Integrative Structure Validation Report

July 22, 2024 - 05:08 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	9A2W
PDB-Dev ID	PDBDEV_00000181
Structure Title	Model of E. coli MtlA 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

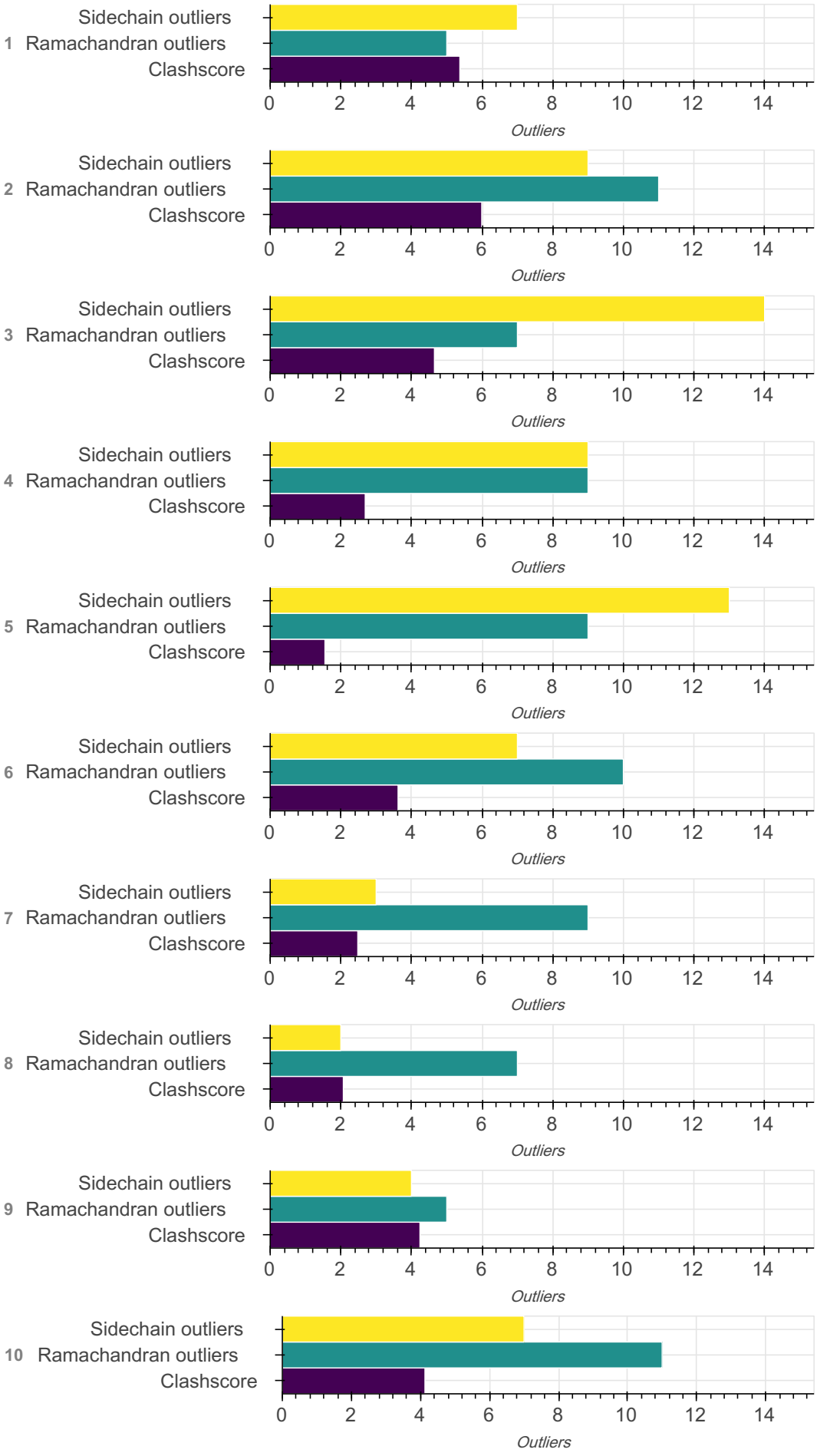
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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	P00550	A	A	637
2	1	1	P00550	A	A	637
3	1	1	P00550	A	A	637
4	1	1	P00550	A	A	637
5	1	1	P00550	A	A	637
6	1	1	P00550	A	A	637
7	1	1	P00550	A	A	637
8	1	1	P00550	A	A	637
9	1	1	P00550	A	A	637
10	1	1	P00550	A	A	637

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	-	1-637

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 49040 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
CG2--HG22	1.09	0.97	1340
CA--HA	1.09	0.97	5700
CB--HB3	1.09	0.97	4360
CB--HB2	1.09	0.97	4360
CG--HG3	1.09	0.97	1540
CG--HG2	1.09	0.97	1540
CA--HA2	1.09	0.97	670
CD1--HD13	1.09	0.97	1210
CG--HG	1.09	0.97	670
CA--HA3	1.09	0.97	670
CD1--HD11	1.09	0.97	1210
CD2--HD23	1.09	0.97	670
CG2--HG21	1.09	0.97	1340
CD--HD2	1.09	0.97	800
OG--HG	0.96	0.84	400
CG1--HG11	1.09	0.97	500
NZ--HZ2	1.01	0.89	310
CD1--HD12	1.09	0.97	1210
CD--HD3	1.09	0.97	800
CG1--HG13	1.09	0.97	1040
CD2--HD22	1.09	0.97	670
CB--HB	1.09	0.97	1340

