Integrative Structure Validation Report

July 22, 2024 - 05:14 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	9A36
PDB-Dev ID	PDBDEV_00000191
Structure Title	Model of E. coli CirA 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

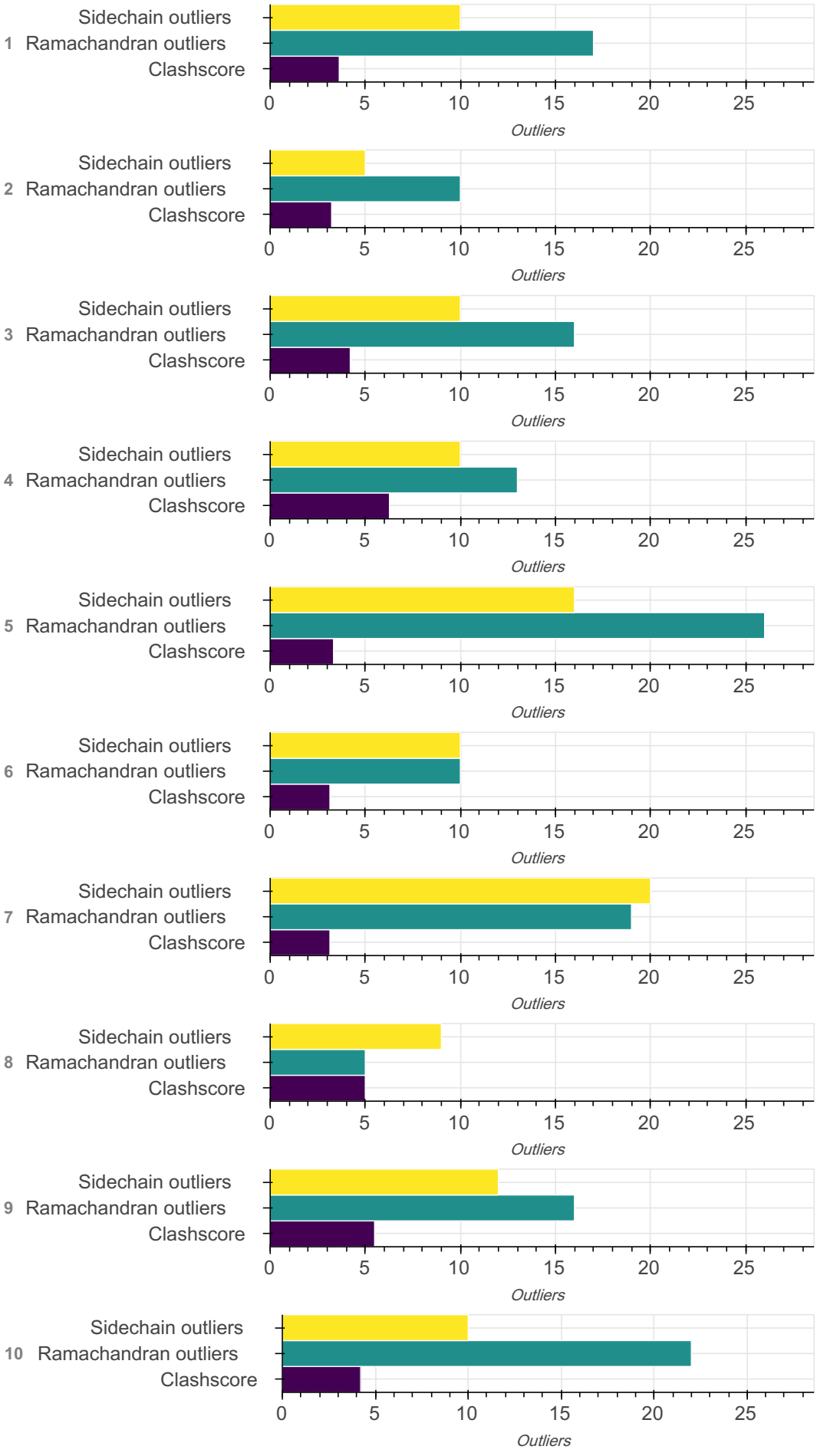
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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

Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 10 unique models, with 1 subunits in each model. A total of 1 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	P17315	A	A	663
2	1	1	P17315	A	A	663
3	1	1	P17315	A	A	663
4	1	1	P17315	A	A	663
5	1	1	P17315	A	A	663
6	1	1	P17315	A	A	663
7	1	1	P17315	A	A	663
8	1	1	P17315	A	A	663
9	1	1	P17315	A	A	663
10	1	1	P17315	A	A	663

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	-	1-663

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 49856 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG2--HG22	1.09	0.97	1260
CB--HB3	1.09	0.97	4780
OG--HG	0.96	0.84	560
CB--HB2	1.09	0.97	4780
CD2--HD21	1.09	0.97	480
CD2--HD22	1.09	0.97	480
CA--HA	1.09	0.97	6040
CG--HG	1.09	0.97	480
CB--HB	1.09	0.97	1260
CD1--HD12	1.09	0.97	730
CA--HA2	1.09	0.97	590
CG--HG3	1.09	0.97	1620
CE--HE3	1.09	0.97	410
CA--HA3	1.09	0.97	590
CG2--HG23	1.09	0.97	1260
NZ--HZ2	1.01	0.89	340
CD--HD2	1.09	0.97	990
CD1--HD13	1.09	0.97	730
CE--HE2	1.09	0.97	410
NZ--HZ1	1.01	0.89	340
CD--HD3	1.09	0.97	990
CG--HG2	1.09	0.97	1620

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--HG12	1.09	0.97	760
OG1--HG1	0.96	0.84	500
CG2--HG21	1.09	0.97	1260
CE--HE1	1.09	0.97	70
CD1--HD11	1.09	0.97	730
NZ--HZ3	1.01	0.89	340
CD2--HD23	1.09	0.97	480
CG1--HG13	1.09	0.97	760
CG1--HG11	1.09	0.97	510
CB--HB1	1.09	0.97	360
OH--HH	0.96	0.84	280
N--H3	1.01	0.89	10
N--H2	1.01	0.89	10
N--H1	1.01	0.89	10
SG--HG	1.33	1.20	6
SG--HG	1.34	1.20	20
CD1--HD1	1.08	0.93	680
CD2--HD2	1.08	0.93	600
N--H	1.01	0.86	6350
NH2--HH22	1.01	0.86	380
NH1--HH12	1.01	0.86	380
NH2--HH21	1.01	0.86	380
NE--HE	1.01	0.86	380

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CZ--HZ	1.08	0.93	230
CE2--HE2	1.08	0.93	510
NE2--HE22	1.01	0.86	190
CE1--HE1	1.08	0.93	600
ND2--HD22	1.01	0.86	410
CE3--HE3	1.08	0.93	170
ND1--HD1	1.01	0.86	76
CZ3--HZ3	1.08	0.93	170
NH1--HH11	1.01	0.86	380
NE2--HE21	1.01	0.86	190
ND2--HD21	1.01	0.86	410
CZ2--HZ2	1.08	0.93	170
CH2--HH2	1.08	0.93	170
NE1--HE1	1.01	0.86	170
NE2--HE2	1.01	0.86	14

