Integrative Structure Validation Report

July 22, 2024 - 05:40 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	9A85
PDB-Dev ID	PDBDEV_00000370
Structure Title	Equilibrated 52-mer bacterial gasdermin pore model from Vitiosangium sp.
Structure Authors	Johnson, A.G.; Mayer, M.L.; Schaefer, S.L.; McNamara-Bordewick, N.K.; Hummer, G.; Kranzusch, P.J.

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

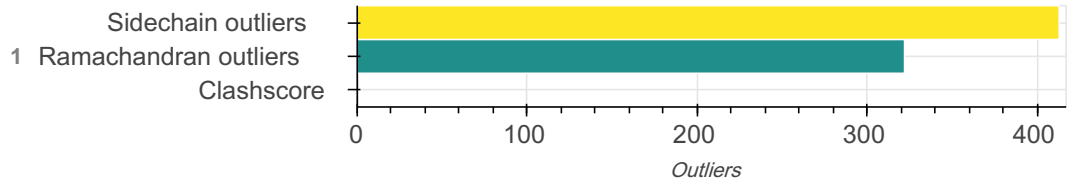
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 52 subunits in each model. A total of 2 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 52 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled None/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Gasdermin bGSDM	AA	a	234
1	2	1	Gasdermin bGSDM	BA	b	234
1	3	1	Gasdermin bGSDM	CA	c	234
1	4	1	Gasdermin bGSDM	DA	d	234
1	5	1	Gasdermin bGSDM	EA	e	234
1	6	1	Gasdermin bGSDM	FA	f	234
1	7	1	Gasdermin bGSDM	GA	g	234

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	8	1	Gasdermin bGSDM	HA	h	234
1	9	1	Gasdermin bGSDM	IA	i	234
1	10	1	Gasdermin bGSDM	JA	j	234
1	11	1	Gasdermin bGSDM	KA	k	234
1	12	1	Gasdermin bGSDM	LA	l	234
1	13	1	Gasdermin bGSDM	MA	m	234
1	14	1	Gasdermin bGSDM	NA	n	234
1	15	1	Gasdermin bGSDM	OA	o	234
1	16	1	Gasdermin bGSDM	PA	p	234
1	17	1	Gasdermin bGSDM	QA	q	234
1	18	1	Gasdermin bGSDM	RA	r	234
1	19	1	Gasdermin bGSDM	SA	s	234
1	20	1	Gasdermin bGSDM	TA	t	234
1	21	1	Gasdermin bGSDM	UA	u	234
1	22	1	Gasdermin bGSDM	VA	v	234

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	23	1	Gasdermin bGSDM	WA	w	234
1	24	1	Gasdermin bGSDM	XA	x	234
1	25	1	Gasdermin bGSDM	YA	y	234
1	26	1	Gasdermin bGSDM	ZA	z	234
1	27	1	Gasdermin bGSDM	A	A	234
1	28	1	Gasdermin bGSDM	B	B	234
1	29	1	Gasdermin bGSDM	C	C	234
1	30	1	Gasdermin bGSDM	D	D	234
1	31	1	Gasdermin bGSDM	E	E	234
1	32	1	Gasdermin bGSDM	F	F	234
1	33	1	Gasdermin bGSDM	G	G	234
1	34	1	Gasdermin bGSDM	H	H	234
1	35	1	Gasdermin bGSDM	I	I	234
1	36	1	Gasdermin bGSDM	J	J	234
1	37	1	Gasdermin bGSDM	K	K	234

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	38	1	Gasdermin bGSDM	L	L	234
1	39	1	Gasdermin bGSDM	M	M	234
1	40	1	Gasdermin bGSDM	N	N	234
1	41	1	Gasdermin bGSDM	O	O	234
1	42	1	Gasdermin bGSDM	P	P	234
1	43	1	Gasdermin bGSDM	Q	Q	234
1	44	1	Gasdermin bGSDM	R	R	234
1	45	1	Gasdermin bGSDM	S	S	234
1	46	1	Gasdermin bGSDM	T	T	234
1	47	1	Gasdermin bGSDM	U	U	234
1	48	1	Gasdermin bGSDM	V	V	234
1	49	1	Gasdermin bGSDM	W	W	234
1	50	1	Gasdermin bGSDM	X	X	234
1	51	1	Gasdermin bGSDM	Y	Y	234
1	52	1	Gasdermin bGSDM	Z	Z	234

Datasets used for modeling

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	8sl0
2	Integrative model	PDB-Dev	PDBDEV_00000369

Representation

This entry has only one representation and includes 0 rigid bodies and 52 flexible units

Chain ID	Rigid bodies	Non-rigid segments
AA	-	1-234
BA	-	1-234
CA	-	1-234
DA	-	1-234
EA	-	1-234
FA	-	1-234
GA	-	1-234
HA	-	1-234
IA	-	1-234
JA	-	1-234
KA	-	1-234
LA	-	1-234
MA	-	1-234
NA	-	1-234
OA	-	1-234

Chain ID	Rigid bodies	Non-rigid segments
PA	-	1-234
QA	-	1-234
RA	-	1-234
SA	-	1-234
TA	-	1-234
UA	-	1-234
VA	-	1-234
WA	-	1-234
XA	-	1-234
YA	-	1-234
ZA	-	1-234
A	-	1-234
B	-	1-234
C	-	1-234
D	-	1-234
E	-	1-234
F	-	1-234
G	-	1-234
H	-	1-234
I	-	1-234
J	-	1-234
K	-	1-234
L	-	1-234

Chain ID	Rigid bodies	Non-rigid segments
M	-	1-234
N	-	1-234
O	-	1-234
P	-	1-234
Q	-	1-234
R	-	1-234
S	-	1-234
T	-	1-234
U	-	1-234
V	-	1-234
W	-	1-234
X	-	1-234
Y	-	1-234
Z	-	1-234

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

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	This model is derivative of the other PDBDEV_00000369 and the protocol is therefore highly similar. However, this particular model resulted from allowing the PDBDEV_00000369 model to equilibrate in an MD simulation with backbone positions restrained, but the rest was allowed to move such that key features (i.e., the palmitoyl) entered more natural conformations.	None	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Python	v3.9.7	model building	https://www.python.org/
2	MDAnalysis	v2.4.2	model building	https://www.mdanalysis.org/
3	Gromacs	v2022.4	MD simulations	https://manual.gromacs.org/2023.4/download.html
4	Charmm	Not available	MD simulations	https://www.charmm.org/

Data quality

Model quality

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

Standard geometry: bond outliers

There are 93184 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.07	0.97	1488
CA--HA2	1.07	0.97	175
CA--HA1	1.07	0.97	174
N--HN2	0.99	0.89	7
N--HN1	0.99	0.89	8
CA--HA2	1.08	0.97	959
CA--HA	1.08	0.97	8311
N--HN2	1.00	0.89	43
CA--HA1	1.08	0.97	965
N--HN1	1.00	0.89	40
OG1--HG1	0.95	0.84	74
OH--HH	0.95	0.84	50
OH--HH	0.96	0.84	292
OG1--HG1	0.96	0.84	390
CA--HA	1.09	0.97	1017
CA--HA1	1.09	0.97	109
CA--HA2	1.09	0.97	114
N--HN1	1.01	0.89	4
N--HN2	1.01	0.89	2
SG--HG1	1.32	1.20	23
N--HN	0.98	0.86	6
OG1--HG1	0.97	0.84	56

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
SG--HG1	1.33	1.20	29
N--HN	0.99	0.86	4215
OH--HH	0.97	0.84	22
CB--HB2	1.10	0.97	819
CD2--HD22	1.10	0.97	115
CD--HD2	1.10	0.97	238
NH2--HH22	0.99	0.86	59
CD--HD1	1.10	0.97	232
NE--HE	0.99	0.86	70
CG1--HG11	1.10	0.97	206
CG--HG2	1.10	0.97	350
ND2--HD22	0.99	0.86	67
CD1--HD13	1.10	0.97	113
CB--HB	1.10	0.97	246
CG--HG1	1.10	0.97	330
NE2--HE21	0.99	0.86	146
CG2--HG21	1.10	0.97	239
ND2--HD21	0.99	0.86	73
CB--HB1	1.10	0.97	790
CG2--HG23	1.10	0.97	225
NE2--HE22	0.99	0.86	129
CD--HD3	1.10	0.97	84
CD2--HD23	1.10	0.97	121

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--HG12	1.10	0.97	176
NH2--HH21	0.99	0.86	65
CB--HB3	1.10	0.97	78
CG2--HG22	1.10	0.97	197
NH1--HH11	0.99	0.86	65
CD1--HD11	1.10	0.97	109
CD2--HD21	1.10	0.97	113
CE--HE1	1.10	0.97	93
CG--HG	1.10	0.97	120
CD1--HD12	1.10	0.97	118
NH1--HH12	0.99	0.86	60
CG1--HG13	1.10	0.97	117
ND1--HD1	0.99	0.86	4
CE--HE2	1.10	0.97	79
CE--HE3	1.10	0.97	5
CB--HB1	1.11	0.97	6375
CD--HD2	1.11	0.97	1940
CD2--HD21	1.11	0.97	938
CG--HG1	1.11	0.97	2696
CE--HE1	1.11	0.97	663
CB--HB2	1.11	0.97	6343
CG--HG2	1.11	0.97	2707
CD--HD3	1.11	0.97	575

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--HB3	1.11	0.97	709
CD--HD1	1.11	0.97	1962
CG2--HG21	1.11	0.97	1889
CG--HG	1.11	0.97	876
CB--HB	1.11	0.97	1898
CG1--HG11	1.11	0.97	1455
CD1--HD13	1.11	0.97	921
CD1--HD11	1.11	0.97	912
CG1--HG12	1.11	0.97	1479
CD2--HD23	1.11	0.97	894
CE--HE2	1.11	0.97	692
CG2--HG23	1.11	0.97	1863
CG2--HG22	1.11	0.97	1880
CD1--HD12	1.11	0.97	888
N--HN	1.00	0.86	7104
ND2--HD21	1.00	0.86	393
NE--HE	1.00	0.86	312
ND2--HD22	1.00	0.86	417
NH2--HH22	1.00	0.86	313
NH1--HH12	1.00	0.86	322
NE2--HE21	1.00	0.86	666
NE2--HE22	1.00	0.86	672
NH1--HH11	1.00	0.86	315

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--HG13	1.11	0.97	851
CD2--HD22	1.11	0.97	910
NH2--HH21	1.00	0.86	307
CE--HE3	1.11	0.97	40
ND1--HD1	1.00	0.86	41
CE1--HE1	1.07	0.93	113
NZ--HZ2	1.03	0.89	123
CE2--HE2	1.07	0.93	112
CD2--HD2	1.07	0.93	127
CD1--HD1	1.07	0.93	117
NZ--HZ1	1.03	0.89	116
NZ--HZ3	1.03	0.89	134
CZ--HZ	1.07	0.93	69
N--H3	1.03	0.89	8
N--H2	1.03	0.89	4
N--H1	1.03	0.89	9
NZ--HZ1	1.04	0.89	643
NZ--HZ2	1.04	0.89	630
N--H2	1.04	0.89	43
CE1--HE1	1.08	0.93	696
NZ--HZ3	1.04	0.89	612
CG2--HG22	1.12	0.97	367
CG--HG2	1.12	0.97	479

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--HB1	1.12	0.97	1207
CD1--HD12	1.12	0.97	190
CG2--HG23	1.12	0.97	356
CG--HG1	1.12	0.97	510
CG1--HG11	1.12	0.97	263
CG--HG	1.12	0.97	200
CD--HD1	1.12	0.97	354
CG2--HG21	1.12	0.97	316
CD--HD2	1.12	0.97	370
CE--HE1	1.12	0.97	128
CB--HB2	1.12	0.97	1210
CD2--HD22	1.12	0.97	171
CG1--HG12	1.12	0.97	269
CD1--HD13	1.12	0.97	162
CD2--HD23	1.12	0.97	181
CG1--HG13	1.12	0.97	176
CE--HE2	1.12	0.97	113
CB--HB3	1.12	0.97	149
CE--HE3	1.12	0.97	7
CD--HD3	1.12	0.97	121
CB--HB	1.12	0.97	300
CD2--HD21	1.12	0.97	145
N--HN	1.01	0.86	167

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE2--HE2	1.08	0.93	696
CD1--HD1	1.08	0.93	686
CD2--HD2	1.08	0.93	720
CZ--HZ	1.08	0.93	411
CD1--HD11	1.12	0.97	175
NE--HE	1.01	0.86	34
NE2--HE22	1.01	0.86	83
ND2--HD22	1.01	0.86	36
NE2--HE21	1.01	0.86	72
ND2--HD21	1.01	0.86	54
NH1--HH11	1.01	0.86	36
NH2--HH22	1.01	0.86	44
NH1--HH12	1.01	0.86	34
ND1--HD1	1.01	0.86	7
NH2--HH21	1.01	0.86	44
N--H3	1.04	0.89	39
N--H1	1.04	0.89	39
NZ--HZ1	1.05	0.89	73
NZ--HZ2	1.05	0.89	79
NZ--HZ3	1.05	0.89	86
CE1--HE1	1.09	0.93	120
CE2--HE2	1.09	0.93	76
CZ--HZ	1.09	0.93	40

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CD1--HD1	1.09	0.93	81
CD2--HD2	1.09	0.93	89
N--H3	1.05	0.89	5
N--H1	1.05	0.89	4
N--H2	1.05	0.89	5
CE1--HE1	1.10	0.93	7