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ1	1.01	0.89	310
CG2--HG23	1.09	0.97	1340
N--H3	1.01	0.89	10
NZ--HZ3	1.01	0.89	310
CG1--HG12	1.09	0.97	1040
CE--HE1	1.09	0.97	250
CB--HB1	1.09	0.97	640
CE--HE2	1.09	0.97	560
CD2--HD21	1.09	0.97	670
OH--HH	0.96	0.84	110
CE--HE3	1.09	0.97	560
OG1--HG1	0.96	0.84	300
N--H1	1.01	0.89	10
N--H2	1.01	0.89	10
SG--HG	1.33	1.20	8
SG--HG	1.34	1.20	32
NH1--HH12	1.01	0.86	230
N--H	1.01	0.86	6100
CD1--HD1	1.08	0.93	440
CD2--HD2	1.08	0.93	530
CE2--HE2	1.08	0.93	400
CE1--HE1	1.08	0.93	530
CZ3--HZ3	1.08	0.93	40

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE1--HE1	1.01	0.86	40
ND2--HD22	1.01	0.86	230
NH2--HH22	1.01	0.86	230
NH1--HH11	1.01	0.86	230
ND2--HD21	1.01	0.86	230
CZ--HZ	1.08	0.93	290
NE--HE	1.01	0.86	230
NE2--HE21	1.01	0.86	150
NH2--HH21	1.01	0.86	230
ND1--HD1	1.01	0.86	105
NE2--HE22	1.01	0.86	150
CZ2--HZ2	1.08	0.93	40
CH2--HH2	1.08	0.93	40
CE3--HE3	1.08	0.93	40
NE2--HE2	1.01	0.86	25

