Integrative Structure Validation Report

July 22, 2024 - 05:11 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	9A31
PDB-Dev ID	PDBDEV_00000186
Structure Title	Model of E. coli fhuA 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

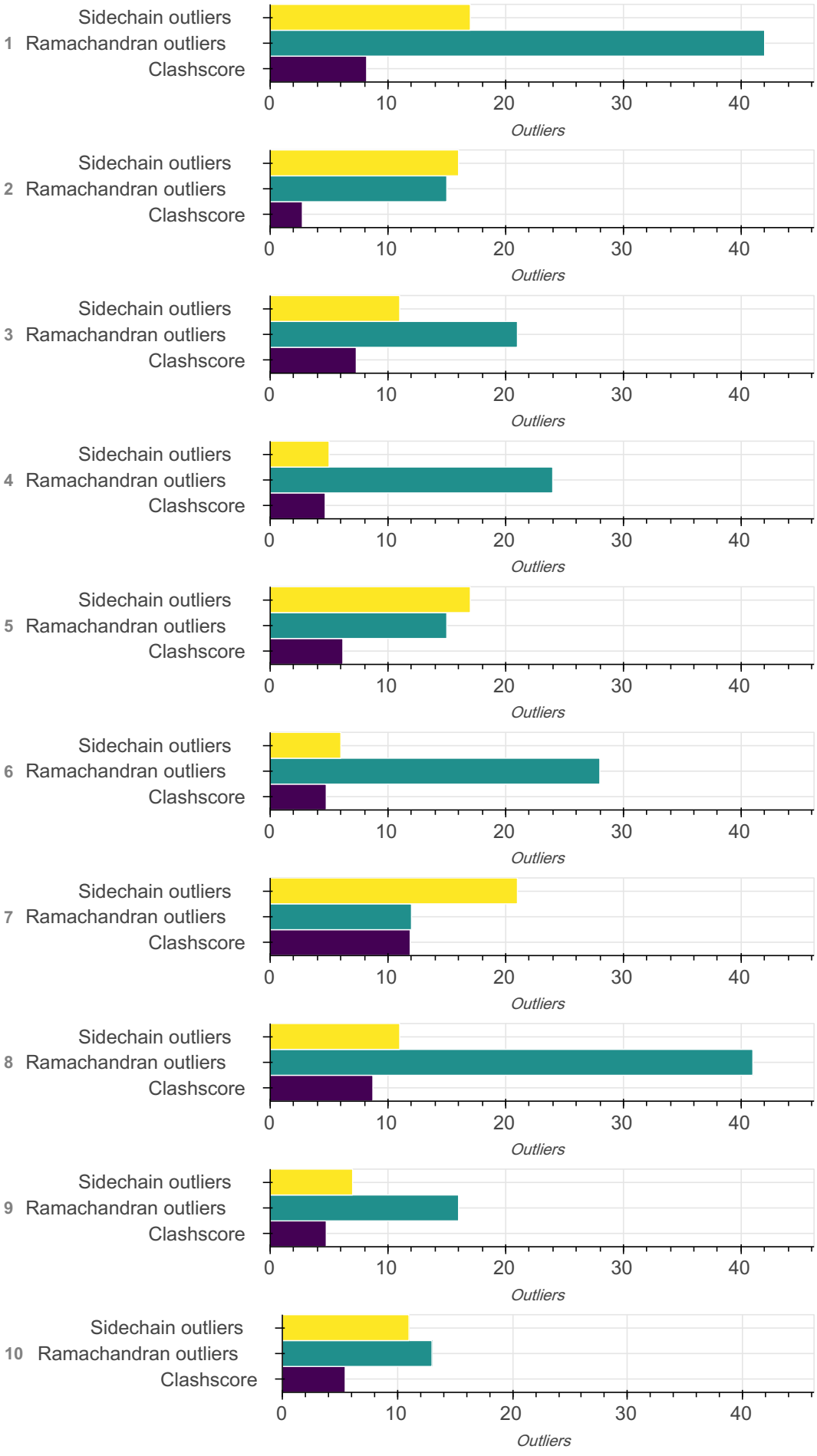
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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
10
20
30
40
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	P06971	A	A	747
2	1	1	P06971	A	A	747
3	1	1	P06971	A	A	747
4	1	1	P06971	A	A	747
5	1	1	P06971	A	A	747
6	1	1	P06971	A	A	747
7	1	1	P06971	A	A	747
8	1	1	P06971	A	A	747
9	1	1	P06971	A	A	747
10	1	1	P06971	A	A	747

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	-	1-747

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 55504 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
CA--HA	1.09	0.97	6850
OG--HG	0.96	0.84	540
CE--HE2	1.09	0.97	520
CD--HD2	1.09	0.97	1100
CB--HB2	1.09	0.97	5500
CD2--HD23	1.09	0.97	460
CG--HG3	1.09	0.97	1900
CG2--HG21	1.09	0.97	1350
CG2--HG22	1.09	0.97	1350
CB--HB3	1.09	0.97	5500
CB--HB1	1.09	0.97	690
CG1--HG11	1.09	0.97	600
CD1--HD13	1.09	0.97	630
CD1--HD11	1.09	0.97	630
CG--HG2	1.09	0.97	1900
CG1--HG12	1.09	0.97	770
CD--HD3	1.09	0.97	1100
CB--HB	1.09	0.97	1350
CD2--HD21	1.09	0.97	460
CG--HG	1.09	0.97	460
CG2--HG23	1.09	0.97	1350
CA--HA3	1.09	0.97	620

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD12	1.09	0.97	630
NZ--HZ3	1.01	0.89	400
CA--HA2	1.09	0.97	620
CE--HE3	1.09	0.97	520
NZ--HZ2	1.01	0.89	400
OG1--HG1	0.96	0.84	580
CG1--HG13	1.09	0.97	770
CD2--HD22	1.09	0.97	460
OH--HH	0.96	0.84	420
CE--HE1	1.09	0.97	120
NZ--HZ1	1.01	0.89	400
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	1
SG--HG	1.34	1.20	3
N--H	1.01	0.86	7090
NH2--HH22	1.01	0.86	330
CE2--HE2	1.08	0.93	780
CE1--HE1	1.08	0.93	860
CD1--HD1	1.08	0.93	870
CZ--HZ	1.08	0.93	360
CD2--HD2	1.08	0.93	860

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND2--HD22	1.01	0.86	430
NH1--HH11	1.01	0.86	330
NE2--HE21	1.01	0.86	330
NE2--HE22	1.01	0.86	330
ND2--HD21	1.01	0.86	430
CZ2--HZ2	1.08	0.93	90
NH2--HH21	1.01	0.86	330
NE--HE	1.01	0.86	330
NH1--HH12	1.01	0.86	330
CH2--HH2	1.08	0.93	90
CZ3--HZ3	1.08	0.93	90
NE1--HE1	1.01	0.86	90
CE3--HE3	1.08	0.93	90
ND1--HD1	1.01	0.86	78
NE2--HE2	1.01	0.86	2

