A:241:LYS:HA	A:291:ILE:HD11	0.409
2	A:537:MET:HE3	A:542:ALA:HB2	0.740
2	A:321:LEU:HD21	A:441:ARG:NH1	0.684
2	A:141:MET:HE2	A:214:PHE:CE1	0.618
2	A:241:LYS:HE3	A:285:PHE:CZ	0.603
2	A:393:MET:HE2	A:402:VAL:HG11	0.584
2	A:537:MET:HE3	A:542:ALA:CB	0.548
2	A:241:LYS:CE	A:285:PHE:CE1	0.534
2	A:241:LYS:HE3	A:285:PHE:CE1	0.503
2	A:335:MET:HE2	A:385:PHE:CZ	0.495
2	A:241:LYS:HE2	A:285:PHE:CE1	0.481
2	A:194:PRO:HD2	A:441:ARG:HH21	0.480
2	A:141:MET:HE2	A:214:PHE:CZ	0.478
2	A:434:VAL:HG23	A:589:ILE:HD11	0.472
2	A:413:TYR:CZ	A:575:LYS:HE2	0.471
2	A:537:MET:SD	A:545:ILE:HD12	0.471
2	A:612:ASN:C	A:614:GLY:H	0.465

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:261:GLY:C	A:529:ARG:HH22	0.456
2	A:237:PHE:CD1	A:285:PHE:CE2	0.455
2	A:335:MET:HB3	A:340:LEU:HD11	0.446
2	A:221:PHE:HB3	A:274:THR:HG21	0.441
2	A:321:LEU:HD21	A:441:ARG:HH12	0.439
2	A:14:VAL:HG11	A:111:LEU:HD21	0.432
2	A:27:SER:C	A:29:GLY:H	0.429
2	A:32:VAL:CG2	A:66:TYR:CD2	0.422
2	A:483:GLU:CD	A:483:GLU:H	0.405
2	A:580:LYS:HE2	A:604:TRP:CH2	0.403
3	A:228:VAL:HG21	A:232:ARG:HE	0.773
3	A:424:LEU:HD21	A:598:VAL:HG11	0.591
3	A:228:VAL:CG2	A:232:ARG:HE	0.566
3	A:27:SER:C	A:29:GLY:H	0.542
3	A:473:ARG:NE	A:485:VAL:HG11	0.537
3	A:473:ARG:HD2	A:485:VAL:HG11	0.529
3	A:478:ILE:HG21	A:568:MET:HE1	0.502
3	A:473:ARG:CD	A:485:VAL:HG11	0.471
3	A:134:PHE:HZ	A:214:PHE:CD1	0.467
3	A:134:PHE:CZ	A:214:PHE:CD1	0.464
3	A:166:GLU:CD	A:315:ARG:HH12	0.459
3	A:413:TYR:CZ	A:575:LYS:HE2	0.459
3	A:8:TRP:CH2	A:119:PHE:CZ	0.445

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:335:MET:HB3	A:340:LEU:HD11	0.445
3	A:421:ILE:HD11	A:564:LEU:HG	0.445
3	A:454:ALA:HB1	A:507:TRP:CZ2	0.441
3	A:434:VAL:HG23	A:589:ILE:HD11	0.432
3	A:526:PHE:O	A:527:LEU:HG	0.419
3	A:279:LEU:HD22	A:312:ARG:HD3	0.413
3	A:474:LEU:HD21	A:557:TYR:CZ	0.407
3	A:478:ILE:HG21	A:568:MET:CE	0.404
4	A:216:ILE:HD11	A:236:MET:SD	0.891
4	A:356:PHE:CE2	A:393:MET:HE3	0.602
4	A:225:PHE:CD1	A:271:ARG:HA	0.598
4	A:225:PHE:CD2	A:271:ARG:HG2	0.584
4	A:170:TYR:HB2	A:184:ILE:HD13	0.583
4	A:473:ARG:CD	A:485:VAL:HG11	0.536
4	A:401:MET:HE3	A:403:MET:SD	0.517
4	A:40:GLU:OE2	A:60:LYS:HE2	0.514
4	A:222:VAL:HA	A:225:PHE:CD2	0.506
4	A:397:GLU:CD	A:438:PRO:HB2	0.499
4	A:412:ALA:HA	A:436:ILE:HG21	0.495
4	A:216:ILE:HD11	A:236:MET:CE	0.487
4	A:221:PHE:CE2	A:250:ILE:HG23	0.483
4	A:237:PHE:CD1	A:281:GLU:HB3	0.483
4	A:433:LYS:HE3	A:441:ARG:HD3	0.479