Standard geometry: angle outliers

There are 293 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
CA-CB-CG	113.80	126.20	1
C-N-CA	121.70	138.45	1
C-N-CA	121.70	137.77	1
CA-CB-CG	112.60	121.19	1
C-N-CA	121.70	136.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	115.34	1
CA-CB-CG2	110.50	122.07	1
CA-CB-CG	113.80	107.03	1
CA-CB-CG	112.60	119.23	1
C-N-CA	121.70	133.57	1
OD1-CG-ND2	122.60	116.05	1
C-N-CA	121.70	133.42	1
C-N-CA	121.70	133.27	1
C-N-CA	121.70	133.22	1
CA-N-CD	112.00	103.14	1
C-N-CA	121.70	132.99	1
CA-CB-CG	113.80	119.95	1
C-N-CA	121.70	132.59	1
C-N-CA	121.70	132.51	1
O-C-N	123.00	113.40	1
OD1-CG-ND2	122.60	116.66	1
CA-CB-CG	113.80	107.87	1
CA-CB-CG2	110.50	120.40	1
C-N-CA	121.70	132.18	1
CA-C-N	116.20	127.82	1
C-N-CA	121.70	132.07	1
C-N-CA	121.70	132.01	1
OD1-CG-ND2	122.60	116.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.97	1
CA-CB-CG	112.60	118.30	1
C-N-CA	121.70	131.89	1
OD1-CG-ND2	122.60	116.99	1
NE-CZ-NH2	119.20	124.24	1
C-N-CA	121.70	131.75	1
C-CA-CB	110.50	118.87	1
C-N-CA	121.70	131.69	1
C-N-CA	121.70	131.67	1
CA-CB-CG	112.60	118.13	1
C-CA-CB	110.10	120.47	1
CA-CB-CG	113.80	119.20	1
OE1-CD-NE2	122.60	117.22	1
OE1-CD-NE2	122.60	117.24	2
OE1-CD-NE2	122.60	117.26	2
OE1-CD-NE2	122.60	117.27	1
CA-CB-CG1	110.40	119.43	1
C-N-CA	121.70	131.23	1
OE1-CD-NE2	122.60	117.31	1
OE1-CD-NE2	122.60	117.32	1
OE1-CD-NE2	122.60	117.33	1
C-N-CA	121.70	131.18	1
NE-CZ-NH2	119.20	123.86	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.45	1
OE1-CD-NE2	122.60	117.46	1
CB-CG-CD2	131.20	124.52	1
N-CA-CB	110.50	101.78	1
N-CA-C	111.00	125.36	1
CA-C-N	116.90	124.59	2
OE1-CD-NE2	122.60	117.50	1
C-N-CA	121.70	130.86	1
O-C-N	123.00	114.91	1
C-N-CA	121.70	130.75	1
C-N-CA	121.70	130.72	1
OE1-CD-NE2	122.60	117.62	1
C-N-CA	121.70	130.62	1
C-N-CA	121.70	130.60	1
OE1-CD-NE2	122.60	117.67	1
O-C-N	123.00	115.13	1
OE1-CD-NE2	122.60	117.70	1
C-N-CA	121.70	130.50	2
OE1-CD-NE2	122.60	117.73	1
C-N-CA	121.70	130.43	1
OE1-CD-NE2	122.60	117.76	1
CB-CG-CD2	131.20	124.94	1
CA-C-N	116.20	125.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	123.53	1
N-CA-C	111.00	124.43	1
C-N-CA	121.70	130.31	1
C-N-CA	121.70	130.29	1
CA-CB-CG	112.60	117.37	1
OE1-CD-NE2	122.60	117.84	1
N-CA-CB	110.50	102.42	1
OE1-CD-NE2	122.60	117.85	1
OE1-CD-NE2	122.60	117.86	1
CA-CB-CG	112.60	117.34	1
OE1-CD-NE2	122.60	117.87	1
C-N-CA	121.70	130.21	1
OE1-CD-NE2	122.60	117.89	1
OE1-CD-NE2	122.60	117.90	2
OD1-CG-ND2	122.60	117.90	1
C-N-CA	121.70	130.11	1
CA-CB-CG	113.80	118.46	1
CB-CG-CD2	131.20	125.14	1
CA-C-N	116.20	125.52	1
CB-CG-CD2	131.20	125.15	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	1
CB-CG-CD2	131.20	125.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	117.46	1
C-N-CA	121.70	130.04	2
OE1-CD-NE2	122.60	117.97	1
CB-CG-CD2	131.20	125.19	1
C-N-CA	121.70	130.01	1
CB-CG-CD2	131.20	125.20	1
CB-CG-CD2	131.20	125.22	1
OE1-CD-NE2	122.60	118.00	1
C-CA-CB	110.50	117.39	1
C-N-CA	121.70	129.96	1
CA-CB-CG	112.60	117.19	1
OE1-CD-NE2	122.60	118.02	1
OE1-CD-NE2	122.60	118.03	2
CB-CG-CD2	131.20	125.26	1
OE1-CD-NE2	122.60	118.04	1
CA-CB-CG	112.60	117.16	1
C-N-CA	121.70	129.91	1
N-CA-CB	110.40	117.24	1
CB-CG-CD2	131.20	125.27	1
CB-CG-CD2	131.20	125.29	1
C-N-CA	121.70	129.87	1
CA-CB-CG	112.60	117.13	1
CB-CG-CD2	131.20	125.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.12	1
CB-CG-CD2	131.20	125.33	2
OE1-CD-NE2	122.60	118.08	1
C-N-CA	121.70	129.82	1
CB-CG-CD2	131.20	125.34	2
CB-CG-CD2	131.20	125.35	2
OE1-CD-NE2	122.60	118.10	1
OE1-CD-NE2	122.60	118.11	1
CB-CG-CD2	131.20	125.37	1
OE1-CD-NE2	122.60	118.12	1
CB-CG-CD2	131.20	125.38	1
OE1-CD-NE2	122.60	118.13	1
CB-CG-CD2	131.20	125.40	1
C-N-CA	121.70	129.73	1
CB-CG-CD2	131.20	125.41	1
C-CA-CB	110.50	117.18	1
OE1-CD-NE2	122.60	118.15	1
N-CA-CB	110.50	102.93	1
OD1-CG-ND2	122.60	118.15	1
CB-CG-CD2	131.20	125.42	2
CB-CG-CD2	131.20	125.43	1
OD1-CG-ND2	122.60	118.17	1
OE1-CD-NE2	122.60	118.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.67	1
C-N-CA	121.70	129.66	1
OE1-CD-NE2	122.60	118.18	1
OE1-CD-NE2	122.60	118.23	2
NE-CZ-NH2	119.20	123.13	1
C-N-CA	121.70	129.55	1
OE1-CD-NE2	122.60	118.24	1
CA-CB-CG	112.60	116.95	1
OE1-CD-NE2	122.60	118.25	1
C-N-CA	121.70	129.52	1
OE1-CD-NE2	122.60	118.26	1
N-CA-CB	110.50	103.13	1
OE1-CD-NE2	122.60	118.27	3
N-CA-CB	111.50	118.86	1
OE1-CD-NE2	122.60	118.28	1
C-N-CA	121.70	129.47	1
C-N-CA	121.70	129.45	1
C-N-CA	121.70	129.44	1
OE1-CD-NE2	122.60	118.30	1
C-N-CD	125.00	107.39	1
CB-CG-CD2	131.20	125.62	3
CA-CB-CG	113.80	118.09	1
OE1-CD-NE2	122.60	118.31	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	118.21	1
OE1-CD-NE2	122.60	118.33	1
N-CA-CB	110.50	117.75	1
C-N-CA	121.70	129.38	1
OE1-CD-NE2	122.60	118.34	1
CA-CB-CG	112.60	116.86	1
CB-CG-CD2	131.20	125.67	1
N-CA-CB	111.50	104.27	1
C-N-CA	121.70	129.36	1
OD1-CG-ND2	122.60	118.35	1
OD1-CG-ND2	122.60	118.36	1
CA-CB-CG	113.80	109.57	1
NH1-CZ-NH2	119.30	113.80	1
N-CA-CB	110.50	103.33	1
CA-C-N	116.20	124.64	1
N-CA-CB	110.50	117.66	1
OE1-CD-NE2	122.60	118.39	1
CB-CG-CD2	131.20	125.73	1
OD1-CG-ND2	122.60	118.39	1
C-N-CA	121.70	129.27	1
N-CA-CB	110.50	117.65	1
OD1-CG-ND2	122.60	118.40	1
OE1-CD-NE2	122.60	118.40	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.41	3
OD1-CG-ND2	122.60	118.41	3
CB-CG-CD2	131.20	125.76	1
OD1-CG-ND2	122.60	118.42	1
CA-CB-CG	112.60	116.78	1
OE1-CD-NE2	122.60	118.43	2
CA-CB-CG	113.80	117.96	1
CB-CG-CD2	131.20	125.79	1
OD1-CG-ND2	122.60	118.44	1
CB-CG-CD2	131.20	125.80	1
CA-CB-CG	113.80	117.95	1
OD1-CG-ND2	122.60	118.45	1
OD1-CG-ND2	122.60	118.46	3
N-CA-CB	110.40	104.19	1
N-CA-CB	103.00	107.55	1
CB-CG-CD2	131.20	125.82	1
OE1-CD-NE2	122.60	118.47	1
CB-CG-CD2	131.20	125.83	1
OD1-CG-ND2	122.60	118.47	1
OD1-CG-ND2	122.60	118.48	1
OE1-CD-NE2	122.60	118.48	2
CB-CG1-CD1	113.80	105.16	1
CA-CB-CG	113.80	117.91	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	124.41	2
NH1-CZ-NH2	119.30	113.96	1
CB-CG-CD2	131.20	125.87	1
CA-CB-CG	112.60	116.69	1
N-CA-CB	110.50	103.56	1
OE1-CD-NE2	122.60	118.52	1
OD1-CG-ND2	122.60	118.52	1
C-CA-CB	110.50	116.62	1
C-N-CA	121.70	129.04	1
C-N-CA	121.70	129.03	1
CB-CG-CD2	131.20	125.91	1
OD1-CG-ND2	122.60	118.53	1
CB-CG-CD2	131.20	125.92	1
N-CA-CB	110.50	117.41	1
OE1-CD-NE2	122.60	118.54	1
OD1-CG-ND2	122.60	118.55	1
OE1-CD-NE2	122.60	118.55	1
CA-C-N	116.90	122.97	1
CB-CG-CD2	131.20	125.94	2
OE1-CD-NE2	122.60	118.56	1
CB-CG-CD2	131.20	125.95	2
C-N-CA	121.70	128.96	1
CA-C-O	120.80	113.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.57	1
OE1-CD-NE2	122.60	118.57	2
C-N-CA	121.70	128.94	1
OD1-CG-ND2	122.60	118.58	1
CA-C-N	116.20	124.23	1
OE1-CD-NE2	122.60	118.59	1
CB-CG-CD2	131.20	125.99	1
CA-CB-OG	111.10	103.09	1
N-CA-HA	97.98	110.00	1
C-N-H	112.23	124.30	1
HZ1-NZ-HZ2	96.91	109.00	1
C-N-H	112.10	124.30	1
C-N-H	112.06	124.30	1
HZ1-NZ-HZ2	96.75	109.00	1
HZ2-NZ-HZ3	96.73	109.00	1
C-N-H	111.89	124.30	1
HZ2-NZ-HZ3	96.50	109.00	1
HZ1-NZ-HZ3	96.34	109.00	1
HZ1-NZ-HZ2	96.27	109.00	1
C-N-H	111.55	124.30	1
HZ1-NZ-HZ2	96.09	109.00	1
C-N-H	111.11	124.30	1
HZ1-NZ-HZ2	95.76	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	110.92	124.30	1
C-N-H	110.54	124.30	1
HB2-CB-HB3	96.05	110.00	1
HH11-NH1-HH12	105.99	120.00	1
C-N-H	109.08	124.30	1
HH11-NH1-HH12	98.96	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	5.37	52
2	5.99	58
3	4.65	45
4	2.69	26
5	1.55	15
6	3.62	35
7	2.48	24
8	2.07	20
9	4.24	41
10	4.13	40

