Integrative Structure Validation Report

July 22, 2024 - 05:02 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	9A2M
PDB-Dev ID	PDBDEV_00000171
Structure Title	Model of E. coli OmpA 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

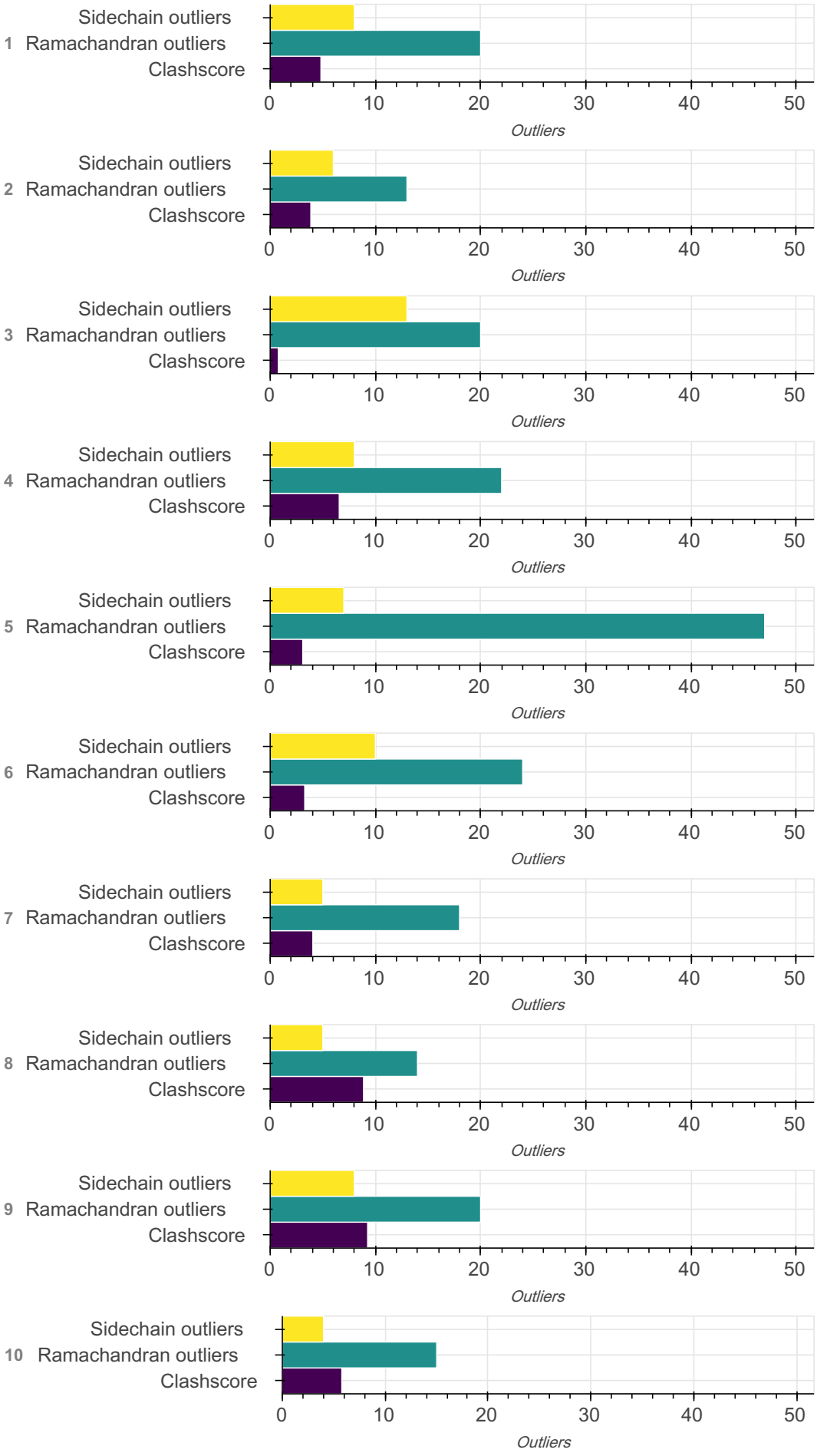
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
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40
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
Clashscore
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Outliers
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Sidechain outliers
Ramachandran outliers
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Sidechain outliers
Ramachandran outliers
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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
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	P0A910	A	A	346
2	1	1	P0A910	A	A	346
3	1	1	P0A910	A	A	346
4	1	1	P0A910	A	A	346
5	1	1	P0A910	A	A	346
6	1	1	P0A910	A	A	346
7	1	1	P0A910	A	A	346
8	1	1	P0A910	A	A	346
9	1	1	P0A910	A	A	346
10	1	1	P0A910	A	A	346

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	-	1-346

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 25618 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
CB--HB3	1.09	0.97	2420
CA--HA	1.09	0.97	3080
CG2--HG23	1.09	0.97	660
CG--HG2	1.09	0.97	870
CB--HB	1.09	0.97	660
CB--HB2	1.09	0.97	2420
NZ--HZ2	1.01	0.89	190
NZ--HZ1	1.01	0.89	190
CG2--HG21	1.09	0.97	660
CD2--HD21	1.09	0.97	230
CE--HE2	1.09	0.97	250
CG--HG3	1.09	0.97	870
CD2--HD23	1.09	0.97	230
CG2--HG22	1.09	0.97	660
CE--HE3	1.09	0.97	250
CG1--HG13	1.09	0.97	430
CD1--HD11	1.09	0.97	390
CD1--HD12	1.09	0.97	390
CA--HA2	1.09	0.97	380
CG1--HG12	1.09	0.97	430
CB--HB1	1.09	0.97	370
CG--HG	1.09	0.97	230