Standard geometry: angle outliers

There are 523 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	139.85	1
CA-CB-CG	112.60	103.33	1
C-N-CA	121.70	138.02	1
C-N-CA	121.70	136.29	1
CA-CB-CG	112.60	104.66	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	114.87	1
C-CA-CB	110.10	124.70	1
C-N-CA	121.70	135.34	1
C-CA-CB	110.10	95.80	1
C-N-CA	121.70	134.96	1
C-N-CA	121.70	134.92	1
CD-NE-CZ	124.40	114.19	1
C-N-CA	121.70	134.82	1
CA-CB-CG2	110.40	122.57	1
OD1-CG-ND2	122.60	115.54	1
C-N-CA	121.70	134.38	1
CA-CB-CG2	110.50	122.42	1
CA-CB-CG	112.60	119.61	1
C-CA-CB	110.10	123.41	1
CA-N-CD	112.00	102.36	1
OE1-CD-NE2	122.60	115.87	1
OE1-CD-NE2	122.60	116.03	1
CA-CB-CG	112.60	119.09	1
C-N-CA	121.70	133.36	1
N-CA-CB	110.50	99.63	1
C-N-CA	121.70	133.17	1
NE-CZ-NH2	119.20	124.92	1
CA-CB-CG2	110.40	121.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	133.01	1
C-N-CA	121.70	132.90	1
OE1-CD-NE2	122.60	116.39	2
CA-CB-CG1	110.40	120.88	1
CA-CB-CG	112.60	106.44	1
CA-CB-OG1	109.60	100.38	1
C-N-CA	121.70	132.71	1
CA-CB-CG	112.60	118.68	1
N-CA-CB	110.50	100.21	1
C-N-CA	121.70	132.58	1
C-CA-CB	110.10	121.55	1
C-N-CA	121.70	132.46	1
C-N-CA	121.70	132.45	1
C-N-CA	121.70	132.43	1
O-C-N	123.00	113.47	1
OE1-CD-NE2	122.60	116.66	1
C-CA-CB	110.10	98.83	1
OG1-CB-CG2	109.30	97.46	1
C-N-CA	121.70	111.08	1
C-N-CA	121.70	132.23	1
C-N-CA	121.70	132.09	1
C-N-CA	121.70	132.08	1
CA-CB-CG1	110.40	120.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.97	1
C-N-CA	121.70	131.91	1
N-CA-CB	103.00	109.21	1
OE1-CD-NE2	122.60	116.96	1
CA-N-CD	112.00	104.11	1
CA-CB-CG	112.60	118.19	1
CA-CB-CG	112.60	118.18	1
C-N-CA	121.70	131.74	1
C-N-CA	121.70	131.69	1
CB-CG-CD	112.60	103.17	1
OE1-CD-NE2	122.60	117.06	1
C-N-CA	121.70	131.65	1
C-N-CA	121.70	131.63	1
C-N-CA	121.70	131.62	1
CA-CB-CG	112.60	107.11	1
C-CA-CB	110.10	120.53	1
CA-CB-CG	112.60	107.12	1
OE1-CD-NE2	122.60	117.12	1
OE1-CD-NE2	122.60	117.13	1
CA-CB-CG	112.60	118.05	1
C-CA-CB	110.10	120.41	1
OE1-CD-NE2	122.60	117.19	1
CB-CG-CD2	131.20	124.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.38	1
OD1-CG-ND2	122.60	117.23	1
C-N-CA	121.70	131.36	1
C-N-CA	121.70	131.35	1
C-CA-CB	110.10	120.28	1
OE1-CD-NE2	122.60	117.25	1
C-N-CA	121.70	131.32	2
OE1-CD-NE2	122.60	117.26	1
C-N-CA	121.70	131.31	1
C-CA-CB	110.10	120.24	1
C-N-CA	121.70	131.25	1
C-CA-CB	109.10	120.74	1
OE1-CD-NE2	122.60	117.35	1
C-N-CA	121.70	131.14	1
NH1-CZ-NH2	119.30	112.49	1
OE1-CD-NE2	122.60	117.36	1
CA-CB-CG	112.60	117.83	1
C-N-CA	121.70	131.10	1
OE1-CD-NE2	122.60	117.38	1
OD1-CG-ND2	122.60	117.42	1
CA-C-N	116.20	126.56	1
CA-CB-CG2	110.40	119.20	1
OE1-CD-NE2	122.60	117.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.61	1
C-N-CA	121.70	130.93	1
CA-CB-CG2	110.40	119.10	1
OE1-CD-NE2	122.60	117.49	1
OD1-CG-ND2	122.60	117.49	1
N-CA-CB	110.50	101.84	1
OE1-CD-NE2	122.60	117.51	2
CD-NE-CZ	124.40	131.52	1
C-N-CA	121.70	130.85	1
CA-CB-CG	112.60	107.52	1
OE1-CD-NE2	122.60	117.52	2
C-N-CA	121.70	130.84	1
N-CA-CB	110.40	102.79	1
CA-CB-CG	113.80	108.73	1
OD1-CG-ND2	122.60	117.53	1
CA-C-N	116.20	126.33	1
N-CA-CB	111.50	120.10	1
OE1-CD-NE2	122.60	117.54	1
C-N-CA	121.70	130.80	1
CA-CB-CG	112.60	107.55	1
N-CA-CB	103.00	108.56	1
OD1-CG-ND2	122.60	117.56	1
N-CA-CB	103.00	108.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	114.67	1
CA-CB-CG	112.60	107.57	1
N-CA-CB	110.50	119.05	1
OE1-CD-NE2	122.60	117.58	1
OD1-CG-ND2	122.60	117.59	1
OE1-CD-NE2	122.60	117.60	1
C-N-CA	121.70	130.66	1
OE1-CD-NE2	122.60	117.62	1
OE1-CD-NE2	122.60	117.63	1
C-N-CA	121.70	130.61	1
C-N-CA	121.70	130.60	1
CA-CB-CG	112.60	117.55	1
OE1-CD-NE2	122.60	117.65	1
OE1-CD-NE2	122.60	117.66	2
N-CA-CB	110.40	102.99	1
C-N-CA	121.70	130.58	1
OE1-CD-NE2	122.60	117.68	1
C-N-CA	121.70	130.55	1
N-CA-CB	103.00	108.40	1
CD1-CG-CD2	110.80	121.61	1
OD1-CG-ND2	122.60	117.70	1
CG-CD-CE	111.30	100.04	1
OE1-CD-NE2	122.60	117.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.49	1
CA-CB-CG2	110.50	118.80	1
CA-C-N	116.20	125.96	1
C-N-CA	121.70	130.47	1
OE1-CD-NE2	122.60	117.74	2
C-N-CA	121.70	130.43	1
OD1-CG-ND2	122.60	117.75	2
OE1-CD-NE2	122.60	117.75	1
OE1-CD-NE2	122.60	117.77	2
OD1-CG-ND2	122.60	117.77	1
C-N-CA	121.70	130.35	1
OD1-CG-ND2	122.60	117.81	1
OE1-CD-NE2	122.60	117.82	2
OE1-CD-NE2	122.60	117.83	2
N-CA-CB	110.50	118.61	1
C-N-CA	121.70	130.28	1
N-CA-C	111.00	124.32	1
OE1-CD-NE2	122.60	117.86	5
CA-C-O	120.80	112.75	1
O-C-N	123.00	115.43	1
C-N-CA	121.70	130.20	1
OE1-CD-NE2	122.60	117.88	1
C-CA-CB	109.10	119.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.40	102.45	1
CD1-CG-CD2	110.80	100.44	1
CA-CB-CG	112.60	107.90	1
C-N-CA	121.70	130.16	1
OE1-CD-NE2	122.60	117.90	1
OE1-CD-NE2	122.60	117.91	1
OD1-CG-ND2	122.60	117.91	1
CA-C-N	116.90	123.93	1
C-N-CA	121.70	130.13	1
CD1-CG-CD2	110.80	121.08	1
OE1-CD-NE2	122.60	117.94	1
N-CA-CB	103.00	108.12	1
CA-CB-CG	112.60	107.95	1
C-N-CA	121.70	130.07	1
CA-CB-CG	114.10	123.40	1
OD1-CG-ND2	122.60	117.95	1
CB-CG-CD2	131.20	125.16	1
C-CA-CB	110.10	118.91	1
OE1-CD-NE2	122.60	117.97	1
OE1-CD-NE2	122.60	117.98	2
C-N-CA	121.70	130.02	1
CA-CB-CG	112.60	107.98	1
N-CA-CB	110.40	103.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.99	1
CG1-CB-CG2	110.80	100.66	1
N-CA-C	112.10	100.59	1
CD-NE-CZ	124.40	130.84	1
OD1-CG-ND2	122.60	118.01	2
CA-N-CD	112.00	105.58	1
O-C-N	123.00	115.66	1
OE1-CD-NE2	122.60	118.02	2
C-CA-CB	110.10	118.81	1
C-N-CA	121.70	129.94	1
O-C-N	123.00	115.68	1
C-N-CA	121.70	113.47	1
CA-CB-CG	112.60	117.17	1
C-N-CA	121.70	129.92	1
CB-CG-CD2	131.20	125.27	1
C-N-CA	121.70	129.91	1
CA-N-CD	112.00	105.62	1
C-N-CA	121.70	129.89	1
OE1-CD-NE2	122.60	118.06	1
N-CA-CB	103.00	107.98	1
CB-CG-CD2	131.20	125.32	1
OE1-CD-NE2	122.60	118.08	2
OD1-CG-ND2	122.60	118.09	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.11	1
OE1-CD-NE2	122.60	118.09	4
CD-NE-CZ	124.40	130.71	1
CA-CB-CG1	110.40	118.06	1
C-N-CA	121.70	129.80	1
NE-CZ-NH1	121.50	117.00	1
CB-CG-CD2	131.20	125.35	1
OD1-CG-ND2	122.60	118.10	1
OE1-CD-NE2	122.60	118.11	3
OD1-CG-ND2	122.60	118.11	1
OE1-CD-NE2	122.60	118.12	2
C-N-CA	121.70	129.76	1
C-CA-CB	110.10	101.60	1
C-N-CA	121.70	129.75	1
OE1-CD-NE2	122.60	118.13	1
CA-CB-CG2	110.40	118.00	1
C-N-CA	121.70	129.73	3
C-CA-CB	110.10	118.58	1
CB-CG-CD2	131.20	125.41	1
C-CA-CB	110.10	118.56	1
CB-CG-CD2	131.20	125.42	1
N-CA-C	111.00	98.54	1
OD1-CG-ND2	122.60	118.15	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	118.54	1
OE1-CD-NE2	122.60	118.16	5
C-N-CA	121.70	129.68	2
OD1-CG-ND2	122.60	118.17	2
N-CA-C	111.00	123.40	1
OE1-CD-NE2	122.60	118.17	1
CA-CB-OG1	109.60	116.24	1
OE1-CD-NE2	122.60	118.18	1
C-N-CA	121.70	129.65	2
N-CA-C	111.00	123.37	1
N-CA-CB	103.00	107.86	1
NE-CZ-NH2	119.20	123.17	1
C-N-CA	121.70	113.75	1
OD1-CG-ND2	122.60	118.19	2
OE1-CD-NE2	122.60	118.19	2
C-N-CA	121.70	129.64	1
N-CA-C	111.00	98.66	1
C-N-CA	121.70	129.63	1
OE1-CD-NE2	122.60	118.20	3
OE1-CD-NE2	122.60	118.21	2
C-N-CA	121.70	129.60	1
CA-CB-CG1	110.40	117.85	1
OE1-CD-NE2	122.60	118.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.23	1
CA-CB-CG2	110.40	117.84	1
C-N-CA	121.70	129.57	1
CB-CG-CD2	131.20	125.52	1
C-N-CA	121.70	129.56	2
NE-CZ-NH2	119.20	123.13	1
N-CA-C	111.00	123.20	1
CA-CB-CG	113.80	118.16	1
CA-CB-CG	113.80	109.45	1
N-CA-CB	103.00	107.79	1
CA-CB-CG	112.60	116.95	1
OD1-CG-ND2	122.60	118.25	1
CA-CB-CG	112.60	108.25	1
OE1-CD-NE2	122.60	118.25	1
OE1-CD-NE2	122.60	118.26	4
C-CA-CB	110.10	118.35	1
N-CA-C	111.00	123.16	1
OE1-CD-NE2	122.60	118.27	3
O-C-N	123.00	116.07	1
CA-CB-CG	113.80	118.13	1
CA-CB-CG2	110.40	117.76	1
C-N-CA	121.70	129.48	1
N-CA-CB	110.50	117.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.28	3
N-CA-CB	103.00	107.75	1
OD1-CG-ND2	122.60	118.28	1
C-N-CA	121.70	129.47	1
C-N-CA	121.70	129.46	1
OE1-CD-NE2	122.60	118.29	1
OD1-CG-ND2	122.60	118.29	1
CD-NE-CZ	124.40	130.43	1
OD1-CG-ND2	122.60	118.30	1
OE1-CD-NE2	122.60	118.30	3
C-N-CA	121.70	129.44	1
CA-C-N	116.20	124.80	1
OE1-CD-NE2	122.60	118.31	1
OD1-CG-ND2	122.60	118.31	1
CD1-CG-CD2	110.80	120.23	1
OD1-CG-ND2	122.60	118.32	1
ND1-CG-CD2	106.10	110.38	1
CG-CD-CE	111.30	101.45	1
OE1-CD-NE2	122.60	118.32	2
C-N-CA	121.70	129.39	1
OE1-CD-NE2	122.60	118.33	4
O-C-N	123.00	116.17	1
C-N-CA	121.70	129.38	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.34	2
C-N-CA	121.70	129.36	3
OD1-CG-ND2	122.60	118.35	1
OE1-CD-NE2	122.60	118.35	4
CB-CG-CD2	131.20	125.68	2
OE1-CD-NE2	122.60	118.36	2
OE1-CD-NE2	122.60	118.37	4
C-N-CA	121.70	129.32	2
CA-CB-CG1	110.40	103.21	1
CA-CB-OG1	109.60	115.94	1
C-N-CA	121.70	129.31	1
C-N-CA	121.70	129.30	1
N-CA-CB	103.00	107.64	1
OD1-CG-ND2	122.60	118.38	1
C-N-CA	121.70	129.28	2
OD1-CG-ND2	122.60	118.39	2
CA-C-N	116.20	124.62	1
OE1-CD-NE2	122.60	118.39	1
OE1-CD-NE2	122.60	118.40	2
CA-CB-CG	112.60	108.40	1
C-N-CA	121.70	129.26	1
CG-CD-CE	111.30	101.65	1
OE1-CD-NE2	122.60	118.41	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.25	1
CB-CG-CD	112.60	105.47	1
C-N-CA	121.70	129.24	1
CA-CB-CG1	110.40	117.52	1
OD1-CG-ND2	122.60	118.42	1
OE1-CD-NE2	122.60	118.42	1
CA-CB-OG	111.10	119.46	1
C-N-CA	121.70	129.22	1
OE1-CD-NE2	122.60	118.43	1
C-N-CA	121.70	129.19	1
OD1-CG-ND2	122.60	118.44	2
OE1-CD-NE2	122.60	118.44	1
C-N-CA	121.70	114.22	1
OD1-CG-ND2	122.60	118.45	1
OE1-CD-NE2	122.60	118.45	2
C-CA-CB	110.10	117.99	1
CD-NE-CZ	124.40	130.21	1
NH1-CZ-NH2	119.30	113.91	1
C-CA-CB	110.50	116.72	1
C-N-CA	121.70	129.16	1
N-CA-CB	103.00	107.55	1
C-N-CA	121.70	129.15	1
CA-CB-CG	112.60	116.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	125.82	1
N-CA-C	111.00	122.57	1
CA-CB-CG	112.60	116.73	1
C-N-CA	121.70	129.13	2
OD1-CG-ND2	122.60	118.47	1
CA-CB-CG	112.60	116.72	3
OE1-CD-NE2	122.60	118.48	1
N-CA-CB	103.00	107.53	2
OD1-CG-ND2	122.60	118.48	1
OD1-CG-ND2	122.60	118.49	1
OE1-CD-NE2	122.60	118.49	4
C-N-CA	121.70	129.10	1
N-CA-CB	103.00	107.52	1
OE1-CD-NE2	122.60	118.50	1
CA-CB-CG	112.60	108.50	1
N-CA-CB	111.50	118.47	1
N-CA-CB	110.50	103.54	1
OD1-CG-ND2	122.60	118.51	2
N-CA-CB	110.50	103.55	1
OE1-CD-NE2	122.60	118.51	1
C-N-CA	121.70	129.06	1
OD1-CG-ND2	122.60	118.52	1
CD-NE-CZ	124.40	130.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.52	1
OD1-CG-ND2	122.60	118.53	2
C-N-CA	121.70	129.02	3
CA-CB-CG	112.60	116.67	1
CA-CB-OG	111.10	102.97	1
CB-CG-ND2	116.40	122.50	1
CA-CB-CG	112.60	116.66	1
CA-C-O	120.80	113.90	1
OD1-CG-ND2	122.60	118.54	3
C-N-CA	121.70	129.00	2
N-CA-C	111.00	122.36	1
N-CA-CB	103.00	107.46	1
OD1-CG-ND2	122.60	118.55	1
C-N-CA	121.70	128.99	1
C-N-CA	121.70	128.98	2
CA-CB-OG1	109.60	115.67	1
CD-NE-CZ	124.40	130.06	1
OD1-CG-ND2	122.60	118.56	1
OE1-CD-NE2	122.60	118.56	1
CD1-CG-CD2	110.80	101.93	1
CA-CB-OG	111.10	103.04	1
OD1-CG-ND2	122.60	118.57	1
OD1-CG-ND2	122.60	118.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	99.74	1
CA-C-N	116.20	124.24	1
N-CA-C	111.00	122.25	1
CB-CG-CD2	131.20	125.98	1
CA-CB-CG	112.60	116.61	1
OE1-CD-NE2	122.60	118.59	2
OD1-CG-ND2	122.60	118.60	1
C-N-H	112.27	124.30	1
C-N-H	112.22	124.30	1
C-CA-HA	96.86	109.00	1
C-N-H	112.10	124.30	1
C-N-H	112.07	124.30	1
C-N-H	112.01	124.30	1
C-N-H	111.98	124.30	1
C-N-H	111.95	124.30	1
C-N-H	111.94	124.30	1
C-N-H	111.92	124.30	1
C-N-H	111.87	124.30	1
C-N-H	111.82	124.30	1
HE21-NE2-HE22	107.49	120.00	1
CG-ND2-HD22	107.39	120.00	1
CZ-NH2-HH22	107.38	120.00	1
HE21-NE2-HE22	107.36	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-H	111.63	124.30	1
C-N-H	111.60	124.30	1
C-N-H	111.41	124.30	1
HZ1-NZ-HZ2	95.36	109.00	1
C-N-H	110.58	124.30	1
C-N-H	110.44	124.30	1
C-N-H	110.40	124.30	1
C-N-H	109.58	124.30	1
CZ-NH1-HH12	105.22	120.00	1
C-N-H	108.83	124.30	1
CD-NE2-HE21	104.45	120.00	1
C-N-H	108.49	124.30	1
CG-ND2-HD21	103.46	120.00	1
C-N-H	107.19	124.30	1
HB2-CB-HB3	91.29	110.00	1
HH21-NH2-HH22	100.39	120.00	1
HE21-NE2-HE22	98.33	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	8.19	93
2	2.73	31

