Integrative Structure Validation Report

July 22, 2024 - 05:12 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	9A32
PDB-Dev ID	PDBDEV_00000187
Structure Title	Model of E. coli OmpC 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

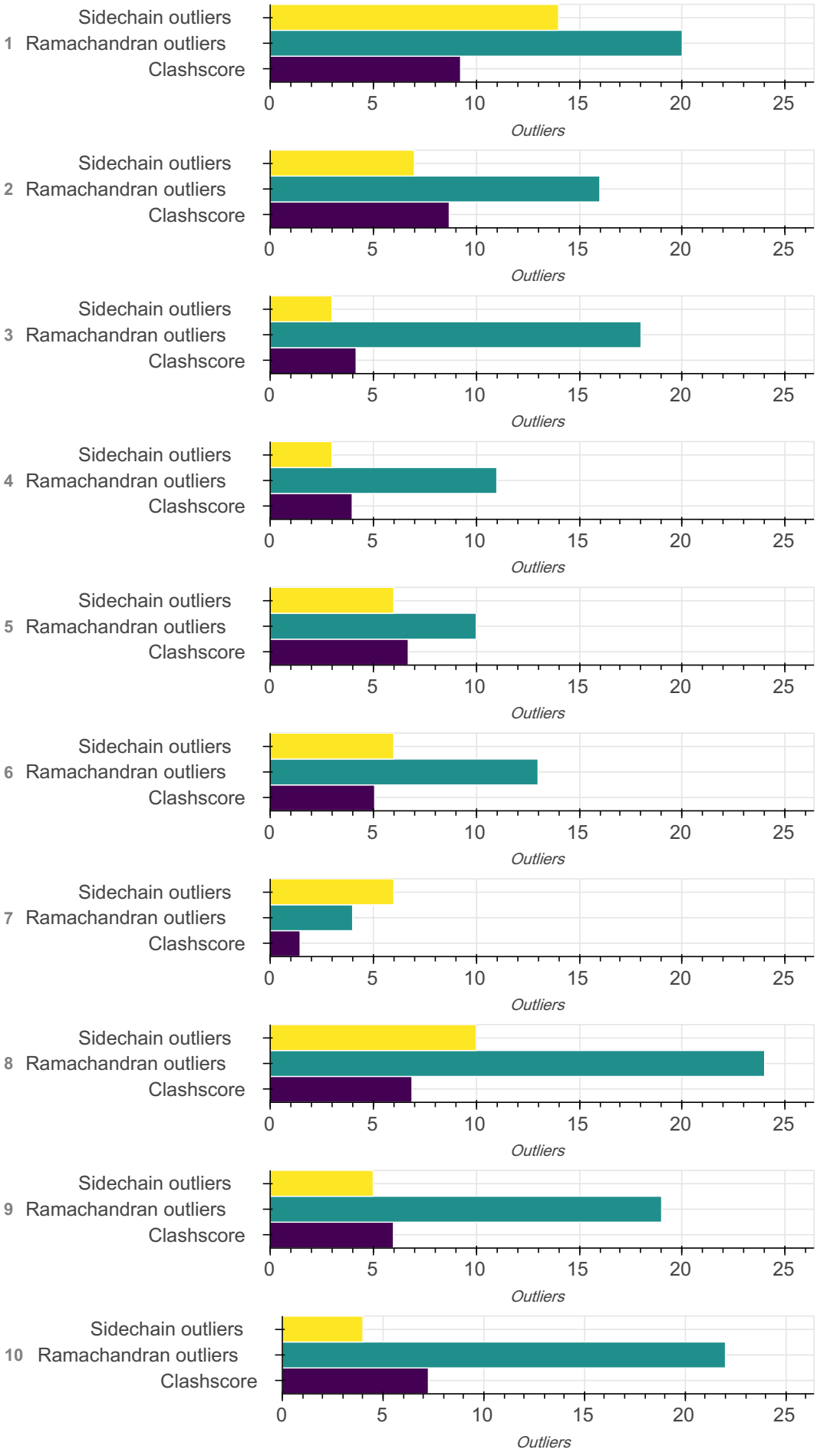
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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Sidechain outliers
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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
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Clashscore
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Sidechain outliers
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Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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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	P06996	A	A	367
2	1	1	P06996	A	A	367
3	1	1	P06996	A	A	367
4	1	1	P06996	A	A	367
5	1	1	P06996	A	A	367
6	1	1	P06996	A	A	367
7	1	1	P06996	A	A	367
8	1	1	P06996	A	A	367
9	1	1	P06996	A	A	367
10	1	1	P06996	A	A	367

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	-	1-367

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 26630 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
CE--HE3	1.09	0.97	210
CB--HB2	1.09	0.97	2600
CG2--HG22	1.09	0.97	590
CA--HA	1.09	0.97	3190
CB--HB3	1.09	0.97	2600
CD1--HD11	1.09	0.97	370
CD1--HD12	1.09	0.97	370
CG2--HG21	1.09	0.97	590
CG--HG	1.09	0.97	270
CG2--HG23	1.09	0.97	590
CG--HG2	1.09	0.97	700
CB--HB1	1.09	0.97	290
CG1--HG12	1.09	0.97	350
NZ--HZ2	1.01	0.89	170
CE--HE2	1.09	0.97	210
NZ--HZ3	1.01	0.89	170
CA--HA3	1.09	0.97	480
CD2--HD22	1.09	0.97	270
CA--HA2	1.09	0.97	480
CG1--HG13	1.09	0.97	350
OH--HH	0.96	0.84	290
CB--HB	1.09	0.97	590