Standard geometry: angle outliers

There are 8109 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
SG-C7-C8	109.23	178.50	1
CB-SG-C7	106.10	172.35	1
SG-C7-C8	109.23	175.29	1
CB-SG-C7	106.10	171.98	1
SG-C7-C8	109.23	171.55	1
CB-SG-C7	106.10	165.58	1
CB-SG-C7	106.10	165.43	1
CB-SG-C7	106.10	164.23	1
CB-SG-C7	106.10	161.77	1
SG-C7-C8	109.23	164.37	1
SG-C7-C8	109.23	164.26	1
CB-SG-C7	106.10	159.16	1
SG-C7-C8	109.23	160.65	1
CB-SG-C7	106.10	156.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-SG-C7	106.10	155.42	1
SG-C7-C8	109.23	156.73	1
SG-C7-C8	109.23	156.58	1
SG-C7-C8	109.23	155.53	1
CB-SG-C7	106.10	151.91	1
CA-CB-CG	112.60	127.26	1
CB-SG-C7	106.10	149.92	1
SG-C7-C8	109.23	152.07	1
SG-C7-C8	109.23	152.04	1
CB-SG-C7	106.10	148.08	1
CB-SG-C7	106.10	147.22	1
CB-SG-C7	106.10	146.41	1
NE-CZ-NH2	119.20	107.88	1
SG-C7-C8	109.23	71.55	1
CA-CB-CG	113.80	101.62	1
CB-SG-C7	106.10	141.73	1
SG-C7-C8	109.23	144.55	1
SG-C7-C8	109.23	144.24	1
SG-C7-C8	109.23	143.74	1
CA-C-N	116.90	133.92	1
SG-C7-C8	109.23	143.13	1
OE1-CD-NE2	122.60	111.34	1
CA-CB-CG	113.80	102.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
SG-C7-C8	109.23	76.01	1
SG-C7-C8	109.23	76.05	1
CB-SG-C7	106.10	139.16	1
NE-CZ-NH1	121.50	132.51	1
NE-CZ-NH1	121.50	132.32	1
SG-C7-C8	109.23	76.88	1
SG-C7-C8	109.23	141.10	1
NE-CZ-NH2	119.20	109.67	1
CA-CB-CG	113.80	124.33	1
CB-SG-C7	106.10	137.43	1
CA-CB-CG	112.60	122.88	1
CA-CB-CG	112.60	122.78	1
CA-CB-CG	112.60	122.54	1
NE-CZ-NH1	121.50	131.44	1
NE-CZ-NH1	121.50	131.42	1
NE-CZ-NH1	121.50	131.33	1
CA-C-N	116.90	131.64	1
NE-CZ-NH1	121.50	131.25	1
CA-CB-CG	112.60	102.85	1
NE-CZ-NH1	121.50	131.23	1
CA-CB-CG	113.80	104.13	1
CA-C-N	116.90	131.34	1
NE-CZ-NH1	121.50	131.12	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	113.00	1
NE-CZ-NH2	119.20	110.57	1
CA-CB-CG	112.60	122.11	1
CA-CB-CG	113.80	104.39	1
NE-CZ-NH2	119.20	110.75	1
CA-CB-CG	112.60	121.98	1
CA-CB-CG	112.60	103.22	1
N-CA-CB	110.50	126.43	1
CA-CB-CG	112.60	121.96	1
CA-CB-CG	112.60	121.93	1
NE-CZ-NH2	119.20	110.81	1
OD1-CG-ND2	122.60	113.28	1
CB-SG-C7	106.10	133.81	1
NE-CZ-NH1	121.50	130.71	1
OE1-CD-NE2	122.60	113.45	1
CB-SG-C7	106.10	133.50	1
OE1-CD-NE2	122.60	113.47	1
SG-C7-C8	109.23	136.46	1
CA-CB-CG	112.60	121.65	1
CA-CB-CG	112.60	121.62	1
OD1-CG-ND2	122.60	113.63	1
OE1-CD-NE2	122.60	113.69	1
CA-CB-CG	113.80	122.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	113.73	1
CA-CB-CG	112.60	121.43	1
CA-CB-CG	112.60	121.42	1
CA-C-N	116.90	130.09	1
CA-CB-CG	112.60	121.34	1
C-N-CA	121.70	137.42	1
CA-CB-CG	112.60	103.90	1
CA-C-N	116.90	129.95	1
SG-C7-C8	109.23	135.31	1
OE1-CD-NE2	122.60	113.93	1
CA-C-N	116.90	129.89	1
NE-CZ-NH1	121.50	130.11	2
CA-CB-CG	112.60	121.21	1
SG-C7-C8	109.23	83.40	1
NE-CZ-NH2	119.20	111.46	1
CA-CB-CG	113.80	105.22	1
OD1-CG-ND2	122.60	114.02	1
NE-CZ-NH1	121.50	130.07	1
OE1-CD-NE2	122.60	114.04	1
CA-CB-CG	112.60	104.06	1
CA-CB-CG	113.80	122.33	1
CA-CB-CG	113.80	105.27	1
CA-CB-CG	113.80	122.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	131.11	1
CA-CB-CG	113.80	122.27	1
NE-CZ-NH2	119.20	126.81	1
N-CA-CB	110.40	97.74	1
C-N-CA	121.70	136.90	1
CA-CB-CG	113.80	105.38	2
N-CA-CB	103.00	112.24	1
CB-CG-CD2	131.20	120.30	1
O-C-N	123.00	109.59	1
CA-CB-CG	112.60	120.97	1
CB-SG-C7	106.10	131.19	1
CA-CB-CG	113.80	122.16	1
NE-CZ-NH2	119.20	126.72	2
C-N-CA	121.70	136.67	1
OE1-CD-NE2	122.60	114.28	1
CA-CB-CG	112.60	120.91	1
OE1-CD-NE2	122.60	114.34	1
CA-CB-CG	112.60	120.86	1
NE-CZ-NH2	119.20	111.78	1
CA-C-N	116.90	129.22	1
OD1-CG-ND2	122.60	114.40	1
NE-CZ-NH2	119.20	126.58	1
NE-CZ-NH1	121.50	129.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	120.77	1
CA-CB-CG	112.60	104.43	1
OE1-CD-NE2	122.60	114.43	1
C-N-CA	121.70	136.40	1
CA-CB-CG	112.60	120.76	1
OE1-CD-NE2	122.60	114.45	1
CG-CD2-NE2	107.20	115.35	1
C-N-CA	121.70	136.33	1
NE-CZ-NH2	119.20	111.88	1
NE-CZ-NH2	119.20	111.90	1
CA-C-N	116.90	129.06	1
CA-CB-CG	113.80	121.91	1
N-CA-CB	110.50	124.28	1
CA-CB-CG	113.80	105.70	1
CG-SD-CE	100.90	83.13	1
N-CA-CB	110.50	124.22	1
CA-CB-CG2	110.50	96.79	1
CA-CB-CG	112.60	120.66	1
NE-CZ-NH1	121.50	129.56	1
CA-CB-CG	113.80	105.75	1
NE-CZ-NH2	119.20	126.44	1
CG-CD-NE2	116.40	128.45	1
CA-CB-CG	112.60	120.63	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	120.60	1
C-CA-CB	110.10	125.30	1
NE-CZ-NH2	119.20	112.00	1
CB-SG-C7	106.10	130.04	1
CA-C-N	116.90	128.87	1
CA-C-N	116.90	128.83	1
OE1-CD-NE2	122.60	130.53	1
N-CA-CB	110.40	98.53	1
CB-SG-C7	106.10	129.80	1
NH1-CZ-NH2	119.30	109.04	1
N-CA-CB	110.50	123.92	1
OD1-CG-ND2	122.60	130.49	1
NE-CZ-NH2	119.20	112.10	1
CA-CB-CG	112.60	120.48	1
C-N-CA	121.70	135.84	1
NE-CZ-NH2	119.20	126.26	1
CA-CB-CG	112.60	104.75	1
OE1-CD-NE2	122.60	114.76	2
CA-CB-CG	112.60	120.44	1
NE-CZ-NH1	121.50	129.31	1
OE1-CD-NE2	122.60	130.41	1
CA-CB-CG	112.60	120.39	1
CA-CB-CG	112.60	104.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	112.20	1
NE-CZ-NH2	119.20	112.21	1
OE1-CD-NE2	122.60	114.84	1
NH1-CZ-NH2	119.30	109.22	1
OD1-CG-ND2	122.60	114.85	1
CA-C-N	116.90	128.51	1
NE-CZ-NH2	119.20	112.24	1
OD1-CG-ND2	122.60	114.87	1
N-CA-CB	110.40	98.81	1
CA-CB-CG	113.80	106.08	1
CA-CB-OG1	109.60	121.16	1
OD1-CG-ND2	122.60	114.90	1
CA-C-N	116.90	128.44	1
CA-CB-CG	112.60	120.30	1
OE1-CD-NE2	122.60	114.91	1
CA-CB-CG	112.60	104.93	1
CD2-NE2-CE1	109.00	101.33	1
C-CA-CB	110.10	124.67	1
CA-C-N	116.90	128.40	1
NE-CZ-NH1	121.50	129.15	1
CA-C-N	116.90	128.37	1
NE-CZ-NH2	119.20	112.32	1
CA-CB-CG	113.80	106.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	104.97	1
CA-CB-CG	113.80	106.17	1
SG-C7-C8	109.23	132.12	1
C-CA-CB	110.10	124.60	1
O-C-N	123.00	110.79	1
OE1-CD-NE2	122.60	114.98	1
CG-CD-NE2	116.40	127.83	1
CA-CB-CG	112.60	104.98	1
OE1-CD-NE2	122.60	114.99	1
OD1-CG-ND2	122.60	114.99	1
NH1-CZ-NH2	119.30	109.41	1
CA-CB-CG	112.60	105.00	1
OD1-CG-ND2	122.60	115.00	1
OE1-CD-NE2	122.60	130.20	1
C-N-CA	121.70	135.36	2
O-C-N	123.00	110.86	1
CA-CB-CG	112.60	120.18	1
CA-CB-CG	113.80	106.23	1
CA-CB-CG	112.60	105.03	1
CA-C-N	116.90	128.24	2
N-CA-CB	103.00	94.69	1
OE1-CD-NE2	122.60	115.05	1
CA-C-O	120.80	107.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	121.35	1
N-CA-CB	111.50	124.31	1
CB-SG-C7	106.10	128.66	1
NE-CZ-NH2	119.20	112.44	1
OD1-CG-ND2	122.60	115.11	1
NE-CZ-NH1	121.50	114.02	1
CA-CB-CG	112.60	120.08	1
C-N-CA	121.70	135.15	1
CA-CB-CG	112.60	105.13	1
CA-CB-CG	112.60	120.07	1
CA-CB-CG	112.60	105.14	1
CA-C-N	116.90	128.08	1
OE1-CD-NE2	122.60	115.15	1
NE-CZ-NH1	121.50	128.94	1
ND1-CE1-NE2	108.40	115.84	1
O-C-N	123.00	111.11	1
N-CA-CB	110.50	123.13	1
NE-CZ-NH2	119.20	112.53	1
CA-C-N	116.90	128.01	1
OE1-CD-NE2	122.60	115.19	1
C-N-CA	121.70	135.02	1
N-CA-CB	110.50	123.03	1
N-CA-CB	110.40	99.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CB-CG2	110.80	126.99	1
CA-CB-CG	113.80	106.45	1
NH1-CZ-NH2	119.30	109.75	1
CA-CB-CG	112.60	119.95	1
CA-CB-OG1	109.60	120.62	1
NE-CZ-NH2	119.20	112.59	1
NE-CZ-NH2	119.20	112.60	1
CA-C-N	116.90	127.89	1
CA-CB-CG2	110.50	98.05	1
CA-CB-CG	112.60	105.29	1
NE-CZ-NH1	121.50	128.81	1
CA-C-N	116.90	127.86	1
CA-C-N	116.90	127.85	1
CA-CB-CG	112.60	105.31	1
CA-C-N	116.90	127.83	1
CA-CB-CG	112.60	105.33	2
N-CA-CB	110.50	122.86	1
CA-CB-CG	112.60	119.87	1
CA-C-N	116.90	127.80	1
O-C-N	123.00	111.38	2
CA-CB-CG	112.60	119.86	1
CA-CB-CG	113.80	121.05	1
CA-CB-CG	112.60	119.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	134.72	1
C-CA-CB	110.50	121.35	1
CA-CB-OG1	109.60	120.45	1
OE1-CD-NE2	122.60	129.83	1
CA-C-N	116.90	127.74	1
CA-CB-CG	113.80	106.58	1
CA-CB-CG	112.60	119.82	1
CA-CB-CG	112.60	119.81	1
CA-CB-CG	113.80	106.60	1
CA-CB-CG	113.80	121.00	1
CA-CB-CG	112.60	119.79	1
NE-CZ-NH2	119.20	112.73	1
C-N-CA	121.70	134.64	1
OE1-CD-NE2	122.60	115.42	1
N-CA-CB	110.50	122.71	1
CA-C-N	116.90	127.66	1
N-CA-CB	110.40	99.64	1
CA-CB-CG	112.60	105.43	1
SG-C7-C8	109.23	130.72	1
CA-C-N	116.90	127.64	1
CB-SG-C7	106.10	127.57	1
O-C-N	123.00	111.56	1
OE1-CD-NE2	122.60	115.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	134.57	1
CA-CB-CG	112.60	119.74	1
CD2-NE2-CE1	109.00	101.86	1
CB-CG-CD2	131.20	140.49	1
NE-CZ-NH2	119.20	112.78	1
CA-C-N	116.90	127.60	1
C-N-CA	121.70	134.52	1
N-CA-CB	110.50	122.60	1
OD1-CG-ND2	122.60	129.72	1
C-N-CA	121.70	134.51	1
OE1-CD-NE2	122.60	115.49	1
NE-CZ-NH1	121.50	128.61	1
CA-CB-CG	114.10	128.32	1
CD2-NE2-CE1	109.00	101.89	1
CB-CG-ND2	116.40	127.06	1
CA-C-N	116.90	127.55	1
SG-C7-C8	109.23	87.93	1
CA-CB-CG1	110.40	122.46	1
NE-CZ-NH2	119.20	125.58	1
CB-SG-C7	106.10	127.33	1
NH1-CZ-NH2	119.30	110.10	1
C-CA-CB	110.50	121.10	1
C-N-CA	121.70	134.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	127.49	1
CA-CB-CG	112.60	105.54	1
C-N-CA	121.70	134.40	2
OE1-CD-NE2	122.60	115.56	1
NE-CZ-NH1	121.50	128.54	1
CA-CB-CG	112.60	119.64	1
NH1-CZ-NH2	119.30	128.44	1
NE-CZ-NH1	121.50	128.53	1
CA-CB-CG	113.80	106.77	1
OD1-CG-ND2	122.60	115.58	1
C-CA-CB	110.10	123.44	1
OE1-CD-NE2	122.60	115.59	1
CA-CB-CG	112.60	119.61	1
C-N-CA	121.70	134.30	1
CA-CB-CG	113.80	106.81	1
CA-C-O	120.80	132.68	1
CA-CB-CG	113.80	120.78	1
OD1-CG-ND2	122.60	115.62	1
CA-CB-OG1	109.60	120.07	1
C-CA-CB	110.10	123.36	1
CA-CB-CG	113.80	106.83	1
C-N-CA	121.70	134.25	1
N-CA-CB	110.50	98.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	120.75	1
OD1-CG-ND2	122.60	115.65	1
CA-CB-OG1	109.60	120.02	1
N-CA-CB	110.50	98.69	1
NE-CZ-NH2	119.20	112.95	1
CA-CB-CG	112.60	105.65	1
OE1-CD-NE2	122.60	115.66	1
NE-CZ-NH1	121.50	128.44	1
CA-C-N	116.90	127.31	1
C-CA-CB	110.50	100.10	1
CA-CB-CG1	110.40	122.18	1
CD-NE-CZ	124.40	134.10	1
CA-CB-CG	112.60	119.52	4
CA-C-N	116.90	127.28	1
O-C-N	123.00	111.93	1
CA-CB-CG	112.60	119.51	1
OD1-CG-ND2	122.60	115.69	1
N-CA-CB	110.50	122.24	1
N-CA-CB	110.40	120.74	1
OD1-CG-ND2	122.60	129.49	1
CA-C-N	116.90	127.24	1
CD2-NE2-CE1	109.00	102.11	2
CA-C-N	116.90	127.23	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	111.99	1
NE-CZ-NH1	121.50	128.38	2
CA-CB-CG	112.60	105.73	1
CA-C-N	116.90	127.20	1
CB-CG-CD1	120.80	110.51	1
SG-C7-C8	109.23	129.81	1
CA-C-N	116.90	127.19	1
OD1-CG-ND2	122.60	115.75	2
NE-CZ-NH1	121.50	128.35	2
CA-CB-CG	112.60	105.75	1
N-CA-CB	103.00	95.47	1
CA-CB-CG	112.60	119.44	1
C-N-CA	121.70	134.02	1
CA-CB-CG	112.60	105.76	2
OD1-CG-ND2	122.60	115.76	1
NE-CZ-NH1	121.50	128.33	1
N-CA-C	111.00	91.88	1
CA-CB-CG	112.60	119.43	1
C-N-CA	121.70	133.99	1
NE-CZ-NH2	119.20	125.35	1
CA-CB-CG	112.60	105.77	1
CG-CD2-NE2	107.20	114.03	1
CA-CB-OG1	109.60	119.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	105.78	2
O-C-N	123.00	112.09	1
OE1-CD-NE2	122.60	115.78	1
C-N-CA	121.70	133.96	2
N-CA-CB	110.50	122.08	1
CD-NE-CZ	124.40	133.92	1
CA-C-O	120.80	109.24	1
O-C-N	123.00	112.12	1
C-N-CA	121.70	133.94	1
NE-CZ-NH2	119.20	125.31	1
OD1-CG-ND2	122.60	115.81	1
C-N-CA	121.70	133.91	1
C-N-CA	121.70	133.90	2
C-CA-CB	110.10	122.98	1
OD1-CG-ND2	122.60	115.82	1
CA-C-N	116.90	127.05	1
C-CA-CB	110.10	122.96	1
O-C-N	123.00	112.18	2
NE-CZ-NH2	119.20	125.29	1
CA-C-N	116.90	127.03	1
C-N-CA	121.70	133.85	1
NE-CZ-NH1	121.50	128.25	1
OD1-CG-ND2	122.60	115.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	133.84	1
N-CA-CB	110.50	121.96	1
CA-C-N	116.20	129.68	1
OE1-CD-NE2	122.60	115.86	2
CA-CB-CG	113.80	120.54	1
ND1-CE1-NE2	108.40	115.14	1
CA-CB-OG1	109.60	119.70	1
OE1-CD-NE2	122.60	129.33	1
CA-CB-CG	113.80	107.08	1
N-CA-CB	103.00	95.61	1
NE-CZ-NH1	121.50	128.22	1
OD1-CG-ND2	122.60	115.89	1
CA-C-N	116.90	126.97	1
CA-C-N	116.90	126.95	1
CA-CB-CG	112.60	119.29	1
C-N-CA	121.70	133.74	1
O-C-N	123.00	112.30	1
C-N-CA	121.70	133.72	1
CA-CB-CG2	110.50	121.85	1
CA-C-N	116.90	126.92	1
CA-C-N	116.90	126.91	3
C-CA-CB	110.10	97.42	1
NE-CZ-NH2	119.20	113.20	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	133.70	1
CA-CB-OG1	109.60	119.59	1
N-CA-CB	110.50	121.83	1
CA-C-N	116.90	126.89	1
C-CA-CB	110.10	122.75	1
O-C-N	123.00	112.36	1
N-CA-CB	103.00	110.31	1
CB-CG-OD1	120.80	134.09	1
N-CA-CB	110.50	121.79	1
CA-CB-CG	112.60	119.24	1
NE-CZ-NH2	119.20	113.23	1
C-N-CA	121.70	133.63	1
CA-C-N	116.90	126.84	1
C-N-CA	121.70	133.62	1
N-CA-CB	103.00	110.28	1
CA-C-N	116.90	126.83	1
CG-CD-NE	112.00	97.45	1
CA-CB-CG	114.10	127.32	1
CA-CB-CG2	110.40	121.63	1
C-N-CA	121.70	133.59	1
N-CA-CB	110.40	120.31	1
C-CA-CB	110.10	122.65	1
N-CA-CB	111.50	122.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	112.44	1
CA-CB-CG	112.60	106.00	1
OE1-CD-NE2	122.60	116.01	1
O-C-N	123.00	112.46	2
CA-CB-CG	113.80	107.21	1
CA-CB-CG	113.80	107.22	1
C-N-CA	121.70	133.55	1
CA-CB-CG	113.80	120.38	2
C-N-CA	121.70	133.54	1
CA-CB-CG	112.60	119.18	1
NH1-CZ-NH2	119.30	110.76	1
CG-CD-OE1	120.80	133.93	1
OE1-CD-NE2	122.60	116.05	1
O-C-N	123.00	112.52	1
CA-C-N	116.90	126.73	1
C-CA-CB	110.10	122.54	1
NE-CZ-NH2	119.20	113.31	1
O-C-N	123.00	112.55	1
CB-SG-C7	106.10	125.68	1
CA-C-N	116.90	126.68	1
N-CA-CB	103.00	110.17	1
C-N-CA	121.70	133.43	1
CB-SG-C7	106.10	125.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	126.67	1
NE-CZ-NH1	121.50	128.01	1
C-N-CA	121.70	133.41	1
C-N-CA	121.70	133.40	1
C-CA-CB	110.10	97.76	1
CA-CB-CG1	110.40	121.44	1
NH1-CZ-NH2	119.30	127.73	1
NH1-CZ-NH2	119.30	110.87	1
CA-CB-CG	112.60	119.08	1
O-C-N	123.00	112.63	1
CA-C-N	116.90	126.62	1
CG-CD2-CE2	121.20	111.48	1
OD1-CG-ND2	122.60	116.12	1
C-CA-CB	110.10	122.40	1
NH1-CZ-NH2	119.30	110.89	1
CA-C-N	116.90	126.60	1
C-N-CA	121.70	133.34	1
CA-C-N	116.90	126.59	1
NH1-CZ-NH2	119.30	110.90	1
N-CA-CB	110.50	121.47	1
O-C-N	123.00	112.68	1
OE1-CD-NE2	122.60	116.15	1
CD2-NE2-CE1	109.00	102.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	116.16	1
NE-CZ-NH1	121.50	127.94	2
CG-CD2-CE2	121.20	111.54	1
N-CA-CB	110.50	121.44	1
N-CA-CB	110.50	121.43	1
NH1-CZ-NH2	119.30	110.95	1
CG-CD-NE2	116.40	126.03	1
N-CA-CB	110.50	99.58	1
OE1-CD-NE2	122.60	116.18	2
SG-C7-C8	109.23	128.49	1
CA-C-N	116.90	126.53	1
CA-CB-CG1	110.40	121.31	1
CA-CB-CG1	110.40	121.30	1
O-C-N	123.00	112.74	1
CA-C-N	116.90	126.52	1
OD1-CG-ND2	122.60	129.01	1
CB-CG-CD	112.60	123.48	1
NE-CZ-NH1	121.50	127.90	1
O-C-N	123.00	112.76	1
CA-CB-CG	112.60	119.00	1
OE1-CD-NE2	122.60	116.20	1
NH1-CZ-NH2	119.30	110.99	1
OD1-CG-ND2	122.60	116.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.21	1
CD-NE-CZ	124.40	115.45	1
NE-CZ-NH1	121.50	127.89	1
N-CA-CB	110.40	100.82	1
C-CA-CB	110.10	122.23	1
CA-CB-CG2	110.40	121.25	1
CB-CG-CD	111.30	125.98	1
OD1-CG-ND2	122.60	116.22	1
O-C-N	123.00	112.80	1
N-CA-CB	110.50	121.34	1
CA-CB-CG	112.60	118.97	2
OD1-CG-ND2	122.60	116.23	1
C-N-CA	121.70	133.17	1
OD1-CG-ND2	122.60	116.24	3
NE-CZ-NH1	121.50	127.86	1
CA-C-N	116.90	126.44	1
C-CA-CB	110.50	100.96	1
O-C-N	123.00	112.83	2
CA-CB-CG	113.80	120.15	1
NE-CZ-NH1	121.50	127.85	1
OE1-CD-NE2	122.60	116.25	1
NE-CZ-NH2	119.20	124.92	1
O-C-N	123.00	112.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	121.29	1
N-CA-CB	110.50	99.71	1
CA-C-N	116.90	126.42	1
NE-CZ-NH2	119.20	113.49	1
C-N-CA	121.70	133.11	1
N-CA-CB	110.50	121.27	1
C-N-CA	121.70	133.10	1
NE-CZ-NH1	121.50	127.83	1
CA-CB-CG	112.60	106.28	1
NE-CZ-NH2	119.20	124.89	1
N-CA-CB	110.50	121.25	1
CG-CD2-NE2	107.20	113.52	2
N-CA-CB	111.50	122.24	1
CA-CB-CG	112.60	118.92	1
NH1-CZ-NH2	119.30	111.09	1
SG-C7-C8	109.23	128.17	1
C-N-CA	121.70	133.06	1
C-CA-CB	110.10	98.11	1
NE-CZ-NH2	119.20	113.52	1
NE-CZ-NH1	121.50	127.81	1