All 356 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:386:ALA:HB1	A:388:MET:HE2	1.040
1	A:161:LEU:HD22	A:214:PHE:CE2	0.713

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:386:ALA:HB1	A:388:MET:CE	0.712
1	A:70:LYS:HE2	A:75:GLU:HA	0.682
1	A:161:LEU:HD22	A:214:PHE:CZ	0.677
1	A:232:MET:HE2	A:244:GLY:HA2	0.674
1	A:65:GLY:HA2	A:388:MET:SD	0.672
1	A:88:VAL:HA	A:96:MET:HE3	0.639
1	A:26:ALA:CA	A:297:PRO:HG3	0.609
1	A:343:ASP:O	A:347:ALA:HB3	0.570
1	A:55:MET:HE1	A:246:ALA:HA	0.567
1	A:59:LEU:HD22	A:255:ILE:HD13	0.562
1	A:459:THR:HG21	A:601:ILE:HG21	0.539
1	A:70:LYS:HE2	A:75:GLU:CA	0.535
1	A:177:ALA:HB3	A:217:ILE:HD11	0.521
1	A:197:ILE:HB	A:216:LEU:HD21	0.520
1	A:417:ILE:HD11	A:437:ALA:HB2	0.511
1	A:26:ALA:HA	A:297:PRO:HG3	0.509
1	A:70:LYS:HE2	A:74:GLY:C	0.508
1	A:92:ALA:HA	A:96:MET:HE2	0.505
1	A:88:VAL:O	A:92:ALA:HB2	0.498
1	A:418:ASN:HD21	A:436:ARG:NH2	0.497
1	A:26:ALA:HA	A:297:PRO:CG	0.491
1	A:70:LYS:HE2	A:75:GLU:N	0.491
1	A:181:VAL:HG11	A:217:ILE:HB	0.485

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:59:LEU:HD22	A:255:ILE:HG21	0.484
1	A:26:ALA:HB2	A:297:PRO:HG3	0.476
1	A:85:THR:HG22	A:89:ILE:HD12	0.476
1	A:449:LEU:HD22	A:457:LEU:HD13	0.468
1	A:198:PHE:CZ	A:216:LEU:HD13	0.463
1	A:554:HIS:CD2	A:600:HIS:CE1	0.463
1	A:94:MET:HE2	A:213:ILE:H	0.450
1	A:30:TRP:CZ2	A:56:ILE:HG23	0.443
1	A:418:ASN:HA	A:440:GLN:HE22	0.440
1	A:282:PHE:CZ	A:286:ILE:HD11	0.437
1	A:600:HIS:CE1	A:604:ILE:HD11	0.435
1	A:220:ASN:O	A:223:PRO:HD2	0.431
1	A:295:ALA:HA	A:306:MET:SD	0.427
1	A:292:VAL:HG21	A:315:ASN:HD21	0.425
1	A:22:PRO:HA	A:296:SER:O	0.424
1	A:198:PHE:CE2	A:216:LEU:HB3	0.422
1	A:26:ALA:CB	A:297:PRO:HG3	0.418
1	A:219:ALA:HB2	A:256:HIS:CD2	0.418
1	A:390:SER:HB2	A:452:PHE:CD2	0.415
1	A:216:LEU:O	A:217:ILE:HG13	0.414
1	A:65:GLY:CA	A:388:MET:SD	0.414
1	A:526:TYR:CD1	A:567:GLY:HA3	0.412
1	A:161:LEU:HD13	A:214:PHE:CD2	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:234:PHE:CD1	A:335:LYS:HE3	0.404
1	A:402:ILE:HG23	A:407:LEU:HB2	0.403
1	A:59:LEU:CD2	A:255:ILE:HG21	0.402
1	A:254:GLY:HA2	A:298:GLY:C	0.401
2	A:180:PHE:CZ	A:197:ILE:HD11	0.955
2	A:174:LEU:CD1	A:179:ILE:HD11	0.847
2	A:34:THR:HG23	A:38:ILE:HD12	0.802
2	A:57:THR:HA	A:96:MET:HE1	0.728
2	A:60:LEU:HD21	A:186:ILE:HG21	0.692
2	A:256:HIS:CG	A:273:VAL:HG13	0.688
2	A:192:ALA:HA	A:197:ILE:HD12	0.649
2	A:40:THR:CG2	A:193:ILE:HG23	0.626
2	A:34:THR:HG23	A:38:ILE:CD1	0.614
2	A:478:VAL:HG13	A:482:LEU:HD12	0.614
2	A:16:LEU:HD21	A:258:ILE:HG21	0.605
2	A:37:PHE:CE1	A:48:LEU:HD23	0.599
2	A:60:LEU:CD2	A:186:ILE:HG21	0.595
2	A:38:ILE:HD11	A:56:ILE:CD1	0.591
2	A:40:THR:HG1	A:42:TRP:CD1	0.586
2	A:37:PHE:CD1	A:48:LEU:HD23	0.585
2	A:184:ALA:HB3	A:187:LEU:HD12	0.580
2	A:16:LEU:HD21	A:258:ILE:CG2	0.572
2	A:189:LEU:HD11	A:227:VAL:HG21	0.563