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--HG3	1.09	0.97	700
CD--HD3	1.09	0.97	340
CD2--HD23	1.09	0.97	270
CD2--HD21	1.09	0.97	270
CD--HD2	1.09	0.97	340
N--H1	1.01	0.89	10
NZ--HZ1	1.01	0.89	170
OG--HG	0.96	0.84	170
CD1--HD13	1.09	0.97	370
OG1--HG1	0.96	0.84	240
CG1--HG11	1.09	0.97	250
N--H3	1.01	0.89	10
CE--HE1	1.09	0.97	40
N--H2	1.01	0.89	10
CD2--HD2	1.08	0.93	490
CE2--HE2	1.08	0.93	480
CD1--HD1	1.08	0.93	520
N--H	1.01	0.86	3620
CE1--HE1	1.08	0.93	490
ND2--HD22	1.01	0.86	320
NE--HE	1.01	0.86	130
NE2--HE21	1.01	0.86	210
ND2--HD21	1.01	0.86	320

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND1--HD1	1.01	0.86	10
CZ--HZ	1.08	0.93	190
CZ2--HZ2	1.08	0.93	40
NH1--HH11	1.01	0.86	130
NH2--HH22	1.01	0.86	130
NE1--HE1	1.01	0.86	40
CZ3--HZ3	1.08	0.93	40
NH1--HH12	1.01	0.86	130
NE2--HE22	1.01	0.86	210
NH2--HH21	1.01	0.86	130
CH2--HH2	1.08	0.93	40
CE3--HE3	1.08	0.93	40