OD1-CG-ND2	122.60	116.29	1
CG-CD2-NE2	107.20	113.51	1
CA-CB-CG	112.60	118.91	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.29	1
C-N-CA	121.70	133.05	1
N-CA-CB	110.50	121.21	1
CA-C-O	120.80	131.51	1
NE-CZ-NH2	119.20	113.53	1
OD1-CG-ND2	122.60	116.30	1
N-CA-CB	110.40	100.95	1
CA-CB-CG	113.80	107.50	1
CB-SG-C7	106.10	124.99	1
CA-C-N	116.90	126.34	1
NE-CZ-NH1	121.50	127.79	1
O-C-N	123.00	112.93	1
CA-CB-CG	112.60	118.89	1
C-N-CA	121.70	132.99	1
N-CA-CB	110.50	121.17	1
NE-CZ-NH2	119.20	124.85	1
CA-C-O	120.80	131.46	1
CA-CB-CG	113.80	107.53	1
C-CA-CB	110.10	122.02	1
CA-C-N	116.90	126.30	1
OD1-CG-ND2	122.60	116.33	1
NH1-CZ-NH2	119.30	111.15	1
O-C-N	123.00	112.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	121.15	1
C-N-CA	121.70	132.97	2
NE-CZ-NH2	119.20	124.83	1
CA-C-N	116.90	126.28	1
CA-CB-CG	113.80	107.55	1
CA-CB-CG	112.60	118.85	2
NE-CZ-NH1	121.50	127.75	1
O-C-N	123.00	113.00	1
N-CA-CB	110.40	101.03	1
CD-NE-CZ	124.40	115.66	1
C-CA-CB	110.50	101.14	1
C-N-CA	121.70	132.94	1
OE1-CD-NE2	122.60	116.36	1
O-C-N	123.00	113.02	1
CB-CG-CD1	120.80	111.44	1
CA-CB-CG	113.80	120.04	1
N-CA-CB	110.50	121.10	1
CA-CB-CG1	110.40	121.00	1
NE-CZ-NH1	121.50	127.73	1
O-C-N	123.00	113.03	1
CA-CB-OG	111.10	123.56	1
CA-CB-CG	113.80	107.57	1
N-CA-CB	110.50	121.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	132.90	2
N-CA-CB	110.50	121.07	1
CA-C-N	116.90	126.23	1
C-N-CA	121.70	132.89	1
C-N-CA	121.70	132.88	1
NH1-CZ-NH2	119.30	111.23	1
N-CA-CB	110.40	101.09	1
CB-CG-CD	112.60	102.05	1
O-C-N	123.00	113.07	1
N-CA-CB	110.40	119.70	1
OD1-CG-ND2	122.60	116.40	1
CA-CB-CG	113.80	107.61	1
ND1-CE1-NE2	108.40	114.59	1
C-N-CA	121.70	132.85	1
N-CA-CB	110.40	101.11	1
NE-CZ-NH2	119.20	113.63	1
C-N-CA	121.70	132.84	1
CA-CB-CG	114.10	126.48	1
NH1-CZ-NH2	119.30	111.26	1
N-CA-CB	110.50	99.99	1
CA-CB-CG1	110.40	120.91	1
C-CA-CB	110.50	101.23	1
N-CA-CB	110.50	121.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	126.17	1
CG-CD-NE2	116.40	125.67	1
N-CA-CB	110.50	120.99	1
C-N-CA	121.70	132.81	1
OE1-CD-NE2	122.60	116.43	1
OE1-CD-NE2	122.60	128.77	1
CB-CG-CD	111.30	125.48	1
OE1-CD-NE2	122.60	116.44	1
NE-CZ-NH1	121.50	127.66	1
N-CA-CB	111.50	121.97	2
N-CA-CB	110.50	120.97	1
CB-SG-C7	106.10	124.57	1
C-N-CA	121.70	132.78	1
C-CA-CB	110.10	121.80	1
O-C-N	123.00	113.16	2
C-N-CA	121.70	132.77	1
CA-CB-OG1	109.60	118.83	1
OE1-CD-NE2	122.60	116.46	2
C-N-CA	121.70	132.76	1
N-CA-CB	111.50	121.94	2
CB-CG-CD	112.60	123.04	1
CA-CB-CG	112.60	118.74	1
O-C-N	123.00	113.18	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-NE-CZ	124.40	132.99	1
C-CA-CB	110.10	121.75	1
CB-CG-CD	112.60	123.03	1
C-N-CA	121.70	132.74	1
CA-CB-OG1	109.60	118.80	1
O-C-N	123.00	113.19	2
C-N-CA	121.70	132.73	1
CA-CB-CG	113.80	119.92	1
CG-CD-CE	111.30	125.37	1
C-CA-CB	110.10	121.72	1
CA-CB-CG1	110.40	120.79	1
OD1-CG-ND2	122.60	116.49	2
C-CA-CB	111.60	99.38	1
CA-CB-CG	112.60	106.49	1
CA-CB-CG	113.80	107.69	2
OE1-CD-NE2	122.60	116.49	1
C-N-CA	121.70	132.69	1
N-CA-CB	110.40	101.25	1
N-CA-CB	110.50	120.87	2
N-CA-CB	103.00	96.29	1
CB-CG-CD	112.60	102.23	1
C-N-CA	121.70	132.67	1
OE1-CD-NE2	122.60	116.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	127.59	1
C-CA-CB	110.50	101.37	1
CA-CB-CG	112.60	106.51	1
CG-CD-OE1	120.80	108.63	1
CA-CB-CG	112.60	106.52	1
CB-CG-ND1	122.70	131.82	1
NH1-CZ-NH2	119.30	111.40	1
O-C-N	123.00	113.27	1
CA-CB-CG2	110.50	100.17	1
N-CA-CB	110.50	100.17	1
C-CA-CB	110.50	119.61	1
O-C-N	123.00	113.28	1
CA-C-O	120.80	110.48	1
N-CA-CB	111.50	121.82	1
C-N-CA	121.70	132.63	1
CA-CB-CG2	110.50	120.81	1
N-CA-CB	111.50	121.81	1
NE-CZ-NH1	121.50	127.56	2
C-N-CA	121.70	132.61	1
N-CA-CB	110.50	100.21	1
OD1-CG-ND2	122.60	116.55	2
CA-CB-CG	113.80	107.75	1
CA-CB-CG	113.80	119.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	116.56	1
CG-CD1-CE1	121.20	112.15	1
C-CA-CB	110.50	119.55	1
O-C-N	123.00	113.35	2
CB-CG-ND1	122.70	131.75	1
CA-CB-CG	112.60	118.63	1
C-N-CA	121.70	132.55	2
C-CA-CB	110.10	121.55	1
CA-CB-CG1	110.40	120.65	1
C-N-CA	121.70	132.54	1
CA-CB-CG	112.60	118.62	1
NE-CZ-NH1	121.50	127.52	1
CA-CB-CG	114.10	126.14	1
CA-CB-CG	113.80	107.78	1
CA-CB-CG2	110.50	100.27	1
C-CA-CB	110.10	121.53	2
CB-CG-CD	111.30	125.14	1
C-N-CA	121.70	132.53	1
CA-C-N	116.90	125.92	2
O-C-N	123.00	113.38	1
CA-CB-CG	112.60	118.61	1
CA-C-N	116.90	125.91	1
C-N-CA	121.70	132.51	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	113.40	3
N-CA-CB	110.50	100.30	1
NE-CZ-NH2	119.20	124.60	1
N-CA-CB	110.50	100.31	1
CA-CB-OG1	109.60	118.59	1
C-CA-CB	110.10	121.49	1
CA-C-N	116.90	125.89	1
N-CA-CB	103.00	96.41	1
C-N-CA	121.70	132.48	1
O-C-N	123.00	113.42	1
CA-CB-CG	113.80	107.81	1
OE1-CD-NE2	122.60	116.61	2
OD1-CG-ND2	122.60	116.62	1
O-C-N	123.00	113.43	1
C-CA-CB	110.50	119.47	1
OE1-CD-NE2	122.60	116.62	1
OD1-CG-ND2	122.60	128.58	1
C-CA-CB	110.50	101.53	1
NE-CZ-NH2	119.20	113.82	1
O-C-N	123.00	113.44	1
CA-C-O	120.80	130.96	1
OD1-CG-ND2	122.60	116.63	1
N-CA-CB	110.40	119.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	102.16	1
N-CA-CB	110.50	120.65	2
C-N-CA	121.70	132.44	1
O-C-N	123.00	113.45	1
CA-CB-CG	112.60	106.64	1
N-CA-CB	110.50	100.36	1
NE-CZ-NH2	119.20	124.57	1
N-CA-CB	111.50	121.64	1
O-C-N	123.00	113.46	1
N-CD-CG	103.20	112.14	1
OE1-CD-NE2	122.60	128.56	1
NE-CZ-NH1	121.50	127.46	1
O-C-N	123.00	113.48	3
CA-C-N	116.90	125.83	1
OD1-CG-ND2	122.60	116.65	1
OE1-CD-NE2	122.60	116.65	1
CA-C-N	116.90	125.82	1
CD2-NE2-CE1	109.00	103.05	1
CD2-NE2-CE1	109.00	103.06	1
OE1-CD-NE2	122.60	128.54	1
C-N-CA	121.70	132.39	1
N-CA-CB	110.50	120.59	1
CA-CB-CG2	110.50	100.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NH1-CZ-NH2	119.30	111.59	1
C-N-CA	121.70	132.37	1
CA-CB-CG2	110.50	120.58	1
O-C-N	123.00	113.52	2
CB-CG-CD1	120.80	111.91	1
CG-CD2-NE2	107.20	113.12	1
NE-CZ-NH1	121.50	127.42	2
C-N-CA	121.70	132.36	1
O-C-N	123.00	113.53	1
OE1-CD-NE2	122.60	116.68	1
N-CA-CB	111.50	121.56	1
C-N-CA	121.70	132.34	2
O-C-N	123.00	113.54	1
NH1-CZ-NH2	119.30	111.62	1
NE-CZ-NH2	119.20	113.88	1
O-C-N	123.00	113.55	1
CA-CB-CG	112.60	118.50	1
C-N-CA	121.70	132.33	1
CA-C-N	116.90	125.76	1
N-CA-CB	110.50	120.54	1
N-CA-CB	111.50	121.54	1
N-CA-CB	110.50	120.53	1
N-CA-CB	103.00	109.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	113.89	1
C-CA-CB	110.50	101.65	1
N-CA-CB	103.00	96.51	1
OE1-CD-NE2	122.60	128.49	1
C-N-CA	121.70	132.31	1
CA-CB-CG	112.60	106.71	1
NE-CZ-NH2	119.20	113.90	1
O-C-N	123.00	113.57	2
C-CA-CB	110.10	121.29	1
C-CA-CB	111.40	122.59	1
OD1-CG-ND2	122.60	116.71	1
CB-CG-ND2	116.40	125.23	1
N-CA-CB	103.00	109.47	1
C-CA-CB	110.10	121.28	1
O-C-N	123.00	113.59	1
CA-CB-CG2	110.50	120.50	1
CA-C-N	116.90	125.72	1
C-CA-CB	111.40	122.56	1
O-C-N	123.00	113.60	1
O-C-N	123.00	113.61	1
CB-CG-CD	112.60	102.62	1
O-C-N	123.00	113.62	2
N-CA-C	111.00	127.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	121.24	1
N-CA-CB	110.50	120.47	1
CA-CB-CG1	110.40	120.37	1
C-N-CA	121.70	132.25	1
CA-C-N	116.90	125.69	1
NH1-CZ-NH2	119.30	111.68	1
C-N-CA	121.70	132.24	2
N-CA-CB	110.50	120.46	1
CB-CG-CD	111.30	124.77	1
CA-CB-CG	112.60	106.75	1
CA-CB-CG	113.80	107.95	2
CA-CB-CG	112.60	118.45	1
N-CA-CB	110.50	120.45	1
NE-CZ-NH2	119.20	113.93	1
NE-CZ-NH1	121.50	127.35	1
OD1-CG-ND2	122.60	116.75	1
N-CD-CG	103.20	111.96	1
C-N-CA	121.70	132.21	3
CA-CB-CG	114.10	125.78	1
O-C-N	123.00	113.66	1
CA-CB-CG	113.80	107.97	1
C-N-CA	121.70	132.20	1
CA-CB-CG	114.10	125.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	120.41	1
N-CA-CB	103.00	109.41	1
OE1-CD-NE2	122.60	116.77	1
NE-CZ-NH2	119.20	124.44	1
CA-CB-CG	112.60	118.42	1
CA-CB-OG1	109.60	118.33	1
CA-CB-CG	114.10	125.74	1
C-N-CA	121.70	132.18	2
CA-C-N	116.90	125.63	1
C-N-CA	121.70	132.17	2
OE1-CD-NE2	122.60	116.78	1
NE-CZ-NH2	119.20	113.96	1
CA-CB-CG	114.10	125.73	1
SG-C7-C8	109.23	126.68	1
CA-CB-CG1	110.40	120.28	1
C-N-CA	121.70	132.16	1
O-C-N	123.00	113.70	3
CA-C-N	116.90	125.62	1
CA-CB-CG	112.60	118.41	1
C-N-CA	121.70	132.15	1
CA-CB-OG1	109.60	118.31	1
OE1-CD-NE2	122.60	116.79	1
O-C-N	123.00	113.71	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	127.30	1
O-C-N	123.00	113.72	1
C-CA-CB	111.40	100.38	1
C-CA-CB	110.50	119.20	1
CA-CB-CG	113.80	119.60	1
CA-CB-CG2	110.40	100.54	1
CA-C-N	116.90	125.60	1
NE-CZ-NH2	119.20	113.99	1
NE-CZ-NH1	121.50	127.29	1
N-CA-CB	111.50	101.65	1
CA-CB-OG	111.10	122.68	1
CA-C-O	120.80	110.95	1
C-N-CA	121.70	132.12	2
CA-CB-CG	112.60	118.39	1
NE-CZ-NH2	119.20	124.41	1
C-CA-CB	110.50	101.82	1
N-CD-CG	103.20	111.87	1
CB-CG-CD	112.60	122.43	1
CA-C-N	116.90	125.57	1
CA-CB-CG	113.80	119.58	2
N-CA-CB	110.50	120.32	2
CA-CB-CG1	110.40	120.22	1
O-C-N	123.00	113.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
ND1-CE1-NE2	108.40	114.18	1
C-N-CA	121.70	132.09	2
N-CA-CB	111.50	121.32	1
CB-CG-CD	112.60	122.41	1
CD-NE-CZ	124.40	116.32	1
N-CA-CB	110.50	120.31	1
CA-CB-CG	113.80	108.03	1
O-C-N	123.00	113.78	1
OE1-CD-NE2	122.60	128.36	1
C-N-CA	121.70	132.07	1
CD1-CG-CD2	110.80	98.14	1
N-CA-CB	103.00	109.33	1
NH1-CZ-NH2	119.30	111.82	1
OD1-CG-ND2	122.60	116.85	1
NE-CZ-NH2	119.20	114.03	1
O-C-N	123.00	113.81	1
C-N-CA	121.70	132.04	1
NE-CZ-NH1	121.50	127.24	1
N-CA-CB	110.50	120.26	1
C-CA-CB	110.10	121.01	1
C-N-CA	121.70	132.03	1
N-CA-CB	110.50	120.25	1
N-CA-CB	110.50	100.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	120.15	1
NE-CZ-NH2	119.20	114.04	1
CA-CB-CG	112.60	118.33	1
C-N-CA	121.70	132.02	1
NE-CZ-NH1	121.50	127.23	1
CA-CB-CG	114.10	125.56	1
C-CA-CB	110.10	99.21	1
O-C-N	123.00	113.83	2
CA-C-N	116.90	125.50	1
N-CA-CB	110.50	120.24	2
N-CA-CB	110.50	100.76	1
OE1-CD-NE2	122.60	116.87	1
C-N-CA	121.70	132.01	1
CB-CG-ND2	116.40	107.81	1
CA-CB-CG	114.10	125.55	1
N-CA-CB	110.40	101.81	1
C-N-CA	121.70	132.00	1
O-C-N	123.00	113.84	1
CA-CB-CG	112.60	118.32	1
OD1-CG-ND2	122.60	116.88	1
N-CA-CB	110.50	100.77	1
CA-CB-CG	113.80	108.08	1
C-CA-CB	110.10	120.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	127.22	1
N-CA-CB	110.50	120.22	2
C-N-CA	121.70	131.99	1
CB-CG-ND2	116.40	107.83	1
CG-CD2-NE2	107.20	112.92	1
NE-CZ-NH2	119.20	114.06	1
N-CA-CB	111.50	121.21	1
CA-C-N	116.90	125.46	1
CB-CG-CD	112.60	102.89	1
OE1-CD-NE2	122.60	116.89	1
N-CA-CB	110.50	120.20	2
CB-CG-CD	111.30	124.42	1
C-CA-CB	110.10	120.94	1
CB-CG-CD	112.60	122.30	1
OE1-CD-NE2	122.60	128.30	1
C-N-CA	121.70	131.96	2
N-CA-CB	110.50	100.81	1
OD1-CG-ND2	122.60	128.30	1
O-C-N	123.00	113.88	1
C-CA-CB	110.10	120.93	1
CA-C-N	116.90	125.45	1
CA-CB-CG	113.90	103.64	1
OE1-CD-NE2	122.60	116.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.95	2
NE-CZ-NH1	121.50	127.19	2
N-CA-CB	103.00	96.74	1
CA-C-N	116.90	125.44	1
CG-CD-CE	111.30	124.39	1
O-C-N	123.00	113.90	2
CB-CG-CD1	120.80	112.27	1
CA-CB-CG2	110.40	100.73	1
C-N-CA	121.70	131.93	1
CB-CG-CD2	120.80	129.33	1
OE1-CD-NE2	122.60	116.92	2
O-C-N	123.00	113.91	1
C-CA-CB	110.50	101.98	1
NE-CZ-NH2	119.20	124.31	1
N-CA-CB	111.50	101.85	1
C-CA-CB	110.50	119.02	1
C-N-CA	121.70	131.92	1
O-C-N	123.00	113.92	1
CG-CD-NE2	116.40	124.91	1
CA-C-O	120.80	130.44	1
CA-CB-CG	112.60	118.27	1
SG-C7-C8	109.23	92.23	1
C-N-CA	121.70	131.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	125.40	1
CA-C-N	116.20	127.53	1
CA-C-O	120.80	130.43	1
CA-CB-CG	112.60	118.26	1
OE1-CD-NE2	122.60	116.94	1
OD1-CG-ND2	122.60	116.94	2
O-C-N	123.00	113.95	1
OE1-CD-NE2	122.60	116.95	2
CG1-CB-CG2	110.80	98.36	1
NE-CZ-NH1	121.50	127.15	1
OD1-CG-ND2	122.60	116.95	3
N-CA-CB	103.00	109.22	1
C-N-CA	121.70	131.87	1
N-CA-CB	110.50	120.10	1
CA-C-N	116.90	125.37	1
CB-CG-CD	111.30	124.28	1
N-CA-CB	103.00	109.21	2
C-N-CA	121.70	131.86	1
OE1-CD-NE2	122.60	128.24	1
CA-C-N	116.90	125.36	1
OD1-CG-ND2	122.60	116.96	1
N-CA-CB	110.50	120.09	2
C-CA-CB	111.40	122.12	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	99.39	1
N-CA-CB	111.50	121.09	1
OE1-CD-NE2	122.60	116.96	1
CA-CB-CG2	110.40	100.82	1
C-CA-CB	110.10	120.81	1
N-CA-CB	111.50	121.08	1
CA-CB-CG	113.90	103.76	1
O-C-N	123.00	132.02	1
NE-CZ-NH1	121.50	127.13	1
N-CD-CG	103.20	94.75	1
N-CA-CB	110.50	120.07	1
N-CA-CB	111.50	121.07	1
CG-CD2-NE2	107.20	112.83	1
C-N-CA	121.70	131.83	1
N-CA-CB	110.50	120.06	1
O-C-N	123.00	114.00	1
C-N-CA	121.70	131.82	1
CB-CG-CD	112.60	122.15	1
N-CA-CB	110.50	120.05	3
CA-CB-CG2	110.50	120.05	1
C-CA-CB	110.10	99.43	1
CG-CD-NE2	116.40	124.83	1
CA-C-N	116.90	125.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	111.30	124.22	1
CA-C-O	120.80	111.25	1
CD2-NE2-CE1	109.00	103.38	1
C-CA-CB	110.10	120.77	3
CA-CB-CG	112.60	118.21	1
N-CA-CB	111.50	121.04	1
CA-CB-OG	111.10	122.32	1
CA-C-N	116.90	125.31	1
CA-C-N	116.20	127.41	1
NE-CZ-NH1	121.50	127.11	1
O-C-N	123.00	114.03	1
OE1-CD-NE2	122.60	128.20	1
CD2-NE2-CE1	109.00	103.40	1
CG-CD-NE	112.00	99.68	1
C-CA-CB	111.60	122.80	1
C-N-CA	121.70	131.77	2
C-CA-CB	110.50	118.89	1
CA-CB-CG1	110.40	119.91	1
CB-CG-ND2	116.40	124.79	1
CA-C-O	120.80	111.29	1
NE-CZ-NH2	119.20	114.17	1
N-CA-CB	110.50	120.01	1
NE-CZ-NH1	121.50	127.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.05	1
O-C-N	123.00	114.06	3
C-N-CA	121.70	131.76	1
CA-C-N	116.90	125.28	1
CA-CB-CG2	110.50	120.00	1
N-CA-CB	110.50	119.99	1
NE-CZ-NH2	119.20	124.23	1
C-N-CA	121.70	111.65	1
CA-C-N	116.90	125.27	1
O-C-N	123.00	114.07	2
C-CA-CB	110.50	118.87	1
C-N-CA	121.70	131.74	2
N-CA-C	112.10	126.05	1
CA-CB-CG1	110.40	119.88	1
OD1-CG-ND2	122.60	128.18	1
N-CA-CB	110.50	119.98	1
C-N-CA	121.70	131.73	1
CB-CG-ND2	116.40	124.76	1
C-N-CA	121.70	111.67	1
O-C-N	123.00	114.08	1
CA-CB-CG	112.60	118.17	1
O-C-N	123.00	114.09	4
CD1-CG-CD2	110.80	98.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	127.07	1
CA-CB-CG1	110.40	119.87	1
N-CA-CB	110.50	119.97	1
C-CA-CB	110.50	102.15	1
CA-CB-CG	113.80	108.23	1
CA-CB-CG1	110.40	119.86	1
C-CA-CB	110.10	120.68	1
CA-C-O	120.80	130.26	1
N-CA-CB	110.50	101.04	1
CB-CG-CD2	120.70	111.24	1
N-CA-CB	110.50	119.96	1
C-CA-CB	110.10	120.67	1
NE-CZ-NH2	119.20	114.20	1
CD2-NE2-CE1	109.00	103.44	1
CA-CB-CG	113.80	108.24	1
OE1-CD-NE2	122.60	128.16	1
C-N-CA	121.70	131.70	1
C-CA-CB	110.50	102.17	1
CB-CG-CD	112.60	122.04	1
CA-C-O	120.80	130.24	1
CA-C-N	116.90	125.23	1
CA-CB-CG	113.80	119.35	1
C-N-CA	121.70	131.69	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.13	2
CA-CB-CG	113.80	119.34	1
OE1-CD-NE2	122.60	117.06	1
CA-C-N	116.90	125.22	1
C-N-CA	121.70	131.67	3
CA-CB-CG2	110.40	119.82	1
CA-CB-CG	112.60	118.14	1
CB-CG-CD1	120.70	111.29	1
OE1-CD-NE2	122.60	128.14	1
O-C-N	123.00	114.14	1
N-CA-CB	110.50	119.91	1
NE-CZ-NH1	121.50	127.04	1
C-N-CA	121.70	131.66	1
N-CA-CB	110.40	102.10	1
CB-CG-CD1	120.80	129.10	1
CB-CG-CD	112.60	122.01	1
OE1-CD-NE2	122.60	117.07	1
CA-C-N	116.20	127.26	1
N-CA-CB	110.50	119.90	2
CA-C-N	116.90	125.20	1
O-C-N	123.00	114.15	1
C-N-CA	121.70	131.65	1
O-C-N	123.00	114.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	119.80	1
CA-CB-OG1	109.60	117.89	1
CA-CB-CG	112.60	118.12	2
NE-CZ-NH2	119.20	124.17	1
CB-SG-C7	106.10	122.65	1
C-N-CA	121.70	131.63	1
OE1-CD-NE2	122.60	117.08	2
C-CA-CB	110.50	102.23	1
CA-C-O	120.80	111.43	2
N-CA-CB	110.50	119.87	1
C-N-CA	121.70	131.62	1
OE1-CD-NE2	122.60	117.09	1
O-C-N	123.00	114.18	1
NE-CZ-NH1	121.50	115.99	1
N-CA-CB	110.50	119.86	1
C-CA-CB	110.10	120.57	1
NE-CZ-NH2	119.20	114.24	1
O-C-N	123.00	114.19	1
CA-CB-CG	113.80	119.31	1
NE-CZ-NH1	121.50	127.00	1