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:40:THR:HG22	A:193:ILE:HG23	0.551
2	A:38:ILE:HD11	A:56:ILE:HD13	0.549
2	A:64:ILE:HD12	A:97:PHE:CD1	0.542
2	A:71:LEU:HA	A:355:MET:HE1	0.534
2	A:34:THR:HG21	A:189:LEU:HD23	0.504
2	A:526:TYR:CD1	A:567:GLY:HA3	0.501
2	A:494:PHE:CE1	A:606:SER:HB3	0.496
2	A:34:THR:CB	A:189:LEU:HD23	0.487
2	A:60:LEU:HD23	A:97:PHE:CZ	0.487
2	A:180:PHE:CZ	A:197:ILE:CD1	0.486
2	A:478:VAL:CG1	A:482:LEU:HD12	0.485
2	A:28:ILE:HG13	A:222:GLY:HA2	0.466
2	A:361:GLY:C	A:363:SER:H	0.465
2	A:35:ALA:HB2	A:227:VAL:HG22	0.449
2	A:88:VAL:HG11	A:99:GLY:HA3	0.448
2	A:197:ILE:HG22	A:215:PHE:CE1	0.448
2	A:174:LEU:HD11	A:179:ILE:HD11	0.445
2	A:174:LEU:HD12	A:179:ILE:HD11	0.445
2	A:60:LEU:HD23	A:97:PHE:HZ	0.443
2	A:168:MET:HE3	A:179:ILE:CD1	0.442
2	A:40:THR:HG22	A:193:ILE:HG12	0.440
2	A:34:THR:CG2	A:189:LEU:HD23	0.435
2	A:95:PRO:CG	A:191:ASN:HD21	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:165:VAL:HA	A:179:ILE:HD12	0.432
2	A:219:ALA:HA	A:224:GLY:HA3	0.432
2	A:218:GLU:CD	A:250:HIS:CE1	0.426
2	A:361:GLY:C	A:363:SER:N	0.426
2	A:34:THR:HB	A:189:LEU:HD23	0.416
2	A:218:GLU:CD	A:254:GLY:H	0.414
2	A:356:LYS:HE2	A:360:LYS:HE3	0.411
2	A:192:ALA:CA	A:197:ILE:HD12	0.410
2	A:478:VAL:HG13	A:482:LEU:CD1	0.410
2	A:128:MET:HE3	A:385:ASP:HB2	0.408
2	A:42:TRP:HZ2	A:198:PHE:CD1	0.404
2	A:197:ILE:CG2	A:215:PHE:CE1	0.404
2	A:38:ILE:CG2	A:193:ILE:HG21	0.403
2	A:38:ILE:HG22	A:193:ILE:HG21	0.402
2	A:94:MET:CB	A:95:PRO:HD3	0.401
2	A:174:LEU:HD13	A:179:ILE:HD11	0.401
3	A:98:LEU:HD13	A:154:VAL:HG22	0.774
3	A:55:MET:HE1	A:84:THR:HG22	0.744
3	A:33:ILE:HD11	A:140:MET:HA	0.723
3	A:181:VAL:HG12	A:185:LYS:HE3	0.658
3	A:56:ILE:HG21	A:213:ILE:HG12	0.621
3	A:150:ILE:HG22	A:154:VAL:HG23	0.558
3	A:111:ILE:HD11	A:135:ALA:HA	0.546

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:16:LEU:HD23	A:97:PHE:CZ	0.528
3	A:16:LEU:CD2	A:97:PHE:CZ	0.521
3	A:19:MET:HE1	A:101:MET:HG2	0.500
3	A:63:LEU:HD11	A:81:GLY:HA3	0.498
3	A:86:MET:HE1	A:185:LYS:HG3	0.497
3	A:97:PHE:CE1	A:101:MET:SD	0.492
3	A:106:LEU:HD23	A:142:LEU:HD22	0.490
3	A:234:PHE:CE1	A:335:LYS:HE3	0.489
3	A:370:VAL:HG21	A:446:HIS:O	0.488
3	A:63:LEU:O	A:67:THR:HG23	0.486
3	A:234:PHE:CD1	A:335:LYS:HE3	0.479
3	A:24:ILE:HG12	A:249:ILE:HD11	0.474
3	A:19:MET:HE1	A:101:MET:HA	0.473
3	A:90:VAL:HG13	A:94:MET:HG3	0.469
3	A:16:LEU:HD23	A:97:PHE:CE2	0.464
3	A:526:TYR:CD1	A:567:GLY:HA3	0.459
3	A:15:PHE:CZ	A:101:MET:HE3	0.456
3	A:76:ARG:HH21	A:172:ASP:CG	0.453
3	A:284:LEU:HD21	A:315:ASN:HA	0.450
3	A:41:GLY:O	A:42:TRP:C	0.446
3	A:19:MET:CE	A:101:MET:HA	0.440
3	A:102:ILE:CD1	A:150:ILE:HD13	0.438
3	A:19:MET:CE	A:101:MET:HG2	0.432