Standard geometry: angle outliers

There are 314 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	129.62	1
C-CA-CB	110.10	131.96	1
CA-CB-CG	112.60	123.61	1
C-N-CA	121.70	139.50	1
C-N-CA	121.70	138.00	1
CA-CB-CG	112.60	121.55	1
OE1-CD-NE2	122.60	114.42	1
C-N-CA	121.70	136.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	110.38	1
OD1-CG-ND2	122.60	115.10	1
O-C-N	123.00	111.25	1
OE1-CD-NE2	122.60	115.30	1
OD1-CG-ND2	122.60	115.34	1
OD1-CG-ND2	122.60	115.53	1
C-N-CA	121.70	134.15	1
CA-CB-CG	112.60	119.35	1
C-N-CA	121.70	133.73	1
CA-CB-CG	112.60	118.98	1
OE1-CD-NE2	122.60	116.29	1
OE1-CD-NE2	122.60	116.38	1
OE1-CD-NE2	122.60	116.39	1
OE1-CD-NE2	122.60	116.40	1
OE1-CD-NE2	122.60	116.46	3
C-N-CA	121.70	132.61	1
C-N-CA	121.70	132.55	1
OE1-CD-NE2	122.60	116.59	1
CA-CB-CG	112.60	106.60	1
C-N-CA	121.70	132.46	1
CA-CB-CG	112.60	118.54	1
OE1-CD-NE2	122.60	116.69	1
OE1-CD-NE2	122.60	116.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	118.60	109.78	1
OD1-CG-ND2	122.60	116.74	1
C-N-CA	121.70	132.20	2
OD1-CG-ND2	122.60	116.78	1
CA-CB-CG	112.60	118.38	1
OE1-CD-NE2	122.60	116.84	1
C-N-CA	121.70	132.06	1
OE1-CD-NE2	122.60	116.85	1
CA-CB-CG	112.60	118.26	1
N-CA-CB	110.50	120.11	1
OE1-CD-NE2	122.60	116.96	1
C-CA-CB	110.10	120.80	1
C-N-CA	121.70	131.79	1
C-N-CA	121.70	131.60	1
N-CA-CB	110.40	102.21	1
OD1-CG-ND2	122.60	117.18	1
NH1-CZ-NH2	119.30	112.26	1
OE1-CD-NE2	122.60	117.20	1
OE1-CD-NE2	122.60	117.21	1
OE1-CD-NE2	122.60	117.22	2
CA-CB-CG	112.60	117.97	1
C-N-CA	121.70	131.36	1
OE1-CD-NE2	122.60	117.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	120.22	1
OG1-CB-CG2	109.30	98.69	1
CA-C-N	116.20	126.78	1
C-N-CA	121.70	131.22	1
OE1-CD-NE2	122.60	117.31	2
C-N-CA	121.70	131.15	1
CA-CB-CG	113.90	123.33	1
OD1-CG-ND2	122.60	117.37	1
CA-CB-CG	112.60	117.82	1
CA-CB-CG	112.60	117.81	1
OE1-CD-NE2	122.60	117.40	1
C-N-CA	121.70	131.06	1
OE1-CD-NE2	122.60	117.43	1
CA-CB-CG	112.60	117.77	1
CA-CB-CG	112.60	117.76	1
C-N-CA	121.70	130.98	1
OE1-CD-NE2	122.60	117.45	3
OE1-CD-NE2	122.60	117.46	1
C-N-CA	121.70	130.94	2
OE1-CD-NE2	122.60	117.48	1
CA-CB-CG	112.60	117.71	1
OE1-CD-NE2	122.60	117.50	1
N-CA-CB	110.50	119.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.53	2
CA-CB-CG	112.60	107.54	1
OE1-CD-NE2	122.60	117.54	1
CA-CB-CG2	110.50	119.08	1
C-N-CA	121.70	130.78	1
OE1-CD-NE2	122.60	117.56	2
OD1-CG-ND2	122.60	117.60	1
OE1-CD-NE2	122.60	117.60	2
OD1-CG-ND2	122.60	117.61	1
CA-CB-CG	112.60	117.56	2
OE1-CD-NE2	122.60	117.64	1
CA-CB-CG	112.60	117.55	1
OE1-CD-NE2	122.60	117.65	1
CA-CB-CG	112.60	117.54	1
C-N-CA	121.70	130.59	1
OE1-CD-NE2	122.60	117.66	1
OE1-CD-NE2	122.60	117.67	1
N-CA-CB	103.00	108.37	1
OD1-CG-ND2	122.60	117.73	1
C-N-CA	121.70	130.46	1
CA-C-N	116.20	125.93	1
CA-CB-CG	112.60	117.46	1
C-N-CA	121.70	130.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.42	1
OE1-CD-NE2	122.60	117.77	1
OE1-CD-NE2	122.60	117.78	2
OE1-CD-NE2	122.60	117.79	1
CA-CB-CG	112.60	107.80	1
CA-CB-CG	113.80	109.00	1
OE1-CD-NE2	122.60	117.81	2
OE1-CD-NE2	122.60	117.82	2
C-N-CA	121.70	130.31	1
C-N-CA	121.70	130.28	1
OD1-CG-ND2	122.60	117.84	1
OE1-CD-NE2	122.60	117.85	1
CA-CB-CG	112.60	117.35	1
CA-CB-CG	112.60	117.34	1
OE1-CD-NE2	122.60	117.88	1
OE1-CD-NE2	122.60	117.90	2
C-N-CA	121.70	130.15	1
N-CA-CB	110.40	103.36	1
OE1-CD-NE2	122.60	117.91	2
C-N-CA	121.70	130.12	1
CA-CB-CG	112.60	117.27	1
OE1-CD-NE2	122.60	117.93	2
C-CA-CB	110.10	118.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.10	1
CA-CB-CG	112.60	117.26	1
OE1-CD-NE2	122.60	117.94	2
OD1-CG-ND2	122.60	117.95	1
C-N-CA	121.70	130.07	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	1
OG1-CB-CG2	109.30	100.04	1
OD1-CG-ND2	122.60	117.98	1
OE1-CD-NE2	122.60	117.99	2
OE1-CD-NE2	122.60	118.00	1
OE1-CD-NE2	122.60	118.01	2
OD1-CG-ND2	122.60	118.01	1
OD1-CG-ND2	122.60	118.02	1
CA-CB-OG1	109.60	116.47	1
OE1-CD-NE2	122.60	118.03	2
CA-CB-CG	112.60	117.17	1
OD1-CG-ND2	122.60	118.03	1
C-N-CA	121.70	129.92	1
OE1-CD-NE2	122.60	118.04	1
OE1-CD-NE2	122.60	118.05	2
NE-CZ-NH1	121.50	126.04	1
OE1-CD-NE2	122.60	118.07	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	123.68	1
OE1-CD-NE2	122.60	118.08	1
CA-CB-CG	112.60	117.11	1
N-CA-C	111.00	123.60	1
CA-CB-CG	112.60	117.10	1
C-N-CA	121.70	129.80	1
OE1-CD-NE2	122.60	118.10	1
OE1-CD-NE2	122.60	118.11	1
C-N-CA	121.70	129.78	1
OE1-CD-NE2	122.60	118.12	2
CA-CB-CG	112.60	117.08	1
C-N-CA	121.70	129.73	1
CA-CB-CG	112.60	117.04	1
OD1-CG-ND2	122.60	118.17	1
OD1-CG-ND2	122.60	118.19	2
C-N-CA	121.70	129.64	1
OE1-CD-NE2	122.60	118.20	1
OE1-CD-NE2	122.60	118.21	1
OD1-CG-ND2	122.60	118.21	1
CA-CB-CG	112.60	116.99	1
CA-CB-CG	112.60	116.98	1
CA-CB-CG	112.60	108.22	1
OD1-CG-ND2	122.60	118.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.59	2
OD1-CG-ND2	122.60	118.23	1
OE1-CD-NE2	122.60	118.23	2
OE1-CD-NE2	122.60	118.24	1
CA-CB-CG	112.60	116.96	1
N-CA-C	111.00	123.16	1
OE1-CD-NE2	122.60	118.26	1
O-C-OXT	118.00	130.96	1
CA-CB-CG	112.60	116.92	1
CA-CB-CG	112.60	108.29	1
OD1-CG-ND2	122.60	118.29	1
OE1-CD-NE2	122.60	118.29	3
CA-CB-CG	112.60	116.90	2
C-CA-CB	110.10	118.26	1
OE1-CD-NE2	122.60	118.31	2
C-N-CA	121.70	129.41	1
C-N-CA	121.70	129.40	1
C-N-CA	121.70	129.39	1
N-CA-CB	110.50	103.25	1
OE1-CD-NE2	122.60	118.34	3
OD1-CG-ND2	122.60	118.34	2
C-N-CA	121.70	129.36	1
OD1-CG-ND2	122.60	118.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG1	109.60	103.23	1
C-N-CA	121.70	129.34	1
OE1-CD-NE2	122.60	118.37	1
C-N-CA	121.70	129.30	1
C-CA-CB	110.50	116.84	1
OE1-CD-NE2	122.60	118.38	2
OD1-CG-ND2	122.60	118.38	2
OG1-CB-CG2	109.30	100.87	1
OD1-CG-ND2	122.60	118.40	1
OE1-CD-NE2	122.60	118.40	1
CA-CB-OG1	109.60	115.89	1
OD1-CG-ND2	122.60	118.41	1
C-N-CA	121.70	129.24	1
CA-CB-CG	113.90	121.44	1
C-CA-CB	110.10	118.05	1
N-CA-C	111.00	122.72	1
C-CA-CB	110.10	118.04	1
OE1-CD-NE2	122.60	118.42	1
CA-C-N	116.20	124.51	1
OE1-CD-NE2	122.60	118.45	1
C-N-CA	121.70	129.17	3
C-CA-CB	110.10	117.98	1
N-CA-CB	111.50	118.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.46	1
CA-CB-CG	112.60	116.74	2
OE1-CD-NE2	122.60	118.46	1
CD-NE-CZ	124.40	130.18	1
OD1-CG-ND2	122.60	118.47	2
CB-CG-CD	111.30	120.79	1
CA-CB-CG	112.60	116.72	2
OE1-CD-NE2	122.60	118.49	3
OD1-CG-ND2	122.60	118.49	1
OE1-CD-NE2	122.60	118.50	1
OD1-CG-ND2	122.60	118.50	2
OE1-CD-NE2	122.60	118.51	2
C-N-CA	121.70	129.04	1
C-N-CA	121.70	129.03	1
CA-CB-CG	112.60	116.67	2
N-CA-CB	110.50	117.41	1
C-CA-CB	110.10	117.83	1
N-CA-C	111.00	122.39	1
CA-CB-CG	113.80	109.73	1
OE1-CD-NE2	122.60	118.53	1
C-N-CA	121.70	129.01	1
CA-CB-CG	112.60	116.66	1
NE-CZ-NH1	121.50	125.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.40	103.69	1
C-N-CA	121.70	129.00	1
C-N-CA	121.70	128.99	1
OD1-CG-ND2	122.60	118.55	1
C-N-CA	121.70	128.97	1
CA-CB-CG	112.60	116.63	1
OE1-CD-NE2	122.60	118.58	1
N-CA-CB	110.50	103.66	1
OD1-CG-ND2	122.60	118.58	2
N-CA-CB	110.50	103.68	1
OE1-CD-NE2	122.60	118.60	1
C-N-H	112.17	124.30	1
C-N-H	111.83	124.30	1
C-N-H	111.66	124.30	1
C-N-H	111.35	124.30	1
HG2-CG-HG3	96.88	110.00	1
C-N-H	111.13	124.30	1
C-N-H	110.87	124.30	1
C-N-H	110.73	124.30	1
C-N-H	110.42	124.30	1
C-N-H	109.71	124.30	1
C-N-H	108.99	124.30	1
C-N-H	108.92	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	108.89	124.30	1
HB2-CB-HB3	91.71	110.00	1
HH21-NH2-HH22	98.35	120.00	1
HH21-NH2-HH22	96.90	120.00	1
HH21-NH2-HH22	93.25	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	9.24	51
2	8.69	48
3	4.17	23
4	3.98	22
5	6.70	37
6	5.07	28
7	1.45	8
8	6.88	38
9	5.98	33
10	7.25	40