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
OH--HH	0.96	0.84	170
OG1--HG1	0.96	0.84	230
N--H3	1.01	0.89	10
CD--HD2	1.09	0.97	510
CD--HD3	1.09	0.97	510
OG--HG	0.96	0.84	160
CD1--HD13	1.09	0.97	390
CA--HA3	1.09	0.97	380
CD2--HD22	1.09	0.97	230
CG1--HG11	1.09	0.97	270
NZ--HZ3	1.01	0.89	190
CE--HE1	1.09	0.97	60
N--H1	1.01	0.89	10
N--H2	1.01	0.89	10
SG--HG	1.33	1.20	4
SG--HG	1.34	1.20	14
ND2--HD21	1.01	0.86	190
N--H	1.01	0.86	3260
CZ2--HZ2	1.08	0.93	50
CD1--HD1	1.08	0.93	310
CD2--HD2	1.08	0.93	310
NH1--HH11	1.01	0.86	130
CE1--HE1	1.08	0.93	310

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.01	0.86	130
NE2--HE22	1.01	0.86	170
CE2--HE2	1.08	0.93	260
ND2--HD22	1.01	0.86	190
NE--HE	1.01	0.86	130
NE2--HE21	1.01	0.86	170
NH1--HH12	1.01	0.86	130
CH2--HH2	1.08	0.93	50
NH2--HH21	1.01	0.86	130
CZ--HZ	1.08	0.93	90
ND1--HD1	1.01	0.86	50
NE1--HE1	1.01	0.86	50
CZ3--HZ3	1.08	0.93	50
CE3--HE3	1.08	0.93	50