Model ID	Clash score	Number of clashes
3	7.31	83
4	4.67	53
5	6.17	70
6	4.76	54
7	11.89	135
8	8.72	99
9	4.76	54
10	5.46	62

All 734 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:158:MET:HE1	A:247:ALA:HB3	0.824
1	A:78:LYS:HA	A:479:LEU:HD21	0.814
1	A:103:LEU:HD11	A:164:ILE:HD11	0.762
1	A:158:MET:CE	A:247:ALA:HB3	0.748
1	A:158:MET:HE3	A:230:LEU:HB3	0.743
1	A:128:PHE:CE1	A:181:LEU:HD13	0.722
1	A:479:LEU:HD23	A:516:ASN:HD22	0.708
1	A:221:GLY:HA2	A:222:VAL:HG23	0.687
1	A:120:TYR:CE2	A:726:PHE:CZ	0.660
1	A:139:LEU:HD12	A:144:LEU:HD11	0.656
1	A:172:LEU:C	A:408:LEU:HD22	0.644
1	A:379:VAL:HG21	A:590:PHE:CZ	0.644
1	A:312:GLU:CD	A:314:MET:HE3	0.614

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:85:VAL:HG11	A:107:PRO:HD2	0.608
1	A:126:ARG:CZ	A:574:TYR:CE1	0.598
1	A:126:ARG:CZ	A:574:TYR:CD1	0.589
1	A:85:VAL:HG21	A:107:PRO:HG2	0.575
1	A:78:LYS:C	A:479:LEU:HD21	0.569
1	A:378:TYR:CE1	A:380:VAL:HG23	0.567
1	A:83:ILE:HG22	A:128:PHE:CE2	0.566
1	A:105:TYR:CE1	A:618:VAL:HG13	0.559
1	A:280:LEU:HD22	A:374:LEU:CD2	0.555
1	A:78:LYS:CA	A:479:LEU:HD21	0.554
1	A:78:LYS:HA	A:479:LEU:CD2	0.553
1	A:85:VAL:HG21	A:107:PRO:CG	0.552
1	A:103:LEU:HD13	A:123:LEU:HD21	0.549
1	A:76:ILE:HB	A:87:THR:HG22	0.537
1	A:185:VAL:HG12	A:187:LYS:N	0.534
1	A:158:MET:SD	A:247:ALA:HB3	0.533
1	A:85:VAL:HB	A:106:THR:HG23	0.531
1	A:83:ILE:CG2	A:128:PHE:CE2	0.526
1	A:158:MET:HE1	A:247:ALA:CB	0.526
1	A:234:ALA:HB3	A:243:GLU:OE2	0.519
1	A:314:MET:HE2	A:336:ALA:HB1	0.516
1	A:83:ILE:HB	A:128:PHE:CZ	0.513
1	A:158:MET:HG2	A:230:LEU:HD22	0.506