All 328 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:120:ASP:H	A:151:THR:HG21	0.908
1	A:149:PHE:HB2	A:258:GLN:CD	0.730

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:346:GLN:HA	A:349:ARG:HE	0.700
1	A:150:ALA:HB1	A:283:VAL:HG21	0.687
1	A:34:LEU:HD23	A:367:PHE:CZ	0.634
1	A:125:THR:HG22	A:334:TYR:CG	0.610
1	A:115:TYR:CE2	A:219:SER:HB3	0.573
1	A:120:ASP:N	A:151:THR:HG21	0.563
1	A:142:MET:HA	A:171:GLN:CD	0.556
1	A:117:VAL:HG11	A:245:GLY:N	0.554
1	A:266:THR:HG1	A:273:TRP:CD1	0.547
1	A:79:TYR:CD2	A:94:THR:HG22	0.534
1	A:133:GLY:CA	A:316:LEU:HD22	0.534
1	A:141:PHE:CD2	A:221:SER:CB	0.534
1	A:141:PHE:CG	A:221:SER:HB2	0.531
1	A:150:ALA:CB	A:283:VAL:HG21	0.528
1	A:117:VAL:HG13	A:215:GLY:C	0.523
1	A:160:LEU:HD12	A:247:LYS:NZ	0.510
1	A:182:PHE:O	A:183:THR:HG23	0.496
1	A:261:GLN:NE2	A:263:TYR:CZ	0.496
1	A:141:PHE:CD1	A:221:SER:HB2	0.493
1	A:175:GLY:HA3	A:190:GLY:HA2	0.492
1	A:133:GLY:HA2	A:316:LEU:HD22	0.487
1	A:300:GLN:HE22	A:317:LYS:HE3	0.486
1	A:49:ASP:O	A:50:VAL:HG23	0.483

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:119:TYR:HB2	A:160:LEU:HD11	0.483
1	A:120:ASP:H	A:151:THR:CG2	0.482
1	A:34:LEU:HB3	A:367:PHE:CZ	0.480
1	A:149:PHE:CG	A:258:GLN:HB3	0.480
1	A:136:TYR:CZ	A:146:GLY:HA3	0.478
1	A:104:GLN:O	A:161:VAL:HG11	0.477
1	A:149:PHE:CD2	A:258:GLN:HB3	0.466
1	A:133:GLY:HA2	A:316:LEU:CD2	0.464
1	A:160:LEU:HD13	A:208:ASP:OD2	0.455
1	A:283:VAL:HG22	A:297:ALA:CB	0.451
1	A:149:PHE:CE1	A:257:ALA:C	0.436
1	A:61:PHE:CE1	A:77:TRP:CE3	0.425
1	A:136:TYR:CE1	A:146:GLY:N	0.425
1	A:139:ASP:O	A:141:PHE:CE2	0.425
1	A:141:PHE:CG	A:221:SER:CB	0.424
1	A:300:GLN:HE22	A:317:LYS:CE	0.424
1	A:97:ALA:HA	A:145:ARG:HH22	0.422
1	A:137:GLY:C	A:139:ASP:H	0.421
1	A:160:LEU:HD12	A:247:LYS:HZ3	0.418
1	A:130:GLU:HG2	A:131:PHE:CZ	0.417
1	A:127:VAL:H	A:127:VAL:HG23	0.408
1	A:33:ASP:CG	A:157:PHE:CE2	0.405
1	A:135:THR:HG21	A:279:ASN:HD21	0.404

