

Integrative Structure Validation Report

July 22, 2024 - 03:43 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	8ZZG
PDB-Dev ID	PDBDEV_00000016
Structure Title	Integrative structure-function mapping of the nucleoporin Nup133
Structure Authors	Kim SJ; Fernandez-Martinez J; Sampathkumar P; Martel A; Matsui T; Tsuruta H; Weiss TM; Shi Y; Markina-Inarrairaegui A; Bonanno JB; Sauder JM; Burley SK; Chait BT; Almo SC; Rout MP; Sali A

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

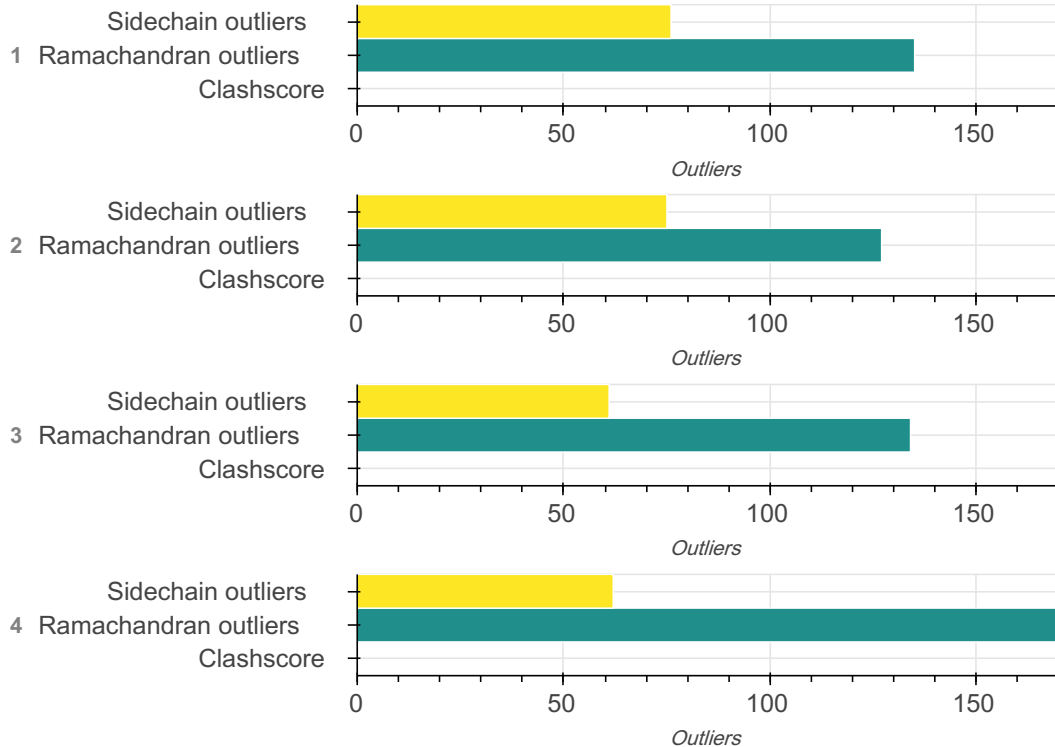
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

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



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 4 unique models, with 1 subunits in each model. A total of 56 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 4 unique types of models in this entry. These models are titled 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	Nup133	A	A	1166
2	1	1	Nup133	A	A	1166
3	1	1	Nup133	A	A	1166

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	1	1	Nup133	A	A	1166

Datasets used for modeling

There are 56 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	SAS data	File	10.5281/zenodo.1209565
2	SAS data	File	10.5281/zenodo.1209565
3	SAS data	File	10.5281/zenodo.1209565
4	SAS data	File	10.5281/zenodo.1209565
5	SAS data	File	10.5281/zenodo.1209565
6	SAS data	File	10.5281/zenodo.1209565
7	SAS data	File	10.5281/zenodo.1209565
8	SAS data	File	10.5281/zenodo.1209565
9	SAS data	File	10.5281/zenodo.1209565
10	SAS data	File	10.5281/zenodo.1209565
11	SAS data	File	10.5281/zenodo.1209565
12	SAS data	File	10.5281/zenodo.1209565
13	SAS data	File	10.5281/zenodo.1209565
14	SAS data	File	10.5281/zenodo.1209565
15	SAS data	File	10.5281/zenodo.1209565
16	SAS data	File	10.5281/zenodo.1209565
17	SAS data	File	10.5281/zenodo.1209565
18	SAS data	File	10.5281/zenodo.1209565

ID	Dataset type	Database name	Data access code
19	SAS data	File	10.5281/zenodo.1209565
20	2DEM class average	File	10.5281/zenodo.1209565
21	2DEM class average	File	10.5281/zenodo.1209565
22	2DEM class average	File	10.5281/zenodo.1209565
23	2DEM class average	File	10.5281/zenodo.1209565
24	2DEM class average	File	10.5281/zenodo.1209565
25	2DEM class average	File	10.5281/zenodo.1209565
26	2DEM class average	File	10.5281/zenodo.1209565
27	2DEM class average	File	10.5281/zenodo.1209565
28	2DEM class average	File	10.5281/zenodo.1209565
29	2DEM class average	File	10.5281/zenodo.1209565
30	2DEM class average	File	10.5281/zenodo.1209565
31	2DEM class average	File	10.5281/zenodo.1209565
32	2DEM class average	File	10.5281/zenodo.1209565
33	2DEM class average	File	10.5281/zenodo.1209565
34	2DEM class average	File	10.5281/zenodo.1209565
35	2DEM class average	File	10.5281/zenodo.1209565
36	2DEM class average	File	10.5281/zenodo.1209565
37	2DEM class average	File	10.5281/zenodo.1209565
38	2DEM class average	File	10.5281/zenodo.1209565
39	2DEM class average	File	10.5281/zenodo.1209565
40	2DEM class average	File	10.5281/zenodo.1209565
41	2DEM class average	File	10.5281/zenodo.1209565

ID	Dataset type	Database name	Data access code
42	2DEM class average	File	10.5281/zenodo.1209565
43	Crosslinking-MS data	File	10.5281/zenodo.1209565
44	Experimental model	PDB	3I4R
45	Experimental model	PDB	3KFO
46	Experimental model	PDB	4Q9T
47	Experimental model	PDB	2JO8
48	Experimental model	PDB	2QIW
49	Experimental model	PDB	3CIG
50	Experimental model	PDB	2ELO
51	Experimental model	PDB	3GUZ
52	Experimental model	PDB	2CIW
53	Experimental model	PDB	1A92
54	Experimental model	PDB	1GDJ
55	Experimental model	PDB	1X4O
56	Comparative model	File	10.5281/zenodo.1209565

Representation ?

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-1166

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	AllosMod	MD-based conformational sampling	None	7000	True	False
2	1	MES	Minimal Ensemble Search	None	4	True	False

There are 6 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HHpred	2.0.16	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred
2	PSIPRED	4.0	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
3	DISOPRED	3	disorder prediction	http://bioinf.cs.ucl.ac.uk/psipred/?disopred=1
4	Integrative Modeling Platform (IMP)	2.2	integrative model building	https://integrativemodeling.org
5	MODELLER	9.13	comparative modeling	https://salilab.org/modeller/
6	AllosMod	Not available	sampling	https://salilab.org/allosmod

Data quality ?

2DEM class average

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobit analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers ?