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:225:PHE:CE1	A:274:THR:HB	0.472
4	A:279:LEU:HD22	A:312:ARG:HD3	0.463
4	A:413:TYR:CZ	A:575:LYS:HE2	0.455
4	A:177:PHE:CD1	A:184:ILE:HD11	0.452
4	A:503:MET:HA	A:507:TRP:CE3	0.448
4	A:433:LYS:HE3	A:441:ARG:CD	0.447
4	A:431:VAL:HG13	A:445:VAL:HG13	0.442
4	A:397:GLU:OE2	A:438:PRO:HB2	0.442
4	A:279:LEU:HD21	A:307:LEU:HD23	0.430
4	A:393:MET:HB2	A:440:GLY:HA2	0.427
4	A:433:LYS:HE2	A:446:THR:OG1	0.424
4	A:216:ILE:HD11	A:236:MET:HE1	0.410
4	A:170:TYR:CD2	A:184:ILE:HD12	0.408
4	A:581:TYR:C	A:583:THR:H	0.408
4	A:237:PHE:CD1	A:285:PHE:CZ	0.402
4	A:170:TYR:CG	A:184:ILE:HD13	0.400
5	A:190:MET:SD	A:199:THR:HG23	0.748
5	A:285:PHE:CE1	A:291:ILE:HD12	0.625
5	A:403:MET:HE1	A:411:THR:CG2	0.586
5	A:412:ALA:O	A:416:ALA:HB3	0.568
5	A:134:PHE:CZ	A:216:ILE:HD11	0.544
5	A:403:MET:HE1	A:411:THR:HG21	0.529
5	A:167:LEU:HD13	A:294:ILE:HD11	0.528

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:134:PHE:CE2	A:216:ILE:HD11	0.495
5	A:27:SER:C	A:29:GLY:H	0.489
5	A:195:GLY:H	A:199:THR:HG21	0.485
5	A:335:MET:HB3	A:340:LEU:HD11	0.478
5	A:351:ARG:O	A:583:THR:HG21	0.476
5	A:198:LYS:HD2	A:296:ALA:HB1	0.464
5	A:174:PRO:HG3	A:185:PRO:HD3	0.457
5	A:241:LYS:HE3	A:285:PHE:CZ	0.457
5	A:389:LYS:HG2	A:393:MET:HE3	0.450
5	A:306:ALA:HB1	A:312:ARG:HH12	0.446
5	A:403:MET:HE2	A:407:GLN:HB3	0.445
5	A:632:ASN:CB	A:633:PRO:HD3	0.443
5	A:256:VAL:HG23	A:278:MET:HE1	0.442
5	A:630:THR:HB	A:631:PRO:CD	0.441
5	A:170:TYR:HA	A:177:PHE:CE2	0.437
5	A:198:LYS:HE2	A:251:ASP:OD1	0.434
5	A:134:PHE:CE1	A:236:MET:HA	0.428
5	A:632:ASN:CG	A:633:PRO:HD3	0.425
5	A:167:LEU:CD1	A:294:ILE:HD11	0.424
5	A:575:LYS:HG3	A:589:ILE:HG21	0.422
5	A:141:MET:HE2	A:214:PHE:CZ	0.419
5	A:141:MET:HE2	A:214:PHE:CE1	0.413
5	A:403:MET:HE1	A:411:THR:HG23	0.413

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:401:MET:CE	A:438:PRO:HB3	0.650
6	A:473:ARG:HH11	A:493:ILE:HD11	0.644
6	A:401:MET:SD	A:438:PRO:HB3	0.552
6	A:415:GLU:CD	A:444:GLY:HA2	0.550
6	A:241:LYS:HA	A:291:ILE:HD11	0.531
6	A:122:GLN:C	A:125:GLY:H	0.517
6	A:139:ALA:HB2	A:216:ILE:HD12	0.510
6	A:222:VAL:CG2	A:256:VAL:HG13	0.487
6	A:335:MET:HB3	A:340:LEU:HD11	0.482
6	A:256:VAL:HG11	A:275:LEU:HG	0.478
6	A:413:TYR:CZ	A:575:LYS:HE2	0.471
6	A:401:MET:CE	A:438:PRO:CB	0.465
6	A:355:GLY:HA3	A:441:ARG:NH1	0.460
6	A:401:MET:HE1	A:438:PRO:HB3	0.437
6	A:178:GLN:HE21	A:288:ASN:HB3	0.426
6	A:335:MET:HE2	A:385:PHE:CZ	0.420
6	A:537:MET:SD	A:545:ILE:HD12	0.402
6	A:131:ALA:HB1	A:140:ARG:HB3	0.401
7	A:478:ILE:HG21	A:568:MET:HE1	0.706
7	A:116:TRP:CZ3	A:120:MET:HE2	0.575
7	A:537:MET:SD	A:545:ILE:HD12	0.537
7	A:503:MET:CE	A:552:LEU:HD13	0.524
7	A:474:LEU:HD21	A:557:TYR:CZ	0.509

