Integrative Structure Validation Report

July 22, 2024 - 05:18 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	9A3C
PDB-Dev ID	PDBDEV_00000197
Structure Title	Model of E. coli Fiu 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

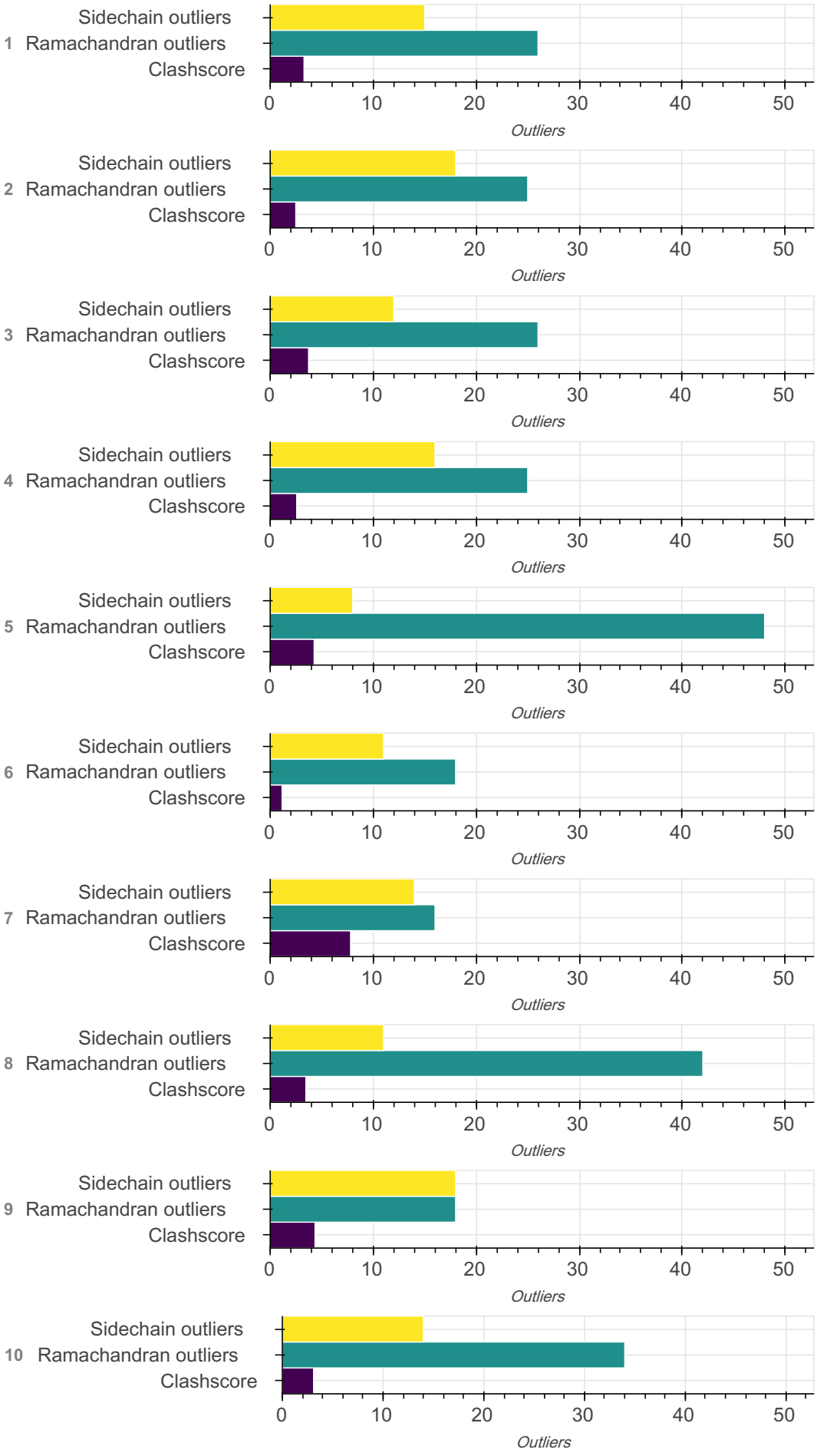
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
10
20
30
40
50
Outliers
2
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
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40
50
Outliers
3
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
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50
Outliers
4
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
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40
50
Outliers
5
Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
6
Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
7
Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
8
Sidechain outliers
Ramachandran outliers
Clashscore
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50
Outliers
9
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
Outliers
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
10
20
30
40
50
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	P75780	A	A	760
2	1	1	P75780	A	A	760
3	1	1	P75780	A	A	760
4	1	1	P75780	A	A	760
5	1	1	P75780	A	A	760
6	1	1	P75780	A	A	760
7	1	1	P75780	A	A	760
8	1	1	P75780	A	A	760
9	1	1	P75780	A	A	760
10	1	1	P75780	A	A	760

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	-	1-760

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 54970 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--HG	1.09	0.97	400
CD1--HD12	1.09	0.97	790
OH--HH	0.96	0.84	330
CB--HB3	1.09	0.97	5170
CA--HA3	1.09	0.97	760
CA--HA	1.09	0.97	6840
CD--HD3	1.09	0.97	920
CG1--HG13	1.09	0.97	840
CG--HG2	1.09	0.97	1580
CB--HB2	1.09	0.97	5170
CE--HE3	1.09	0.97	380
CG2--HG21	1.09	0.97	1670
CG1--HG12	1.09	0.97	840
CG--HG3	1.09	0.97	1580
CD1--HD11	1.09	0.97	790
CD1--HD13	1.09	0.97	790
CB--HB	1.09	0.97	1670
CD--HD2	1.09	0.97	920
CG2--HG23	1.09	0.97	1670
CG2--HG22	1.09	0.97	1670
CA--HA2	1.09	0.97	760
CG1--HG11	1.09	0.97	450

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OG--HG	0.96	0.84	560
CE--HE1	1.09	0.97	110
CD2--HD22	1.09	0.97	400
NZ--HZ1	1.01	0.89	270
CD2--HD23	1.09	0.97	400
OG1--HG1	0.96	0.84	830
CD2--HD21	1.09	0.97	400
CB--HB1	1.09	0.97	670
NZ--HZ3	1.01	0.89	270
NZ--HZ2	1.01	0.89	270
CE--HE2	1.09	0.97	380
N--H2	1.01	0.89	10
N--H1	1.01	0.89	10
N--H3	1.01	0.89	10
SG--HG	1.33	1.20	2
SG--HG	1.34	1.20	8
CZ--HZ	1.08	0.93	260
N--H	1.01	0.86	7280
CZ2--HZ2	1.08	0.93	90
ND2--HD21	1.01	0.86	570
CD2--HD2	1.08	0.93	750
CD1--HD1	1.08	0.93	680
NH2--HH22	1.01	0.86	340

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE1--HE1	1.08	0.93	750
NE2--HE22	1.01	0.86	310
ND2--HD22	1.01	0.86	570
NH2--HH21	1.01	0.86	340
NE--HE	1.01	0.86	340
CE2--HE2	1.08	0.93	590
NE2--HE21	1.01	0.86	310
CZ3--HZ3	1.08	0.93	90
NH1--HH12	1.01	0.86	340
NH1--HH11	1.01	0.86	340
CH2--HH2	1.08	0.93	90
NE1--HE1	1.01	0.86	90
ND1--HD1	1.01	0.86	148
CE3--HE3	1.08	0.93	90
NE2--HE2	1.01	0.86	12