Standard geometry: angle outliers

There are 394 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	146.08	1
N-CA-CB	110.40	130.06	1
C-CA-CB	110.50	92.31	1
CA-CB-CG	112.60	121.68	1
CA-CB-CG2	110.40	124.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	136.41	1
C-N-CA	121.70	136.28	1
C-N-CA	121.70	135.11	1
C-CA-CB	110.50	121.55	1
OD1-CG-ND2	122.60	115.38	1
CA-CB-CG	113.80	120.72	1
C-N-CA	121.70	134.01	1
C-N-CA	121.70	133.93	1
CG1-CB-CG2	110.80	125.20	1
CA-CB-CG	112.60	119.13	1
CA-CB-CG	112.60	118.99	1
OE1-CD-NE2	122.60	116.30	1
OE1-CD-NE2	122.60	116.31	1
N-CA-C	111.00	128.40	1
OE1-CD-NE2	122.60	116.41	1
OE1-CD-NE2	122.60	116.46	1
C-N-CA	121.70	132.75	1
OE1-CD-NE2	122.60	116.49	1
NE-CZ-NH2	119.20	124.69	1
C-N-CA	121.70	132.66	1
C-CA-CB	110.50	119.58	1
OE1-CD-NE2	122.60	116.60	1
C-N-CA	121.70	132.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.46	1
C-N-CA	121.70	132.42	1
C-N-CA	121.70	132.35	1
CB-CG-CD2	131.20	123.58	1
C-CA-CB	110.50	119.26	1
OE1-CD-NE2	122.60	116.76	1
CG-CD2-CE3	133.90	139.70	1
C-N-CA	121.70	132.13	1
C-N-CA	121.70	132.08	1
CA-CB-CG	112.60	118.34	1
OD1-CG-ND2	122.60	116.93	1
CA-CB-CG	113.80	119.47	1
CA-CB-CG	112.60	118.26	2
OE1-CD-NE2	122.60	116.99	1
OE1-CD-NE2	122.60	117.05	1
C-N-CA	121.70	131.68	1
NE-CZ-NH2	119.20	124.15	1
OE1-CD-NE2	122.60	117.10	1
OD1-CG-ND2	122.60	117.16	1
C-N-CA	121.70	131.50	1
N-CA-CB	111.50	120.74	1
CA-CB-CG	112.60	118.03	1
CA-CB-CG	113.80	119.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.46	1
OE1-CD-NE2	122.60	117.19	1
C-N-CA	121.70	131.44	1
C-N-CA	121.70	131.42	1
OE1-CD-NE2	122.60	117.22	1
CB-CG-CD2	131.20	124.23	1
CA-CB-CG	112.60	117.95	1
OE1-CD-NE2	122.60	117.26	1
C-N-CA	121.70	131.30	1
OE1-CD-NE2	122.60	117.27	1
OE1-CD-NE2	122.60	117.28	1
OD1-CG-ND2	122.60	117.31	1
C-N-CA	121.70	131.21	1
OE1-CD-NE2	122.60	117.32	1
CA-CB-CG	112.60	117.87	1
OE1-CD-NE2	122.60	117.33	1
O-C-N	123.00	114.57	1
OE1-CD-NE2	122.60	117.34	2
OE1-CD-NE2	122.60	117.35	1
OD1-CG-ND2	122.60	117.35	1
OD1-CG-ND2	122.60	117.36	2
CA-CB-CG1	110.40	101.50	1
CA-CB-CG	112.60	117.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.82	1
CA-CB-CG	112.60	117.81	1
C-N-CA	121.70	131.07	2
OE1-CD-NE2	122.60	117.39	1
OE1-CD-NE2	122.60	117.42	2
C-N-CA	121.70	131.01	1
OE1-CD-NE2	122.60	117.43	1
OD1-CG-ND2	122.60	117.44	1
OD1-CG-ND2	122.60	117.45	1
OE1-CD-NE2	122.60	117.45	3
OE1-CD-NE2	122.60	117.46	1
OE1-CD-NE2	122.60	117.47	1
C-N-CA	121.70	130.93	1
C-N-CA	121.70	130.88	1
C-N-CA	121.70	130.87	1
OE1-CD-NE2	122.60	117.52	1
CB-CG-CD2	131.20	124.61	1
NE-CZ-NH2	119.20	123.76	1
OE1-CD-NE2	122.60	117.54	1
OD1-CG-ND2	122.60	117.55	1
CB-CG-CD2	131.20	124.64	1
OE1-CD-NE2	122.60	117.56	1
C-N-CA	121.70	130.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	117.57	1
C-N-CA	121.70	130.74	1
CD-NE-CZ	124.40	131.38	1
C-N-CA	121.70	130.67	2
OD1-CG-ND2	122.60	117.63	1
OE1-CD-NE2	122.60	117.64	1
C-N-CA	121.70	130.62	1
OE1-CD-NE2	122.60	117.66	1
CD-NE-CZ	124.40	131.30	1
N-CA-CB	103.00	108.42	1
OD1-CG-ND2	122.60	117.68	1
CA-CB-CG	112.60	117.52	1
OE1-CD-NE2	122.60	117.68	1
C-CA-CB	110.10	119.44	1
C-CA-CB	111.40	120.74	1
OD1-CG-ND2	122.60	117.69	1
OE1-CD-NE2	122.60	117.69	1
C-N-CA	121.70	130.52	1
C-N-CA	121.70	130.51	1
OE1-CD-NE2	122.60	117.71	1
OD1-CG-ND2	122.60	117.72	1
C-N-CA	121.70	130.48	1
OE1-CD-NE2	122.60	117.73	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.74	1
OD1-CG-ND2	122.60	117.74	1
CA-C-N	116.20	125.91	1
OE1-CD-NE2	122.60	117.75	1
OE1-CD-NE2	122.60	117.76	2
OD1-CG-ND2	122.60	117.76	1
OD1-CG-ND2	122.60	117.77	1
C-N-CA	121.70	130.39	1
C-N-CA	121.70	130.38	1
OE1-CD-NE2	122.60	117.78	1
OD1-CG-ND2	122.60	117.79	1
CA-CB-CG	113.80	118.61	1
O-C-N	123.00	115.30	1
OD1-CG-ND2	122.60	117.80	1
C-N-CA	121.70	130.34	1
CA-CB-CG	112.60	117.39	1
OE1-CD-NE2	122.60	117.81	1
CB-CG-CD2	131.20	124.98	1
OE1-CD-NE2	122.60	117.82	1
OE1-CD-NE2	122.60	117.83	1
OE1-CD-NE2	122.60	117.84	1
CD2-CE2-CZ2	122.40	117.64	1
NE-CZ-NH1	121.50	126.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.27	1
CD-NE-CZ	124.40	131.06	1
CA-CB-CG2	110.50	118.58	1
NE-CZ-NH2	119.20	123.46	1
OE1-CD-NE2	122.60	117.87	3
CB-CG-CD2	131.20	125.06	1
C-CA-CB	111.40	120.37	1
OD1-CG-ND2	122.60	117.89	1
OE1-CD-NE2	122.60	117.90	2
OE1-CD-NE2	122.60	117.91	2
CA-CB-CG	112.60	117.27	1
OE1-CD-NE2	122.60	117.94	2
OD1-CG-ND2	122.60	117.95	1
OE1-CD-NE2	122.60	117.96	2
C-N-CA	121.70	130.06	1
OD1-CG-ND2	122.60	117.97	1
OE1-CD-NE2	122.60	117.97	1
C-N-CA	121.70	130.03	1
OE1-CD-NE2	122.60	117.98	1
CA-C-N	116.20	125.43	1
OD1-CG-ND2	122.60	117.99	1
OE1-CD-NE2	122.60	117.99	2
CB-CG-CD	112.60	120.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.00	1
C-N-CA	121.70	129.97	2
OE1-CD-NE2	122.60	118.01	2
CA-CB-CG	112.60	108.01	1