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:126:ARG:HH22	A:603:VAL:C	0.505
1	A:126:ARG:NH2	A:574:TYR:CE1	0.502
1	A:185:VAL:CG1	A:188:ARG:H	0.497
1	A:223:TYR:CD1	A:252:PHE:CZ	0.481
1	A:694:LEU:HD13	A:712:HIS:CE1	0.479
1	A:175:LYS:HG2	A:176:SER:HA	0.473
1	A:459:LEU:HD22	A:496:ARG:HH21	0.473
1	A:155:ASP:CG	A:232:ARG:HH11	0.472
1	A:187:LYS:HZ3	A:249:ALA:HB3	0.469
1	A:171:VAL:HG22	A:512:ARG:CZ	0.463
1	A:280:LEU:HD22	A:374:LEU:HD23	0.463
1	A:158:MET:HE3	A:230:LEU:CB	0.462
1	A:143:LYS:HE2	A:537:SER:CB	0.461
1	A:143:LYS:HE2	A:537:SER:OG	0.461
1	A:201:ALA:HA	A:206:LEU:CD2	0.461
1	A:164:ILE:C	A:166:ARG:N	0.460
1	A:118:ASN:CG	A:156:PRO:HG3	0.459
1	A:81:GLN:C	A:83:ILE:H	0.454
1	A:201:ALA:HA	A:206:LEU:HD22	0.454
1	A:162:ALA:C	A:164:ILE:N	0.453
1	A:140:ASN:HB3	A:334:ARG:NH1	0.452
1	A:143:LYS:HE2	A:537:SER:HB3	0.452
1	A:676:TYR:CE1	A:681:ASN:OD1	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:206:LEU:CD2	A:207:PHE:HA	0.448
1	A:156:PRO:HG2	A:157:TYR:CD2	0.447
1	A:140:ASN:HB3	A:334:ARG:CZ	0.441
1	A:103:LEU:HD13	A:123:LEU:CD2	0.440
1	A:105:TYR:CD1	A:608:LYS:HB2	0.438
1	A:139:LEU:HD13	A:312:GLU:OE2	0.438
1	A:187:LYS:HE2	A:228:THR:HG21	0.438
1	A:280:LEU:HD22	A:374:LEU:HD21	0.438
1	A:114:ARG:NH1	A:723:ALA:HA	0.430
1	A:105:TYR:CE1	A:618:VAL:HG22	0.428
1	A:276:TYR:CE1	A:303:ALA:O	0.428
1	A:278:GLY:HA3	A:299:PHE:HB3	0.428
1	A:157:TYR:CE1	A:200:LYS:NZ	0.424
1	A:426:TYR:CD2	A:447:ALA:HB1	0.424
1	A:167:GLY:O	A:168:PRO:C	0.424
1	A:86:VAL:HB	A:166:ARG:HH12	0.423
1	A:83:ILE:HB	A:128:PHE:CE1	0.422
1	A:432:LEU:HD21	A:445:PHE:CE2	0.421
1	A:178:PRO:CB	A:414:MET:HE3	0.419
1	A:175:LYS:HB2	A:512:ARG:NH2	0.418
1	A:559:LYS:HE2	A:561:VAL:CG2	0.418
1	A:142:LEU:HD22	A:387:ASN:ND2	0.416
1	A:164:ILE:HG22	A:166:ARG:HA	0.415

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:178:PRO:HB3	A:414:MET:SD	0.411
1	A:348:TYR:O	A:375:ALA:HB3	0.411
1	A:661:SER:HB3	A:701:ARG:CZ	0.411
1	A:103:LEU:HD13	A:123:LEU:HD11	0.408
1	A:126:ARG:CZ	A:604:GLU:CD	0.407
1	A:118:ASN:CB	A:156:PRO:HG3	0.405
1	A:317:TYR:CE1	A:333:LEU:HB3	0.405
1	A:172:LEU:O	A:408:LEU:HD13	0.405
1	A:168:PRO:O	A:169:VAL:C	0.405
1	A:276:TYR:OH	A:304:LYS:HA	0.404
1	A:175:LYS:HB2	A:512:ARG:HH21	0.403
2	A:142:LEU:HD13	A:178:PRO:HD3	0.644
2	A:109:VAL:HG12	A:110:SER:HB2	0.574
2	A:131:GLU:CD	A:727:ASN:H	0.566
2	A:126:ARG:HA	A:622:THR:HG21	0.506
2	A:83:ILE:HG23	A:85:VAL:HG22	0.504
2	A:83:ILE:HG21	A:526:TYR:CD2	0.501
2	A:83:ILE:HG21	A:526:TYR:CE2	0.496
2	A:143:LYS:HE3	A:414:MET:SD	0.495
2	A:111:VAL:H	A:123:LEU:HD13	0.481
2	A:70:THR:HG22	A:255:ARG:NH2	0.470
2	A:114:ARG:HH12	A:713:VAL:C	0.466
2	A:195:LYS:HE2	A:214:SER:O	0.458

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	A:76:ILE:HG21	A:89:GLU:HB3	0.456
2	A:128:PHE:CD1	A:138:TYR:CZ	0.451
2	A:725:CYS:HA	A:731:CYS:HA	0.450
2	A:142:LEU:HD13	A:178:PRO:CD	0.449
2	A:83:ILE:HA	A:84:SER:C	0.444
2	A:70:THR:HG21	A:253:THR:HB	0.442
2	A:154:ILE:HD11	A:165:MET:HE2	0.438
2	A:198:GLN:HE21	A:742:THR:HG23	0.432
2	A:83:ILE:CG2	A:85:VAL:HG22	0.428
2	A:111:VAL:H	A:123:LEU:CD1	0.428
2	A:694:LEU:HD13	A:712:HIS:CE1	0.427
2	A:114:ARG:CZ	A:712:HIS:HB3	0.424
2	A:83:ILE:HG23	A:85:VAL:CG2	0.420
2	A:146:GLY:HA3	A:151:ASP:HA	0.416
2	A:142:LEU:HB3	A:178:PRO:HD3	0.413
2	A:82:SER:HB2	A:553:GLN:CD	0.411
2	A:114:ARG:HH12	A:713:VAL:CA	0.411
2	A:149:TYR:HB3	A:308:TYR:CE2	0.407
2	A:172:LEU:CD1	A:408:LEU:HD13	0.404
3	A:158:MET:HE3	A:247:ALA:HB3	0.931
3	A:99:VAL:HG21	A:610:ALA:HB2	0.834
3	A:71:LYS:HZ3	A:265:LEU:HD22	0.824
3	A:158:MET:CE	A:247:ALA:HB3	0.784

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:113:THR:HG21	A:723:ALA:CB	0.744
3	A:113:THR:HG21	A:723:ALA:HB1	0.717
3	A:119:THR:CG2	A:153:VAL:HG11	0.649
3	A:276:TYR:CE1	A:304:LYS:HA	0.648
3	A:71:LYS:HZ3	A:265:LEU:CD2	0.646
3	A:99:VAL:CG2	A:610:ALA:HB2	0.636
3	A:455:PRO:O	A:497:VAL:HG21	0.608
3	A:158:MET:SD	A:247:ALA:HB3	0.607
3	A:583:MET:HE2	A:634:TYR:CE2	0.601
3	A:103:LEU:HD13	A:568:VAL:HG23	0.593
3	A:88:ALA:H	A:109:VAL:HG11	0.587
3	A:70:THR:HG21	A:163:GLU:CD	0.586
3	A:641:GLN:HE22	A:725:CYS:H	0.561
3	A:176:SER:HB3	A:485:ARG:HD3	0.556
3	A:106:THR:HG23	A:606:GLU:OE2	0.552
3	A:72:THR:HG21	A:173:TYR:CE1	0.548
3	A:105:TYR:C	A:608:LYS:HZ1	0.545
3	A:119:THR:HG23	A:153:VAL:HG11	0.539
3	A:237:GLN:NE2	A:736:GLU:H	0.536
3	A:113:THR:HG21	A:723:ALA:HB3	0.533
3	A:103:LEU:HD22	A:568:VAL:HB	0.526
3	A:566:PRO:HG2	A:610:ALA:HB3	0.526
3	A:176:SER:HB3	A:485:ARG:CD	0.522

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:276:TYR:CD1	A:304:LYS:HA	0.522
3	A:279:TRP:CD1	A:279:TRP:H	0.517
3	A:721:TYR:CZ	A:734:GLY:HA3	0.517
3	A:641:GLN:NE2	A:725:CYS:H	0.517
3	A:289:LEU:HD21	A:293:LYS:O	0.514
3	A:119:THR:HG21	A:153:VAL:HG11	0.512
3	A:90:GLU:CD	A:94:HIS:CD2	0.505
3	A:109:VAL:HG13	A:123:LEU:HD23	0.499
3	A:559:LYS:HE2	A:561:VAL:HG21	0.498
3	A:71:LYS:HE3	A:187:LYS:O	0.494
3	A:174:GLY:HA2	A:468:TYR:CZ	0.493
3	A:126:ARG:HE	A:604:GLU:CD	0.493
3	A:314:MET:HG3	A:334:ARG:HE	0.492
3	A:170:SER:HB2	A:179:GLY:HA3	0.487
3	A:99:VAL:HG21	A:610:ALA:CB	0.482
3	A:281:PRO:HG3	A:296:PRO:HG3	0.477
3	A:566:PRO:CG	A:610:ALA:HB3	0.477
3	A:144:LEU:CD1	A:184:MET:HE3	0.472
3	A:694:LEU:HD13	A:712:HIS:CE1	0.471
3	A:109:VAL:HG22	A:123:LEU:CD2	0.470
3	A:423:TRP:CH2	A:425:GLY:HA3	0.458
3	A:75:PRO:C	A:77:GLN:H	0.454
3	A:136:ASN:HD21	A:534:GLU:CD	0.454

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:109:VAL:HG22	A:123:LEU:HD22	0.452
3	A:139:LEU:HD11	A:157:TYR:HE2	0.452
3	A:139:LEU:HD13	A:156:PRO:CG	0.449
3	A:78:LYS:O	A:479:LEU:HD23	0.446
3	A:462:GLN:HG3	A:491:GLN:HE22	0.442
3	A:158:MET:HE3	A:247:ALA:CB	0.438
3	A:103:LEU:CD1	A:568:VAL:HG23	0.438
3	A:103:LEU:HD13	A:568:VAL:CG2	0.437
3	A:80:PRO:HG2	A:514:GLY:CA	0.436
3	A:165:MET:HE2	A:185:VAL:CG2	0.433
3	A:86:VAL:HG12	A:109:VAL:HG21	0.428
3	A:66:SER:C	A:68:THR:H	0.427
3	A:125:ILE:HD12	A:182:LEU:CD2	0.426
3	A:295:LEU:HD12	A:733:TRP:CD1	0.426
3	A:86:VAL:HG21	A:106:THR:C	0.425
3	A:81:GLN:HB2	A:168:PRO:HD2	0.423
3	A:295:LEU:HD11	A:733:TRP:H	0.423
3	A:423:TRP:CH2	A:443:PHE:CZ	0.421
3	A:75:PRO:C	A:77:GLN:N	0.420
3	A:281:PRO:CB	A:286:VAL:CG2	0.418
3	A:165:MET:HE1	A:173:TYR:CE2	0.415
3	A:138:TYR:CD2	A:180:GLY:N	0.414
3	A:279:TRP:NE1	A:346:TYR:CD1	0.414