There are 3419 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
CB-CG-OD1	120.80	35.84	1
CB-CG-OD1	120.80	41.81	1
CB-CG-OD1	120.80	43.01	1
CG-CD-OE1	120.80	43.17	1
CG-CD-OE1	120.80	48.94	1
CA-CB-CG	113.80	94.74	1
CA-CB-CG	112.60	94.03	1
CA-CB-CG	113.80	95.83	1
CA-CB-CG-CD-NE2	116.40	89.74	1
OE1-CD-NE2	122.60	140.06	1
CA-CB-CG	113.80	96.59	1
CG-CD-NE2	116.40	91.13	1
CA-CB-CG	113.80	97.01	1
OD1-CG-ND2	122.60	139.36	1
CA-CB-CG	113.80	97.91	1
CA-CB-CG	113.80	98.50	1
CA-CB-CG	113.80	98.51	1
NE-CZ-NH2	119.20	105.46	1
CA-CB-CG	112.60	97.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	99.37	1
OD1-CG-ND2	122.60	136.95	1
NE-CZ-NH2	119.20	106.38	1
CB-CG-ND2	116.40	95.54	1
CA-CB-CG	113.80	100.28	1
CB-CG-ND2	116.40	96.36	1
CA-CB-CG	112.60	99.41	1
CA-CB-CG	113.80	100.66	1
CA-CB-CG	113.80	100.72	1
CA-CB-CG	112.60	99.57	1
CA-CB-CG	113.80	100.79	1
CA-CB-CG	112.60	99.59	1
CA-CB-CG	112.60	99.71	1
NE-CZ-NH1	121.50	108.66	1
CA-CB-CG	112.60	99.89	1
NE-CZ-NH1	121.50	109.16	1
CA-CB-CG	112.60	100.28	2
CA-CB-CG	113.80	101.52	1
CA-CB-CG	112.60	100.35	1
CA-CB-CG	113.80	101.56	1
CD-NE-CZ	124.40	107.47	1
CA-CB-CG	112.60	100.56	1
CA-CB-CG	112.60	100.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	134.53	1
CA-CB-CG	112.60	124.49	1
CA-CB-CA-CB-NE-CZ-NH1	121.50	109.68	1
CA-CB-CG	112.60	100.81	1
CA-CB-CG	113.80	102.01	1
CA-CB-CG	112.60	100.87	1
CA-CB-CG	112.60	100.89	1
CA-CB-CG	112.60	100.91	1
CB-CG-ND2	116.40	98.90	1
CA-CB-CA-CB-CG	112.60	100.95	1
CA-CB-CG	112.60	100.99	1
CA-CB-CG	112.60	101.07	1
CA-CB-CG	112.60	101.10	1
CA-CB-CA-CB-CG	112.60	101.19	1
CA-CB-CG	113.80	102.39	1
CA-CB-CG	112.60	101.25	1
CA-CB-CG	113.80	102.47	1
CA-CB-CG	112.60	101.28	1
CA-CB-NE-CZ-CA-CB-CG	113.80	102.58	1
CA-CB-CG	113.80	102.64	1
CA-CB-CG	113.80	102.73	1
CA-CB-CG	112.60	101.56	1
CA-CB-CG	113.80	102.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	101.74	1
CA-CB-CA-CB-CG	112.60	101.80	1
CA-CB-CG	112.60	101.87	1
CA-CB-CA-CB-CG	112.60	101.88	1
CA-CB-CG	112.60	101.91	2
CA-CB-CG	112.60	101.96	1
C-N-CA	121.70	102.63	1
CA-CB-CG	112.60	102.04	1
CA-CB-CG	113.80	103.28	1
CA-CB-CG	113.80	103.30	1
CA-CB-CG	112.60	102.11	1
CA-CB-NE-CZ-NH1	121.50	111.06	1
CA-CB-CG	113.80	103.37	1
CA-CB-CG	112.60	102.22	1
CA-CB-CG	113.80	103.42	1
CD2-NE2-CE1	109.00	98.63	1
CA-CB-CG	112.60	102.28	1
CA-CB-CG	112.60	102.29	1
CA-CB-CG	112.60	102.30	2
CA-CB-CG	112.60	102.37	1
CA-CB-CG	112.60	102.41	1
CA-CB-CD2-NE2-CA-CB-CA-CB-CG	112.60	102.45	1
C-CA-CB	110.10	90.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	103.73	1
CA-CB-CG	113.80	103.85	1
CB-CG-CD	112.60	95.70	1
CA-CB-CG	112.60	102.66	1
NE-CZ-NH2	119.20	128.14	1
CA-CB-CG	113.80	103.90	1
CA-CB-CG	112.60	102.72	1
CA-CB-CG	113.80	103.92	1
NE-CZ-NH2	119.20	128.09	1
OE1-CD-NE2	122.60	132.46	1
CA-CB-CG	113.80	103.94	1
OD1-CG-ND2	122.60	132.45	1
CA-CB-CG	113.80	103.96	1
CA-CB-OD1-CG-ND2	122.60	132.43	1
CA-CB-CG	112.60	102.80	1
CA-CB-CG	112.60	102.82	1
CA-CB-CG	113.80	104.03	1
CD2-NE2-CE1	109.00	99.27	1
CA-CB-CG	112.60	102.87	1
CB-CG-ND2	116.40	101.83	1
CA-CB-CG	112.60	102.92	1
CA-CB-CG	113.80	104.17	1
CA-CB-CG	112.60	102.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	103.03	1
CA-CB-CG	112.60	122.14	1
OD1-CG-CG-CD2-NE2	107.20	116.74	1
CB-CG-CA-CB-CG	112.60	103.09	1
CA-CB-CG	113.80	104.29	2
CA-CB-CG	113.90	96.79	1
CG-SD-CE	100.90	80.01	1
CA-CB-CG	113.80	104.32	1
CA-CB-CG	112.60	103.12	2
CD-NE-CZ	124.40	111.14	1
CA-CB-CG	113.80	104.33	1
OD1-CG-ND2	122.60	113.13	1
CA-CB-OD1-CG-ND2	122.60	132.04	1
C-N-CA	121.70	138.67	1
CA-CB-CA-CB-CA-CB-CG	112.60	103.27	1
CA-CB-CG	113.80	104.49	2
CA-CB-CG	112.60	103.30	2
CA-CB-NE-CZ-NH2	119.20	127.55	1
CA-CB-CG	112.60	103.34	1
OD1-CG-ND2	122.60	113.34	1
CA-CB-CG	113.80	104.55	1
CA-CB-CG	112.60	121.82	1
CA-CB-CG	112.60	103.39	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	103.40	1
CA-CB-CA-CB-CB-CG-CD	112.60	97.03	1
CA-CB-CG	112.60	103.44	1
CA-CB-CG	113.80	122.92	1
CA-CB-CG	112.60	103.48	1
NE-CZ-CA-CB-CA-CB-CA-CB-CG	112.60	103.62	1
CA-CB-CG	113.80	104.83	1
C-CA-CB	110.50	97.06	1
CD2-NE2-CE1	109.00	100.05	1
CA-CB-CG	112.60	103.66	1
N-CA-CB	110.50	125.68	1
CA-CB-CG	112.60	121.52	1
CA-CB-CG	113.80	104.89	1
CA-CB-CG	113.80	104.90	1
C-N-CA	121.70	105.68	1
CA-CB-OD1-CG-ND2	122.60	113.74	1
CA-CB-CG	112.60	103.75	1
CA-CB-CD2-NE2-CA-CB-CG	112.60	103.76	1
CA-CB-CG	112.60	103.78	1
CA-CB-CG	112.60	103.79	1
CD-NE-CZ	124.40	112.06	1
CD2-NE2-CA-CB-CG	113.80	105.04	1
NE-CZ-NH2	119.20	127.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-C-N-CA	121.70	105.96	1
OD1-CG-ND2	122.60	131.34	1
CA-CB-CG	113.80	105.07	1
OD1-CG-ND2	122.60	131.29	1
CA-CB-CG	113.80	105.12	1
CA-CB-CG	112.60	103.93	1
NH1-CZ-CA-CB-CG	112.60	103.95	1
CA-CB-CG	112.60	103.96	1
CA-CB-CA-CB-CG	113.80	105.18	1
C-N-CA	121.70	106.19	1
CA-CB-CG	112.60	103.99	1
CB-CG-CD	112.60	98.00	1
CA-CB-CG	112.60	104.01	1
CA-CB-CG	112.60	104.03	1
CA-CB-CG	113.80	105.24	1
CA-C-N	116.90	104.08	1
CA-CB-CG	112.60	104.06	1
CA-CB-CA-CB-CG	112.60	121.12	1
CA-CB-CG	112.60	104.09	1
CA-CB-CG	112.60	104.10	1
CA-CB-CA-CB-CG	113.80	105.34	1
CB-CG-C-N-CA	121.70	106.52	1
OD1-CG-ND2	122.60	114.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-C-N-CA	121.70	106.57	1
CA-CB-CG	113.80	105.40	1
CG-SD-ND1-CE1-NE2	108.40	116.79	1
CA-CB-CG	112.60	104.23	1
CA-CB-OE1-CD-CB-CG-CD	112.60	98.38	1
CB-CG-OD1-CG-ND2	122.60	130.94	1
C-N-CA	121.70	106.68	1
CA-CB-CG	113.80	105.46	1
N-CA-CA-CB-CG	113.80	105.46	1
CA-CB-CG	112.60	104.26	1
CA-CB-CG	113.80	105.47	2
ND1-CE1-NE2	108.40	116.73	1
CB-CG-CD	112.60	98.47	1
C-N-CA	121.70	136.65	1
NE-CZ-NH2	119.20	111.73	1
CA-CB-CG	113.80	105.51	1
C-N-CA	121.70	136.63	1
CA-CB-CG	112.60	120.89	1
OE1-CD-NE2	122.60	114.32	1
CB-CG-CD	112.60	98.52	1
CB-CG-OD1	120.80	137.35	1
N-CA-CB	103.00	112.10	1
CA-CB-CG	112.60	104.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	106.85	1
CA-CB-CG	112.60	104.36	1
CA-CB-CG	113.80	105.58	1
CA-CB-CG	113.80	105.59	1
CD-NE-CZ	124.40	112.90	1
CA-CB-CB-CG-CD	112.60	98.64	1
CG-SD-CE	100.90	82.84	1
CA-CB-CG	113.90	99.13	1
CA-CB-CG	113.80	105.60	1
OD1-CG-ND2	122.60	130.80	1
CA-CB-CG	112.60	104.40	1
CA-CB-CG	113.80	105.61	2
CA-CB-CG	112.60	104.41	1
CB-CG-CD	112.60	98.72	1
CA-CB-CG	113.80	105.64	1
C-CA-CB	110.10	94.60	1
CA-CB-CG	112.60	104.44	1
CD-NE-CZ	124.40	112.99	1
CA-CB-CG	112.60	104.45	1
CA-CB-CG	113.80	105.66	1
NH1-CZ-NH2	119.30	129.88	1
CA-CB-CA-CB-CG	112.60	104.50	1
C-N-CA	121.70	107.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	105.71	1
CA-CB-CG	112.60	104.52	2
CA-CB-CG	113.80	105.72	1
C-N-CA	121.70	107.21	2
CA-CB-CG	112.60	104.55	1
C-N-CA	121.70	136.17	1
CA-CB-CG	112.60	104.56	1
NE-CZ-NH2	119.20	111.98	1
C-N-CA	121.70	107.26	1
CA-CB-CA-CB-CG	112.60	120.59	1
CA-CB-CG	112.60	120.59	1
CA-C-N	116.90	104.92	1
C-N-CG-CD2-NE2	107.20	115.17	1
CA-CB-CG	113.90	99.55	1
CB-CG-CD	112.60	99.06	1
CA-CB-CG	113.80	105.83	1
CD2-NE2-CE1	109.00	101.04	1
CA-CB-CG	112.60	104.64	1
CB-CG-OD1-CG-ND2	122.60	114.65	1
C-CA-N-CA-CB	110.40	122.32	1
CD-NE-CZ	124.40	113.28	1
CA-CB-CG	112.60	104.66	2
CA-CB-CG	113.80	105.86	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	123.99	1
CB-CG-NE-CZ-NH2	119.20	126.33	1
CB-CG-CD	112.60	99.14	2
CA-CB-CG	113.80	105.90	1
CA-CB-CG	113.80	105.91	1
OE1-CD-NE2	122.60	114.72	1
CA-CB-CG	112.60	104.74	1
CB-CG-CD	112.60	99.24	1
CA-CB-CG	112.60	104.75	1
NE-CZ-NH1	121.50	113.66	1
NE-CZ-CA-CB-CG	112.60	104.77	1
CA-CB-CG	113.80	105.98	1
C-N-CA	121.70	107.66	1
CB-CG-CD	112.60	99.35	1
CB-CG-CD	112.60	99.36	1
CA-CB-CG	112.60	104.82	1
CB-CG-CD	112.60	99.39	1
CA-CB-CG	113.80	121.56	1
C-N-CA	121.70	107.77	1
CG-CD2-NE2	107.20	114.94	1
CA-CB-CG	112.60	120.34	1
OD1-CG-ND2	122.60	130.33	1
CA-CB-CG	112.60	104.87	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	95.42	1
CA-CB-CG	113.80	106.08	1
CG-CD2-NE2	107.20	114.92	1
C-N-CA	121.70	107.84	1
C-CA-CB	110.10	95.49	1
NE-CZ-C-CA-CB	110.10	95.50	1
C-CA-CA-CB-CG	113.80	106.13	1
CA-CB-OD1-CG-ND2	122.60	130.26	1
CA-CB-CG	113.80	106.14	1
N-CA-CB	103.00	111.42	1
C-N-CA	121.70	135.48	1
CA-CB-CG	113.80	106.15	1
C-N-CA	121.70	107.93	2
CB-CG-ND2	116.40	104.94	1
NE-CZ-CA-CB-CG	113.80	106.16	1
CB-CG-CD	112.60	99.62	1
C-N-CA	121.70	107.98	1
CA-C-N	116.90	105.46	1
CB-CG-CD	112.60	99.65	1
ND1-CE1-NE2	108.40	116.02	1
CB-CG-CD	112.60	99.66	1
CG-SD-CE	100.90	84.15	1
CA-CB-CG	113.80	106.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	99.67	1
C-CA-CB	110.10	95.66	1
OD1-CG-ND2	122.60	115.00	1
CA-CB-CG	112.60	105.00	1
CG-CD2-CE3	133.90	126.33	1
CG-SD-CE	100.90	84.25	1
N-CA-CB	110.50	123.37	1
CA-CB-CG	112.60	105.03	1
CA-C-N	116.90	128.25	1
CA-CB-CG	113.90	100.33	1
CA-CB-CG	113.80	106.27	1
C-CA-CB	111.40	97.10	1
CA-CB-CG	112.60	105.08	2
OE1-CD-NE2	122.60	130.11	1
CA-CB-CG	112.60	105.09	1
N-CA-CA-CB-OD1-CG-ND2	122.60	115.11	1
CA-CB-CG	112.60	105.12	1
CB-CG-OD1	120.80	135.75	1
CA-CB-CG	113.80	106.33	2
OG1-CB-CG2	109.30	124.24	1
CA-CB-CG	112.60	105.13	1
CB-CG-CD	112.60	99.92	1
C-N-CA	121.70	108.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	125.90	1
C-N-CA	121.70	108.33	1
CA-CB-CG	113.80	106.38	1
CA-CB-CD-NE-ND1-CE1-CA-CB-CG	112.60	105.21	1
N-CA-CB	110.50	123.07	1
CA-CB-CG	113.80	106.41	1
CA-CB-CG	113.80	121.19	1
CB-CG-CA-CB-CA-CB-CG	113.80	121.17	1
OD1-CG-ND2	122.60	115.23	1
CG-CD2-NE2	107.20	114.56	2
C-N-CA	121.70	108.45	1
C-N-CG-CD2-CE3	133.90	126.55	1
CD2-NE2-CE1	109.00	101.65	1
NE-CZ-CB-CG-ND2	116.40	105.38	1
CA-CB-CG	113.90	100.68	1
CA-CB-CG	113.80	106.46	1
O-C-N	123.00	111.26	1
CA-CB-OG1	109.60	120.61	1
C-CA-CB	111.60	96.92	1
CG-CD-NE2	116.40	127.40	1
CA-C-N	116.90	127.90	1
NE-CZ-C-CA-CB	110.10	96.18	1
CA-CB-CG	112.60	105.28	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	122.94	1
CG-CD-NE2	116.40	105.43	1
CD2-NE2-CE1	109.00	101.69	1
C-N-CA	121.70	108.55	1
CA-CB-CG	113.90	100.75	1
CA-CB-CG	112.60	105.30	1
CD-NE-CZ	124.40	114.18	1
N-CA-CB	110.50	122.91	1
ND1-CE1-NE2	108.40	115.69	1
C-N-CA	121.70	108.58	1
CA-CB-CG	113.80	106.52	2
CB-CG-CD	112.60	100.22	1
CA-CB-CG	112.60	105.32	1
OE1-CD-NE2	122.60	129.87	1
CA-CB-CG	112.60	105.33	1
CA-CB-CG	112.60	119.87	1
CA-CB-CG	113.80	106.53	1
CA-CB-CG	113.80	106.54	1
CA-CB-CG	112.60	105.34	1
C-N-CA	121.70	108.64	1
OD1-CG-ND2	122.60	115.34	1
CA-CB-CG	112.60	119.85	1
OD1-CG-ND2	122.60	129.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	108.67	1
CA-CB-CG	113.80	106.56	1
CA-CB-CA-CB-CG	112.60	105.37	1
CD2-NE2-CE1	109.00	101.78	1
C-CA-NE-CZ-NH1	121.50	128.71	1
NE-CZ-NH2	119.20	125.69	1
OE1-CD-NE2	122.60	129.80	1
OD1-CG-ND2	122.60	115.40	1
CA-CB-OE1-CD-NE2	122.60	129.80	1
CA-CB-CG	114.10	99.71	1
CA-CB-CG	113.80	106.61	1
CA-CB-CG	112.60	105.41	1
CA-C-N	116.90	106.13	1
CA-CB-CG	113.80	106.62	1
CD2-NE2-CE1	109.00	101.82	1
N-CA-CB-CG-CD2	120.80	131.56	1
CA-CB-CA-CB-C-CA-CB	110.10	96.48	1
CA-CB-CG	112.60	119.77	1
NE-CZ-NH1	121.50	128.67	1
NH1-CZ-NH2	119.30	128.61	1
N-CA-CB	111.50	123.67	1
CD2-NE2-C-N-CA	121.70	108.84	1
CA-CB-CG	112.60	105.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	122.63	1
N-CA-CB	110.40	121.10	1
C-N-CA	121.70	108.86	1
CG-CD2-CE3	133.90	126.77	1
CA-CB-CG	112.60	105.47	1
ND1-CG-CD2	106.10	98.98	1
C-CA-CB	111.60	97.36	1
N-CA-CB	103.00	110.83	1
CB-CG-OD1	120.80	106.58	1
CD-NE-CZ	124.40	114.45	1
CB-CG-CD	112.60	100.53	1
OD1-CG-ND2	122.60	115.50	1
CE2-CD2-CE3	118.80	125.89	1
CD-NE-CZ	124.40	114.48	1
C-N-CA	121.70	108.95	1
CG-CD2-ND1-CE1-NE2	108.40	115.48	1
CA-CB-CG2	110.40	98.37	1
N-CA-CB	110.50	122.52	1
CD2-NE2-OD1-CG-ND2	122.60	129.67	1
CB-CG-CD	112.60	100.59	1
CA-CB-CG	113.80	106.74	1
CA-CB-CG	113.80	120.85	1
CA-CB-CG	112.60	105.56	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	120.84	1
CA-CB-CG	113.80	106.76	2
C-N-CA	121.70	109.03	1
CB-CG-CD	112.60	100.65	1
CB-CG-CD	112.60	100.67	1
C-CA-CB	111.60	97.57	1
CD2-NE2-CB-CG-CD1	126.90	137.41	1
NH1-CZ-NH2	119.30	110.20	1
CA-CB-CG	112.60	105.61	2
C-N-CA	121.70	109.11	1
CB-CG-CD	112.60	100.72	1
CD2-NE2-CE1	109.00	102.01	1
C-N-CA	121.70	109.13	1
CA-CB-CG	112.60	105.62	1
CG-CD-NE2	116.40	126.87	1
NE-CZ-NH2	119.20	125.47	1
CA-CB-CG	113.80	106.83	1
C-N-CA	121.70	109.16	1
C-CA-CB	111.40	98.17	1
CB-CG-CD1	120.80	110.36	1
CA-CB-CG	113.80	106.84	1
CB-CG-CD	112.60	100.77	1
C-N-CA	121.70	109.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OG1-CB-C-N-CA	121.70	134.20	1
OE1-CD-NE2	122.60	129.54	2
CG-SD-CE	100.90	85.65	1
C-N-OD1-CG-ND2	122.60	115.68	1
CB-CG-CA-CB-CG1	110.40	122.13	1
CB-CG-CD	112.60	100.88	1
C-N-CA-CB-CG	112.60	105.71	1
N-CA-CB	103.00	110.57	1
OD1-CG-ND2	122.60	115.72	1
CA-CB-CG	112.60	105.72	1
N-CA-CB	110.50	122.17	1
C-CA-CB	110.50	100.21	1
OD1-CG-CB-CG-CD	112.60	100.95	1
CA-CB-CG	112.60	105.75	1
CE2-CD2-CE3	118.80	125.65	1
NE-CZ-NH1	121.50	114.65	1
CG-SD-CE	100.90	85.83	1
CG-SD-CE	100.90	85.84	1
CA-CB-CG	114.10	100.42	1
C-CA-CB	110.10	97.13	1
CA-CB-CG	113.80	106.97	2
CA-CB-CG	112.60	105.78	1
CG-SD-CE	100.90	85.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-NE-CZ	124.40	114.85	1
CA-CB-CA-CB-CG	112.60	105.79	1
CA-CB-CG2	110.50	98.92	1
CA-CB-CG	113.80	106.99	1
CA-CB-CG	112.60	105.79	1
CB-CG-N-CA-CB	110.50	122.08	1
CD-NE-CZ	124.40	114.87	1
C-CA-CB	110.10	97.17	1
C-N-CA	121.70	109.45	1
CA-CB-CG	112.60	119.40	1
CA-CB-CG	112.60	105.81	1
N-CA-CB	110.50	122.05	1
CB-CG-CD	112.60	101.05	1
CD2-NE2-CE1	109.00	102.21	1
NE-CZ-CB-CG-CD	112.60	101.06	1
CD1-CG-CD2	118.60	108.42	1
CA-CB-CG	113.80	107.02	1
C-N-CA	121.70	133.90	1
N-CA-CB	110.50	122.02	1
CA-CB-CG	112.60	105.82	1
OD1-CG-ND2	122.60	129.38	1
C-N-CA	121.70	109.52	1
CA-CB-CG	113.80	120.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	97.25	1
C-N-CG-CD2-CE2	120.70	132.19	1
OD1-CG-ND2	122.60	115.84	1
NH1-CZ-NH2	119.30	110.52	1
N-CA-CB	111.50	122.98	1
CA-CB-CG	112.60	105.85	2
C-N-CA	121.70	109.55	1
N-CA-CB	111.50	122.96	1
CB-CG-CD	112.60	101.15	1
CB-CG-CA-CB-CG	112.60	105.86	1
CA-CB-CG	113.80	107.07	1
NE-CZ-NH2	119.20	125.26	1
C-CA-CB	111.60	98.16	1
C-CA-CB	110.10	97.34	1
N-CA-CB	110.50	121.92	1
C-N-CA	121.70	109.61	1
CA-CB-CG	114.10	127.53	1
CD2-CE2-CZ	120.00	132.08	1
CA-CB-CG	112.60	105.90	1
C-N-CA	121.70	133.75	1
CD2-NE2-C-CA-CB	111.60	98.23	1
N-CA-CB	110.50	121.87	1
ND1-CE1-NE2	108.40	115.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	122.53	1
C-N-CA	121.70	133.70	1
CA-CB-CG	112.60	105.93	1
CB-CG-OE1-CD-NE2	122.60	115.94	1
OE1-CD-NE2	122.60	115.94	1
CB-CG-CD	112.60	101.28	1
ND1-CE1-NE2	108.40	115.06	1
C-N-CA	121.70	109.72	3
CA-CB-CG	112.60	105.95	1
N-CA-CB	110.50	121.81	2
N-CA-N-CA-CB	110.50	121.80	1
CD-NE-CZ	124.40	115.10	1
C-N-CA	121.70	109.75	1
N-CA-CB	110.50	121.78	1
N-CA-CB	110.40	120.35	1
CA-CB-CG	113.80	107.17	1
OE1-CD-NE2	122.60	115.97	1
CA-CB-CG	112.60	105.97	1
N-CA-CB	103.00	110.29	1
CB-CG-CD	112.60	101.34	2
C-N-CA	121.70	109.80	1
C-N-N-CA-CB	103.00	110.27	1
CA-CB-N-CA-CB	110.50	121.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	121.72	1
CB-CG-CD	112.60	101.38	1
C-N-CA	121.70	109.82	1
CA-CB-CG	112.60	106.01	1
CA-CB-CG	113.90	102.04	1
C-N-CA	121.70	109.84	2
CA-CB-CG1	110.40	99.20	1
CG-CD2-NE2	107.20	113.78	1
C-N-N-CA-CB	110.40	120.27	1
C-N-CA	121.70	109.86	1
CB-CG-CD	112.60	101.44	1
CA-CB-OD1-CG-ND2	122.60	116.04	1
CA-CB-CG	113.90	102.11	1
CA-CB-NH1-CZ-NH2	119.30	127.81	1
C-N-CA	121.70	109.92	1
CB-CG-CA-CB-CG	112.60	106.06	1
CB-CG-ND1	122.70	132.50	1
CA-CB-CA-CB-CG2	110.40	99.29	1
CB-CG-CD	112.60	101.50	1
CA-CB-CG	113.90	102.15	1
CA-CB-N-CA-CB	110.50	121.58	1
CG-CD2-CE2	121.20	130.98	1
CA-CB-CG	113.80	107.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	100.72	1
ND1-CE1-NE2	108.40	114.92	1
C-N-CA-CB-CG	112.60	106.09	1
CA-CB-CG	113.80	120.31	1
CA-CB-CG	113.90	102.19	1
CA-CB-CG	112.60	106.10	1
CA-CB-CG-CD2-NE2	107.20	113.70	1
CE2-CD2-CE3	118.80	125.29	1
CB-CG-ND2	116.40	126.14	1
CA-CB-CG	113.80	107.31	1
CA-CB-C-N-C-CA-CB	110.10	97.78	1
OD1-CG-ND2	122.60	129.08	1
C-N-CA	121.70	110.04	2
OE1-CD-NE2	122.60	116.12	1
CA-CB-NH1-CZ-NH2	119.30	110.89	1
CG-CD2-CE3	133.90	127.43	1
C-N-CA	121.70	110.05	1
CD2-NE2-CE1	109.00	102.53	1
CD-NE-CZ	124.40	115.34	1
O-C-CA-C-N	116.90	107.22	1
CB-CG-CD	112.60	101.64	1
C-N-CA	121.70	110.10	1
CA-CB-CG	113.80	107.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	101.65	1
C-CA-CB	110.10	97.86	1
CD2-NE2-CE1	109.00	102.56	1
C-N-CA	121.70	110.12	1
C-N-CA	121.70	110.13	1
NE-CZ-NH2	119.20	124.99	1
CB-CG-CD	112.60	101.67	1
CA-CB-CG	113.80	107.37	1
CB-CG-CD	112.60	101.68	1
O-C-CA-CB-CG	112.60	106.18	1
CA-CB-CG	112.60	106.18	1
NE-CZ-NH1	121.50	127.92	1
CB-CG-CD	112.60	101.70	1
C-CA-CB	111.60	98.78	1
C-N-CA	121.70	110.16	1
CG-CD-OE1	120.80	133.60	1
C-N-CA	121.70	110.19	2
C-CA-CB	110.10	97.95	1
N-CA-CB	110.40	119.99	1
C-CA-CB-CG-CD	112.60	101.74	1
C-CA-CB	110.10	97.97	1
N-CA-CB	110.50	121.35	1
CD-NE-CA-CB-CG	112.60	106.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-NE-CZ	124.40	115.47	1
CA-CB-CG	112.60	118.97	1
CB-CG-ND2	116.40	125.96	1
CB-CG-CD	112.60	101.77	2
CD2-NE2-CE1	109.00	102.63	1
C-N-CA	121.70	110.24	1
N-CA-CB	110.50	121.32	1
NH1-CZ-NH2	119.30	127.57	1
N-CA-CB	111.50	122.32	1
CA-CB-CG1	110.40	99.59	1