OD1-CG-ND2	122.60	118.02	2
OE1-CD-NE2	122.60	118.02	1
C-N-CA	121.70	129.93	1
C-CA-CB	110.10	118.77	1
CA-CB-CG	112.60	117.16	1
OE1-CD-NE2	122.60	118.04	1
C-N-CA	121.70	129.91	1
C-N-CA	121.70	129.89	1
OE1-CD-NE2	122.60	118.05	1
CA-C-N	116.20	125.29	1
OD1-CG-ND2	122.60	118.06	1
C-N-CA	121.70	129.86	1
OD1-CG-ND2	122.60	118.07	1
OE1-CD-NE2	122.60	118.07	1
CA-CB-CG	112.60	117.13	1
NE-CZ-NH2	119.20	115.13	1
CA-CB-CG	112.60	117.12	1
NE-CZ-NH2	119.20	123.26	1
O-C-N	123.00	115.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.09	1
OE1-CD-NE2	122.60	118.11	1
CB-CG-CD2	131.20	125.36	1
N-CA-CB	103.00	107.94	1
N-CA-CB	110.50	102.89	1
OE1-CD-NE2	122.60	118.13	1
CA-CB-CG	112.60	117.07	1
OD1-CG-ND2	122.60	118.14	1
NH1-CZ-NH2	119.30	113.51	1
OE1-CD-NE2	122.60	118.15	2
CA-CB-CG	112.60	117.05	1
OD1-CG-ND2	122.60	118.16	2
OE1-CD-NE2	122.60	118.16	1
CA-CB-CG	112.60	117.03	1
CD1-CG-CD2	110.80	120.54	1
OD1-CG-ND2	122.60	118.18	1
NH1-CZ-NH2	119.30	113.56	1
C-N-CA	121.70	129.64	1
C-N-CA	121.70	129.63	1
NE-CZ-NH2	119.20	123.16	2
OE1-CD-NE2	122.60	118.20	4
CA-CB-CG	112.60	117.00	1
CA-CB-CG	112.60	116.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	123.27	1
CB-CG-CD2	131.20	125.51	1
OE1-CD-NE2	122.60	118.22	2
OE1-CD-NE2	122.60	118.23	1
C-N-CA	121.70	129.57	1
CA-CB-CG	112.60	116.97	1
NE-CZ-NH1	121.50	125.87	1
C-N-CA	121.70	129.56	1
CB-CG-CD2	131.20	125.53	1
OE1-CD-NE2	122.60	118.24	1
C-N-CA	121.70	129.55	1
OD1-CG-ND2	122.60	118.24	1
OD1-CG-ND2	122.60	118.26	1
OE1-CD-NE2	122.60	118.28	4
CB-CG-CD2	131.20	125.59	1
N-CA-C	111.00	123.09	1
OE1-CD-NE2	122.60	118.29	1
OE1-CD-NE2	122.60	118.30	3
CB-CG-CD2	131.20	125.62	1
C-CA-CB	110.10	118.26	1
OE1-CD-NE2	122.60	118.31	1
CA-CB-CG	112.60	116.89	1
O-C-N	123.00	116.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.32	2
C-N-CA	121.70	129.40	1
CA-CB-CG	112.60	116.88	1
CA-CB-CG	112.60	116.87	2
C-N-CA	121.70	129.39	1
OE1-CD-NE2	122.60	118.33	3
OE1-CD-NE2	122.60	118.34	2
NE-CZ-NH1	121.50	125.76	1
C-N-CA	121.70	129.35	1
OE1-CD-NE2	122.60	118.35	1
OD1-CG-ND2	122.60	118.35	2
OE1-CD-NE2	122.60	118.36	1
CA-CB-CG	114.10	105.62	1
C-CA-CB	110.10	118.16	1
CB-CG-CD2	131.20	125.69	1
CD-NE-CZ	124.40	130.33	1
OD1-CG-ND2	122.60	118.37	1
OE1-CD-NE2	122.60	118.37	1
N-CA-CB	110.50	103.31	1
C-CA-CB	110.10	118.12	1
OE1-CD-NE2	122.60	118.38	1
CA-CB-CG2	110.40	117.57	1
CB-CG-CD2	131.20	125.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	118.39	1
C-N-CA	121.70	129.28	1
CA-C-N	116.20	124.62	1
OE1-CD-NE2	122.60	118.39	1
OE1-CD-NE2	122.60	118.40	1
C-N-CA	121.70	129.25	1
C-CA-CB	110.10	118.06	1
C-N-CA	121.70	129.24	1
NH1-CZ-NH2	119.30	113.87	2
OE1-CD-NE2	122.60	118.43	1
OD1-CG-ND2	122.60	118.43	1
CB-CG-CD2	131.20	125.79	1
CA-C-N	116.90	123.14	1
C-CA-CB	110.10	117.98	1
OD1-CG-ND2	122.60	118.46	2
C-N-CA	121.70	129.15	1
OE1-CD-NE2	122.60	118.46	1
CE2-CD2-CE3	118.80	114.66	1
OE1-CD-NE2	122.60	118.47	1
OE1-CD-NE2	122.60	118.48	1
OD1-CG-ND2	122.60	118.49	1
OE1-CD-NE2	122.60	118.49	2
C-N-CA	121.70	129.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	104.25	1
CB-CG-CD2	131.20	125.87	3
OD1-CG-ND2	122.60	118.50	1
C-N-CA	121.70	129.06	2
OE1-CD-NE2	122.60	118.51	1
C-N-CA	121.70	129.05	4
OE1-CD-NE2	122.60	118.52	3
CA-CB-CG	112.60	116.68	1
C-N-CA	121.70	129.04	1
CA-CB-CG	113.80	109.73	1
CD-NE-CZ	124.40	130.10	1
C-N-CA	121.70	129.03	1
CA-CB-CG2	110.50	117.42	1
NE-CZ-NH2	119.20	122.86	1
N-CA-CB	103.00	107.48	1
CA-CB-CG	112.60	116.67	1
OD1-CG-ND2	122.60	118.54	1
CA-CB-CG	112.60	108.54	1
OE1-CD-NE2	122.60	118.54	2
C-N-CA	121.70	129.01	1
CB-CG-CD2	131.20	125.93	1
CA-C-N	116.20	124.30	1
C-N-CA	121.70	128.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	122.32	1
OE1-CD-NE2	122.60	118.56	2
C-N-CA	121.70	128.97	1
N-CA-C	111.00	122.30	1
OD1-CG-ND2	122.60	118.57	1
C-N-CA	121.70	128.95	2
CD-NE-CZ	124.40	130.03	1
C-N-CA	121.70	128.93	1
CA-CB-CG	112.60	116.62	1
OD1-CG-ND2	122.60	118.58	1
CB-CG-CD2	131.20	125.98	1
CA-CB-CG	112.60	116.61	1
CA-CB-CG	113.80	117.81	1
C-N-H	112.22	124.30	1
C-CA-HA	96.87	109.00	1
C-N-H	112.06	124.30	1
C-N-H	111.95	124.30	1
C-CA-HA	96.54	109.00	1
C-N-H	111.53	124.30	1
C-N-H	111.34	124.30	1
C-N-H	111.33	124.30	1
C-N-H	111.14	124.30	1
CD-NE2-HE21	106.69	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	110.67	124.30	1
C-CA-HA	95.14	109.00	1
HH11-NH1-HH12	105.80	120.00	1
HH21-NH2-HH22	105.41	120.00	1
C-N-H	109.69	124.30	1
HD21-ND2-HD22	105.36	120.00	1
CB-CA-HA	94.33	109.00	1
C-N-H	108.91	124.30	1
HB2-CB-HB3	94.22	110.00	1
C-N-H	108.44	124.30	1
N-CA-HA	93.01	110.00	1
CB-CA-HA	91.48	109.00	1
C-N-H	106.20	124.30	1
C-CA-HA	89.31	109.00	1
CG1-CB-HB	87.99	108.00	1
HH21-NH2-HH22	95.60	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	3.63	37
2	3.23	33
3	4.21	43