Standard geometry: angle outliers

There are 516 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-N-CD	112.00	99.98	1
C-N-CA	121.70	134.90	1
C-N-CA	121.70	133.86	1
C-N-CA	121.70	133.79	1
C-N-CA	121.70	133.62	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.08	1
CA-CB-CG	112.60	119.11	1
CA-CB-OG1	109.60	119.35	1
OE1-CD-NE2	122.60	116.14	1
OD1-CG-ND2	122.60	116.14	1
C-N-CA	121.70	133.05	1
C-N-CA	121.70	133.04	1
C-N-CA	121.70	132.94	1
OD1-CG-ND2	122.60	116.36	1
CA-CB-CG	112.60	118.79	1
C-CA-CB	110.50	119.67	1
C-N-CA	121.70	132.61	1
NE-CZ-NH2	119.20	124.65	1
OE1-CD-NE2	122.60	116.57	1
CA-CB-CG	112.60	118.62	1
C-N-CA	121.70	132.38	1
C-N-CA	121.70	132.37	1
OE1-CD-NE2	122.60	116.69	1
CA-CB-CG	112.60	118.50	1
OE1-CD-NE2	122.60	116.70	1
OE1-CD-NE2	122.60	116.74	1
C-N-CA	121.70	132.22	1
OE1-CD-NE2	122.60	116.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	118.40	1
C-N-CA	121.70	132.13	1
NE-CZ-NH2	119.20	124.34	1
C-N-CA	121.70	131.94	1
CA-CB-CG	112.60	118.28	1
OE1-CD-NE2	122.60	116.92	1
CA-N-CD	112.00	104.10	1
OE1-CD-NE2	122.60	116.96	1
C-N-CA	121.70	131.82	1
C-N-CA	121.70	131.77	1
OD1-CG-ND2	122.60	117.02	1
CA-CB-CG	112.60	118.16	1
OE1-CD-NE2	122.60	117.04	1
OE1-CD-NE2	122.60	117.06	1
OE1-CD-NE2	122.60	117.10	2
CA-CB-CG	112.60	107.10	1
OD1-CG-ND2	122.60	117.15	1
OE1-CD-NE2	122.60	117.16	1
CA-CB-CG1	110.40	119.63	1
C-N-CA	121.70	131.46	1
C-N-CA	121.70	131.43	1
C-N-CA	121.70	131.41	1
OE1-CD-NE2	122.60	117.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.23	2
CA-CB-CG	112.60	117.96	1
OE1-CD-NE2	122.60	117.26	2
C-CA-CB	110.50	118.50	1
CB-CG-CD2	131.20	124.27	1
OE1-CD-NE2	122.60	117.27	1
C-N-CA	121.70	131.26	1
C-N-CA	121.70	131.24	1
OE1-CD-NE2	122.60	117.30	1
CA-CB-CG	112.60	107.32	1
C-N-CA	121.70	131.20	1
OE1-CD-NE2	122.60	117.33	2
CA-CB-CG	113.80	119.05	1
O-C-N	123.00	114.62	1
C-N-CA	121.70	131.11	1
OE1-CD-NE2	122.60	117.38	1
NE-CZ-NH2	119.20	123.89	1
OE1-CD-NE2	122.60	117.41	2
CA-C-N	116.20	126.55	1
OE1-CD-NE2	122.60	117.43	1
OD1-CG-ND2	122.60	117.45	1
OE1-CD-NE2	122.60	117.46	1
N-CA-CB	110.50	101.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.47	1
C-N-CA	121.70	130.93	1
C-N-CA	121.70	130.92	1
CD-NE-CZ	124.40	131.56	1
CA-CB-CG	112.60	117.71	1
OE1-CD-NE2	122.60	117.50	1
OE1-CD-NE2	122.60	117.51	1
OE1-CD-NE2	122.60	117.52	1
CA-CB-CG	112.60	107.53	1
OE1-CD-NE2	122.60	117.54	2
CB-CG-CD2	131.20	124.63	1
OE1-CD-NE2	122.60	117.55	1
OE1-CD-NE2	122.60	117.56	1
C-N-CA	121.70	130.77	1
C-N-CA	121.70	130.76	1
OE1-CD-NE2	122.60	117.58	2
CB-CG-CD2	131.20	124.68	1
OE1-CD-NE2	122.60	117.60	1
C-N-CA	121.70	130.69	1
OE1-CD-NE2	122.60	117.61	1
C-N-CA	121.70	130.68	1
C-N-CA	121.70	130.67	1
OD1-CG-ND2	122.60	117.62	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.57	2
OE1-CD-NE2	122.60	117.65	1
N-CA-C	111.00	124.85	1
CD-NE-CZ	124.40	131.32	1
OE1-CD-NE2	122.60	117.66	1
C-N-CA	121.70	130.59	1
OD1-CG-ND2	122.60	117.66	1
CA-CB-CG	114.10	123.96	1
OE1-CD-NE2	122.60	117.67	1
C-N-CA	121.70	130.55	1
CA-C-N	116.20	126.02	1
C-N-CA	121.70	130.53	1
OE1-CD-NE2	122.60	117.70	3
OD1-CG-ND2	122.60	117.70	1
NE-CZ-NH2	119.20	123.60	1
OE1-CD-NE2	122.60	117.71	1
OE1-CD-NE2	122.60	117.72	1
C-N-CA	121.70	130.48	2
C-N-CA	121.70	112.94	1
C-N-CA	121.70	130.46	1
OE1-CD-NE2	122.60	117.74	1
OE1-CD-NE2	122.60	117.75	3
OE1-CD-NE2	122.60	117.76	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.77	2
C-N-CA	121.70	130.39	1
OE1-CD-NE2	122.60	117.79	1
OE1-CD-NE2	122.60	117.80	2
CA-CB-CG	112.60	117.40	1
OE1-CD-NE2	122.60	117.82	1
C-N-CA	121.70	130.30	1
OD1-CG-ND2	122.60	117.82	1
C-N-CA	121.70	130.29	1
OD1-CG-ND2	122.60	117.83	1
OE1-CD-NE2	122.60	117.83	2
C-N-CA	121.70	130.27	1
OE1-CD-NE2	122.60	117.84	1
C-N-CA	121.70	130.26	1
CA-CB-CG	112.60	117.35	1
C-CA-CB	110.10	119.12	1
OE1-CD-NE2	122.60	117.86	3
C-N-CA	121.70	130.23	1
OE1-CD-NE2	122.60	117.87	1
C-N-CA	121.70	130.20	1
OE1-CD-NE2	122.60	117.89	1
C-CA-CB	110.50	117.56	1
CA-CB-CG	112.60	117.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.91	3
C-N-CA	121.70	130.14	1
O-C-N	123.00	115.51	1
C-N-CA	121.70	130.13	1
OE1-CD-NE2	122.60	117.93	2
CD-NE-CZ	124.40	130.94	1
CA-CB-OG1	109.60	116.58	1
OE1-CD-NE2	122.60	117.95	2
CD-NE-CZ	124.40	130.90	1
OE1-CD-NE2	122.60	117.96	1
NE-CZ-NH2	119.20	123.37	1
OD1-CG-ND2	122.60	117.97	1
OE1-CD-NE2	122.60	117.97	3
OE1-CD-NE2	122.60	117.98	4
CB-CG-CD2	131.20	125.20	1
CB-CG-CD2	131.20	125.21	1
N-CA-C	111.00	123.90	1
C-N-CA	121.70	129.99	1
OE1-CD-NE2	122.60	118.00	3
CB-CG-CD2	131.20	125.22	2
CA-C-N	116.90	123.79	1
OD1-CG-ND2	122.60	118.01	1
OE1-CD-NE2	122.60	118.01	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.66	1
OE1-CD-NE2	122.60	118.02	3
OE1-CD-NE2	122.60	118.03	1
C-N-CA	121.70	129.92	1
OE1-CD-NE2	122.60	118.04	2
OD1-CG-ND2	122.60	118.05	1
OD1-CG-ND2	122.60	118.06	1
CA-CB-CG	112.60	117.13	1
OE1-CD-NE2	122.60	118.07	1
OD1-CG-ND2	122.60	118.07	1
N-CA-CB	110.40	103.61	1
OE1-CD-NE2	122.60	118.08	1
OD1-CG-ND2	122.60	118.08	1
CA-CB-CG	112.60	117.12	1
CA-CB-CG	113.80	109.28	1
C-N-CA	121.70	129.82	1
C-CA-CB	110.50	117.26	1
N-CA-CB	103.00	107.96	1
OD1-CG-ND2	122.60	118.09	1
OD1-CG-ND2	122.60	118.10	1
OE1-CD-NE2	122.60	118.10	1
N-CA-CB	110.50	102.86	1
OD1-CG-ND2	122.60	118.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.12	1
OD1-CG-ND2	122.60	118.12	1
OE1-CD-NE2	122.60	118.13	3
CB-CG-CD2	131.20	125.39	1
CB-CG-CD2	131.20	125.40	1
N-CA-C	111.00	123.49	1
OE1-CD-NE2	122.60	118.14	2
CA-CB-CG2	110.50	118.08	1
C-N-CA	121.70	129.72	1
C-N-CA	121.70	129.71	1
NE-CZ-NH2	119.20	123.21	1
CA-CB-CG	112.60	117.05	1
CB-CG-CD2	131.20	125.42	1
N-CA-C	111.00	123.43	1
OE1-CD-NE2	122.60	118.16	1