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:434:VAL:HG23	A:589:ILE:HD11	0.502
7	A:116:TRP:CH2	A:120:MET:HE2	0.498
7	A:224:MET:HE3	A:232:ARG:HH12	0.488
7	A:505:THR:HG22	A:545:ILE:HD13	0.477
7	A:537:MET:HE3	A:542:ALA:CB	0.448
7	A:478:ILE:CG2	A:568:MET:HE1	0.424
7	A:335:MET:HE1	A:349:ILE:HD12	0.419
7	A:419:ALA:HB2	A:434:VAL:HG21	0.418
7	A:581:TYR:C	A:583:THR:H	0.411
7	A:519:ALA:C	A:521:GLU:H	0.406
7	A:413:TYR:CZ	A:575:LYS:HE2	0.405
8	A:398:ARG:NH2	A:437:ILE:HG23	0.744
8	A:537:MET:HE3	A:542:ALA:HB2	0.638
8	A:434:VAL:HG23	A:589:ILE:HD11	0.550
8	A:429:ASP:CG	A:448:PHE:CD1	0.538
8	A:429:ASP:HB2	A:448:PHE:CD1	0.538
8	A:413:TYR:CZ	A:575:LYS:HE2	0.506
8	A:443:LEU:HD22	A:491:ASN:CG	0.493
8	A:421:ILE:O	A:425:VAL:HG22	0.488
8	A:419:ALA:HB2	A:434:VAL:HG21	0.474
8	A:443:LEU:HD22	A:491:ASN:ND2	0.470
8	A:586:ALA:HB3	A:587:PRO:HD3	0.465
8	A:412:ALA:HA	A:436:ILE:HG21	0.464

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:537:MET:HE3	A:542:ALA:CB	0.448
8	A:429:ASP:HB3	A:430:PRO:HD2	0.443
8	A:611:ASN:C	A:613:SER:H	0.441
8	A:513:LEU:HD13	A:516:LEU:HD11	0.439
8	A:27:SER:C	A:29:GLY:H	0.437
8	A:260:ARG:HA	A:268:HIS:CE1	0.427
8	A:335:MET:HB3	A:340:LEU:HD11	0.416
8	A:133:SER:HB2	A:136:LYS:HB2	0.412
8	A:335:MET:HE2	A:385:PHE:CZ	0.405
8	A:221:PHE:HB3	A:274:THR:HG21	0.402
8	A:412:ALA:HA	A:436:ILE:CG2	0.402
8	A:534:ALA:C	A:536:HIS:N	0.402
9	A:443:LEU:HD11	A:488:GLY:C	0.840
9	A:241:LYS:HE2	A:285:PHE:CZ	0.660
9	A:393:MET:CE	A:447:PHE:CE1	0.610
9	A:191:VAL:HG11	A:316:GLN:HE21	0.609
9	A:401:MET:HE1	A:440:GLY:N	0.597
9	A:170:TYR:CE2	A:184:ILE:HD13	0.575
9	A:393:MET:CE	A:447:PHE:CZ	0.544
9	A:221:PHE:HB3	A:274:THR:HG21	0.517
9	A:414:HIS:NE2	A:443:LEU:HD13	0.465
9	A:335:MET:HB3	A:340:LEU:HD11	0.457
9	A:443:LEU:HD21	A:488:GLY:HA3	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:413:TYR:CZ	A:575:LYS:HE2	0.453
9	A:393:MET:HE3	A:447:PHE:CE1	0.446
9	A:443:LEU:CG	A:488:GLY:HA3	0.437
9	A:412:ALA:HB2	A:436:ILE:HD11	0.422
9	A:241:LYS:NZ	A:285:PHE:CE1	0.421
9	A:401:MET:HB2	A:401:MET:HE3	0.414
9	A:286:GLU:C	A:288:ASN:H	0.410
9	A:393:MET:HE2	A:447:PHE:CZ	0.409
9	A:426:PRO:CG	A:460:GLN:HE21	0.408
10	A:601:PRO:HD2	A:604:TRP:CG	0.632
10	A:170:TYR:CE2	A:184:ILE:HD13	0.620
10	A:601:PRO:HD2	A:604:TRP:CD2	0.583
10	A:505:THR:HB	A:518:TYR:CZ	0.557
10	A:335:MET:HB3	A:340:LEU:HD11	0.552
10	A:601:PRO:HD2	A:604:TRP:CD1	0.548
10	A:505:THR:HB	A:518:TYR:CE2	0.543
10	A:413:TYR:CZ	A:575:LYS:HE2	0.536
10	A:19:PHE:O	A:23:GLY:HA3	0.521
10	A:473:ARG:HH11	A:493:ILE:HD11	0.510
10	A:601:PRO:HD2	A:604:TRP:CE2	0.496
10	A:191:VAL:HG21	A:316:GLN:HE21	0.494
10	A:27:SER:C	A:29:GLY:H	0.484
10	A:526:PHE:CZ	A:528:GLY:HA2	0.479