Model ID	Atom-1	Atom-2	Clash overlap (Å)
3	A:72:THR:C	A:74:THR:N	0.414
3	A:158:MET:SD	A:247:ALA:C	0.413
3	A:144:LEU:CD2	A:334:ARG:HH12	0.411
3	A:208:GLN:CD	A:230:LEU:HD11	0.410
3	A:267:TYR:CZ	A:269:GLN:HB2	0.410
3	A:178:PRO:HD3	A:532:SER:HB2	0.407
3	A:93:LEU:CD2	A:200:LYS:HZ1	0.406
3	A:281:PRO:HB3	A:296:PRO:HG3	0.403
3	A:412:ASP:OD2	A:485:ARG:NH1	0.403
3	A:561:VAL:HG22	A:568:VAL:HG22	0.402
4	A:173:TYR:CZ	A:178:PRO:HB3	0.796
4	A:173:TYR:CE1	A:178:PRO:HB3	0.784
4	A:172:LEU:HB3	A:173:TYR:CE1	0.670
4	A:172:LEU:HB3	A:173:TYR:CZ	0.666
4	A:100:LYS:HE2	A:113:THR:HG22	0.643
4	A:719:ARG:H	A:737:ARG:CZ	0.637
4	A:719:ARG:H	A:737:ARG:NH1	0.598
4	A:100:LYS:CE	A:113:THR:HG22	0.588
4	A:173:TYR:CG	A:178:PRO:HA	0.580
4	A:173:TYR:CE2	A:178:PRO:HG3	0.564
4	A:374:LEU:HB2	A:435:LEU:HD21	0.546
4	A:100:LYS:HE3	A:111:VAL:CG1	0.545
4	A:281:PRO:HB2	A:435:LEU:HD22	0.543

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:280:LEU:HD21	A:733:TRP:CZ2	0.540
4	A:378:TYR:HE2	A:445:PHE:CD1	0.538
4	A:128:PHE:CD1	A:578:LYS:HD2	0.536
4	A:172:LEU:C	A:173:TYR:CG	0.532
4	A:172:LEU:CB	A:173:TYR:CZ	0.530
4	A:172:LEU:HD21	A:470:GLN:NE2	0.515
4	A:143:LYS:HD2	A:175:LYS:HE3	0.514
4	A:295:LEU:HD13	A:299:PHE:HB3	0.514
4	A:281:PRO:CB	A:435:LEU:HD22	0.511
4	A:719:ARG:C	A:737:ARG:HH22	0.502
4	A:172:LEU:HD21	A:470:GLN:HE22	0.501
4	A:172:LEU:O	A:173:TYR:CD2	0.499
4	A:173:TYR:CZ	A:178:PRO:CB	0.495
4	A:721:TYR:CZ	A:723:ALA:HA	0.492
4	A:70:THR:HA	A:172:LEU:HD22	0.491
4	A:173:TYR:CE2	A:178:PRO:CG	0.489
4	A:638:THR:H	A:681:ASN:HD21	0.474
4	A:343:ASN:HB3	A:445:PHE:CD1	0.458
4	A:691:VAL:O	A:715:ASN:HA	0.458
4	A:138:TYR:CD2	A:180:GLY:N	0.453
4	A:719:ARG:H	A:737:ARG:NH2	0.453
4	A:173:TYR:CZ	A:178:PRO:HG3	0.452
4	A:127:GLY:C	A:128:PHE:CD2	0.451

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	A:688:TYR:CD2	A:721:TYR:CE2	0.448
4	A:126:ARG:HD2	A:574:TYR:CE2	0.443
4	A:721:TYR:CE2	A:723:ALA:HA	0.442
4	A:100:LYS:HE3	A:111:VAL:HG13	0.439
4	A:422:ALA:HB1	A:424:PHE:CE2	0.439
4	A:349:GLY:HA2	A:729:TYR:CE2	0.430
4	A:295:LEU:CD1	A:299:PHE:HB3	0.423
4	A:134:SER:HB3	A:151:ASP:OD1	0.422
4	A:169:VAL:HG13	A:512:ARG:HH11	0.421
4	A:100:LYS:CE	A:111:VAL:HG13	0.419
4	A:174:GLY:HA2	A:468:TYR:CE1	0.417
4	A:172:LEU:HB2	A:173:TYR:CE2	0.411
4	A:93:LEU:O	A:694:LEU:HD22	0.411
4	A:295:LEU:HD13	A:299:PHE:CB	0.410
4	A:661:SER:HB3	A:701:ARG:CZ	0.405
4	A:145:GLN:CD	A:416:MET:SD	0.403
4	A:711:LEU:HD11	A:739:VAL:CG1	0.403
5	A:75:PRO:CD	A:171:VAL:HG13	0.776
5	A:75:PRO:HD2	A:171:VAL:HG13	0.740
5	A:124:ILE:HG21	A:642:VAL:HG13	0.656
5	A:74:THR:HG22	A:171:VAL:HA	0.628
5	A:94:HIS:HB3	A:105:TYR:CZ	0.623
5	A:166:ARG:HH11	A:169:VAL:HG22	0.594

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:92:ALA:HB1	A:712:HIS:NE2	0.593
5	A:163:GLU:CD	A:189:PRO:HA	0.585
5	A:72:THR:HG22	A:76:ILE:HD12	0.571
5	A:265:LEU:HD12	A:314:MET:HE1	0.552
5	A:194:LEU:HD22	A:746:ARG:NH2	0.549
5	A:459:LEU:HD21	A:461:LYS:HE3	0.543
5	A:70:THR:C	A:72:THR:H	0.542
5	A:191:THR:H	A:226:ARG:HH12	0.538
5	A:170:SER:CB	A:174:GLY:H	0.534
5	A:126:ARG:HB3	A:576:LEU:CD1	0.532
5	A:374:LEU:C	A:430:VAL:HG11	0.525
5	A:172:LEU:O	A:408:LEU:HD23	0.521
5	A:71:LYS:H	A:106:THR:HG23	0.506
5	A:165:MET:HE1	A:333:LEU:O	0.505
5	A:422:ALA:HB3	A:456:TYR:CZ	0.505
5	A:277:TYR:CZ	A:303:ALA:HB1	0.504
5	A:74:THR:HG22	A:171:VAL:CA	0.502
5	A:127:GLY:HA2	A:642:VAL:HG21	0.502
5	A:294:ARG:HH21	A:297:THR:HG21	0.499
5	A:159:LEU:CD1	A:198:GLN:HB3	0.493
5	A:159:LEU:HD13	A:210:GLY:C	0.491
5	A:262:PHE:CE1	A:264:PHE:CZ	0.491
5	A:49:ALA:O	A:50:PRO:C	0.490

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:75:PRO:HD3	A:171:VAL:HG13	0.488
5	A:533:PHE:CE2	A:548:PRO:HB2	0.487
5	A:171:VAL:HG12	A:172:LEU:HG	0.479
5	A:533:PHE:CE2	A:548:PRO:CB	0.475
5	A:120:TYR:HB3	A:724:SER:HB3	0.467
5	A:373:TYR:HB3	A:430:VAL:HG13	0.466
5	A:299:PHE:CE1	A:348:TYR:HA	0.465
5	A:91:MET:HE2	A:618:VAL:HG21	0.462
5	A:131:GLU:CD	A:628:TYR:CZ	0.458
5	A:144:LEU:HD13	A:416:MET:HE1	0.458
5	A:504:ARG:HH11	A:545:ILE:HG22	0.458
5	A:198:GLN:OE1	A:200:LYS:HE3	0.454
5	A:267:TYR:HB3	A:314:MET:HE3	0.452
5	A:75:PRO:HD3	A:171:VAL:HG22	0.444
5	A:78:LYS:CB	A:479:LEU:HD21	0.444
5	A:171:VAL:C	A:172:LEU:HG	0.439
5	A:126:ARG:HD3	A:576:LEU:HD11	0.436
5	A:70:THR:HA	A:106:THR:CG2	0.435
5	A:71:LYS:CE	A:183:ASN:O	0.435
5	A:78:LYS:CG	A:479:LEU:HD21	0.433
5	A:721:TYR:CZ	A:734:GLY:HA3	0.432
5	A:120:TYR:HB3	A:724:SER:CB	0.430
5	A:166:ARG:HH11	A:169:VAL:CG2	0.428

Model ID	Atom-1	Atom-2	Clash overlap (Å)
5	A:447:ALA:C	A:449:ASP:H	0.428
5	A:160:GLU:CG	A:230:LEU:HD22	0.427
5	A:432:LEU:HD13	A:445:PHE:HB3	0.427
5	A:451:ALA:HB2	A:497:VAL:HG22	0.426
5	A:133:GLN:HE21	A:582:LEU:HB2	0.426
5	A:597:GLU:HB3	A:630:THR:HG23	0.426
5	A:277:TYR:CZ	A:303:ALA:CB	0.421
5	A:168:PRO:HD3	A:332:ASN:HB2	0.420
5	A:424:PHE:CE2	A:456:TYR:CE1	0.420
5	A:424:PHE:CD2	A:456:TYR:CE1	0.418
5	A:176:SER:O	A:414:MET:HE2	0.415
5	A:661:SER:HB3	A:701:ARG:CZ	0.415
5	A:159:LEU:HD11	A:198:GLN:HB3	0.414
5	A:99:VAL:HG23	A:616:ASN:OD1	0.410
5	A:116:ALA:HB1	A:121:ASP:CG	0.407
5	A:583:MET:HG2	A:595:GLY:HA3	0.407
5	A:114:ARG:NH1	A:204:ASP:CB	0.406
5	A:126:ARG:HB3	A:576:LEU:HD12	0.403
6	A:295:LEU:HD21	A:731:CYS:HB2	0.776
6	A:244:GLN:H	A:274:THR:HG21	0.743
6	A:641:GLN:HE21	A:725:CYS:H	0.724
6	A:326:THR:HG23	A:397:LYS:O	0.645
6	A:280:LEU:HD22	A:348:TYR:OH	0.627

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:267:TYR:HB3	A:314:MET:HE2	0.590
6	A:106:THR:HG21	A:164:ILE:HD12	0.570
6	A:139:LEU:HB2	A:144:LEU:HD11	0.570
6	A:295:LEU:HD21	A:731:CYS:CB	0.567
6	A:458:ILE:HD13	A:495:ASN:HA	0.557
6	A:459:LEU:HD22	A:496:ARG:HH21	0.553
6	A:153:VAL:HB	A:310:ARG:HH22	0.536
6	A:66:SER:HB2	A:75:PRO:HA	0.517
6	A:303:ALA:C	A:305:ASN:H	0.517
6	A:272:PRO:O	A:274:THR:HG23	0.513
6	A:349:GLY:HA3	A:445:PHE:CE2	0.505
6	A:362:CYS:HB2	A:374:LEU:HD11	0.503
6	A:135:GLN:O	A:143:LYS:HE2	0.500
6	A:583:MET:HE1	A:634:TYR:CE2	0.499
6	A:88:ALA:HB2	A:160:GLU:O	0.493
6	A:378:TYR:CD2	A:424:PHE:CE1	0.493
6	A:661:SER:HB3	A:701:ARG:CZ	0.486
6	A:169:VAL:HG11	A:181:LEU:HD12	0.478
6	A:439:VAL:HG12	A:440:ASN:ND2	0.472
6	A:294:ARG:O	A:439:VAL:HG13	0.468
6	A:641:GLN:HE21	A:725:CYS:N	0.466
6	A:358:TYR:CD2	A:447:ALA:HB1	0.465
6	A:70:THR:HB	A:172:LEU:HD13	0.464

