Integrative Structure Validation Report

July 22, 2024 - 05:16 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	9A39
PDB-Dev ID	PDBDEV_00000194
Structure Title	Model of E. coli LptD 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

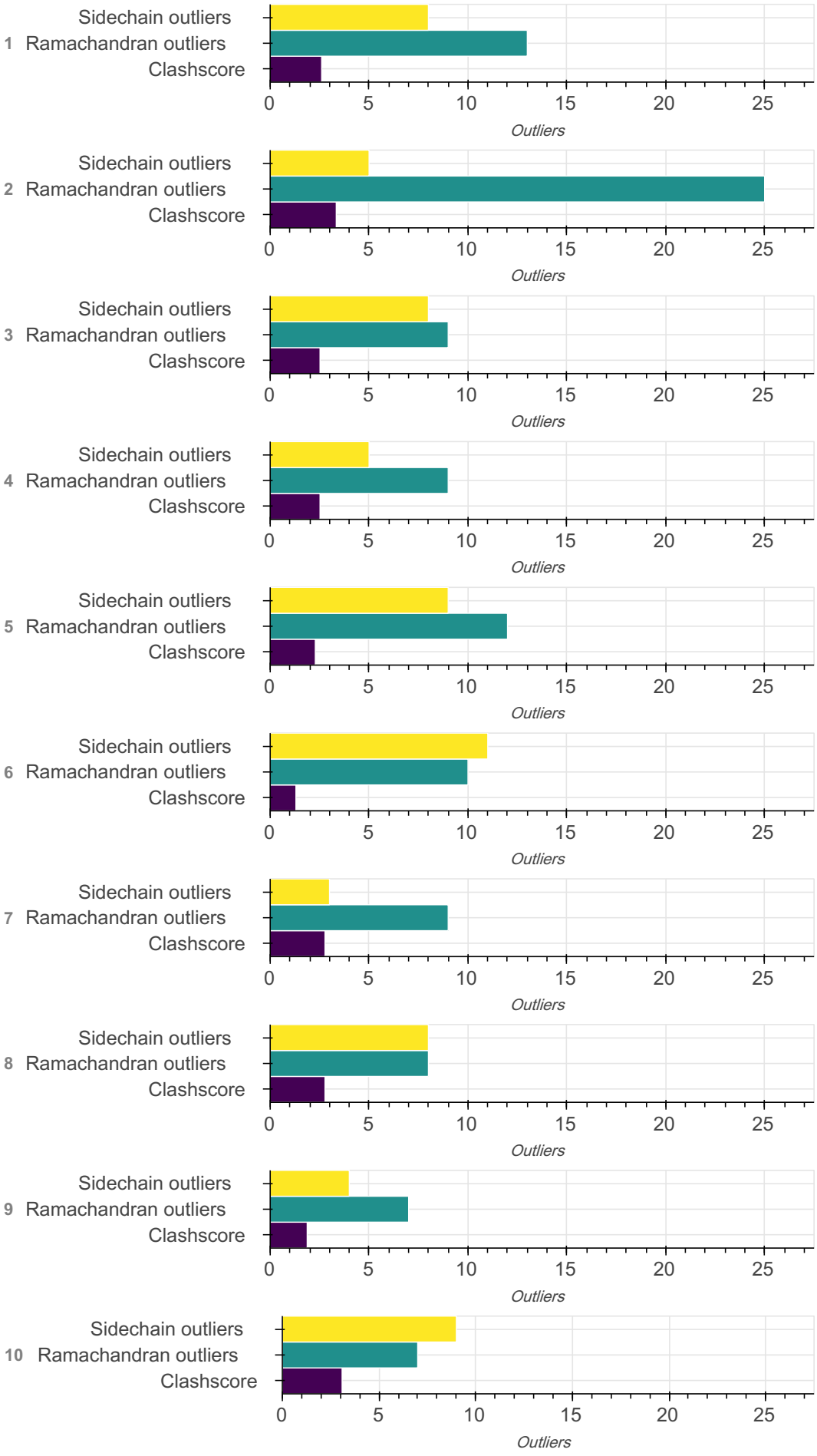
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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


Sidechain outliers
1 Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
Sidechain outliers
2 Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
Sidechain outliers
3 Ramachandran outliers
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6 Ramachandran outliers
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0 5 10 15 20 25
Outliers
Sidechain outliers
7 Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
Sidechain outliers
8 Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
Sidechain outliers
9 Ramachandran outliers
Clashscore
0 5 10 15 20 25
Outliers
Sidechain outliers
10 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	P31554	A	A	784
2	1	1	P31554	A	A	784
3	1	1	P31554	A	A	784
4	1	1	P31554	A	A	784
5	1	1	P31554	A	A	784
6	1	1	P31554	A	A	784
7	1	1	P31554	A	A	784
8	1	1	P31554	A	A	784
9	1	1	P31554	A	A	784
10	1	1	P31554	A	A	784

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	-	1-784

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 59530 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
CD2--HD22	1.09	0.97	540
CA--HA	1.09	0.97	7300
CG2--HG22	1.09	0.97	1340
CG2--HG21	1.09	0.97	1340
CB--HB3	1.09	0.97	5960
CD1--HD11	1.09	0.97	880
CB--HB	1.09	0.97	1340
CE--HE3	1.09	0.97	450
CG2--HG23	1.09	0.97	1340
CD1--HD12	1.09	0.97	880
CD--HD3	1.09	0.97	1060
CG--HG3	1.09	0.97	2030
CG--HG2	1.09	0.97	2030
OH--HH	0.96	0.84	580
CD1--HD13	1.09	0.97	880
CB--HB2	1.09	0.97	5960
CG1--HG12	1.09	0.97	840
CG1--HG13	1.09	0.97	840
CD--HD2	1.09	0.97	1060
CG--HG	1.09	0.97	540
CD2--HD21	1.09	0.97	540
CE--HE2	1.09	0.97	450