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:389:LYS:HG2	A:393:MET:HE2	0.461
10	A:403:MET:SD	A:443:LEU:HD22	0.456
10	A:601:PRO:CD	A:604:TRP:CE2	0.446
10	A:421:ILE:HD11	A:564:LEU:HG	0.445
10	A:221:PHE:HB3	A:274:THR:HG21	0.442
10	A:134:PHE:CZ	A:141:MET:HB2	0.437
10	A:586:ALA:HB3	A:587:PRO:HD3	0.433
10	A:421:ILE:O	A:425:VAL:HG22	0.432
10	A:425:VAL:HG23	A:428:HIS:HB2	0.421
10	A:335:MET:HE1	A:349:ILE:HD12	0.414
10	A:134:PHE:CD1	A:239:GLN:OE1	0.413
10	A:443:LEU:HD12	A:487:THR:HB	0.402

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	642	592	32	18
2	642	595	36	11
3	642	580	41	21
4	642	586	39	17
5	642	587	44	11
6	642	567	48	27
7	642	594	38	10
8	642	592	39	11

Model ID	Analyzed	Favored	Allowed	Outliers
9	642	576	49	17
10	642	594	32	16

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	527	508	15	4
2	527	508	13	6
3	527	507	14	6
4	527	500	18	9
5	527	498	14	15
6	527	506	16	5
7	527	498	20	9
8	527	506	13	8
9	527	503	17	7
10	527	511	10	6

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	5	LEU
1	A	112	LEU
1	A	483	GLU
1	A	526	PHE
2	A	5	LEU
2	A	119	PHE

Model ID	Chain	Residue ID	Residue type
2	A	483	GLU
2	A	530	SER
2	A	630	THR
2	A	641	LEU
3	A	5	LEU
3	A	98	LEU
3	A	134	PHE
3	A	530	SER
3	A	597	ASP
3	A	636	THR
4	A	5	LEU
4	A	98	LEU
4	A	111	LEU
4	A	112	LEU
4	A	228	VAL
4	A	401	MET
4	A	433	LYS
4	A	509	PHE
4	A	510	SER
5	A	5	LEU
5	A	98	LEU
5	A	111	LEU
5	A	112	LEU

Model ID	Chain	Residue ID	Residue type
5	A	258	ARG
5	A	424	LEU
5	A	429	ASP
5	A	431	VAL
5	A	474	LEU
5	A	499	LEU
5	A	583	THR
5	A	584	ILE
5	A	592	LEU
5	A	604	TRP
5	A	630	THR
6	A	9	LEU
6	A	16	MET
6	A	98	LEU
6	A	630	THR
6	A	641	LEU
7	A	5	LEU
7	A	19	PHE
7	A	103	PHE
7	A	112	LEU
7	A	120	MET
7	A	134	PHE
7	A	445	VAL

Model ID	Chain	Residue ID	Residue type
7	A	453	ASP
7	A	613	SER
8	A	1	MET
8	A	5	LEU
8	A	98	LEU
8	A	166	GLU
8	A	425	VAL
8	A	429	ASP
8	A	445	VAL
8	A	456	SER
9	A	5	LEU
9	A	9	LEU
9	A	98	LEU
9	A	132	MET
9	A	517	LEU
9	A	526	PHE
9	A	636	THR
10	A	1	MET
10	A	5	LEU
10	A	9	LEU
10	A	19	PHE
10	A	103	PHE
10	A	112	LEU

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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