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:459:LEU:HD22	A:496:ARG:NH2	0.459
6	A:116:ALA:HB2	A:279:TRP:CZ3	0.450
6	A:276:TYR:CE1	A:304:LYS:HA	0.449
6	A:343:ASN:OD1	A:377:LYS:HE3	0.447
6	A:81:GLN:HE21	A:83:ILE:HD11	0.445
6	A:174:GLY:HA3	A:468:TYR:CZ	0.444
6	A:638:THR:H	A:681:ASN:HD21	0.444
6	A:276:TYR:CD1	A:304:LYS:HA	0.443
6	A:280:LEU:HD22	A:348:TYR:CZ	0.441
6	A:106:THR:HG22	A:166:ARG:HH21	0.435
6	A:438:PRO:C	A:440:ASN:H	0.435
6	A:597:GLU:HB3	A:630:THR:HG23	0.434
6	A:66:SER:CB	A:75:PRO:HA	0.430
6	A:133:GLN:CD	A:136:ASN:HD22	0.430
6	A:174:GLY:HA3	A:468:TYR:CE1	0.425
6	A:242:GLU:O	A:274:THR:HB	0.423
6	A:262:PHE:CE1	A:264:PHE:CZ	0.422
6	A:262:PHE:CE1	A:264:PHE:CE2	0.420
6	A:267:TYR:CB	A:314:MET:HE2	0.420
6	A:149:TYR:CE2	A:378:TYR:CE1	0.418
6	A:365:LEU:HD21	A:432:LEU:HD13	0.416
6	A:566:PRO:HG2	A:610:ALA:HB3	0.415
6	A:726:PHE:CE1	A:732:PHE:CE2	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	A:726:PHE:CE1	A:730:GLY:HA3	0.408
6	A:378:TYR:CE1	A:380:VAL:HG23	0.405
6	A:280:LEU:HD21	A:345:VAL:CG1	0.403
7	A:60:THR:HB	A:64:ARG:CZ	0.793
7	A:139:LEU:HD21	A:598:ILE:HD12	0.782
7	A:138:TYR:CD1	A:181:LEU:HD22	0.765
7	A:598:ILE:HD11	A:628:TYR:CE1	0.712
7	A:58:ALA:HB2	A:746:ARG:NH2	0.702
7	A:83:ILE:HD13	A:185:VAL:HG21	0.679
7	A:59:ALA:H	A:194:LEU:HD22	0.673
7	A:641:GLN:HE22	A:724:SER:HA	0.662
7	A:108:GLY:CA	A:184:MET:HE2	0.652
7	A:109:VAL:HG22	A:184:MET:HE1	0.652
7	A:63:ALA:H	A:226:ARG:HH11	0.652
7	A:79:VAL:HG12	A:81:GLN:H	0.647
7	A:85:VAL:HG11	A:124:ILE:HB	0.640
7	A:128:PHE:CD1	A:642:VAL:HG22	0.640
7	A:108:GLY:HA2	A:184:MET:HE2	0.614
7	A:109:VAL:HB	A:162:ALA:HB3	0.614
7	A:377:LYS:HE2	A:426:TYR:CE1	0.605
7	A:265:LEU:HD12	A:314:MET:HE1	0.596
7	A:106:THR:CG2	A:186:SER:HA	0.595
7	A:83:ILE:HD13	A:185:VAL:CG2	0.591

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:566:PRO:HG2	A:610:ALA:HB3	0.590
7	A:79:VAL:HG13	A:171:VAL:HG21	0.581
7	A:99:VAL:CG2	A:610:ALA:HB2	0.564
7	A:171:VAL:HG13	A:481:THR:HG21	0.563
7	A:59:ALA:H	A:194:LEU:CD2	0.560
7	A:58:ALA:HB2	A:746:ARG:HH21	0.557
7	A:277:TYR:CD1	A:303:ALA:CB	0.555
7	A:99:VAL:HG21	A:610:ALA:HB2	0.551
7	A:286:VAL:HG23	A:731:CYS:SG	0.551
7	A:59:ALA:HB3	A:196:GLU:CD	0.549
7	A:58:ALA:HA	A:194:LEU:HD22	0.547
7	A:128:PHE:CD1	A:642:VAL:CG2	0.545
7	A:64:ARG:NH2	A:189:PRO:HG2	0.545
7	A:106:THR:HG23	A:186:SER:HA	0.537
7	A:139:LEU:CD2	A:598:ILE:HD12	0.536
7	A:60:THR:CB	A:64:ARG:CZ	0.531
7	A:67:ALA:O	A:68:THR:HG23	0.528
7	A:54:ALA:HB1	A:55:TRP:CD1	0.527
7	A:60:THR:N	A:194:LEU:HD13	0.526
7	A:76:ILE:HB	A:187:LYS:CE	0.521
7	A:129:ALA:HB3	A:641:GLN:O	0.521
7	A:158:MET:HE1	A:247:ALA:C	0.520
7	A:606:GLU:OE1	A:608:LYS:HE3	0.520

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:76:ILE:HB	A:187:LYS:HE2	0.518
7	A:180:GLY:C	A:182:LEU:H	0.515
7	A:64:ARG:HH22	A:189:PRO:HB2	0.515
7	A:173:TYR:CE1	A:393:GLN:NE2	0.514
7	A:47:ALA:HB1	A:48:PRO:CD	0.511
7	A:290:PRO:CG	A:436:TYR:CD1	0.508
7	A:158:MET:SD	A:249:ALA:HB3	0.507
7	A:638:THR:H	A:681:ASN:HD21	0.507
7	A:103:LEU:HD22	A:568:VAL:CG2	0.505
7	A:109:VAL:CG2	A:164:ILE:HD12	0.504
7	A:63:ALA:H	A:226:ARG:NH1	0.503
7	A:114:ARG:CZ	A:735:ALA:HB3	0.500
7	A:377:LYS:HE2	A:426:TYR:CZ	0.500
7	A:346:TYR:CD1	A:376:ARG:CZ	0.498
7	A:491:GLN:HE21	A:535:PRO:HB3	0.495
7	A:60:THR:HG21	A:64:ARG:NH2	0.494
7	A:136:ASN:HA	A:538:GLN:CD	0.493
7	A:141:GLY:C	A:142:LEU:HG	0.493
7	A:167:GLY:HA2	A:185:VAL:HG13	0.492
7	A:95:GLN:HB3	A:696:ARG:HH11	0.488
7	A:59:ALA:N	A:194:LEU:HD13	0.488
7	A:677:GLY:HA3	A:683:PHE:CZ	0.485
7	A:114:ARG:NH1	A:735:ALA:H	0.483

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:153:VAL:HG12	A:155:ASP:HA	0.482
7	A:171:VAL:HG12	A:470:GLN:HE22	0.482
7	A:64:ARG:NH2	A:189:PRO:HB2	0.482
7	A:598:ILE:HD13	A:639:PRO:HG3	0.481
7	A:283:GLU:OE2	A:732:PHE:CD1	0.479
7	A:128:PHE:CZ	A:626:ALA:HB1	0.474
7	A:114:ARG:NH2	A:735:ALA:HB3	0.474
7	A:283:GLU:CD	A:732:PHE:HA	0.471
7	A:174:GLY:O	A:485:ARG:HD2	0.469
7	A:79:VAL:HG13	A:171:VAL:CG2	0.468
7	A:372:HIS:CD2	A:436:TYR:CE2	0.462
7	A:728:THR:HB	A:729:TYR:CE2	0.462
7	A:91:MET:SD	A:102:ALA:HB1	0.461
7	A:139:LEU:HD21	A:598:ILE:CD1	0.461
7	A:606:GLU:CD	A:608:LYS:HE3	0.459
7	A:159:LEU:HD21	A:210:GLY:HA3	0.458
7	A:120:TYR:CE2	A:238:GLN:NE2	0.457
7	A:60:THR:H	A:194:LEU:CD1	0.457
7	A:106:THR:HG23	A:187:LYS:N	0.456
7	A:61:ILE:H	A:226:ARG:NH2	0.456
7	A:661:SER:HB3	A:701:ARG:CZ	0.454
7	A:83:ILE:HD13	A:185:VAL:CB	0.452
7	A:81:GLN:HE22	A:178:PRO:HB2	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:353:ASP:O	A:359:SER:HB2	0.452
7	A:566:PRO:CG	A:610:ALA:HB3	0.451
7	A:76:ILE:HD12	A:187:LYS:HE3	0.450
7	A:352:SER:HB2	A:729:TYR:CE2	0.449
7	A:156:PRO:HB3	A:162:ALA:HB2	0.448
7	A:240:GLY:O	A:277:TYR:CD2	0.447
7	A:137:ASN:CG	A:582:LEU:C	0.445
7	A:281:PRO:C	A:283:GLU:H	0.444
7	A:295:LEU:HD21	A:435:LEU:HD22	0.444
7	A:59:ALA:CA	A:194:LEU:HD13	0.440
7	A:83:ILE:CD1	A:185:VAL:HG21	0.440
7	A:83:ILE:CG1	A:185:VAL:HB	0.439
7	A:83:ILE:CD1	A:185:VAL:CG2	0.439
7	A:597:GLU:HB3	A:630:THR:HG23	0.437
7	A:84:SER:HA	A:107:PRO:CG	0.436
7	A:60:THR:N	A:194:LEU:CD1	0.436
7	A:128:PHE:CE1	A:626:ALA:CB	0.435
7	A:237:GLN:OE1	A:735:ALA:HB2	0.434
7	A:114:ARG:HH12	A:735:ALA:H	0.433
7	A:109:VAL:CG2	A:184:MET:HE1	0.430
7	A:131:GLU:OE2	A:732:PHE:CD2	0.430
7	A:82:SER:C	A:83:ILE:HD12	0.428
7	A:120:TYR:CE1	A:131:GLU:CD	0.428