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA2	1.09	0.97	540
OG1--HG1	0.96	0.84	500
CG1--HG11	1.09	0.97	500
CA--HA3	1.09	0.97	540
CB--HB1	1.09	0.97	490
NZ--HZ2	1.01	0.89	270
CD2--HD23	1.09	0.97	540
NZ--HZ1	1.01	0.89	270
OG--HG	0.96	0.84	560
CE--HE1	1.09	0.97	180
NZ--HZ3	1.01	0.89	270
N--H2	1.01	0.89	10
N--H3	1.01	0.89	10
N--H1	1.01	0.89	10
N--H	1.01	0.86	7490
NH1--HH11	1.01	0.86	450
CE2--HE2	1.08	0.93	820
NH2--HH21	1.01	0.86	450
ND2--HD21	1.01	0.86	540
CE3--HE3	1.08	0.93	180
CZ2--HZ2	1.08	0.93	180
NE2--HE2	1.01	0.86	8
CE1--HE1	1.08	0.93	940

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.01	0.86	450
ND2--HD22	1.01	0.86	540
NE--HE	1.01	0.86	450
CD1--HD1	1.08	0.93	1000
NE2--HE22	1.01	0.86	440
NH1--HH12	1.01	0.86	450
NE2--HE21	1.01	0.86	440
CD2--HD2	1.08	0.93	940
CH2--HH2	1.08	0.93	180
CZ--HZ	1.08	0.93	240
NE1--HE1	1.01	0.86	180
CZ3--HZ3	1.08	0.93	180
ND1--HD1	1.01	0.86	112