OE1-CD-NE2	122.60	118.17	1
CD-NE-CZ	124.40	130.59	1
OE1-CD-NE2	122.60	118.18	2
OD1-CG-ND2	122.60	118.18	2
OD1-CG-ND2	122.60	118.19	1
CD-NE-CZ	124.40	130.58	1
OE1-CD-NE2	122.60	118.19	1
CD1-CG-CD2	110.80	101.10	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.01	1
NE-CZ-NH2	119.20	123.16	1
OE1-CD-NE2	122.60	118.20	3
C-N-CA	121.70	129.62	1
OD1-CG-ND2	122.60	118.20	1
CD-NE-CZ	124.40	130.56	1
C-N-CA	121.70	129.61	1
OD1-CG-ND2	122.60	118.21	1
OE1-CD-NE2	122.60	118.21	2
OD1-CG-ND2	122.60	118.22	1
OE1-CD-NE2	122.60	118.23	1
NH1-CZ-NH2	119.30	113.62	1
OD1-CG-ND2	122.60	118.23	1
CB-CG-CD2	131.20	125.53	1
OE1-CD-NE2	122.60	118.24	2
CD-NE-CZ	124.40	130.50	1
OD1-CG-ND2	122.60	118.24	1
OE1-CD-NE2	122.60	118.25	1
C-N-CA	121.70	129.52	2
O-C-N	123.00	116.05	1
C-N-CA	121.70	129.51	2
OE1-CD-NE2	122.60	118.26	3
OD1-CG-ND2	122.60	118.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	123.10	1
OE1-CD-NE2	122.60	118.27	5
OD1-CG-ND2	122.60	118.27	1
CD-NE-CZ	124.40	130.46	1
CA-CB-OG1	109.60	116.09	1
OD1-CG-ND2	122.60	118.28	2
NE-CZ-NH2	119.20	123.09	1
OE1-CD-NE2	122.60	118.28	2
NE-CZ-NH2	119.20	123.08	1
OD1-CG-ND2	122.60	118.29	2
OE1-CD-NE2	122.60	118.29	1
OD1-CG-ND2	122.60	118.30	1
OD1-CG-ND2	122.60	118.31	2
N-CA-C	111.00	123.02	1
CA-C-N	116.20	124.78	1
OD1-CG-ND2	122.60	118.32	2
C-N-CA	121.70	129.41	1
OD1-CG-ND2	122.60	118.33	3
NH1-CZ-NH2	119.30	113.76	2
CA-CB-CG	113.80	118.06	1
CA-CB-CG	112.60	116.86	2
OE1-CD-NE2	122.60	118.34	5
OD1-CG-ND2	122.60	118.34	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.36	1
CA-CB-CG	113.90	121.55	1
C-N-CA	121.70	129.35	1
OE1-CD-NE2	122.60	118.35	2
OD1-CG-ND2	122.60	118.35	1
C-N-CA	121.70	129.34	2
CB-CG-CD2	131.20	125.68	1
CB-CG-CD2	131.20	125.69	1
OE1-CD-NE2	122.60	118.36	1
N-CA-CB	110.50	103.31	1
CD2-NE2-CE1	109.00	104.77	1
CB-CG-CD2	131.20	125.70	1
OE1-CD-NE2	122.60	118.37	1
C-CA-CB	110.50	116.84	1
OD1-CG-ND2	122.60	118.37	1
CA-CB-CG	112.60	116.83	1
C-N-CA	121.70	129.30	1
OE1-CD-NE2	122.60	118.38	1
CB-CG-CD2	131.20	125.71	1
NE-CZ-NH1	121.50	125.72	1
OD1-CG-ND2	122.60	118.39	4
C-N-CA	121.70	129.28	2
OE1-CD-NE2	122.60	118.39	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.73	1
CA-CB-CG2	110.50	117.65	1
OE1-CD-NE2	122.60	118.40	3
OD1-CG-ND2	122.60	118.40	1
CA-CB-CG	112.60	108.40	1
OD1-CG-ND2	122.60	118.41	2
C-N-CA	121.70	129.25	1
CA-CB-CG	113.80	117.99	1
OD1-CG-ND2	122.60	118.42	3
C-N-CA	121.70	129.23	1
CB-CG-CD2	131.20	125.77	1
CD-NE-CZ	124.40	130.24	1
OE1-CD-NE2	122.60	118.43	3
OD1-CG-ND2	122.60	118.43	2
CA-CB-CG2	110.50	117.59	1
CB-CG-CD2	131.20	125.78	1
C-N-CA	121.70	129.20	1
OD1-CG-ND2	122.60	118.44	1
CD-NE-CZ	124.40	130.23	1
C-N-CA	121.70	129.18	1
OD1-CG-ND2	122.60	118.45	3
NH1-CZ-NH2	119.30	113.90	1
CA-CB-CG	112.60	116.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.46	2
OD1-CG-ND2	122.60	118.46	1
C-N-CA	121.70	129.15	1
CD-NE-CZ	124.40	130.19	1
CA-CB-CG	112.60	116.74	1
C-N-CA	121.70	129.14	1
OD1-CG-ND2	122.60	118.47	2
O-C-N	123.00	116.39	1
OE1-CD-NE2	122.60	118.47	2
CA-CB-CG	112.60	116.73	1
C-N-CA	121.70	129.12	1
CG1-CB-CG2	110.80	101.73	1
N-CA-C	111.00	122.54	1
CA-CB-CG	112.60	116.72	1
OE1-CD-NE2	122.60	118.48	3
OD1-CG-ND2	122.60	118.48	1
C-CA-CB	110.10	102.28	1
C-N-CA	121.70	129.11	1
C-N-CA	121.70	129.10	1
NE-CZ-NH1	121.50	125.61	1
NH1-CZ-NH2	119.30	113.96	1
OD1-CG-ND2	122.60	118.49	1
C-N-CA	121.70	129.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.50	2
OD1-CG-ND2	122.60	118.51	2
OE1-CD-NE2	122.60	118.51	2
CB-CG-CD2	131.20	125.89	1
C-N-CA	121.70	129.05	2
OE1-CD-NE2	122.60	118.52	4
CD-NE-CZ	124.40	130.11	1
CB-CG-CD2	131.20	125.90	1
C-N-CA	121.70	129.04	1
CG-CD-CE	111.30	101.92	1
C-N-CA	121.70	129.03	1
CA-C-O	120.80	113.88	1
OE1-CD-NE2	122.60	118.53	3
CA-CB-CG	112.60	116.67	1
CB-CG-CD2	131.20	125.91	1
OD1-CG-ND2	122.60	118.53	1
OE1-CD-NE2	122.60	118.54	1
OD1-CG-ND2	122.60	118.54	1
CB-CG-CD2	131.20	125.93	1
CD-NE-CZ	124.40	130.08	1
NE-CZ-NH2	119.20	115.55	1
OE1-CD-NE2	122.60	118.55	2
NE-CZ-NH2	119.20	122.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.55	2
CA-CB-CG	112.60	116.65	1
C-N-CA	121.70	128.99	1
OD1-CG-ND2	122.60	118.56	1
CA-CB-CG	112.60	116.64	1
C-N-CA	121.70	128.97	1
OE1-CD-NE2	122.60	118.57	2
O-C-N	123.00	116.55	1
C-N-CA	121.70	128.95	1
OD1-CG-ND2	122.60	118.57	4
CD-NE-CZ	124.40	130.04	1
CB-CG-CD2	131.20	125.97	1
NE-CZ-NH1	121.50	125.53	1
N-CA-C	111.00	122.27	1
C-CA-CB	110.50	116.54	1
OD1-CG-ND2	122.60	118.58	1
C-N-CA	121.70	128.93	3
O-C-N	123.00	116.57	1
OE1-CD-NE2	122.60	118.58	1
OE1-CD-NE2	122.60	118.59	1
CD-NE-CZ	124.40	130.01	1
NE-CZ-NH2	119.20	122.81	1
OE1-CD-NE2	122.60	118.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	128.91	1
C-N-CA	121.70	128.90	2
NH1-CZ-NH2	119.30	114.10	1
OD1-CG-ND2	122.60	118.60	1
C-N-H	112.09	124.30	1
C-N-H	111.94	124.30	1
HH11-NH1-HH12	107.56	120.00	1
C-CA-HA2	96.55	109.00	1
C-N-H	111.61	124.30	1
HZ1-NZ-HZ2	96.22	109.00	1
C-N-H	111.42	124.30	1
C-N-H	111.37	124.30	1
C-N-H	111.34	124.30	1
HH21-NH2-HH22	106.91	120.00	1
HH11-NH1-HH12	106.66	120.00	1
C-N-H	110.91	124.30	1
HZ2-NZ-HZ3	95.22	109.00	1
C-N-H	110.46	124.30	1
C-N-H	110.27	124.30	1
C-N-H	110.09	124.30	1
CZ-NH2-HH21	105.25	120.00	1
C-N-H	109.43	124.30	1
C-N-H	109.16	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	109.15	124.30	1
C-N-H	109.10	124.30	1
C-N-H	108.63	124.30	1
C-N-H	108.46	124.30	1
C-N-H	108.27	124.30	1
C-N-H	108.11	124.30	1
C-N-H	107.61	124.30	1
C-N-H	107.44	124.30	1
HH21-NH2-HH22	100.68	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	3.28	37
2	2.48	28
3	3.72	42
4	2.57	29
5	4.26	48
6	1.15	13
7	7.80	88
8	3.46	39
9	4.35	49
10	3.10	35