Model ID	Atom-1	Atom-2	Clash overlap (Å)
7	A:116:ALA:HB3	A:239:LYS:HE3	0.427
7	A:428:ASP:HA	A:445:PHE:CD2	0.427
7	A:142:LEU:HD23	A:532:SER:HB3	0.423
7	A:60:THR:CB	A:64:ARG:NH2	0.422
7	A:143:LYS:HE2	A:145:GLN:HG3	0.421
7	A:339:LYS:HE3	A:384:LYS:HE3	0.419
7	A:70:THR:CB	A:330:ARG:HD3	0.415
7	A:99:VAL:HG21	A:610:ALA:CA	0.415
7	A:158:MET:HE1	A:248:ILE:HA	0.414
7	A:352:SER:HG	A:729:TYR:HD2	0.412
7	A:711:LEU:HD11	A:739:VAL:CG1	0.410
7	A:158:MET:SD	A:249:ALA:CB	0.407
7	A:64:ARG:NH2	A:189:PRO:CG	0.407
7	A:128:PHE:CZ	A:600:ALA:HB2	0.406
7	A:83:ILE:HG21	A:185:VAL:H	0.404
7	A:121:ASP:C	A:122:HIS:CG	0.404
7	A:311:ASN:OD1	A:313:LYS:HE3	0.404
7	A:158:MET:HB2	A:228:THR:HG21	0.403
7	A:103:LEU:HD22	A:568:VAL:HB	0.403
7	A:353:ASP:O	A:359:SER:CB	0.403
7	A:356:ASN:HA	A:587:GLU:HA	0.401
7	A:60:THR:CG2	A:161:ARG:HH11	0.401
7	A:136:ASN:HA	A:538:GLN:NE2	0.400

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:157:TYR:CG	A:230:LEU:HD22	0.809
8	A:110:SER:HB3	A:124:ILE:HD12	0.772
8	A:157:TYR:CE1	A:230:LEU:HD13	0.716
8	A:68:THR:HG23	A:100:LYS:CE	0.703
8	A:277:TYR:CE1	A:298:ASP:HA	0.696
8	A:171:VAL:HG21	A:512:ARG:CZ	0.689
8	A:157:TYR:CD1	A:230:LEU:HD22	0.688
8	A:171:VAL:HG11	A:512:ARG:NH2	0.687
8	A:694:LEU:HD13	A:712:HIS:CE1	0.679
8	A:138:TYR:CD2	A:180:GLY:HA3	0.675
8	A:191:THR:C	A:193:PRO:HD3	0.666
8	A:107:PRO:CG	A:109:VAL:HG22	0.663
8	A:87:THR:HG21	A:121:ASP:CG	0.654
8	A:84:SER:HA	A:166:ARG:CZ	0.651
8	A:68:THR:HG23	A:100:LYS:HE3	0.648
8	A:129:ALA:HA	A:182:LEU:HD11	0.635
8	A:346:TYR:CE2	A:377:LYS:HE3	0.624
8	A:157:TYR:CE1	A:189:PRO:HA	0.613
8	A:172:LEU:HD11	A:472:GLN:CD	0.612
8	A:70:THR:HG21	A:79:VAL:HG21	0.611
8	A:72:THR:HA	A:173:TYR:CD2	0.611
8	A:103:LEU:HA	A:608:LYS:HZ2	0.602
8	A:141:GLY:HA3	A:165:MET:HE2	0.598

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:68:THR:HG23	A:100:LYS:HE2	0.592
8	A:171:VAL:HG11	A:512:ARG:HH21	0.586
8	A:172:LEU:HD21	A:472:GLN:HG3	0.575
8	A:157:TYR:CD2	A:230:LEU:HD22	0.573
8	A:70:THR:HG21	A:79:VAL:CG2	0.571
8	A:103:LEU:HA	A:608:LYS:NZ	0.569
8	A:153:VAL:H	A:310:ARG:NH2	0.568
8	A:462:GLN:CD	A:491:GLN:HE22	0.566
8	A:608:LYS:HE3	A:618:VAL:HG13	0.558
8	A:295:LEU:HD21	A:435:LEU:HD22	0.557
8	A:100:LYS:HA	A:103:LEU:HD12	0.537
8	A:379:VAL:HG22	A:424:PHE:CD1	0.531
8	A:173:TYR:CE1	A:330:ARG:NH1	0.517
8	A:86:VAL:CG2	A:105:TYR:HA	0.516
8	A:164:ILE:HA	A:185:VAL:HG11	0.516
8	A:191:THR:HB	A:193:PRO:HD3	0.513
8	A:67:ALA:O	A:100:LYS:HE2	0.509
8	A:223:TYR:CE1	A:255:ARG:CZ	0.508
8	A:215:ASP:HB3	A:225:TYR:CE1	0.506
8	A:107:PRO:CB	A:109:VAL:HG22	0.505
8	A:141:GLY:N	A:165:MET:HE2	0.502
8	A:94:HIS:CE1	A:190:THR:OG1	0.500
8	A:141:GLY:CA	A:165:MET:HE2	0.497

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:23:ALA:O	A:24:VAL:HG23	0.496
8	A:86:VAL:HG21	A:105:TYR:CD1	0.496
8	A:638:THR:H	A:681:ASN:HD21	0.495
8	A:339:LYS:HE3	A:384:LYS:HE3	0.493
8	A:85:VAL:O	A:86:VAL:HG23	0.491
8	A:119:THR:HG22	A:232:ARG:NH2	0.489
8	A:67:ALA:C	A:100:LYS:HE2	0.488
8	A:141:GLY:C	A:177:SER:HB3	0.488
8	A:269:GLN:HG2	A:270:ASN:H	0.487
8	A:139:LEU:CD2	A:154:ILE:HD12	0.483
8	A:181:LEU:CD1	A:578:LYS:HE3	0.483
8	A:267:TYR:CG	A:268:PHE:N	0.481
8	A:85:VAL:HG21	A:123:LEU:HD22	0.473
8	A:106:THR:HG1	A:606:GLU:CD	0.472
8	A:721:TYR:CZ	A:734:GLY:HA3	0.467
8	A:103:LEU:HD11	A:568:VAL:HB	0.464
8	A:103:LEU:CD1	A:568:VAL:HB	0.459
8	A:110:SER:CB	A:124:ILE:HD12	0.454
8	A:79:VAL:HG12	A:81:GLN:H	0.443
8	A:181:LEU:HD13	A:578:LYS:CE	0.441
8	A:200:LYS:HE2	A:740:VAL:HG13	0.440
8	A:128:PHE:CE2	A:576:LEU:HD23	0.435
8	A:86:VAL:HG21	A:105:TYR:HA	0.434

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:348:TYR:CD2	A:377:LYS:HE2	0.434
8	A:252:PHE:CE1	A:254:TRP:HB2	0.433
8	A:245:ARG:O	A:268:PHE:HA	0.431
8	A:86:VAL:HG11	A:105:TYR:HD1	0.424
8	A:103:LEU:CD2	A:568:VAL:HB	0.424
8	A:70:THR:HG21	A:79:VAL:CB	0.421
8	A:247:ALA:O	A:266:SER:HA	0.420
8	A:71:LYS:HE3	A:165:MET:HA	0.419
8	A:71:LYS:C	A:72:THR:CG2	0.418
8	A:191:THR:CB	A:193:PRO:HD3	0.418
8	A:317:TYR:CE1	A:333:LEU:HB3	0.416
8	A:295:LEU:CD2	A:435:LEU:HD22	0.415
8	A:248:ILE:HG23	A:265:LEU:O	0.414
8	A:117:SER:C	A:119:THR:H	0.413
8	A:85:VAL:C	A:86:VAL:HG23	0.411
8	A:193:PRO:HG2	A:196:GLU:CD	0.411
8	A:171:VAL:HG21	A:512:ARG:NH2	0.410
8	A:86:VAL:HB	A:105:TYR:HA	0.408
8	A:107:PRO:CG	A:109:VAL:CG2	0.408
8	A:138:TYR:CE2	A:180:GLY:CA	0.408
8	A:141:GLY:HA3	A:165:MET:CE	0.408
8	A:249:ALA:HB3	A:265:LEU:HD12	0.408
8	A:70:THR:O	A:72:THR:N	0.407

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	A:191:THR:HB	A:193:PRO:CD	0.406
8	A:246:TYR:CE1	A:268:PHE:CD2	0.405
8	A:145:GLN:NE2	A:537:SER:HB3	0.405
8	A:109:VAL:HG12	A:110:SER:C	0.404
8	A:243:GLU:O	A:270:ASN:HA	0.404
8	A:133:GLN:HE22	A:641:GLN:CD	0.403
8	A:200:LYS:HE2	A:740:VAL:CG1	0.400
9	A:459:LEU:HD22	A:496:ARG:HH21	0.693
9	A:18:VAL:O	A:19:VAL:HG23	0.672
9	A:566:PRO:HG2	A:610:ALA:HB3	0.657
9	A:100:LYS:NZ	A:113:THR:HG23	0.650
9	A:58:ALA:HB1	A:610:ALA:HB2	0.638
9	A:109:VAL:HG21	A:164:ILE:HD13	0.634
9	A:168:PRO:HB3	A:532:SER:HB3	0.620
9	A:276:TYR:CE1	A:277:TYR:CD2	0.601
9	A:276:TYR:CZ	A:277:TYR:CE2	0.601
9	A:280:LEU:HD11	A:733:TRP:HE1	0.594
9	A:459:LEU:HD22	A:496:ARG:NH2	0.591
9	A:362:CYS:SG	A:375:ALA:HB2	0.588
9	A:295:LEU:HD21	A:435:LEU:HB3	0.579
9	A:165:MET:SD	A:173:TYR:CZ	0.575
9	A:276:TYR:CZ	A:277:TYR:CZ	0.574
9	A:721:TYR:CZ	A:734:GLY:HA3	0.573