Standard geometry: angle outliers

There are 410 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	112.60	121.44	1
CA-CB-CG	112.60	120.41	1
C-N-CA	121.70	135.23	1
CD-NE-CZ	124.40	134.90	1
OE1-CD-NE2	122.60	116.02	1
OE1-CD-NE2	122.60	116.03	1
CA-CB-CG	112.60	118.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	133.15	1
CA-CB-CG	112.60	118.95	1
OE1-CD-NE2	122.60	116.28	1
C-CA-CB	110.50	119.95	1
C-N-CA	121.70	133.04	1
C-N-CA	121.70	133.02	1
OE1-CD-NE2	122.60	116.41	1
C-N-CA	121.70	132.79	1
C-N-CA	121.70	132.78	1
OE1-CD-NE2	122.60	116.52	1
OE1-CD-NE2	122.60	116.56	1
OD1-CG-ND2	122.60	116.57	1
C-N-CA	121.70	132.43	1
C-N-CA	121.70	132.22	1
OE1-CD-NE2	122.60	116.76	1
CA-CB-CG	112.60	106.82	1
OD1-CG-ND2	122.60	116.85	1
C-N-CA	121.70	132.02	1
CA-CB-CG	112.60	118.32	1
OE1-CD-NE2	122.60	116.88	1
C-N-CA	121.70	131.98	1
OE1-CD-NE2	122.60	116.89	1
C-N-CA	121.70	131.92	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	116.93	1
OE1-CD-NE2	122.60	116.93	1
C-N-CA	121.70	131.86	1
OD1-CG-ND2	122.60	116.97	1
CA-CB-CG	112.60	118.17	1
OD1-CG-ND2	122.60	117.04	1
OE1-CD-NE2	122.60	117.06	2
OD1-CG-ND2	122.60	117.11	1
OE1-CD-NE2	122.60	117.13	1
CA-CB-CG	112.60	118.02	1
OE1-CD-NE2	122.60	117.22	1
OE1-CD-NE2	122.60	117.25	1
OD1-CG-ND2	122.60	117.26	1
OD1-CG-ND2	122.60	117.30	1
CA-CB-CG	112.60	107.31	1
CA-CB-CG	112.60	117.88	1
OE1-CD-NE2	122.60	117.33	1
OD1-CG-ND2	122.60	117.34	1
CA-N-CD	112.00	104.66	1
OE1-CD-NE2	122.60	117.38	1
OD1-CG-ND2	122.60	117.38	1
CA-CB-CG	112.60	117.77	1
NE-CZ-NH2	119.20	123.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	101.76	1
CA-CB-CG	112.60	117.74	1
C-N-CA	121.70	130.91	1
OD1-CG-ND2	122.60	117.51	1
OE1-CD-NE2	122.60	117.51	1
NH1-CZ-NH2	119.30	112.69	1
CA-CB-CG	112.60	117.67	1
OE1-CD-NE2	122.60	117.55	1
OE1-CD-NE2	122.60	117.56	1
N-CA-CB	103.00	108.53	1
CA-CB-CG	112.60	117.62	1
CA-CB-CG	112.60	117.59	2
OE1-CD-NE2	122.60	117.65	2
OE1-CD-NE2	122.60	117.67	3
CA-CB-CG	112.60	117.53	1
CA-CB-CG	112.60	117.52	1
CA-CB-CG	112.60	117.51	1
CB-CG-CD2	131.20	124.83	1
C-N-CA	121.70	130.49	2
C-N-CA	121.70	130.48	1
OD1-CG-ND2	122.60	117.73	1
OE1-CD-NE2	122.60	117.75	1
CA-CB-CG	112.60	107.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	117.76	1
OE1-CD-NE2	122.60	117.76	1
OE1-CD-NE2	122.60	117.78	2
C-N-CA	121.70	130.37	1
OE1-CD-NE2	122.60	117.79	1
OE1-CD-NE2	122.60	117.80	2
OE1-CD-NE2	122.60	117.81	1
C-N-CA	121.70	130.31	1
OE1-CD-NE2	122.60	117.82	2
OD1-CG-ND2	122.60	117.83	1
OD1-CG-ND2	122.60	117.84	1
CB-CG-CD2	131.20	125.01	1
OE1-CD-NE2	122.60	117.84	1
OE1-CD-NE2	122.60	117.85	2
OE1-CD-NE2	122.60	117.87	1
OE1-CD-NE2	122.60	117.90	2
OE1-CD-NE2	122.60	117.91	4
CA-CB-CG	112.60	117.29	1
OD1-CG-ND2	122.60	117.94	1
OE1-CD-NE2	122.60	117.94	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	1
OE1-CD-NE2	122.60	117.97	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.98	2
OE1-CD-NE2	122.60	117.99	1
NE-CZ-NH2	119.20	123.34	1
OE1-CD-NE2	122.60	118.00	1
CA-CB-CG	112.60	117.20	1
OD1-CG-ND2	122.60	118.00	1
OE1-CD-NE2	122.60	118.02	2
OE1-CD-NE2	122.60	118.03	2
NE-CZ-NH1	121.50	126.07	1
OE1-CD-NE2	122.60	118.04	2
CA-CB-CG	112.60	117.16	1
CA-CB-CG	112.60	108.05	2
OE1-CD-NE2	122.60	118.05	1
NE-CZ-NH1	121.50	126.05	1
OE1-CD-NE2	122.60	118.06	3
OD1-CG-ND2	122.60	118.06	1
CA-CB-CG	112.60	117.13	1
NE-CZ-NH2	119.20	123.27	1
C-N-CA	121.70	129.83	1
OE1-CD-NE2	122.60	118.08	3
OE1-CD-NE2	122.60	118.09	3
N-CA-C	111.00	123.62	1
CA-CB-CG	112.60	117.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.09	2
C-N-CA	121.70	129.77	2
OE1-CD-NE2	122.60	118.12	1
CA-C-N	116.90	123.61	1
OE1-CD-NE2	122.60	118.13	2
C-N-CA	121.70	129.74	1
C-N-CA	121.70	129.73	1
OD1-CG-ND2	122.60	118.14	1
OE1-CD-NE2	122.60	118.14	2
OE1-CD-NE2	122.60	118.15	1
OE1-CD-NE2	122.60	118.16	1
C-N-CA	121.70	129.70	1
C-N-CA	121.70	129.68	2
OE1-CD-NE2	122.60	118.17	2
OD1-CG-ND2	122.60	118.17	1
OE1-CD-NE2	122.60	118.18	3
CA-CB-CG	112.60	108.18	1
N-CA-CB	110.50	102.99	1
OE1-CD-NE2	122.60	118.19	1
CA-CB-CG	112.60	117.01	1
NE-CZ-NH2	119.20	123.16	1
OD1-CG-ND2	122.60	118.20	4
OE1-CD-NE2	122.60	118.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.21	1
C-N-CA	121.70	129.61	1
CA-CB-CG	112.60	116.98	1
OE1-CD-NE2	122.60	118.23	4
CA-CB-CG	112.60	116.97	1
CA-CB-CG	112.60	116.96	1
OE1-CD-NE2	122.60	118.24	4
OE1-CD-NE2	122.60	118.25	2
CA-CB-CG	112.60	116.95	3
OD1-CG-ND2	122.60	118.25	1
CB-CG-CD2	131.20	125.55	1
OE1-CD-NE2	122.60	118.26	4
OD1-CG-ND2	122.60	118.26	1
NE-CZ-NH2	119.20	123.10	1
OE1-CD-NE2	122.60	118.27	2
OD1-CG-ND2	122.60	118.28	2
CA-CB-OG1	109.60	116.08	1
C-CA-CB	110.10	118.31	1
C-N-CA	121.70	129.47	1
OE1-CD-NE2	122.60	118.29	3
CA-CB-CG	112.60	116.91	1
OD1-CG-ND2	122.60	118.29	1
NE-CZ-NH2	119.20	115.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.30	2
CA-CB-CG	112.60	116.90	1
OE1-CD-NE2	122.60	118.31	1
C-N-CA	121.70	129.43	1
OE1-CD-NE2	122.60	118.32	4
C-CA-CB	110.10	118.23	1
OD1-CG-ND2	122.60	118.32	1
OE1-CD-NE2	122.60	118.33	3
OD1-CG-ND2	122.60	118.33	1
OE1-CD-NE2	122.60	118.34	2
C-N-CA	121.70	129.37	1
N-CA-CB	110.50	117.73	1
OE1-CD-NE2	122.60	118.35	3
CA-N-CD	112.00	106.05	1
NE-CZ-NH2	119.20	115.38	1
OE1-CD-NE2	122.60	118.36	3
N-CA-CB	103.00	107.66	1
CA-CB-OG	111.10	102.63	1
OE1-CD-NE2	122.60	118.37	2
CB-CG-CD1	110.70	123.38	1
CA-CB-CG	112.60	116.82	1
CA-C-N	116.20	124.64	1
OE1-CD-NE2	122.60	118.38	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	99.21	1
OD1-CG-ND2	122.60	118.39	1
OE1-CD-NE2	122.60	118.39	3
OE1-CD-NE2	122.60	118.40	4
OD1-CG-ND2	122.60	118.40	2
CA-CB-CG	112.60	116.80	1
OE1-CD-NE2	122.60	118.41	5
CA-CB-CG	112.60	116.79	1
C-N-CA	121.70	129.24	1
OD1-CG-ND2	122.60	118.42	2
NH1-CZ-NH2	119.30	113.86	1
OE1-CD-NE2	122.60	118.42	4
OE1-CD-NE2	122.60	118.43	1
C-CA-CB	110.10	118.02	1
OE1-CD-NE2	122.60	118.44	1
OD1-CG-ND2	122.60	118.44	1
CA-C-N	116.20	124.50	1
CA-C-N	116.90	123.12	1
NE-CZ-NH1	121.50	125.64	2
OE1-CD-NE2	122.60	118.46	2
OE1-CD-NE2	122.60	118.47	2
NH1-CZ-NH2	119.30	113.93	1
CA-CB-CG	112.60	116.73	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.47	2
CB-CG-CD2	131.20	125.83	1
N-CA-C	111.00	122.56	1
OE1-CD-NE2	122.60	118.48	3
OD1-CG-ND2	122.60	118.48	2
C-N-CA	121.70	129.11	1
CA-CB-CG	112.60	116.71	1
CA-C-N	116.20	124.43	1
OE1-CD-NE2	122.60	118.49	3
C-CA-CB	111.40	103.59	1
OE1-CD-NE2	122.60	118.50	3
OE1-CD-NE2	122.60	118.51	4
OD1-CG-ND2	122.60	118.51	3
C-N-CA	121.70	129.06	2
NE-CZ-NH2	119.20	122.88	1
OE1-CD-NE2	122.60	118.52	3
OD1-CG-ND2	122.60	118.52	4
CA-CB-CG	112.60	116.68	1
N-CA-C	111.00	122.42	1
OD1-CG-ND2	122.60	118.53	5
OE1-CD-NE2	122.60	118.53	2
CA-C-N	116.20	124.34	2
CA-CB-CG	112.60	116.67	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	104.59	1
OE1-CD-NE2	122.60	118.54	2
OD1-CG-ND2	122.60	118.54	1
OD1-CG-ND2	122.60	118.55	2
O-C-OXT	118.00	130.16	1
OE1-CD-NE2	122.60	118.55	3
OE1-CD-NE2	122.60	118.56	6
OD1-CG-ND2	122.60	118.56	2
CA-CB-CG	112.60	116.64	3
OE1-CD-NE2	122.60	118.57	5
C-N-CA	121.70	128.96	1
C-N-CA	121.70	128.95	1
OE1-CD-NE2	122.60	118.58	2
OE1-CD-NE2	122.60	118.59	3
OD1-CG-ND2	122.60	118.59	2
CB-CG-CD2	131.20	125.99	1
CA-C-N	116.20	124.21	1
OE1-CD-NE2	122.60	118.60	3
OD1-CG-ND2	122.60	118.60	1
NH1-CZ-NH2	119.30	114.10	1
HH11-NH1-HH12	107.69	120.00	1
CZ-NH1-HH11	107.58	120.00	1
C-N-H	111.73	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CZ-NH1-HH11	107.32	120.00	1
HZ1-NZ-HZ2	96.18	109.00	1
CZ-NH1-HH11	107.15	120.00	1
HZ1-NZ-HZ3	96.14	109.00	1
HZ1-NZ-HZ3	96.09	109.00	1
HH11-NH1-HH12	107.09	120.00	1
HZ2-NZ-HZ3	96.05	109.00	1
HZ1-NZ-HZ3	96.05	109.00	1
HZ1-NZ-HZ2	96.01	109.00	1
HH11-NH1-HH12	106.97	120.00	1
HZ1-NZ-HZ3	95.93	109.00	1
HZ2-NZ-HZ3	95.81	109.00	1
C-N-H	110.47	124.30	1
HH11-NH1-HH12	105.90	120.00	1
HH11-NH1-HH12	105.37	120.00	1
HH11-NH1-HH12	104.95	120.00	1
CZ-NH1-HH11	104.55	120.00	1
C-N-H	106.56	124.30	1
HH21-NH2-HH22	101.48	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