Standard geometry: angle outliers

There are 346 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	137.06	1
C-N-CA	121.70	136.87	1
C-N-CA	121.70	136.09	1
O-C-N	123.00	110.33	1
C-N-CA	121.70	135.45	1
C-N-CA	121.70	135.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	135.17	1
C-N-CA	121.70	108.69	1
C-N-CA	121.70	134.51	1
C-N-CA	121.70	134.23	2
CA-C-N	116.90	127.30	1
C-N-CA	121.70	134.14	1
C-CA-CB	110.10	122.90	1
OD1-CG-ND2	122.60	115.89	1
C-N-CA	121.70	133.67	1
C-N-CA	121.70	133.51	1
C-CA-CB	110.10	122.12	1
CA-CB-CG	112.60	118.90	1
C-N-CA	121.70	132.96	1
C-N-CA	121.70	132.88	1
CA-CB-CG	112.60	118.81	1
CA-CB-CG	112.60	118.79	1
CA-CB-CG	112.60	118.72	1
C-CA-CB	110.10	121.72	1
C-N-CA	121.70	132.61	1
OE1-CD-NE2	122.60	116.59	1
CA-C-N	116.90	125.90	1
C-N-CA	121.70	132.42	1
C-N-CA	121.70	132.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	121.34	1
OE1-CD-NE2	122.60	116.71	1
C-N-CA	121.70	132.22	1
OE1-CD-NE2	122.60	116.76	2
C-N-CA	121.70	132.18	2
OE1-CD-NE2	122.60	116.82	1
OE1-CD-NE2	122.60	116.83	1
OE1-CD-NE2	122.60	116.84	1
C-N-CA	121.70	132.04	1
C-N-CA	121.70	131.98	1
C-N-CA	121.70	131.95	1
OE1-CD-NE2	122.60	116.91	1
CA-CB-CG	116.30	135.98	1
C-N-CA	121.70	131.81	2
OE1-CD-NE2	122.60	117.01	1
OE1-CD-NE2	122.60	117.02	1
C-N-CA	121.70	131.74	1
C-N-CA	121.70	131.61	1
C-N-CA	121.70	131.60	2
CA-CB-CG1	110.40	119.75	1
N-CA-C	111.00	126.39	1
C-N-CA	121.70	131.59	1
OE1-CD-NE2	122.60	117.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	108.98	1
C-N-CA	121.70	131.46	1
OD1-CG-ND2	122.60	117.20	1
OE1-CD-NE2	122.60	117.21	1
C-N-CA	121.70	131.38	1
C-N-CA	121.70	131.32	1
C-N-CA	121.70	131.29	1
C-N-CA	121.70	131.24	1
C-N-CA	121.70	131.21	1
C-N-CA	121.70	131.19	1
C-N-CA	121.70	131.16	1
C-N-CA	121.70	131.10	1
OE1-CD-NE2	122.60	117.39	1
C-N-CA	121.70	131.08	2
CA-CB-CG	112.60	117.80	1
OD1-CG-ND2	122.60	117.42	1
C-N-CA	121.70	130.99	1
O-C-N	123.00	114.75	1
C-N-CA	121.70	130.97	1
C-N-CA	121.70	130.96	1
OE1-CD-NE2	122.60	117.47	1
OE1-CD-NE2	122.60	117.49	1
OE1-CD-NE2	122.60	117.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.54	1
C-N-CA	121.70	130.79	1
C-N-CA	121.70	130.78	1
OE1-CD-NE2	122.60	117.58	2
C-N-CA	121.70	130.73	1
CA-C-O	120.80	112.29	1
CA-CB-CG1	110.40	118.89	1
OE1-CD-NE2	122.60	117.61	1
C-N-CA	121.70	130.67	1
C-N-CA	121.70	130.66	1
NE-CZ-NH2	119.20	123.68	1
OE1-CD-NE2	122.60	117.63	1
OE1-CD-NE2	122.60	117.64	1
C-N-CA	121.70	130.62	1
CA-CB-CG2	110.50	118.90	1
OE1-CD-NE2	122.60	117.66	1
CA-CB-CG2	110.50	118.89	1
OD1-CG-ND2	122.60	117.67	1
CA-C-N	116.20	126.04	1
C-N-CA	121.70	130.55	1
OE1-CD-NE2	122.60	117.70	2
CA-CB-CG	112.60	117.50	1
C-N-CA	121.70	130.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.72	1
OE1-CD-NE2	122.60	117.73	2
N-CA-CB	110.40	103.10	1
OE1-CD-NE2	122.60	117.75	2
C-N-CA	121.70	130.42	1
C-N-CA	121.70	130.37	1
CA-CB-CG	114.10	104.48	1
OE1-CD-NE2	122.60	117.80	1
OD1-CG-ND2	122.60	117.80	1
CA-C-N	116.90	124.09	1
C-N-CA	121.70	130.29	1
C-N-CA	121.70	130.27	1
C-N-CA	121.70	130.25	2
OE1-CD-NE2	122.60	117.86	1
OD1-CG-ND2	122.60	117.86	1
OE1-CD-NE2	122.60	117.88	1
C-N-CA	121.70	130.19	1
N-CA-C	111.00	97.79	1
C-N-CA	121.70	130.18	1
OE1-CD-NE2	122.60	117.89	1
CA-C-N	116.20	125.61	1
OE1-CD-NE2	122.60	117.91	1
C-CA-CB	110.10	118.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.12	1
OE1-CD-NE2	122.60	117.92	2
OE1-CD-NE2	122.60	117.93	1
OE1-CD-NE2	122.60	117.94	1
C-N-CA	121.70	130.09	1
CA-CB-CG	112.60	117.26	1
OD1-CG-ND2	122.60	117.95	1
OE1-CD-NE2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	5
C-N-CA	121.70	130.04	1
OE1-CD-NE2	122.60	117.97	1
OE1-CD-NE2	122.60	117.98	1
N-CA-C	111.00	123.93	1
OE1-CD-NE2	122.60	117.99	3
OE1-CD-NE2	122.60	118.00	1
C-N-CA	121.70	129.98	1
C-N-CA	121.70	129.96	1
OE1-CD-NE2	122.60	118.02	2
NE-CZ-NH2	119.20	123.32	1
OD1-CG-ND2	122.60	118.02	1
C-N-CA	121.70	129.94	1
CA-C-N	116.20	125.35	1
CB-CG-CD2	131.20	125.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.03	1
C-N-CA	121.70	129.92	1
CA-CB-CG	112.60	117.16	1