ND1-CG-CD2	106.10	100.60	1
O-C-N	123.00	114.20	1
C-N-CA	121.70	131.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	107.10	2
N-CA-CB	103.00	96.95	1
CB-CG-CD	112.60	121.95	1
CA-CB-CG	114.10	125.10	1
CA-CB-CG	112.60	118.10	1
OD1-CG-ND2	122.60	117.10	1
CA-CB-CG	113.80	108.30	1
CA-CB-CG	112.60	118.09	2
C-N-CA	121.70	131.59	1
NE-CZ-NH2	119.20	114.26	2
N-CD-CG	103.20	111.44	1
C-CA-CB	110.10	120.53	1
CA-CB-CG2	110.50	101.17	1
CB-CG-CD2	120.80	129.03	1
CA-C-O	120.80	111.47	1
O-C-N	123.00	114.22	2
C-N-CA	121.70	131.58	1
CA-CB-CG	113.80	108.31	1
C-CA-CB	110.10	120.52	1
C-N-CA	121.70	131.57	2
CG-CD-NE2	116.40	108.18	1
CA-CB-CG1	110.40	119.71	1
C-N-CA	121.70	131.56	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	119.81	1
OE1-CD-NE2	122.60	117.12	1
O-C-N	123.00	114.24	2
CA-CB-CG	113.80	108.33	1
CG-CD2-NE2	107.20	112.67	1
CA-C-O	120.80	130.10	1
OE1-CD-NE2	122.60	117.13	1
N-CA-CB	110.50	119.80	1
C-N-CA	121.70	131.54	2
CA-CB-CG	112.60	118.07	1
NH1-CZ-NH2	119.30	112.19	1
O-C-N	123.00	114.26	1
CA-C-O	120.80	130.09	1
N-CA-CB	110.50	119.79	1
CA-C-N	116.90	125.09	3
CB-CG-OD1	120.80	131.72	1
CA-CB-CG	112.60	118.06	1
N-CA-CB	110.50	119.78	3
NE-CZ-NH2	119.20	114.29	1
C-N-CA	121.70	131.52	2
O-C-N	123.00	114.27	2
CA-C-N	116.20	127.11	1
CA-CB-CG	114.10	125.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.28	1
C-CA-CB	110.10	99.74	1
OE1-CD-NE2	122.60	117.15	1
C-CA-CB	111.40	121.75	1
CA-CB-CG2	110.40	119.66	1
CA-C-N	116.90	125.07	1
C-CA-CB	110.10	120.45	1
CD-NE-CZ	124.40	132.02	1
OE1-CD-NE2	122.60	117.16	2
N-CA-CB	110.50	119.75	1
OD1-CG-ND2	122.60	117.16	1
O-C-N	123.00	114.30	1
C-CA-CB	110.10	99.77	1
CA-CB-CG	114.10	124.97	1
CG-CD-NE	112.00	100.04	1
O-C-N	123.00	114.31	2
CA-CB-CG2	110.40	101.16	1
CA-C-N	116.90	125.05	1
CB-CG-ND2	116.40	124.55	1
N-CA-CB	110.50	119.73	1
CB-CG-CD	112.60	103.37	1
CA-CB-CG	112.60	107.17	1
C-CA-CB	110.10	120.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	119.63	1
NE-CZ-NH2	119.20	124.09	1
CA-C-O	120.80	111.57	1
O-C-N	123.00	114.32	2
CD-NE-CZ	124.40	116.81	1
CB-CG-CD1	120.80	112.66	1
CA-CB-CG	112.60	107.18	1
C-N-CA	121.70	131.46	4
O-C-N	123.00	114.33	1
C-CA-CB	110.10	99.80	1
C-N-CA	121.70	131.45	1
N-CA-CB	111.50	120.71	1
OE1-CD-NE2	122.60	128.02	1
CA-CB-CG	112.60	118.01	2
OE1-CD-NE2	122.60	128.01	1
CA-C-O	120.80	130.00	1
C-CA-CB	110.10	120.38	1
CA-CB-CG1	110.40	119.60	1
CA-CB-CG2	110.40	101.20	1
CB-CG-ND2	116.40	108.29	1
N-CA-CB	110.50	119.70	1
O-C-N	123.00	114.35	1
OE1-CD-NE2	122.60	117.19	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	102.39	1
OD1-CG-ND2	122.60	117.19	1
CA-CB-CG	112.60	118.00	1
OD1-CG-ND2	122.60	117.20	1
OE1-CD-NE2	122.60	117.20	1
CA-CB-CG	113.80	108.40	1
CA-C-O	120.80	129.98	1
CB-CG-OD1	118.40	130.81	1
NH1-CZ-NH2	119.30	112.28	1
C-CA-CB	110.10	120.35	1
N-CA-CB	110.50	119.67	1
O-C-N	123.00	114.37	3
CA-C-O	120.80	111.63	1
CA-CB-CG	112.60	117.99	1
CD2-NE2-CE1	109.00	103.61	1
O-C-N	123.00	114.38	3
C-N-CA	121.70	131.40	2
OD1-CG-ND2	122.60	117.21	1
CB-CG-CD2	120.80	112.72	1
NH1-CZ-NH2	119.30	112.30	1
CA-CB-CG	114.10	124.87	1
N-CA-C	111.00	95.92	1
CA-C-N	116.90	124.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	119.66	1
C-N-CA	121.70	131.39	2
O-C-N	123.00	114.39	1
CA-C-N	116.90	124.97	1
OD1-CG-ND2	122.60	117.22	1
CA-CB-CG2	110.40	101.25	1
N-CA-CB	110.50	119.65	1
CB-CG-CD	112.60	103.45	1
OE1-CD-NE2	122.60	117.22	1
CB-CG-ND1	122.70	114.63	1
NE-CZ-NH1	121.50	126.88	1
CA-CB-OG	111.10	121.86	1
N-CA-CB	110.50	101.36	1
ND1-CE1-NE2	108.40	113.78	1
C-N-CA	121.70	131.38	1
N-CA-CB	110.50	119.64	1
CA-CB-CG	112.60	117.97	2
C-CA-CB	110.10	120.31	1
C-N-CA	121.70	131.37	3
N-CA-CB	110.50	119.63	1
C-CA-CB	110.50	102.45	1
CG-CD-OE1	120.80	131.53	1
C-CA-CB	110.50	118.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.95	1
C-N-CA	121.70	131.36	1
N-CA-CB	111.50	120.62	1
NE-CZ-NH1	121.50	126.86	1
CA-CB-CG	112.60	107.24	1
N-CA-CB	110.50	119.62	2
O-C-N	123.00	114.42	1
C-N-CA	121.70	131.35	1
CA-CB-CG	114.10	124.82	1
CA-C-N	116.90	124.94	1
C-N-CA	121.70	131.34	1
C-CA-CB	110.10	120.28	1
OE1-CD-NE2	122.60	117.24	1
CA-CB-CG	113.80	119.16	1
CB-CG-CD2	120.70	129.80	1
O-C-N	123.00	131.57	1
CA-CB-CG1	110.40	119.50	1
CG-CD-OE1	120.80	110.10	1
N-CA-CB	110.50	119.59	1
CA-C-N	116.90	124.92	2
CB-CG-CD1	120.80	112.78	1
C-N-CA	121.70	131.32	1
N-CA-CB	110.50	101.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	118.51	1
O-C-N	123.00	114.46	2
NE-CZ-NH1	121.50	116.16	1
CD2-NE2-CE1	109.00	103.66	1
CG-CD-NE2	116.40	124.41	1
OE1-CD-NE2	122.60	117.26	1
CB-CG-CD2	131.20	124.26	1
C-N-CA	121.70	131.30	1
CA-CB-OG1	109.60	117.60	1
C-CA-CB	110.10	120.23	1
C-CA-CB	111.40	121.53	1
CB-CG-CD2	120.70	129.76	1
CA-C-N	116.90	124.89	2
CA-CB-CG	114.10	124.76	1
CA-CB-CG	113.80	119.13	1
CB-CG-OD1	120.80	110.15	1
NE-CZ-NH2	119.20	123.99	2
C-N-CA	121.70	131.29	1
CA-CB-CG2	110.40	101.35	1
CB-CG-ND2	116.40	108.42	1
C-N-CA	121.70	131.28	2
O-C-N	123.00	114.48	1
N-CA-CB	110.50	119.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	119.12	1
CB-CG-OD1	120.80	131.44	1
OD1-CG-ND2	122.60	117.28	2
O-C-N	123.00	114.49	1
CA-CB-CG	112.60	107.28	1
CA-CB-CG	113.80	108.48	1
C-N-CA	121.70	131.27	1
C-CA-CB	110.50	118.47	1
CA-CB-CG1	110.40	119.44	1
CG-CD-NE2	116.40	124.37	1
CA-CB-CG2	110.40	119.43	1
CB-CG-ND2	116.40	124.37	1
CB-CG-CD1	120.80	112.83	1
CA-CB-CG	114.10	124.72	1
C-N-CA	121.70	131.26	1
C-N-CA	121.70	112.14	1
N-CA-CB	110.50	119.53	1
CA-C-N	116.90	124.86	3
CA-CB-CG1	110.40	119.43	1
CB-CG-CD1	120.70	129.72	1
CA-C-O	120.80	129.82	1
C-N-CA	121.70	131.25	1
OD1-CG-ND2	122.60	117.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	120.52	1
CG-CD2-NE2	107.20	112.51	1
CG-CD-NE2	116.40	108.45	1
C-CA-CB	111.40	121.47	1
CA-CB-CG	112.60	117.90	2
O-C-N	123.00	114.52	1
CA-CB-CG	113.80	108.50	1
CA-CB-CG	113.90	104.37	1
OE1-CD-NE2	122.60	117.30	1
C-N-CA	121.70	131.23	2
O-C-N	123.00	114.53	2
CB-CG-CD	111.30	123.48	1
CA-C-O	120.80	111.80	1
N-CA-CB	111.50	120.50	1
N-CA-CB	110.50	119.49	2
N-CA-CB	103.00	97.18	1
O-C-N	123.00	114.54	2
CA-C-O	120.80	129.79	1
CA-CB-CG	112.60	117.89	1
CA-C-N	116.90	124.83	1
CA-CB-CG	113.80	119.09	1
OE1-CD-NE2	122.60	117.32	1
C-CA-CB	110.50	118.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.40	119.38	1
CA-C-N	116.20	126.77	1
N-CA-CB	110.50	119.48	2
CA-CB-CG	113.80	108.52	1
CA-CB-CG	112.60	117.88	1
CA-C-O	120.80	111.83	1
C-CA-CB	110.10	120.12	2
CB-CG-CD	112.60	121.57	1
CA-CB-CG	112.60	117.87	1
C-CA-CB	110.50	118.41	1
C-CA-CB	110.10	100.08	1
N-CA-CB	110.50	119.46	2
O-C-N	123.00	114.56	1
NE-CZ-NH2	119.20	123.95	1
CA-CB-CG	114.10	124.64	1
OD1-CG-ND2	122.60	117.33	2
CA-C-N	116.90	124.80	3
C-CA-CB	110.10	100.09	1
CB-CG-CD	112.60	103.65	2
NH1-CZ-NH2	119.30	112.46	1
CA-CB-CG	114.10	124.63	1
O-C-N	123.00	114.58	3
C-N-CA	121.70	131.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	120.44	1
CA-CB-OG	111.10	121.61	1
CD-NE-CZ	124.40	117.04	1
C-N-CA	121.70	131.16	3
O-C-N	123.00	114.60	2
C-N-CA	121.70	131.15	5
N-CA-CB	110.50	119.43	2
N-CA-CB	103.00	108.77	1
N-CA-CB	110.50	119.42	2
CB-CG-CD1	120.70	129.62	1
CA-CB-CG	112.60	107.36	1
CB-CG-ND2	116.40	124.27	1
C-N-CA	121.70	131.14	2
O-C-N	123.00	114.61	1
N-CA-CB	110.50	119.41	2
C-CA-CB	110.50	102.64	1
NH1-CZ-NH2	119.30	112.49	1
O-C-N	123.00	114.62	1
OD1-CG-ND2	122.60	117.36	1
N-CA-CB	103.00	108.76	1
C-N-CA	121.70	131.12	1
N-CA-CB	110.50	101.60	1
CA-CB-CG1	110.40	119.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	103.63	1
CA-CB-CG	113.80	108.57	2
O-C-N	123.00	114.63	1
NE-CZ-NH2	119.20	114.49	1
N-CA-CB	110.50	101.61	1
CA-CB-OG	111.10	121.56	1
N-CA-CB	110.50	119.39	1
CA-CB-CG2	110.50	101.61	1
C-N-CA	121.70	131.11	1
C-CA-CB	110.50	102.66	1
CB-CG-CD1	120.80	112.96	1
OD1-CG-ND2	122.60	117.37	2
OE1-CD-NE2	122.60	117.38	1
CG-CD-NE2	116.40	108.56	1
CA-CB-CG	112.60	117.82	2
CD2-NE2-CE1	109.00	103.78	1
N-CA-CB	110.50	119.37	1
C-CA-CB	110.10	120.02	1
CA-CB-CG2	110.40	119.27	1
CA-CB-CG	114.10	124.54	1
CA-C-N	116.20	126.64	1
O-C-N	123.00	114.65	3
CA-C-O	120.80	111.93	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	123.89	1
C-N-CA	121.70	131.09	3
CA-C-N	116.90	124.72	1
O-C-N	123.00	114.66	3
C-N-CA	121.70	131.08	1
CA-CB-CG	114.10	103.68	1
N-CD-CG	103.20	111.02	1
N-CA-CB	111.50	120.35	1
CA-CB-OG1	109.60	117.41	1
C-CA-CB	110.10	120.00	1
OE1-CD-NE2	122.60	117.39	1
O-C-N	123.00	114.67	1
C-CA-CB	110.10	100.21	1
N-CA-CB	110.50	101.65	1
CA-CB-CG2	110.50	119.35	1
N-CA-CB	110.50	119.35	1
CA-C-O	120.80	129.64	1
CA-C-N	116.20	126.60	1
N-CA-C	111.00	96.44	1
OD1-CG-ND2	122.60	117.40	1
C-CA-CB	110.10	119.98	1
N-CA-CB	110.40	102.60	2
CB-CG-CD2	120.80	128.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.70	2
CA-CB-CG2	110.50	119.34	1
CA-CB-CG	112.60	117.80	1
N-CA-CB	111.50	120.33	2
C-CA-CB	111.60	101.21	1
O-C-N	123.00	114.69	2
CB-CG-CD	112.60	103.77	1
C-N-CA	121.70	131.05	4
CA-C-N	116.90	124.69	1
CG-CD-NE2	116.40	124.19	1
CG-SD-CE	100.90	89.47	1
CA-CB-CG1	110.40	119.23	1
OE1-CD-NE2	122.60	117.41	1
N-CA-CB	111.50	120.32	2
C-CA-CB	110.10	119.96	1
O-C-N	123.00	114.70	4
CA-C-N	116.20	126.58	1
CG1-CB-CG2	110.80	99.38	1
N-CA-CB	110.50	119.32	2
C-N-CA	121.70	131.04	1
CB-CG-CD	112.60	103.78	1
NE-CZ-NH2	119.20	114.53	2
CG-CD-CE	111.30	123.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	118.99	1
C-CA-CB	110.10	100.25	1
O-C-N	123.00	114.71	2
C-N-CA	121.70	131.03	2
CB-CG-ND2	116.40	108.62	1
CA-CB-CG	113.90	104.57	1
CB-CG-CD	112.60	103.79	1
CA-CB-OG1	109.60	117.37	1
NH1-CZ-NH2	119.30	112.56	1
OE1-CD-NE2	122.60	117.42	1
CB-CG-CD	112.60	121.41	1
C-N-CA	121.70	131.02	1
CA-CB-CG	114.10	124.46	1
CG1-CB-CG2	110.80	99.41	1
CB-CG-CD1	120.70	129.50	1
CA-CB-CG	112.60	117.78	1
CA-CB-CG	113.80	118.97	1
C-N-CA	121.70	131.01	3
OE1-CD-NE2	122.60	117.43	1
N-CA-CB	110.50	119.29	2
O-C-N	123.00	114.72	2
NE-CZ-NH1	121.50	126.67	1
CB-CG-CD2	120.80	128.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	118.16	1
O-C-N	123.00	114.73	2
CA-CB-CG1	110.40	119.19	1
OE1-CD-NE2	122.60	127.77	1
N-CA-CB	103.00	108.69	1
CA-CB-CG	113.80	108.63	1
CD-NE-CZ	124.40	131.64	1
C-N-CA	121.70	131.00	2
N-CA-CB	110.50	119.28	1
N-CA-CB	110.50	101.72	1
C-CA-CB	110.10	119.92	1
CA-C-O	120.80	129.58	1
CA-C-N	116.90	124.65	1
O-C-N	123.00	114.74	1
OD1-CG-ND2	122.60	117.44	2
CA-C-O	120.80	112.02	1
CA-CB-OG1	109.60	117.35	1
CG-CD-CE	111.30	123.18	1
N-CA-CB	111.50	120.28	2
CA-C-N	116.90	124.64	2
C-N-CA	121.70	130.99	3
NE-CZ-NH2	119.20	123.84	1
CA-CB-CG1	110.40	119.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.75	1
N-CA-CB	110.50	119.27	1
CA-CB-CG	114.10	124.42	1
C-N-CA	121.70	130.98	2
CA-CB-CG	112.60	117.75	1
C-CA-CB	110.10	119.89	1
OE1-CD-NE2	122.60	117.45	1
C-CA-CB	111.40	121.19	1
N-CA-CB	110.50	119.26	2
C-N-CA	121.70	130.97	3
CA-CB-CG2	110.50	119.26	1
O-C-N	123.00	114.76	2
C-CA-CB	111.40	101.62	1
NE-CZ-NH2	119.20	114.57	1
CA-CB-CG1	110.40	119.15	3
NE-CZ-NH1	121.50	126.65	1
N-CA-CB	111.50	120.25	1
N-CA-CB	110.50	101.75	1
CA-CB-CG	113.80	108.65	1
CA-CB-CG	114.10	124.39	1
CA-C-O	120.80	112.05	1
CD-NE-CZ	124.40	117.20	1
CA-CB-CG	113.90	123.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.61	1
CA-CB-CG	113.90	104.65	1
CB-CG-CD	112.60	121.34	1
O-C-N	123.00	114.77	1
C-CA-CB	110.10	119.87	1
OD1-CG-ND2	122.60	117.46	1
N-CA-CB	110.40	118.11	1
CA-CB-OG1	109.60	117.31	1
O-C-N	123.00	114.78	4
N-CA-CB	110.50	119.24	1
C-N-CA	121.70	130.95	1
CA-CB-CG	112.60	107.46	1
CA-CB-CG	113.80	108.66	1
N-CA-CB	110.50	119.23	2
CA-CB-CG1	110.40	119.13	1
CB-CG-CD2	120.70	111.97	1
CB-CG-OD1	120.80	110.53	1
OD1-CG-ND2	122.60	117.47	1
CA-CB-CG	112.60	117.73	2
OE1-CD-NE2	122.60	117.47	2
C-CA-CB	110.50	102.80	1
CG-CD-NE	112.00	100.71	1
N-CA-CB	110.50	119.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	126.46	1
CB-CG-CD	112.60	121.32	1
C-N-CA	121.70	130.93	3
CG-CD2-NE2	107.20	112.33	1
O-C-N	123.00	114.79	1
C-CA-CB	110.10	100.35	1
C-CA-CB	110.10	119.84	1
O-C-N	123.00	114.80	2
C-CA-CB	110.50	118.19	1
CA-CB-CG1	110.40	119.12	1
N-CA-CB	110.50	119.21	1
CA-C-O	120.80	112.09	1
CB-CG-ND2	116.40	124.09	1
N-CA-CB	103.00	108.64	1
CA-CB-CG	112.60	107.48	1
NE-CZ-NH1	121.50	126.62	1
N-CA-CB	111.50	120.21	2
C-N-CA	121.70	130.92	1
ND1-CE1-NE2	108.40	113.52	1
C-CA-CB	110.10	119.83	1
C-CA-CB	111.40	121.13	1
CB-CG-ND2	116.40	124.08	1
N-CA-CB	110.50	101.80	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	114.81	1
C-N-CA	121.70	130.91	1
CA-C-N	116.90	124.58	1
N-CA-CB	110.40	102.72	1
CB-CG-CD1	120.80	113.12	1
CA-C-O	120.80	129.50	1
CA-CB-OG	111.10	121.33	1
CG-CD2-NE2	107.20	112.32	1
CA-C-N	116.90	124.57	1
O-C-N	123.00	114.82	3
N-CA-CB	110.50	119.19	2
CA-CB-CG	113.80	108.69	1
C-N-CA	121.70	130.90	1
N-CA-CB	103.00	108.62	1
C-CA-CB	111.40	121.11	1
NE-CZ-NH2	119.20	123.80	1
C-CA-CB	110.50	102.84	1
CA-CB-CG2	110.40	101.72	1
CA-C-O	120.80	129.48	1
C-N-CA	121.70	130.89	1
CB-CG-CD	112.60	103.92	1
O-C-N	123.00	114.83	1
C-CA-CB	110.10	119.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	117.50	1
CA-CB-CG2	110.50	119.18	1
CA-C-N	116.20	126.40	1
CA-CB-CG2	110.40	119.07	1
N-CA-CB	110.50	119.17	1
O-C-N	123.00	114.84	3
CB-CG-CD	112.60	103.93	1
C-N-CA	121.70	130.88	1
NE-CZ-NH2	119.20	114.61	1
CA-CB-CG	113.90	104.72	1
CA-CB-CG	112.60	107.50	1
CG-CD1-CE1	121.20	128.85	1
CA-CB-CG2	110.50	119.16	1
C-CA-CB	110.10	119.78	1
C-CA-CB	110.50	118.15	1
CA-C-O	120.80	129.46	1
N-CA-CB	111.50	120.16	1
O-C-N	123.00	114.85	4
CA-CB-CG1	110.40	119.06	1
NE-CZ-NH1	121.50	126.60	1
CB-CG-CD2	120.70	129.36	1
CA-C-N	116.20	126.39	1
C-N-CA	121.70	130.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	117.51	2
N-CA-CB	110.50	119.16	1
O-C-N	123.00	114.86	4
CA-CB-CG	113.80	118.89	1
NH1-CZ-NH2	119.30	112.68	1
C-N-CA	121.70	130.86	3
NH1-CZ-NH2	119.30	112.69	1
CA-CB-CG2	110.50	119.15	1
N-CD-CG	103.20	110.83	1
C-N-CA	121.70	130.85	4
CD-NE-CZ	124.40	117.28	1
N-CA-CB	111.50	120.14	1
N-CA-CB	103.00	97.41	1
N-CA-CB	110.50	119.14	1
O-C-N	123.00	114.87	1
CB-CG-CD	112.60	121.24	1
OE1-CD-NE2	122.60	117.52	1
N-CA-CB	110.50	101.86	1
OE1-CD-NE2	122.60	127.68	1
N-CA-CB	110.50	119.13	4
OD1-CG-ND2	122.60	117.52	1
C-N-CA	121.70	130.84	3
N-CA-CB	110.40	118.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	100.45	1
CA-CB-CG	113.80	108.73	1
N-CA-CB	110.50	119.12	1
CD1-CG-CD2	110.80	99.64	1
CA-CB-CG	113.90	104.77	1
C-N-CA	121.70	130.83	1
CA-CB-CG1	110.40	119.02	1
C-CA-CB	110.10	119.74	1
CA-CB-CG	113.90	123.03	1
O-C-N	123.00	114.89	1
N-CD-CG	103.20	110.80	1
CB-CG-CD1	120.80	113.20	1
CA-C-N	116.20	126.33	1
N-CA-C	112.10	124.76	1
NH1-CZ-NH2	119.30	112.71	1
N-CA-CB	110.50	101.89	1
CA-CB-CG	113.80	118.86	1
NE-CZ-NH1	121.50	126.56	1
C-N-CA	121.70	130.81	4
O-C-N	123.00	114.90	1
C-CA-CB	111.40	121.02	1
CG-CD-CE	111.30	122.94	1
CA-C-N	116.90	124.49	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.50	102.91	1
O-C-N	123.00	114.91	2
CA-CB-CG	112.60	107.55	1
C-N-CA	121.70	130.80	1
C-N-CA	121.70	130.79	2
N-CA-CB	110.50	119.09	1
NE-CZ-NH1	121.50	126.55	1
CA-CB-CG2	110.50	101.92	1
OD1-CG-ND2	122.60	127.65	1
CA-CB-CG1	110.40	118.98	1
N-CA-CB	110.40	102.83	1
N-CA-CB	111.50	120.08	1
CG1-CB-CG2	110.80	99.70	1
N-CA-CB	110.40	117.97	1
C-CA-CB	110.50	102.93	1
C-N-CA	121.70	130.78	1
CA-CB-CG	114.10	104.01	1
NH1-CZ-NH2	119.30	112.74	1
C-CA-CB	111.40	101.82	1
OD1-CG-ND2	122.60	117.56	1
ND1-CG-CD2	106.10	101.06	1
N-CA-C	111.00	96.89	1