All 408 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:156:PRO:HG3	A:534:ALA:HB3	0.780
1	A:156:PRO:CG	A:534:ALA:HB3	0.771
1	A:137:ILE:HD12	A:333:VAL:HG23	0.750
1	A:137:ILE:CD1	A:333:VAL:HG23	0.712
1	A:602:ASP:CG	A:741:GLY:HA3	0.604
1	A:602:ASP:OD2	A:741:GLY:HA3	0.603
1	A:414:THR:CG2	A:433:THR:HG23	0.566
1	A:604:THR:HG21	A:646:ASP:HB2	0.553
1	A:414:THR:HG23	A:433:THR:HG23	0.552
1	A:548:ALA:HB2	A:561:PHE:HZ	0.552
1	A:86:GLN:NE2	A:97:ASN:HD22	0.537
1	A:548:ALA:HB2	A:561:PHE:CZ	0.520
1	A:735:ALA:HB2	A:747:GLY:HA2	0.508
1	A:156:PRO:HG2	A:534:ALA:HB3	0.505
1	A:137:ILE:HA	A:374:ILE:HD12	0.504
1	A:293:HIS:O	A:342:ILE:HD11	0.503
1	A:332:ARG:NH2	A:334:LYS:HE2	0.483
1	A:604:THR:CG2	A:646:ASP:HB2	0.473
1	A:332:ARG:CZ	A:334:LYS:HE3	0.465
1	A:468:LEU:HD21	A:513:MET:CE	0.459
1	A:106:ALA:HB2	A:117:ALA:CB	0.457
1	A:106:ALA:HB2	A:117:ALA:HB2	0.455
1	A:164:SER:C	A:538:GLN:HE22	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:194:PHE:CD2	A:220:THR:HG22	0.448
1	A:605:TYR:OH	A:655:LEU:HD11	0.448
1	A:604:THR:HG21	A:646:ASP:CB	0.447
1	A:733:TYR:CZ	A:747:GLY:HA3	0.432
1	A:106:ALA:CB	A:117:ALA:HB2	0.420
1	A:130:TYR:CE1	A:161:TYR:HB3	0.417
1	A:606:SER:C	A:608:TYR:H	0.416
1	A:588:LEU:HD23	A:616:TYR:HB3	0.415
1	A:53:LEU:HD12	A:629:GLN:HE22	0.405
1	A:137:ILE:HD11	A:333:VAL:HG23	0.404
1	A:598:GLU:HB2	A:605:TYR:CD2	0.403
1	A:349:ILE:CD1	A:418:VAL:HG22	0.402
1	A:109:ASN:HA	A:226:ASP:OD2	0.402
1	A:297:GLY:HA2	A:301:ASP:OD2	0.401
2	A:225:ARG:CZ	A:737:ILE:HG23	0.779
2	A:489:ILE:HD13	A:503:THR:HG21	0.693
2	A:114:THR:HG21	A:261:THR:HG21	0.668
2	A:282:ALA:HB1	A:290:VAL:HG13	0.663
2	A:405:GLN:CD	A:549:GLN:HE22	0.612
2	A:489:ILE:CD1	A:503:THR:HG21	0.611
2	A:282:ALA:CB	A:290:VAL:HG13	0.602
2	A:134:ILE:HB	A:329:ARG:HH11	0.560
2	A:109:ASN:HA	A:264:GLY:H	0.527