CB-CG-CD	112.60	101.81	2
C-N-CA	121.70	110.27	1
N-CA-CB	110.50	121.29	1
N-CA-CB	110.50	121.27	1
C-CA-CB	110.10	98.06	1
C-N-CA	121.70	133.10	1
OD1-CG-ND2	122.60	116.28	1
N-CA-CB	110.50	121.24	1
N-CA-CB	103.00	109.95	1
OD1-CG-ND2	122.60	128.91	1
N-CA-CA-CB-CG	112.60	106.29	1
CG-SD-CE	100.90	87.02	1
CA-CB-CG	113.90	102.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CD-CG	103.20	112.66	1
CD2-CE2-CZ2	122.40	116.09	1
CG-CD-CA-CB-CG	112.60	106.30	1
C-CA-CB	111.40	99.43	1
CD-NE-ND1-CE1-NE2	108.40	114.70	1
CA-CB-CG2	110.40	99.70	1
C-N-CA	121.70	110.38	1
OD1-CG-ND2	122.60	128.88	1
C-N-CA	121.70	110.39	1
CB-CG-C-N-CA	121.70	110.41	1
CA-CB-CG-SD-CE	100.90	87.11	1
C-N-CA	121.70	110.41	1
CA-CB-C-CA-CB	110.10	98.19	1
CG-CD-NE2	116.40	107.00	1
C-N-CA	121.70	110.43	1
CD-NE-CZ	124.40	115.63	1
CD2-NE2-CE1	109.00	102.74	1
CE2-CD2-CE3	118.80	125.06	1
CA-C-O	120.80	131.44	1
CD-NE-N-CA-CB	110.50	121.14	1
N-CA-CB	103.00	109.88	1
C-N-CA	121.70	110.44	1
CB-CG-CD	112.60	101.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	98.22	1
CD-NE-CZ	124.40	115.65	1
CD2-NE2-C-N-ND1-CE1-NE2	108.40	114.65	1
N-CA-CB	103.00	109.87	1
CB-CG-CD	112.60	101.99	1
CD2-NE2-CG-CD1-CE1	120.70	131.30	1
C-CA-CB	110.10	98.26	1
CD-NE-CZ	124.40	115.68	1
CB-CG-CD1	120.80	130.15	1
N-CA-CB	110.50	121.09	1
CB-CG-CD2	120.70	131.29	1
CB-CG-ND1	122.70	113.36	1
NE-CZ-NH2	119.20	113.60	1
OD1-CG-ND2	122.60	116.37	1
CB-CG-OD1	120.80	108.35	1
ND1-CE1-NE2	108.40	114.63	1
C-CA-CB	110.10	98.28	1
CA-CB-CG	112.60	106.38	1
OD1-CG-ND2	122.60	116.38	1
CA-CB-CG	113.90	102.71	1
CB-CG-CA-CB-CG	113.90	102.72	1
CA-CB-CG	113.90	102.72	1
CA-C-O	120.80	131.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.88	1
N-CA-CB	110.50	121.06	1
N-CA-CB	110.50	121.05	1
CB-CG-CD	112.60	102.05	1
CD-NE-CZ	124.40	115.71	1
CB-CG-CA-C-N	116.90	126.20	1
CA-C-N	116.90	126.20	2
CA-CB-CG	112.60	106.40	1
C-N-CA	121.70	110.54	1
CD2-NE2-C-N-CA	121.70	110.54	1
OD1-CG-N-CA-CB	110.50	121.03	1
C-N-CA	121.70	110.56	1
OE1-CD-NE2	122.60	128.79	1
N-CA-CB	103.00	109.81	1
C-N-CA	121.70	110.57	1
CA-CB-CG	113.80	107.62	1
CA-CB-CG	113.90	102.77	1
CD2-NE2-CE1	109.00	102.82	1
C-N-CA	121.70	110.58	1
N-CA-CB	111.50	122.00	2
C-CA-CB	110.10	98.37	1
OD1-CG-ND2	122.60	116.43	1
C-CA-CA-CB-CG	112.60	106.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD1-CE1	120.70	110.21	1
C-N-CA-CB-CG	112.60	106.44	1
CB-CG-CD2	120.80	130.05	1
CB-CG-CD	112.60	102.12	1
CA-CB-CG	112.60	106.44	4
CD2-NE2-CE1	109.00	102.84	1
C-CA-CB	110.10	98.40	1
N-CA-CB	110.50	120.97	1
CG-CD-NE2	116.40	125.62	1
CA-CB-CG	112.60	106.45	1
CD2-CE3-CZ3	118.60	110.61	1
CE3-CZ3-CH2	121.10	113.12	1
CA-CB-C-N-CA	121.70	110.66	1
C-CA-CB	110.50	101.30	1
NE-CZ-NH1	121.50	115.37	1
C-N-CA	121.70	110.67	2
CB-CG-CD	112.60	102.19	1
CA-CB-C-N-CD1-CG-N-CA-CA-CB-CG2	110.50	100.10	1
O-C-N	123.00	132.78	1
C-N-OE1-CD-NE2	122.60	116.49	1
CA-CB-CG1	110.40	120.78	1
C-N-CA	121.70	110.72	2
CG-CD-NE2	116.40	125.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	120.87	1
CA-CB-CG	112.60	106.51	1
N-CA-CB	111.50	121.86	1
N-CA-CB	110.50	120.85	2
C-N-CA	121.70	132.66	1
C-CA-CB	110.10	98.53	1
CB-CG-CD	112.60	102.25	1
C-N-CA	121.70	132.65	1
CA-CB-CG	112.60	106.52	2
N-CA-CB	110.50	120.83	1
CA-C-N	116.90	126.02	1
CA-CB-C-N-CA-C-NE-CZ-NH1	121.50	115.43	1
CB-CG-CD	112.60	102.29	1
N-CA-N-CA-CB	103.00	109.67	1
CD2-NE2-CE1	109.00	102.94	1
C-CA-CB	110.10	98.59	2
C-N-CA	121.70	110.80	1
C-N-CA	121.70	110.81	1
CA-CB-CG	112.60	106.55	1
C-CA-CB	110.10	98.60	1
CG-CD2-CG-CD-OE1	120.80	108.71	1
N-CA-CB	111.50	121.78	1
CA-CB-CG	112.60	106.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	102.33	1
OD1-CG-ND2	122.60	128.64	1
C-N-CA	121.70	132.57	1
N-CA-CB	110.50	120.77	1
CG-CD2-CE2	121.20	130.26	1
C-N-CA	121.70	110.83	2
CA-CB-CG	113.80	107.76	1
C-CA-CB	110.10	98.64	1
C-N-CA	121.70	132.55	1
CA-C-N	116.90	107.85	1
CA-C-O	120.80	110.55	1
N-CA-CA-C-O	120.80	131.05	1
C-N-CA	121.70	110.86	1
CB-CG-CD	112.60	102.36	1
N-CA-CB	110.50	120.74	2
N-CA-CB	111.50	121.74	1
N-CA-CB	110.50	120.73	3
CA-CB-CG-SD-CE	100.90	87.67	1
C-CA-CB	111.60	99.58	1
ND1-CE1-NE2	108.40	114.41	1
C-CA-CB	110.10	98.69	3
C-N-CA	121.70	110.89	1
N-CA-C-N-CA	121.70	110.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.51	1
CA-CB-CG	113.80	107.80	2
CA-CB-CG	112.60	106.60	1
N-CA-CB	110.50	120.70	1
CB-CG-N-CA-CB	110.50	120.70	1
CG-CD2-NE2	107.20	113.19	1
CA-CB-CG1-CB-CG2	110.80	123.97	1
CA-CB-CG	112.60	106.61	1
OE1-CD-NE2	122.60	116.62	1
CG-CD2-NE2	107.20	113.18	1
CD1-CE1-CZ	120.00	109.23	1
ND1-CE1-NE2	108.40	114.38	1
CG1-CB-O-C-N	123.00	132.57	1
OD1-CG-ND2	122.60	116.62	1
C-N-CA	121.70	110.94	1
C-N-CA	121.70	132.46	1
CB-CG-CD	112.60	102.44	1
OE1-CD-NE2	122.60	128.57	1
C-N-CA	121.70	110.95	1
CA-CB-CG	112.60	106.63	1
CB-CG-CD	112.60	102.45	2
OD1-CG-ND2	122.60	116.63	1
C-N-C-N-CA	121.70	110.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	110.96	1
ND1-CE1-CB-CG-C-N-CA	121.70	132.43	1
O-C-C-N-CA	121.70	110.98	1
N-CA-CB	110.50	120.63	1
CA-CB-CD-NE-CZ	124.40	116.07	1
CB-CG-OD1	120.80	108.90	1
CA-CB-CG	112.60	118.55	1
CB-CG-C-N-CA	121.70	111.00	1
C-N-CA	121.70	111.00	1
C-N-CA	121.70	111.01	1
CA-CB-CA-CB-CG	112.60	106.67	1
C-N-CA	121.70	111.02	1
CA-CB-CG	112.60	106.67	1
CG-CD1-CE1	121.20	130.09	1
CB-CG-CA-C-C-N-CA	121.70	111.03	1
CD-NE-CZ	124.40	116.11	1
C-CA-CB	110.10	121.35	1
C-N-CA	121.70	132.36	1
CA-CB-CG	113.90	103.24	1
C-N-CA	121.70	111.05	1
CA-C-O	120.80	110.74	1
N-CA-CB	110.50	120.55	1
C-N-CA	121.70	111.07	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.33	1
C-N-CA	121.70	132.32	1
CA-CB-CG	113.80	107.90	1
CB-CG-ND2	116.40	107.55	1
CA-CB-CG	113.80	119.70	1
CA-CB-CG	112.60	106.71	3
N-CA-C	113.30	96.22	1
CB-CG-ND2	116.40	107.57	1
N-CA-CB	110.50	120.51	1
CA-CB-CG	113.80	107.91	1
C-N-CA	121.70	111.10	1
C-N-CA	121.70	132.30	1
CD1-CE1-CZ	120.00	130.60	1
NE-CZ-N-CA-CB	110.50	120.51	1
CA-CB-CG	114.10	102.33	1
CA-CB-CG	112.60	106.72	1
CD2-NE2-CE1	109.00	103.12	1
CB-CG-ND2	116.40	125.22	1
C-N-CA	121.70	111.12	1
CB-CG-CD	112.60	102.61	1
C-CA-CB	110.10	98.94	1
N-CA-CB	111.50	121.48	1
CA-CB-CG	113.80	107.93	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.27	1
CG-CD2-NE2	107.20	113.07	1
N-CA-CB	110.50	120.48	1
CG-CD1-C-N-CA	121.70	132.25	1
CG-CD-NE2	116.40	107.61	1
CB-CG-CD2	120.80	112.02	1
CB-CG-ND2	116.40	107.62	1
CA-CB-CG	113.90	103.37	1
C-CA-CB-CG-ND2	116.40	107.63	1
CA-CB-CG	112.60	106.75	1
ND1-CE1-NE2	108.40	114.24	1
O-C-CD1-CE1-CZ	119.60	130.11	1
C-N-CA	121.70	111.19	1
CB-CG-CD	112.60	102.68	1
CA-CB-CG2	110.50	120.42	1
N-CA-CB	110.50	120.42	1
CA-C-C-N-CA	121.70	111.21	1
C-CA-CB	110.10	99.03	1
C-CA-CB	110.50	101.77	1
C-CA-N-CA-CB	110.50	120.39	1
CB-CG-ND1-CE1-NE2	108.40	114.21	1
CB-CG-CD	112.60	102.72	1
CA-CB-CG	113.90	103.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.40	100.52	1
N-CA-CB-CG-CA-CB-C-N-CA	121.70	111.25	1
C-N-CA	121.70	111.25	1
N-CA-CB	110.50	120.37	1
C-N-CA-C-O	120.80	130.66	1
OD1-CG-ND2	122.60	116.80	1
CA-CB-CG	114.10	125.69	1
CG-CD-NE	112.00	99.26	1
N-CA-CB	110.50	120.34	1
CE1-CZ-CE2	120.00	109.58	1
CA-CB-OG1	109.60	100.92	1
CB-CG-CD	112.60	102.76	2
C-CA-CB	111.40	100.41	1
C-N-CA	121.70	111.29	1
C-CA-CB	110.10	99.11	1
CG-CD-OE1	120.80	109.23	1
C-CA-CB	110.50	101.83	1
CG-SD-CE	100.90	88.18	1
CG-CD-NE2	116.40	107.73	1
CB-CG-CD	112.60	102.78	1
C-CA-CB	110.10	121.08	1
O-C-N	123.00	113.76	1
CD2-NE2-CE1	109.00	103.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
ND1-CE1-NE2	108.40	114.17	1
C-N-C-N-CA	121.70	111.32	1
C-N-CA	121.70	111.33	2
N-CA-CB	111.50	121.29	1
N-CA-CB	103.00	109.33	2
CA-CB-CG2	110.50	100.72	1
C-N-CA	121.70	111.34	1
N-CA-CB	110.50	120.28	1
CA-CB-CG	113.90	103.55	1
ND1-CE1-NE2	108.40	114.15	1
C-N-CA	121.70	111.35	1
N-CA-CB	110.50	120.27	2
NH1-CZ-N-CA-CB	110.50	120.27	1
C-CA-CB	110.10	99.18	1
N-CA-C-CA-CB	110.10	99.19	1
C-N-CA	121.70	111.36	1
C-N-CA-CB-C-CA-CB	110.10	99.20	1
CG-CD2-CE3	133.90	128.16	1
N-CA-CB	110.50	120.25	1
C-N-CA	121.70	111.38	1
CA-CB-CG	113.80	108.06	1
NH1-CZ-NH2	119.30	126.76	1
C-CA-CB	110.10	99.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-ND2	116.40	107.80	1
CA-CB-C-N-CA	121.70	111.39	1
C-N-CA	121.70	111.39	1
N-CA-CB	110.50	120.24	1
CD-NE-CZ	124.40	116.38	1
CA-CB-CA-C-CB-CG-N-CA-CB	110.50	120.22	1
CB-CG-CD2-NE2-CE1	109.00	103.29	1
C-CA-CB	110.10	99.24	1
CG-SD-CE	100.90	88.33	1
C-CA-CB	110.10	99.25	1
C-N-CA	121.70	111.43	3
CB-CG-CD1	120.70	130.40	1
CA-CB-CD2-NE2-CE1	109.00	103.30	1
N-CA-CB	110.50	120.20	1
C-CA-CB	110.50	101.95	1
N-CA-CB	110.50	120.19	1
CA-CB-CG	113.80	108.10	1
CA-CB-CG	114.10	125.50	1
CA-CB-CG1	110.40	100.71	1
N-CA-CB	110.40	118.95	1
C-N-CA	121.70	111.44	1
C-N-CA	121.70	111.45	1
C-CA-CB	110.10	99.28	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	102.92	1
CB-CG-CA-CB-CG	113.80	108.11	1
CG-CD-NE	112.00	99.49	1
CA-CB-CG	112.60	106.92	1
C-N-CA	121.70	111.47	1
CA-CB-CG	113.90	103.68	2
CA-CB-CG	113.80	108.12	1
C-N-CB-CG1-CD1	113.80	125.72	1
OD1-CG-ND2	122.60	116.93	1
CA-CB-CG	113.80	108.13	1
CG-CD-OE2	118.40	131.45	1
CA-CB-CA-C-O	120.80	111.16	1
N-CA-CB	110.50	120.14	1
C-CA-CB	111.60	100.26	1
CA-CB-CG	113.90	103.72	1
CA-CB-C-CA-CB	110.10	99.35	1
CB-CG-ND2	116.40	107.92	1
CG-CD-NE2	116.40	107.92	1
C-N-CA-CB-CG	113.80	108.15	1
CA-CB-CG	112.60	106.95	1
C-N-CA	121.70	111.52	1
CB-CG-C-N-CA	121.70	111.53	1
C-CA-CB	110.10	99.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-N-CA-CB	110.50	120.09	1
CA-CB-CG-CD2-NE2	107.20	112.84	1
N-CA-CB	110.50	120.09	1
CB-CG-NE-CZ-NH1	121.50	115.86	1
CG-CD2-NE2	107.20	112.84	1
C-N-CA	121.70	111.56	1
CA-CB-CG	112.60	118.24	1
C-CA-CB	110.50	102.05	1
N-CA-CB	110.50	120.07	1
C-N-C-N-CA	121.70	111.58	1
CA-CB-CG	113.80	108.18	1
CG-CD2-NE2	107.20	112.82	1
CA-C-CG-CD2-NE2	107.20	112.82	1
N-CA-CB	110.50	120.06	1
OE1-CD-NE2	122.60	116.98	1
CG-CD2-C-N-CA-CB-CG2	110.50	100.95	1
CG1-CB-CG2	110.80	123.16	1
N-CA-C	111.00	95.27	1
C-CA-CB	110.10	99.43	1
OD1-CG-CB-CG-ND2	116.40	107.99	1
C-N-CA	121.70	131.80	1
CA-C-N	116.20	127.42	1
N-CA-CB	110.50	120.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	108.19	1
ND1-CE1-N-CA-CB	111.50	101.98	1
N-CA-CB	110.50	120.02	1
C-N-CA	121.70	111.62	1
C-CA-CB	110.10	99.47	1
CA-CB-CG	112.60	107.01	1
C-N-CA	121.70	111.63	1
CA-CB-N-CA-N-CA-CB	110.50	120.00	1
CB-CG-CA-CB-CG2	110.40	100.90	1
CG-CD-CE	111.30	124.15	1
CB-CG-CA-CB-C-N-CA	121.70	111.65	1
CA-CB-CG	112.60	107.02	2
C-CA-CB	110.10	99.49	1
C-N-CA	121.70	111.65	1
CB-CG-CD	112.60	103.11	1
CA-CB-CA-CB-CG	113.90	103.86	1
C-N-CA	121.70	131.73	1
C-CA-CB	110.10	99.51	1
C-N-C-CA-C-N-CA	121.70	131.73	1
CG-CD2-CD2-NE2-CE1	109.00	103.43	1
C-CA-CB	110.10	99.52	1
CA-CB-CG	113.80	108.23	1
N-CA-CB	111.50	120.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-NE-CZ	124.40	116.61	1
N-CA-C	111.00	95.41	1
N-CA-CB	111.50	120.96	1
CB-CG-OD1	120.80	131.93	1
CA-CB-CG	112.60	107.04	3
CA-CB-CG	113.90	103.89	1
OD1-CG-N-CA-CB	110.50	119.95	1
CA-CB-N-CA-CB	110.50	119.95	1
C-N-CA	121.70	111.70	1
N-CA-CB	110.50	119.94	1
CB-CG-CD	111.30	124.08	1
CA-C-CA-CB-CA-CB-CG2	110.50	101.06	1
O-C-N	123.00	114.12	1
C-N-CA	121.70	111.71	2
CG-SD-CE	100.90	88.69	1
N-CA-CB	110.50	119.93	1
CD1-CG-CD2	110.80	123.00	1
N-CA-C	111.00	95.48	1
N-CA-CB	111.50	120.92	1
CD2-CE2-CZ	120.00	110.02	1
NE-CZ-NH2	119.20	114.21	1
C-N-CA	121.70	111.73	1
CB-CG1-CD1	113.80	102.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-OD1	118.40	131.14	1
OD1-CG-ND2	122.60	128.14	1
CA-CB-CG	114.10	103.02	1
O-C-N	123.00	114.14	1
N-CD-CG	103.20	111.50	1
C-N-CA	121.70	111.74	1
N-CA-CB	111.50	120.91	1
OE1-CD-NE2	122.60	117.07	1
CA-CB-C-N-CA	121.70	111.74	1
N-CA-CB	110.50	119.90	1
CD-NE-CZ	124.40	116.66	1
CA-CB-CG	112.60	107.07	2
C-N-CA	121.70	131.65	1
C-N-CA	121.70	111.75	1
OD1-CG-C-N-CA	121.70	131.64	1
N-CA-CB	110.50	119.89	1
C-N-CA	121.70	111.76	2
C-N-CA	121.70	131.64	1
N-CA-CB	110.50	119.88	1
OD1-CG-CA-CB-CG2	110.50	101.12	1
C-CA-CB	110.10	99.61	1
C-N-N-CA-C-CA-CB	111.40	100.92	1
CE2-CD2-CE3	118.80	124.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	120.80	112.53	1
OD1-CG-C-N-C-N-C-CA-CB	110.10	99.64	1
CA-CB-CG	113.80	108.30	1
CE1-CZ-CE2	120.00	110.10	1
C-N-CA	121.70	111.81	2
C-N-CA	121.70	131.59	1
C-N-CB-CG-CD1	120.70	111.36	1
CA-CB-CG	112.60	107.11	2
C-CA-CB	110.10	99.67	1
CA-CB-CG	113.80	108.31	1
CB-CG-CG-CD2-CG-CD2-NE2	107.20	112.69	1
CG-CD2-C-N-CA	121.70	111.83	1
C-N-CA	121.70	111.83	2
CD2-NE2-CA-CB-CG	113.80	108.32	1
CG-CD2-CB-CG-ND2	116.40	124.62	1
CB-CG-CD1	126.90	135.12	1
O-C-N	123.00	114.23	1
CB-CG-OD1	120.80	131.76	1
C-CA-CB	110.10	99.69	1
C-N-CA	121.70	111.84	1
CB-CG-CB-CG-CD	112.60	103.28	1
N-CA-CB-CG-C-N-CA	121.70	131.56	1
CG-CD-OE2	118.40	105.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-ND2	116.40	108.19	1
CA-CB-CG1	110.40	101.09	1
C-N-CA	121.70	131.55	1
CD1-CG-CD2	118.60	110.39	1
N-CA-CA-C-CD1-CG-CD2	110.80	122.84	1
C-N-OE1-CD-NE2	122.60	117.13	1
CD2-NE2-CE1	109.00	103.53	1
CD-NE-CZ	124.40	116.75	2
OE1-CD-NE2	122.60	117.14	1
CD2-NE2-CE1	109.00	103.54	1
CB-CG-CD	112.60	103.32	2
N-CA-CB	110.50	119.78	1
C-N-CA	121.70	131.53	1
CB-CG-CG-CD-CE	111.30	123.85	1
C-N-CA	121.70	111.88	1
N-CA-CB	110.50	119.77	1
C-CA-CB	111.40	101.04	1
CG-CD-OE1	120.80	131.71	1
CA-CB-CG	112.60	107.15	1
CB-CG-ND2	116.40	108.23	1
N-CA-CB	110.50	119.76	1
N-CA-CB	103.00	108.99	1
C-N-CA	121.70	111.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	103.34	1
CA-CB-CG	112.60	107.16	1
CA-CB-CG	114.10	103.22	1
CA-CB-CG	113.80	108.37	1
CA-CB-CG	113.90	104.12	1
OE1-CD-NE2	122.60	117.17	1
NH1-CZ-NH2	119.30	126.36	1
C-CA-CB	111.60	100.75	1
C-N-CA	121.70	131.47	1
C-CA-CB	109.10	97.16	1
CA-C-O	120.80	130.02	1
C-N-CA	121.70	111.94	1
CD2-NE2-CE1	109.00	103.58	1
N-CA-CB	110.50	119.71	1
CG-CD2-NE2	107.20	112.62	1
C-N-CA	121.70	131.46	1
CD1-CG-CD2	110.80	122.72	1
C-N-CA	121.70	131.45	1
CA-CB-CG	112.60	107.18	1
ND1-CE1-NE-CZ-NH2	119.20	124.07	1
OD1-CG-ND2	122.60	128.01	1
CD1-CG-CA-CB-CG1	110.40	101.21	1
C-N-CA	121.70	111.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	102.39	1
N-CA-CB	103.00	108.95	1
CB-CG-ND2	116.40	124.51	1
C-CA-CB	111.60	100.79	1
CA-CB-CG	112.60	107.20	1
CA-CB-CG	113.80	108.40	1
OD1-CG-ND2	122.60	117.20	1
CA-C-O	120.80	129.98	1
N-CA-CA-CB-CG	113.80	119.20	1
CA-N-CB-CG-OD1	120.80	131.60	1
C-N-CA	121.70	131.41	1
CB-CG-CD	112.60	103.43	1
CB-CG-C-CA-CB	110.10	99.85	1
O-C-N	123.00	114.37	1
NE-CZ-NH1	121.50	126.89	1
CD2-NE2-CE1	109.00	103.61	1
C-N-CA	121.70	112.00	1
CA-CB-CA-CB-CG2	110.50	101.34	1
N-CA-C-N-CA	121.70	131.39	1
C-N-CA	121.70	131.39	1
C-N-CA	121.70	112.01	1
N-CA-CB	110.50	119.65	1
CG-CD2-CE2	120.70	129.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	119.18	1
C-N-CB-CG-C-N-CA	121.70	112.02	1
CA-CB-OG	111.10	100.35	1
CB-CG-CD	112.60	103.46	1
C-CA-CB	110.10	99.89	1
CA-C-N	116.20	126.95	1
CB-CG-OD1	120.80	131.55	1
CB-CG-CD	112.60	103.47	1
CG1-CB-CG2	110.80	122.62	1
CD2-NE2-CE1	109.00	103.63	1
OD1-CG-ND2	122.60	127.97	1
CG-CD-NE2	116.40	108.35	1
CA-CB-CG	112.60	107.23	1
C-CA-CB	110.10	99.91	1
C-N-N-CA-CB	103.00	108.90	1
N-CA-CB	110.50	119.62	1
C-CA-N-CA-CB	110.50	119.62	1
OG1-CB-CG2	109.30	120.02	1
N-CA-CB	103.00	108.90	1
C-CA-CB	109.10	97.31	1
C-N-CA	121.70	131.35	1
C-N-CA	121.70	112.05	1
ND1-CE1-NE2	108.40	113.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	99.92	1
C-CA-CB	110.10	99.93	1
OE1-CD-NE2	122.60	117.25	1
CA-C-C-CA-CB	110.10	99.93	1
N-CA-CG-CD-NE	112.00	100.23	1
N-CA-CB	110.50	119.59	2
C-N-CA	121.70	131.32	1
C-N-CA	121.70	112.08	4
CB-CG-ND2	116.40	124.42	1
N-CA-C	112.10	98.74	1
C-CA-CB	111.60	100.91	1
CB-CG-ND2	116.40	108.38	1
C-N-CA	121.70	112.09	3
CA-CB-CG	112.60	107.26	1
CB-CG-OD1	120.80	131.47	1
CB-CG-N-CA-C	111.00	96.07	1
CD2-NE2-CE1	109.00	103.67	1
N-CA-CB	110.40	118.40	1
CA-CB-CG	112.60	107.27	1
C-N-CA	121.70	131.29	1
CB-CG-CD	112.60	103.54	1
CA-CB-CG2	110.50	101.44	1
CA-CB-OG1	109.60	117.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-C-CA-CB	110.10	99.98	1
C-N-CA	121.70	112.11	1
C-CA-CB	110.10	99.98	1
CB-CG1-CD1	113.80	124.98	1
CB-CG-O-C-N	123.00	131.52	1
C-N-CA	121.70	112.12	2
N-CA-CB	110.50	119.55	1
N-CA-CB	110.50	119.54	2
C-CA-CB	110.10	99.99	1
CA-CB-CG	112.60	107.28	1
C-N-CA	121.70	112.13	3
C-N-CA	121.70	131.27	1
CA-CB-CG	113.90	104.33	1
CB-CG-CD	112.60	103.56	1
CA-C-O	120.80	111.77	1
CA-CB-OG1	109.60	101.63	1
C-N-CA	121.70	112.14	1
C-CA-C-N-CA	121.70	112.14	1
CA-CB-C-N-CA	121.70	131.26	1
CA-CB-CG1	110.40	119.42	1
CA-CB-CG	113.80	108.49	1
C-N-CA	121.70	112.15	2
CA-CB-C-CA-C-CA-CB	110.10	100.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	103.69	1
CA-CB-CG	113.80	108.50	1
CA-CB-CA-C-N	116.90	108.95	1
CD2-NE2-CE1	109.00	103.70	1
C-CA-CB	109.10	97.44	1
N-CA-C	111.00	96.16	1
CB-CG-ND2	116.40	124.35	1
N-CA-CB	103.00	108.83	1
CG-CD2-CE3	133.90	128.60	1
C-N-CA	121.70	112.17	1
CD1-CE1-CZ	120.00	110.47	1
CD1-CE1-CZ	119.60	110.07	1
CA-CB-CA-CB-CG	113.80	108.51	1
CA-C-N	116.90	124.84	1
C-N-CA	121.70	131.22	1
N-CA-CB	110.50	119.49	1
CB-CG-CD1	120.70	129.69	1
N-CA-C-N-CA	121.70	112.19	1
CA-CB-C-N-CA	121.70	112.19	1
N-CA-CB-CG-CD2	131.20	124.33	1