Model ID	Clash score	Number of clashes
4	6.27	64
5	3.33	34
6	3.14	32
7	3.14	32
8	5.00	51
9	5.49	56
10	4.21	43

All 425 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:160:ILE:HG21	A:198:VAL:HG11	0.760
1	A:63:PRO:CB	A:656:PHE:CE1	0.589
1	A:93:GLY:HA3	A:552:ASN:HD21	0.568
1	A:54:ILE:HD11	A:74:VAL:CG2	0.548
1	A:63:PRO:HB2	A:656:PHE:CE1	0.543
1	A:494:VAL:CG1	A:504:VAL:HG11	0.531
1	A:63:PRO:CB	A:656:PHE:CZ	0.527
1	A:173:THR:HG23	A:183:THR:HG23	0.519
1	A:63:PRO:HB3	A:656:PHE:CZ	0.509
1	A:93:GLY:CA	A:552:ASN:HD21	0.494
1	A:37:ALA:CB	A:143:LEU:HB3	0.489
1	A:63:PRO:HB3	A:656:PHE:CE1	0.488
1	A:277:TYR:CE2	A:296:GLY:HA3	0.485
1	A:37:ALA:HB2	A:144:TYR:CE2	0.481

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:629:LEU:CD2	A:659:VAL:HG22	0.474
1	A:349:LEU:HB2	A:355:SER:CB	0.472
1	A:349:LEU:HB2	A:355:SER:HB3	0.472
1	A:293:LYS:HB3	A:295:TYR:CE2	0.467
1	A:54:ILE:HD11	A:74:VAL:HG22	0.459
1	A:115:PHE:CE1	A:431:THR:HG22	0.455
1	A:393:HIS:CD2	A:418:PHE:CE2	0.451
1	A:349:LEU:HD12	A:355:SER:HB2	0.449
1	A:111:ARG:HD2	A:339:ARG:HH22	0.445
1	A:28:ASP:C	A:30:GLY:H	0.444
1	A:143:LEU:HD21	A:397:ARG:NH2	0.437
1	A:390:TYR:CE2	A:421:PRO:HD2	0.435
1	A:64:VAL:HG21	A:70:VAL:HG22	0.433
1	A:526:ALA:HB1	A:565:LEU:HD11	0.433
1	A:338:TRP:CD1	A:362:TYR:CE1	0.432
1	A:491:THR:O	A:516:PRO:HB3	0.424
1	A:350:THR:C	A:352:GLY:H	0.423
1	A:349:LEU:O	A:350:THR:HG23	0.414
1	A:31:GLU:CD	A:43:ASN:HD22	0.413
1	A:494:VAL:HG12	A:504:VAL:HG11	0.413
1	A:308:SER:HB3	A:345:ASP:OD2	0.410
1	A:108:VAL:HG11	A:120:PHE:CD2	0.407
1	A:467:TRP:CZ3	A:468:LEU:HD21	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:54:ILE:HD13	A:70:VAL:HG12	0.667
2	A:430:TRP:CH2	A:432:SER:HB3	0.662
2	A:54:ILE:HD11	A:74:VAL:CG2	0.634
2	A:68:LYS:HB3	A:122:LEU:HD13	0.626
2	A:63:PRO:HG2	A:590:TYR:CE1	0.582
2	A:430:TRP:CZ3	A:432:SER:HB3	0.571
2	A:603:SER:HB3	A:606:ALA:HB3	0.525
2	A:63:PRO:CG	A:590:TYR:CE1	0.516
2	A:491:THR:HG21	A:503:PHE:HB2	0.513
2	A:97:SER:HA	A:118:ASN:ND2	0.496
2	A:603:SER:CB	A:606:ALA:HB3	0.494
2	A:97:SER:HA	A:118:ASN:CG	0.484
2	A:227:PRO:HB2	A:436:ARG:HH11	0.484
2	A:235:ARG:HH22	A:259:ARG:CZ	0.484
2	A:596:THR:CG2	A:612:TYR:CZ	0.478
2	A:180:ARG:NH2	A:229:ILE:HD11	0.464
2	A:643:ARG:HA	A:649:ASN:ND2	0.459
2	A:390:TYR:CE2	A:421:PRO:HD2	0.458
2	A:489:SER:HB2	A:521:TYR:CE1	0.452
2	A:7:PHE:O	A:8:VAL:HG23	0.449
2	A:85:ASN:ND2	A:232:PHE:CZ	0.446
2	A:485:ARG:NH1	A:565:LEU:HD13	0.444
2	A:180:ARG:CZ	A:229:ILE:HD11	0.436

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:367:GLU:CD	A:397:ARG:HH21	0.435
2	A:453:GLU:CD	A:455:TRP:CZ2	0.426
2	A:649:ASN:H	A:649:ASN:ND2	0.423
2	A:35:VAL:HG11	A:51:ILE:HG21	0.422
2	A:430:TRP:CZ2	A:432:SER:HB3	0.416
2	A:235:ARG:HH22	A:259:ARG:NH1	0.413
2	A:34:VAL:HG22	A:41:GLU:CG	0.410
2	A:467:TRP:CZ3	A:468:LEU:HD21	0.409
2	A:308:SER:CB	A:346:ALA:HB3	0.405
2	A:554:GLY:HA3	A:568:LEU:HD13	0.400
3	A:160:ILE:HD12	A:242:ALA:HB3	0.742
3	A:115:PHE:CD1	A:430:TRP:CH2	0.663
3	A:37:ALA:HB3	A:143:LEU:HD23	0.655
3	A:54:ILE:HD13	A:70:VAL:HG12	0.654
3	A:64:VAL:HG21	A:70:VAL:HG22	0.654
3	A:63:PRO:HB2	A:656:PHE:CZ	0.643
3	A:143:LEU:HD22	A:397:ARG:HH22	0.620
3	A:54:ILE:HD11	A:74:VAL:CG2	0.615
3	A:424:LEU:HD13	A:430:TRP:HE3	0.610
3	A:33:MET:HE2	A:53:VAL:CG2	0.580
3	A:424:LEU:HD13	A:430:TRP:CE3	0.563
3	A:143:LEU:HD22	A:397:ARG:NH2	0.557
3	A:8:VAL:HG12	A:10:VAL:HG23	0.555