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:107:GLY:C	A:109:ASN:H	0.519
2	A:129:ILE:HD12	A:142:ARG:CZ	0.518
2	A:130:TYR:CE1	A:161:TYR:HB3	0.511
2	A:653:SER:HB2	A:697:THR:HG23	0.510
2	A:647:VAL:HG13	A:652:SER:OG	0.506
2	A:284:LEU:HD22	A:288:GLY:O	0.505
2	A:476:ASP:OD1	A:502:THR:HG23	0.498
2	A:130:TYR:CZ	A:161:TYR:HB3	0.497
2	A:479:THR:HB	A:489:ILE:HD12	0.465
2	A:62:PRO:HB2	A:382:THR:HG21	0.449
2	A:267:PRO:HB3	A:295:PHE:CE1	0.447
2	A:120:MET:HB3	A:125:THR:HG21	0.445
2	A:653:SER:HB2	A:697:THR:CG2	0.443
2	A:225:ARG:HH21	A:737:ILE:HG12	0.428
2	A:86:GLN:NE2	A:97:ASN:HD22	0.417
2	A:156:PRO:CG	A:534:ALA:HB3	0.416
2	A:165:ALA:N	A:543:ASN:HD21	0.413
2	A:334:LYS:HZ3	A:336:ASP:CG	0.405
2	A:433:THR:C	A:435:ASN:H	0.400
3	A:159:THR:HG22	A:451:PHE:CE1	0.712
3	A:598:GLU:HB3	A:608:TYR:CE2	0.697
3	A:156:PRO:HG2	A:534:ALA:HB3	0.651
3	A:92:THR:HG23	A:103:ALA:HB1	0.636

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:598:GLU:CB	A:608:TYR:CE2	0.616
3	A:159:THR:HG21	A:516:LYS:HD3	0.611
3	A:439:ALA:HB1	A:546:ALA:HB1	0.588
3	A:439:ALA:CB	A:546:ALA:HB1	0.579
3	A:159:THR:HG21	A:516:LYS:CD	0.575
3	A:133:GLY:HA2	A:161:TYR:CD1	0.568
3	A:134:ILE:HB	A:329:ARG:HH11	0.563
3	A:417:ALA:H	A:431:GLY:HA2	0.560
3	A:145:PHE:CD1	A:216:MET:SD	0.551
3	A:272:PRO:CG	A:418:VAL:HG21	0.525
3	A:476:ASP:OD1	A:503:THR:HG23	0.524
3	A:219:LYS:HE2	A:221:HIS:CE1	0.520
3	A:272:PRO:HG3	A:418:VAL:HG21	0.517
3	A:132:ASP:HB3	A:313:ARG:HH22	0.507
3	A:159:THR:HG21	A:516:LYS:CE	0.507
3	A:271:LEU:HD12	A:359:TRP:CZ2	0.493
3	A:282:ALA:HB3	A:290:VAL:HG22	0.491
3	A:108:GLU:HG2	A:735:ALA:HB3	0.481
3	A:162:GLY:O	A:467:ARG:CD	0.474
3	A:475:TYR:CE2	A:545:PHE:HB3	0.473
3	A:504:VAL:HG11	A:549:GLN:OE1	0.459
3	A:558:ARG:NH2	A:605:TYR:CG	0.451
3	A:133:GLY:CA	A:161:TYR:CD1	0.450

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:156:PRO:CG	A:534:ALA:HB3	0.447
3	A:161:TYR:CE2	A:171:ASN:HB2	0.442
3	A:598:GLU:HB2	A:608:TYR:CE2	0.433
3	A:142:ARG:NH1	A:254:LEU:HD23	0.431
3	A:473:THR:CG2	A:475:TYR:CE2	0.431
3	A:595:ASN:HB3	A:607:GLN:NE2	0.429
3	A:271:LEU:HD12	A:359:TRP:CH2	0.425
3	A:43:THR:C	A:45:VAL:H	0.417
3	A:59:SER:O	A:173:ILE:HG21	0.417
3	A:351:GLN:HA	A:352:PRO:HD3	0.408
3	A:222:ASP:HA	A:227:LYS:HA	0.407
3	A:261:THR:O	A:302:TYR:HA	0.406
3	A:297:GLY:HA3	A:342:ILE:HD12	0.405
3	A:145:PHE:CE1	A:216:MET:SD	0.401
3	A:548:ALA:HB2	A:605:TYR:CE2	0.400
4	A:701:THR:HG21	A:745:HIS:CE1	0.863
4	A:689:LYS:HE2	A:701:THR:HG22	0.743
4	A:112:SER:HA	A:140:VAL:HG22	0.671
4	A:68:VAL:HG22	A:75:MET:CE	0.648
4	A:689:LYS:CE	A:701:THR:HG22	0.629
4	A:606:SER:HB3	A:608:TYR:CE2	0.611
4	A:606:SER:CB	A:608:TYR:CE2	0.578
4	A:68:VAL:HG22	A:75:MET:HE2	0.551

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:51:PRO:C	A:53:LEU:H	0.510
4	A:639:ALA:HB1	A:655:LEU:HD12	0.505
4	A:406:THR:HG21	A:408:TYR:CE2	0.502
4	A:274:TYR:CE2	A:737:ILE:HG23	0.492
4	A:276:ALA:HB1	A:281:THR:HB	0.491
4	A:701:THR:HB	A:745:HIS:CD2	0.488
4	A:78:ILE:HD11	A:98:VAL:HG22	0.473
4	A:339:MET:HE1	A:432:LEU:HD13	0.470
4	A:165:ALA:HB1	A:168:GLY:C	0.465
4	A:104:PHE:CZ	A:657:TYR:HB3	0.458
4	A:581:ARG:HH12	A:625:THR:HA	0.457
4	A:225:ARG:HD2	A:295:PHE:CZ	0.455
4	A:734:VAL:CG1	A:737:ILE:HD12	0.449
4	A:258:GLN:NE2	A:260:ASN:HD21	0.443
4	A:153:ILE:CD1	A:161:TYR:CE2	0.440
4	A:112:SER:HB2	A:335:GLN:CD	0.436
4	A:406:THR:CG2	A:408:TYR:CE2	0.429
4	A:165:ALA:HB1	A:168:GLY:O	0.416
4	A:82:VAL:HG12	A:86:GLN:HE21	0.412
4	A:339:MET:HE1	A:432:LEU:HD22	0.412
4	A:105:PHE:CG	A:109:ASN:HB2	0.400
5	A:68:VAL:HG22	A:75:MET:HE3	0.800
5	A:156:PRO:CB	A:534:ALA:HB3	0.680

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:131:ILE:HG23	A:659:PRO:HD2	0.659
5	A:54:TYR:CE1	A:82:VAL:HG22	0.626
5	A:363:ARG:HH11	A:418:VAL:HG11	0.621
5	A:166:PRO:CB	A:566:ALA:HB3	0.607
5	A:78:ILE:HD11	A:98:VAL:CG2	0.580
5	A:166:PRO:HB3	A:566:ALA:HB3	0.568
5	A:156:PRO:HB2	A:534:ALA:HB3	0.557
5	A:54:TYR:CZ	A:82:VAL:HG22	0.550
5	A:156:PRO:HB3	A:534:ALA:HB3	0.533
5	A:338:LEU:HD21	A:429:PRO:CG	0.531
5	A:57:GLN:O	A:68:VAL:HG23	0.527
5	A:86:GLN:NE2	A:97:ASN:HD22	0.521
5	A:159:THR:HG21	A:534:ALA:HB1	0.519
5	A:104:PHE:CZ	A:657:TYR:CD1	0.512
5	A:269:ILE:HG22	A:271:LEU:HG	0.511
5	A:53:LEU:HD22	A:81:GLN:HG2	0.496
5	A:166:PRO:HB2	A:566:ALA:HB3	0.487
5	A:17:PHE:CD1	A:18:PHE:CE2	0.484
5	A:109:ASN:HD21	A:748:GLU:HG2	0.483
5	A:68:VAL:HG22	A:75:MET:CE	0.479
5	A:266:ILE:HG21	A:423:PRO:CB	0.479
5	A:102:GLY:HA3	A:131:ILE:HD12	0.474
5	A:135:ARG:HG3	A:165:ALA:HB2	0.467