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:217:ILE:O	A:218:GLU:C	0.431
3	A:16:LEU:HD12	A:187:LEU:HD11	0.430
3	A:16:LEU:CD2	A:97:PHE:CE2	0.423
3	A:27:PHE:CD1	A:255:ILE:CD1	0.422
3	A:55:MET:HE1	A:84:THR:CG2	0.420
3	A:220:ASN:O	A:223:PRO:HD2	0.418
3	A:16:LEU:CD1	A:187:LEU:HD13	0.414
3	A:402:ILE:HG23	A:407:LEU:HB2	0.413
3	A:282:PHE:CZ	A:286:ILE:HD11	0.409
3	A:33:ILE:HD11	A:140:MET:CA	0.407
3	A:16:LEU:CD1	A:187:LEU:CD1	0.406
3	A:390:SER:HB2	A:452:PHE:CD2	0.406
3	A:307:THR:HG23	A:315:ASN:ND2	0.406
3	A:106:LEU:CD2	A:142:LEU:HD22	0.405
3	A:449:LEU:HD22	A:457:LEU:HD13	0.400
4	A:259:TYR:CD1	A:273:VAL:HG22	0.814
4	A:20:VAL:HG11	A:260:PHE:CZ	0.702
4	A:307:THR:HG23	A:315:ASN:HD22	0.634
4	A:259:TYR:CE1	A:273:VAL:HG22	0.633
4	A:307:THR:CG2	A:315:ASN:HD22	0.621
4	A:86:MET:O	A:90:VAL:HG23	0.567
4	A:107:GLY:HA2	A:142:LEU:CD1	0.555
4	A:260:PHE:CZ	A:264:LEU:HD11	0.523

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:20:VAL:CG1	A:260:PHE:CZ	0.520
4	A:34:THR:HG23	A:38:ILE:HD12	0.469
4	A:260:PHE:CE1	A:264:LEU:HD11	0.469
4	A:92:ALA:HB2	A:96:MET:HE2	0.458
4	A:253:GLY:O	A:298:GLY:HA3	0.457
4	A:98:LEU:HB2	A:154:VAL:HG11	0.455
4	A:114:PHE:CE1	A:118:VAL:HG21	0.448
4	A:52:VAL:HG13	A:56:ILE:HD12	0.441
4	A:48:LEU:O	A:52:VAL:HG23	0.437
4	A:526:TYR:CD1	A:567:GLY:HA3	0.432
4	A:181:VAL:CG1	A:185:LYS:HE3	0.425
4	A:114:PHE:CZ	A:118:VAL:HG21	0.418
4	A:90:VAL:HG22	A:201:LEU:HD22	0.417
4	A:554:HIS:CD2	A:600:HIS:NE2	0.409
4	A:101:MET:HE3	A:191:ASN:CB	0.407
4	A:417:ILE:HD11	A:437:ALA:HB2	0.406
4	A:390:SER:HB2	A:452:PHE:CD2	0.404
4	A:28:ILE:HD11	A:222:GLY:CA	0.403
5	A:219:ALA:HB1	A:296:SER:CB	0.583
5	A:86:MET:HE2	A:96:MET:SD	0.581
5	A:219:ALA:HB1	A:296:SER:HB2	0.572
5	A:219:ALA:HB1	A:296:SER:H	0.554
5	A:90:VAL:HG23	A:91:GLY:O	0.529

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:222:GLY:HA2	A:273:VAL:CG1	0.517
5	A:297:PRO:HB2	A:302:ALA:HB3	0.454
5	A:20:VAL:HG13	A:24:ILE:HB	0.450
5	A:15:PHE:CZ	A:19:MET:SD	0.429
5	A:558:GLU:CD	A:558:GLU:H	0.422
5	A:133:PHE:CE1	A:137:ILE:HD11	0.419
5	A:61:PRO:HB2	A:89:ILE:HD11	0.408
5	A:90:VAL:HG21	A:96:MET:HE1	0.402
5	A:282:PHE:CZ	A:286:ILE:HD11	0.402
5	A:297:PRO:HB2	A:302:ALA:CB	0.402
6	A:16:LEU:HD22	A:101:MET:HE2	0.770
6	A:369:ASP:CG	A:601:ILE:HG23	0.711
6	A:1:MET:HE3	A:5:ILE:HG22	0.635
6	A:95:PRO:HD2	A:154:VAL:CG1	0.613
6	A:417:ILE:HD11	A:437:ALA:HB2	0.610
6	A:95:PRO:CD	A:154:VAL:CG1	0.587
6	A:28:ILE:HA	A:255:ILE:HD11	0.568
6	A:95:PRO:CD	A:154:VAL:HG12	0.564
6	A:186:ILE:HD13	A:263:VAL:HG11	0.524
6	A:369:ASP:OD1	A:601:ILE:HG23	0.523
6	A:27:PHE:CZ	A:60:LEU:HD21	0.512
6	A:19:MET:HE1	A:101:MET:HA	0.510
6	A:24:ILE:HG22	A:388:MET:SD	0.496

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:370:VAL:CG1	A:374:LEU:HD21	0.492
6	A:370:VAL:CG2	A:447:ILE:HG12	0.487
6	A:27:PHE:CE2	A:60:LEU:HD21	0.479
6	A:94:MET:SD	A:195:HIS:HB2	0.472
6	A:343:ASP:O	A:347:ALA:HB3	0.467
6	A:176:LEU:HD23	A:278:MET:HE3	0.459
6	A:478:VAL:HG12	A:482:LEU:HD12	0.453
6	A:21:MET:HA	A:388:MET:HE1	0.449
6	A:162:ALA:HA	A:197:ILE:CD1	0.427
6	A:225:MET:HE3	A:251:PHE:HB2	0.424
6	A:20:VAL:C	A:21:MET:O	0.424
6	A:30:TRP:HZ3	A:60:LEU:HD22	0.420
6	A:95:PRO:HD3	A:154:VAL:HG12	0.420
6	A:368:GLY:H	A:434:THR:HG21	0.417
6	A:225:MET:HG2	A:323:MET:HE2	0.414
6	A:526:TYR:CD1	A:565:LYS:HE3	0.414
6	A:88:VAL:HG11	A:99:GLY:HA3	0.410
6	A:95:PRO:HD2	A:154:VAL:HG12	0.410
6	A:12:PHE:CE1	A:16:LEU:HD11	0.407
6	A:526:TYR:CD1	A:567:GLY:HA3	0.405
6	A:521:LEU:HD22	A:594:ALA:HB2	0.403
6	A:343:ASP:O	A:347:ALA:CB	0.402
7	A:239:ALA:HA	A:345:ILE:HD11	0.724