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:142:MET:SD	A:171:GLN:CB	0.403
1	A:312:ASP:C	A:314:ASP:H	0.403
1	A:334:TYR:CE1	A:362:GLY:HA3	0.401
2	A:98:PHE:CZ	A:127:VAL:HG22	0.697
2	A:127:VAL:HG21	A:169:GLN:NE2	0.695
2	A:345:ASN:HA	A:348:THR:HG22	0.661
2	A:16:ALA:HB1	A:331:MET:SD	0.644
2	A:347:PHE:CD2	A:350:ASP:CG	0.643
2	A:347:PHE:CE2	A:350:ASP:HB2	0.633
2	A:124:TRP:HD1	A:135:THR:HG21	0.627
2	A:133:GLY:N	A:217:ALA:HB3	0.620
2	A:223:ARG:NH1	A:233:ILE:HG22	0.591
2	A:124:TRP:CD1	A:135:THR:HG21	0.589
2	A:267:ARG:HB2	A:273:TRP:CZ2	0.587
2	A:347:PHE:CB	A:349:ARG:HA	0.583
2	A:306:LEU:HD11	A:314:ASP:CG	0.582
2	A:347:PHE:CD1	A:349:ARG:C	0.581
2	A:347:PHE:CD1	A:349:ARG:CA	0.577
2	A:16:ALA:HB2	A:365:TYR:OH	0.566
2	A:21:ALA:HB1	A:367:PHE:CD1	0.550
2	A:347:PHE:CD1	A:349:ARG:CB	0.539
2	A:150:ALA:HA	A:293:ARG:HH22	0.538
2	A:347:PHE:CG	A:350:ASP:N	0.534

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:127:VAL:HG21	A:169:GLN:CD	0.532
2	A:347:PHE:CD1	A:349:ARG:HB3	0.524
2	A:353:ILE:HG22	A:355:THR:HG23	0.524
2	A:227:GLN:O	A:233:ILE:HD12	0.521
2	A:223:ARG:CZ	A:233:ILE:HG22	0.499
2	A:128:LEU:HB2	A:132:GLY:HA3	0.493
2	A:347:PHE:HA	A:350:ASP:OD1	0.493
2	A:98:PHE:CE1	A:127:VAL:HG13	0.491
2	A:347:PHE:CE1	A:349:ARG:C	0.491
2	A:267:ARG:HB2	A:273:TRP:CH2	0.487
2	A:121:VAL:HG12	A:135:THR:HG21	0.483
2	A:47:ASN:HD21	A:342:LEU:HD12	0.479
2	A:267:ARG:CB	A:273:TRP:CZ2	0.470
2	A:233:ILE:HA	A:273:TRP:CH2	0.463
2	A:141:PHE:CD1	A:358:ILE:CD1	0.454
2	A:140:ASN:HD21	A:271:LEU:HD12	0.453
2	A:347:PHE:CE2	A:350:ASP:CB	0.453
2	A:150:ALA:HA	A:293:ARG:NH2	0.446
2	A:347:PHE:CG	A:349:ARG:HA	0.444
2	A:273:TRP:CD1	A:273:TRP:N	0.434
2	A:96:VAL:HB	A:98:PHE:CE2	0.432
2	A:273:TRP:C	A:306:LEU:HD23	0.418
2	A:227:GLN:HA	A:233:ILE:HD12	0.417

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:345:ASN:HA	A:348:THR:CG2	0.416
2	A:141:PHE:CE1	A:340:ASN:ND2	0.409
2	A:129:PRO:HD2	A:204:SER:OG	0.408
2	A:133:GLY:H	A:217:ALA:HB3	0.404
2	A:140:ASN:HB2	A:141:PHE:CE2	0.401
3	A:127:VAL:HG11	A:297:ALA:HB2	0.963
3	A:316:LEU:HD13	A:342:LEU:HD12	0.597
3	A:268:VAL:HG22	A:277:ALA:HB2	0.573
3	A:136:TYR:CZ	A:269:GLY:HA3	0.541
3	A:128:LEU:HD22	A:334:TYR:CE2	0.540
3	A:131:PHE:CE2	A:364:VAL:HG13	0.536
3	A:151:THR:HG21	A:153:ARG:NH1	0.509
3	A:19:ALA:HB2	A:367:PHE:CZ	0.496
3	A:268:VAL:CG2	A:277:ALA:HB2	0.496
3	A:299:LEU:HD23	A:318:TYR:CD2	0.480
3	A:127:VAL:C	A:129:PRO:HD3	0.467
3	A:271:LEU:HD21	A:342:LEU:CD1	0.465
3	A:297:ALA:HB3	A:320:ASP:HB3	0.461
3	A:58:ARG:HH22	A:134:ASP:CG	0.458
3	A:136:TYR:CE2	A:269:GLY:HA3	0.457
3	A:268:VAL:HG22	A:277:ALA:CB	0.454
3	A:233:ILE:CG2	A:305:ASN:HB3	0.437
3	A:233:ILE:HG22	A:275:ASN:HB2	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:95:ARG:HH21	A:145:ARG:NH1	0.423
3	A:44:PHE:HE1	A:359:VAL:HG23	0.418
3	A:5:VAL:HG12	A:9:LEU:HD12	0.414
3	A:143:GLN:NE2	A:262:THR:HG21	0.406
3	A:35:TYR:CZ	A:60:GLY:HA3	0.403
4	A:37:LYS:HE2	A:58:ARG:CZ	0.646
4	A:223:ARG:HH22	A:231:ALA:CB	0.633
4	A:34:LEU:HD11	A:59:LEU:HD11	0.617
4	A:19:ALA:HB1	A:367:PHE:CE1	0.610
4	A:95:ARG:HH21	A:145:ARG:NH2	0.601
4	A:128:LEU:HD12	A:131:PHE:CE2	0.588
4	A:52:GLY:HA2	A:86:ALA:HB2	0.575
4	A:128:LEU:HD11	A:297:ALA:HB3	0.555
4	A:128:LEU:HD11	A:297:ALA:CB	0.545
4	A:34:LEU:HD13	A:61:PHE:CE1	0.539
4	A:143:GLN:HE22	A:279:ASN:ND2	0.522
4	A:239:ALA:HB1	A:265:ALA:HB2	0.510
4	A:223:ARG:HH22	A:231:ALA:HB3	0.505
4	A:233:ILE:HD11	A:307:GLY:CA	0.490
4	A:137:GLY:HA3	A:144:GLN:HE21	0.487
4	A:114:ASN:ND2	A:157:PHE:CE2	0.469
4	A:54:GLN:HE21	A:84:ASN:ND2	0.466
4	A:278:GLN:OE1	A:304:LYS:HE3	0.463