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:541:GLY:C	A:543:ASN:H	0.460
5	A:336:ASP:HB3	A:432:LEU:HD11	0.459
5	A:266:ILE:HD11	A:363:ARG:NH1	0.455
5	A:106:ALA:HB1	A:111:ASN:H	0.440
5	A:689:LYS:HB3	A:699:ALA:O	0.439
5	A:122:GLY:HA3	A:403:GLU:CD	0.427
5	A:544:ASN:ND2	A:605:TYR:CE2	0.427
5	A:451:PHE:CD1	A:516:LYS:HE2	0.425
5	A:44:LEU:HD23	A:46:VAL:CG2	0.423
5	A:363:ARG:HD2	A:418:VAL:HG22	0.422
5	A:606:SER:HB2	A:608:TYR:CE2	0.422
5	A:611:LYS:HE3	A:656:PRO:HG3	0.422
5	A:338:LEU:HD21	A:429:PRO:HG3	0.418
5	A:343:MET:C	A:348:ASN:HD22	0.418
5	A:727:ASN:HD21	A:748:GLU:HB2	0.418
5	A:78:ILE:HD11	A:98:VAL:HG21	0.415
5	A:135:ARG:CG	A:165:ALA:HB2	0.415
5	A:368:LYS:HE3	A:549:GLN:NE2	0.413
5	A:266:ILE:HD13	A:423:PRO:HB2	0.412
5	A:337:TYR:CE2	A:339:MET:HB2	0.412
5	A:239:VAL:HG11	A:241:PHE:CZ	0.407
5	A:368:LYS:HE2	A:370:VAL:HG21	0.407
5	A:110:GLY:O	A:111:ASN:C	0.405

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:270:GLY:HA2	A:280:GLY:HA3	0.545
6	A:26:THR:HG22	A:27:PRO:HD2	0.489
6	A:270:GLY:HA2	A:280:GLY:CA	0.474
6	A:682:ARG:HH21	A:706:VAL:HG11	0.452
6	A:406:THR:HG21	A:408:TYR:CZ	0.434
6	A:547:LEU:HB3	A:605:TYR:CE2	0.432
6	A:54:TYR:CD2	A:622:GLY:HA2	0.422
6	A:475:TYR:CE2	A:546:ALA:HA	0.420
6	A:261:THR:HB	A:262:PRO:HD2	0.414
6	A:733:TYR:CE1	A:737:ILE:HD12	0.413
6	A:176:GLN:HE22	A:252:ASN:ND2	0.412
6	A:52:SER:C	A:54:TYR:H	0.410
6	A:506:THR:HG21	A:559:THR:HB	0.404
7	A:512:LEU:HD11	A:539:PRO:HD3	0.900
7	A:145:PHE:CD1	A:216:MET:HE2	0.742
7	A:161:TYR:CD2	A:451:PHE:CE1	0.731
7	A:161:TYR:CE2	A:451:PHE:CD1	0.702
7	A:123:ALA:HB3	A:167:THR:CG2	0.684
7	A:161:TYR:CD2	A:451:PHE:CZ	0.670
7	A:145:PHE:CE1	A:216:MET:HE2	0.660
7	A:156:PRO:HB2	A:534:ALA:HB3	0.659
7	A:53:LEU:HD21	A:245:THR:HA	0.641
7	A:125:THR:HG22	A:167:THR:OG1	0.637

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:512:LEU:CD1	A:539:PRO:HD3	0.632
7	A:541:GLY:HA2	A:545:PHE:CE2	0.625
7	A:512:LEU:HD11	A:539:PRO:CD	0.623
7	A:108:GLU:OE1	A:339:MET:HE1	0.611
7	A:706:VAL:HG22	A:733:TYR:CZ	0.602
7	A:53:LEU:HD11	A:245:THR:HG22	0.595
7	A:548:ALA:HB2	A:605:TYR:OH	0.590
7	A:156:PRO:HB3	A:568:THR:HB	0.581
7	A:332:ARG:CZ	A:334:LYS:HE3	0.579
7	A:749:PRO:O	A:751:THR:HG23	0.575
7	A:145:PHE:CG	A:216:MET:HE2	0.573
7	A:160:ASP:O	A:161:TYR:CD2	0.573
7	A:113:THR:HG22	A:368:LYS:HZ2	0.571
7	A:688:HIS:CD2	A:690:GLY:H	0.552
7	A:479:THR:HB	A:489:ILE:HD11	0.546
7	A:153:ILE:HG22	A:158:GLY:HA2	0.540
7	A:689:LYS:HE2	A:737:ILE:HG23	0.539
7	A:121:ARG:O	A:613:VAL:HG11	0.538
7	A:68:VAL:HG13	A:75:MET:CE	0.537
7	A:53:LEU:HD11	A:245:THR:HA	0.536
7	A:482:GLY:O	A:497:LYS:HE3	0.535
7	A:107:GLY:H	A:225:ARG:NH1	0.534
7	A:342:ILE:HG21	A:361:TRP:CD2	0.533

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:541:GLY:CA	A:545:PHE:CE2	0.529
7	A:161:TYR:CE2	A:451:PHE:CE1	0.526
7	A:742:TYR:HB3	A:744:TYR:CD2	0.521
7	A:695:VAL:HG21	A:740:SER:HB2	0.520
7	A:123:ALA:HB3	A:167:THR:HG21	0.518
7	A:145:PHE:CZ	A:216:MET:CE	0.504
7	A:113:THR:HG21	A:547:LEU:HD13	0.498
7	A:107:GLY:H	A:225:ARG:HH12	0.497
7	A:160:ASP:C	A:161:TYR:CD2	0.494
7	A:68:VAL:HG13	A:75:MET:HE2	0.486
7	A:54:TYR:CZ	A:208:THR:HA	0.483
7	A:156:PRO:CB	A:568:THR:HB	0.483
7	A:471:TYR:CD1	A:539:PRO:HG3	0.470
7	A:650:ASP:HB3	A:698:PRO:CG	0.467
7	A:332:ARG:NH2	A:334:LYS:HE2	0.463
7	A:71:THR:C	A:73:ARG:H	0.462
7	A:361:TRP:CE2	A:420:ILE:HD11	0.462
7	A:368:LYS:HE2	A:370:VAL:CG2	0.460
7	A:161:TYR:CZ	A:451:PHE:CD1	0.458
7	A:192:ALA:HB1	A:221:HIS:O	0.457
7	A:78:ILE:HD11	A:98:VAL:HG21	0.456
7	A:153:ILE:CG2	A:158:GLY:HA2	0.455
7	A:689:LYS:HE2	A:737:ILE:CG2	0.455