Model ID	Clash score	Number of clashes
1	2.60	32
2	3.34	41
3	2.52	31
4	2.52	31
5	2.28	28
6	1.30	16
7	2.77	34
8	2.77	34
9	1.87	23
10	3.09	38

All 308 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:533:LEU:HD13	A:550:ASP:H	0.818
1	A:474:LEU:HD13	A:526:TYR:CE1	0.673
1	A:482:MET:HE3	A:517:VAL:HG22	0.673
1	A:530:SER:HA	A:533:LEU:HD12	0.648
1	A:406:PHE:CZ	A:408:THR:HG23	0.642
1	A:341:ASN:OD1	A:351:THR:HG22	0.605
1	A:533:LEU:HD22	A:550:ASP:CB	0.581
1	A:406:PHE:CE1	A:408:THR:HG23	0.539
1	A:533:LEU:CD1	A:550:ASP:H	0.521
1	A:530:SER:HA	A:533:LEU:CD1	0.498
1	A:530:SER:HA	A:533:LEU:HG	0.492

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:700:VAL:CG2	A:777:ILE:HD11	0.492
1	A:232:ASN:HB3	A:244:TYR:CZ	0.467
1	A:265:HIS:CE1	A:266:ARG:HG3	0.467
1	A:391:GLU:CD	A:413:GLN:HE21	0.466
1	A:230:ILE:HD13	A:757:GLU:HG3	0.457
1	A:431:HIS:CE1	A:532:LEU:HD21	0.456
1	A:354:TYR:CD2	A:377:PHE:CD1	0.449
1	A:415:VAL:HG21	A:429:ARG:HH21	0.449
1	A:526:TYR:HB2	A:528:TYR:CE1	0.448
1	A:474:LEU:HD22	A:526:TYR:HE1	0.443
1	A:526:TYR:CB	A:528:TYR:CE1	0.439
1	A:148:ARG:HH12	A:175:PRO:N	0.437
1	A:406:PHE:CE2	A:436:ILE:HG23	0.426
1	A:480:ARG:HD2	A:525:ILE:HD11	0.426
1	A:148:ARG:HH12	A:174:LEU:C	0.422
1	A:545:THR:HB	A:546:TYR:CD2	0.420
1	A:140:TYR:CE1	A:165:LEU:HD13	0.418
1	A:533:LEU:HD22	A:550:ASP:CG	0.418
1	A:595:ILE:HG22	A:597:TRP:CD1	0.410
1	A:511:ARG:HB3	A:540:LEU:CD2	0.401
1	A:572:VAL:CG1	A:615:ARG:HH11	0.400
2	A:419:ASN:HD22	A:424:MET:HB3	0.674
2	A:355:ALA:HB2	A:380:PHE:CE2	0.637