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:127:VAL:CG2	A:283:VAL:HG11	0.448
4	A:95:ARG:HH21	A:145:ARG:CZ	0.439
4	A:115:TYR:CZ	A:145:ARG:CZ	0.412
4	A:128:LEU:HB2	A:131:PHE:CD2	0.406
5	A:348:THR:HG23	A:354:ASN:HD22	0.747
5	A:129:PRO:HB2	A:334:TYR:CG	0.632
5	A:128:LEU:HD21	A:338:LYS:HE2	0.616
5	A:149:PHE:CZ	A:262:THR:HG23	0.601
5	A:348:THR:HG23	A:354:ASN:ND2	0.568
5	A:129:PRO:HA	A:132:GLY:H	0.566
5	A:348:THR:CG2	A:354:ASN:HB2	0.565
5	A:141:PHE:CE1	A:316:LEU:HD11	0.551
5	A:19:ALA:HA	A:367:PHE:CZ	0.547
5	A:128:LEU:CD2	A:338:LYS:HE2	0.543
5	A:189:ASN:HD22	A:191:ARG:HH21	0.538
5	A:128:LEU:HD11	A:338:LYS:HE2	0.515
5	A:311:ASP:C	A:313:GLU:H	0.512
5	A:348:THR:HG23	A:354:ASN:HB2	0.512
5	A:127:VAL:HG13	A:285:GLN:HE21	0.505
5	A:114:ASN:HA	A:152:TYR:CG	0.502
5	A:149:PHE:CZ	A:262:THR:CG2	0.500
5	A:230:ALA:C	A:232:TYR:H	0.493
5	A:114:ASN:C	A:152:TYR:HB3	0.485

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:118:VAL:HG12	A:122:THR:HG23	0.479
5	A:128:LEU:CD1	A:338:LYS:HE2	0.477
5	A:129:PRO:HD2	A:336:ASP:OD1	0.472
5	A:365:TYR:CE1	A:367:PHE:CE2	0.472
5	A:149:PHE:CE1	A:239:ALA:HB1	0.464
5	A:149:PHE:CZ	A:239:ALA:HB1	0.461
5	A:62:LYS:HE3	A:157:PHE:CZ	0.450
5	A:43:TYR:CD1	A:50:VAL:HG12	0.447
5	A:19:ALA:HA	A:367:PHE:CE2	0.433
5	A:183:THR:C	A:185:GLY:H	0.432
5	A:114:ASN:CA	A:152:TYR:HB3	0.430
5	A:126:ASP:OD1	A:131:PHE:CD2	0.414
5	A:150:ALA:HB1	A:171:GLN:OE1	0.414
5	A:151:THR:C	A:152:TYR:CG	0.412
5	A:149:PHE:CZ	A:265:ALA:HB3	0.411
5	A:115:TYR:C	A:152:TYR:HB2	0.407
5	A:141:PHE:CD1	A:316:LEU:HD11	0.406
5	A:127:VAL:HG21	A:297:ALA:HB2	0.405
6	A:141:PHE:HB3	A:262:THR:HG21	0.799
6	A:146:GLY:HA3	A:149:PHE:CE2	0.586
6	A:146:GLY:HA2	A:149:PHE:CZ	0.585
6	A:131:PHE:CD1	A:338:LYS:HE3	0.562
6	A:128:LEU:HD11	A:297:ALA:CB	0.548