N-CA-CB	110.50	119.07	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.40	101.83	1
N-CA-CB	110.50	101.94	2
CA-CB-CG1	110.40	118.96	1
O-C-N	123.00	114.94	2
N-CA-CB	110.50	119.06	1
N-CD-CG	103.20	110.75	1
CG-CD-NE2	116.40	108.85	1
C-N-CA	121.70	130.76	1
OE1-CD-NE2	122.60	117.57	1
C-CA-CB	110.10	119.66	1
CA-CB-OG1	109.60	117.15	1
N-CA-CB	110.50	119.05	1
CA-CB-CG	112.60	117.63	2
O-C-N	123.00	114.95	1
CB-CG-CD	111.30	122.87	1
C-N-CA	121.70	130.75	1
CG-CD-NE2	116.40	123.94	1
C-CA-CB	110.10	119.65	1
CA-C-N	116.90	124.44	1
O-C-N	123.00	131.04	1
O-C-N	123.00	114.96	2
N-CA-CB	110.50	119.04	1
CA-CB-CG	113.80	108.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	114.68	1
OE1-CD-NE2	122.60	117.58	3
C-N-CA	121.70	130.74	1
CB-CG-CD	112.60	121.14	1
OD1-CG-ND2	122.60	117.58	1
CA-CB-CG2	110.50	101.97	1
N-CA-CB	111.50	120.03	2
C-N-CA	121.70	112.67	1
CA-C-N	116.90	124.43	1
CA-CB-CG1	110.40	118.93	1
C-N-CA	121.70	130.73	2
N-CA-CB	110.50	119.03	2
CA-CB-CG	114.10	124.13	2
C-CA-CB	110.10	119.63	2
N-CA-CB	110.50	119.02	2
CA-C-N	116.90	124.42	1
C-N-CA	121.70	130.72	1
C-CA-CB	110.10	119.62	1
CG-CD-NE2	116.40	123.92	1
ND1-CE1-NE2	108.40	113.41	1
CB-CG-CD1	120.70	129.22	1
CA-CB-CG	114.10	104.08	1
O-C-N	123.00	114.98	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH2	119.20	114.69	1
CA-CB-OG1	109.60	117.11	1
N-CA-CB	110.50	101.99	1
CA-CB-CG1	110.40	118.91	2
CD1-CG-CD2	110.80	99.78	1
O-C-N	123.00	114.99	1
CA-C-O	120.80	129.31	1
C-N-CA	121.70	130.71	1
CA-CB-CG	112.60	117.60	1
CA-N-CD	112.00	105.00	1
O-C-N	123.00	115.00	3
C-N-CA	121.70	130.70	2
CA-CB-CG1	110.40	101.90	1
C-CA-CB	111.40	120.90	1
CA-CB-CG1	110.40	118.90	1
CA-CB-OG1	109.60	117.10	1
CG-CD-NE	112.00	101.00	1
CD1-CG-CD2	110.80	99.80	1
NE-CZ-NH1	121.50	126.50	1
N-CA-CB	111.50	120.00	1
CB-SG-C7	106.10	121.09	1
N-CA-CB	110.50	102.00	1
C-CA-CB	110.10	119.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OD1-CG-ND2	122.60	117.60	1
C-N-CA	121.70	130.69	4
N-CA-CB	110.40	102.91	1
O-C-N	123.00	115.01	2
N-CA-C	111.00	124.98	1
C-CA-CB	110.10	119.58	1
CA-C-N	116.20	126.18	1
CA-C-O	120.80	129.29	1
N-CA-CB	110.50	118.98	3
NE-CZ-NH2	119.20	114.71	1
N-CA-CB	110.40	117.88	1
N-CA-C	111.00	124.97	1
CA-CB-CG	113.80	118.79	1
O-C-N	123.00	115.02	1
C-N-CA	121.70	130.68	1
N-CA-CB	111.50	119.98	1
CA-CB-CG	112.60	107.62	1
O-C-N	123.00	115.03	3
CB-CG-CD	111.30	122.76	1
CB-CG-CD	112.60	121.07	2
C-CA-CB	111.40	120.86	1
C-CA-CB	110.50	103.03	1
CA-CB-CG	113.80	108.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.37	1
CA-CB-CG	113.80	118.78	1
CD2-NE2-CE1	109.00	104.02	1
N-CA-CB	111.50	119.96	1
N-CA-CB	103.00	97.53	1
C-N-CA	121.70	130.66	1
CA-CB-OG	111.10	121.05	1
O-C-N	123.00	115.04	1
N-CA-CB	110.50	118.96	1
CA-CB-CG	113.80	108.83	1
CA-CB-CG1	110.40	101.95	1
CA-C-N	116.90	124.36	1
CA-CB-CG	113.80	118.77	1
N-CA-CB	110.50	118.95	1
C-N-CA	121.70	130.65	2
CA-CB-CG	112.60	117.57	1
O-C-N	123.00	115.05	3
CA-CB-CG2	110.40	118.85	1
C-N-CA	121.70	130.64	3
CB-CG-ND2	116.40	123.85	1
NH1-CZ-NH2	119.30	112.85	2
C-N-CA	121.70	130.63	4
N-CA-CB	103.00	108.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD1	120.80	113.36	1
CA-CB-CG	114.10	104.18	1
CA-CB-CG2	110.50	102.07	1
O-C-N	123.00	115.06	1
NE-CZ-NH1	121.50	126.46	1
CG-CD-CE	111.30	122.71	1
N-CA-CB	110.50	118.93	2
CA-CB-OG1	109.60	117.04	1
C-CA-CB	110.10	100.68	1
CA-CB-CG	112.60	117.56	1
O-C-N	123.00	115.07	2
C-N-CA	121.70	130.62	1
OE1-CD-NE2	122.60	117.64	1
CD2-NE2-CE1	109.00	104.04	1
CB-CG-ND2	116.40	123.83	1
C-CA-CB	110.10	100.69	1
N-CA-CB	111.50	103.08	1
NE-CZ-NH2	119.20	123.66	1
CB-CG-CD	111.30	122.69	1
CB-CG-CD1	120.70	129.12	1
C-N-CA	121.70	130.61	3
CA-C-N	116.20	126.10	1
CB-CG-CD1	120.70	129.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	119.50	3
CA-CB-CG	112.60	117.55	1
N-CA-CB	110.50	118.91	1
CG-CD-CE	111.30	122.68	1
N-CA-CB	111.50	119.91	1
C-N-CA	121.70	130.60	2
CD-NE-CZ	124.40	131.32	1
OD1-CG-ND2	122.60	127.55	1
CA-CB-CG	113.90	105.00	1
CA-CB-CG	112.60	107.66	1
OD1-CG-ND2	122.60	117.66	1
C-CA-CB	110.10	119.49	1
N-CA-CB	110.50	118.90	1
C-N-CA	121.70	130.59	4
CA-C-N	116.20	126.08	1
NE-CZ-NH1	121.50	126.44	1
C-CA-CB	110.50	103.09	1
OE1-CD-NE2	122.60	117.66	1
CA-C-O	120.80	112.40	1
CA-CB-CG	113.80	108.86	1
CA-C-O	120.80	112.41	1
O-C-N	123.00	115.10	3
NE-CZ-NH2	119.20	123.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	112.81	1
CA-C-N	116.90	124.30	2
N-CA-CB	110.50	118.89	1
NH1-CZ-NH2	119.30	112.89	2
N-CA-CB	110.50	102.11	1
C-N-CA	121.70	130.58	3
CB-CG1-CD	113.80	124.16	1
O-C-N	123.00	115.11	5
C-CA-CB	110.10	119.47	2
N-CA-CB	110.50	102.12	1
N-CA-CB	110.50	118.88	1
OD1-CG-ND2	122.60	117.67	1
CA-CB-CG	114.10	104.24	1
CA-CB-CG	112.60	117.53	2
CA-C-N	116.90	124.29	1
C-CA-CB	110.10	119.46	2
C-N-CA	121.70	130.57	2
CA-CB-CG2	110.40	118.78	1
O-C-N	123.00	115.12	1
CA-CB-CG	113.80	118.73	1
N-CA-CB	110.50	118.87	1
N-CA-CB	111.50	119.87	1
NE-CZ-NH1	121.50	126.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG	111.10	120.94	1
O-C-N	123.00	115.13	3
CA-CB-CG2	110.50	118.87	1
C-N-CA	121.70	130.56	2
CA-CB-CG2	110.50	118.86	1
CA-C-N	116.90	124.28	2
C-CA-CB	110.10	119.45	1
CG-CD-NE	112.00	101.18	1
CG-CD-NE2	116.40	109.02	1
CA-CB-CG	112.60	117.52	1
NH1-CZ-NH2	119.30	112.91	1
CA-CB-CG	114.10	123.93	1
CA-C-O	120.80	129.16	2
N-CA-CB	110.50	118.86	1
CA-CB-CG	113.90	105.05	1
C-CA-CB	110.10	119.44	1
O-C-N	123.00	115.14	2
C-N-CA	121.70	130.54	2
C-CA-CB	110.10	100.77	1
CA-C-N	116.20	126.02	1
N-CA-C	111.00	97.25	1
C-CA-CB	110.50	117.87	1
N-CA-CB	110.50	118.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.26	2
CA-CB-CG	113.80	108.89	2
CA-CB-CG	112.60	117.51	1
OG1-CB-CG2	109.30	99.48	1
OD1-CG-ND2	122.60	117.69	1
O-C-N	123.00	115.15	1
CA-N-CD	112.00	118.87	1
C-CA-CB	110.10	119.42	2
CA-C-O	120.80	129.14	1
N-CA-CB	103.00	97.60	1
C-CA-CB	110.10	100.78	1
CA-C-N	116.20	126.01	1
CA-CB-CG	114.10	123.91	1
CG-CD-CE	111.30	122.57	1
O-C-N	123.00	115.16	4
CA-C-N	116.90	124.25	1
N-CA-CB	110.50	102.17	2
N-CA-CB	111.50	119.83	1
C-CA-CB	110.10	119.41	1
CA-C-O	120.80	129.13	1
N-CA-C	111.00	124.72	1
CA-CB-OG	111.10	120.90	1
CA-C-O	120.80	112.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.52	1
OE1-CD-NE2	122.60	117.70	1
C-N-CA	121.70	130.51	3
N-CA-CB	110.50	118.82	1
CG-CD-NE	112.00	101.23	1
C-CA-CB	110.50	117.84	1
N-CA-CB	110.40	117.74	1
CG-CD-NE2	116.40	123.74	1
NH1-CZ-NH2	119.30	112.94	2
CA-CB-CG2	110.50	102.18	1
CB-CG-CD	111.30	122.55	1
N-CA-CB	111.50	119.82	1
C-N-CA	121.70	112.90	1
O-C-N	123.00	115.17	1
O-C-N	123.00	115.18	2
C-N-CA	121.70	130.50	2
C-CA-CB	110.10	119.38	1
CA-C-N	116.20	125.97	1
CA-CB-OG1	109.60	116.93	1
C-CA-CB	110.50	117.83	1
C-N-CA	121.70	130.49	1
CA-C-O	120.80	129.10	1
N-CA-CB	103.00	108.37	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.40	118.70	1
O-C-N	123.00	115.19	5
N-CA-CB	110.50	118.80	1
CA-CB-CG	114.10	123.86	1
CG1-CB-CG2	110.80	100.06	1
C-N-CA	121.70	130.48	3
CA-C-O	120.80	129.09	1
CA-CB-CG	112.60	117.48	1
CA-C-N	116.20	125.95	1
O-C-N	123.00	115.20	5
CA-CB-CG	112.60	107.72	1
CB-CG-CD	112.60	120.89	1
N-CA-CB	110.50	118.78	2
C-N-CA	121.70	130.47	2
CG-CD-NE2	116.40	109.09	1
CA-CB-CG2	110.50	102.22	1
CA-CB-CG	112.60	117.47	2
OE1-CD-NE2	122.60	117.73	1
N-CA-CB	103.00	108.36	1
N-CA-CB	110.50	102.22	1
O-C-N	123.00	115.21	4
CA-C-N	116.20	125.94	1
C-N-CA	121.70	130.46	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	119.35	1
CA-C-O	120.80	112.52	1
CB-CG-CD1	120.70	112.43	1
CA-CB-CG	114.10	123.83	1
N-CA-CB	110.50	118.77	3
NE-CZ-NH1	121.50	126.37	1
CA-C-N	116.90	124.20	1
NH1-CZ-NH2	119.30	112.98	1
CA-C-O	120.80	129.07	1
OE1-CD-NE2	122.60	117.74	2
C-CA-CB	110.10	100.86	1
CA-CB-OG1	109.60	116.89	1
N-CA-C	112.10	124.26	1
CB-CG-OD1	120.80	130.52	1
OD1-CG-ND2	122.60	117.74	1
C-N-CA	121.70	130.45	1
CA-CB-CG	112.60	117.46	1
N-CA-CB	110.50	118.76	1
O-C-N	123.00	115.23	2
C-N-CA	121.70	130.44	4
N-CA-CB	111.50	103.24	1
N-CA-CB	111.50	119.75	2
N-CA-CB	110.50	118.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	123.81	1
CA-CB-CG	112.60	117.45	2
NH1-CZ-NH2	119.30	125.61	1
CA-N-CD	112.00	105.21	1
CA-CB-CG1	110.40	118.65	2
O-C-N	123.00	115.24	1
CG-CD-OE1	120.80	130.50	1
OE1-CD-NE2	122.60	117.75	2
C-CA-CB	110.10	100.88	1
CA-C-O	120.80	129.05	1
OG1-CB-CG2	109.30	99.60	1
CA-CB-CG	113.80	108.95	1
CA-CB-CG	113.80	118.65	1
CA-C-O	120.80	129.04	2
CA-CB-CG	114.10	123.79	1
CA-C-N	116.90	124.17	1
N-CA-CB	111.50	119.74	1
NH1-CZ-NH2	119.30	113.00	1
CA-CB-CG2	110.50	118.74	1
CA-CB-CG1	110.40	118.64	1
C-N-CA	121.70	130.42	2
N-CA-CB	110.50	118.74	1
C-CA-CB	110.10	119.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	129.03	1
O-C-N	123.00	115.25	1
N-CA-CB	110.50	102.27	1
C-N-CA	121.70	130.41	4
C-CA-CB	110.10	119.29	1
CA-CB-CG	112.60	117.44	1
C-CA-CB	110.50	103.24	1
CB-CG-OD1	120.80	130.47	1
C-CA-CB	110.10	100.91	1
CA-C-O	120.80	112.58	1
CG-CD-NE	112.00	101.36	1
CD1-CG-CD2	118.60	125.85	1
C-N-CA	121.70	130.40	1
N-CA-CB	110.50	102.28	1
N-CA-CB	103.00	108.32	1
CA-CB-CG1	110.40	118.62	1
CA-CB-CG	113.80	108.97	1
CA-CB-OG1	109.60	116.85	2
CA-C-N	116.90	124.15	1
O-C-N	123.00	115.27	3
CB-CG-OD1	120.80	130.46	1
CB-CG-CD	111.30	122.41	1
CA-C-O	120.80	129.01	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	119.28	1
CA-CB-CG1	110.40	118.61	1
OE1-CD-NE2	122.60	117.77	1
C-N-CA	121.70	130.39	4
CG-CD-NE	112.00	101.38	1
N-CA-CB	110.50	118.71	1
CA-CB-CG	114.10	123.76	1
OD1-CG-ND2	122.60	127.43	1
O-C-N	123.00	115.28	3
CA-CB-CG2	110.40	102.19	1
CD2-NE2-CE1	109.00	104.17	1
CB-CG-CD2	120.80	113.56	1
NH1-CZ-NH2	119.30	113.03	1
CA-C-N	116.90	124.14	1
NE-CZ-NH1	121.50	126.32	1
C-CA-CB	110.10	119.27	1
C-N-CA	121.70	130.38	4
C-CA-CB	110.10	100.94	1
CA-CB-CG	113.80	118.62	2
N-CA-CB	110.50	102.30	1
N-CA-CB	110.50	118.70	1
O-C-N	123.00	115.29	2
CA-CB-CG1	110.40	118.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-NE2	107.20	112.02	1
CA-C-O	120.80	128.99	1
CB-CG-CD	112.60	120.79	2
CB-CG-CD	111.30	122.38	1
C-CA-CB	109.10	119.70	1
C-CA-CB	110.10	119.25	1
CA-C-O	120.80	112.61	1
N-CA-CB	111.50	119.69	2
N-CA-CB	110.50	118.69	1
N-CA-CB	110.40	103.18	1
C-N-CA	121.70	130.37	1
CA-CB-CG	112.60	117.41	1
CA-C-O	120.80	128.98	1
OE1-CD-NE2	122.60	127.41	1
N-CA-CB	103.00	97.71	1
N-CA-CB	111.50	119.68	1
C-N-CA	121.70	130.36	1
O-C-N	123.00	115.31	5
CA-C-N	116.20	125.82	1
N-CA-CB	111.50	103.32	1
CA-CB-OG1	109.60	116.81	1
N-CA-CB	110.50	102.33	1
C-N-CA	121.70	130.35	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	128.97	2
CA-CB-CG2	110.40	102.23	2
N-CA-CB	110.50	118.67	1
OG1-CB-CG2	109.30	99.69	1
O-C-N	123.00	115.32	3
CB-CG-CD	112.60	104.44	1
NH1-CZ-NH2	119.30	113.06	1
N-CA-CB	110.50	102.34	1
N-CA-CB	110.50	118.66	1
CA-CB-CG	113.80	118.60	2
CA-CB-CG	112.60	117.40	2
NE-CZ-NH2	119.20	114.88	1
CG-CD-CE	111.30	122.34	1
N-CA-CB	110.40	117.60	1
N-CA-CB	111.50	119.66	1
CB-CG1-CD	113.80	123.88	1
C-N-CA	121.70	130.34	1
N-CA-CB	111.50	103.34	1
C-CA-CB	110.10	119.22	1
OE1-CD-NE2	122.60	117.81	1
C-N-CA	121.70	130.33	3
O-C-N	123.00	115.33	2
CB-CG-CD	111.30	122.32	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.65	1
N-CA-CB	110.50	102.35	1
CA-C-N	116.20	125.78	3
C-N-CA	121.70	130.32	1
O-C-N	123.00	115.34	2
N-CA-C	111.00	97.59	1
SG-C7-C8	109.23	123.60	1
N-CD-CG	103.20	110.38	3
N-CA-CB	111.50	119.64	1
C-CA-CB	110.10	119.20	1
CB-CG-ND2	116.40	123.58	1
N-CA-CB	110.50	102.36	1
C-CA-CB	110.50	117.68	1
CA-CB-CG1	110.40	118.54	1
CB-CG-OD1	120.80	111.22	1
CG-CD-NE	112.00	101.47	1
CA-CB-CG	112.60	117.39	1
N-CA-CB	110.50	118.64	1
C-N-CA	121.70	130.31	3
C-CA-CB	110.10	119.19	1
NE-CZ-NH1	121.50	126.28	2
O-C-N	123.00	115.35	7
CA-CB-OG1	109.60	116.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-OE1	120.80	130.36	1
CB-CG-CD	112.60	120.73	1
OD1-CG-ND2	122.60	127.38	1
CA-C-N	116.20	125.76	1
C-CA-CB	110.10	119.18	2
CB-CG-CD	111.30	122.29	1
C-N-CA	121.70	130.30	1
CA-CB-CG	113.80	109.02	1
C-CA-CB	110.10	101.02	1
C-CA-CB	111.40	120.48	1
N-CA-CB	110.50	102.38	1
OE1-CD-NE2	122.60	117.82	1
O-C-N	123.00	115.36	4
N-CA-C	111.00	97.63	1
N-CA-CB	110.40	117.56	1
CA-CB-CG2	110.40	102.28	1
CA-C-O	120.80	130.83	1
CB-CG-CD1	120.70	128.82	1
CA-C-N	116.90	124.06	1
CA-C-O	120.80	128.92	1
CA-CB-CG	112.60	117.37	1
CA-CB-CG2	110.40	118.52	1
N-CA-CB	110.50	118.62	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	113.11	1
N-CA-CB	110.50	118.61	1
N-CA-CB	111.50	119.61	1
CA-CB-CG1	110.40	118.51	1
CA-CB-OG1	109.60	116.76	1
C-CA-CB	110.10	119.16	2
C-CA-CB	110.50	103.35	1
O-C-N	123.00	115.37	2
NE-CZ-NH2	119.20	114.91	1
O-C-N	123.00	115.38	4
CA-CB-CG	114.10	123.63	1
C-N-CA	121.70	130.28	1
N-CA-CB	110.50	118.60	1
N-CA-CB	110.50	102.40	1
CA-CB-CG2	110.40	102.31	1
CG-CD-CE	111.30	122.25	1
OE1-CD-NE2	122.60	117.84	1
NE-CZ-NH2	119.20	114.92	1
N-CA-CB	110.50	102.41	1
CA-CB-CG	113.90	105.33	1
CA-CB-CG	112.60	117.36	1
CG-CD-OE1	120.80	130.32	1
N-CA-CB	111.50	119.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.39	2
N-CA-CB	110.50	118.59	2
C-N-CA	121.70	113.13	1
CB-CG-CD	111.30	122.24	1
CA-CB-OG1	109.60	116.74	1
CA-C-O	120.80	128.89	1
N-CA-C	111.00	97.68	1
N-CA-CB	110.50	118.58	1
CA-CB-CG	113.80	118.56	1
C-N-CA	121.70	130.26	1
CB-CG-CD2	120.80	113.67	2
CA-CB-CG	112.60	107.85	1
O-C-N	123.00	115.40	2
CB-CG-ND2	116.40	123.53	1
C-CA-CB	110.10	119.13	1
CA-CB-CG2	110.50	102.42	1
CA-C-N	116.20	125.70	1
CA-C-O	120.80	128.87	2
CD-NE-CZ	124.40	131.05	1
CB-CG-ND2	116.40	123.52	1
C-N-CA	121.70	130.25	1
C-CA-CB	110.10	119.12	1
CG-CD-CE	111.30	122.22	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.24	4
O-C-N	123.00	115.41	3
CA-CB-CG	113.80	109.05	2
CD-NE-CZ	124.40	131.04	1
CA-CB-CG	113.80	118.54	1
CA-CB-CG	113.80	109.06	2
N-CA-CB	111.50	119.56	1
N-CA-CB	110.50	102.44	1
CA-C-O	120.80	128.86	1
CA-C-N	116.90	124.01	1
C-CA-CB	110.50	103.39	1
O-C-N	123.00	115.42	6
CA-C-O	120.80	128.85	1
OE1-CD-NE2	122.60	117.86	2
CG-CD-CE	111.30	122.19	1
C-N-CA	121.70	130.22	1
SG-C7-C8	109.23	123.43	1
C-CA-CB	110.10	119.10	1
C-CA-CB	110.10	101.11	1
CB-CG-CD	112.60	120.65	1
C-CA-CB	110.10	119.09	2
C-N-CA	121.70	113.18	1
CG-CD-OE1	120.80	111.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NH1-CZ-NH2	119.30	113.15	1
CA-CB-CG	114.10	104.64	1
CA-CB-OG1	109.60	116.69	1
N-CA-CB	111.50	103.46	1
C-N-CA	121.70	130.21	2
C-CA-CB	110.10	119.08	1
N-CA-CB	110.50	118.54	1
NH1-CZ-NH2	119.30	125.45	1
O-C-N	123.00	115.44	2
CB-CG-CD	112.60	104.56	1
CA-CB-CG	114.10	123.55	1
CA-CB-CG	113.80	118.53	1
C-N-CA	121.70	130.20	1
N-CA-CB	110.50	118.53	1
N-CA-C	111.00	124.23	1
C-CA-CB	110.10	119.07	2
CA-CB-CG1	110.40	118.43	2
NE-CZ-NH2	119.20	114.95	2
CA-CB-CG	113.90	105.40	1
CB-CG-CD2	120.80	127.88	1
O-C-N	123.00	115.45	3
CB-CG-CD	112.60	120.63	1
N-CA-CB	110.50	102.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	111.60	102.16	1
CB-CG-CD	111.30	122.15	1
CB-CG1-CD	113.80	123.71	1
C-N-CA	121.70	130.19	4
CA-CB-CG	113.80	109.08	1
N-CA-CB	111.50	119.52	1
CA-C-N	116.20	125.63	2
N-CA-CB	110.50	118.52	1
C-CA-CB	110.10	101.14	1
CA-CB-OG1	109.60	116.67	3
N-CA-CB	110.40	103.33	1
CB-CG-CD	112.60	120.61	1
C-N-CA	121.70	130.18	4
CA-C-N	116.90	123.97	1
CA-C-O	120.80	112.79	1
O-C-N	123.00	115.46	2
CB-CG-CD2	120.70	128.71	1
CA-CB-CG	114.10	123.52	1
C-CA-CB	110.10	119.05	1
CA-CB-OG1	109.60	116.66	1
CA-C-N	116.20	125.62	1
N-CA-CB	110.50	118.51	1
O-C-N	123.00	115.47	6