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:236:THR:HG22	A:751:ALA:HB2	0.620
2	A:75:ILE:HD11	A:87:VAL:HG11	0.612
2	A:355:ALA:HB2	A:380:PHE:CZ	0.586
2	A:700:VAL:HG23	A:773:LEU:HD21	0.563
2	A:352:ASP:HB2	A:354:TYR:CE2	0.557
2	A:352:ASP:CB	A:354:TYR:CE2	0.527
2	A:419:ASN:ND2	A:424:MET:HB3	0.525
2	A:711:LYS:HE2	A:739:TRP:CZ3	0.517
2	A:153:LEU:HD21	A:155:LYS:HE3	0.511
2	A:700:VAL:CG2	A:773:LEU:HD21	0.504
2	A:145:ARG:HH22	A:194:GLN:NE2	0.500
2	A:419:ASN:HD22	A:424:MET:CB	0.498
2	A:423:ASP:C	A:465:TRP:CZ2	0.486
2	A:424:MET:HG3	A:526:TYR:CE1	0.486
2	A:234:LYS:HE2	A:751:ALA:CB	0.464
2	A:480:ARG:HH11	A:522:GLN:HG2	0.463
2	A:151:ALA:HB2	A:164:ILE:HG23	0.458
2	A:34:GLY:C	A:141:GLN:HE22	0.452
2	A:532:LEU:HD22	A:667:THR:HG22	0.451
2	A:537:TYR:CZ	A:578:SER:HB3	0.450
2	A:203:PHE:CE2	A:761:LEU:HD11	0.449
2	A:519:TYR:CE2	A:589:ARG:HB2	0.442
2	A:23:LEU:HA	A:26:ASP:HB2	0.441

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:151:ALA:CB	A:164:ILE:HG23	0.441
2	A:151:ALA:HB2	A:164:ILE:CG2	0.436
2	A:424:MET:CE	A:528:TYR:CD1	0.428
2	A:117:VAL:HG11	A:162:TYR:CE1	0.422
2	A:425:PRO:HB3	A:463:LEU:HD23	0.422
2	A:153:LEU:CD2	A:155:LYS:HE3	0.421
2	A:139:ASP:OD1	A:150:LYS:HE2	0.415
2	A:597:TRP:CE3	A:631:ARG:HB3	0.412
2	A:164:ILE:HD11	A:189:HIS:CD2	0.411
2	A:733:GLU:CG	A:751:ALA:HB3	0.409
2	A:632:LEU:HD22	A:662:GLU:CB	0.408
2	A:391:GLU:HA	A:392:PRO:HA	0.407
2	A:310:ARG:HH12	A:342:ASP:CG	0.407
2	A:140:TYR:HB3	A:154:MET:SD	0.406
2	A:30:GLN:HA	A:33:LEU:HD12	0.402
2	A:234:LYS:HE2	A:751:ALA:HB1	0.401
3	A:584:TYR:CE2	A:606:LEU:HD12	0.835
3	A:472:THR:HG21	A:523:SER:HB2	0.692
3	A:700:VAL:HG23	A:773:LEU:HD21	0.678
3	A:584:TYR:CZ	A:606:LEU:HD12	0.640
3	A:195:VAL:HG13	A:225:ARG:CZ	0.628
3	A:189:HIS:CD2	A:220:VAL:HG21	0.627
3	A:480:ARG:CZ	A:525:ILE:HD12	0.560