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:128:LEU:HD13	A:320:ASP:OD2	0.544
6	A:34:LEU:HD13	A:61:PHE:CE1	0.530
6	A:231:ALA:HB3	A:233:ILE:CG1	0.509
6	A:131:PHE:CG	A:338:LYS:HE3	0.508
6	A:145:ARG:HG2	A:197:ASN:ND2	0.507
6	A:52:GLY:HA3	A:86:ALA:HB2	0.504
6	A:141:PHE:CZ	A:277:ALA:CB	0.503
6	A:196:GLN:HB2	A:224:THR:HG21	0.497
6	A:299:LEU:HD22	A:316:LEU:CD2	0.489
6	A:146:GLY:CA	A:149:PHE:CE2	0.482
6	A:145:ARG:HB3	A:171:GLN:HE22	0.480
6	A:128:LEU:HD11	A:297:ALA:HB2	0.467
6	A:271:LEU:CD1	A:347:PHE:CE2	0.464
6	A:34:LEU:HD23	A:367:PHE:CZ	0.442
6	A:141:PHE:CZ	A:277:ALA:HB2	0.441
6	A:145:ARG:HA	A:197:ASN:ND2	0.437
6	A:145:ARG:CG	A:197:ASN:ND2	0.430
6	A:146:GLY:CA	A:149:PHE:CZ	0.426
6	A:135:THR:HG23	A:281:GLU:OE1	0.425
6	A:319:VAL:HG23	A:341:LEU:HD11	0.416
6	A:128:LEU:HD11	A:297:ALA:HB3	0.413
6	A:149:PHE:CD1	A:169:GLN:NE2	0.411
6	A:261:GLN:CD	A:276:LYS:HE3	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:258:GLN:HE21	A:281:GLU:CD	0.455
7	A:5:VAL:C	A:7:SER:H	0.430
7	A:146:GLY:HA3	A:149:PHE:CZ	0.430
7	A:278:GLN:OE1	A:304:LYS:HE3	0.430
7	A:128:LEU:HD11	A:297:ALA:CB	0.428
7	A:142:MET:HE2	A:201:VAL:N	0.416
7	A:141:PHE:CE1	A:171:GLN:NE2	0.404
7	A:141:PHE:CD1	A:171:GLN:NE2	0.401
8	A:342:LEU:HD12	A:355:THR:HG22	0.879
8	A:191:ARG:HA	A:194:LEU:HD12	0.698
8	A:342:LEU:CD1	A:355:THR:HG22	0.583
8	A:271:LEU:HD13	A:312:ASP:HB2	0.582
8	A:37:LYS:HE2	A:39:ASP:OD2	0.546
8	A:271:LEU:HD13	A:312:ASP:CB	0.535
8	A:122:THR:HG23	A:145:ARG:HH12	0.529
8	A:91:ASN:HB3	A:93:TRP:CE2	0.504
8	A:113:ARG:NH2	A:157:PHE:CE2	0.499
8	A:305:ASN:HD21	A:354:ASN:HD22	0.494
8	A:310:TYR:HB2	A:355:THR:HG23	0.475
8	A:271:LEU:HD13	A:312:ASP:H	0.470
8	A:169:GLN:NE2	A:171:GLN:HE21	0.468
8	A:149:PHE:CE1	A:167:ALA:HB3	0.466
8	A:264:ASN:C	A:266:THR:H	0.455

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:342:LEU:HD12	A:355:THR:CG2	0.449
8	A:311:ASP:O	A:342:LEU:HD13	0.447
8	A:194:LEU:HD13	A:228:ASN:CG	0.446
8	A:115:TYR:HB2	A:152:TYR:CE1	0.444
8	A:270:SER:C	A:271:LEU:HG	0.441
8	A:310:TYR:CB	A:355:THR:CG2	0.439
8	A:258:GLN:NE2	A:279:ASN:HD21	0.431
8	A:51:ASP:C	A:53:ASP:H	0.428
8	A:35:TYR:CE2	A:62:LYS:HE2	0.427
8	A:99:ALA:HB3	A:114:ASN:HB2	0.427
8	A:64:GLU:HB3	A:74:TYR:CE1	0.426
8	A:194:LEU:HD13	A:228:ASN:OD1	0.425
8	A:39:ASP:CG	A:58:ARG:HH21	0.418
8	A:25:TYR:CE2	A:32:LEU:HB2	0.417
8	A:41:LEU:HD11	A:56:TYR:CD2	0.417
8	A:181:GLY:C	A:183:THR:H	0.417
8	A:25:TYR:CZ	A:32:LEU:HB2	0.415
8	A:310:TYR:HB3	A:355:THR:CG2	0.413
8	A:194:LEU:CD2	A:223:ARG:HH11	0.409
8	A:122:THR:HG23	A:145:ARG:NH1	0.405
8	A:164:LEU:HD21	A:166:PHE:CZ	0.403
8	A:271:LEU:CD1	A:312:ASP:HB2	0.403
8	A:305:ASN:ND2	A:354:ASN:HD22	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:269:GLY:HA2	A:347:PHE:CE2	0.691
9	A:316:LEU:HD12	A:342:LEU:HG	0.681
9	A:266:THR:HG23	A:273:TRP:CH2	0.643
9	A:269:GLY:CA	A:347:PHE:CE2	0.614
9	A:316:LEU:HD11	A:340:ASN:HD21	0.609
9	A:141:PHE:CE1	A:239:ALA:HB1	0.576
9	A:316:LEU:HD12	A:342:LEU:CG	0.569
9	A:19:ALA:HB1	A:21:ALA:HB2	0.566
9	A:136:TYR:CE1	A:267:ARG:CZ	0.553
9	A:303:GLY:N	A:315:ILE:HD12	0.532
9	A:316:LEU:HD23	A:318:TYR:HD1	0.522
9	A:23:GLU:CD	A:26:ASN:HB2	0.507
9	A:136:TYR:OH	A:316:LEU:HD13	0.501
9	A:155:THR:HG21	A:165:ASN:OD1	0.500
9	A:316:LEU:HD23	A:318:TYR:CD1	0.496
9	A:48:LYS:HE2	A:344:ASP:CA	0.492
9	A:48:LYS:HE2	A:344:ASP:HA	0.481
9	A:21:ALA:C	A:367:PHE:CZ	0.469
9	A:87:GLU:C	A:89:GLU:H	0.468
9	A:269:GLY:HA3	A:347:PHE:CZ	0.440
9	A:77:TRP:CH2	A:79:TYR:HB2	0.438
9	A:316:LEU:HD12	A:342:LEU:CD1	0.436
9	A:129:PRO:HB2	A:334:TYR:CE2	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:334:TYR:CE1	A:362:GLY:HA3	0.427
9	A:95:ARG:NH2	A:145:ARG:HH11	0.427
9	A:48:LYS:NZ	A:344:ASP:HA	0.423
9	A:208:ASP:OD1	A:247:LYS:CE	0.422
9	A:95:ARG:HH22	A:145:ARG:CD	0.409
9	A:20:ASN:C	A:22:ALA:H	0.407
9	A:143:GLN:HE21	A:241:THR:HG21	0.405
9	A:266:THR:HG23	A:273:TRP:CZ2	0.405
9	A:348:THR:HG23	A:353:ILE:O	0.405
9	A:95:ARG:HH22	A:145:ARG:HD3	0.401
10	A:316:LEU:HD21	A:319:VAL:HG23	0.669
10	A:95:ARG:CZ	A:149:PHE:CE1	0.655
10	A:147:ASN:HB2	A:149:PHE:CZ	0.652
10	A:299:LEU:HD22	A:318:TYR:CE2	0.647
10	A:348:THR:HG21	A:355:THR:CG2	0.606
10	A:316:LEU:HD21	A:319:VAL:CG2	0.595
10	A:136:TYR:CD1	A:273:TRP:CZ3	0.593
10	A:271:LEU:HD22	A:310:TYR:HE2	0.585
10	A:42:HIS:CD2	A:44:PHE:CZ	0.583
10	A:144:GLN:HE22	A:241:THR:HG21	0.551
10	A:122:THR:HG21	A:144:GLN:OE1	0.544
10	A:348:THR:HG21	A:355:THR:HG21	0.535
10	A:42:HIS:CD2	A:44:PHE:CE1	0.533