OE1-CD-NE2	122.60	118.04	1
C-N-CA	121.70	129.90	1
CA-C-N	116.20	125.31	1
OE1-CD-NE2	122.60	118.05	1
C-CA-CB	110.10	118.72	1
OE1-CD-NE2	122.60	118.07	1
CB-CG-CD2	131.20	125.31	1
C-N-CA	121.70	129.85	1
N-CA-CB	103.00	107.98	1
CB-CG-CD2	131.20	125.32	1
N-CA-CB	111.50	103.83	1
CA-CB-CG	113.80	109.29	1
C-N-CA	121.70	129.80	1
CD1-CG-CD2	110.80	120.70	1
CA-CB-CG	113.80	109.31	1
CA-C-N	116.20	125.16	1
OE1-CD-NE2	122.60	118.12	2
C-N-CA	121.70	129.76	1
OE1-CD-NE2	122.60	118.13	3
OE1-CD-NE2	122.60	118.14	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.41	1
OE1-CD-NE2	122.60	118.15	1
C-CA-CB	110.10	118.53	1
C-N-CA	121.70	129.68	1
OE1-CD-NE2	122.60	118.17	2
N-CA-CB	110.50	102.97	1
N-CA-C	111.00	98.61	1
OE1-CD-NE2	122.60	118.18	2
OE1-CD-NE2	122.60	118.19	2
N-CA-C	111.00	123.35	1
C-N-CA	121.70	129.62	1
N-CA-CB	103.00	107.84	1
C-CA-CB	110.50	117.10	1
OE1-CD-NE2	122.60	118.21	1
OE1-CD-NE2	122.60	118.22	1
CA-CB-CG	113.80	109.42	1
C-N-CA	121.70	129.56	1
OE1-CD-NE2	122.60	118.24	2
CA-CB-CG	113.80	109.44	1
OD1-CG-ND2	122.60	118.24	1
CB-CG-CD2	131.20	125.54	2
C-CA-CB	110.50	117.03	1
OD1-CG-ND2	122.60	118.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-CD	112.00	105.91	1
OE1-CD-NE2	122.60	118.26	2
C-N-CA	121.70	129.51	1
N-CA-CB	103.00	107.77	1
N-CA-C	111.00	123.12	2
C-CA-CB	110.10	118.33	1
C-N-CA	121.70	129.48	1
OE1-CD-NE2	122.60	118.28	4
OG1-CB-CG2	109.30	100.65	1
CA-N-CD	112.00	105.96	1
OE1-CD-NE2	122.60	118.29	2
CA-CB-OG1	109.60	116.07	1
C-N-CA	121.70	129.46	1
OE1-CD-NE2	122.60	118.31	2
OE1-CD-NE2	122.60	118.32	1
O-C-N	123.00	116.15	1
C-N-CA	121.70	129.40	1
OD1-CG-ND2	122.60	118.33	1
CB-CG-CD2	131.20	125.66	2
OE1-CD-NE2	122.60	118.34	1
C-N-CA	121.70	129.35	2
OE1-CD-NE2	122.60	118.35	1
CB-CG-CD2	131.20	125.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.36	1
OE1-CD-NE2	122.60	118.37	1
C-N-CA	121.70	129.32	2
NE-CZ-NH2	119.20	123.00	1
N-CA-C	111.00	122.82	1
OE1-CD-NE2	122.60	118.38	2
OE1-CD-NE2	122.60	118.39	2
C-N-CA	121.70	129.28	1
CA-C-N	116.20	124.61	1
C-N-CA	121.70	129.26	1
CA-C-N	116.20	124.59	1
OD1-CG-ND2	122.60	118.41	2
O-C-N	123.00	116.31	1
O-C-N	123.00	116.32	1
OE1-CD-NE2	122.60	118.43	1
O-C-N	123.00	116.33	1
CA-CB-CG	113.80	109.64	1
O-C-N	123.00	116.36	1
CA-C-N	116.90	123.13	1
C-N-CA	121.70	129.17	1
OE1-CD-NE2	122.60	118.45	1
CA-CB-CG1	110.40	117.45	1
CD1-CG-CD2	110.80	101.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.66	1
C-N-CA	121.70	129.14	1
C-N-CA	121.70	129.13	1
OE1-CD-NE2	122.60	118.47	1
C-N-CA	121.70	129.12	2
OE1-CD-NE2	122.60	118.48	1
C-N-CA	121.70	129.11	1
CA-C-N	116.20	124.43	1
N-CA-C	111.00	122.51	1
OD1-CG-ND2	122.60	118.50	1
C-CA-CB	110.10	117.90	1
CA-C-N	116.20	124.40	1
OE1-CD-NE2	122.60	118.51	1
CB-CG-CD2	131.20	125.89	1
C-N-CA	121.70	129.04	1
C-N-CA	121.70	129.03	2
CA-CB-CG1	110.40	117.32	1
OD1-CG-ND2	122.60	118.53	1
N-CA-CB	103.00	107.47	1
OE1-CD-NE2	122.60	118.53	1
C-N-CA	121.70	129.00	1
OE1-CD-NE2	122.60	118.54	1
CA-CB-SG	114.40	105.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.56	1
C-N-CA	121.70	128.96	1
OE1-CD-NE2	122.60	118.57	3
O-C-N	123.00	116.56	1
OE1-CD-NE2	122.60	118.58	1
C-N-CA	121.70	128.93	1
N-CA-C	111.00	122.25	1
OE1-CD-NE2	122.60	118.59	3
N-CA-C	111.00	122.23	1
C-N-CA	121.70	128.91	1
CA-CB-CG	113.90	106.70	1
C-N-CA	121.70	128.90	1
C-N-H	112.08	124.30	1
C-CA-HA	96.76	109.00	1
C-N-H	111.97	124.30	1
C-N-H	111.87	124.30	1
C-CA-HA	96.55	109.00	1
C-N-H	111.78	124.30	1
C-N-H	111.74	124.30	1
N-CA-HA	97.41	110.00	1
C-N-H	111.64	124.30	1
C-N-H	111.63	124.30	1
C-N-H	111.53	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	111.51	124.30	1
C-N-H	111.48	124.30	1
C-N-H	111.40	124.30	1
C-N-H	111.00	124.30	1
C-N-H	110.87	124.30	1
C-N-H	110.50	124.30	1
C-N-H	110.47	124.30	1
C-N-H	109.94	124.30	1
C-N-H	109.52	124.30	1
C-N-H	109.44	124.30	1
C-N-H	108.85	124.30	1
C-N-H	108.41	124.30	1
C-N-H	106.38	124.30	1
C-N-H	105.99	124.30	1
CG-CB-HB3	89.00	108.00	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	4.82	25
2	3.86	20
3	0.77	4
4	6.56	34