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:143:LEU:HD13	A:397:ARG:NH2	0.547
3	A:160:ILE:HD12	A:242:ALA:CB	0.547
3	A:570:PHE:CE1	A:572:THR:HG23	0.546
3	A:345:ASP:OD1	A:347:VAL:HG22	0.544
3	A:33:MET:HE2	A:53:VAL:HG23	0.517
3	A:33:MET:SD	A:51:ILE:HG21	0.513
3	A:489:SER:HB2	A:521:TYR:CE1	0.501
3	A:620:ALA:HB1	A:628:LYS:HE2	0.495
3	A:340:HIS:NE2	A:342:LYS:HE3	0.491
3	A:63:PRO:CB	A:656:PHE:CZ	0.473
3	A:160:ILE:HG12	A:232:PHE:CE2	0.473
3	A:48:PRO:O	A:140:MET:HG3	0.455
3	A:35:VAL:HG11	A:48:PRO:HD2	0.448
3	A:35:VAL:HG12	A:36:THR:HG23	0.445
3	A:143:LEU:HD11	A:365:PHE:CD2	0.445
3	A:144:TYR:CD2	A:152:VAL:HG21	0.438
3	A:56:GLN:HE21	A:60:GLN:NE2	0.434
3	A:308:SER:HB3	A:346:ALA:CB	0.431
3	A:390:TYR:CE2	A:421:PRO:HD2	0.428
3	A:63:PRO:HD3	A:590:TYR:CE1	0.424
3	A:111:ARG:CZ	A:272:LEU:HD12	0.424
3	A:64:VAL:HG21	A:70:VAL:CG2	0.417
3	A:164:TRP:HB3	A:193:PRO:HG3	0.417

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:63:PRO:CD	A:590:TYR:CE1	0.415
3	A:393:HIS:CD2	A:418:PHE:CE2	0.415
3	A:491:THR:HG21	A:503:PHE:HB2	0.415
3	A:36:THR:HG21	A:140:MET:HE3	0.412
3	A:35:VAL:HG13	A:51:ILE:HD11	0.411
3	A:54:ILE:HD11	A:74:VAL:HG22	0.407
3	A:238:ASN:OD1	A:256:GLY:HA3	0.403
4	A:105:GLY:HA2	A:150:GLY:HA3	0.683
4	A:70:VAL:HG11	A:133:ILE:CD1	0.657
4	A:144:TYR:CD2	A:152:VAL:HG21	0.655
4	A:84:ASP:CG	A:113:ALA:HB2	0.640
4	A:84:ASP:OD1	A:113:ALA:HB2	0.640
4	A:44:LEU:HD22	A:53:VAL:HG11	0.620
4	A:105:GLY:CA	A:150:GLY:HA3	0.596
4	A:646:TYR:HB3	A:648:TYR:CD2	0.574
4	A:94:LEU:HD22	A:124:TRP:CZ2	0.556
4	A:33:MET:HE3	A:35:VAL:HG21	0.542
4	A:105:GLY:HA2	A:150:GLY:CA	0.538
4	A:117:HIS:CG	A:428:PRO:HD2	0.530
4	A:143:LEU:HD13	A:397:ARG:NH2	0.521
4	A:105:GLY:CA	A:150:GLY:CA	0.512
4	A:128:ASP:OD2	A:167:THR:HG21	0.511
4	A:117:HIS:HA	A:119:ASP:H	0.509

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:108:VAL:HA	A:555:ARG:HH12	0.508
4	A:116:ARG:HH21	A:488:ILE:HD12	0.508
4	A:56:GLN:HE21	A:60:GLN:NE2	0.504
4	A:94:LEU:CD2	A:99:THR:HG23	0.503
4	A:102:LEU:CD2	A:152:VAL:HG22	0.498
4	A:71:LEU:CD1	A:122:LEU:HD13	0.492
4	A:107:ARG:CZ	A:550:THR:HG21	0.489
4	A:390:TYR:CE2	A:421:PRO:HD2	0.489
4	A:267:LEU:HD21	A:433:ASN:OD1	0.484
4	A:185:ASN:HD21	A:187:GLN:NE2	0.484
4	A:75:PRO:CB	A:548:ASN:HD21	0.477
4	A:117:HIS:CE1	A:428:PRO:O	0.475
4	A:107:ARG:NH2	A:550:THR:HG21	0.475
4	A:646:TYR:HB3	A:648:TYR:CE2	0.475
4	A:568:LEU:HD12	A:600:ARG:C	0.473
4	A:340:HIS:NE2	A:342:LYS:HE3	0.471
4	A:75:PRO:HB3	A:548:ASN:HD21	0.468
4	A:393:HIS:CD2	A:418:PHE:CE2	0.465
4	A:644:ASP:C	A:646:TYR:H	0.461
4	A:418:PHE:CE2	A:449:PRO:HB3	0.459
4	A:568:LEU:CD1	A:600:ARG:C	0.456
4	A:91:ILE:HG21	A:94:LEU:HD21	0.455
4	A:610:GLY:HA2	A:646:TYR:OH	0.447

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:33:MET:HE1	A:371:ARG:HD2	0.446
4	A:94:LEU:HD13	A:124:TRP:CZ2	0.446
4	A:143:LEU:HD13	A:397:ARG:HH22	0.446
4	A:146:SER:HA	A:418:PHE:O	0.446
4	A:94:LEU:HD23	A:99:THR:HG23	0.443
4	A:91:ILE:CG2	A:94:LEU:HD21	0.442
4	A:54:ILE:HD13	A:77:VAL:CG2	0.429
4	A:268:ASP:HB2	A:304:PRO:CB	0.422
4	A:117:HIS:CB	A:428:PRO:HD2	0.419
4	A:350:THR:HG23	A:442:VAL:HG21	0.419
4	A:434:SER:C	A:436:ARG:H	0.419
4	A:70:VAL:HG13	A:74:VAL:HG21	0.416
4	A:122:LEU:HD23	A:124:TRP:HE1	0.414
4	A:104:ASP:OD2	A:106:LYS:HE3	0.413
4	A:102:LEU:HD23	A:152:VAL:HG22	0.412
4	A:94:LEU:HD22	A:124:TRP:CH2	0.412
4	A:54:ILE:CD1	A:77:VAL:CG2	0.411
4	A:107:ARG:C	A:555:ARG:HH12	0.409
4	A:568:LEU:HD11	A:601:ALA:HA	0.409
4	A:107:ARG:O	A:555:ARG:NH2	0.407
4	A:33:MET:HE3	A:35:VAL:CG2	0.406
4	A:44:LEU:HD21	A:132:ARG:HD3	0.406
4	A:75:PRO:CB	A:548:ASN:ND2	0.404