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:1:MET:HE3	A:5:ILE:HG22	0.643
7	A:97:PHE:CE2	A:195:HIS:HB3	0.587
7	A:96:MET:SD	A:154:VAL:HG12	0.560
7	A:188:PHE:CZ	A:356:LYS:HE3	0.559
7	A:239:ALA:HB2	A:265:MET:HE1	0.545
7	A:88:VAL:HG11	A:99:GLY:HA3	0.530
7	A:503:LEU:HD21	A:629:VAL:HG21	0.519
7	A:188:PHE:CE1	A:356:LYS:HE3	0.516
7	A:15:PHE:CZ	A:19:MET:SD	0.499
7	A:96:MET:CE	A:154:VAL:HG12	0.489
7	A:1:MET:CE	A:5:ILE:HG22	0.484
7	A:97:PHE:CD2	A:195:HIS:HB3	0.476
7	A:188:PHE:CE1	A:356:LYS:CE	0.476
7	A:357:ALA:HB1	A:362:ALA:O	0.476
7	A:133:PHE:CE1	A:137:ILE:HD11	0.474
7	A:526:TYR:CD1	A:567:GLY:HA3	0.473
7	A:251:PHE:CD2	A:300:ILE:HD12	0.472
7	A:485:SER:O	A:486:PHE:CD2	0.455
7	A:23:ASN:HB3	A:27:PHE:CE2	0.449
7	A:282:PHE:CZ	A:286:ILE:HD11	0.430
7	A:370:VAL:HG22	A:447:ILE:HG12	0.421
7	A:161:LEU:HD13	A:197:ILE:HD11	0.407
7	A:418:ASN:HA	A:440:GLN:HE22	0.404

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:19:MET:HE1	A:101:MET:HA	0.673
8	A:186:ILE:HD11	A:273:VAL:HG21	0.666
8	A:19:MET:HE3	A:68:GLY:HA3	0.663
8	A:370:VAL:HG11	A:374:LEU:HD21	0.647
8	A:337:SER:HB3	A:339:VAL:HG23	0.637
8	A:98:LEU:HD22	A:187:LEU:O	0.619
8	A:6:LYS:NZ	A:339:VAL:HG22	0.585
8	A:173:MET:HE2	A:176:LEU:HD12	0.502
8	A:526:TYR:CD1	A:567:GLY:HA3	0.494
8	A:251:PHE:CD2	A:300:ILE:HD12	0.483
8	A:337:SER:C	A:339:VAL:H	0.483
8	A:418:ASN:HA	A:440:GLN:HE22	0.454
8	A:347:ALA:HA	A:350:ARG:HB2	0.450
8	A:366:SER:C	A:368:GLY:H	0.449
8	A:342:GLU:HA	A:347:ALA:HB1	0.429
8	A:526:TYR:CD1	A:565:LYS:HE3	0.424
8	A:282:PHE:CZ	A:286:ILE:HD11	0.416
8	A:217:ILE:HG12	A:281:VAL:HG22	0.405
8	A:339:VAL:HG13	A:343:ASP:HB3	0.402
8	A:417:ILE:HD11	A:437:ALA:HB2	0.400
9	A:265:MET:HE1	A:348:ALA:HB2	0.731
9	A:265:MET:HE1	A:348:ALA:CB	0.693
9	A:203:ILE:HD11	A:291:LEU:H	0.690

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:42:TRP:CZ2	A:234:PHE:CD2	0.660
9	A:30:TRP:NE1	A:56:ILE:HD11	0.660
9	A:30:TRP:HE1	A:56:ILE:HD11	0.652
9	A:42:TRP:CH2	A:234:PHE:CD2	0.592
9	A:190:ASN:OD1	A:193:ILE:HD12	0.575
9	A:357:ALA:HB1	A:362:ALA:O	0.567
9	A:42:TRP:CH2	A:234:PHE:CE2	0.556
9	A:181:VAL:HG12	A:185:LYS:HE3	0.552
9	A:233:PHE:HB2	A:234:PHE:CD2	0.552
9	A:185:LYS:HE2	A:194:ASN:ND2	0.536
9	A:14:ARG:HH21	A:264:LEU:HD22	0.531
9	A:1:MET:HE2	A:5:ILE:CG2	0.524
9	A:418:ASN:HA	A:440:GLN:HE22	0.513
9	A:193:ILE:HG12	A:250:HIS:CE1	0.511
9	A:1:MET:HE2	A:5:ILE:HG21	0.510
9	A:19:MET:HE1	A:101:MET:HA	0.505
9	A:42:TRP:CZ2	A:234:PHE:CG	0.495
9	A:89:ILE:O	A:89:ILE:HG22	0.483
9	A:526:TYR:CD1	A:567:GLY:HA3	0.480
9	A:259:TYR:C	A:261:PRO:HD2	0.472
9	A:19:MET:HE3	A:68:GLY:HA3	0.461
9	A:33:ILE:CG2	A:52:VAL:HG21	0.461
9	A:42:TRP:CE2	A:234:PHE:CB	0.461