Model ID	Clash score	Number of clashes
5	3.09	16
6	3.28	17
7	4.05	21
8	8.87	46
9	9.26	48
10	5.78	30

All 261 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:322:ASP:C	A:324:LEU:HB2	0.856
1	A:322:ASP:O	A:324:LEU:HB2	0.647
1	A:278:ALA:HB1	A:297:ALA:HB1	0.646
1	A:323:CYS:N	A:324:LEU:HB2	0.617
1	A:39:TYR:CZ	A:178:PRO:CG	0.556
1	A:39:TYR:CZ	A:178:PRO:HG3	0.538
1	A:250:PRO:HG2	A:338:LYS:HE3	0.535
1	A:321:ILE:HG23	A:323:CYS:SG	0.523
1	A:319:ALA:C	A:321:ILE:H	0.509
1	A:311:CYS:SG	A:322:ASP:CG	0.488
1	A:322:ASP:C	A:324:LEU:CB	0.475
1	A:319:ALA:HB1	A:321:ILE:O	0.473
1	A:258:LEU:HD23	A:329:ARG:HA	0.470
1	A:258:LEU:CD2	A:329:ARG:HA	0.466
1	A:321:ILE:HG12	A:323:CYS:SG	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:197:ALA:O	A:198:PRO:C	0.440
1	A:201:ALA:O	A:202:PRO:C	0.433
1	A:196:ALA:O	A:197:ALA:C	0.429
1	A:45:ILE:HD12	A:173:THR:HG21	0.424
1	A:329:ARG:CZ	A:331:GLU:CD	0.422
1	A:231:LYS:HB3	A:233:GLU:OE2	0.417
1	A:33:LYS:HE3	A:182:MET:HE1	0.416
1	A:282:VAL:HG13	A:295:ILE:HG21	0.406
1	A:39:TYR:CZ	A:178:PRO:HG2	0.405
1	A:257:VAL:O	A:330:VAL:HB	0.402
2	A:209:GLU:CB	A:217:LEU:HB3	0.620
2	A:306:VAL:O	A:307:THR:HG23	0.550
2	A:43:GLY:HA3	A:176:THR:HG21	0.546
2	A:209:GLU:HB3	A:217:LEU:HB3	0.529
2	A:3:LYS:O	A:4:THR:HG23	0.504
2	A:209:GLU:CD	A:217:LEU:HD22	0.504
2	A:333:GLU:OE1	A:335:LYS:HE3	0.502
2	A:255:VAL:HG21	A:337:ILE:CD1	0.493
2	A:255:VAL:HG21	A:337:ILE:HD12	0.483
2	A:209:GLU:OE1	A:217:LEU:HD22	0.472
2	A:248:LEU:C	A:250:PRO:HD3	0.451
2	A:280:SER:O	A:284:TYR:HB2	0.445
2	A:117:ARG:HH21	A:161:GLU:CD	0.441

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:310:THR:C	A:312:ASP:H	0.432
2	A:245:LEU:HD22	A:337:ILE:HG21	0.431
2	A:44:PHE:CD2	A:82:MET:HE1	0.420
2	A:245:LEU:HD21	A:337:ILE:HD13	0.413
2	A:231:LYS:HB3	A:233:GLU:OE2	0.407
2	A:209:GLU:HB2	A:217:LEU:HB3	0.405
2	A:43:GLY:CA	A:176:THR:HG21	0.404
3	A:286:ILE:HG13	A:295:ILE:HD12	0.488
3	A:28:TRP:CE3	A:188:SER:HB3	0.477
3	A:227:LYS:C	A:229:THR:H	0.423
3	A:31:GLY:HA2	A:61:PHE:CZ	0.409
4	A:241:LEU:HD22	A:340:VAL:HG21	0.699
4	A:258:LEU:CD2	A:300:MET:HE2	0.642
4	A:248:LEU:HD11	A:339:ASP:HB2	0.596
4	A:286:ILE:HG12	A:295:ILE:HD12	0.574
4	A:111:ASP:CG	A:143:VAL:HG13	0.573
4	A:33:LYS:C	A:35:GLY:H	0.562
4	A:287:SER:C	A:346:ALA:HB3	0.554
4	A:282:VAL:HG13	A:295:ILE:HG21	0.547
4	A:290:ILE:HG21	A:295:ILE:HD11	0.541
4	A:258:LEU:HD22	A:300:MET:HE2	0.524
4	A:230:LEU:HD12	A:284:TYR:CG	0.520
4	A:286:ILE:CG1	A:295:ILE:HD12	0.520

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:202:PRO:HA	A:338:LYS:HE3	0.498
4	A:309:ASN:O	A:310:THR:HG23	0.497
4	A:230:LEU:CD1	A:284:TYR:CG	0.483
4	A:263:ARG:N	A:324:LEU:HD11	0.479
4	A:112:LEU:HD12	A:187:VAL:HG13	0.471
4	A:104:LEU:HD13	A:108:ILE:CD1	0.464
4	A:129:SER:C	A:131:VAL:H	0.454
4	A:230:LEU:HD12	A:284:TYR:CD2	0.453
4	A:67:ASN:HD22	A:190:ARG:HA	0.441
4	A:286:ILE:C	A:288:LYS:H	0.428
4	A:115:TYR:CZ	A:186:GLY:HA3	0.427
4	A:263:ARG:HB2	A:324:LEU:HD12	0.423
4	A:104:LEU:HD13	A:108:ILE:HD12	0.422
4	A:47:ASN:O	A:48:ASN:CG	0.418
4	A:132:TYR:CE1	A:167:ASN:OD1	0.418
4	A:57:GLY:C	A:59:GLY:H	0.417
4	A:248:LEU:HD13	A:339:ASP:O	0.416
4	A:104:LEU:C	A:106:TYR:H	0.414
4	A:33:LYS:C	A:35:GLY:N	0.411
4	A:64:TYR:CE1	A:190:ARG:NH2	0.411
4	A:64:TYR:CD1	A:190:ARG:NH2	0.410
4	A:320:LEU:HB3	A:323:CYS:SG	0.406
5	A:101:THR:HG22	A:119:GLY:HA3	0.657