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:98:TYR:CE2	A:154:ASN:CG	0.402
4	A:121:ASP:C	A:123:ASN:H	0.401
5	A:21:TRP:CD2	A:21:TRP:CE2	1.600
5	A:21:TRP:CD2	A:21:TRP:CG	1.548
5	A:21:TRP:CE2	A:21:TRP:NE1	1.543
5	A:21:TRP:CD1	A:21:TRP:NE1	1.474
5	A:21:TRP:CG	A:23:VAL:HB	1.384
5	A:21:TRP:CD2	A:23:VAL:CB	1.210
5	A:21:TRP:CD2	A:23:VAL:CG2	1.209
5	A:21:TRP:CE2	A:23:VAL:CG2	1.199
5	A:21:TRP:CG	A:23:VAL:CG2	1.191
5	A:21:TRP:CD1	A:23:VAL:CG2	1.189
5	A:21:TRP:CE2	A:23:VAL:CB	1.175
5	A:21:TRP:CD1	A:23:VAL:CB	1.172
5	A:21:TRP:CG	A:23:VAL:CB	1.169
5	A:21:TRP:CD2	A:23:VAL:HB	1.025
5	A:21:TRP:NE1	A:23:VAL:CG2	0.987
5	A:21:TRP:NE1	A:23:VAL:CB	0.976
5	A:21:TRP:CD2	A:23:VAL:HG21	0.873
5	A:21:TRP:CG	A:23:VAL:HG23	0.767
5	A:21:TRP:CE2	A:23:VAL:CG1	0.762
5	A:21:TRP:CD1	A:23:VAL:HG23	0.758
5	A:21:TRP:CD1	A:23:VAL:CA	0.746

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:21:TRP:CD1	A:23:VAL:HA	0.699
5	A:21:TRP:NE1	A:23:VAL:HG22	0.640
5	A:21:TRP:CD1	A:21:TRP:CE2	0.635
5	A:21:TRP:CD1	A:21:TRP:CD2	0.631
5	A:21:TRP:CD2	A:23:VAL:CG1	0.604
5	A:21:TRP:CE2	A:21:TRP:CG	0.552
5	A:21:TRP:NE1	A:23:VAL:HA	0.520
5	A:21:TRP:CD2	A:23:VAL:HG11	0.493
5	A:21:TRP:CE2	A:23:VAL:HG22	0.487
5	A:21:TRP:CE2	A:23:VAL:HG11	0.455
5	A:38:SER:C	A:320:LYS:HE3	0.425
5	A:202:LYS:HE2	A:204:TYR:CE1	0.421
5	A:23:VAL:HG13	A:24:LEU:N	0.405
6	A:78:GLN:HE22	A:572:THR:HG21	0.806
6	A:140:MET:HE1	A:399:TYR:CE1	0.740
6	A:78:GLN:NE2	A:572:THR:HG21	0.670
6	A:285:TRP:CZ3	A:292:LEU:HD21	0.610
6	A:521:TYR:CE1	A:523:VAL:HG22	0.592
6	A:49:ALA:HA	A:140:MET:HE2	0.579
6	A:140:MET:HE1	A:399:TYR:CZ	0.570
6	A:116:ARG:HA	A:424:LEU:HD13	0.567
6	A:349:LEU:HD22	A:428:PRO:O	0.548
6	A:116:ARG:HA	A:424:LEU:CD1	0.521

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:74:VAL:HG11	A:135:VAL:HG21	0.503
6	A:49:ALA:CB	A:140:MET:HE2	0.497
6	A:149:LEU:HD11	A:452:SER:HB2	0.497
6	A:149:LEU:HD11	A:452:SER:CB	0.490
6	A:56:GLN:OE1	A:158:LYS:HE2	0.483
6	A:63:PRO:HD3	A:590:TYR:CE1	0.477
6	A:494:VAL:HG11	A:519:SER:CB	0.463
6	A:59:LEU:CD2	A:70:VAL:HG13	0.450
6	A:49:ALA:CA	A:140:MET:HE2	0.448
6	A:285:TRP:CE3	A:292:LEU:HD21	0.442
6	A:289:THR:C	A:291:GLU:H	0.441
6	A:34:VAL:HG21	A:51:ILE:HD12	0.436
6	A:399:TYR:CD1	A:413:GLY:HA3	0.433
6	A:146:SER:HB2	A:420:ALA:H	0.432
6	A:59:LEU:HD21	A:70:VAL:HG13	0.418
6	A:387:HIS:CE1	A:390:TYR:OH	0.417
6	A:140:MET:CE	A:399:TYR:CZ	0.404
6	A:338:TRP:CD1	A:362:TYR:CE1	0.403
6	A:397:ARG:HE	A:399:TYR:HE2	0.403
6	A:117:HIS:C	A:119:ASP:H	0.402
6	A:54:ILE:HD11	A:74:VAL:HA	0.401
6	A:121:ASP:O	A:124:TRP:CD1	0.401
7	A:22:PRO:CG	A:37:ALA:HA	1.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:22:PRO:CB	A:22:PRO:CG	1.260
7	A:22:PRO:CD	A:22:PRO:N	1.257
7	A:22:PRO:CD	A:22:PRO:CG	1.250
7	A:22:PRO:CA	A:22:PRO:CB	1.249
7	A:22:PRO:CA	A:22:PRO:N	1.243
7	A:22:PRO:CD	A:37:ALA:HA	1.175
7	A:22:PRO:CD	A:37:ALA:CA	1.093
7	A:22:PRO:CA	A:37:ALA:CA	1.091
7	A:22:PRO:CB	A:37:ALA:CA	1.085
7	A:22:PRO:CG	A:37:ALA:CA	1.080
7	A:22:PRO:CB	A:37:ALA:N	0.998
7	A:22:PRO:CA	A:37:ALA:N	0.987
7	A:22:PRO:CD	A:37:ALA:N	0.982
7	A:22:PRO:CG	A:37:ALA:N	0.975
7	A:22:PRO:N	A:37:ALA:CA	0.935
7	A:22:PRO:N	A:37:ALA:N	0.848
7	A:22:PRO:HG3	A:37:ALA:HA	0.811
7	A:22:PRO:HB3	A:37:ALA:CB	0.788
7	A:22:PRO:CB	A:37:ALA:CB	0.784
7	A:22:PRO:N	A:37:ALA:H	0.732
7	A:22:PRO:HB3	A:37:ALA:HB2	0.656
7	A:22:PRO:N	A:37:ALA:C	0.652
7	A:22:PRO:CG	A:36:THR:C	0.558