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG	111.10	120.52	1
C-N-CA	121.70	130.17	2
N-CA-CB	110.50	118.50	1
CA-C-O	120.80	128.80	1
CD2-NE2-CE1	109.00	104.29	1
CA-C-N	116.90	123.96	1
CA-N-CD	112.00	105.41	1
C-CA-CB	110.10	101.16	1
O-C-N	123.00	115.48	3
CA-CB-CG	113.80	109.10	1
N-CA-CB	110.50	118.49	2
N-CA-CB	111.50	119.49	2
C-N-CA	121.70	130.16	5
CA-CB-CG	113.80	118.50	1
OE1-CD-NE2	122.60	117.90	2
NH1-CZ-NH2	119.30	125.41	1
CB-CG-OD1	120.80	130.20	1
CA-CB-CG	112.60	117.30	2
NE-CZ-NH2	119.20	114.97	1
C-N-CA	121.70	130.15	5
O-C-N	123.00	115.49	6
C-CA-CB	110.10	101.18	1
ND1-CE1-NE2	108.40	113.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG1	109.60	116.64	1
CA-C-O	120.80	112.82	2
CB-CG-CD	111.30	122.09	1
C-N-CA	121.70	113.25	1
CG-CD-OE1	120.80	130.18	1
N-CA-CB	110.50	118.47	1
C-N-CA	121.70	130.14	1
CA-C-O	120.80	130.65	1
CA-CB-CG	114.10	123.48	1
O-C-N	123.00	115.50	6
CG-CD-NE2	116.40	123.43	2
CA-C-N	116.90	123.93	2
CG-CD-NE	112.00	101.69	1
CE1-CZ-CE2	120.00	111.56	1
CB-CG-CD1	120.80	127.83	1
CA-CB-CG1	110.40	118.37	1
C-CA-CB	110.10	119.00	1
C-N-CA	121.70	130.13	5
OE1-CD-NE2	122.60	117.91	1
CD2-NE2-CE1	109.00	104.32	1
O-C-N	123.00	115.51	4
CA-CB-CG	114.10	104.73	1
C-CA-CB	110.50	103.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.12	1
N-CA-C	112.10	123.81	1
N-CA-CB	110.40	103.38	1
CA-CB-CG	112.60	117.28	2
N-CA-CB	111.50	119.46	1
OD1-CG-ND2	122.60	117.92	1
C-N-CA	121.70	130.12	1
OE1-CD-NE2	122.60	117.92	1
NH1-CZ-NH2	119.30	113.22	1
CA-CB-CG	112.60	107.92	1
CA-C-N	116.20	125.55	1
C-CA-CB	111.40	102.51	1
C-CA-CB	110.10	118.99	1
CA-CB-CG	114.10	123.45	1
CA-C-N	116.90	123.91	1
CB-CG-CD	112.60	120.55	1
CA-CB-CG2	110.40	118.35	1
CB-CG-CD	111.30	122.05	1
C-CA-CB	111.40	120.28	1
CA-CB-OG1	109.60	116.61	1
C-N-CA	121.70	130.11	3
CA-CB-CG1	110.40	118.35	1
CA-C-O	120.80	112.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.52	1
CA-CB-CG1	110.40	118.34	2
N-CA-CB	110.50	102.56	2
CA-CB-CG	113.80	109.13	1
N-CA-CB	103.00	108.14	1
C-CA-CB	110.50	103.49	1
N-CA-CB	110.50	118.44	1
O-C-N	123.00	115.53	2
N-CA-CB	111.50	119.44	1
CG-CD2-NE2	107.20	111.87	1
C-N-CA	121.70	130.10	2
N-CD-CG	103.20	110.20	1
CA-CB-CG1	110.40	118.33	1
N-CA-CB	110.50	118.43	3
N-CA-CB	111.50	119.43	1
CA-C-N	116.20	125.53	1
N-CA-CB	110.40	103.40	1
NE-CZ-NH1	121.50	116.84	1
C-CA-CB	111.40	102.54	1
N-CA-CB	110.40	103.41	1
C-CA-CB	110.10	118.96	1
OE1-CD-NE2	122.60	127.26	1
CA-CB-OG	111.10	120.42	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NH1-CZ-NH2	119.30	113.24	1
CA-C-O	120.80	128.73	1
N-CA-CB	110.50	118.42	1
CB-CG-CD	111.30	122.02	1
N-CA-CB	110.50	102.58	1
C-N-CA	121.70	130.09	2
O-C-N	123.00	115.54	1
CA-CB-CG1	110.40	118.32	1
CB-CG-CD	112.60	120.52	1
CB-CG-CD2	120.80	127.79	1
N-CA-C	111.00	97.96	1
CA-C-N	116.20	125.51	1
CA-C-O	120.80	112.88	1
OD1-CG-ND2	122.60	117.94	1
CA-CB-CG	112.60	117.26	1
CA-C-O	120.80	128.71	1
C-N-CA	121.70	130.08	4
N-CA-CB	110.50	118.41	2
O-C-N	123.00	115.55	2
CB-CG-CD	112.60	104.69	1
CB-CG-CD1	120.80	127.78	1
N-CA-C	111.00	97.97	1
O-C-N	123.00	115.56	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	123.40	2
C-N-CA	121.70	130.07	4
OE1-CD-NE2	122.60	117.95	2
CA-CB-CG1	110.40	118.30	1
CB-CG-CD1	120.70	112.80	1
OD1-CG-ND2	122.60	117.95	2
CG-CD-NE	112.00	101.77	1
N-CA-CB	110.50	102.60	1
C-CA-CB	109.10	98.88	1
C-CA-CB	110.50	103.53	1
CA-CB-CG2	110.40	102.50	1
NE-CZ-NH2	119.20	115.02	1
CA-CB-CG2	110.50	102.61	1
C-CA-CB	110.50	117.46	2
N-CA-C	111.00	98.00	1
CA-C-N	116.20	125.49	1
O-C-N	123.00	115.57	1
N-CA-CB	110.50	102.61	2
C-N-CA	121.70	130.05	2
OE1-CD-NE2	122.60	127.24	1
CA-CB-CG	113.90	105.55	1
O-C-N	123.00	115.58	3
CG-CD-OE1	120.80	130.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-NE2	116.40	109.44	1
CA-C-N	116.20	125.48	2
N-CA-CB	110.40	103.44	1
CB-CG-CD2	120.70	112.81	1
NE-CZ-NH2	119.20	123.37	2
CB-SG-C7	106.10	92.19	1
C-CA-CB	111.60	120.87	1
CG-SD-CE	100.90	90.70	1
CB-CG-CD	112.60	104.72	1
CD-NE-CZ	124.40	130.89	1
C-CA-CB	110.50	117.45	1
NH1-CZ-NH2	119.30	113.27	1
CG-CD-NE2	116.40	109.45	1
C-N-CA	121.70	130.04	7
CA-C-N	116.20	125.47	1
NE-CZ-NH1	121.50	126.13	1
N-CA-CB	103.00	97.90	1
N-CA-CB	110.50	118.38	2
CB-CG-CD	111.30	121.96	1
C-CA-CB	110.50	103.55	1
CA-CB-CG2	110.50	118.38	1
CG-CD-OE1	118.40	129.05	1
C-CA-CB	110.10	118.90	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	127.23	1
CA-C-N	116.90	123.85	1
C-CA-CB	110.10	101.30	3
O-C-N	123.00	115.59	4
N-CA-CB	110.50	102.63	1
N-CA-CB	110.50	118.37	1
CA-CB-OG1	109.60	102.66	1
C-N-CA	121.70	130.03	3
CA-CB-CG2	110.40	118.26	2
N-CA-CB	110.40	103.46	1
C-CA-CB	110.10	118.88	1
N-CA-CB	110.50	118.36	1
O-C-N	123.00	115.60	2
N-CD-CG	103.20	110.13	1
CA-CB-CG	114.10	123.34	1
C-CA-CB	111.40	102.62	2
CA-CB-CG1	110.40	118.26	1
C-N-CA	121.70	130.02	1
CA-CB-CG	113.80	109.18	1
O-C-N	123.00	115.61	3
NH1-CZ-NH2	119.30	113.30	1
CA-CB-OG	111.10	101.86	1
CA-CB-CG	114.10	104.86	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	130.01	3
N-CA-C	113.30	99.91	1
C-CA-CB	110.10	118.87	1
OD1-CG-ND2	122.60	117.98	1
CA-CB-CG	112.60	117.22	1
CA-C-N	116.90	123.82	1
O-C-N	123.00	115.62	4
ND1-CE1-NE2	108.40	113.01	1
CA-CB-OG1	109.60	116.52	1
N-CA-CB	110.50	118.34	2
CA-CB-CG2	110.40	118.24	1
N-CA-CB	110.50	102.66	1
N-CA-CB	110.40	103.48	1
CG-CD2-NE2	107.20	111.81	1
C-CA-CB	110.10	118.86	2
C-N-CA	121.70	130.00	1
CB-CG-CD	111.30	121.90	1
C-CA-CB	111.60	102.38	1
CB-CG-ND2	116.40	123.31	1
N-CA-CB	110.50	118.33	1
CA-CB-CG	112.60	107.99	1
C-N-CA	121.70	129.99	2
CA-CB-CG	113.80	118.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.63	6
NE-CZ-NH1	121.50	126.11	1
CG-CD-NE	112.00	101.87	1
N-CA-CB	111.50	119.33	1
N-CA-CB	110.50	102.67	1
OE1-CD-NE2	122.60	118.00	1
CG-CD-CE	111.30	121.89	1
CA-C-O	120.80	128.63	1
CA-CB-CG	114.10	123.31	1
CA-CB-CG	113.80	109.20	2
C-CA-CB	110.10	118.85	1
OE1-CD-NE2	122.60	127.20	2
C-CA-CB	111.40	102.66	1
CA-CB-CG	113.80	118.40	1
O-C-N	123.00	115.64	1
C-CA-CB	111.40	120.14	1
CD2-CE2-CZ	120.00	111.72	1
N-CA-CB	111.50	119.32	1
C-CA-CB	110.10	118.84	1
C-CA-CB	110.50	117.40	1
C-CA-CB	110.10	101.36	1
C-N-CA	121.70	129.98	1
CA-C-N	116.90	123.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	123.88	1
NE-CZ-NH1	121.50	126.10	2
C-CA-CB	110.50	103.60	1
CA-CB-CG1	110.40	118.22	1
N-CA-C	111.00	98.13	1
N-CD-CG	103.20	110.10	1
C-CA-CB	110.10	101.37	1
CA-CB-OG1	109.60	116.50	1
C-N-CA	121.70	129.97	3
CA-CB-CG2	110.40	102.59	1
CB-CG-CD1	120.70	112.89	1
OD1-CG-ND2	122.60	118.00	1
C-CA-CB	110.10	118.83	2
CA-C-N	116.20	125.39	1
N-CA-CB	103.00	108.06	1
CA-C-O	120.80	128.61	1
O-C-N	123.00	115.65	2
N-CA-CB	110.50	118.31	1
C-CA-CB	110.50	117.39	1
CA-C-N	116.90	123.79	1
N-CA-CB	111.50	119.31	1
N-CA-CB	111.50	103.69	1
N-CA-C	111.00	98.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.50	102.69	1
N-CA-C	111.00	123.86	1
N-CA-CB	103.00	97.95	1
NE-CZ-NH1	121.50	126.09	1
CD-NE-CZ	124.40	130.83	1
OE1-CD-NE2	122.60	118.01	1
N-CA-CB	110.40	117.28	1
C-N-CA	121.70	129.96	3
O-C-N	123.00	115.66	1
C-CA-CB	110.50	117.38	1
CA-C-N	116.90	123.78	1
OE1-CD-NE2	122.60	127.19	1
CG-CD-CE	111.30	121.85	1
CB-CG-CD1	120.70	112.91	1
O-C-N	123.00	115.67	5
CA-C-O	120.80	128.59	1
CA-C-N	116.20	125.37	1
C-CA-CB	110.10	118.81	1
N-CA-C	111.00	123.83	1
CA-CB-CG	113.90	105.65	1
CB-CG-CD2	131.20	125.24	1
C-N-CA	121.70	129.95	3
CA-C-O	120.80	113.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-NE2	116.40	109.53	1
CB-CG-OD1	120.80	129.96	1
C-N-CA	121.70	129.94	2
CG-CD-NE2	116.40	123.27	1
N-CA-CB	111.50	119.29	1
C-CA-CB	110.10	101.40	1
N-CA-CB	110.50	102.71	1
CA-C-N	116.20	125.36	1
C-CA-CB	110.10	118.80	1
CG-CD-OE1	120.80	129.96	1
N-CA-CB	110.40	103.53	1
C-CA-CB	111.40	120.10	1
CB-CG-CD	111.30	121.83	1
O-C-N	123.00	115.68	3
OD1-CG-ND2	122.60	118.02	1
OD1-CG-ND2	122.60	127.18	1
CB-CG-ND2	116.40	123.26	1
CB-CG-CD	111.30	121.82	1
CA-CB-CG1	110.40	118.18	2
CA-CB-CG	112.60	117.17	1
OE1-CD-NE2	122.60	118.03	1
CA-CB-CG	113.80	109.23	2
CA-CB-OG1	109.60	116.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	128.57	2
O-C-N	123.00	115.69	3
CA-C-N	116.90	123.76	1
C-CA-CB	110.10	101.42	1
N-CA-CB	111.50	119.27	1
CA-CB-CG	113.90	105.67	1
N-CA-CB	110.50	118.27	1
CA-N-CD	112.00	105.61	1
N-CA-CB	110.50	118.26	4
CB-CG-CD	111.30	121.80	1
C-N-CA	121.70	129.92	2
N-CA-CB	110.50	102.74	1
O-C-N	123.00	115.70	1
OD1-CG-ND2	122.60	127.16	1
C-N-CA	121.70	129.91	2
CB-CG-CD2	120.80	127.64	1
CB-CG-CD	112.60	104.85	1
CA-C-N	116.20	125.32	1
CA-CB-CG	113.90	105.69	1
NH1-CZ-NH2	119.30	113.37	2
N-CA-CB	111.50	119.25	1
CD-NE-CZ	124.40	130.78	1
OG1-CB-CG2	109.30	100.18	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.25	1
C-CA-CB	110.10	118.76	1
O-C-N	123.00	115.71	2
CG-CD-OE1	120.80	111.69	1
CA-CB-CG	114.10	123.21	1
CA-C-N	116.20	125.31	1
CA-CB-CG	113.80	109.24	1
C-N-CA	121.70	129.90	4
CD1-CG-CD2	110.80	100.78	1
N-CA-CB	111.50	119.24	1
CB-CG-OD1	120.80	111.69	1
CA-CB-OG	111.10	120.21	1
CA-CB-CG1	110.40	118.14	1
C-N-CA	121.70	129.89	5
CB-CG-CD	111.30	121.77	1
C-CA-CB	111.40	102.75	1
CA-CB-CG	112.60	108.05	1
N-CA-CB	110.50	118.24	1
O-C-N	123.00	115.72	3
NH1-CZ-NH2	119.30	113.39	1
CA-CB-CG	113.80	109.25	1
CA-C-O	120.80	128.53	1
CA-CB-CG1	110.40	118.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.50	102.77	1
C-CA-CB	110.10	101.46	1
CA-C-N	116.90	123.72	2
NE-CZ-NH1	121.50	126.05	2
C-CA-CB	110.50	117.32	1
O-C-N	123.00	115.73	1
CA-C-O	120.80	113.08	1
C-N-CA	121.70	129.88	2
N-CA-CB	111.50	119.22	1
CA-C-N	116.20	125.29	2
CA-CB-CG	112.60	108.06	2
C-N-CA	121.70	129.87	3
C-CA-CB	110.10	118.73	2
N-CA-CB	110.50	118.22	1
CA-CB-CG	113.80	118.34	1
O-C-N	123.00	115.74	3
N-CA-C	111.00	98.29	1
CA-CB-CG	113.90	122.07	1
CA-CB-CG	112.60	117.14	1
C-CA-CB	111.60	102.53	1
NE-CZ-NH1	121.50	126.04	1
N-CA-C	111.00	123.70	1
C-N-CA	121.70	129.86	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	118.72	1
CB-CG-CD2	120.70	112.99	1
C-CA-CB	110.10	118.71	1
O-C-N	123.00	115.75	2
CA-CB-CG	114.10	123.16	1
N-CA-CB	111.50	103.80	1
OE1-CD-NE2	122.60	127.13	2
CA-C-O	120.80	128.50	1
O-C-N	123.00	115.76	2
NH1-CZ-NH2	119.30	113.41	1
CD2-NE2-CE1	109.00	104.47	1
CA-CB-CG	112.60	117.13	1
C-CA-CB	110.50	117.29	1
CB-CG-ND2	116.40	123.19	1
CA-C-O	120.80	113.11	2
C-N-CA	121.70	129.85	2
CA-CB-CG1	110.40	118.09	1
N-CA-CB	110.50	102.81	1
CG-CD-OE1	120.80	129.85	1
CG-CD-NE	112.00	102.05	1
C-CA-CB	110.50	117.28	1
N-CA-CB	110.50	118.19	2
CA-C-O	120.80	128.49	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.08	2
C-N-CA	121.70	129.84	1
ND1-CE1-NE2	108.40	112.92	1
CA-CB-CG	114.10	123.14	2
CB-CG-CD	112.60	104.92	1
O-C-N	123.00	115.77	2
N-CA-CB	110.50	118.18	1
C-CA-CB	110.50	103.72	1
CA-C-N	116.20	125.24	1
CA-CB-OG1	109.60	116.38	1
CA-CB-CG	112.60	108.08	1
N-CD-CG	103.20	109.98	1
CG-CD2-NE2	107.20	111.72	1
C-N-CA	121.70	129.83	3
CD-NE-CZ	124.40	118.08	1
CG-CD-CE	111.30	121.68	1
O-C-N	123.00	115.78	5
CA-C-O	120.80	128.47	1
C-CA-CB	110.10	101.53	1
OE1-CD-NE2	122.60	127.11	1
CG-CD-NE	112.00	102.07	1
CD-NE-CZ	124.40	130.72	1
C-N-CA	121.70	129.82	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	102.83	1
CD1-CG-CD2	110.80	100.88	1
NE-CZ-NH1	121.50	116.99	1
CB-CG-CD1	120.80	114.04	1
N-CA-CB	110.50	102.84	2
N-CA-CB	110.40	103.64	1
C-CA-CB	110.10	101.54	1
C-N-CA	121.70	129.81	7
CA-CB-CG	113.90	105.79	1
O-C-N	123.00	115.79	2
C-CA-CB	110.10	118.66	3
CA-CB-CG1	110.40	102.74	1
CB-CG-OD1	120.80	129.81	1
N-CA-CB	110.50	118.16	4
CA-CB-CG1	110.40	118.06	1
CA-CB-CG	112.60	117.10	2
N-CA-C	111.00	123.61	1
N-CA-CB	110.50	118.15	1
CA-CB-CG	114.10	123.10	1
CG-CD-CE	111.30	121.65	1
N-CA-CB	111.50	119.15	1
CG-CD-OE1	120.80	129.80	1
CG-CD-NE2	116.40	123.15	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	104.95	1
O-C-N	123.00	115.80	3
CA-CB-CG2	110.40	102.75	1
C-CA-CB	110.10	118.65	1
C-N-CA	121.70	113.61	1
C-CA-CB	110.10	118.64	4
O-C-N	123.00	115.81	4
C-N-CA	121.70	129.79	1
CA-C-O	120.80	128.44	3
CA-C-O	120.80	111.36	1
NH1-CZ-NH2	119.30	113.46	1
CB-CG-CD1	120.70	113.06	1
OE1-CD-NE2	122.60	118.11	1
CD1-CE1-CZ	119.60	127.69	1
CG-CD-NE2	116.40	109.66	1
CA-CB-CG1	110.40	118.04	1
CB-CG-CD	111.30	121.63	1
CB-CG-CD	112.60	120.24	1
CA-CB-CG	114.10	123.08	1
N-CA-CB	110.50	102.86	1
CA-C-N	116.20	125.18	1
CA-C-O	120.80	128.43	2
C-CA-CB	110.50	103.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	112.60	120.23	1
N-CA-CB	110.50	102.87	1
N-CA-CB	110.50	118.13	3
NH1-CZ-NH2	119.30	113.47	1
C-N-CA	121.70	129.78	3
O-C-N	123.00	115.82	2
NE-CZ-NH1	121.50	125.99	1
C-CA-CB	111.40	102.87	1
C-CA-CB	110.10	118.62	1
OD1-CG-ND2	122.60	127.09	1
CA-CB-CG	114.10	123.07	1
OD1-CG-ND2	122.60	118.11	1
N-CA-C	111.00	98.44	1
N-CD-CG	103.20	109.93	1
CD1-CG-CD2	110.80	120.66	1
C-CA-CB	110.10	101.58	1
O-C-N	123.00	115.83	2
N-CA-CB	110.40	103.68	1
N-CA-CB	110.50	118.12	1
N-CA-C	111.00	98.46	1
NH1-CZ-NH2	119.30	113.48	1
C-CA-CB	110.10	101.59	1
CA-C-N	116.90	123.62	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	118.61	1
CA-CB-OG1	109.60	116.32	1
CA-CB-CG	112.60	117.08	1
CA-CB-CG	113.80	118.28	1
OE1-CD-NE2	122.60	118.12	1
CA-CB-CG1	110.40	118.01	1
O-C-N	123.00	130.16	1
CB-CG-CD	111.30	121.60	1
N-CA-CB	110.50	118.11	1
C-N-CA	121.70	129.76	1
C-N-CA	121.70	113.64	1
O-C-N	123.00	115.84	2
C-CA-CB	110.10	118.60	1
C-N-CA	121.70	129.75	3
CB-CG-OD1	120.80	129.75	1
CA-C-O	120.80	128.40	1
CA-CB-CG	113.90	105.85	1
C-CA-CB	111.40	102.90	1
O-C-N	123.00	115.85	6
N-CA-CB	111.50	119.10	1
CA-CB-CG	114.10	123.04	2
C-CA-CB	110.50	103.79	1
C-CA-CB	110.10	118.59	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	113.20	2
C-CA-CB	110.50	117.20	1
OE1-CD-NE2	122.60	118.13	1
CG-CD1-CE1	121.20	114.50	1
CA-CB-OG1	109.60	116.30	1
CG-CD-OE1	118.40	128.68	1
N-CA-CB	110.50	118.09	2
CG-CD-OE1	120.80	129.73	1
C-N-CA	121.70	129.74	2
CA-CB-CG1	110.40	102.81	1
C-CA-CB	111.60	102.67	1
CA-CB-CG2	110.40	117.99	1
C-N-CA	121.70	129.73	2
O-C-N	123.00	115.86	6
OG1-CB-CG2	109.30	100.37	1
CA-C-N	116.20	125.12	1
N-CA-C	111.00	123.49	1
C-CA-CB	110.10	118.57	4
CA-CB-CG	112.60	117.06	1
C-CA-CB	110.50	117.19	1
O-C-N	123.00	115.87	4
CA-CB-CG1	110.40	117.98	1
N-CA-C	112.10	123.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.72	3
CA-C-O	128.33	114.96	1
NE-CZ-NH1	121.50	125.96	1
C-N-CA	121.70	113.68	1
CA-CB-CG1	110.40	102.82	1
CA-C-N	116.20	125.11	1
CA-CB-CG2	110.40	117.98	1
N-CA-CB	111.50	119.07	1
CB-CG-CD	112.60	120.17	2
N-CD-CG	103.20	109.88	1
CA-CB-CG	112.60	108.15	1
ND1-CE1-NE2	108.40	112.85	1
CA-C-O	120.80	113.23	1
CA-CB-CG2	110.40	102.83	1
C-CA-CB	110.10	118.56	3
CA-CB-CG1	110.40	117.97	2
N-CA-CB	110.50	118.07	1
O-C-N	123.00	115.88	3
C-N-CA	121.70	129.71	2
CA-CB-OG1	109.60	116.27	1
OE1-CD-NE2	122.60	118.15	1
CG1-CB-CG2	110.80	101.02	1
N-CA-CB	110.50	118.06	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.70	3
CA-C-O	120.80	128.36	1
OD1-CG-ND2	122.60	118.15	1
OE1-CD-NE2	122.60	118.16	1
N-CA-CB	110.50	102.94	1
CA-C-O	120.80	113.24	1
ND1-CG-CD2	106.10	101.66	1
C-CA-CB	110.10	101.66	1
CA-CB-CG2	110.50	118.05	1
N-CA-CB	111.50	119.05	1
CA-CB-CG	114.10	105.22	1
CG-CD-CE	111.30	121.52	1
OD1-CG-ND2	122.60	127.04	1
C-N-CA	121.70	129.69	4
C-CA-CB	110.10	118.54	2
CG-CD-OE2	118.40	108.19	1
OD1-CG-ND2	122.60	118.16	1
CA-C-O	120.80	113.25	1
O-C-N	123.00	115.90	2
N-CA-CB	110.50	118.05	2
CA-CB-OG	111.10	119.98	1
NH1-CZ-NH2	119.30	125.07	1
CA-CB-CG	112.60	117.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	113.71	1
N-CA-CB	110.50	118.04	1
N-CA-CB	110.40	103.74	1
N-CA-CB	110.40	117.06	1
C-CA-CB	111.60	102.73	1
CB-CG-CD2	120.70	113.16	1
C-CA-CB	110.10	118.53	1
NH1-CZ-NH2	119.30	113.53	1
O-C-N	123.00	115.91	5
CA-CB-CG1	110.40	117.94	1
C-N-CA	121.70	129.68	6