CA-CB-CG	113.80	108.52	1
N-CA-CB	110.50	119.48	1
CB-CG-ND2	116.40	108.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	120.70	129.67	1
CB-CG-CD	112.60	103.63	1
O-C-N	123.00	114.56	1
N-CA-CB	110.50	119.47	1
NE-CZ-NH2	119.20	123.95	1
C-N-CA	121.70	112.21	2
N-CA-CB	110.50	119.46	2
N-CA-CB	111.50	120.46	1
N-CA-C	111.00	96.24	1
CB-CG-CD	112.60	103.64	1
OD1-CG-ND2	122.60	127.87	1
OD1-CG-ND2	122.60	117.33	1
CA-C-O	120.80	129.76	1
C-CA-CB	110.10	100.09	1
N-CA-CB	110.50	119.45	1
C-N-CD1-CG-C-CA-CB	111.40	101.40	1
N-CA-CB	110.50	119.44	1
C-CA-CB	110.10	120.09	1
O-C-N	123.00	114.59	1
CG-CD2-NE2	107.20	112.46	1
C-N-C-CA-CB	110.50	102.62	1
C-N-CA	121.70	112.25	1
CE1-CZ-CE2	120.00	110.55	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-CB-OG	111.10	100.60	1
C-CA-C-CA-CB	110.10	100.13	1
N-CA-C	111.00	96.30	1
C-CA-CB	111.40	101.43	1
C-CA-CB	110.10	100.13	1
N-CA-CB	110.40	118.27	1
O-C-N	123.00	131.39	1
N-CA-CB-CG-ND2	116.40	108.53	1
CA-CB-SG	114.40	102.34	1
OE1-CD-NE2	122.60	127.84	1
C-CA-CB	110.10	100.14	2
C-CA-CB	110.50	102.64	1
C-N-CA-CB-CG	112.60	107.36	1
CA-C-N	116.90	109.04	1
CB-CG-CD1	120.80	112.94	1
C-N-CA	121.70	112.27	2
CA-CB-CG	114.10	124.57	1
CA-CB-CD2-NE2-CE1	109.00	103.77	1
C-CA-CB	110.10	100.15	1
OE1-CD-NE2	122.60	127.83	1
C-N-N-CA-N-CA-C-CA-CB	111.40	101.46	1
N-CA-CB	110.50	119.39	2
C-CA-CB	110.10	100.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CB-CG-CD	112.60	103.72	1
CD2-NE2-CE1	109.00	103.77	1
O-C-N	123.00	114.64	1
C-CA-CB	110.10	120.03	1
CG-CD2-NE2	107.20	112.42	1
CB-CG-CA-CB-CG2	110.50	101.62	1
CA-CB-CG2	110.40	101.52	1
N-CA-CB	110.50	119.37	1
CB-CG-CD	112.60	103.73	1
CA-CB-CG	114.10	124.53	1
C-CA-CB	110.10	100.19	1
C-N-CA	121.70	112.31	1
CB-CG-CD	112.60	103.74	1
N-CA-CB	110.50	119.36	1
CG-CD-OE1	118.40	106.41	1
C-N-CA	121.70	112.32	2
CA-CB-CG	112.60	107.39	1
O-C-N	123.00	114.66	1
CG-CD-OE2	118.40	130.38	1
N-CA-CB	110.50	119.35	1
N-CA-CD2-NE2-CE1	109.00	103.79	1
C-N-CA	121.70	112.33	2
C-CA-CB	111.60	101.19	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	111.30	99.33	1
NE-CZ-NH1	121.50	116.30	1
CG-CD-NE	112.00	100.56	1
N-CA-CB	110.50	119.33	1
C-N-CA	121.70	112.35	3
CA-C-O	120.80	129.63	1
CA-CB-CG	112.60	107.41	1
CA-CB-CG	112.60	117.79	1
C-CA-CB	110.10	100.23	2
C-CA-CB	110.50	102.71	1
CA-CB-CG2	110.50	101.67	1
N-CA-CB	110.50	119.32	1
CD2-CE2-CZ2	122.40	117.21	1
CG-CD2-CE2	120.70	129.52	1
CA-CB-CG1	110.40	101.59	1
NE-CZ-NH2	119.20	114.54	1
N-CA-CB	110.50	119.30	1
C-CA-CB	110.10	100.26	1
OD1-CG-ND2	122.60	127.77	1
O-C-N	123.00	114.72	2
C-CA-O-C-N	123.00	114.72	1
CB-CG-CD1	120.70	111.91	1
N-CA-CB	110.50	119.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	117.77	1
C-CA-CB	110.10	100.28	2
CB-CG-CA-CB-CG	114.10	124.44	1
CA-CB-CG	112.60	107.43	1
CD1-CG-C-CA-CB	110.10	100.28	1
CB-CG-OD2	118.40	106.52	1
CA-CB-CG2	110.50	101.72	1
CG-CD2-NE2	107.20	112.37	1
C-N-CA	121.70	112.41	2
N-CA-CB	111.50	120.28	1
N-CA-CB	110.50	119.27	1
CG-CD2-C-CA-C-N-CA	121.70	130.99	1
C-CA-CB	110.10	100.30	1
CA-CB-CG	112.60	107.44	1
C-N-CA	121.70	112.42	1
CA-CB-CG	113.80	108.64	1
CG-CD-OE1	120.80	131.11	1
N-CA-CB	110.50	119.26	3
CB-CG-OD1	120.80	131.11	1
CB-CG-C-N-CA	121.70	130.98	1
N-CA-C-N-CA	121.70	112.42	1
C-CA-CB	110.10	100.31	1
CG-CD2-NE2	107.20	112.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.76	1
N-CD-CG	103.20	110.92	1
CA-CB-CG	112.60	107.45	1
C-N-CA	121.70	130.97	1
C-N-CA	121.70	112.44	1
C-CA-CB	110.10	100.32	1
OD1-CG-ND2	122.60	127.75	1
OD1-CG-ND2	122.60	117.46	1
N-CA-CB	110.50	119.25	1
CB-CG-CD	112.60	103.86	1
CG-CD2-CE3	133.90	128.76	1
CB-CG-OD1	120.80	110.51	1
CD1-CG-CD2	110.80	122.11	1
CG-CD-C-N-CA	121.70	112.45	1
C-N-CA	121.70	112.46	1
C-CA-C-CA-CB	110.10	100.34	1
CA-CB-CG	114.10	124.37	1
N-CA-N-CA-CB	111.50	102.78	1
C-CA-CB	110.10	100.35	1
N-CA-CB	110.50	119.22	1
CA-CB-CG2	110.50	101.78	1
C-N-CA	121.70	112.47	1
CD2-NE2-CE1	109.00	103.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CB-CG2	110.80	122.08	1
CA-CB-CG	112.60	107.47	1
CA-CB-CG	114.10	124.35	1
CG-CD2-CE3	133.90	128.78	1
C-N-CA	121.70	112.48	1
CA-CB-CG2	110.40	101.70	1
CA-CB-CG	114.10	103.87	1
C-N-CA	121.70	130.91	1
O-C-N	123.00	114.82	1
N-CA-CB	110.50	119.19	1
CA-CB-CG	112.60	107.49	1
N-CA-CB-CG-CD	112.60	103.91	1
C-N-CA	121.70	112.50	1
N-CA-CB	103.00	108.62	1
CG-CD2-CE2	121.20	128.86	1
CE1-CZ-CE2	120.00	129.20	1
C-CA-CB	110.10	100.39	1
CB-CG-CD	112.60	103.92	1
CG-CD-NE2	116.40	124.06	1
CA-CB-OG	111.10	100.88	1
CA-CB-CG2	110.50	101.82	1
C-N-CD1-CG-CD2	118.60	110.94	1
N-CA-CB	110.50	119.17	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	103.90	1
CA-CB-CG	112.60	117.70	1
C-N-CA	121.70	130.88	1
C-N-CA	121.70	112.52	1
OD1-CG-ND2	122.60	127.70	1
CB-CG-ND2	116.40	108.75	1
N-CA-CB	110.50	119.16	1
N-CA-CB	111.50	120.16	2
OE1-CD-CB-CG-CD1	126.90	134.54	1
C-N-CA	121.70	112.53	1
C-N-C-CA-CB	110.10	100.42	1
CA-CB-CG	113.90	104.73	1
N-CA-CB	111.50	120.15	1
C-N-CA	121.70	112.54	2
CG-CD1-CE1	120.70	129.35	1
N-CA-CB	110.50	119.15	1
CB-CG-ND2	116.40	124.03	1
ND1-CE1-N-CA-C-N-CA	121.70	112.55	1
N-CA-CB	110.50	119.14	1
CA-CB-CG	113.80	108.72	1
C-N-CA	121.70	112.56	2
CA-CB-CG	113.60	123.25	1
N-CA-CB-CG-OD1	120.80	110.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CA-CB-CG	112.60	107.53	1
CD1-CE1-CZ	120.00	129.13	1
ND1-CE1-CD1-CG-CD2	118.10	110.49	1
CG-CD-NE	112.00	100.85	1
OD1-CG-C-N-CA	121.70	112.58	1
ND1-CE1-NE2	108.40	113.47	1
N-CA-CB	110.50	119.12	1
CA-CB-CG	113.80	108.73	1
C-N-CA	121.70	112.58	2
CG-CD-CE	111.30	122.95	1
C-CA-CG-CD2-CB-CG-CD2	120.70	129.31	1
CA-CB-OG1	109.60	117.19	2
CB-CG-O-C-N	123.00	114.90	1
C-N-CA	121.70	130.81	1
CA-CB-CG	113.90	104.79	1
ND1-CE1-CG-SD-CE	100.90	89.77	1
CB-CG-CD	111.30	122.93	1
C-CA-CB	110.10	100.49	1
CB-CG-OD1	120.80	110.69	1
CD1-CG-CA-CB-C-N-CA	121.70	112.61	1
C-N-CA	121.70	112.61	1
O-C-N	123.00	114.92	1
N-CA-CB	110.50	119.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	104.02	2
CE2-CD2-CE3	118.80	123.85	1
CG-CD-C-CA-CB	110.10	100.52	1
CD1-CG-CD2	110.80	121.89	1
C-CA-CB	110.50	102.94	1
C-N-CA	121.70	112.63	1
CA-CB-CG	112.60	117.64	1
CA-CB-CG	113.80	108.76	1
C-N-CD-NE-CA-CB-CG	113.80	108.76	1
C-CA-CB	110.10	100.53	1
N-CA-CB	110.50	119.06	2
CA-CB-CG	113.80	108.77	1
CB-CG-CD	112.60	121.16	1
N-CA-CB	110.50	119.05	1
O-C-N	123.00	131.05	1
CB-CG-OD1	118.40	106.83	1
CA-CB-OG1	109.60	117.14	1
C-N-CA	121.70	112.65	1
CA-C-C-N-CA	121.70	112.66	1
CG-CD2-NE2	107.20	112.22	1
O-C-OG1-CB-CA-CB-CG	112.60	107.58	1
C-N-C-CA-C-N-CA	121.70	130.73	1
C-CA-CB	110.10	100.57	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	112.67	2
N-CA-CB	111.50	120.03	1
CA-CB-CG	112.60	117.62	2
ND1-CE1-NE2	108.40	113.42	1
CB-CG-CD2	120.80	113.28	1
N-CA-CB	111.50	120.02	1
CE2-CD2-CE3	118.80	123.81	1
CA-CB-OE1-CD-C-CA-CB	110.50	102.98	1
C-N-CA	121.70	112.68	1
O-C-N	123.00	114.99	1
CA-C-N-CA-CB	110.50	119.01	1
CA-C-O	120.80	129.31	1
CG-CD-C-N-CA	121.70	130.71	1
C-N-CA	121.70	112.69	1
C-CA-CB	110.10	119.61	1
CG-CD1-CE1	120.70	112.19	1
ND1-CE1-N-CA-C	111.00	96.99	1
CB-CG-ND1	122.70	130.20	1
NE-CZ-NH1	121.50	116.50	1
C-N-CA	121.70	112.70	1
CA-C-O	120.80	129.30	1
N-CA-CB	110.50	119.00	1
CA-CB-CG2	110.50	102.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	112.30	1
C-CA-CB	110.10	100.60	1
CG-CD-CE	111.30	122.79	1
CD2-NE2-CE1	109.00	104.00	1
CA-CB-CG	112.60	117.60	1
N-CA-C	111.00	97.01	1
C-N-N-CA-N-CA-C-CA-CB	111.40	101.91	1
NE-CZ-N-CA-CB	103.00	108.49	1
CA-CB-CG	112.60	107.61	1
N-CA-C	112.10	99.62	1
CA-CB-CG2	110.50	102.02	1
N-CA-CB	110.50	118.98	1
CB-CG-CD	112.60	104.12	1
C-CA-CB	110.10	100.63	2
C-N-CA	121.70	112.73	2
C-CA-CB	109.10	98.13	1
N-CA-CD2-CE2-CZ	119.60	110.63	1
CB-CG-CD	112.60	104.13	1
N-CA-CB	110.50	118.97	1
N-CA-CB	111.50	119.97	1
CA-CB-CG	113.90	104.94	1
C-CA-CB	110.10	100.64	1
N-CA-CB	111.50	119.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-OD1-CG-ND2	122.60	117.62	1
OD1-CG-ND2	122.60	117.63	1
NE-CZ-NH2	119.20	114.72	1
N-CA-CB	110.50	118.95	1
CA-CB-CG1	110.40	118.85	1
CD1-CG-CD2	110.80	99.86	1
CD2-NE2-N-CA-CB	110.50	118.95	1
CG-CD-NE2	116.40	123.85	1
C-N-CA	121.70	112.76	1
N-CA-CB	110.50	118.94	2
OE1-CD-NE2	122.60	127.57	1
C-CA-CB	110.10	100.67	2
CA-CB-CG	113.80	108.84	2
CA-CB-CG	112.60	107.64	1
O-C-N	123.00	115.06	1
N-CA-CB-CG-CD1	120.70	129.14	1
N-CA-CB	110.50	118.93	2
C-N-CA	121.70	112.77	1
CA-CB-CA-CB-CG	114.10	124.02	1
CG-CD2-NE2	107.20	112.16	1
CB-CG-CD2	120.70	129.13	1
CB-CG1-CD1	113.80	124.21	1
C-CA-CB	110.10	100.68	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	112.78	5
CG-CD-NE	112.00	101.10	1
CG1-CB-CG2	110.80	121.70	1
CG-SD-CE	100.90	90.01	1
CB-CG-CD2	126.80	119.87	1
CE2-CD2-CE3	118.80	123.75	1
CG1-CB-CG2	110.80	121.68	1
N-CA-CB	103.00	108.44	1
CA-CB-CG	112.60	107.65	1
N-CA-CB	111.50	119.91	1
N-CA-CB	110.50	118.91	1
CG-CD1-CA-CB-CG	113.80	108.86	1
CA-C-O	120.80	112.39	1
CA-CB-CA-CB-CG	112.60	107.66	1
CA-CB-CG2	110.40	102.00	1
C-CA-CB	111.40	102.02	1
C-N-CA	121.70	130.59	1
CA-C-N	116.20	126.07	1
CG-CD2-NE-CZ-NH1	121.50	126.44	1
CA-CB-O-C-N	123.00	130.89	1
N-CA-CA-C-O	120.80	112.41	1
CA-CB-CG	112.60	107.67	2
C-N-CA	121.70	112.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.60	122.96	1
N-CA-CB	110.50	118.88	1
CA-CB-CG1	110.40	118.78	1
N-CA-CB-CG-ND2	116.40	109.01	1
N-CA-CB	110.50	118.87	1
OD1-CG-ND2	122.60	117.68	1
C-CA-CB	110.50	103.12	1
CA-CB-CG	112.60	117.52	1
CA-CB-CG	113.80	108.88	1
C-CA-CB	110.10	100.76	5
C-N-CA	121.70	112.85	2
CA-CB-N-CA-C	111.00	97.24	1
O-C-N	123.00	115.13	1
CG-SD-CE	100.90	90.09	1
O-C-N	123.00	115.14	1
CG-CD1-CE1	121.20	113.83	1
C-CA-CB	110.10	119.44	1
CE2-CZ2-CH2	117.50	111.11	1
N-CA-CB	111.50	119.85	1
OE1-CD-NE2	122.60	117.69	1
CG-CD-OE1	120.80	110.97	1
C-CA-CB	110.10	100.77	1
CB-CG-C-CA-CB	110.10	100.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	97.25	1
CD-NE-CZ	124.40	117.53	1
N-CA-CB	110.50	102.16	1
N-CA-C-CA-CB	110.10	100.78	1
C-N-CA	121.70	112.87	1
CB-CG-ND2	116.40	123.75	1
O-C-C-N-CA-CB-CG	114.10	104.30	1
CA-CB-CG	113.90	105.08	1
NE-CZ-NH1	121.50	116.60	1
C-N-CA	121.70	112.88	1
CB-CG-CD2	120.70	129.03	1
C-CA-CB	111.60	101.81	1
CA-CB-CG2	110.40	102.07	1
C-N-CA	121.70	130.51	1
N-CA-CB	110.50	118.82	2
ND1-CE1-NE2	108.40	113.30	1
N-CA-C-CA-CB	110.10	100.80	1
CA-CB-CG	112.60	107.71	1
NE-CZ-NH2	119.20	114.80	1
N-CA-CB	103.00	108.38	1
OD1-CG-ND2	122.60	117.71	1
C-CA-CA-CB-N-CA-CB-CG-CD2	120.70	112.39	1
CG-CD-OE2	118.40	107.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-NE-CZ-NH2	119.20	123.60	1
CB-CG-CD	112.60	104.30	1
CD-NE-O-C-N	123.00	115.19	1
C-N-CA	121.70	130.48	1
C-N-N-CA-CB	103.00	108.37	1
CA-CB-CG1	110.40	118.69	1
CA-CB-CG1	110.40	102.11	1
C-CA-CB	110.10	100.83	1
C-N-CA	121.70	112.92	1
N-CA-CB	110.50	118.78	2
O-C-N	123.00	115.21	2
C-CA-CB	110.10	119.35	1
C-CA-CB	110.10	100.85	1
N-CA-CB	103.00	108.36	1
CA-CB-CG2	110.50	102.22	1
C-N-CA	121.70	112.94	2
N-CA-CB	110.50	118.77	1
N-CA-C	111.00	97.37	1
CG-CD2-NE2	107.20	112.07	1
C-CA-N-CA-CB	103.00	108.35	1
CA-CB-CG	113.90	105.14	1
CD1-CG-CD2	118.60	111.30	1
CA-CB-CG2	110.50	102.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.40	102.16	1
CA-CB-CD1-CG-CD2	118.60	125.89	1
C-N-CA	121.70	130.45	1
O-C-N	123.00	115.22	1
N-CA-CB	110.50	118.76	4
CB-CG-CD2	131.20	124.88	1
C-N-CA	121.70	112.95	1
N-CA-CB	103.00	108.35	1
CA-CB-OG1	109.60	116.89	1
CG-CD-NE2	116.40	109.11	1
C-CA-CB	111.60	101.88	1
C-CA-CB	110.50	117.79	1
C-N-CA	121.70	112.96	2
CD-NE-CZ	124.40	117.60	2
ND1-CE1-NE2	108.40	113.26	1
C-CA-CB	110.10	100.88	2
O-C-N	123.00	130.76	1
CB-CG-OD1	120.80	111.10	1
O-C-N	123.00	115.24	1
C-CA-CB	110.10	100.89	1
N-CA-CB-CG-N-CA-CB	110.50	118.74	1
N-CA-N-CA-C	111.00	97.43	1
N-CA-C	111.00	97.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.25	1
C-N-CA	121.70	112.98	1
N-CA-CB	111.50	119.73	1
N-CA-CB	110.50	118.73	1
C-N-CA	121.70	112.99	1
N-CD-CG	103.20	110.46	1
CA-C-O	120.80	129.03	1
CA-C-N	116.90	109.64	1
CD2-NE2-CE1	109.00	104.16	1
CA-CB-C-CA-CB	110.10	100.91	1
CA-CB-CA-CB-CG	116.30	99.37	1
CB-CG-CD2	120.80	128.06	1
C-N-CA	121.70	130.41	1
C-N-CA	121.70	113.00	1
CB-CG-CD	112.60	104.38	1
CB-CG-CD	112.60	104.39	1
C-CA-CB	111.60	101.94	1
CA-CB-CG	113.80	108.97	1
CD2-CE2-C-N-CA	121.70	130.39	1
N-CA-CB	110.50	118.71	1
CG-CD-CE	111.30	122.41	1
C-N-CA	121.70	113.01	2
C-CA-CB	111.60	101.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CA-CB-CG	112.60	107.77	1
CB-CG-CD	112.60	104.40	1
C-CA-CB	110.10	100.94	1
O-C-N	123.00	115.28	1
N-CA-CB	110.50	118.70	1
CA-CB-CG2	110.50	102.31	1
C-N-CA	121.70	113.03	2
CG-CD2-CE3	133.90	129.08	1
CA-C-ND1-CG-CD2	106.10	101.28	1
C-CA-CB	110.10	119.25	1
CA-CB-CG	113.80	108.98	1
CB-CG-ND1	122.70	115.48	1
OD1-CG-ND2	122.60	117.79	2
N-CA-CB	110.50	118.68	2
C-CA-CB	110.10	100.96	1
O-C-N	123.00	115.30	1
CG-CD2-NE2	107.20	112.01	1
O-C-N	123.00	115.31	1
CA-CB-CG1	110.40	102.23	1
N-CA-CG-CD-CG-CD2-CE2	120.70	128.87	1
CD-NE-CZ	124.40	117.67	1
O-C-CA-CB-CG	112.60	107.80	1
C-N-CA	121.70	130.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	107.80	1
C-CA-CB	110.10	100.97	1
CA-CB-CG-CD-CE	111.30	122.34	1
N-CA-CB	110.50	118.66	2
CA-C-N	116.90	124.10	1
C-N-CA	121.70	113.06	2
C-CA-CB	110.10	100.98	3
CB-CG-OD1	118.40	107.36	1
N-CA-CB	110.50	118.65	4
C-N-CA	121.70	130.33	1
CD2-NE2-CE1	109.00	104.20	1
CD1-CG-N-CA-CB	110.50	118.65	1
C-N-CA	121.70	113.07	1
CB-CG-ND2	116.40	109.21	1
CA-CB-CG	112.60	107.81	2
C-N-CA	121.70	113.08	1
N-CA-CB	110.50	118.64	2
CB-CG-CD	112.60	104.46	1
C-CA-CB	110.10	101.00	1
OD1-CG-ND2	122.60	117.81	1
CA-CB-CG2	110.40	102.26	1
CB-CG-CD	111.30	122.31	1
CA-CB-OG	111.10	101.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	112.67	1
CA-CB-CG	113.80	109.02	1
N-CA-CB	110.50	118.63	1
C-CA-CB	110.10	101.01	1
O-C-N	123.00	115.35	1
C-N-CA	121.70	113.09	1
C-N-CA	121.70	113.10	2
O-C-N	123.00	115.36	1
N-CA-CB	110.50	118.62	1
C-CA-CB	110.10	101.03	1
CA-CB-CD1-CG-C-N-CA	121.70	130.29	1
C-N-CA	121.70	113.11	3
N-CA-CB	110.40	117.56	1
C-N-CA	121.70	130.29	1
CA-CB-CG	113.90	105.32	1
CA-CB-CG	112.60	117.37	1
N-CA-CB	111.50	119.61	1
C-CA-CB	110.10	101.04	2
CB-CG-CD	112.60	104.50	1
OE1-CD-NE2	122.60	127.37	1
CG-CD2-NE2	107.20	111.96	1
C-CA-CB	110.10	101.05	1
C-N-CA	121.70	130.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.27	1
C-N-CA	121.70	113.13	5
CA-CB-CG	112.60	107.84	2
O-C-N	123.00	115.38	1
CE1-CZ-CE2	120.00	128.57	1
C-CA-CB	110.10	101.06	1
CB-CG-CG-CD2-N-CA-CB	110.50	118.59	1
CA-CB-CG	114.10	123.62	2
CA-CB-CG	113.90	105.33	1
CA-C-C-CA-C-N-CA	121.70	113.14	1
CA-CB-CG	112.60	107.85	1
CD-NE-CZ	124.40	117.75	1
NH1-CZ-NH2	119.30	113.12	1
N-CA-CB	110.40	117.53	1
CA-CB-CG1	110.40	102.32	1
C-CA-CB	110.10	101.07	1
CD2-CE2-CZ	120.00	128.55	1
OD1-CG-ND2	122.60	127.35	1
OD1-CG-ND2	122.60	117.85	1
C-N-CA	121.70	113.15	1
CG-SD-CE	100.90	90.46	1
CD1-CG-CD2	110.80	121.24	2
CG-CD-NE2	116.40	109.28	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.05	1
CB-CG-CD	112.60	104.53	1
N-CA-CB	110.50	118.57	1
C-N-CA	121.70	113.16	1
CB-CG-CA-CB-CG	112.60	107.86	1
N-CA-N-CA-CB	110.50	118.56	1
N-CA-CB	110.50	118.56	1
C-CA-CB	110.10	101.09	1
C-N-CA	121.70	113.17	2
CA-C-N	116.20	125.68	1
CB-CG-CD1	120.70	128.76	1
C-CA-CB	111.60	102.13	1
CG-CD2-CE2	120.70	112.65	1
CA-CB-CG	113.80	109.07	1
CA-CB-CG1	110.40	102.35	1
C-N-CA	121.70	130.22	1
C-CA-CB	110.50	103.40	1
C-CA-C-N-CA	121.70	113.19	1
CG-CD2-NE2	107.20	111.93	1
C-CA-CB	111.60	102.14	1
C-CA-CB	110.10	101.12	1
CB-CG-CD1	120.80	113.71	1
CB-CG-OD2	118.40	107.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-N-CA-C-N-CA	121.70	130.20	1
CG-CD-OE2	118.40	107.54	1
CE1-CZ-CE2	120.30	129.75	1
OD1-CG-ND2	122.60	127.32	1
C-N-CA	121.70	113.20	3
C-CA-C-CA-CB	110.10	101.13	1
CA-CB-CG	113.80	109.08	1
CB-CG-CD	112.60	104.58	1
CG-SD-C-N-CA	121.70	113.21	1
N-CA-CB	110.40	117.48	1
C-N-CA	121.70	130.19	1
C-CA-CB	111.60	102.17	1
CB-CG-ND2	116.40	109.33	1
N-CA-CB	110.50	118.51	1
OE1-CD-NE2	122.60	117.89	1
CA-CB-CG2	110.40	118.41	1
C-N-CA	121.70	113.22	2
O-C-N	123.00	115.46	1
C-N-CA	121.70	130.18	1
CA-C-O	120.80	128.81	1
CG1-CB-CG-CD-NE2	116.40	109.34	1
CB-CG-CD2	120.70	112.70	1
C-N-CA	121.70	113.23	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.50	1
CA-CB-CG	112.60	117.31	1
CB-CG-CD	112.60	104.60	1
OD1-CG-ND2	122.60	117.90	1
CA-CB-CG	112.60	117.30	1
CB-CG-CD	111.30	122.12	1
C-N-CA	121.70	113.24	2
CA-CB-CG	112.60	107.90	1
ND1-CE1-NE2	108.40	113.10	1
CG-CD2-CB-CG-CD1	120.70	112.71	1
C-N-CA	121.70	130.15	2
CA-CB-OG	111.10	101.71	1
O-C-N	123.00	130.51	1
N-CA-CB	110.50	118.48	1
O-C-N	123.00	115.49	1
NH1-CZ-NH2	119.30	125.40	1
N-CA-CB-CG-C-CA-CB	110.50	103.46	1
CA-C-O	120.80	112.83	1
N-CA-CB	103.00	108.16	2
CA-CB-CG	113.80	109.11	1
C-N-CA	121.70	130.14	1
C-N-CA	121.70	113.26	1
N-CA-CB	110.50	118.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	120.70	128.67	1
NE-CZ-NH2	119.20	123.42	1
CD1-CG-CD2	118.60	111.57	1
N-CA-C	111.00	97.88	1
C-CA-CB	111.60	102.23	1
OD1-CG-ND2	122.60	127.29	1
CA-C-O	120.80	112.84	1
CB-CG-CD	111.30	122.07	1
N-CA-CB	110.50	118.46	1
C-CA-CB	110.10	101.21	1
C-CA-CB	110.10	118.99	1
O-C-N	123.00	115.51	1