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:95:ARG:NH1	A:149:PHE:CE1	0.506
10	A:233:ILE:HD12	A:267:ARG:NH2	0.493
10	A:152:TYR:CE1	A:364:VAL:HG11	0.491
10	A:136:TYR:CE1	A:273:TRP:CZ3	0.490
10	A:122:THR:HG22	A:258:GLN:OE1	0.488
10	A:274:ALA:C	A:276:LYS:H	0.488
10	A:131:PHE:CE2	A:338:LYS:HB2	0.485
10	A:95:ARG:NH2	A:149:PHE:CE1	0.477
10	A:261:GLN:NE2	A:263:TYR:CZ	0.476
10	A:152:TYR:CE1	A:364:VAL:CG1	0.461
10	A:273:TRP:NE1	A:347:PHE:CZ	0.453
10	A:144:GLN:NE2	A:241:THR:HG21	0.443
10	A:261:GLN:NE2	A:263:TYR:CE2	0.439
10	A:267:ARG:HG2	A:268:VAL:N	0.439
10	A:334:TYR:CZ	A:362:GLY:HA3	0.437
10	A:117:VAL:HG21	A:202:GLY:C	0.431
10	A:223:ARG:HH12	A:234:GLY:CA	0.426
10	A:233:ILE:O	A:233:ILE:HG22	0.423
10	A:188:ASN:C	A:190:GLY:H	0.422
10	A:80:GLN:CD	A:93:TRP:CZ2	0.421
10	A:147:ASN:HB2	A:149:PHE:CE2	0.411
10	A:233:ILE:O	A:267:ARG:HG3	0.411
10	A:34:LEU:HD13	A:61:PHE:CE1	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:223:ARG:HH22	A:234:GLY:HA3	0.408
10	A:153:ARG:CZ	A:157:PHE:CG	0.404
10	A:26:ASN:ND2	A:30:ASN:HD22	0.404
10	A:233:ILE:N	A:267:ARG:HD2	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	365	313	32	20
2	365	328	21	16
3	365	314	33	18
4	365	335	19	11
5	365	335	20	10
6	365	332	20	13
7	365	343	18	4
8	365	308	33	24
9	365	323	23	19
10	365	323	20	22

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	290	262	14	14
2	290	268	15	7

Model ID	Analyzed	Favored	Allowed	Outliers
3	290	278	9	3
4	290	283	4	3
5	290	275	9	6
6	290	278	6	6
7	290	275	9	6
8	290	266	14	10
9	290	279	6	5
10	290	273	13	4

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	1	MET
1	A	6	LEU
1	A	8	LEU
1	A	13	LEU
1	A	122	THR
1	A	142	MET
1	A	149	PHE
1	A	157	PHE
1	A	183	THR
1	A	186	VAL
1	A	268	VAL
1	A	316	LEU
1	A	320	ASP

Model ID	Chain	Residue ID	Residue type
1	A	343	ASP
2	A	1	MET
2	A	121	VAL
2	A	122	THR
2	A	151	THR
2	A	178	SER
2	A	182	PHE
2	A	273	TRP
3	A	130	GLU
3	A	135	THR
3	A	151	THR
4	A	50	VAL
4	A	136	TYR
4	A	270	SER
5	A	6	LEU
5	A	50	VAL
5	A	118	VAL
5	A	127	VAL
5	A	344	ASP
5	A	348	THR
6	A	135	THR
6	A	136	TYR
6	A	142	MET

Model ID	Chain	Residue ID	Residue type
6	A	169	GLN
6	A	186	VAL
6	A	232	TYR
7	A	6	LEU
7	A	7	SER
7	A	8	LEU
7	A	50	VAL
7	A	85	SER
7	A	142	MET
8	A	6	LEU
8	A	8	LEU
8	A	71	LEU
8	A	109	PHE
8	A	122	THR
8	A	136	TYR
8	A	139	ASP
8	A	268	VAL
8	A	270	SER
8	A	355	THR
9	A	128	LEU
9	A	182	PHE
9	A	266	THR
9	A	312	ASP

Model ID	Chain	Residue ID	Residue type
9	A	316	LEU
10	A	8	LEU
10	A	151	THR
10	A	233	ILE
10	A	343	ASP

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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