NE-CZ-NH2	119.20	115.21	1
CB-CG-CD	111.30	121.50	1
N-CA-CB	110.50	118.03	4
CA-C-N	116.90	123.55	1
C-CA-CB	110.10	118.52	1
C-CA-CB	111.40	119.82	1
OG1-CB-CG2	109.30	100.44	1
CA-C-O	120.80	128.33	1
CB-CG-CD	111.30	121.49	1
CA-CB-CG2	110.40	117.93	1
O-C-N	123.00	115.92	4
CD-NE-CZ	124.40	130.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	119.03	1
CA-CB-CG1	110.40	117.92	2
CB-CG-ND2	116.40	109.76	1
OE1-CD-NE2	122.60	118.17	1
N-CA-CB	110.50	118.02	1
C-CA-CB	110.50	103.87	1
C-N-CA	121.70	129.66	4
O-C-N	123.00	115.93	6
CB-CG-CD	111.30	121.47	1
C-CA-CB	110.50	117.13	1
C-CA-CB	110.10	101.70	1
N-CA-CB	110.50	118.01	5
CA-CB-CG	112.60	108.18	1
CA-C-N	116.20	125.04	1
C-N-CA	121.70	113.75	1
C-N-CA	121.70	129.65	2
N-CA-CB	110.50	102.99	1
CA-CB-OG1	109.60	116.23	1
N-CA-C	111.00	98.63	1
CG-CD-OE1	120.80	129.64	1
N-CA-CB	110.40	117.03	1
NE-CZ-NH2	119.20	115.23	1
N-CA-CB	103.00	98.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.94	3
CD-NE-CZ	124.40	130.58	1
CA-CB-CG2	110.50	103.00	1
ND1-CE1-NE2	108.40	112.81	1
N-CA-CB	110.40	103.78	1
C-N-CA	121.70	129.64	5
N-CA-C	112.10	123.13	1
N-CA-CB	103.00	107.85	1
CB-CG-CD	112.60	120.10	1
N-CA-CB	110.50	103.00	1
OD1-CG-ND2	122.60	118.19	1
CA-CB-CG	112.60	117.01	1
O-C-N	123.00	115.95	8
CB-CG-CD	112.60	105.10	1
N-CA-CB	110.50	117.99	2
CA-C-N	116.90	123.51	1
N-CA-CB	110.40	103.79	1
C-N-CA	121.70	129.63	4
C-CA-CB	110.10	118.47	1
CG-CD-NE	112.00	102.31	1
CA-CB-OG1	109.60	116.21	1
CA-CB-CG2	110.50	103.01	1
CA-C-O	120.80	113.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	101.73	1
CB-CG-CD	112.60	120.08	1
N-CA-C	111.00	98.67	1
C-N-CA	121.70	129.62	3
CD1-CG-CD2	110.80	120.49	1
N-CA-CB	110.50	117.98	1
N-CA-CB	110.40	117.00	1
O-C-N	123.00	115.96	5
CA-CB-CG	114.10	122.90	1
N-CA-CB	110.50	103.02	1
CA-C-N	116.20	125.00	1
CA-CB-CG	113.80	109.40	2
CA-CB-CG	112.60	117.00	1
CB-CG-ND2	116.40	123.00	1
C-CA-CB	110.10	118.46	1
CA-CB-OG1	109.60	116.20	1
OE1-CD-NE2	122.60	118.20	1
C-N-CA	121.70	129.61	3
CA-C-N	116.90	123.50	1
CD2-NE2-CE1	109.00	104.60	1
CA-C-N	116.20	124.99	3
O-C-N	123.00	115.97	4
CB-CG-CD	112.60	105.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	101.75	3
CG-CD-OE1	120.80	129.59	1
CA-C-N	116.90	123.49	1
C-CA-CB	110.10	118.45	1
CA-CB-CG	113.80	118.19	1
NE-CZ-NH2	119.20	115.25	1
C-N-CA	121.70	113.79	1
CA-CB-CG1	110.40	117.87	1
OG1-CB-CG2	109.30	100.52	1
C-N-CA	121.70	129.60	4
N-CA-CB	111.50	118.96	1
CB-CG1-CD	113.80	123.02	1
CA-CB-CG2	110.40	117.86	1
C-CA-CB	110.50	117.08	1
OE1-CD-NE2	122.60	126.99	1
CB-CG-CD1	120.80	127.38	1
O-C-N	123.00	115.98	1
CB-CG-CD	111.30	121.39	2
CA-C-N	116.90	123.48	1
OE1-CD-NE2	122.60	118.21	1
CD-NE-CZ	124.40	118.26	1
N-CA-CB	110.50	117.96	1
C-CA-CB	111.60	102.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	113.34	1
C-CA-CB	110.10	101.77	2
CA-CB-CG	113.80	109.41	1
C-CA-CB	110.10	118.43	1
CA-C-N	116.20	124.97	2
C-N-CA	121.70	129.59	3
OE1-CD-NE2	122.60	118.22	3
CG-CD-NE2	116.40	109.82	1
C-CA-CB	110.50	103.92	1
CA-C-O	120.80	128.25	1
CB-CG-CD	112.60	105.15	1
N-CA-CB	110.50	117.95	1
O-C-N	123.00	115.99	6
CB-CG-CD	111.30	121.38	1
C-CA-CB	110.50	103.93	1
O-C-N	123.00	130.01	1
CA-CB-CG	112.60	108.22	3
CA-C-O	120.80	113.35	1
OD1-CG-ND2	122.60	118.22	1
CA-CB-CG1	110.40	117.85	1
CB-CG-OD1	120.80	129.56	1
CG-CD-NE2	116.40	122.97	1
C-N-CA	121.70	129.58	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.42	1
CG-CD2-NE2	107.20	111.58	1
N-CD-CG	103.20	109.77	1
CA-CB-CG	112.60	116.98	2
N-CA-CB	110.50	103.06	1
O-C-N	123.00	116.00	4
CA-CB-CG	113.90	106.02	1
CA-CB-SG	114.40	124.47	1
CB-CG-CD2	120.70	113.26	1
CA-CB-CG1	110.40	117.84	1
CA-CB-CG	113.90	106.03	2
CA-C-N	116.20	124.95	1
CB-CG-CD1	120.80	114.24	1
C-CA-CB	110.10	101.79	1
CD1-CG-CD2	118.60	125.16	1
CA-CB-CG	112.60	108.23	1
NH1-CZ-NH2	119.30	113.61	1
CA-C-O	120.80	128.23	2
C-CA-CB	110.50	117.06	1
O-C-N	123.00	116.01	5
CB-CG-OD1	120.80	129.54	1
CA-CB-CG1	110.40	117.83	1
CA-CB-OG	111.10	119.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.57	1
N-CA-CB	110.50	103.07	1
N-CA-CB	110.50	117.93	2
C-N-CA	121.70	129.56	5
N-CD-CG	103.20	109.75	1
O-C-N	123.00	129.99	1
C-CA-CB	110.10	101.80	1
N-CA-CB	110.50	103.08	1
CG-CD-NE2	116.40	109.85	1
CA-CB-CG	113.90	121.76	1
O-C-N	123.00	116.02	3
C-CA-CB	110.10	101.81	2
CA-CB-OG1	109.60	116.15	1
N-CA-CB	110.50	117.92	3
CA-C-N	116.90	123.45	2
C-CA-CB	110.10	118.39	1
CB-CG-CD	111.30	121.34	1
O-C-N	123.00	129.98	1
C-N-CA	121.70	129.55	3
NH1-CZ-NH2	119.30	113.63	1
CA-CB-CG1	110.40	117.82	1
CA-C-N	116.20	124.92	1
CG-CD-NE	112.00	102.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-CD	112.00	105.90	1
N-CA-CB	110.50	117.91	1
CA-C-O	120.80	113.39	1
CA-CB-OG	111.10	119.82	1
C-CA-CB	110.50	103.96	1
CA-CB-CG1	110.40	102.99	1
O-C-N	123.00	116.03	3
CB-CG-OD1	120.80	129.51	1
C-N-CA	121.70	129.54	4
CB-CG-CD2	120.80	127.34	1
N-CA-CB	111.50	118.91	1
CA-C-N	116.20	124.91	1
C-CA-CB	110.10	118.37	1
CG-CD2-CE2	120.70	113.30	1
N-CA-CB	111.50	118.90	1
OG1-CB-CG2	109.30	100.59	1
N-CA-CB	110.50	117.90	3
O-C-N	123.00	116.04	2
OE1-CD-NE2	122.60	118.25	1
OG1-CB-CG2	109.30	100.60	1
N-CA-C	113.30	125.92	1
CA-C-N	116.20	124.90	1
CG1-CB-CG2	110.80	101.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.89	6
C-N-CA	121.70	129.53	3
CA-CB-CG	113.80	109.45	1
C-CA-CB	110.10	101.84	1
CA-CB-CG	112.60	108.25	1
C-CA-CB	110.10	118.36	1
CA-CB-OG	111.10	119.80	1
CB-CG-CD2	120.70	128.09	1
OD1-CG-ND2	122.60	118.25	1
O-C-N	123.00	116.05	5
CB-CG-CD	111.30	121.30	1
CG-CD-NE2	116.40	122.92	1
CA-C-N	116.90	123.42	2
CA-CB-CG	113.80	118.15	1
C-CA-CB	111.40	119.65	1
CA-CB-CG	112.60	116.94	1
N-CA-CB	111.50	118.88	1
C-N-CA	121.70	129.52	2
OD1-CG-ND2	122.60	118.26	2
CA-C-N	116.20	124.88	1
NH1-CZ-NH2	119.30	113.66	1
O-C-N	123.00	116.06	5
N-CA-C	112.10	122.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	118.34	1
CA-CB-CG2	110.40	117.78	1
C-N-CA	121.70	129.51	3
N-CA-CB	110.50	117.88	1
CB-CG-CD	111.30	121.28	1
CG-CD-CE	111.30	121.28	1
CB-CG-CD	112.60	119.97	2
CA-CB-CG	114.10	122.77	1
N-CA-C	111.00	123.14	1
CA-CB-CG	112.60	108.26	1
C-N-CA	121.70	129.50	2
N-CA-CB	110.50	117.87	1
CA-N-CD	112.00	105.93	1
C-CA-CB	110.50	104.00	1
CA-CB-CG1	110.40	117.77	1
O-C-N	123.00	116.07	5
CA-C-O	120.80	128.17	1
CD2-NE2-CE1	109.00	104.67	1
CD1-CG-CD2	118.10	124.60	1
NE-CZ-NH1	121.50	125.83	2
N-CA-CB	110.50	117.86	1
CA-CB-CG	114.10	122.76	1
C-CA-CB	110.10	101.88	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CB-CG2	110.80	120.32	1
O-C-N	123.00	116.08	6
C-CA-CB	110.10	118.32	2
C-N-CA	121.70	129.49	3
CA-C-O	120.80	113.44	1
C-CA-CB	111.40	103.18	1
OD1-CG-ND2	122.60	118.27	1
N-CA-C	111.00	98.89	1
N-CA-CB	110.50	117.85	2
CB-CG-CD	111.30	121.25	2
CA-C-N	116.90	123.39	1
NH1-CZ-NH2	119.30	113.68	1
CD-NE-CZ	124.40	118.35	1
CA-CB-CG	113.80	118.12	1
C-CA-CB	110.10	118.31	2
CA-C-N	116.20	124.85	1
CD-NE-CZ	124.40	130.45	1
C-N-CA	121.70	129.48	2
OE1-CD-NE2	122.60	118.28	1
CA-CB-CG	114.10	122.74	1
O-C-N	123.00	116.09	4
CA-C-N	116.20	124.84	1
NE-CZ-NH1	121.50	125.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD1	120.80	127.28	1
N-CA-CB	111.50	118.84	1
N-CA-CB	110.50	103.16	2
N-CA-CB	110.50	117.84	3
N-CA-CB	103.00	107.75	1
CB-CG-ND1	122.70	116.22	1
C-N-CA	121.70	129.47	5
CA-C-O	120.80	113.46	2
CB-CG-OD1	118.40	128.33	1
C-CA-CB	110.10	118.30	2
C-CA-CB	110.50	116.98	1
CA-C-N	116.90	123.38	1
CA-C-N	116.90	123.37	1
CA-C-O	120.80	128.13	1
CB-CG-CD	112.60	105.27	1
C-CA-CB	110.10	118.29	1
C-N-CA	121.70	129.46	4
CB-CG-CD2	120.70	113.37	1
C-CA-CB	110.10	101.91	1
N-CA-CB	110.50	103.17	1
N-CA-CB	110.50	117.83	4
CA-CB-OG1	109.60	116.07	1
CB-CG-ND2	116.40	122.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	114.10	105.48	1
O-C-N	123.00	116.10	4
C-N-CA	121.70	113.94	1
CA-CB-CG	113.90	106.14	1
CA-CB-CG	113.80	109.49	1
CB-CG-CD	112.60	119.92	1
CA-C-O	120.80	128.12	1
O-C-N	123.00	116.11	3
CA-C-N	116.20	124.81	2
C-N-CA	121.70	129.45	4
CG-CD2-NE2	107.20	111.51	1
C-CA-CB	110.10	101.92	1
OE1-CD-NE2	122.60	118.29	1
C-CA-CB	110.10	118.28	2
CB-CG-ND2	116.40	109.94	1
N-CA-CB	110.50	103.18	1
C-N-CA	121.70	113.95	1
OG1-CB-CG2	109.30	100.69	1
CA-CB-CG2	110.50	103.18	1
CA-CB-CG	112.60	116.90	1
N-CA-CB	111.50	118.82	1
N-CA-CB	110.40	103.94	1
ND1-CE1-NE2	108.40	112.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.12	3
N-CA-C	112.10	122.86	1
C-CA-CB	110.10	118.27	1
CB-CG-CD1	120.70	128.01	1
NE-CZ-NH1	121.50	125.80	2
C-CA-CB	110.10	101.93	2
N-CA-C	111.00	98.96	1
CA-C-O	120.80	128.11	1
CA-C-N	116.20	124.80	1
CA-C-N	116.90	123.35	2
C-N-CA	121.70	129.44	1
CG-CD-CE	111.30	121.19	1
N-CA-CB	111.50	118.81	1
CB-CG-ND1	122.70	129.15	1
NE-CZ-NH2	119.20	115.33	1
N-CA-CB	110.50	117.81	1
C-CA-CB	111.40	103.24	1
O-C-N	123.00	129.88	1
CB-CG-OD1	120.80	129.39	1
CA-C-N	116.90	123.34	1
N-CA-CB	110.50	117.80	2
CB-CG-CD2	131.20	125.62	1
CA-C-N	116.20	124.79	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	120.80	127.24	1
N-CA-CB	111.50	118.80	2
O-C-N	123.00	116.13	3
CA-C-O	120.80	128.10	1
C-N-CA	121.70	129.43	3
NE-CZ-NH2	119.20	115.34	1
N-CA-CB	110.50	103.20	1
N-CD-CG	103.20	109.64	1
CA-CB-CG	112.60	116.89	2
CB-CG-CD	111.30	121.17	1
N-CA-CB	110.50	117.79	2
C-CA-CB	110.10	118.25	2
C-N-CA	121.70	129.42	3
CA-CB-OG1	109.60	116.03	1
CG-CD-OE1	120.80	129.38	1
N-CA-CB	103.00	107.72	1
NE-CZ-NH1	121.50	125.79	1
CA-C-N	116.20	124.78	1
OD1-CG-ND2	122.60	118.31	1
CB-CG-CD	111.30	121.16	1
CA-C-N	116.90	123.33	2
CA-C-O	120.80	128.09	1
N-CA-CB	110.40	103.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	109.51	1
CA-CB-CG	112.60	108.31	1
CD-NE-CZ	124.40	118.40	1
O-C-N	123.00	116.14	5
CB-SG-C7	106.10	118.96	1
CA-CB-CG	113.90	121.62	1
CA-C-N	116.20	124.77	1
N-CA-CB	111.50	118.79	1
N-CA-CB	111.50	118.78	1
C-N-CA	121.70	129.41	3
CG1-CB-CG2	110.80	101.38	1
CA-CB-CG1	110.40	117.68	2
NE-CZ-NH2	119.20	115.35	1
C-CA-CB	110.10	101.96	1
N-CA-CB	110.50	117.78	1
CA-CB-CG	113.90	106.19	1
CG-CD-NE2	116.40	109.98	1
O-C-N	123.00	116.15	3
C-N-CA	121.70	129.40	6
CD1-CG-CD2	110.80	101.39	2
CA-CB-CG1	110.40	117.67	2
CA-CB-CG	112.60	116.88	1
CA-CB-OG	111.10	119.66	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG2	110.50	103.23	1
N-CD-CG	103.20	109.62	1
N-CA-CB	103.00	98.29	1
N-CA-CB	111.50	118.77	1
CA-C-O	120.80	128.07	1
O-C-N	123.00	116.16	3
CG-CD-NE2	116.40	122.81	1
N-CA-CB	110.50	117.77	1
CA-CB-CG2	110.40	117.67	1
NE-CZ-NH1	121.50	125.78	1
CG-CD-CE	111.30	121.13	1
CB-CG-CD	112.60	105.33	1
CA-C-N	116.90	123.31	2
C-CA-CB	110.10	118.22	2
N-CA-CB	110.50	103.23	1
N-CA-CB	103.00	98.30	1
CB-CG-CD	112.60	119.86	2
N-CA-CB	110.50	117.76	2
CG-CD2-NE2	107.20	111.47	1
C-N-CA	121.70	114.01	1
CB-CG-CD2	110.70	123.52	1
CA-C-N	116.20	124.74	1
CA-CB-CG2	110.40	103.14	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.17	4
C-N-CA	121.70	129.39	2
CB-CG-CD2	110.70	123.51	1
CG-CD-CE	111.30	121.12	1
CB-CG-CD	111.30	121.12	2
C-CA-CB	111.40	119.51	1
CA-CB-OG1	109.60	116.00	2
C-N-CA	121.70	129.38	5
C-CA-CB	110.10	118.21	1
C-CA-CB	110.10	101.99	1
N-CA-CB	110.50	117.75	5
CA-CB-CG	112.60	116.87	1
CA-CB-CG2	110.40	103.15	1
C-CA-CB	110.50	116.90	1
OE1-CD-NE2	122.60	118.34	1
CG1-CB-CG2	110.80	101.42	1
CA-CB-CG	112.60	116.86	1
CB-CG-OD1	120.80	129.32	1
CA-C-N	116.90	123.29	1
N-CA-CB	111.50	118.74	1
CA-C-O	120.80	128.04	1
O-C-N	123.00	116.18	1
N-CA-CB	110.50	117.74	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	113.30	100.94	1
CA-C-N	116.20	124.72	2
C-CA-CB	110.10	118.19	2
O-C-N	123.00	116.19	3
C-CA-CB	110.10	102.01	3
OE1-CD-NE2	122.60	126.86	1
C-N-CA	121.70	129.36	2
CA-CB-OG	111.10	119.62	1
C-N-CA	121.70	114.04	1
C-CA-CB	109.10	118.47	1
NH1-CZ-NH2	119.30	113.77	1
CB-CG-CD	112.60	119.84	1
OD1-CG-ND2	122.60	118.34	1
CG-SD-CE	100.90	91.54	1
CA-C-O	120.80	113.57	2
N-CA-CB	110.50	117.73	1
CA-CB-CG1	110.40	117.63	2
CB-CG-CD1	120.70	113.47	1
CA-C-N	116.20	124.71	1
CG-CD-CE	111.30	121.08	2
CG1-CB-CG2	110.80	101.44	1
C-CA-CB	110.10	118.18	2
N-CA-CB	110.50	103.27	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.35	2
CA-CB-CG	112.60	108.35	1
CA-CB-CG	113.80	109.55	1
CA-CB-CG	114.10	105.60	1
CB-CG-CD	112.60	105.37	1
CE1-CZ-CE2	120.30	111.80	1
CG-CD-NE2	116.40	122.78	1
CA-C-N	116.20	124.70	1
CG-CD2-NE2	107.20	111.45	1
CB-CG-CD2	120.70	113.48	1
CA-CB-CG2	110.40	103.18	1
O-C-N	123.00	116.20	1
N-CA-CB	110.40	116.77	1
CA-C-O	120.80	113.58	1
N-CA-CB	110.50	117.72	2
NE-CZ-NH2	119.20	123.02	1
CA-CB-CG	114.10	122.60	1
N-CA-CB	110.50	103.28	1
C-CA-CB	110.10	102.03	1
CG-CD-CE	111.30	121.07	1
C-N-CA	121.70	129.34	3
CA-CB-CG	114.10	105.61	1
CB-CG-CD	112.60	119.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
ND1-CE1-NE2	108.40	112.65	1
CB-CG-OD1	120.80	129.29	1
N-CA-C	111.00	122.89	1
O-C-N	123.00	116.21	3
CA-C-N	116.20	107.71	1
N-CA-CB	111.50	118.71	2
CB-CG-CD1	120.80	127.17	1
CA-C-O	120.80	128.01	2
OD1-CG-ND2	122.60	126.84	1
CD-NE-CZ	124.40	130.34	1
NE-CZ-NH2	119.20	115.38	1
CD2-CE2-CZ	120.00	112.36	1
N-CA-CB	110.50	117.71	1
OE1-CD-NE2	122.60	118.36	1
C-N-CA	121.70	129.33	1
C-CA-CB	110.10	102.04	2
CD1-CG-CD2	110.80	101.47	1
CA-CB-CG	113.80	109.56	1
CA-CB-OG	111.10	119.58	1
CA-CB-CG1	110.40	103.19	1
OG1-CB-CG2	109.30	100.82	1
O-C-N	123.00	116.22	4
N-CA-CB	110.40	104.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	102.05	1
CB-CG-CD	112.60	119.80	1
CA-CB-CG	114.10	122.58	1
CB-CG-CD	111.30	121.05	1
CA-C-N	116.20	124.67	1
CG-CD-NE2	116.40	110.05	1
CB-CG-ND2	116.40	110.05	1
CA-CB-CG	114.10	122.57	1
N-CA-C	111.00	99.14	1
N-CA-CB	103.00	107.66	1
C-N-CA	121.70	129.32	4
N-CA-CB	110.50	117.70	2
CB-CG1-CD	113.80	104.91	1
CA-C-O	120.80	127.99	1
CA-C-O	120.80	113.61	1
N-CA-CB	110.40	116.75	1
C-CA-CB	110.10	118.14	2
O-C-N	123.00	116.23	2
N-CA-CB	111.50	118.69	1
C-CA-CB	110.10	102.06	1
N-CA-C	111.00	99.15	1
NH1-CZ-NH2	119.30	124.80	1
CB-CG-CD	112.60	119.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	136.70	1
CA-CB-CG	113.90	106.29	1
CG-CD-NE2	116.40	122.74	3
N-CA-C	112.10	122.67	1
CA-CB-CG	112.60	116.83	2
C-N-CA	121.70	129.31	2
CB-CG-OD1	120.80	129.26	1
CA-CB-CG2	110.50	103.31	1
CG-CD-NE	112.00	102.70	1
O-C-N	123.00	116.24	6
N-CA-C	113.30	101.04	1
C-CA-CB	110.10	118.13	2
CA-CB-OG1	109.60	115.94	2
N-CA-CB	110.50	117.68	5
N-CA-C	111.00	122.83	1
CA-C-N	116.90	123.23	2
NE-CZ-NH1	121.50	125.72	2
NH1-CZ-NH2	119.30	113.81	1
N-CA-C	111.00	122.82	1
C-N-CA	121.70	129.30	2
CA-CB-CG	112.60	108.38	1
C-CA-CB	111.40	119.42	1
OE1-CD-NE2	122.60	118.38	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	104.07	1
CA-CB-CG1	110.40	117.58	1
C-N-CA	121.70	114.10	1
N-CA-CB	111.50	118.67	2
O-C-N	123.00	116.25	4
C-CA-CB	110.10	102.08	1
CB-CG-CD	112.60	119.77	1
CA-CB-CG	113.90	106.31	1
CA-C-O	120.80	113.63	3
CB-CG-CD	111.30	121.00	1
C-CA-CB	109.10	118.38	1
C-N-CA	121.70	129.29	3
CA-CB-CG	113.80	109.58	1
C-CA-CB	111.40	119.41	2
CG-CD-NE	112.00	102.72	1
CG-CD-OE2	118.40	108.70	1
N-CA-CB	103.00	107.64	1
C-CA-CB	110.50	104.18	1
N-CA-CB	110.50	117.67	2
O-C-N	123.00	116.26	11
CA-CB-CG	113.80	109.59	1
N-CA-CB	111.50	118.66	3
CB-CG-CD1	120.80	114.48	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	124.63	1
CD1-CG-CD2	110.80	101.53	1
C-N-CA	121.70	129.28	4
N-CA-CB	110.50	117.66	1
CA-CB-CG	112.60	116.81	1
CA-CB-CG2	110.40	117.56	1
C-CA-CB	110.10	102.09	1
CA-C-O	120.80	127.96	2
CA-CB-CG1	110.40	117.56	1
N-CA-CB	110.50	103.34	2
CG-CD-NE	112.00	102.73	1
CA-C-N	116.20	124.62	2
N-CA-CB	110.40	116.72	1
CA-CB-CG	114.10	122.52	1
N-CA-CB	103.00	107.63	1
CD2-NE2-CE1	109.00	104.79	1
CA-CB-CG	113.80	118.01	1
CG-CD-OE1	120.80	129.22	1
CA-C-O	120.80	113.64	1
CA-C-N	116.90	123.21	4
CA-CB-OG1	109.60	115.91	1
CB-CG1-CD	113.80	122.64	1
O-C-N	123.00	116.27	8