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:333:GLU:O	A:334:VAL:HG23	0.635
5	A:211:GLN:O	A:212:THR:HG23	0.634
5	A:302:GLU:CD	A:320:LEU:HD11	0.634
5	A:24:LYS:H	A:193:GLN:NE2	0.584
5	A:144:PHE:HB2	A:164:TRP:CD1	0.563
5	A:39:TYR:CE1	A:53:GLU:HB2	0.557
5	A:122:VAL:HG23	A:143:VAL:CG2	0.514
5	A:153:THR:HB	A:154:PRO:HD2	0.503
5	A:152:ILE:HD11	A:158:THR:HG23	0.475
5	A:108:ILE:HD11	A:114:ILE:CD1	0.469
5	A:20:GLN:CD	A:154:PRO:HB3	0.459
5	A:33:LYS:HE3	A:77:ASP:OD1	0.455
5	A:207:ALA:HB3	A:260:TYR:CD2	0.424
5	A:282:VAL:HG22	A:295:ILE:HG22	0.419
5	A:108:ILE:HD11	A:114:ILE:HD12	0.417
6	A:43:GLY:CA	A:176:THR:HG21	0.605
6	A:19:ALA:HA	A:191:PHE:CZ	0.545
6	A:43:GLY:HA2	A:176:THR:HG21	0.536
6	A:206:PRO:HB2	A:345:GLN:CD	0.488
6	A:235:GLN:HG2	A:284:TYR:CZ	0.465
6	A:175:GLY:O	A:176:THR:HG23	0.455
6	A:117:ARG:HD3	A:159:ARG:HH22	0.452
6	A:165:THR:CG2	A:168:ILE:HD11	0.446

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:117:ARG:HH21	A:161:GLU:CD	0.441
6	A:324:LEU:HA	A:328:ARG:CD	0.441
6	A:171:ALA:HB2	A:177:ARG:HH21	0.428
6	A:206:PRO:C	A:345:GLN:NE2	0.425
6	A:250:PRO:HA	A:337:ILE:HD13	0.425
6	A:37:SER:HB3	A:180:ASN:HD21	0.417
6	A:41:ASP:HB2	A:50:PRO:HD2	0.415
6	A:115:TYR:CE2	A:159:ARG:NH2	0.411
6	A:23:PRO:HD2	A:28:TRP:CE2	0.403
7	A:278:ALA:HB1	A:297:ALA:HB1	0.608
7	A:230:LEU:HD11	A:284:TYR:CZ	0.587
7	A:19:ALA:HA	A:191:PHE:CZ	0.560
7	A:121:MET:HE2	A:123:TRP:HB3	0.533
7	A:282:VAL:HG13	A:295:ILE:HG21	0.511
7	A:19:ALA:HA	A:191:PHE:CE1	0.500
7	A:15:PHE:CE2	A:30:THR:HG23	0.496
7	A:40:HIS:CE1	A:52:HIS:CE1	0.483
7	A:230:LEU:CD2	A:284:TYR:CE2	0.483
7	A:121:MET:SD	A:165:THR:HG21	0.461
7	A:282:VAL:HG22	A:295:ILE:HG21	0.459
7	A:223:PHE:CZ	A:277:ARG:HG2	0.454
7	A:91:GLY:HA2	A:128:LYS:O	0.445
7	A:334:VAL:HG11	A:337:ILE:HD12	0.436

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:211:GLN:HB3	A:212:THR:HG23	0.432
7	A:282:VAL:HG22	A:295:ILE:CG2	0.429
7	A:164:TRP:HE1	A:179:ASP:CG	0.419
7	A:89:GLU:C	A:91:GLY:H	0.414
7	A:230:LEU:HD22	A:284:TYR:CE2	0.413
7	A:230:LEU:CD1	A:284:TYR:CZ	0.412
7	A:214:HIS:CD2	A:214:HIS:H	0.403
8	A:238:LEU:HB3	A:285:LEU:HD21	0.768
8	A:258:LEU:CD2	A:330:VAL:H	0.765
8	A:261:THR:HG22	A:273:LEU:CD2	0.763
8	A:238:LEU:CB	A:285:LEU:HD21	0.678
8	A:209:GLU:HB3	A:217:LEU:HD13	0.641
8	A:261:THR:HG22	A:273:LEU:HD23	0.639
8	A:258:LEU:HD22	A:329:ARG:HA	0.633
8	A:210:VAL:O	A:217:LEU:HD12	0.612
8	A:215:PHE:CE2	A:217:LEU:HD11	0.580
8	A:258:LEU:HD22	A:330:VAL:H	0.568
8	A:39:TYR:CD2	A:82:MET:HE1	0.565
8	A:199:VAL:C	A:201:ALA:H	0.550
8	A:197:ALA:O	A:198:PRO:C	0.545
8	A:278:ALA:HB1	A:297:ALA:HB1	0.539
8	A:215:PHE:HE2	A:217:LEU:HD11	0.534
8	A:39:TYR:CD2	A:82:MET:SD	0.513