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:367:GLU:CD	A:397:ARG:HH22	0.529
7	A:22:PRO:CA	A:37:ALA:H	0.506
7	A:68:LYS:HB3	A:68:LYS:HZ3	0.481
7	A:92:ARG:HH12	A:456:GLU:CD	0.469
7	A:184:TYR:CE2	A:209:LYS:HE3	0.460
7	A:22:PRO:CB	A:36:THR:C	0.455
7	A:22:PRO:C	A:37:ALA:N	0.438
7	A:340:HIS:CD2	A:342:LYS:HE3	0.416
8	A:195:ILE:HD12	A:244:THR:HG21	0.922
8	A:160:ILE:CG2	A:195:ILE:HD11	0.779
8	A:103:VAL:HG21	A:125:ILE:HD11	0.743
8	A:37:ALA:HB3	A:143:LEU:HD23	0.655
8	A:160:ILE:HG23	A:195:ILE:HD11	0.650
8	A:160:ILE:HG22	A:195:ILE:HD11	0.635
8	A:144:TYR:CD2	A:152:VAL:HG21	0.596
8	A:24:LEU:HD11	A:132:ARG:NH1	0.586
8	A:143:LEU:N	A:397:ARG:HH12	0.557
8	A:564:PRO:HB3	A:600:ARG:CD	0.553
8	A:140:MET:HE1	A:367:GLU:OE2	0.542
8	A:26:VAL:HG13	A:30:GLY:HA2	0.541
8	A:63:PRO:CD	A:616:ASN:HD21	0.536
8	A:74:VAL:HG11	A:135:VAL:HG21	0.526
8	A:343:LEU:HD23	A:346:ALA:HB2	0.523

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:37:ALA:HB2	A:144:TYR:CD2	0.513
8	A:338:TRP:CD1	A:362:TYR:CE1	0.506
8	A:86:ARG:HD2	A:114:VAL:HG23	0.494
8	A:103:VAL:HG23	A:108:VAL:HG11	0.489
8	A:113:ALA:CB	A:424:LEU:HD13	0.489
8	A:612:TYR:CD1	A:641:LEU:HD21	0.486
8	A:262:ARG:NH2	A:307:SER:H	0.486
8	A:564:PRO:CB	A:600:ARG:HD3	0.485
8	A:92:ARG:NH1	A:478:PHE:CE2	0.479
8	A:48:PRO:HG2	A:140:MET:HE2	0.473
8	A:243:TRP:CH2	A:245:PRO:HG3	0.473
8	A:489:SER:HB3	A:521:TYR:CE2	0.471
8	A:149:LEU:HD22	A:417:ALA:CB	0.470
8	A:103:VAL:HG23	A:108:VAL:CG1	0.462
8	A:414:TRP:CZ2	A:416:THR:HG23	0.450
8	A:86:ARG:CZ	A:114:VAL:HG22	0.448
8	A:564:PRO:CB	A:600:ARG:CD	0.448
8	A:26:VAL:HG12	A:27:ASP:O	0.445
8	A:46:ASP:CG	A:371:ARG:HH22	0.444
8	A:564:PRO:HB3	A:600:ARG:HD3	0.441
8	A:262:ARG:HH22	A:307:SER:H	0.435
8	A:108:VAL:HG21	A:120:PHE:CE2	0.434
8	A:63:PRO:HB3	A:656:PHE:CD1	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:142:SER:C	A:397:ARG:HH12	0.432
8	A:115:PHE:CE1	A:347:VAL:HB	0.431
8	A:469:GLU:O	A:538:PRO:HA	0.423
8	A:81:ASN:ND2	A:648:TYR:CD1	0.423
8	A:438:ALA:H	A:515:ILE:CG2	0.421
8	A:438:ALA:O	A:517:VAL:HA	0.419
8	A:81:ASN:ND2	A:648:TYR:CG	0.418
8	A:202:LYS:HE3	A:240:GLU:CD	0.414
8	A:94:LEU:CD1	A:150:GLY:HA2	0.410
8	A:421:PRO:HG2	A:443:GLY:HA2	0.409
8	A:78:GLN:HE22	A:552:ASN:HD21	0.405
8	A:1:MET:O	A:2:PHE:CD2	0.403
8	A:8:VAL:HG12	A:10:VAL:HG23	0.403
9	A:33:MET:HE1	A:55:THR:HG22	0.727
9	A:496:ALA:HA	A:500:TYR:CE2	0.674
9	A:64:VAL:HG23	A:127:VAL:HG11	0.668
9	A:115:PHE:CE2	A:272:LEU:HD22	0.666
9	A:418:PHE:CE2	A:449:PRO:CB	0.644
9	A:393:HIS:CG	A:418:PHE:CE2	0.631
9	A:243:TRP:CH2	A:251:PHE:CG	0.627
9	A:71:LEU:HD12	A:122:LEU:HD22	0.614
9	A:63:PRO:HG3	A:590:TYR:CE1	0.606
9	A:426:LEU:HD23	A:441:ILE:HG23	0.606

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:243:TRP:CE3	A:251:PHE:HA	0.600
9	A:393:HIS:CD2	A:418:PHE:CZ	0.596
9	A:243:TRP:CH2	A:251:PHE:CD1	0.590
9	A:61:ARG:HG2	A:580:LYS:HE3	0.574
9	A:89:VAL:CG2	A:122:LEU:HD21	0.564
9	A:444:SER:HB2	A:483:LYS:HE2	0.557
9	A:393:HIS:CD2	A:418:PHE:CE2	0.548
9	A:349:LEU:HD22	A:428:PRO:HB3	0.543
9	A:48:PRO:HA	A:399:TYR:CZ	0.541
9	A:579:TRP:CE2	A:589:PHE:HB2	0.541
9	A:243:TRP:CZ2	A:251:PHE:CD2	0.538
9	A:349:LEU:HA	A:439:CYS:SG	0.534
9	A:490:ARG:NH1	A:612:TYR:CE1	0.522
9	A:418:PHE:CE2	A:449:PRO:HB3	0.516
9	A:33:MET:HE1	A:55:THR:CG2	0.502
9	A:160:ILE:HD12	A:242:ALA:HB3	0.499
9	A:59:LEU:CD2	A:70:VAL:HG13	0.497
9	A:243:TRP:CZ3	A:251:PHE:HB2	0.484
9	A:228:ARG:HB2	A:265:ASP:HB3	0.473
9	A:349:LEU:HD13	A:428:PRO:HG3	0.468
9	A:349:LEU:HD22	A:428:PRO:CG	0.461
9	A:63:PRO:HG3	A:590:TYR:CZ	0.458
9	A:432:SER:C	A:434:SER:H	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:390:TYR:CE1	A:447:LEU:O	0.453
9	A:504:VAL:HG11	A:516:PRO:HB3	0.453
9	A:121:ASP:HB3	A:124:TRP:CE2	0.452
9	A:61:ARG:HG2	A:580:LYS:CE	0.450
9	A:141:SER:HB2	A:152:VAL:HG23	0.449
9	A:33:MET:SD	A:132:ARG:HD3	0.448
9	A:314:SER:HB2	A:424:LEU:HD11	0.446
9	A:243:TRP:CZ2	A:251:PHE:CE2	0.442
9	A:460:TYR:CE1	A:462:MET:HG2	0.430
9	A:59:LEU:HD22	A:70:VAL:HG13	0.428
9	A:484:ASP:CG	A:524:ASN:HA	0.425
9	A:38:SER:C	A:40:VAL:H	0.423
9	A:349:LEU:HD22	A:428:PRO:CB	0.423
9	A:390:TYR:CE2	A:421:PRO:HD2	0.423
9	A:67:LEU:HD21	A:155:ILE:HD13	0.421
9	A:568:LEU:HD12	A:599:LYS:HB2	0.416
9	A:49:ALA:HB3	A:456:GLU:OE1	0.415
9	A:54:ILE:HG21	A:74:VAL:HG22	0.414
9	A:120:PHE:HD1	A:122:LEU:HD23	0.414
9	A:71:LEU:CD1	A:122:LEU:HD22	0.411
9	A:426:LEU:CD2	A:441:ILE:HG23	0.408
9	A:149:LEU:HD13	A:419:LYS:CB	0.405
9	A:486:ILE:HD12	A:565:LEU:CD1	0.402