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:156:PRO:HG3	A:568:THR:HB	0.453
7	A:163:ARG:CZ	A:539:PRO:HD2	0.452
7	A:120:MET:CE	A:170:ILE:HG13	0.450
7	A:122:GLY:HA3	A:658:THR:HG23	0.442
7	A:342:ILE:HD13	A:361:TRP:CE3	0.442
7	A:123:ALA:HB3	A:167:THR:HG22	0.438
7	A:449:TYR:CD2	A:451:PHE:CZ	0.437
7	A:113:THR:HG22	A:368:LYS:NZ	0.436
7	A:482:GLY:O	A:497:LYS:CE	0.434
7	A:734:VAL:HB	A:746:PRO:HD2	0.433
7	A:216:MET:HE1	A:234:GLY:HA3	0.432
7	A:650:ASP:HB3	A:698:PRO:HG2	0.430
7	A:639:ALA:CB	A:658:THR:HG21	0.429
7	A:407:ASN:HD22	A:547:LEU:HA	0.424
7	A:145:PHE:CE1	A:216:MET:CE	0.422
7	A:339:MET:HE3	A:341:ALA:HB2	0.419
7	A:734:VAL:CG2	A:746:PRO:HD2	0.418
7	A:122:GLY:CA	A:658:THR:HG23	0.417
7	A:477:SER:HB3	A:549:GLN:NE2	0.417
7	A:156:PRO:HD3	A:568:THR:HG21	0.416
7	A:487:GLY:HA2	A:553:GLY:HA3	0.416
7	A:471:TYR:CG	A:539:PRO:HG3	0.414
7	A:526:ASN:OD1	A:580:LYS:HE2	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:749:PRO:O	A:750:ARG:C	0.409
7	A:342:ILE:HD13	A:361:TRP:CZ3	0.407
7	A:113:THR:CB	A:547:LEU:HD13	0.406
7	A:648:ALA:HB3	A:650:ASP:OD1	0.406
7	A:449:TYR:HB2	A:451:PHE:CZ	0.405
7	A:104:PHE:CE1	A:687:MET:HE1	0.405
7	A:113:THR:OG1	A:547:LEU:HD13	0.403
7	A:450:ALA:C	A:451:PHE:CD1	0.400
7	A:554:ASN:HD22	A:604:THR:CG2	0.400
8	A:611:LYS:HE3	A:655:LEU:HD11	0.902
8	A:54:TYR:CE1	A:631:ILE:HD11	0.729
8	A:547:LEU:HD13	A:605:TYR:CZ	0.729
8	A:54:TYR:HE1	A:631:ILE:HD11	0.721
8	A:547:LEU:HD13	A:605:TYR:CE1	0.686
8	A:116:ASP:O	A:140:VAL:HG21	0.670
8	A:547:LEU:HD22	A:605:TYR:OH	0.660
8	A:269:ILE:HD12	A:361:TRP:CZ3	0.652
8	A:611:LYS:HE3	A:655:LEU:CD1	0.643
8	A:363:ARG:HH21	A:415:LEU:HD13	0.595
8	A:641:ILE:HD11	A:655:LEU:HD23	0.567
8	A:342:ILE:HD13	A:361:TRP:CE3	0.561
8	A:295:PHE:CE2	A:420:ILE:HG22	0.550
8	A:441:GLY:HA3	A:545:PHE:CD1	0.550

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:722:GLN:HE21	A:724:ASN:HD21	0.529
8	A:295:PHE:CZ	A:342:ILE:HD11	0.518
8	A:54:TYR:CE1	A:82:VAL:HG22	0.515
8	A:468:LEU:HD21	A:513:MET:CE	0.507
8	A:738:ASN:CG	A:743:ARG:HA	0.497
8	A:639:ALA:CB	A:655:LEU:HD12	0.496
8	A:267:PRO:CG	A:342:ILE:HD12	0.494
8	A:53:LEU:HD12	A:629:GLN:HE22	0.487
8	A:266:ILE:HD13	A:278:SER:CB	0.472
8	A:267:PRO:HG3	A:342:ILE:HD12	0.463
8	A:451:PHE:CD1	A:516:LYS:HE2	0.440
8	A:92:THR:HG23	A:103:ALA:CB	0.435
8	A:53:LEU:HD13	A:81:GLN:HG2	0.429
8	A:400:PHE:CE1	A:446:PHE:CD2	0.422
8	A:639:ALA:HB1	A:655:LEU:CD1	0.418
8	A:166:PRO:HB3	A:566:ALA:HB2	0.415
8	A:487:GLY:HA2	A:553:GLY:HA3	0.415
8	A:279:ALA:HA	A:292:THR:HG21	0.412
8	A:136:ASP:CG	A:142:ARG:HH21	0.411
8	A:188:SER:HB3	A:753:LEU:HD11	0.410
8	A:156:PRO:HD3	A:568:THR:HG21	0.409
8	A:157:SER:HG	A:164:SER:CB	0.409
8	A:552:SER:C	A:554:ASN:H	0.408

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:639:ALA:HB1	A:655:LEU:HG	0.402
8	A:338:LEU:HD21	A:429:PRO:HG2	0.401
9	A:123:ALA:HB2	A:167:THR:HG21	0.866
9	A:140:VAL:HG22	A:333:VAL:CG2	0.770
9	A:140:VAL:HG22	A:333:VAL:HG23	0.759
9	A:72:THR:HG22	A:520:LEU:HD22	0.670
9	A:140:VAL:HG13	A:307:THR:HG23	0.633
9	A:228:VAL:HG22	A:262:PRO:HA	0.606
9	A:271:LEU:HD22	A:359:TRP:CZ3	0.576
9	A:581:ARG:HH22	A:625:THR:CA	0.574
9	A:226:ASP:HB2	A:228:VAL:HG23	0.568
9	A:131:ILE:HG21	A:134:ILE:HD12	0.540
9	A:78:ILE:HD11	A:98:VAL:HG21	0.536
9	A:78:ILE:HD11	A:98:VAL:CG2	0.529
9	A:194:PHE:CD2	A:220:THR:HG22	0.523
9	A:72:THR:HG22	A:520:LEU:HD13	0.521
9	A:123:ALA:CB	A:167:THR:HG21	0.519
9	A:581:ARG:HH22	A:625:THR:HA	0.516
9	A:482:GLY:O	A:497:LYS:HE3	0.514
9	A:119:TYR:CE1	A:124:ASP:HB3	0.490
9	A:104:PHE:CE1	A:687:MET:SD	0.484
9	A:130:TYR:CE2	A:163:ARG:HD2	0.481
9	A:167:THR:HG22	A:591:THR:HG21	0.481

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:137:ILE:HG22	A:140:VAL:HG21	0.480
9	A:72:THR:CG2	A:520:LEU:HD22	0.480
9	A:64:PHE:CD1	A:173:ILE:HD11	0.474
9	A:221:HIS:NE2	A:229:LYS:HE2	0.469
9	A:473:THR:HG23	A:545:PHE:CZ	0.462
9	A:298:THR:HB	A:339:MET:CE	0.461
9	A:135:ARG:HH12	A:538:GLN:CD	0.455
9	A:130:TYR:HB2	A:165:ALA:HB2	0.452
9	A:137:ILE:HA	A:374:ILE:HD13	0.449
9	A:598:GLU:HB2	A:608:TYR:CZ	0.449
9	A:123:ALA:HB1	A:128:SER:HB2	0.445
9	A:54:TYR:CE2	A:242:GLY:HA3	0.441
9	A:105:PHE:CD1	A:225:ARG:NH1	0.434
9	A:71:THR:C	A:73:ARG:H	0.432
9	A:473:THR:CG2	A:545:PHE:CE1	0.425
9	A:581:ARG:HH22	A:624:ILE:C	0.425
9	A:482:GLY:O	A:497:LYS:CE	0.422
9	A:338:LEU:HD21	A:415:LEU:HD11	0.421
9	A:137:ILE:HA	A:374:ILE:CD1	0.419
9	A:400:PHE:CE1	A:446:PHE:CD2	0.417
9	A:591:THR:HG22	A:593:ILE:HG13	0.415
9	A:38:THR:HB	A:39:ASN:CG	0.412
9	A:338:LEU:HD22	A:429:PRO:HG3	0.412