CA-C-N	116.90	109.88	1
C-N-CA	121.70	113.28	2
C-N-CA	121.70	130.12	1
CA-CB-CG	112.60	107.92	1
CA-CB-CG	112.60	107.93	2
CA-CB-C-CA-CB	111.60	102.26	1
CA-C-O	120.80	112.86	1
C-N-CA	121.70	130.11	1
CG-CD-NE2	116.40	109.40	1
N-CA-CB	110.50	118.44	1
CD1-CE1-CZ	120.00	111.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	118.33	1
N-CA-CB	110.50	118.43	3
CA-CB-CG	113.80	109.13	1
CA-C-O	120.80	112.87	1
CA-CB-CG2	110.50	102.57	1
C-CA-CB	110.10	101.23	1
C-N-CA	121.70	113.30	1
CD1-CG-CA-CB-CG2	110.50	102.57	1
CA-CB-CG	113.80	109.14	3
CB-CG-CA-CB-CG	112.60	107.94	1
CA-C-N	116.90	109.91	1
OD1-CG-ND2	122.60	127.26	1
N-CA-CB	110.50	118.42	2
CA-C-C-CA-CB	111.40	102.55	1
CG-CD-OE1	120.80	111.48	1
CB-CG-CD	112.60	104.68	1
C-CA-CB	110.10	101.25	2
CG-SD-CE	100.90	90.65	1
CD2-CE2-C-N-CB-CG-ND1	122.70	129.69	1
CB-CG-CA-CB-CG	112.60	117.26	1
CD2-NE2-CE1	109.00	104.34	1
N-CA-CG-CD1-NE1	110.20	104.15	1
O-C-N	123.00	115.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	108.12	2
CA-CB-CG	113.80	109.15	1
N-CA-C	111.00	97.97	1
C-N-CA	121.70	113.33	1
CB-CG-ND2	116.40	109.42	1
CB-CG-CD2	120.80	127.78	1
N-CA-CB	110.50	118.41	1
N-CA-C	111.00	97.98	1
C-CA-CB	110.10	101.27	1
N-CA-CB	110.50	118.40	3
CB-CG-OD2	118.40	107.71	1
OE1-CD-NE2	122.60	127.25	1
C-N-CA	121.70	113.34	1
CB-CG-CD2	131.20	137.24	1
OG1-CB-CG2	109.30	118.59	1
CB-CG-OD2	118.40	107.72	1
O-C-N	123.00	115.57	1
NE-CZ-NH2	119.20	115.02	1
N-CA-C-CA-CB	111.60	102.32	1
CB-CG-CD	112.60	104.71	1
OE1-CD-NE2	122.60	127.24	1
N-CA-C	113.30	99.85	1
O-C-N	123.00	115.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-ND1	122.70	129.66	1
CA-CB-CG	113.90	105.55	1
N-CA-CB	110.40	117.36	1
CA-CB-CG2	110.40	102.52	1
CG-CD2-CE2	121.20	128.15	1
N-CA-CB	110.50	118.38	1
CD2-NE2-CE1	109.00	104.36	1
C-N-CA	121.70	113.36	3
CB-CG-CD	111.30	121.96	1
CG-CD2-CE3	133.90	129.27	1
C-CA-CB	110.10	101.30	1
N-CA-CB	111.50	119.37	1
CB-CG1-CD1	113.80	123.53	1
C-N-CA	121.70	130.04	1
N-CA-C	111.00	98.03	1
O-C-N	123.00	130.41	1
CA-CB-CG	112.60	107.97	1
CG-CD2-C-CA-CB	110.10	118.89	1
N-CA-C-N-CA	121.70	113.38	1
CA-CB-CG	112.60	107.98	2
CB-CG-ND2	116.40	109.46	1
CB-CG-CD	112.60	104.74	1
C-N-CA	121.70	113.38	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	98.06	1
N-CA-CB	111.50	119.36	1
CD-NE-CZ	124.40	117.93	1
CD2-CE2-CZ	120.00	111.68	1
CB-CG-CD1	120.70	112.84	1
CA-CB-CG	113.90	105.58	1
NH1-CZ-NH2	119.30	125.30	1
CG-CD-NE2	116.40	123.33	1
ND1-CE1-NE2	108.40	113.02	1
CA-CB-CG1	110.40	102.55	1
C-N-OE1-CD-NE2	122.60	127.22	1
C-N-C-CA-CB	111.40	102.63	1
CD1-CG-CD2	110.80	120.96	2
C-CA-CB	110.10	101.33	1
C-CA-C-CA-CB	110.10	101.34	1
C-N-CA	121.70	113.40	1
N-CA-CB	110.50	118.34	1
NE-CZ-CB-CG1-CD1	113.80	104.12	1
CA-CB-CG	112.60	107.99	1
CG1-CB-CG2	110.70	124.53	1
C-CA-CB	110.50	103.59	2
CG-CD1-CE1	120.70	128.54	1
CA-C-N	116.90	109.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CA-CB-CG	112.60	107.99	1
C-N-CA	121.70	113.41	2
C-N-CA-CB-CG	113.80	109.19	1
N-CD-C-N-CA	121.70	113.41	1
CB-CG-CD1	120.70	112.87	1
N-CA-CB	110.50	118.33	1
N-CA-C	111.00	98.11	1
CG-CD1-CE1	121.20	114.30	1
O-C-N-CA-CB	110.50	118.32	1
C-CA-CB	110.10	101.36	1
O-C-N	123.00	115.64	1
C-N-CA	121.70	129.98	1
C-N-CA	121.70	113.42	2
CD2-CE2-CZ	120.00	128.28	1
CG-SD-CE	100.90	90.79	1
C-CA-CB	109.10	98.99	1
N-CA-C	111.00	98.13	1
OG1-CB-O-C-N	123.00	130.35	1
CB-CG1-CD1	113.80	104.15	1
CE1-CZ-CE2	120.00	111.73	1
CD2-CE3-CZ3	118.60	112.63	1
CA-C-N	116.20	125.39	1
CG-CD2-CB-CG-ND2	116.40	109.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	128.60	1
CB-CG-CD	111.30	121.85	1
C-N-CA	121.70	129.96	2
C-CA-CB	110.10	101.39	1
N-CA-CB	110.50	118.30	2
OE1-CD-NE2	122.60	118.01	1
N-CA-CB	103.00	108.04	1
C-CA-C-N-CA	121.70	129.95	1
N-CA-C-CA-CB	110.10	101.39	1
CA-CB-CG1	110.40	102.61	1
CB-CG-CD	112.60	104.81	1
CA-CB-CG	113.80	109.22	1
C-N-CA	121.70	113.45	1
CB-CG-CG-CD-CE	111.30	121.83	1
C-N-CA	121.70	129.94	1
C-N-CA	121.70	113.46	1
C-CA-CB	111.60	102.44	1
CA-CB-CG2	110.50	102.72	1
C-CA-CB	110.10	101.40	1
CD2-CE2-CZ	120.00	128.24	1
OD1-CG-ND2	122.60	118.02	1
NE-CZ-NH1	121.50	116.92	1
CB-CG-CD	112.60	104.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-N-CD-CG	103.20	110.06	1
CA-C-N	116.90	123.76	1
N-CA-CB	110.50	118.28	1
O-C-N	123.00	115.68	1
C-N-CA	121.70	129.93	1
N-CA-CB	110.50	118.27	3
CB-CG-C-N-CA	121.70	113.47	1
NH1-CZ-NH2	119.30	125.24	1
CA-CB-OG	111.10	101.96	1
C-N-CA	121.70	113.47	1
C-N-CA	121.70	113.48	1
CB-CG1-CD1	113.80	123.39	1
C-CA-CB	110.10	101.42	1
CD2-NE2-CE1	109.00	104.43	1
CB-CG-OD1	118.40	107.90	1
CA-CB-CG	113.90	105.68	1
CA-CB-OG1	109.60	102.75	1
NH1-CZ-NH2	119.30	113.37	1
C-N-CB-CG-CD2	131.20	125.27	1
CB-CG-CD	112.60	104.84	2
N-CA-CB	110.50	118.26	1
CG-CD1-CE1	120.70	112.94	1
C-N-CA	121.70	129.91	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CG-CD2-CE2	121.20	128.04	1
CG1-CB-CG2	110.80	120.83	1
N-CA-CB	110.50	118.25	1
O-C-N	123.00	115.71	1
C-CA-CB	110.10	101.44	1
CB-CG-CD2	120.70	128.45	1
CD1-CG-CD2	118.60	125.43	1
CA-CB-CG	113.60	122.26	1
CB-CG-O-C-N	123.00	130.29	1
CA-C-O	120.80	128.55	1
CB-CG-CA-C-O	120.80	113.06	1
CB-CG-CD	112.60	104.86	1
N-CA-CB	110.50	118.24	2
C-CA-CG-CD-NE2	116.40	123.23	1
CB-CG-OD1	120.80	129.91	1
CB-CG-CD	111.30	121.77	1
CB-CG1-CD1	113.80	123.36	1
CB-CG-CD1	120.70	128.44	1
O-C-OD1-CG-ND2	122.60	118.05	1
C-N-CA	121.70	113.51	1
CA-CB-CG2	110.50	102.77	1
O-C-N	123.00	115.72	2
CG-SD-CA-CB-CG2	110.50	118.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.23	1
N-CA-C	113.30	100.11	1
C-CA-CB	110.10	118.74	2
CG-CD-OE1	118.40	107.94	1
C-N-CA	121.70	113.52	2
CA-C-O	120.80	128.53	1
N-CA-CB	110.40	117.22	1
N-CA-CB	111.50	119.23	1
C-CA-CB	109.10	99.10	1
N-CA-CD2-CE3-CZ3	118.60	112.69	1
CD1-CG-CD2	110.80	120.79	1
C-CA-CB	110.10	101.47	1
CA-CB-CG	112.60	108.06	1
O-C-CA-CB-CG	112.60	108.06	1
CA-CB-CG	113.90	105.73	1
N-CA-C	111.00	98.29	1
CB-CG-CD	112.60	104.88	1
C-CA-CB	110.10	101.48	2
N-CA-CB	110.50	118.21	2
CD1-CE1-CZ	120.00	111.84	1
CB-CG-CD1	120.70	112.99	1
N-CA-C	112.10	100.77	1
CB-CG-CD1	120.70	128.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.60	102.53	1
O-C-N	123.00	115.75	1
CA-CB-CG	113.80	109.27	1
CG1-CB-CG2	110.80	120.77	1
CG-CD2-CE2	120.70	128.40	1
C-CA-CB	110.10	101.49	2
CB-CG-CD1	120.70	128.40	1
C-N-CA	121.70	113.55	2
OG1-CB-C-N-CA	121.70	113.55	1
CA-C-O	120.80	113.10	1
CA-C-N	116.20	125.26	1
N-CA-N-CA-CB	110.50	118.20	1
CB-CG-CD	111.30	121.71	1
CA-CB-CG1	110.40	102.70	1
N-CA-C-CA-CB	110.10	101.50	1
OD1-CG-ND2	122.60	118.07	1
C-CA-CB	109.10	99.14	1
C-CA-CB	110.10	101.50	1
O-C-CB-CG-CD	112.60	104.91	1
CB-CG-CD2	120.80	114.01	1
CA-CB-CG	112.60	108.08	1
N-CA-CB	110.50	118.19	1
CA-CB-CA-C-CA-CB-CG	112.60	108.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	104.48	1
N-CA-CB	110.50	118.18	1
CA-C-O	120.80	128.48	1
CE3-CZ3-CH2	121.10	126.98	1
N-CA-CB	103.00	107.97	1
C-CA-CB	111.40	102.81	1
C-CA-CB	111.60	102.56	1
C-CA-C-N-CA	121.70	113.57	1
C-N-CA	121.70	113.57	1
CB-CG-ND1	122.70	129.48	1
O-C-N-CA-C	111.00	98.36	1
CB-CG-CD2	126.80	120.48	1
C-CA-CA-CB-CG2	110.50	102.83	1
N-CA-CB	110.50	118.17	2
CG-CD2-CE2	121.20	127.97	1
O-C-N	123.00	115.78	2
CA-CB-CG	112.60	108.09	1
ND1-CE1-NE2	108.40	112.91	1
CA-CB-CG	113.80	109.29	1
CA-CB-CG	113.90	105.78	1
CB-CG-ND2	116.40	109.64	1
CA-C-O	120.80	128.46	1
CG-CD-CB-CG-ND1	122.70	129.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE1-CZ-CE2	120.30	111.29	1
N-CA-O-C-N	123.00	130.21	1
CA-CB-OG	111.10	102.09	1
CA-CB-CG	113.90	105.79	1
CB-CG-CD2	131.20	125.34	1
CA-C-N	116.20	125.21	1
CA-CB-CG	113.80	109.30	1
CA-CB-CG2	110.50	102.85	1
CB-CG-CA-C-N	116.90	110.15	1
CA-CB-CG1	110.40	118.05	1
C-CA-N-CA-CB-CG1-CD1	113.80	104.35	1
N-CA-CB	110.50	118.15	1
N-CA-CB	103.00	107.95	1
CA-CB-CG	113.90	105.81	1
C-N-CA	121.70	113.61	2
N-CA-CB	110.50	118.14	1
C-CA-CB	110.10	101.56	2
CA-CB-OG1	109.60	102.86	1
CA-CB-CG2	110.40	102.76	1
CD-NE-CZ	124.40	118.11	1
C-N-CA	121.70	129.79	1
N-CA-CB-CG-ND2	116.40	109.66	1
N-CA-CB	111.50	119.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CB-CG1-CD1	113.80	104.37	1
CA-CB-CG-SD-CE	100.90	91.02	1
N-CA-N-CA-CB	110.50	118.13	1
CE2-CZ2-CH2	117.50	111.66	1
C-N-CA	121.70	129.78	1
C-N-CA	121.70	113.62	2
CA-CB-CG	112.60	108.11	1
CA-C-O	120.80	113.17	1
CB-CG-CB-CG-CD	112.60	104.97	1
CB-CG-CA-CB-CG2	110.50	118.13	1
N-CA-N-CA-CB	111.50	119.13	1
CA-CB-N-CA-CB	110.50	118.13	1
N-CA-CB	111.50	119.13	1
C-CA-CB	110.10	101.58	2
CA-CB-CG	112.60	108.12	2
C-N-CA	121.70	113.63	2
O-C-N	123.00	130.17	1
N-CA-CB	110.50	118.12	2
N-CA-CB	103.00	107.93	1
NE-CZ-N-CA-CB	110.50	118.12	1
C-N-CA	121.70	129.77	2
N-CA-C	112.10	100.89	1
C-N-CB-CG-CD2	120.70	128.32	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CB-N-CA-C	111.00	98.45	1
CG-CD-OE2	118.40	128.71	1
CA-CB-CG2	110.50	118.12	1
CG1-CB-CG2	110.80	120.66	1
C-CA-CB	110.10	101.59	1
CB-CG-CD1	120.70	128.32	1
CG1-CB-N-CA-CB	110.50	118.12	1
OD1-CG-ND2	122.60	127.08	1
N-CA-CB	110.50	118.11	2
C-N-CA	121.70	113.64	1
C-N-CA	121.70	113.65	1
CD2-NE2-CE1	109.00	104.53	1
N-CA-CB	110.50	118.10	2
CA-C-O	120.80	113.20	1
CA-CB-CG2	110.50	102.90	2
C-CA-CB	110.10	118.60	1
C-CA-CB	110.10	101.60	1
CA-CB-CG	112.60	108.13	1
CB-CG-CD1	110.70	97.29	1
CB-CG-CD	112.60	105.00	1
CG-CD2-CE2	120.70	113.10	1
CA-CB-CA-CB-CG2	110.40	102.80	1
CB-CG1-CD1	113.80	123.18	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	107.91	2
N-CA-CB	110.50	118.09	1
CB-CG-CD	112.60	105.01	1
C-N-CA	121.70	113.66	1
N-CA-N-CA-C-N-N-CA-CB	110.50	102.91	1
CD2-CE2-CZ2	122.40	117.94	1
C-CA-CB	110.10	101.62	1
CA-CB-CG2	110.40	102.82	1
N-CA-CB	110.50	118.08	2
CG-CD-C-N-CA	121.70	113.67	1
O-C-CA-CB-OG1	109.60	102.91	1
N-CA-C	111.00	98.51	1
CA-C-O	120.80	113.22	1
CB-CG-ND1	122.70	129.39	1
N-CD-CG	103.20	109.89	1
CG1-CB-CB-CG-CD	112.60	105.02	1
C-N-CA-C-CA-CB-OG1	109.60	116.29	1
CG-CD1-CE1	120.70	128.28	1
OD1-CG-ND2	122.60	118.14	1
CD-NE-CZ	124.40	118.16	1
N-CA-CB	111.50	119.07	1
CB-CG1-CD1	113.80	104.44	1
CA-CB-CG	112.60	108.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	136.99	1
CB-CG-CD2	131.20	125.41	1
C-CA-CA-CB-CG2	110.40	102.83	1
CA-CB-CG	112.60	108.15	1
CB-CG-OD1	120.80	111.89	1
CG-CD-OE2	118.40	108.16	1
CB-CG-CA-C-N	116.90	110.22	1
C-N-CA	121.70	113.69	1
CB-CG-CD1	120.80	114.13	1
OE1-CD-NE2	122.60	127.05	1
N-CA-CB	103.00	107.89	1
CD1-CE1-CZ	120.00	128.01	1
CB-CG-CA-CB-CG	113.90	105.89	1
CG-CD1-CE1	120.70	128.26	1
CA-CB-CG	113.80	109.35	1
N-CA-CB	110.50	118.06	1
C-CA-CB	110.10	101.65	1
CB-CG-CD	111.30	121.52	1
C-CA-N-CA-CB	110.50	118.06	1
C-CA-CB	110.10	101.66	2
CG-CD2-CE2	120.70	113.15	1
CA-CB-CG2	110.40	102.85	1
CG1-CB-CG2	110.80	120.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	118.10	111.44	1
CA-CB-CG	113.80	109.36	1
CB-CG-OD1	120.80	129.68	1
CG-CD2-CA-CB-CG1	110.40	102.85	1
ND1-CG-CD2	106.10	110.54	1
O-C-N	123.00	115.90	1
C-CA-CB	110.10	118.53	1
CA-CB-CG1	110.40	102.86	1
N-CA-ND1-CG-C-N-CA	121.70	113.72	1
N-CA-N-CA-CB	110.50	118.04	1
CB-CG-CD	112.60	105.06	1
N-CA-CB	103.00	107.88	1
N-CA-C-N-CA	121.70	113.72	1
C-CA-CB	110.10	118.52	2
O-C-N	123.00	130.09	1
CA-C-O	120.80	113.27	1
O-C-N	123.00	115.91	1
CB-CG-CD1	120.80	114.15	1
CA-C-O	120.80	128.33	1
CA-CB-CG	113.80	109.37	1
C-N-CA	121.70	113.73	1
C-N-CA	121.70	129.67	1
CG-SD-CE	100.90	91.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-OD1	120.80	129.65	1
CA-CB-CG	114.10	122.95	1
N-CA-C	113.30	100.47	1
N-CA-CB	111.50	119.02	1
O-C-N	123.00	115.93	3
CG-CD2-CE3	133.90	129.48	1
C-CA-CB	110.10	101.70	1
CG1-CB-CG2	110.80	120.52	1
CB-CG-OD1	120.80	111.96	1
CB-CG-OD1	120.80	129.64	1
CA-CB-O-C-N	123.00	115.93	1
C-CA-CB	111.60	102.77	1
C-CA-CB	110.10	101.71	2
C-N-CA	121.70	113.75	1
N-CA-C-N-CA	121.70	113.76	1
N-CA-C	113.30	100.51	1
CA-C-N	116.90	123.52	1
N-CA-CB	110.50	118.00	1
C-CA-CB	111.40	103.02	1
O-C-N	123.00	130.06	1
O-C-N	123.00	115.94	1
C-CA-CB	110.10	101.72	1
CA-CB-CG2	110.40	117.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.99	2
CA-CB-CG	112.60	108.19	1
CD-NE-CZ	124.40	118.23	1
CB-CG-CD	111.30	121.44	1
CZ2-CH2-CZ3	121.50	127.23	1
C-N-CA	121.70	113.77	2
N-CA-CA-CB-OG1	109.60	116.21	1
C-CA-CB	110.10	101.73	1
N-CA-CB	110.50	103.02	1
CG-CD2-CE2	120.70	113.22	1
C-CA-N-CA-C	111.00	98.68	1
C-N-CA	121.70	129.62	1
C-N-CA	121.70	113.78	1
CG-CD1-CE1	121.20	114.60	1
C-N-CA	121.70	129.61	2
CB-CG-ND2	116.40	109.81	1
CG1-CB-O-C-N	123.00	115.97	1
NE-CZ-NH1	121.50	125.89	1
C-CA-CB	110.10	101.75	1
CD1-CG-CD2	118.10	124.69	1
CE1-CZ-CE2	120.00	127.91	1
C-N-CA	121.70	129.60	1
CA-CB-CG	112.60	108.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.96	2
OE1-CD-NE2	122.60	118.21	1
O-C-N	123.00	115.98	1
CG-CD1-CE1	121.20	114.62	1
CB-CG-CD	112.60	105.14	2
C-N-CA	121.70	113.80	3
CA-CB-CG1	110.40	102.94	1
CA-CB-CG	114.10	122.87	2
CA-CB-C-CA-CB	111.60	102.83	1
CD2-CE2-CZ	120.00	127.89	1
N-CA-C	111.00	98.72	1
C-N-CA	121.70	113.81	1
CA-CB-CG2	110.50	103.05	2
CG-CD1-CE1	121.20	114.63	1
C-CA-CB	110.10	101.78	3
O-C-N	123.00	115.99	1
N-CA-N-CA-C	111.00	98.74	1
C-CA-CB	110.10	118.42	2
CA-CB-CG	112.60	108.22	2
N-CA-CA-C-O	120.80	128.24	1
CA-CB-CG	113.90	106.02	1
CA-C-C-CA-CB	110.10	101.78	1
C-CA-CG-CD-C-N-CA	121.70	113.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.94	1
C-N-CA	121.70	113.82	1
C-N-CA	121.70	129.57	1
CA-CB-CG2	110.40	102.96	1
O-C-N	123.00	116.00	1
C-N-CA	121.70	113.83	1
CB-CG-ND2	116.40	109.84	1
OD1-CG-ND2	122.60	118.23	2
NE-CZ-NH1	121.50	125.87	1
N-CA-C	111.00	98.76	1
C-CA-CB	110.10	101.79	1
CA-CB-CG	113.80	109.43	1
N-CA-CB	110.50	117.93	2
CA-CB-CG2	110.40	102.97	1
C-CA-N-CA-CB	110.50	117.93	1
CB-CG-CD	112.60	105.17	1
C-CA-CB	111.60	102.86	1
CB-CG-CD1	120.70	113.27	1
C-N-CA	121.70	129.56	1
CA-CB-CG	112.60	116.97	1
CD2-NE2-CE1	109.00	104.63	1
CD1-CG-CD2	118.60	125.15	1
N-CA-CB	110.50	117.92	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	107.47	1
O-C-N	123.00	116.02	3
C-CA-CB	110.10	101.81	3
CA-CB-CG2	110.50	117.92	1
CA-CB-CG	112.60	108.24	2
C-N-N-CA-O-C-N	123.00	116.02	1
CB-CG-ND2	116.40	122.95	1
N-CA-C	112.10	101.19	1
CA-CB-CG1	110.40	102.98	1
CB-CG-CD	112.60	105.18	1
CA-CB-C-N-CA	121.70	113.85	1
N-CA-CB	103.00	107.80	1
CA-CB-CG	113.90	106.05	1
N-CA-C	111.00	98.79	1
N-CA-CB	110.50	117.91	1
N-CA-CB	110.40	116.94	1
C-N-CA-C-N	116.20	124.92	1
O-C-N	123.00	116.03	1
C-CA-CB	110.50	103.96	1
N-CA-C	111.00	98.80	1
C-CA-CB	110.10	101.82	1
CA-CB-SG	114.40	104.38	1
CD2-CE3-CZ3	118.60	112.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	113.86	1
CB-CG-OD2	118.40	108.38	1
O-C-N	123.00	129.97	1
N-CA-CB	110.50	117.90	1
C-CA-CB	110.10	101.83	3
CD2-NE2-CE1	109.00	104.65	1
CA-C-O	120.80	128.20	1
C-N-CA	121.70	113.87	2
C-N-CG-CD1-CE1	120.70	128.10	1
N-CA-CB	111.50	118.90	1
CB-CG-CD	112.60	105.20	1
C-CA-CB	111.40	103.13	1
N-CA-CB	111.50	118.89	1
CA-CB-CG1	110.40	117.79	1
CA-CB-CG	113.80	109.45	1
O-C-N	123.00	129.96	1
C-N-CA	121.70	113.88	2
CB-CG-CG-CD1-CE1	121.20	114.68	1
CB-CG-CB-CG-CD2	126.80	120.72	1
N-CA-C	111.00	98.83	1
CB-CG-OD1	120.80	129.49	1
CG-CD-OE1	118.40	108.41	2
NE-CZ-NH1	121.50	125.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-CE-NZ	111.90	98.00	1
C-CA-CB	110.10	101.85	2
CD1-CG-CD2	110.80	120.36	1
CA-CB-CA-C-O	120.80	113.42	1
N-CA-CB	110.50	117.88	2
CB-CG1-CD1	113.80	104.68	1
CB-CG-CD1	120.80	127.31	1
CG-CD1-CE1	121.20	127.71	1
CG1-CB-CG2	110.80	120.35	1
CB-CG-CD	112.60	105.22	2
NE-CZ-C-CA-CG-CD-NE	112.00	102.45	1
CA-CB-CG1	110.40	103.03	1
C-N-CA	121.70	113.89	1
CA-C-CD-NE-C-CA-CB	110.10	101.86	1
CA-CB-CG	113.80	109.46	1
C-CA-CB	111.40	103.16	1
C-N-CA	121.70	129.50	3
N-CA-CB	110.50	117.87	2
C-N-CA	121.70	113.90	1
N-CA-CB	110.50	117.86	3
O-C-N	123.00	129.93	1
CE2-CD2-CE3	118.80	123.13	1
C-CA-CB	110.10	101.87	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	118.86	3
O-C-N	123.00	116.07	1
CA-C-O	120.80	113.44	1
CB-CG-ND1	122.70	129.20	1
CD2-CE2-CZ2	122.40	118.07	1
N-CA-CB	103.00	107.76	2
CB-CG-CD	112.60	105.24	1
N-CA-C-N-CA	121.70	113.91	1
C-N-CA	121.70	129.49	2
CG-CD2-CE2	120.70	113.34	1
NE-CZ-CB-CG-CD1	120.80	127.29	1
OD1-CG-ND2	122.60	126.93	1
N-CA-CB	110.50	117.85	1
CA-CB-CG	114.10	122.75	1
CG-CD-NE2	116.40	122.89	1
CB-CG-ND2	116.40	109.91	1
C-N-CD1-CE1-C-CA-CB	110.10	101.89	1
O-C-N	123.00	116.08	1
CG-CD-CE	111.30	121.24	1
C-N-N-CA-CB	110.50	117.85	1
CA-CB-CG2	110.50	117.85	1
CD1-CE1-CZ	120.00	112.22	1
CD1-CG-CD2	110.80	120.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-CE2	120.70	113.35	1
O-C-N	123.00	116.09	1
ND1-CG-CD2	106.10	110.42	1
N-CA-CB	110.50	117.84	1
CB-CG-CD	111.30	121.23	1
C-N-CA	121.70	113.93	2
CA-CB-CG	113.60	121.80	1
CG-CD-NE	112.00	102.50	1
CB-CG1-CD1	113.80	104.74	1
CG-CD2-N-CA-CB	110.50	117.84	1
N-CA-CB	103.00	107.75	1
CA-C-N-CA-CB	110.50	117.84	1
CD1-CG-CA-CB-CG	112.60	108.29	1
CA-CB-CG	113.80	109.49	1
CA-C-O	120.80	113.47	1
C-N-CB-CG-CA-CB-CG	112.60	108.29	1
C-N-CA	121.70	113.94	3
N-CA-CB	111.50	118.83	1
C-CA-CB	110.10	101.91	1
O-C-N	123.00	116.10	1
N-CA-CB	110.50	117.83	1
CA-C-O	120.80	113.48	1
CA-CB-CG	114.10	105.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	129.89	1
N-CA-C-N-CA	121.70	113.95	1