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:181:VAL:HG12	A:185:LYS:CE	0.460
9	A:233:PHE:HB2	A:234:PHE:CE2	0.446
9	A:390:SER:HB2	A:452:PHE:CD2	0.446
9	A:219:ALA:HB1	A:223:PRO:HG2	0.442
9	A:84:THR:HG23	A:142:LEU:HB3	0.436
9	A:86:MET:HA	A:89:ILE:HD12	0.431
9	A:265:MET:HE1	A:348:ALA:HB1	0.430
9	A:57:THR:O	A:89:ILE:HG23	0.425
9	A:98:LEU:HD23	A:154:VAL:HG13	0.425
9	A:259:TYR:C	A:261:PRO:CD	0.418
9	A:33:ILE:HG21	A:52:VAL:HG21	0.416
9	A:6:LYS:CE	A:267:PRO:HG2	0.411
9	A:6:LYS:HE3	A:267:PRO:CG	0.406
9	A:90:VAL:HG21	A:147:PHE:CD2	0.405
9	A:196:GLY:HA2	A:246:ALA:HA	0.403
10	A:98:LEU:HD23	A:192:ALA:HB1	0.878
10	A:198:PHE:HB3	A:214:PHE:CZ	0.802
10	A:242:SER:HB2	A:388:MET:HE2	0.707
10	A:198:PHE:CG	A:214:PHE:CE2	0.633
10	A:186:ILE:HD11	A:301:LEU:HB2	0.598
10	A:219:ALA:HB1	A:224:GLY:HA3	0.552
10	A:186:ILE:HD11	A:301:LEU:CB	0.543
10	A:243:ALA:HB1	A:246:ALA:O	0.541

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:87:GLY:HA3	A:96:MET:CE	0.533
10	A:251:PHE:HB2	A:257:GLU:HB3	0.518
10	A:181:VAL:HG22	A:198:PHE:CZ	0.516
10	A:184:ALA:C	A:193:ILE:CD1	0.507
10	A:34:THR:HG22	A:38:ILE:CD1	0.498
10	A:34:THR:HG22	A:38:ILE:HD11	0.480
10	A:193:ILE:HG22	A:198:PHE:CD2	0.477
10	A:174:LEU:HD13	A:213:ILE:HG21	0.474
10	A:251:PHE:HB2	A:257:GLU:CG	0.471
10	A:210:GLY:O	A:245:GLY:HA2	0.461
10	A:376:HIS:CE1	A:445:GLN:HE21	0.456
10	A:98:LEU:HD22	A:188:PHE:HB3	0.454
10	A:87:GLY:H	A:96:MET:HE1	0.453
10	A:184:ALA:C	A:193:ILE:HD11	0.452
10	A:188:PHE:O	A:192:ALA:HB3	0.451
10	A:161:LEU:HD13	A:184:ALA:HB2	0.443
10	A:215:PHE:CD2	A:247:ALA:O	0.443
10	A:184:ALA:HB1	A:193:ILE:HD13	0.442
10	A:27:PHE:CZ	A:255:ILE:HD12	0.431
10	A:107:GLY:HA2	A:142:LEU:CD1	0.428
10	A:98:LEU:HD23	A:192:ALA:CB	0.425
10	A:42:TRP:NE1	A:260:PHE:CE1	0.425
10	A:96:MET:HB3	A:96:MET:HE2	0.424

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:218:GLU:HB3	A:250:HIS:O	0.423
10	A:98:LEU:HD21	A:192:ALA:C	0.420
10	A:526:TYR:CD1	A:567:GLY:HA3	0.419
10	A:198:PHE:HB3	A:214:PHE:CE2	0.416
10	A:402:ILE:HG23	A:407:LEU:HB2	0.415
10	A:184:ALA:HB1	A:193:ILE:CD1	0.411
10	A:219:ALA:HB1	A:224:GLY:CA	0.408
10	A:251:PHE:HB2	A:257:GLU:CB	0.406
10	A:27:PHE:CE1	A:255:ILE:HD12	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	635	610	20	5
2	635	595	29	11
3	635	603	25	7
4	635	595	31	9
5	635	603	23	9
6	635	596	29	10
7	635	608	18	9
8	635	611	17	7
9	635	614	16	5
10	635	603	21	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	506	488	11	7
2	506	485	12	9
3	506	479	13	14
4	506	490	7	9
5	506	480	13	13
6	506	487	12	7
7	506	495	8	3
8	506	498	6	2
9	506	491	11	4
10	506	491	8	7

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	60	LEU
1	A	66	TYR
1	A	198	PHE
1	A	214	PHE
1	A	216	LEU
1	A	471	HIS
1	A	493	LEU
2	A	42	TRP
2	A	176	LEU
2	A	189	LEU

Model ID	Chain	Residue ID	Residue type
2	A	216	LEU
2	A	292	VAL
2	A	365	LEU
2	A	366	SER
2	A	493	LEU
2	A	608	THR
3	A	34	THR
3	A	51	LEU
3	A	62	LEU
3	A	84	THR
3	A	93	ASP
3	A	94	MET
3	A	117	TRP
3	A	129	LEU
3	A	182	GLU
3	A	201	LEU
3	A	207	HIS
3	A	213	ILE
3	A	471	HIS
3	A	480	ASP
4	A	30	TRP
4	A	48	LEU
4	A	60	LEU

Model ID	Chain	Residue ID	Residue type
4	A	62	LEU
4	A	197	ILE
4	A	292	VAL
4	A	471	HIS
4	A	472	THR
4	A	480	ASP
5	A	1	MET
5	A	24	ILE
5	A	48	LEU
5	A	86	MET
5	A	189	LEU
5	A	199	SER
5	A	213	ILE
5	A	215	PHE
5	A	216	LEU
5	A	220	ASN
5	A	292	VAL
5	A	485	SER
5	A	493	LEU
6	A	24	ILE
6	A	43	LEU
6	A	343	ASP
6	A	363	SER

Model ID	Chain	Residue ID	Residue type
6	A	388	MET
6	A	493	LEU
6	A	601	ILE
7	A	1	MET
7	A	487	ASP
7	A	493	LEU
8	A	343	ASP
8	A	370	VAL
9	A	43	LEU
9	A	90	VAL
9	A	260	PHE
9	A	481	SER
10	A	30	TRP
10	A	62	LEU
10	A	198	PHE
10	A	220	ASN
10	A	251	PHE
10	A	252	LEU
10	A	471	HIS

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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