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:415:VAL:HG21	A:429:ARG:HH21	0.550
3	A:42:LEU:HD23	A:115:ASN:HD22	0.544
3	A:664:ILE:HD12	A:681:GLY:HA2	0.533
3	A:454:LEU:HD13	A:552:ILE:CD1	0.518
3	A:653:GLN:HE22	A:781:GLN:NE2	0.516
3	A:584:TYR:CD2	A:606:LEU:HD12	0.514
3	A:429:ARG:HH11	A:550:ASP:CG	0.474
3	A:517:VAL:HG11	A:552:ILE:HG21	0.472
3	A:38:TYR:CE2	A:115:ASN:HA	0.466
3	A:75:ILE:HD11	A:87:VAL:HG11	0.454
3	A:111:HIS:CE1	A:120:LYS:HE2	0.452
3	A:140:TYR:CE1	A:165:LEU:HD13	0.452
3	A:225:ARG:HA	A:250:ASN:CB	0.444
3	A:700:VAL:CG2	A:773:LEU:HD21	0.443
3	A:234:LYS:HA	A:752:ILE:O	0.442
3	A:458:TYR:OH	A:550:ASP:CG	0.442
3	A:472:THR:HG21	A:523:SER:CB	0.437
3	A:454:LEU:HD13	A:552:ILE:HD13	0.436
3	A:230:ILE:HG21	A:756:ILE:HB	0.433
3	A:145:ARG:CZ	A:221:GLY:HA2	0.431
3	A:225:ARG:HA	A:250:ASN:HB3	0.424
3	A:139:ASP:OD1	A:150:LYS:HE2	0.417
3	A:700:VAL:HG21	A:773:LEU:HG	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:645:ARG:CZ	A:651:LEU:HD13	0.409
4	A:700:VAL:HG21	A:773:LEU:CD1	0.966
4	A:700:VAL:HG21	A:773:LEU:HD11	0.841
4	A:700:VAL:HG21	A:773:LEU:HD13	0.798
4	A:413:GLN:NE2	A:549:LEU:HD12	0.630
4	A:375:LYS:HE2	A:377:PHE:CZ	0.607
4	A:472:THR:HG21	A:523:SER:HB2	0.576
4	A:546:TYR:CE2	A:553:ALA:HB2	0.560
4	A:354:TYR:CE1	A:379:VAL:HG13	0.553
4	A:375:LYS:HE2	A:377:PHE:CE2	0.527
4	A:224:ARG:HB2	A:248:TYR:CE1	0.507
4	A:375:LYS:CE	A:377:PHE:CE2	0.507
4	A:406:PHE:CE1	A:408:THR:HG23	0.500
4	A:312:LEU:HB2	A:339:TYR:CZ	0.498
4	A:700:VAL:CG2	A:773:LEU:HD11	0.497
4	A:482:MET:CE	A:552:ILE:HD12	0.496
4	A:764:ASN:C	A:766:GLY:H	0.481
4	A:140:TYR:CE1	A:165:LEU:HD13	0.477
4	A:194:GLN:C	A:220:VAL:HG22	0.469
4	A:596:THR:C	A:598:GLU:H	0.468
4	A:664:ILE:HD12	A:681:GLY:HA2	0.460
4	A:232:ASN:HB3	A:244:TYR:CZ	0.458
4	A:600:ASP:C	A:602:LYS:H	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:234:LYS:HE3	A:242:GLU:OE2	0.449
4	A:700:VAL:HG11	A:773:LEU:HD11	0.443
4	A:347:TYR:HB3	A:772:MET:HE3	0.442
4	A:230:ILE:H	A:230:ILE:HD12	0.439
4	A:454:LEU:HD22	A:552:ILE:CD1	0.420
4	A:375:LYS:CE	A:377:PHE:CZ	0.417
4	A:232:ASN:HB3	A:244:TYR:CE2	0.414
4	A:378:GLN:HE21	A:385:THR:HG21	0.404
4	A:454:LEU:HD22	A:552:ILE:HD11	0.400
5	A:700:VAL:HG11	A:773:LEU:HD13	0.667
5	A:553:ALA:HB2	A:590:THR:HG23	0.661
5	A:375:LYS:HE2	A:377:PHE:CZ	0.638
5	A:267:ARG:HH22	A:342:ASP:HB3	0.616
5	A:326:ARG:NH1	A:364:ALA:HB3	0.569
5	A:298:TYR:CD1	A:310:ARG:HD2	0.562
5	A:267:ARG:HH22	A:342:ASP:CB	0.554
5	A:413:GLN:NE2	A:549:LEU:HD12	0.537
5	A:142:MET:HE3	A:189:HIS:CE1	0.510
5	A:75:ILE:HD11	A:87:VAL:HG11	0.509
5	A:632:LEU:HD22	A:662:GLU:HB2	0.506
5	A:234:LYS:HE2	A:751:ALA:HB1	0.478
5	A:472:THR:HG21	A:523:SER:HB2	0.470
5	A:140:TYR:CE1	A:165:LEU:HD13	0.468

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:379:VAL:HG21	A:387:SER:OG	0.461
5	A:581:GLN:HE21	A:606:LEU:HD22	0.453
5	A:111:HIS:CE1	A:118:ILE:HG23	0.451
5	A:700:VAL:HG11	A:773:LEU:CD1	0.447
5	A:519:TYR:CE2	A:589:ARG:HB2	0.439
5	A:700:VAL:CG1	A:773:LEU:HD13	0.431
5	A:645:ARG:CZ	A:651:LEU:HD13	0.424
5	A:429:ARG:HD3	A:458:TYR:CE1	0.423
5	A:375:LYS:CE	A:377:PHE:CZ	0.420
5	A:139:ASP:OD1	A:150:LYS:HE2	0.419
5	A:43:VAL:HG12	A:44:GLN:O	0.413
5	A:423:ASP:HB2	A:465:TRP:CD1	0.412
5	A:632:LEU:HD22	A:662:GLU:CB	0.411
5	A:230:ILE:CG2	A:755:ASN:HD21	0.401
6	A:461:THR:HG22	A:473:LYS:HE3	0.877
6	A:461:THR:HG22	A:473:LYS:CE	0.606
6	A:422:ASP:HA	A:466:TYR:CE1	0.563
6	A:375:LYS:HE2	A:377:PHE:CZ	0.542
6	A:117:VAL:HG11	A:156:GLN:NE2	0.514
6	A:454:LEU:HD13	A:552:ILE:HD13	0.514
6	A:376:GLN:HE21	A:391:GLU:CD	0.507
6	A:140:TYR:CE1	A:165:LEU:HD13	0.501
6	A:43:VAL:HG11	A:50:LEU:HD11	0.489