N-CA-CB	110.50	117.82	2
C-CA-CB	109.10	99.63	1
C-CA-CB	110.10	101.92	1
CA-CB-CG	112.60	108.29	1
CG-CD2-CA-CB-CG	113.80	109.50	1
CB-CG-CD	111.30	101.40	1
CB-CG-CD	112.60	105.28	1
C-N-CA	121.70	129.44	2
C-N-CA	121.70	113.96	2
CG-CD1-CE1	121.20	127.65	1
CB-CG-CD2	131.20	125.61	1
N-CA-C-N-CA	121.70	113.96	1
CA-C-O	120.80	128.11	1
CD1-CG-CD2	118.60	125.05	1
N-CA-C	111.00	98.96	1
C-CA-CB	110.10	101.93	1
CA-CB-OG	111.10	102.50	1
CA-C-N	116.20	124.79	1
N-CA-CB	111.50	104.20	1
C-CA-CB	110.10	101.94	2
N-CA-CB	110.50	117.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-C-CA-CB	110.10	101.94	1
O-C-N	123.00	129.87	1
CB-CG-C-CA-CB	110.10	101.94	1
N-CA-CB	111.50	118.80	1
CB-CG-CD1	120.80	127.24	1
C-N-CA	121.70	113.97	2
CB-CG-CD2	120.70	128.00	1
CB-CG-C-N-CA	121.70	113.98	1
C-N-CA	121.70	113.98	1
C-N-N-CA-C	111.00	98.99	1
N-CA-CB-CG-CD	111.30	121.16	1
O-C-N	123.00	116.14	1
CD1-CE1-CZ	119.60	127.32	1
N-CA-CB	110.50	117.79	3
CB-CG-CD1	126.90	133.33	1
NE-CZ-NH1	121.50	117.21	1
N-CA-C	111.00	99.00	1
C-CA-CB	110.10	118.24	1
CD1-CG-CD2	110.80	120.23	1
CA-CB-OG	111.10	102.53	1
C-N-CA	121.70	129.41	2
N-CA-CB	111.50	118.79	1
C-N-CA	121.70	113.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	126.80	120.80	1
CB-CG-CD2	131.20	136.77	1
CG1-CB-CG2	110.80	120.22	1
C-CA-CB	110.10	101.96	1
CE1-CZ-OH	119.90	132.75	1
CB-CG-OD2	118.40	128.25	1
CB-CG-CD	112.60	105.32	1
N-CA-C-N-CA	121.70	113.99	1
C-CA-CB	110.10	101.97	1
CA-CB-O-C-N-CA-CB	110.50	117.77	1
CB-CG1-CD1	113.80	104.82	2
C-CA-CB	110.10	118.23	1
C-N-CB-CG-CD1	120.80	127.21	1
CA-CB-CG	113.90	106.20	1
C-N-CA	121.70	114.00	1
NE-CZ-NH1	121.50	117.22	1
C-N-CA-C-N-CA-C-CA-CB	111.60	103.05	1
N-CA-CB	110.50	117.77	1
CG-CD2-CE2	120.70	127.97	1
C-CA-CB	110.10	101.98	2
CA-C-O	120.80	113.54	1
CD2-CE3-CZ3	118.60	113.05	2
C-N-N-CA-CB	111.50	118.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.40	103.14	1
CB-CG-CD	112.60	105.34	1
O-C-CA-CB-CG	112.60	108.33	1
CA-CB-CG	114.10	122.64	1
O-C-N	123.00	116.17	1
N-CA-C	111.00	99.05	1
CG-CD-CE	111.30	121.11	1
CB-CG-OD1	120.80	112.27	1
OD1-CG-ND2	122.60	118.33	1
C-CA-CB	110.10	101.99	1
CB-CG1-CD1	113.80	122.76	1
N-CA-CB	110.50	117.75	1
CB-CG-OD1	120.80	129.33	1
C-N-CA	121.70	114.02	1
O-C-N	123.00	116.18	1
CD1-CG-CD2	110.80	120.18	1
C-N-CA	121.70	129.37	1
CA-CB-CG	114.10	105.57	1
O-C-N	123.00	129.82	1
CA-CB-OG	111.10	102.57	1
N-CA-CA-CB-CG1	110.40	117.65	1
CA-CB-CG	113.90	106.23	2
N-CA-CB	110.50	117.74	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CB-CG2	110.80	120.18	1
C-N-CA	121.70	114.03	2
CG-SD-CE	100.90	91.53	1
CG-CD-OE1	120.80	129.32	1
CA-CB-CG2	110.50	103.26	1
N-CA-CB	103.00	107.68	1
CG-CD-CE	111.30	121.09	1
CB-CG-CD1-CG-CD2	110.80	120.17	1
CG-CD2-NE2	107.20	111.46	1
C-CA-CB	110.10	118.19	1
C-CA-CB	110.10	102.01	1
ND1-CE1-NE2	108.40	112.66	1
CA-CB-CG	112.60	108.34	1
O-C-N	123.00	129.81	1
O-C-CA-C-N-CA-N-CA-CB	111.50	118.73	1
CA-CB-CG	114.10	122.61	1
CG-CD-NE	112.00	102.64	1
CA-CB-CG	112.60	108.35	2
C-N-CA	121.70	129.35	1
CA-CB-CA-CB-CG1	110.40	103.17	1
CB-CG-CD	112.60	105.38	1
C-N-CA	121.70	114.05	1
C-CA-CB	110.10	102.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG1	109.60	115.97	1
O-C-N	123.00	116.20	1
CE2-CD2-CE3	118.80	123.05	1
N-CA-CB	111.50	118.72	1
CA-C-O	120.80	113.58	1
CA-C-O	120.80	128.02	1
C-N-CA	121.70	114.06	2
N-CA-CB	110.50	103.28	1
N-CA-CB	110.50	117.72	1
CG-CD2-CE3	133.90	129.65	1
CA-CB-CA-CB-CG1	110.40	103.19	1
CD-NE-CZ	124.40	118.46	1
C-CA-CB	110.10	102.04	4
CA-N-CD	112.00	106.06	1
N-CA-C	111.00	99.12	1
C-N-CA	121.70	129.33	1
O-C-N	123.00	116.21	1
CG-CD-CE	111.30	121.05	1
CB-CG-ND2	116.40	110.04	1
OE1-CD-OE2	122.90	133.08	1
CA-CB-CG	113.80	109.56	1
C-CA-CB	110.10	102.05	1
C-N-C-CA-CB	110.10	102.05	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.70	3
CA-C-O	120.80	128.00	2
CA-CB-OG1	109.60	103.25	1
CA-CB-CG	114.10	105.63	1
CA-CB-CG	113.80	109.57	1
CB-CG-OD1	120.80	129.26	1
ND1-CG-CA-CB-CG	112.60	108.37	1
CA-CB-CG2	110.50	103.31	1
C-N-C-CA-CB	110.10	102.06	1
CD1-CG-CD2	110.80	120.11	1
CA-CB-CG	114.10	105.64	1
CD2-CE2-CZ	119.60	111.99	1
N-CA-CB	110.50	117.69	1
CD1-CE1-CZ	120.00	127.61	1
CB-CG-CD	111.30	121.03	1
CA-CB-CG	112.60	108.37	1
CA-C-N	116.20	124.66	1
CG-CD-NE2	116.40	110.06	1
CA-CB-OG1	109.60	115.94	1
C-N-CA	121.70	114.09	1
CA-C-N	116.20	124.65	1
CB-CG-ND2	116.40	110.06	1
N-CA-O-C-N	123.00	116.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CE2-CD2-CE3	118.80	123.03	1
N-CA-CB	103.00	107.65	1
N-CA-CB	110.50	117.68	1
C-CA-CA-CB-C-N-CA	121.70	114.10	1
CD1-CE1-CZ	120.00	112.40	1
CB-CG-CD	112.60	105.42	1
CG-CD-OE1	120.80	129.24	1
O-C-N	123.00	116.25	1
O-C-CD-NE-CZ	124.40	118.49	1
CA-C-O	120.80	113.63	1
CA-CB-CG	114.10	122.54	1
CA-C-O	120.80	127.97	1
CB-CG-CD	112.60	119.77	1
N-CA-CB	111.50	118.67	1
ND1-CE1-O-C-N	123.00	129.75	1
C-N-CA	121.70	114.11	1
N-CA-CA-CB-CG	112.60	108.38	1
ND1-CE1-NE2	108.40	112.61	1
N-CA-C-N-CA	121.70	114.12	1
CA-CB-CG2	110.40	117.56	1
OE1-CD-NE2	122.60	118.39	1
C-N-CA	121.70	114.12	2
N-CA-CB	111.50	104.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	118.10	124.42	1
CA-CB-CG	113.90	106.32	1
CA-C-N	116.20	124.62	1
CB-CG-CA-CB-CG	114.10	105.68	1
CA-C-C-CA-CB	110.10	102.10	1
CB-CG1-CD1	113.80	122.64	1
O-C-N	123.00	116.26	1
C-N-CA	121.70	129.27	3
N-CA-C	111.00	99.22	3
N-CA-N-CA-CB	110.50	117.65	1
CA-CB-CG	114.10	105.69	3
N-CA-CB	110.50	117.65	2
O-C-N	123.00	129.73	1
CB-CG-CD	112.60	105.45	1
C-CA-CB	110.10	118.09	1
CA-CB-CG	112.60	108.40	2
C-N-CA-CB-OG	111.10	102.69	1
CA-C-N	116.20	124.61	1
C-N-N-CD-C-N-CA	121.70	129.27	1
O-C-N	123.00	129.72	1
C-CA-CB	110.10	102.12	2
CA-CB-CG	114.10	122.50	1
C-N-CA	121.70	114.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	103.26	1
CA-CB-CG2	110.40	117.54	1
OG1-CB-CG-CD-NE2	116.40	110.10	1
CA-CB-CG2	110.40	103.26	1
N-CA-C	111.00	99.24	2
C-N-CA	121.70	129.26	2
OD1-CG-ND2	122.60	126.80	1
CA-C-N	116.90	123.20	1
ND1-CE1-NE2	108.40	112.60	1
C-CA-CB	109.10	99.87	1
C-CA-CB	111.60	103.21	1
C-CA-CB	110.10	102.13	2
N-CA-CB	110.50	117.63	2
CA-CB-CG	112.60	108.41	1
CB-CG-CD2	120.80	127.09	1
N-CA-CB	111.50	118.63	1
CG-CD2-NE2	107.20	111.39	1
CB-CG-ND2	116.40	110.11	1
CG-CD-OE1	120.80	129.18	1
O-C-N	123.00	116.29	1
CE1-CZ-CE2	120.00	112.46	1
N-CA-ND1-CE1-NE2	108.40	112.59	1
CD2-CE2-CZ	120.00	112.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	99.27	1
CB-CG-OD2	118.40	128.03	1
CG-CD-NE2	116.40	122.68	1
N-CA-C-CA-CB	110.10	102.14	1
O-C-N	123.00	116.30	1
N-CA-CB	110.50	117.62	1
N-CA-CB	111.50	104.38	1
N-CA-C	111.00	99.28	1
CB-CG-CD2	120.70	127.82	1
CA-CB-OG1	109.60	115.88	1
CA-CB-CG	113.80	109.62	2
CA-C-O	120.80	127.91	1
N-CA-C	112.10	101.64	1
C-N-CA	121.70	114.17	1
CD1-CG-CD2	118.10	124.37	1
N-CA-C	111.00	99.29	1
N-CA-CA-C-N	116.90	123.17	1
CA-CB-CD2-NE2-CE1	109.00	104.82	1
CB-CG-ND2	116.40	122.67	1
N-CA-CB	110.50	117.61	1
CA-C-N	116.20	107.84	1
N-CA-CB	111.50	118.61	1
CA-CB-CG1	110.40	117.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	99.30	1
C-CA-CB	110.10	102.16	1
CA-CB-CG	112.60	108.42	1
N-CA-C	111.00	99.31	2
CA-CB-C-CA-CB	110.10	118.03	1
CB-CG1-CD1	113.80	122.57	1
N-CA-CB	110.50	117.60	2
C-N-CA	121.70	114.19	3
CB-CG-ND2	116.40	122.66	2
C-CA-CB	110.10	102.17	1
O-C-N	123.00	116.32	1
CB-CG-CD1	120.70	127.79	1
N-CA-CB	110.50	117.59	2
CA-CB-CG2	110.40	103.31	1
C-CA-CB	111.60	103.26	2
CA-CB-OG1	109.60	115.86	1
CB-CG-CD	112.60	105.51	1
CG-ND1-C-CA-CB	110.10	102.18	1
CA-CB-CG	114.10	105.76	1
N-CA-C-CA-CB	110.10	118.02	1
CD2-CE2-CZ	120.00	127.50	1
CB-CG-ND2	116.40	122.65	1
O-C-N	123.00	116.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.20	1
CA-CB-CG	114.10	122.43	1
CD2-NE2-CE1	109.00	104.83	1
CB-CG-O-C-N	123.00	116.34	1
CB-CG-ND2	116.40	110.15	1
CG-CD-OE1	118.40	108.82	1
N-CA-C-N-CA	121.70	114.20	1
CA-CB-CG2	110.50	103.42	1
N-CA-CB	110.50	117.58	3
CB-CG-CD2	126.80	120.97	1
CD-NE-CZ	124.40	118.57	1
N-CA-CG-CD-OE1	118.40	127.97	1
N-CA-CB	111.50	118.58	1
C-N-CA	121.70	114.21	2
CB-CG-CD	111.30	120.87	1
CA-CB-CG	114.10	105.78	2
CG-CD2-NE2	107.20	111.36	1
N-CA-CB	110.50	117.57	1
C-CA-CB	110.10	102.20	1
CD1-CG-CD2	110.80	119.95	1
NE-CZ-NH2	119.20	115.46	1
C-CA-CB	111.60	103.28	1
CB-CG-CD2	131.20	125.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.35	1
N-CA-CB	111.50	118.57	1
CD1-CG-CD2	118.60	124.83	1
CG1-CB-CG2	110.70	123.17	1
CG-CD1-CE1	120.70	113.64	1
CA-C-O	120.80	127.86	1
C-N-CA	121.70	114.22	1
CG1-CB-CG2	110.80	119.94	1
C-CA-CA-C-O	120.80	127.86	1
CA-C-C-CA-CB	110.10	102.21	1
CA-CB-CG	112.60	108.45	1
CG-CD2-NE2	107.20	111.35	1
C-CA-CB	110.10	102.21	2
CA-CB-CG	114.10	122.40	1
C-CA-CB	111.40	103.51	1
O-C-N	123.00	116.36	1
C-N-CA	121.70	129.17	1
CA-C-O	120.80	127.85	1
CA-CB-CG	113.80	109.65	1
N-CA-CB	110.50	117.55	2
CB-CG-ND2	116.40	122.62	1
CG1-CB-CG2	110.70	123.14	1
OD1-CG-ND2	122.60	118.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	114.24	4
CD2-CE2-CZ2	122.40	118.25	1
N-CA-CB	103.00	107.56	1
CB-CG-CD2	120.70	127.74	1
C-CA-CB	111.40	103.53	1
C-CA-CG-CD-NE2	116.40	110.18	1
C-CA-CA-C-O	120.80	113.76	1
CA-CB-CG	112.60	108.46	1
CA-C-O	120.80	127.84	1
CB-CG-OD1	120.80	129.08	1
CA-CB-CG2	110.50	103.46	1
O-C-N	123.00	116.38	1
N-CA-CB	110.50	117.54	1
CB-CG1-CD1	113.80	122.49	1
CG-CD-NE2	116.40	110.19	1
C-CA-CG-CD-OE1	120.80	129.08	1
N-CA-CB	110.50	103.47	1
C-CA-CA-C-O	120.80	113.77	1
C-CA-CA-C-CA-CB-CG2	110.40	103.37	1
C-N-CA	121.70	114.26	3
C-CA-CB	111.40	103.54	1
CG-CD-CE	111.30	120.81	1
CB-CG-CD2	131.20	136.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.52	1
OD1-CG-ND2	122.60	126.73	1
CG-CD2-CE2	121.20	115.01	1
OE1-CD-O-C-N	123.00	129.61	1
C-CA-CB	110.10	102.26	2
CA-C-N-CA-CB	110.50	117.52	1
O-C-N	123.00	116.40	1
CG-CD2-CE2	120.70	127.72	1
CB-CG-OD1	120.80	112.55	2
C-N-CA	121.70	114.27	1
N-CA-CB	110.50	117.51	5
CD1-CG-C-N-CA	121.70	114.28	1
C-N-CA	121.70	129.12	2
CG1-CB-CG2	110.80	119.87	1
CG-CD2-NE2	107.20	111.32	1
CA-CB-CG2	110.40	103.39	2
N-CA-C-CA-CB	110.10	102.27	1
C-N-CA	121.70	114.28	2
CG-CD-OE1	118.40	127.88	1
CA-CB-CG2	110.50	103.49	1
N-CA-N-CA-CB	110.50	117.51	1
N-CA-CB	110.50	117.50	1
CB-CG-CD2	131.20	136.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.48	1
CA-C-N	116.20	107.96	1
CD1-CE1-CZ	120.00	112.59	1
CB-CG-CD2	126.80	121.04	1
CG-CD-OE1	120.80	112.57	1
C-N-CA	121.70	129.11	1
CA-CB-CG2	110.50	103.50	1
C-CA-CB	110.10	102.28	3
CB-CG-ND2	116.40	122.57	1
C-N-CA	121.70	114.29	1
CA-C-CA-CB-OG	111.10	119.33	1
NH1-CZ-NH2	119.30	124.65	1
C-N-CD	125.00	108.14	1
CD2-NE2-CE1	109.00	104.89	1
O-C-N	123.00	116.42	2
C-N-CA	121.70	129.10	2
CA-C-N-CA-CB	110.50	117.49	1
N-CA-CB	110.50	117.49	3
NH1-CZ-NH2	119.30	124.64	1
CD2-CE2-CZ	119.60	127.00	1
CA-CB-OG	111.10	102.88	1
CA-CB-CG2	110.50	117.48	1
C-CA-CB	110.10	102.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-CA-O-C-N	123.00	116.43	1
CB-CG-OD1	120.80	129.01	1
N-CD-CG	103.20	109.36	1
O-C-N	123.00	129.57	1
C-CA-CB	110.10	117.90	1
NE-CZ-NH1	121.50	125.60	1
N-CA-CB	110.50	117.48	1
N-CA-CB	110.40	116.56	1
CD1-CE1-CZ	120.00	127.39	1
CA-CB-CG	114.10	105.89	1
OG1-CB-CG2	109.30	117.51	1
CG1-CB-CG2	110.70	123.01	1
C-CA-CB	110.10	102.31	1
CA-CB-CG	114.10	122.30	1
CD1-CG-CD2	110.80	119.82	1
CA-CB-N-CA-CB	110.40	116.55	1
CA-CB-OG	111.10	102.90	1
O-C-N	123.00	116.44	2
N-CA-C	111.00	99.52	2
N-CA-CB	110.50	117.47	3
N-CA-CB	110.50	103.53	1
C-N-CA	121.70	114.32	1
C-CA-CB	111.40	103.61	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	136.53	1
CA-CB-CG	113.80	117.90	1
C-N-CA	121.70	114.33	3
CA-C-O	120.80	113.84	1
N-CA-CB	111.50	118.46	1
C-CA-O-C-N	123.00	116.45	1
CA-C-N	116.20	124.39	1
N-CA-CA-CB-CG2	110.50	103.54	1
CD1-CG-CD2	118.60	124.74	1
C-N-CA	121.70	129.07	1
N-CA-CB	110.50	117.46	1
C-CA-CA-CB-C-N-CA	121.70	114.34	1
CB-CG1-CG-CD-CE	111.30	120.71	1
CD1-CG-CD2	110.80	119.80	1
CG1-CB-CG2	110.80	119.80	1
CA-C-N	116.20	124.38	2
C-N-CA	121.70	129.06	2
CA-CB-CG	113.90	121.26	1
C-N-CA	121.70	114.34	1
CA-C-O	120.80	127.75	1
CD1-CE1-N-CA-CB	111.50	118.45	1
CA-CB-CG	112.60	108.51	1
OE1-CD-NE2	122.60	126.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-CB-CG1	110.40	103.45	1
CA-C-O	120.80	113.85	1
C-CA-CB	110.10	117.86	1
CD1-CG-CD2	118.10	124.23	1
C-N-CA	121.70	114.35	1
C-CA-CB	110.10	102.34	1
C-N-CA	121.70	129.05	3
CA-CB-CG1	110.40	103.46	1
CA-CB-CA-CB-CG-CD1-CE1	121.20	127.33	1
CB-CG-ND2	116.40	110.27	1
CA-CB-CG1	110.40	117.34	1
CB-CG1-CD1	113.80	122.37	1
CA-C-N	116.90	123.02	1
C-CA-CB	110.10	102.35	1
CE1-CZ-CB-CG-N-CA-C	111.00	99.58	1
O-C-N	123.00	116.47	1
CD1-CG-CD2	110.80	119.77	1
N-CA-C	111.00	99.58	1
CB-CG-CD	112.60	105.67	1
CG-CD1-CE1	120.70	127.63	1
CA-CB-C-N-CA	121.70	129.04	1
CG-CD1-CE1	121.20	127.31	1
C-CA-CB	110.10	102.36	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	118.60	112.49	1
N-CA-CA-N-CD	112.00	106.29	1
OD1-CG-ND2	122.60	118.53	1
CE1-CZ-CE2	120.00	127.33	1
N-CA-CB	110.40	116.51	1
N-CA-C	111.00	99.60	2
CD2-NE2-CE1	109.00	104.93	1
CD-NE-CZ	124.40	118.70	1
CD1-CE1-CZ	120.00	127.33	1
CB-CG-CD	112.60	105.68	2
C-CA-CB	110.50	104.39	1
C-N-CA	121.70	114.37	1
N-CA-CB	110.50	117.42	1
CA-C-O	120.80	127.72	1
O-C-N	123.00	116.49	1
OD1-CG-CB-CG-ND2	116.40	110.30	1
N-CA-CB	110.50	117.41	4
CA-CB-OG1	109.60	115.70	1
C-N-CA	121.70	114.38	1
CA-CB-C-N-CA	121.70	129.02	1
C-N-CG-CD-CE	111.30	120.65	1
C-CA-CB	111.40	103.68	1
CA-C-O	120.80	113.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.01	1
CA-CB-OG	111.10	102.97	1
CB-CG-C-N-CA	121.70	114.39	1
C-N-CA	121.70	114.39	1
CA-CB-CG2	110.50	103.60	1
C-N-O-C-N	123.00	129.50	1
N-CA-CB	111.50	118.40	1
C-CA-CB	110.50	104.41	1
CE2-CZ2-CH2	117.50	122.78	1
CB-CG-CD1	120.70	113.80	1
N-CA-CB	110.40	116.49	1
OD1-CG-CE2-CD2-CE3	118.80	122.86	1
CA-CB-CG	112.60	108.54	1
CA-CB-CG2	110.40	103.50	1
C-CA-CB	110.10	102.39	1
CA-CB-CG1	110.40	103.51	1
CA-CB-CG	114.10	105.99	1
C-N-CA	121.70	129.00	1
C-N-CA	121.70	114.40	1
CA-CB-CG2	110.40	103.51	1
CB-CG-N-CD-CG	103.20	109.28	1
O-C-N	123.00	129.48	1
CB-CG1-CD1	113.80	105.29	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N-CA-C-CA-CB	110.10	102.40	1
C-CA-CB	110.10	117.80	1
CD1-CE1-CZ	120.00	127.29	1
C-CA-N-CA-CB	111.50	104.62	1
C-CA-CB	110.10	102.41	1
CG-CD2-CB-CG-SD	112.70	124.84	1
CD1-CE1-CZ	120.00	112.71	1
CD1-CG-CD2	110.80	101.90	1
OD1-CG-ND2	122.60	126.65	1
CD2-CE2-CZ	119.60	126.88	1
CA-CB-CG	113.80	109.75	1
N-CA-CB	111.50	118.38	2
CA-CB-CG	113.90	106.62	1
CA-CB-CG2	110.50	103.62	1
N-CA-C	111.00	99.68	2
C-CA-CB	110.10	102.42	2
CE3-CZ3-CH2	121.10	126.36	1
C-N-CA	121.70	128.98	2
CA-CB-CG1	110.40	103.53	1
NE-CZ-NH1	121.50	117.46	1
C-CA-CB	111.60	103.51	1
CB-CG-OD1	120.80	128.88	1
CG-CD2-CE2	121.20	127.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	103.00	107.45	1
CA-CB-CG	113.90	106.63	1
O-C-CA-C-O	120.80	127.67	1
CA-C-O	120.80	113.93	1
N-CA-CB	110.50	117.37	1
CB-CG-CD	112.60	105.74	1
N-CA-CA-C-O	120.80	113.94	1
NE-CZ-NH2	119.20	122.83	1
C-CA-CB	110.10	102.43	2
CG-CD-OE1	120.80	128.87	1
N-CA-CB	110.50	117.36	3
CA-C-O	120.80	127.66	1
CG1-CB-CG2	110.70	122.80	1
C-CA-CB	111.60	103.53	1
C-CA-CB	110.10	102.44	1
CG-CD2-CE2	120.70	113.84	1
CG-CD-CE	111.30	120.58	1
O-C-N	123.00	129.45	2
O-C-N	123.00	116.55	1
N-CA-CB	110.50	117.35	2
N-CA-CB-CG-OD1	120.80	128.86	1
C-N-CA	121.70	114.45	2
CA-C-O	120.80	127.65	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-N-CA	121.70	114.45	1
C-CA-CB	110.10	102.45	1
OD1-CG-ND2	122.60	118.57	1
CG-CD1-CE1	121.20	115.16	1
CG-CD2-CE2	121.20	127.24	1
CG-CD-CE	111.30	120.56	1
N-CA-CA-C-O	120.80	127.64	1
C-CA-CB	111.40	103.75	1
OD1-CG-OD2	122.90	132.56	1
N-CA-CB	110.50	117.34	2
C-CA-CB	110.10	102.46	1
N-CA-CB	111.50	118.34	1
CG-CD2-NE2	107.20	111.22	1
C-N-CA	121.70	128.94	1
C-CA-CB	109.10	117.95	1
N-CA-C	111.00	99.74	1
CB-CG-OD1	120.80	128.84	1
CB-CG-CD	112.60	105.76	1
CA-C-O	120.80	113.96	1
CG-CD2-CE2	120.70	113.86	1
CA-CB-OG	111.10	119.14	1
N-CA-CB	110.50	117.33	1
CA-CB-CG	113.80	109.78	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	114.46	1
CB-CG-CA-C-N	116.20	124.24	1
O-C-N	123.00	129.43	1
CD1-CE1-CZ	120.00	112.77	1
N-CA-CB-CG-N-CA-C	113.30	101.65	1
C-CA-CB	110.10	117.73	1
OG1-CB-CG2	109.30	101.27	1
CB-CG-OD1	120.80	128.83	1
CA-C-CD1-CE1-CZ	119.60	112.37	1
CG-CD2-CE2	120.70	127.52	1
O-C-C-N-CA	121.70	128.93	1
N-CA-CB	110.50	117.32	2
C-N-CA	121.70	114.48	1
OD1-CG-ND2	122.60	118.59	1
CA-CB-C-N-C-CA-CB	110.10	102.48	1
C-CA-CB	110.10	102.48	2
N-CA-C-CA-CB	110.50	104.48	1
CA-CB-CG	112.60	108.59	1
CG-CD-CA-C-O	120.80	113.98	1
CA-CB-C-N-CA	121.70	114.48	1
O-C-CD2-CE2-CZ	120.00	112.78	1
N-CA-CB	111.50	118.32	1
O-C-N	123.00	129.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	105.79	1
C-N-CA	121.70	114.49	1
CA-CB-CG	116.30	102.28	1
C-CA-CB	111.60	103.59	1
O-C-N	123.00	116.59	1
N-CA-C	111.00	99.79	1
CB-CG-ND2	116.40	122.41	1
N-CA-CB	110.50	117.31	1
CA-C-N-CA-CB	110.50	117.30	1
CA-CB-CG	114.10	122.10	1
C-N-CA	121.70	114.50	1
CB-CG-O-C-N	123.00	116.60	1
CB-CG-OD1	120.80	128.80	1
O-C-N	123.00	129.40	1
N-CA-CB	110.50	117.30	1
CB-CG-CD1	120.80	126.80	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	0.00	0
2	0.00	0
3	0.00	0