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:153:ILE:HG21	A:158:GLY:HA2	0.411
9	A:250:TYR:CZ	A:252:ASN:HB2	0.404
9	A:140:VAL:O	A:307:THR:HG21	0.403
9	A:542:GLY:HA2	A:545:PHE:CD2	0.401
9	A:135:ARG:NH1	A:538:GLN:CD	0.400
10	A:140:VAL:HG12	A:333:VAL:HG11	0.788
10	A:140:VAL:CG1	A:333:VAL:HG11	0.750
10	A:60:ALA:HB1	A:313:ARG:NH1	0.725
10	A:123:ALA:HB3	A:167:THR:CG2	0.686
10	A:72:THR:HG21	A:463:ASN:HD21	0.653
10	A:123:ALA:HB3	A:167:THR:HG21	0.577
10	A:140:VAL:HB	A:333:VAL:HG21	0.577
10	A:134:ILE:HG23	A:374:ILE:CD1	0.543
10	A:239:VAL:HG11	A:241:PHE:CZ	0.517
10	A:547:LEU:HD21	A:605:TYR:CD2	0.516
10	A:722:GLN:HE21	A:724:ASN:HD21	0.506
10	A:200:ASP:CG	A:214:ASN:HD21	0.502
10	A:544:ASN:HA	A:547:LEU:HB2	0.495
10	A:134:ILE:HG23	A:374:ILE:HD12	0.480
10	A:258:GLN:NE2	A:260:ASN:HD21	0.479
10	A:72:THR:HG21	A:463:ASN:ND2	0.475
10	A:472:HIS:CE1	A:507:ALA:HB1	0.475
10	A:121:ARG:O	A:613:VAL:HG11	0.450

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:56:PRO:O	A:57:GLN:C	0.446
10	A:53:LEU:HD13	A:621:ALA:HB1	0.444
10	A:109:ASN:HB2	A:743:ARG:HH21	0.443
10	A:547:LEU:CD2	A:605:TYR:CD2	0.440
10	A:161:TYR:O	A:467:ARG:HD2	0.432
10	A:547:LEU:HD23	A:605:TYR:CE2	0.432
10	A:406:THR:CG2	A:408:TYR:CE2	0.431
10	A:74:THR:HG21	A:617:GLU:OE1	0.428
10	A:92:THR:HG23	A:103:ALA:CB	0.423
10	A:405:GLN:HB3	A:545:PHE:CE1	0.423
10	A:161:TYR:O	A:467:ARG:CD	0.420
10	A:547:LEU:HD21	A:605:TYR:CG	0.420
10	A:526:ASN:OD1	A:580:LYS:HE2	0.414
10	A:119:TYR:CD1	A:124:ASP:HB2	0.412
10	A:92:THR:HG23	A:103:ALA:HB3	0.410
10	A:451:PHE:CD1	A:516:LYS:HE2	0.408
10	A:407:ASN:HD21	A:549:GLN:NE2	0.407

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	758	676	56	26
2	758	669	64	25
3	758	682	50	26

Model ID	Analyzed	Favored	Allowed	Outliers
4	758	668	65	25
5	758	666	44	48
6	758	681	59	18
7	758	694	48	16
8	758	662	54	42
9	758	696	44	18
10	758	649	75	34

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	617	587	15	15
2	617	578	21	18
3	617	588	17	12
4	617	578	23	16
5	617	591	18	8
6	617	581	25	11
7	617	585	18	14
8	617	592	14	11
9	617	583	16	18
10	617	578	25	14

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	15	LEU

Model ID	Chain	Residue ID	Residue type
1	A	17	PHE
1	A	21	LEU
1	A	26	THR
1	A	43	THR
1	A	44	LEU
1	A	50	THR
1	A	128	SER
1	A	275	SER
1	A	337	TYR
1	A	422	HIS
1	A	433	THR
1	A	503	THR
1	A	664	THR
1	A	692	ASP
2	A	14	SER
2	A	15	LEU
2	A	21	LEU
2	A	26	THR
2	A	43	THR
2	A	54	TYR
2	A	164	SER
2	A	281	THR
2	A	300	SER

Model ID	Chain	Residue ID	Residue type
2	A	338	LEU
2	A	350	THR
2	A	356	VAL
2	A	360	THR
2	A	658	THR
2	A	664	THR
2	A	688	HIS
2	A	697	THR
2	A	740	SER
3	A	14	SER
3	A	15	LEU
3	A	17	PHE
3	A	26	THR
3	A	44	LEU
3	A	50	THR
3	A	113	THR
3	A	275	SER
3	A	298	THR
3	A	356	VAL
3	A	360	THR
3	A	751	THR
4	A	15	LEU
4	A	16	THR

Model ID	Chain	Residue ID	Residue type
4	A	21	LEU
4	A	26	THR
4	A	44	LEU
4	A	50	THR
4	A	59	SER
4	A	286	HIS
4	A	350	THR
4	A	356	VAL
4	A	360	THR
4	A	422	HIS
4	A	695	VAL
4	A	697	THR
4	A	731	THR
4	A	745	HIS
5	A	15	LEU
5	A	17	PHE
5	A	21	LEU
5	A	26	THR
5	A	225	ARG
5	A	337	TYR
5	A	503	THR
5	A	697	THR
6	A	15	LEU

Model ID	Chain	Residue ID	Residue type
6	A	21	LEU
6	A	25	ILE
6	A	28	VAL
6	A	65	SER
6	A	112	SER
6	A	140	VAL
6	A	440	ASN
6	A	503	THR
6	A	567	ASN
6	A	730	ASP
7	A	14	SER
7	A	16	THR
7	A	17	PHE
7	A	21	LEU
7	A	50	THR
7	A	53	LEU
7	A	160	ASP
7	A	216	MET
7	A	350	THR
7	A	489	ILE
7	A	503	THR
7	A	506	THR
7	A	539	PRO

Model ID	Chain	Residue ID	Residue type
7	A	695	VAL
8	A	15	LEU
8	A	26	THR
8	A	28	VAL
8	A	44	LEU
8	A	50	THR
8	A	157	SER
8	A	216	MET
8	A	269	ILE
8	A	503	THR
8	A	601	ASP
8	A	697	THR
9	A	15	LEU
9	A	21	LEU
9	A	26	THR
9	A	43	THR
9	A	50	THR
9	A	137	ILE
9	A	159	THR
9	A	191	SER
9	A	216	MET
9	A	221	HIS
9	A	275	SER

Model ID	Chain	Residue ID	Residue type
9	A	292	THR
9	A	298	THR
9	A	333	VAL
9	A	342	ILE
9	A	356	VAL
9	A	433	THR
9	A	697	THR
10	A	15	LEU
10	A	21	LEU
10	A	26	THR
10	A	43	THR
10	A	44	LEU
10	A	52	SER
10	A	116	ASP
10	A	160	ASP
10	A	274	TYR
10	A	356	VAL
10	A	505	ASP
10	A	664	THR
10	A	736	SER
10	A	744	TYR

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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