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:103:LEU:HD22	A:164:ILE:HD11	0.567
9	A:280:LEU:CD1	A:733:TRP:HE1	0.549
9	A:312:GLU:OE1	A:314:MET:HE3	0.540
9	A:641:GLN:NE2	A:725:CYS:H	0.537
9	A:106:THR:HG21	A:164:ILE:HD12	0.531
9	A:424:PHE:CZ	A:590:PHE:CD2	0.527
9	A:100:LYS:HZ3	A:113:THR:HG23	0.522
9	A:638:THR:H	A:681:ASN:HD21	0.515
9	A:566:PRO:CG	A:610:ALA:HB3	0.502
9	A:153:VAL:CG2	A:310:ARG:HH12	0.501
9	A:153:VAL:HG23	A:310:ARG:HH12	0.490
9	A:123:LEU:CD1	A:182:LEU:HD22	0.488
9	A:348:TYR:CE1	A:375:ALA:HB1	0.481
9	A:106:THR:HG22	A:166:ARG:HH21	0.478
9	A:169:VAL:HG23	A:181:LEU:HD12	0.476
9	A:100:LYS:HZ2	A:113:THR:HG23	0.470
9	A:425:GLY:HA2	A:453:SER:CB	0.468
9	A:425:GLY:CA	A:453:SER:CB	0.467
9	A:58:ALA:CB	A:610:ALA:HB2	0.464
9	A:425:GLY:HA2	A:453:SER:HB3	0.462
9	A:165:MET:CB	A:169:VAL:HG21	0.461
9	A:425:GLY:CA	A:453:SER:HB3	0.453
9	A:169:VAL:HG23	A:181:LEU:CD1	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
9	A:135:GLN:O	A:143:LYS:HE3	0.451
9	A:171:VAL:HG12	A:470:GLN:HB2	0.444
9	A:424:PHE:CZ	A:590:PHE:CE2	0.443
9	A:131:GLU:O	A:148:PHE:CE1	0.442
9	A:128:PHE:CE2	A:576:LEU:HD23	0.439
9	A:167:GLY:O	A:169:VAL:HG22	0.438
9	A:720:GLU:HB3	A:733:TRP:CZ3	0.438
9	A:165:MET:SD	A:173:TYR:CE2	0.425
9	A:165:MET:SD	A:169:VAL:HG21	0.423
9	A:425:GLY:CA	A:453:SER:HB2	0.423
9	A:271:GLU:CD	A:310:ARG:HH21	0.415
9	A:46:ALA:O	A:47:ALA:C	0.410
9	A:100:LYS:HB2	A:121:ASP:CG	0.408
9	A:119:THR:HG22	A:245:ARG:NH2	0.408
9	A:100:LYS:CG	A:111:VAL:HG11	0.407
10	A:67:ALA:HB2	A:161:ARG:HH21	0.776
10	A:67:ALA:HB2	A:161:ARG:NH2	0.717
10	A:721:TYR:HB3	A:734:GLY:HA3	0.691
10	A:393:GLN:HE21	A:408:LEU:HD22	0.655
10	A:299:PHE:CE1	A:733:TRP:CZ2	0.639
10	A:171:VAL:HG22	A:512:ARG:CD	0.597
10	A:171:VAL:HG22	A:512:ARG:HD2	0.592
10	A:128:PHE:CE1	A:578:LYS:HB2	0.574

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:445:PHE:HA	A:448:LYS:HE3	0.572
10	A:174:GLY:HA3	A:468:TYR:CD1	0.559
10	A:70:THR:HG21	A:74:THR:O	0.549
10	A:138:TYR:CE2	A:181:LEU:HD22	0.548
10	A:128:PHE:CE2	A:178:PRO:HG2	0.547
10	A:113:THR:HG21	A:735:ALA:HB2	0.545
10	A:119:THR:HG21	A:310:ARG:HH22	0.545
10	A:721:TYR:CB	A:734:GLY:HA3	0.541
10	A:68:THR:HG21	A:183:ASN:ND2	0.537
10	A:238:GLN:NE2	A:299:PHE:CE2	0.516
10	A:68:THR:O	A:173:TYR:CE2	0.505
10	A:128:PHE:CD1	A:578:LYS:HD2	0.497
10	A:596:GLY:H	A:632:THR:HG21	0.497
10	A:285:THR:HB	A:296:PRO:CG	0.495
10	A:297:THR:HA	A:299:PHE:CE2	0.493
10	A:139:LEU:HB2	A:144:LEU:HD11	0.491
10	A:178:PRO:HD3	A:532:SER:HB2	0.483
10	A:688:TYR:CZ	A:721:TYR:CE2	0.480
10	A:171:VAL:HG22	A:512:ARG:CG	0.471
10	A:549:SER:HB2	A:578:LYS:HE3	0.463
10	A:93:LEU:O	A:694:LEU:HD22	0.455
10	A:174:GLY:HA3	A:468:TYR:CE1	0.454
10	A:71:LYS:HE3	A:173:TYR:CZ	0.452

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:93:LEU:HD21	A:652:ASP:OD2	0.444
10	A:100:LYS:HD2	A:121:ASP:HB2	0.444
10	A:174:GLY:HA3	A:468:TYR:CG	0.443
10	A:167:GLY:O	A:179:GLY:HA2	0.443
10	A:128:PHE:CD1	A:578:LYS:CD	0.438
10	A:395:GLN:HA	A:408:LEU:HD23	0.438
10	A:549:SER:HB2	A:578:LYS:CE	0.438
10	A:351:CYS:SG	A:728:THR:HG21	0.436
10	A:171:VAL:HB	A:470:GLN:CD	0.435
10	A:178:PRO:HB3	A:532:SER:CB	0.431
10	A:459:LEU:HD22	A:496:ARG:HH21	0.431
10	A:238:GLN:OE1	A:299:PHE:CD2	0.424
10	A:168:PRO:HA	A:178:PRO:HA	0.422
10	A:135:GLN:O	A:143:LYS:HE3	0.419
10	A:455:PRO:O	A:497:VAL:HG21	0.419
10	A:583:MET:CE	A:634:TYR:CE2	0.419
10	A:339:LYS:HE3	A:382:ASP:OD1	0.418
10	A:126:ARG:CZ	A:574:TYR:CG	0.414
10	A:198:GLN:OE1	A:200:LYS:HE3	0.414
10	A:167:GLY:C	A:179:GLY:HA3	0.412
10	A:18:VAL:O	A:18:VAL:HG12	0.410
10	A:119:THR:HG22	A:153:VAL:HG21	0.409
10	A:337:GLU:CD	A:384:LYS:HE3	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:172:LEU:HD23	A:408:LEU:CD1	0.406
10	A:691:VAL:O	A:715:ASN:HA	0.406
10	A:128:PHE:CE1	A:578:LYS:CB	0.403
10	A:171:VAL:HG21	A:483:GLY:HA3	0.403
10	A:100:LYS:CD	A:121:ASP:HB2	0.402
10	A:172:LEU:HA	A:408:LEU:HD12	0.402
10	A:103:LEU:HD22	A:164:ILE:CD1	0.401
10	A:171:VAL:HB	A:470:GLN:OE1	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
1	745	638	65	42
2	745	679	51	15
3	745	668	56	21
4	745	659	62	24
5	745	693	37	15
6	745	648	69	28
7	745	697	36	12
8	745	632	72	41
9	745	682	47	16
10	745	691	41	13

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	616	576	23	17
2	616	569	31	16
3	616	590	15	11
4	616	603	8	5
5	616	577	22	17
6	616	595	15	6
7	616	569	26	21
8	616	582	23	11
9	616	598	11	7
10	616	587	18	11

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	6	THR
1	A	22	THR
1	A	28	SER
1	A	41	THR
1	A	53	SER
1	A	66	SER
1	A	83	ILE
1	A	113	THR
1	A	153	VAL
1	A	164	ILE
1	A	171	VAL

Model ID	Chain	Residue ID	Residue type
1	A	177	SER
1	A	203	THR
1	A	206	LEU
1	A	414	MET
1	A	633	THR
1	A	728	THR
2	A	6	THR
2	A	41	THR
2	A	45	THR
2	A	82	SER
2	A	85	VAL
2	A	86	VAL
2	A	89	GLU
2	A	114	ARG
2	A	119	THR
2	A	123	LEU
2	A	142	LEU
2	A	164	ILE
2	A	173	TYR
2	A	216	SER
2	A	325	ASP
2	A	328	THR
3	A	6	THR

Model ID	Chain	Residue ID	Residue type
3	A	22	THR
3	A	41	THR
3	A	60	THR
3	A	93	LEU
3	A	119	THR
3	A	358	TYR
3	A	374	LEU
3	A	378	TYR
3	A	435	LEU
3	A	439	VAL
4	A	22	THR
4	A	41	THR
4	A	45	THR
4	A	169	VAL
4	A	173	TYR
5	A	6	THR
5	A	22	THR
5	A	41	THR
5	A	45	THR
5	A	76	ILE
5	A	111	VAL
5	A	119	THR
5	A	123	LEU

Model ID	Chain	Residue ID	Residue type
5	A	139	LEU
5	A	144	LEU
5	A	173	TYR
5	A	182	LEU
5	A	214	SER
5	A	414	MET
5	A	433	LEU
5	A	633	THR
5	A	728	THR
6	A	6	THR
6	A	22	THR
6	A	41	THR
6	A	45	THR
6	A	169	VAL
6	A	728	THR
7	A	6	THR
7	A	19	VAL
7	A	22	THR
7	A	24	VAL
7	A	41	THR
7	A	43	THR
7	A	44	VAL
7	A	45	THR

Model ID	Chain	Residue ID	Residue type
7	A	131	GLU
7	A	151	ASP
7	A	166	ARG
7	A	177	SER
7	A	186	SER
7	A	265	LEU
7	A	344	SER
7	A	351	CYS
7	A	433	LEU
7	A	582	LEU
7	A	598	ILE
7	A	728	THR
7	A	737	ARG
8	A	4	SER
8	A	6	THR
8	A	41	THR
8	A	60	THR
8	A	68	THR
8	A	93	LEU
8	A	109	VAL
8	A	165	MET
8	A	171	VAL
8	A	177	SER

Model ID	Chain	Residue ID	Residue type
8	A	186	SER
9	A	6	THR
9	A	22	THR
9	A	45	THR
9	A	113	THR
9	A	169	VAL
9	A	171	VAL
9	A	527	PHE
10	A	6	THR
10	A	22	THR
10	A	41	THR
10	A	45	THR
10	A	122	HIS
10	A	169	VAL
10	A	171	VAL
10	A	414	MET
10	A	453	SER
10	A	682	SER
10	A	721	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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