Model ID	Clash score	Number of clashes
4	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Analysed	Favored	Allowed	Outliers
1	1164	703	326	135
2	1164	702	335	127
3	1164	714	316	134
4	1164	648	346	170

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	Analysed	Favored	Allowed	Outliers
1	1096	897	123	76
2	1096	907	114	75
3	1096	910	125	61
4	1096	909	125	62

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	10	LEU
1	A	11	ARG
1	A	12	LEU
1	A	42	MET
1	A	53	LEU

Model ID	Chain	Residue ID	Residue type
1	A	61	LYS
1	A	66	ASN
1	A	76	THR
1	A	96	ILE
1	A	105	LYS
1	A	142	LEU
1	A	168	ILE
1	A	169	ILE
1	A	189	LYS
1	A	190	LEU
1	A	200	LEU
1	A	212	LEU
1	A	223	LEU
1	A	244	LEU
1	A	262	ILE
1	A	272	LEU
1	A	318	ILE
1	A	325	LEU
1	A	334	LYS
1	A	350	LEU
1	A	368	ILE
1	A	386	ASN
1	A	398	LYS

Model ID	Chain	Residue ID	Residue type
1	A	421	MET
1	A	432	ASN
1	A	448	ILE
1	A	450	SER
1	A	452	ARG
1	A	467	LEU
1	A	472	LYS
1	A	490	LYS
1	A	537	SER
1	A	548	ILE
1	A	581	ILE
1	A	589	LEU
1	A	590	ILE
1	A	592	LYS
1	A	647	ILE
1	A	649	LYS
1	A	665	GLN
1	A	670	ASN
1	A	671	VAL
1	A	692	ARG
1	A	747	ILE
1	A	762	ILE
1	A	816	LEU