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:491:THR:HG23	A:504:VAL:HG21	0.890
10	A:93:GLY:CA	A:552:ASN:HD21	0.700
10	A:143:LEU:HD13	A:397:ARG:NH2	0.700
10	A:349:LEU:HD13	A:431:THR:H	0.695
10	A:614:ILE:HD12	A:646:TYR:CZ	0.632
10	A:26:VAL:HG13	A:30:GLY:C	0.590
10	A:614:ILE:HD11	A:641:LEU:CD1	0.587
10	A:25:ALA:HB1	A:33:MET:HB2	0.583
10	A:143:LEU:HD13	A:397:ARG:HH22	0.583
10	A:295:TYR:CZ	A:316:THR:HB	0.566
10	A:93:GLY:N	A:552:ASN:HD21	0.555
10	A:614:ILE:HD11	A:641:LEU:HD12	0.520
10	A:143:LEU:HD11	A:365:PHE:CD2	0.513
10	A:349:LEU:CD1	A:431:THR:H	0.507
10	A:185:ASN:HD21	A:187:GLN:NE2	0.504
10	A:24:LEU:C	A:26:VAL:H	0.499
10	A:80:THR:CG2	A:568:LEU:HD21	0.497
10	A:564:PRO:HB2	A:601:ALA:HB2	0.494
10	A:114:VAL:HG11	A:301:ASN:HD22	0.492
10	A:491:THR:HG23	A:504:VAL:CG2	0.488
10	A:37:ALA:HB3	A:143:LEU:HD23	0.486
10	A:59:LEU:CD2	A:70:VAL:HG13	0.485
10	A:111:ARG:NH2	A:124:TRP:HB3	0.484

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:521:TYR:CE2	A:523:VAL:HG22	0.484
10	A:390:TYR:CE2	A:421:PRO:HD2	0.476
10	A:37:ALA:HB2	A:144:TYR:CE2	0.470
10	A:430:TRP:CZ3	A:432:SER:CB	0.470
10	A:74:VAL:HG11	A:135:VAL:HG21	0.468
10	A:430:TRP:CZ3	A:432:SER:HB2	0.467
10	A:81:ASN:HD21	A:643:ARG:HG2	0.466
10	A:308:SER:HB3	A:346:ALA:HB3	0.463
10	A:26:VAL:HG13	A:30:GLY:CA	0.447
10	A:521:TYR:CD2	A:523:VAL:HG22	0.444
10	A:108:VAL:HG13	A:274:ARG:NH2	0.441
10	A:487:SER:HB3	A:523:VAL:HG21	0.441
10	A:92:ARG:O	A:528:ILE:HG21	0.425
10	A:59:LEU:HD22	A:70:VAL:HG13	0.424
10	A:144:TYR:CD2	A:152:VAL:HG21	0.422
10	A:54:ILE:HG22	A:133:ILE:HB	0.417
10	A:80:THR:HG22	A:568:LEU:HD21	0.408
10	A:48:PRO:O	A:140:MET:HG3	0.404
10	A:521:TYR:CE2	A:523:VAL:HG13	0.401
10	A:625:LYS:HE3	A:626:ASP:OD2	0.401

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	661	591	53	17
2	661	606	45	10
3	661	616	29	16
4	661	611	37	13
5	661	589	46	26
6	661	580	71	10
7	661	588	54	19
8	661	603	53	5
9	661	601	44	16
10	661	580	59	22

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	568	536	22	10
2	568	548	15	5
3	568	548	10	10
4	568	538	20	10
5	568	517	35	16
6	568	544	14	10
7	568	513	35	20
8	568	540	19	9
9	568	540	16	12

Model ID	Analyzed	Favored	Allowed	Outliers
10	568	546	12	10

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	12	LEU
1	A	14	LEU
1	A	24	LEU
1	A	164	TRP
1	A	195	ILE
1	A	219	THR
1	A	220	THR
1	A	589	PHE
1	A	605	THR
1	A	642	SER
2	A	12	LEU
2	A	117	HIS
2	A	118	ASN
2	A	226	THR
2	A	649	ASN
3	A	12	LEU
3	A	24	LEU
3	A	173	THR
3	A	183	THR
3	A	221	THR

Model ID	Chain	Residue ID	Residue type
3	A	226	THR
3	A	430	TRP
3	A	431	THR
3	A	608	THR
3	A	660	ASP
4	A	1	MET
4	A	12	LEU
4	A	14	LEU
4	A	77	VAL
4	A	95	ASP
4	A	121	ASP
4	A	491	THR
4	A	494	VAL
4	A	608	THR
4	A	644	ASP
5	A	21	TRP
5	A	23	VAL
5	A	24	LEU
5	A	68	LYS
5	A	80	THR
5	A	104	ASP
5	A	164	TRP
5	A	173	THR

Model ID	Chain	Residue ID	Residue type
5	A	217	ASN
5	A	345	ASP
5	A	481	ASP
5	A	517	VAL
5	A	524	ASN
5	A	540	ASN
5	A	576	THR
5	A	660	ASP
6	A	12	LEU
6	A	27	ASP
6	A	54	ILE
6	A	326	THR
6	A	424	LEU
6	A	429	ASP
6	A	434	SER
6	A	491	THR
6	A	523	VAL
6	A	608	THR
7	A	24	LEU
7	A	29	ASP
7	A	54	ILE
7	A	57	GLU
7	A	68	LYS

Model ID	Chain	Residue ID	Residue type
7	A	119	ASP
7	A	142	SER
7	A	212	LYS
7	A	226	THR
7	A	250	ASP
7	A	258	ASP
7	A	260	GLN
7	A	325	LEU
7	A	326	THR
7	A	389	THR
7	A	434	SER
7	A	439	CYS
7	A	446	ASP
7	A	495	ASN
7	A	567	ASP
8	A	12	LEU
8	A	14	LEU
8	A	103	VAL
8	A	226	THR
8	A	430	TRP
8	A	491	THR
8	A	494	VAL
8	A	608	THR

Model ID	Chain	Residue ID	Residue type
8	A	644	ASP
9	A	14	LEU
9	A	24	LEU
9	A	28	ASP
9	A	115	PHE
9	A	221	THR
9	A	226	THR
9	A	234	SER
9	A	243	TRP
9	A	251	PHE
9	A	347	VAL
9	A	491	THR
9	A	608	THR
10	A	12	LEU
10	A	38	SER
10	A	149	LEU
10	A	220	THR
10	A	226	THR
10	A	491	THR
10	A	494	VAL
10	A	523	VAL
10	A	608	THR
10	A	650	GLU

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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