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:256:VAL:HA	A:331:GLU:HA	0.513
8	A:39:TYR:CD2	A:82:MET:CE	0.512
8	A:199:VAL:C	A:201:ALA:N	0.509
8	A:261:THR:HG22	A:273:LEU:HD22	0.499
8	A:167:ASN:HA	A:177:ARG:HB3	0.487
8	A:230:LEU:HG	A:284:TYR:CE2	0.485
8	A:162:TYR:CE1	A:164:TRP:CE2	0.484
8	A:256:VAL:HG22	A:331:GLU:CG	0.479
8	A:278:ALA:CB	A:297:ALA:HB1	0.477
8	A:117:ARG:HH21	A:161:GLU:CD	0.461
8	A:258:LEU:CD2	A:329:ARG:HA	0.460
8	A:211:GLN:HG2	A:217:LEU:H	0.452
8	A:256:VAL:HG22	A:331:GLU:HG3	0.452
8	A:39:TYR:HD2	A:82:MET:HE1	0.449
8	A:165:THR:CG2	A:168:ILE:HD11	0.446
8	A:286:ILE:HD13	A:295:ILE:HD13	0.442
8	A:40:HIS:CD2	A:52:HIS:CE1	0.437
8	A:39:TYR:CE2	A:180:ASN:ND2	0.429
8	A:343:GLN:HB3	A:344:PRO:HD2	0.428
8	A:258:LEU:HD22	A:330:VAL:N	0.425
8	A:282:VAL:HG13	A:286:ILE:HD12	0.421
8	A:165:THR:HB	A:168:ILE:HD11	0.419
8	A:196:ALA:O	A:197:ALA:C	0.413

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:202:PRO:O	A:203:ALA:C	0.413
8	A:167:ASN:HA	A:177:ARG:CB	0.405
8	A:302:GLU:OE1	A:320:LEU:HD21	0.405
8	A:162:TYR:CD1	A:164:TRP:CZ2	0.402
8	A:171:ALA:C	A:173:THR:H	0.401
8	A:201:ALA:O	A:202:PRO:C	0.401
8	A:203:ALA:O	A:204:PRO:C	0.400
9	A:230:LEU:HD22	A:284:TYR:CE1	0.901
9	A:217:LEU:HA	A:345:GLN:HA	0.819
9	A:258:LEU:HD22	A:329:ARG:HA	0.674
9	A:123:TRP:CZ2	A:169:GLY:HA2	0.673
9	A:165:THR:HB	A:168:ILE:HD11	0.644
9	A:39:TYR:CE1	A:82:MET:HE2	0.628
9	A:200:VAL:HG13	A:269:TYR:CE2	0.604
9	A:123:TRP:CZ2	A:169:GLY:CA	0.590
9	A:230:LEU:HD22	A:284:TYR:CD1	0.569
9	A:123:TRP:HZ3	A:125:ALA:HB2	0.564
9	A:230:LEU:HB3	A:284:TYR:CE2	0.553
9	A:124:ARG:HH21	A:136:HIS:CE1	0.552
9	A:217:LEU:HD23	A:345:GLN:HA	0.552
9	A:218:LYS:C	A:346:ALA:HA	0.546
9	A:306:VAL:O	A:307:THR:HG23	0.545
9	A:123:TRP:CH2	A:169:GLY:HA3	0.537

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:282:VAL:HG22	A:295:ILE:CG2	0.535
9	A:155:GLU:CG	A:194:GLY:HA3	0.529
9	A:217:LEU:HA	A:345:GLN:CA	0.525
9	A:216:THR:HB	A:345:GLN:CD	0.511
9	A:213:LYS:O	A:214:HIS:CD2	0.507
9	A:217:LEU:HD23	A:345:GLN:H	0.498
9	A:217:LEU:HD23	A:345:GLN:N	0.497
9	A:168:ILE:HD12	A:180:ASN:HB2	0.492
9	A:274:SER:HB3	A:299:GLY:CA	0.489
9	A:274:SER:CB	A:299:GLY:HA3	0.487
9	A:123:TRP:CZ3	A:125:ALA:HB2	0.468
9	A:255:VAL:HG23	A:337:ILE:HB	0.467
9	A:245:LEU:HD23	A:248:LEU:HD12	0.461
9	A:202:PRO:O	A:203:ALA:C	0.461
9	A:155:GLU:OE1	A:194:GLY:HA3	0.460
9	A:230:LEU:HB3	A:284:TYR:CZ	0.449
9	A:200:VAL:HG13	A:269:TYR:CD2	0.448
9	A:217:LEU:HD23	A:345:GLN:CA	0.447
9	A:117:ARG:HH21	A:161:GLU:CD	0.443
9	A:168:ILE:HD12	A:180:ASN:CB	0.439
9	A:282:VAL:HG22	A:295:ILE:HG21	0.439
9	A:256:VAL:HG13	A:331:GLU:HA	0.436
9	A:230:LEU:CB	A:284:TYR:CE2	0.429