Model ID	Chain	Residue ID	Residue type
1	A	820	LEU
1	A	833	LEU
1	A	843	LYS
1	A	908	ILE
1	A	915	LYS
1	A	921	GLU
1	A	931	LEU
1	A	941	LEU
1	A	949	ILE
1	A	953	LEU
1	A	982	ILE
1	A	989	LEU
1	A	994	LYS
1	A	995	SER
1	A	1004	LEU
1	A	1011	LEU
1	A	1026	VAL
1	A	1029	ASN
1	A	1047	ILE
1	A	1049	LEU
1	A	1059	LEU
1	A	1119	ILE
1	A	1139	ILE

Model ID	Chain	Residue ID	Residue type
1	A	1142	VAL
1	A	1160	GLU
2	A	7	LYS
2	A	16	LEU
2	A	42	MET
2	A	53	LEU
2	A	71	VAL
2	A	74	LEU
2	A	80	SER
2	A	89	ASN
2	A	100	LEU
2	A	109	ILE
2	A	122	ILE
2	A	142	LEU
2	A	150	GLU
2	A	161	ASP
2	A	175	ILE
2	A	223	LEU
2	A	245	LYS
2	A	251	ASN
2	A	261	LYS
2	A	270	VAL
2	A	308	LYS

Model ID	Chain	Residue ID	Residue type
2	A	382	THR
2	A	384	ARG
2	A	392	ILE
2	A	428	ILE
2	A	432	ASN
2	A	458	ILE
2	A	490	LYS
2	A	497	LYS
2	A	510	ASN
2	A	518	LEU
2	A	522	ILE
2	A	529	ILE
2	A	535	LEU
2	A	553	ASN
2	A	555	LEU
2	A	559	LEU
2	A	580	LYS
2	A	601	LYS
2	A	605	ILE
2	A	607	ARG
2	A	626	THR
2	A	631	LEU
2	A	659	LEU

Model ID	Chain	Residue ID	Residue type
2	A	666	ASN
2	A	668	LYS
2	A	673	ASN
2	A	707	LYS
2	A	717	LEU
2	A	720	ILE
2	A	757	GLN
2	A	760	ILE
2	A	797	VAL
2	A	804	ILE
2	A	806	ILE
2	A	843	LYS
2	A	853	LEU
2	A	862	LEU
2	A	873	LEU
2	A	890	ILE
2	A	906	LYS
2	A	908	ILE
2	A	935	LEU
2	A	941	LEU
2	A	946	LEU
2	A	949	ILE
2	A	956	ILE

Model ID	Chain	Residue ID	Residue type
2	A	973	ILE
2	A	1058	LYS
2	A	1060	LEU
2	A	1095	GLU
2	A	1106	ILE
2	A	1122	VAL
2	A	1138	THR
2	A	1144	LYS
3	A	26	GLU
3	A	89	ASN
3	A	106	LYS
3	A	141	ILE
3	A	175	ILE
3	A	235	ILE
3	A	241	LYS
3	A	248	LYS
3	A	250	LEU
3	A	252	LYS
3	A	264	ASN
3	A	269	VAL
3	A	299	LEU
3	A	310	ILE
3	A	322	LEU

Model ID	Chain	Residue ID	Residue type
3	A	379	ILE
3	A	398	LYS
3	A	434	LYS
3	A	437	SER
3	A	442	ARG
3	A	474	MET
3	A	482	LYS
3	A	490	LYS
3	A	518	LEU
3	A	534	LYS
3	A	589	LEU
3	A	600	ILE
3	A	612	LEU
3	A	631	LEU
3	A	649	LYS
3	A	684	LEU
3	A	689	LYS
3	A	720	ILE
3	A	737	LEU
3	A	747	ILE
3	A	760	ILE
3	A	771	ASN
3	A	777	ILE

Model ID	Chain	Residue ID	Residue type
3	A	794	LEU
3	A	796	LYS
3	A	799	LEU
3	A	833	LEU
3	A	858	LYS
3	A	862	LEU
3	A	873	LEU
3	A	926	LEU
3	A	938	LYS
3	A	953	LEU
3	A	973	ILE
3	A	978	LYS
3	A	1001	LEU
3	A	1029	ASN
3	A	1032	ASN
3	A	1036	LYS
3	A	1047	ILE
3	A	1083	VAL
3	A	1086	LEU
3	A	1089	LYS
3	A	1091	LEU
3	A	1114	GLU
3	A	1135	LEU

Model ID	Chain	Residue ID	Residue type
4	A	14	LYS
4	A	51	LEU
4	A	52	ARG
4	A	70	ILE
4	A	105	LYS
4	A	112	ILE
4	A	170	LYS
4	A	175	ILE
4	A	180	ILE
4	A	190	LEU
4	A	202	ILE
4	A	209	LYS
4	A	212	LEU
4	A	273	ARG
4	A	277	ILE
4	A	291	LYS
4	A	293	ILE
4	A	299	LEU
4	A	335	ILE
4	A	389	MET
4	A	392	ILE
4	A	457	ILE
4	A	474	MET

Model ID	Chain	Residue ID	Residue type
4	A	490	LYS
4	A	580	LYS
4	A	585	LEU
4	A	586	LYS
4	A	587	LEU
4	A	589	LEU
4	A	617	GLU
4	A	625	LEU
4	A	631	LEU
4	A	685	GLU
4	A	692	ARG
4	A	702	GLU
4	A	741	LYS
4	A	744	LEU
4	A	746	LYS
4	A	759	LYS
4	A	800	LYS
4	A	801	GLU
4	A	806	ILE
4	A	813	LEU
4	A	858	LYS
4	A	863	ILE
4	A	919	LEU

Model ID	Chain	Residue ID	Residue type
4	A	930	LYS
4	A	948	LYS
4	A	949	ILE
4	A	953	LEU
4	A	956	ILE
4	A	965	LYS
4	A	968	LYS
4	A	973	ILE
4	A	989	LEU
4	A	994	LYS
4	A	1007	LEU
4	A	1017	LEU
4	A	1029	ASN
4	A	1047	ILE
4	A	1086	LEU
4	A	1112	ARG

Fit of model to data used for modeling

2DEM class average

Validation for this section is under development.

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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