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:230:ILE:HG23	A:756:ILE:O	0.482
6	A:664:ILE:HD12	A:681:GLY:HA2	0.482
6	A:234:LYS:HE2	A:236:THR:HG22	0.460
6	A:234:LYS:HE2	A:751:ALA:HB1	0.436
6	A:716:MET:SD	A:778:LEU:HD23	0.423
6	A:606:LEU:CD2	A:608:TRP:HE1	0.410
6	A:597:TRP:C	A:599:ASN:H	0.406
7	A:234:LYS:HE2	A:751:ALA:HB1	0.787
7	A:75:ILE:HD11	A:87:VAL:HG11	0.595
7	A:375:LYS:HE2	A:377:PHE:CZ	0.593
7	A:733:GLU:HG2	A:751:ALA:HB3	0.577
7	A:733:GLU:CG	A:751:ALA:HB3	0.547
7	A:584:TYR:CD2	A:606:LEU:HD12	0.525
7	A:584:TYR:CE2	A:606:LEU:HD12	0.525
7	A:423:ASP:HA	A:465:TRP:CZ3	0.515
7	A:153:LEU:HD21	A:155:LYS:HE3	0.495
7	A:544:ARG:HH12	A:549:LEU:HD23	0.476
7	A:423:ASP:HA	A:465:TRP:CH2	0.471
7	A:704:TYR:OH	A:777:ILE:HG23	0.457
7	A:232:ASN:HB3	A:244:TYR:CZ	0.450
7	A:116:GLN:HE22	A:191:ARG:NH1	0.449
7	A:702:ALA:HB2	A:777:ILE:HD11	0.442
7	A:116:GLN:HE22	A:191:ARG:CZ	0.440

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:393:GLN:HG2	A:415:VAL:HG13	0.440
7	A:664:ILE:HD12	A:681:GLY:HA2	0.440
7	A:773:LEU:HD23	A:777:ILE:HD12	0.440
7	A:234:LYS:HE2	A:236:THR:HG22	0.438
7	A:234:LYS:CE	A:751:ALA:HB1	0.437
7	A:153:LEU:CD2	A:155:LYS:HE3	0.436
7	A:764:ASN:O	A:765:TYR:CD2	0.436
7	A:161:ARG:HH21	A:188:ILE:HD13	0.435
7	A:310:ARG:NH1	A:336:ASP:OD2	0.418
7	A:332:THR:HB	A:355:ALA:HB1	0.417
7	A:298:TYR:CE2	A:310:ARG:NH1	0.415
7	A:650:ARG:HG2	A:692:PRO:HD2	0.415
7	A:454:LEU:HD13	A:552:ILE:HD13	0.413
7	A:546:TYR:CE2	A:590:THR:HG21	0.413
7	A:743:LYS:HB3	A:745:HIS:CE1	0.410
7	A:234:LYS:HE2	A:751:ALA:CB	0.409
7	A:349:SER:C	A:351:THR:H	0.408
7	A:743:LYS:CB	A:745:HIS:CE1	0.406
8	A:27:LEU:HB3	A:696:ARG:HH12	0.748
8	A:664:ILE:HG23	A:668:LEU:HD12	0.641
8	A:590:THR:HG21	A:597:TRP:CD1	0.620
8	A:664:ILE:HG21	A:678:TYR:HB3	0.617
8	A:195:VAL:HG11	A:225:ARG:NE	0.569

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:27:LEU:CB	A:696:ARG:HH12	0.535
8	A:379:VAL:HG21	A:387:SER:HB3	0.526
8	A:664:ILE:HD12	A:681:GLY:HA2	0.520
8	A:665:GLN:HA	A:673:SER:HB2	0.509
8	A:123:LYS:HE3	A:136:TRP:CG	0.500
8	A:375:LYS:HE2	A:377:PHE:CZ	0.491
8	A:379:VAL:HG21	A:387:SER:CB	0.478
8	A:189:HIS:CD2	A:220:VAL:HG21	0.475
8	A:386:SER:HB3	A:424:MET:HE1	0.460
8	A:481:VAL:H	A:520:ARG:NH1	0.457
8	A:140:TYR:CE1	A:165:LEU:HD13	0.453
8	A:75:ILE:HD11	A:87:VAL:HG11	0.446
8	A:482:MET:HE1	A:552:ILE:HB	0.438
8	A:386:SER:CB	A:424:MET:HE1	0.436
8	A:375:LYS:HE2	A:377:PHE:CE1	0.428
8	A:775:SER:CB	A:777:ILE:H	0.428
8	A:775:SER:CB	A:777:ILE:HB	0.428
8	A:178:ASP:O	A:206:GLY:HA2	0.427
8	A:425:PRO:HG3	A:526:TYR:CE2	0.426
8	A:230:ILE:HD13	A:757:GLU:HA	0.424
8	A:546:TYR:CD2	A:589:ARG:NH1	0.421
8	A:718:GLY:CA	A:769:THR:HG21	0.420
8	A:491:MET:HE2	A:493:PHE:CZ	0.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:553:ALA:C	A:589:ARG:HE	0.411
8	A:480:ARG:NE	A:482:MET:HE2	0.407
8	A:718:GLY:HA3	A:769:THR:HG21	0.407
8	A:553:ALA:HB1	A:589:ARG:HG2	0.405
8	A:589:ARG:HB3	A:590:THR:HA	0.404
8	A:197:GLU:HG2	A:217:GLN:HE21	0.400
9	A:465:TRP:CZ2	A:469:ARG:CZ	0.613
9	A:375:LYS:HE2	A:377:PHE:CZ	0.565
9	A:142:MET:HE3	A:189:HIS:CG	0.531
9	A:423:ASP:HB3	A:465:TRP:CE2	0.512
9	A:423:ASP:HB3	A:465:TRP:CZ2	0.502
9	A:465:TRP:CE2	A:469:ARG:NH2	0.501
9	A:251:ILE:HG21	A:255:MET:HE3	0.500
9	A:230:ILE:HG21	A:756:ILE:O	0.492
9	A:230:ILE:CD1	A:758:LEU:H	0.486
9	A:234:LYS:HE2	A:751:ALA:HB1	0.468
9	A:376:GLN:HE21	A:391:GLU:CD	0.466
9	A:33:LEU:HA	A:35:VAL:H	0.458
9	A:377:PHE:CD2	A:387:SER:HB3	0.451
9	A:664:ILE:HG23	A:668:LEU:HD12	0.446
9	A:142:MET:HE3	A:189:HIS:CD2	0.434
9	A:236:THR:HG22	A:751:ALA:HB2	0.434
9	A:465:TRP:CE2	A:469:ARG:CZ	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:234:LYS:HE2	A:236:THR:HG22	0.432
9	A:234:LYS:HE2	A:751:ALA:CB	0.431
9	A:774:ARG:HG2	A:778:LEU:HD12	0.431
9	A:117:VAL:HG11	A:156:GLN:NE2	0.427
9	A:75:ILE:HD11	A:87:VAL:HG11	0.424
9	A:140:TYR:CE1	A:165:LEU:HD13	0.422
10	A:581:GLN:HE21	A:606:LEU:HD22	0.764
10	A:474:LEU:HD13	A:526:TYR:CE1	0.653
10	A:688:VAL:HG11	A:777:ILE:HG23	0.620
10	A:466:TYR:CE1	A:474:LEU:HD11	0.598
10	A:688:VAL:HG11	A:777:ILE:CG2	0.581
10	A:474:LEU:HD13	A:526:TYR:HE1	0.554
10	A:581:GLN:HE21	A:606:LEU:CD2	0.531
10	A:501:ALA:HB1	A:502:PRO:HD2	0.530
10	A:28:ALA:HB1	A:32:MET:HE2	0.529
10	A:123:LYS:HE3	A:136:TRP:CG	0.528
10	A:87:VAL:HG13	A:104:VAL:HG13	0.516
10	A:465:TRP:CE2	A:469:ARG:NH2	0.514
10	A:119:LEU:HD11	A:156:GLN:HE21	0.508
10	A:350:SER:C	A:352:ASP:H	0.491
10	A:549:LEU:HD11	A:666:ALA:HB1	0.474
10	A:729:ARG:HD3	A:769:THR:HG21	0.474
10	A:716:MET:HE1	A:777:ILE:HG13	0.473