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:255:VAL:HG23	A:337:ILE:O	0.414
9	A:282:VAL:HG22	A:295:ILE:HG22	0.414
9	A:324:LEU:HA	A:328:ARG:NE	0.413
9	A:324:LEU:HD23	A:328:ARG:NH1	0.412
9	A:230:LEU:HD22	A:284:TYR:CZ	0.411
9	A:274:SER:HB3	A:299:GLY:HA3	0.409
9	A:323:CYS:HB3	A:328:ARG:NH2	0.409
9	A:204:PRO:O	A:205:ALA:C	0.405
9	A:218:LYS:H	A:345:GLN:C	0.402
10	A:230:LEU:HD22	A:284:TYR:CE1	0.887
10	A:230:LEU:HD13	A:284:TYR:CD2	0.860
10	A:286:ILE:HD13	A:295:ILE:HD13	0.820
10	A:258:LEU:CD2	A:330:VAL:H	0.666
10	A:94:LYS:HE3	A:126:ASP:HB2	0.643
10	A:230:LEU:HD13	A:284:TYR:CG	0.643
10	A:42:THR:HG21	A:82:MET:HE1	0.593
10	A:230:LEU:HD22	A:284:TYR:CD1	0.579
10	A:230:LEU:HD13	A:284:TYR:CE2	0.573
10	A:341:VAL:O	A:342:THR:HG23	0.561
10	A:230:LEU:HB2	A:284:TYR:CZ	0.532
10	A:19:ALA:HA	A:28:TRP:CD1	0.521
10	A:278:ALA:HB1	A:297:ALA:HB1	0.506
10	A:230:LEU:CB	A:284:TYR:CZ	0.503

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:238:LEU:HD13	A:285:LEU:CD2	0.497
10	A:337:ILE:O	A:337:ILE:HG22	0.486
10	A:51:THR:C	A:53:GLU:H	0.467
10	A:282:VAL:HG21	A:297:ALA:HB2	0.460
10	A:238:LEU:CD1	A:285:LEU:CD2	0.449
10	A:238:LEU:HD13	A:285:LEU:HD23	0.447
10	A:258:LEU:HD22	A:329:ARG:HA	0.443
10	A:45:ILE:CD1	A:175:GLY:HA3	0.437
10	A:255:VAL:HG21	A:337:ILE:O	0.430
10	A:286:ILE:HD13	A:295:ILE:CD1	0.430
10	A:258:LEU:HD23	A:330:VAL:H	0.416
10	A:255:VAL:HG21	A:337:ILE:HB	0.411
10	A:317:ARG:O	A:321:ILE:HD12	0.410
10	A:241:LEU:HD21	A:337:ILE:HG23	0.406
10	A:117:ARG:HH21	A:161:GLU:CD	0.402
10	A:197:ALA:O	A:198:PRO:C	0.402

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	344	288	36	20
2	344	303	28	13
3	344	298	26	20
4	344	243	79	22

Model ID	Analyzed	Favored	Allowed	Outliers
5	344	236	61	47
6	344	281	39	24
7	344	296	30	18
8	344	304	26	14
9	344	296	28	20
10	344	286	43	15

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	271	248	15	8
2	271	255	10	6
3	271	249	9	13
4	271	244	19	8
5	271	255	9	7
6	271	252	9	10
7	271	260	6	5
8	271	258	8	5
9	271	259	4	8
10	271	256	11	4

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	4	THR
1	A	173	THR

Model ID	Chain	Residue ID	Residue type
1	A	238	LEU
1	A	248	LEU
1	A	310	THR
1	A	320	LEU
1	A	323	CYS
1	A	340	VAL
2	A	4	THR
2	A	18	VAL
2	A	222	LEU
2	A	241	LEU
2	A	314	VAL
2	A	327	ASP
3	A	4	THR
3	A	51	THR
3	A	77	ASP
3	A	84	TYR
3	A	113	ASP
3	A	116	THR
3	A	138	THR
3	A	158	THR
3	A	173	THR
3	A	185	LEU
3	A	241	LEU

Model ID	Chain	Residue ID	Residue type
3	A	261	THR
3	A	295	ILE
4	A	4	THR
4	A	164	TRP
4	A	173	THR
4	A	185	LEU
4	A	248	LEU
4	A	262	ASP
4	A	273	LEU
4	A	339	ASP
5	A	131	VAL
5	A	164	TRP
5	A	222	LEU
5	A	225	PHE
5	A	241	LEU
5	A	306	VAL
5	A	307	THR
6	A	4	THR
6	A	17	THR
6	A	206	PRO
6	A	212	THR
6	A	219	SER
6	A	230	LEU

Model ID	Chain	Residue ID	Residue type
6	A	241	LEU
6	A	263	ARG
6	A	307	THR
6	A	311	CYS
7	A	88	VAL
7	A	217	LEU
7	A	222	LEU
7	A	267	ASP
7	A	341	VAL
8	A	219	SER
8	A	225	PHE
8	A	230	LEU
8	A	241	LEU
8	A	343	GLN
9	A	4	THR
9	A	51	THR
9	A	127	THR
9	A	172	HIS
9	A	230	LEU
9	A	241	LEU
9	A	303	SER
9	A	314	VAL
10	A	225	PHE

Model ID	Chain	Residue ID	Residue type
10	A	226	ASN
10	A	269	TYR
10	A	274	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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