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:486:LYS:HE2	A:488:ASP:OD2	0.471
10	A:344:ASP:C	A:346:LYS:H	0.460
10	A:463:LEU:HD11	A:474:LEU:HB2	0.460
10	A:465:TRP:CZ2	A:469:ARG:CZ	0.460
10	A:552:ILE:HD11	A:631:ARG:NH1	0.453
10	A:474:LEU:HD22	A:526:TYR:CE1	0.449
10	A:709:ALA:HB1	A:711:LYS:HE2	0.442
10	A:407:ASP:HB3	A:437:ASN:HB2	0.441
10	A:581:GLN:NE2	A:606:LEU:HD22	0.441
10	A:552:ILE:HD12	A:584:TYR:CD1	0.435
10	A:729:ARG:CD	A:769:THR:HG21	0.431
10	A:425:PRO:HD3	A:466:TYR:CD2	0.421
10	A:526:TYR:CB	A:528:TYR:CE1	0.421
10	A:460:GLN:NE2	A:526:TYR:CE2	0.421
10	A:537:TYR:CZ	A:627:GLN:CD	0.420
10	A:653:GLN:HE22	A:781:GLN:NE2	0.420
10	A:709:ALA:CB	A:711:LYS:HE2	0.417
10	A:458:TYR:CD2	A:478:VAL:HG23	0.414
10	A:501:ALA:HB1	A:502:PRO:CD	0.411
10	A:552:ILE:HD12	A:584:TYR:CG	0.407
10	A:140:TYR:CE1	A:165:LEU:HD13	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	782	737	32	13
2	782	716	41	25
3	782	747	26	9
4	782	741	32	9
5	782	741	29	12
6	782	739	33	10
7	782	739	34	9
8	782	738	36	8
9	782	733	42	7
10	782	738	37	7

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	681	656	17	8
2	681	655	21	5
3	681	657	16	8
4	681	653	23	5
5	681	652	20	9
6	681	657	13	11
7	681	661	17	3
8	681	657	16	8
9	681	657	20	4
10	681	654	18	9

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	9	LEU
1	A	15	THR
1	A	148	ARG
1	A	240	TYR
1	A	265	HIS
1	A	294	SER
1	A	408	THR
1	A	550	ASP
2	A	9	LEU
2	A	15	THR
2	A	532	LEU
2	A	578	SER
2	A	769	THR
3	A	9	LEU
3	A	38	TYR
3	A	374	THR
3	A	531	SER
3	A	630	THR
3	A	671	TYR
3	A	700	VAL
3	A	769	THR
4	A	9	LEU
4	A	374	THR

Model ID	Chain	Residue ID	Residue type
4	A	532	LEU
4	A	600	ASP
4	A	783	THR
5	A	7	THR
5	A	8	LEU
5	A	9	LEU
5	A	148	ARG
5	A	554	SER
5	A	590	THR
5	A	600	ASP
5	A	771	GLU
5	A	783	THR
6	A	9	LEU
6	A	11	THR
6	A	15	THR
6	A	27	LEU
6	A	33	LEU
6	A	244	TYR
6	A	387	SER
6	A	472	THR
6	A	603	THR
6	A	651	LEU
6	A	769	THR

Model ID	Chain	Residue ID	Residue type
7	A	9	LEU
7	A	385	THR
7	A	600	ASP
8	A	9	LEU
8	A	18	TYR
8	A	27	LEU
8	A	38	TYR
8	A	472	THR
8	A	540	LEU
8	A	545	THR
8	A	775	SER
9	A	9	LEU
9	A	15	THR
9	A	27	LEU
9	A	769	THR
10	A	8	LEU
10	A	9	LEU
10	A	148	ARG
10	A	237	THR
10	A	453	LEU
10	A	511	ARG
10	A	535	SER
10	A	538	SER

Model ID	Chain	Residue ID	Residue type
10	A	660	SER

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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