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.27	6
CA-C-O	120.80	113.65	2
CG-CD2-CE2	121.20	114.89	1
C-CA-CB	110.10	118.09	1
CA-C-O	120.80	127.95	1
CA-CB-CG2	110.40	117.55	1
CA-C-N	116.20	124.61	2
C-CA-CB	110.50	104.19	1
N-CD-CG	103.20	109.51	1
CB-CG-OD2	118.40	108.73	1
N-CA-C	111.00	122.77	1
CB-CG-CD	112.60	119.75	1
N-CA-CB	110.50	117.65	1
CG-CD-CE	111.30	120.97	1
CA-CB-CG1	110.40	117.55	1
O-C-N	123.00	116.28	5
CA-CB-CG2	110.50	117.64	1
CA-CB-OG	111.10	119.51	1
C-N-CA	121.70	129.26	1
CA-CB-CG1	110.40	117.54	1
NE-CZ-NH2	119.20	122.98	2
CA-C-O	120.80	113.66	1
N-CA-C	111.00	99.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.64	1
C-CA-CB	110.10	102.12	2
CA-CB-CG	113.90	106.34	1
CB-CG-CD	112.60	105.46	1
CD-NE-CZ	124.40	130.28	1
N-CA-CB	110.50	117.63	5
CA-CB-OG1	109.60	115.90	1
C-N-CA	121.70	129.25	7
O-C-N	123.00	116.29	1
CB-CG-CD1	120.80	114.51	1
N-CA-C	113.30	101.13	1
C-CA-CB	111.40	103.43	1
CD1-CG-CD2	118.60	112.31	1
CB-CG-ND2	116.40	110.11	1
CA-CB-CG	114.10	105.71	1
N-CA-CB	111.50	118.63	2
CG-CD-NE2	116.40	122.69	1
NE-CZ-NH1	121.50	125.69	1
CG-CD-NE2	116.40	110.11	1
CA-C-O	120.80	127.93	2
CA-C-O	120.80	113.67	2
N-CA-CB	110.40	116.69	2
C-CA-CB	110.10	102.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OG1-CB-CG2	109.30	100.91	1
N-CA-CB	110.50	103.37	1
C-CA-CB	110.50	104.21	2
CA-CB-CG	113.90	106.36	1
C-N-CA	121.70	129.24	1
N-CA-CB	110.50	103.38	1
N-CA-C	111.00	122.73	1
CA-C-O	128.33	115.76	1
N-CA-CB	103.00	107.61	1
CB-CG-CD1	120.80	127.08	1
CA-CB-CG	113.80	117.99	1
CA-C-N	116.20	124.58	1
N-CA-C	111.00	99.27	1
C-CA-CB	110.50	116.78	1
CA-C-O	120.80	127.92	1
CB-CG-CD	111.30	120.93	1
CA-C-N	116.20	107.82	1
O-C-N	123.00	116.30	3
N-CA-CB	110.50	117.62	3
CA-C-N	116.20	124.57	2
CA-C-N	116.90	123.18	1
OE1-CD-NE2	122.60	118.41	1
CD-NE-CZ	124.40	130.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	113.30	101.16	1
CB-CG-CD1	120.70	113.58	1
C-N-CA	121.70	129.23	4
CA-C-O	120.80	127.91	2
CB-CG-CD	112.60	105.49	2
CA-CB-CG2	110.50	117.61	1
O-C-N	123.00	116.31	7
CA-CB-OG1	109.60	115.88	1
C-CA-CB	110.10	118.05	1
N-CA-CB	110.50	117.61	3
C-CA-CB	111.40	119.35	1
CD1-CG-CD2	118.60	124.87	1
CA-C-O	120.80	113.69	1
CA-CB-OG1	109.60	103.33	1
C-CA-CB	110.10	102.16	1
CB-CG-CD	112.60	119.71	1
CA-C-N	116.90	123.17	1
CA-C-N	116.20	124.56	1
CG-CD-NE2	116.40	122.67	2
N-CA-CB	110.50	117.60	5
C-CA-CB	110.50	104.23	1
CB-CG-CD1	120.80	127.07	1
CA-CB-CG	113.90	106.38	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD	111.30	120.91	1
N-CA-C	111.00	122.70	1
CA-CB-CG	112.60	108.42	1
CA-CB-CG2	110.40	117.50	1
C-CA-CB	110.10	118.04	1
N-CA-CB	103.00	107.59	1
CA-CB-CG	114.10	122.45	2
N-CA-C	113.30	101.19	2
CG-CD-NE	112.00	102.81	1
CB-CG-CD	112.60	105.50	1
O-C-N	123.00	116.32	3
N-CA-CB	110.40	104.14	1
CB-CG-CD1	120.70	113.60	1
CG-CD-NE2	116.40	122.66	1
OE1-CD-NE2	122.60	118.42	1
C-CA-CB	109.10	118.28	1
OE1-CD-NE2	122.60	118.43	1
N-CA-CB	110.50	117.59	2
OE1-CD-NE2	122.60	126.77	1
C-CA-CB	110.10	118.03	1
CA-C-N	116.20	124.55	1
CA-CB-CG	114.10	122.44	1
N-CA-CB	110.50	103.41	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	113.30	101.20	1
O-C-N	123.00	116.33	5
C-N-CA	121.70	129.21	3
CA-C-N	116.20	124.54	1
CB-CG-ND2	116.40	110.14	1
CB-CG-CD1	110.70	98.19	1
NH1-CZ-NH2	119.30	113.88	1
CA-CB-CG1	110.40	117.49	1
CA-CB-CG2	110.50	103.41	1
NE-CZ-NH2	119.20	122.95	1
N-CA-CB	111.50	118.59	2
CB-CG-CD	111.30	120.89	1
C-N-CA	121.70	129.20	4
CA-CB-OG1	109.60	115.85	1
N-CA-CB	110.50	103.42	2
C-CA-CB	110.10	118.02	1
CB-CG-CD	112.60	105.52	1
CB-CG-CD1	120.70	127.78	1
CA-C-O	120.80	113.72	1
N-CD-CG	103.20	109.45	1
NE-CZ-NH1	121.50	125.67	1
C-CA-CB	110.10	102.19	2
N-CA-CB	110.50	117.58	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-CE2-CZ	119.60	127.10	1
CB-CG-CD1	120.70	113.62	1
NE-CZ-NH1	121.50	117.34	1
C-CA-CB	111.40	119.31	1
NE-CZ-NH2	119.20	115.45	1
N-CA-C	111.00	122.66	1
O-C-N	123.00	116.34	7
OG1-CB-CG2	109.30	100.97	1
CA-C-N	116.20	124.53	1
CA-CB-CG2	110.50	117.58	1
C-CA-CB	110.10	118.01	1
C-N-CA	121.70	129.19	1
C-CA-CB	110.50	104.26	3
CA-CB-CG	114.10	122.42	1
N-CA-CB	110.50	103.43	2
CG1-CB-CG2	110.80	101.65	1
NH1-CZ-NH2	119.30	113.89	1
C-CA-CB	110.50	116.74	1
CA-CB-CG1	110.40	117.47	2
CB-CG-CD2	120.70	113.63	1
CB-CG-ND1	122.70	128.94	1
C-CA-CB	110.10	118.00	1
OE1-CD-NE2	122.60	118.44	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	117.57	2
CA-C-O	120.80	127.87	1
O-C-N	123.00	116.35	7
CA-CB-CG2	110.50	103.43	1
CA-CB-CG	112.60	108.44	1
NE-CZ-NH1	121.50	125.66	1
CG-CD-OE1	120.80	129.11	1
N-CD-CG	103.20	109.43	1
C-N-CA	121.70	129.18	3
N-CA-C	111.00	122.64	1
C-CA-CB	110.10	102.20	1
NE-CZ-NH2	119.20	115.46	1
C-CA-CB	110.50	116.73	1
CB-CG-OD1	120.80	129.11	2
CA-CB-OG1	109.60	115.83	1
CA-CB-CG1	110.40	117.46	2
NH1-CZ-NH2	119.30	113.90	1
CA-CB-CG	114.10	122.41	1
C-N-CA	121.70	129.17	3
N-CA-CB	110.50	117.56	1
N-CA-CB	110.50	103.44	1
N-CA-CB	103.00	107.57	1
CA-C-O	120.80	127.86	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.36	3
CA-C-N	116.20	124.50	3
N-CA-CB	110.50	117.55	4
CA-CB-CG	113.90	106.43	1
CA-C-O	120.80	127.85	1
C-CA-CB	110.10	117.98	1
CG-CD-NE2	116.40	122.62	1
NH1-CZ-NH2	119.30	113.91	2
OE1-CD-NE2	122.60	118.45	1
C-N-CA	121.70	129.16	4
O-C-N	123.00	116.37	6
CB-CG-CD2	131.20	125.81	1
CG-CD-NE	112.00	102.88	2
CA-C-N	116.20	124.49	2
CA-CB-OG	111.10	119.39	1
CA-C-N	116.90	123.12	1
N-CD-CG	103.20	109.42	1
C-CA-CB	110.10	117.97	2
CA-CB-CG2	110.40	117.44	1
CA-CB-CG	112.60	116.74	1
N-CA-CB	111.50	118.54	2
C-N-CA	121.70	114.24	1
N-CA-CB	110.50	117.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	124.48	1
CA-CB-CG	113.80	109.66	1
C-N-CA	121.70	129.15	5
O-C-N	123.00	116.38	6
C-N-CA	121.70	114.25	1
CA-C-O	120.80	127.84	1
CA-C-N	116.90	123.11	1
CA-CB-CG2	110.40	103.36	1
N-CA-CB	110.50	103.46	1
CA-CB-CG	112.60	108.46	1
CA-CB-CG	113.80	117.94	1
CA-C-N	116.20	124.47	1
C-CA-CB	111.40	103.54	1
C-N-CA	121.70	129.14	4
N-CA-CB	111.50	118.53	2
C-CA-CB	110.10	117.96	1
N-CA-CB	110.50	117.53	2
CA-CB-OG	111.10	119.37	1
CG-CD-NE2	116.40	122.60	1
C-CA-CB	110.50	104.30	1
CA-CB-CG	113.80	109.67	1
CG-CD-NE2	116.40	110.20	1
CB-CG-CD	112.60	105.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	116.39	1
C-CA-CB	111.60	119.86	1
CA-C-N	116.20	124.46	1
CA-CB-CG2	110.50	117.52	1
N-CA-CB	110.50	103.48	2
CG-CD2-CE2	120.70	127.72	1
N-CA-CB	103.00	107.54	1
CD1-CG-CD2	118.60	112.40	1
C-N-CA	121.70	129.13	4
CG-CD-CE	111.30	120.80	1
NH1-CZ-NH2	119.30	113.93	1
C-CA-CB	110.10	117.95	1
CB-CG-OD1	120.80	129.06	1
N-CA-CB	110.50	117.52	1
O-C-N	123.00	116.40	9
CB-CG-CD1	120.80	126.99	1
CA-CB-OG	111.10	119.35	1
CB-CG-CD	112.60	119.61	2
CA-C-O	120.80	127.81	1
C-CA-CB	110.10	117.94	1
CG-CD-CE	111.30	120.79	1
CA-CB-CG1	110.40	117.41	1
OE1-CD-NE2	122.60	118.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	99.45	1
CB-CG-CD2	120.70	127.71	1
C-N-CA	121.70	129.12	5
OD1-CG-ND2	122.60	118.48	2
CA-CB-CG2	110.50	103.49	1
N-CA-C	113.30	101.34	1
N-CA-CB	111.50	118.51	1
N-CA-CB	110.50	117.51	3
N-CA-CB	110.40	104.22	1
C-CA-CB	111.40	119.23	1
CA-CB-CG	114.10	122.34	2
C-CA-CB	111.40	103.57	1
CB-CG-CD	112.60	105.59	1
O-C-N	123.00	116.41	9
OE1-CD-OE2	122.90	113.01	1
N-CA-CB	110.50	117.50	2
CB-CG-CD	111.30	120.77	1
CA-CB-CG	113.80	109.68	1
N-CA-CB	110.50	103.50	1
CB-CG-CD	112.60	119.60	2
C-N-CA	121.70	129.11	2
N-CA-CB	110.40	116.58	1
CG-CD-NE2	116.40	122.58	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	104.23	2
CA-C-N	116.20	124.43	1
N-CA-C	111.00	122.52	1
C-CA-CB	110.10	117.92	1
CA-CB-CG	112.60	116.71	1
CA-C-O	120.80	113.81	3
N-CA-CB	110.50	117.49	3
NE-CZ-NH2	119.20	122.90	1
CA-CB-CG	113.80	117.91	1
OE1-CD-NE2	122.60	126.71	1
CA-CB-OG1	109.60	115.77	2
CD1-CG-CD2	110.80	101.75	1
O-C-N	123.00	116.42	6
N-CD-CG	103.20	109.37	1
C-N-CA	121.70	129.10	5
CA-C-N	116.90	123.07	1
CA-C-N	116.20	124.42	1
N-CA-C	113.30	101.38	1
C-CA-CB	110.10	117.91	1
CA-CB-CG1	110.40	117.39	1
C-CA-CB	110.50	104.33	1
C-CA-CB	110.10	102.29	1
CA-CB-CG2	110.40	117.39	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	104.24	1
CA-CB-CG	114.10	122.32	1
OD1-CG-ND2	122.60	118.49	1
CG-CD2-CE2	121.20	127.36	1
O-C-N	123.00	116.43	7
CA-C-O	120.80	127.78	2
C-N-CA	121.70	129.09	5
CA-CB-CG	114.10	105.88	1
N-CA-CB	110.50	103.52	2
CA-C-N	116.90	123.06	1
CG-CD-OE1	120.80	129.01	1
N-CA-CB	111.50	118.48	1
NE-CZ-NH2	119.20	115.50	1
N-CA-CB	110.50	117.48	2
C-CA-CB	110.10	117.90	1
C-CA-CB	111.40	119.20	1
CA-C-N	116.20	124.41	2
CA-CB-CG2	110.50	103.52	1
CG-CD-CE	111.30	120.74	1
CB-SG-C7	106.10	93.79	1
C-CA-CB	110.10	102.30	1
CA-CB-CG	113.80	117.90	1
CG-CD-NE	112.00	102.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	110.80	119.83	1
N-CA-CB	110.50	117.47	6
N-CA-CB	110.50	103.53	1
O-C-N	123.00	116.44	9
CA-CB-CG1	110.40	103.43	1
CG-CD1-CE1	120.70	113.73	1
NE-CZ-NH2	119.20	122.89	1
NH1-CZ-NH2	119.30	113.97	1
CA-CB-CG	114.10	122.30	1
C-CA-CB	110.10	117.89	3
C-N-CA	121.70	129.08	7
CB-CG-CD	111.30	120.73	2
CA-CB-CG1	110.40	117.37	2
CD1-CG-CD2	118.60	112.45	1
N-CA-CB	111.50	118.47	1
N-CA-C	111.00	99.52	1
CG-CD-CE	111.30	120.73	1
CA-C-O	120.80	127.77	2
N-CA-CB	110.40	104.25	1
O-C-N	123.00	129.56	1
CA-C-O	120.80	129.41	1
OE1-CD-NE2	122.60	118.50	1
CA-C-O	120.80	113.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.07	3
C-CA-CB	110.10	117.88	1
CA-CB-CG	114.10	122.29	1
O-C-N	123.00	116.45	4
CA-C-N	116.90	123.04	1
N-CA-CB	110.40	104.26	2
CA-CB-OG	111.10	119.29	1
CD1-CG-CD2	118.60	112.46	1
CA-C-N	116.20	124.39	2
CA-C-O	120.80	113.84	1
CG-CD-NE	112.00	102.99	1
CG-CD-CE	111.30	120.72	1
N-CA-CB	111.50	118.46	1
C-CA-CB	110.50	116.64	1
CA-CB-CG	112.60	108.50	1
CA-CB-CG	112.60	108.51	2
CA-CB-CG	113.80	117.89	1
CA-CB-CG2	110.50	117.46	1
CB-CG-CD2	120.80	126.94	1
CA-CB-CG	114.10	105.91	1
CG-CD-NE2	116.40	110.26	1
C-CA-CB	111.40	103.62	1
CA-C-O	120.80	127.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OG1	109.60	115.74	1
CA-C-N	116.20	124.38	1
CB-CG-CD	111.30	120.71	1
CD-NE-CZ	124.40	118.67	1
C-CA-CB	110.10	102.33	2
C-N-CA	121.70	129.06	2
C-CA-CB	111.40	103.63	1
CG-CD-CE	111.30	120.71	1
C-CA-CB	110.10	117.87	1
O-C-N	123.00	116.46	4
CA-C-O	120.80	113.85	1
CA-N-CD	112.00	106.28	1
OE1-CD-NE2	122.60	126.69	1
CA-CB-CG2	110.50	117.45	1
CB-CG-ND2	116.40	122.53	2
N-CA-CB	111.50	118.45	3
N-CA-CB	110.50	103.55	2
CB-CG-CD	111.30	120.70	2
C-CA-CB	110.50	116.63	1
NH1-CZ-NH2	119.30	113.99	1
C-N-CA	121.70	129.05	5
OE1-CD-NE2	122.60	118.51	1
N-CA-CB	110.50	103.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	99.56	1
CG-CD1-CE1	121.20	115.07	1
CG1-CB-CG2	110.80	101.82	1
CA-C-N	116.90	123.02	1
C-N-CA	121.70	114.35	1
CB-CG-CD	112.60	119.54	1
OD1-CG-ND2	122.60	118.52	2
O-C-N	123.00	116.47	3
C-CA-CB	111.60	103.44	1
O-C-N	123.00	129.53	1
N-CA-C	111.00	122.43	1
CA-C-O	120.80	127.74	1
N-CA-CB	103.00	107.49	1
N-CA-CB	111.50	118.44	1
CG-CD1-CE1	120.70	113.76	1
C-CA-CB	111.40	103.65	1
CA-C-O	120.80	127.73	2
N-CA-CB	110.50	103.57	1
C-N-CA	121.70	129.04	5
O-C-N	123.00	116.48	5
N-CA-CB	110.50	117.43	2
CB-CG-CD	112.60	119.53	1
CG-CD-CE	111.30	120.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG1	110.40	117.33	1
C-CA-CB	110.10	102.35	1
C-CA-CB	110.50	104.39	1
N-CA-CB	111.50	118.43	1
N-CA-CB	110.40	104.29	1
C-CA-CB	111.40	103.66	1
CB-CG1-CD	113.80	105.24	1
C-N-CA	121.70	129.03	8
N-CA-CB	111.50	118.42	1
CA-CB-CG	113.80	109.73	1
CA-C-O	120.80	127.72	4
C-CA-CB	110.10	117.84	2
CB-CG-CD	112.60	119.52	1
CA-CB-CG1	110.40	117.32	1
N-CA-CB	110.50	103.58	3
CA-C-N	116.20	124.34	1
CA-CB-CG2	110.50	117.42	1
CG-CD2-CE2	121.20	115.09	1
O-C-N	123.00	116.49	3
C-N-CA	121.70	114.37	1
N-CA-CB	110.50	117.42	1
NE-CZ-NH2	119.20	115.54	1
NE-CZ-NH1	121.50	125.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	108.06	1
CA-C-O	120.80	113.88	1
N-CA-CB	110.40	104.30	1
C-N-CA	121.70	129.02	5
CG-CD-CE	111.30	120.66	1
CA-CB-CG	113.80	117.87	1
CA-N-CD	112.00	106.31	1
CA-C-O	120.80	127.71	4
N-CA-CB	110.50	117.41	2
CA-CB-CG2	110.50	117.41	1
C-CA-CB	110.10	117.83	1
CA-CB-OG	111.10	119.23	1
N-CA-CB	111.50	118.41	2
CB-CG-CD	111.30	120.65	1
CG-CD-NE	112.00	103.05	1
CA-CB-CG2	110.40	103.49	2
N-CA-C	111.00	99.61	1
CB-CG-CD	112.60	119.51	1
CG-CD-NE2	116.40	122.50	1
O-C-N	123.00	116.50	10
CA-CB-CG2	110.50	103.59	2
CA-C-O	120.80	113.89	2
CB-CG-ND2	116.40	122.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	114.39	1
CG-CD1-CE1	120.70	113.79	1
CA-CB-OG1	109.60	115.70	1
CG-CD-NE	112.00	103.06	1
CA-CB-CG1	110.40	117.31	1
N-CA-C	111.00	99.62	1
CA-C-N	116.90	122.99	2
CG-CD-NE2	116.40	110.31	1
CA-CB-CG	113.80	109.74	1
CG-CD-NE2	116.40	122.49	1
C-CA-CB	111.40	103.68	1
CD2-NE2-CE1	109.00	104.94	1
N-CA-CB	110.50	103.60	3
N-CA-CB	110.50	117.40	3
C-CA-CB	110.10	117.81	2
C-N-CA	121.70	129.01	1
O-C-N	123.00	116.51	1
N-CA-C	111.00	99.63	1
N-CA-CB	111.50	118.40	1
C-CA-CB	110.10	102.39	1
CB-CG-CD2	120.70	113.80	1
N-CA-CB	110.40	116.49	1
CB-CG-CD	112.60	119.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-OE1	118.40	127.73	1
CA-C-O	120.80	127.70	1
CA-CB-CG	114.10	122.21	1
N-CA-C	111.00	122.36	1
C-CA-CB	111.60	119.71	1
OG1-CB-CG2	109.30	101.19	1
O-C-N	123.00	129.49	1
C-CA-CB	110.10	117.80	3
CA-CB-CG2	110.50	117.39	1
C-CA-CB	110.10	102.40	1
CG-CD-NE2	116.40	122.48	1
C-N-CA	121.70	129.00	2
CA-C-N	116.90	122.98	2
CA-CB-CG	112.60	116.65	1
CA-C-N	116.20	124.30	1
O-C-N	123.00	116.52	5
CE1-CZ-CE2	120.30	112.20	1
N-CA-CB	110.50	117.39	1
N-CA-C	113.30	101.55	1
CA-C-O	120.80	113.91	1
N-CA-C	112.10	122.23	1
CG-CD-CE	111.30	120.62	1
NE-CZ-NH1	121.50	125.55	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	108.55	1
N-CA-CB	110.50	103.62	1
CA-CB-CG1	110.40	117.28	1
OE1-CD-NE2	122.60	118.55	1
C-CA-CB	110.50	104.43	1
C-N-CA	121.70	128.99	1
CA-CB-CG	113.80	109.75	1
N-CA-C	111.00	99.66	1
CD1-CG-CD2	110.80	101.90	2
N-CA-C	111.00	99.67	1
C-CA-CB	110.10	117.79	1
CB-CG-CD1	120.70	127.58	1
CB-CG-ND2	116.40	110.33	2
CA-C-O	120.80	127.68	1
C-N-CA	121.70	128.98	3
CA-CB-OG1	109.60	115.67	1
CG-CD-OE1	120.80	128.89	1
CG-CD-NE	112.00	103.10	1
CA-CB-OG	111.10	119.19	1
CA-CB-CG2	110.40	103.52	1
N-CA-CB	110.50	117.38	1
O-C-N	123.00	116.53	1
CA-C-O	120.80	127.67	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OE1-CD-NE2	122.60	118.56	2
CA-CB-CG1	110.40	117.27	1
OD1-CG-ND2	122.60	118.56	1
CB-CG-CD1	120.80	114.74	1
N-CA-C	111.00	122.32	1
NE-CZ-NH1	121.50	125.54	2
CA-CB-OG1	109.60	115.66	1
N-CA-CB	111.50	104.63	1
CA-CB-CG	114.10	106.02	2
CB-CG-CD	111.30	120.59	1
CA-CB-CG2	110.50	117.37	1
O-C-N	123.00	116.54	6
CA-C-N	116.20	124.28	3
C-CA-CB	111.40	103.73	1
N-CA-CB	110.50	117.37	1
CA-CB-CG	112.60	116.64	2
C-N-CA	121.70	128.97	4
N-CA-C	111.00	99.69	1
NH1-CZ-NH2	119.30	124.55	1
CA-C-O	120.80	127.66	4
CA-C-O	120.80	113.94	3
N-CA-CB	111.50	118.36	1
OE1-CD-NE2	122.60	126.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	117.77	1
C-CA-CB	110.50	104.44	1
CA-CB-CG1	110.40	117.26	1
C-CA-CB	110.10	102.43	1
N-CA-CB	110.50	117.36	1
CB-CG-CD	112.60	105.74	1
CA-CB-CG1	110.40	103.54	1
O-C-N	123.00	116.55	5
C-N-CA	121.70	128.96	7
OD1-CG-ND2	122.60	118.57	1
C-CA-CB	110.10	117.76	2
CA-C-N	116.20	124.27	1
CG-CD-OE1	120.80	128.87	1
OE1-CD-NE2	122.60	126.63	1
CB-CG-OD1	120.80	112.73	1
CB-CG-CD	112.60	119.46	1
CA-CB-CG1	110.40	117.25	1
N-CA-CB	110.50	117.35	3
CA-CB-CG	112.60	116.63	1
OG1-CB-CG2	109.30	101.24	1
CB-CG-CD1	120.80	114.75	1
CA-N-CD	112.00	106.36	1
OE1-CD-OE2	122.90	113.23	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	129.45	1
N-CA-C	111.00	99.71	1
CG-CD1-CE1	121.20	115.15	1
CA-C-O	120.80	113.95	1
NE-CZ-NH2	119.20	115.57	1
NE-CZ-NH1	121.50	125.53	1
C-N-CA	121.70	128.95	3
CA-CB-CG	114.10	106.04	1
C-CA-CB	110.50	104.46	1
N-CA-CB	111.50	118.35	1
CG-CD-CE	111.30	120.56	1
CA-CB-CG2	110.40	117.25	1
N-CA-CB	103.00	107.43	1
N-CA-CB	110.50	103.65	1
CB-CG-CD	112.60	105.75	1
CA-CB-OG	111.10	119.15	1
CA-CB-CG2	110.40	103.55	1
CA-CB-CG1	110.40	103.55	1
O-C-N	123.00	116.56	1
CD1-CG-CD2	118.60	112.56	1
C-CA-CB	110.10	102.45	1
CB-CG-CD	112.60	105.76	1
OG1-CB-CG2	109.30	101.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	122.27	1
CD1-CG-CD2	118.60	124.64	1
C-CA-CB	111.60	103.55	1
C-N-CA	121.70	128.94	2
CA-C-O	120.80	113.96	1
CG-CD1-CE1	120.70	127.54	1
CA-CB-CG	112.60	116.62	2
N-CA-CB	110.50	117.34	1
CA-C-O	120.80	127.64	2
C-CA-CB	110.10	117.74	3
CB-CG-CD	111.30	120.55	1
NE-CZ-NH1	121.50	117.48	1
CB-CG-ND2	116.40	110.37	1
CA-CB-OG	111.10	119.14	1
C-CA-CB	110.10	102.46	1
N-CA-CB	110.50	117.33	4
N-CA-C	111.00	99.74	1
CA-C-O	120.80	113.97	1
C-CA-CB	111.60	103.56	1
CA-C-N	116.90	122.93	2
C-N-CA	121.70	128.93	2
CA-C-N	116.20	124.24	1
CA-CB-CG	113.80	109.78	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE-CZ-NH1	121.50	125.52	1
O-C-N	123.00	116.57	3
CA-CB-CG	113.90	121.13	1
CA-CB-CG	113.80	117.82	1
O-C-N	123.00	129.43	1
NE-CZ-NH2	119.20	115.58	1
C-CA-CB	110.10	117.73	2
CB-CG-OD1	118.40	127.64	1
CA-C-N	116.90	122.92	1
O-C-N	123.00	116.58	4
CA-CB-CG	114.10	122.13	1
OE1-CD-NE2	122.60	118.59	3
CA-CB-CG	114.10	106.07	1
NE-CZ-NH2	119.20	122.81	1
N-CA-CB	111.50	118.32	2
CG-CD-NE2	116.40	122.42	1
NH1-CZ-NH2	119.30	114.08	2
CA-CB-CG2	110.50	103.68	1
C-N-CA	121.70	128.92	5
N-CA-CB	110.50	117.32	1
N-CA-CB	111.50	104.68	1
O-C-N	123.00	129.42	2
CG-CD-CE	111.30	120.53	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	104.38	1
CA-CB-CG	113.80	109.79	1
CA-C-N	116.20	124.22	1
CA-CB-CG	112.60	116.61	1
CD1-CG-CD2	118.60	112.58	1
N-CA-CB	103.00	107.41	1
C-CA-CB	110.10	117.72	1
CA-CB-CG	113.80	117.81	1
C-CA-CB	110.10	102.48	1
CA-C-O	120.80	113.98	1
CB-CG-OD1	120.80	112.78	1
O-C-N	123.00	116.59	8
NE-CZ-NH1	121.50	125.51	1
C-CA-CB	110.50	116.51	1
CD1-CG-CD2	110.80	101.98	1
C-N-CA	121.70	128.91	3
C-CA-CB	109.10	117.91	1
CA-C-O	120.80	127.61	2
CB-CG-ND1	122.70	128.71	1
CA-CB-CG1	110.40	117.21	1
CG-CD-OE1	120.80	112.79	1
N-CA-CB	110.50	117.31	1
C-N-CA	121.70	114.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD1-CG-CD2	110.80	101.99	1
CA-CB-CG	113.80	109.80	1
N-CA-CB	110.50	117.30	1
CB-CG-CD	112.60	105.80	1
C-CA-CB	110.10	102.50	1
C-N-CA	121.70	128.90	2
CG1-CB-CG2	110.80	102.00	1
C-CA-CB	109.10	117.90	1
CB-CG-CD2	120.80	126.80	1
CA-C-O	120.80	127.60	1
CG-CD2-NE2	107.20	111.20	1
O-C-N	123.00	116.60	1
C-N-HN	112.30	124.30	1
CD-CG-HG1	120.00	108.00	1
HB1-CB-HB2	98.00	110.00	1
HD21-CD2-HD22	98.00	110.00	1
CB-CG2-HG21	121.00	109.00	1
C-N-HN	112.29	124.30	4
CE-CD-HD1	120.01	108.00	1
CA-N-HN	126.01	114.00	2
N-CA-HA	97.99	110.00	1
C-CA-HA	121.01	109.00	1
HB1-CB-HB2	97.99	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CB-HB1	95.99	108.00	1
CB-CG-HG2	121.01	109.00	1
CG-CB-HB2	120.01	108.00	1
HH11-NH1-HH12	132.01	120.00	1
HH21-NH2-HH22	132.01	120.00	1
HB2-CB-HB3	97.99	110.00	1
C-CA-HA	96.99	109.00	1
CG-CB-HB1	120.01	108.00	1
HG11-CG1-HG13	97.98	110.00	1
C-CA-HA1	96.98	109.00	1
HG21-CG2-HG23	97.98	110.00	1
C-N-HN	112.28	124.30	2
HB2-CB-HB3	97.98	110.00	1
HE21-NE2-HE22	132.02	120.00	1
C-CA-HA	96.98	109.00	2
HB1-CB-HB2	122.02	110.00	1
HG21-CG2-HG22	122.02	110.00	1
CB-CG1-HG12	121.02	109.00	1
CB-CA-HA	96.98	109.00	1
CA-N-HN	126.03	114.00	2
HA1-CA-HA2	121.03	109.00	1
CB-CA-HA	121.03	109.00	2
CG-CD-HD1	121.03	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	96.97	109.00	2
CB-CG2-HG23	121.03	109.00	1
CB-CA-HA	96.97	109.00	1
C-N-HN	112.27	124.30	1
CG-CB-HB2	122.03	110.00	1
N-CD-HD2	121.03	109.00	1
HD12-CD1-HD13	97.96	110.00	1
HD22-CD2-HD23	97.96	110.00	1
C-N-HN	112.26	124.30	4
HG11-CG1-HG12	97.96	110.00	1
HB1-CB-HB2	97.96	110.00	1
HD22-CD2-HD23	97.95	110.00	1
N-CA-HA2	97.95	110.00	1
CA-CB-HB1	96.95	109.00	1
HG12-CG1-HG13	97.95	110.00	1
N-CA-HA	97.95	110.00	3
HG22-CG2-HG23	97.95	110.00	1
HB1-CB-HB2	97.95	110.00	2
HD21-ND2-HD22	132.05	120.00	1
C-CA-HA	96.95	109.00	1
CB-CG2-HG22	97.95	110.00	1
C-N-HN	112.25	124.30	1
HD12-CD1-HD13	97.95	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE1-ND1-HD1	113.30	125.35	1
C-N-HN	112.24	124.30	3
CA-CB-HB2	121.06	109.00	1
N-CA-HA	97.94	110.00	2
HD1-CD-HD3	97.94	110.00	1
CA-CB-HB1	96.94	109.00	1
CB-CG1-HG13	121.06	109.00	1
HG11-CG1-HG12	97.94	110.00	1
HB1-CB-HB2	97.94	110.00	1
N-CA-HA1	97.94	110.00	1
NE2-CD2-HD2	114.34	126.40	1
C-CA-HA	96.94	109.00	1
CZ-NH2-HH22	107.94	120.00	1
C-N-HN	112.23	124.30	3
CD-CE-HE2	121.06	109.00	1
CG-CD2-HD21	96.94	109.00	1
CA-CB-HB1	96.93	109.00	2
HB1-CB-HB3	97.93	110.00	1
HB1-CB-HB2	97.93	110.00	1
HZ2-NZ-HZ3	96.93	109.00	1
CA-N-HN	126.07	114.00	1
CG-CD2-HD21	121.07	109.00	1
HB1-CB-HB2	97.92	110.00	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD1-HD11	121.08	109.00	1
CE-CD-HD2	120.08	108.00	1
CB-CG-HG1	121.08	109.00	1
CB-CG2-HG21	121.08	109.00	1
CD-CG-HG2	97.92	110.00	1
CB-CG-HG2	96.92	109.00	1
OG1-CB-HB	96.92	109.00	1
N-CA-HA	97.92	110.00	1
HG1-CG-HG2	97.92	110.00	2
HD11-CD1-HD13	97.92	110.00	1
CB-CA-HA	96.92	109.00	1
CG-CB-HB1	120.08	108.00	1
HZ1-NZ-HZ3	96.92	109.00	1
C-N-HN	112.22	124.30	2
HD22-CD2-HD23	97.92	110.00	1
CA-CB-HB	121.09	109.00	1
CA-N-HN	101.91	114.00	1
CA-CB-HB1	96.91	109.00	1
C-N-HN	112.21	124.30	1
HG22-CG2-HG23	96.91	109.00	1
CB-CG-HG	121.09	109.00	1
HB2-CB-HB3	97.91	110.00	1
N-CA-HA2	97.91	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HA1-CA-HA2	121.09	109.00	1
CB-CG-HG2	121.09	109.00	1
CB-CG1-HG11	96.91	109.00	1
CG-CB-HB1	95.91	108.00	1
C-CA-HA	96.91	109.00	2
HG1-CG-HG2	97.91	110.00	1
CG-CB-HB2	120.09	108.00	1
N-CA-HA	122.10	110.00	1
CD-CG-HG1	120.10	108.00	1
C-N-HN	112.20	124.30	3
HD1-CD-HD3	97.90	110.00	1
CA-N-HN	126.10	114.00	1
CZ-NH1-HH12	107.90	120.00	1
CB-CG-HG1	96.90	109.00	1
HB1-CB-HB2	97.90	110.00	1
CG-CD-HD1	121.11	109.00	1
CA-CB-HB1	96.89	109.00	2
HG21-CG2-HG23	97.89	110.00	1
N-CA-HA1	97.89	110.00	2
HB1-CB-HB2	122.11	110.00	1
C-CA-HA1	96.89	109.00	1
HG1-CG-HG2	97.89	110.00	1
HG11-CG1-HG12	97.89	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	112.19	124.30	1
HD1-CD-HD2	97.88	110.00	1
CG-CD1-HD11	121.12	109.00	1
C-N-HN	112.18	124.30	1
CA-N-HN	126.12	114.00	3
CD-CG-HG2	95.88	108.00	1
HB1-CB-HB2	97.88	110.00	1
CA-CB-HB2	96.88	109.00	1
C-CA-HA	96.88	109.00	1
OG-CB-HB2	121.12	109.00	1
CG-CD1-HD1	107.52	119.65	1
HG11-CG1-HG12	97.87	110.00	2
CB-CG1-HG12	121.13	109.00	1
HD22-CD2-HD23	97.87	110.00	1
CB-OG1-HG1	97.87	110.00	1
HD2-CD-HD3	97.87	110.00	1
C-CA-HA	96.87	109.00	2
CB-CA-HA	121.13	109.00	1
C-N-HN	112.17	124.30	1
CB-CA-HA	96.87	109.00	1
HG12-CG1-HG13	97.87	110.00	1
CB-CG2-HG23	121.13	109.00	1
HE1-CE-HE3	97.86	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD1-CD-HD2	97.86	110.00	1
C-N-HN	112.16	124.30	5
C-CA-HA	121.14	109.00	2
CA-N-HN	126.14	114.00	1
CB-CA-HA	96.86	109.00	1
HB1-CB-HB2	97.86	110.00	1
CA-CB-HB3	121.14	109.00	1
HG21-CG2-HG23	97.86	110.00	1
CG-CD2-HD21	121.14	109.00	1
HB2-CB-HB3	97.86	110.00	1
HG1-CG-HG2	97.86	110.00	1
CB-CG-HG1	121.14	109.00	1
HG21-CG2-HG23	96.86	109.00	1
CB-CG2-HG21	122.14	110.00	1
CG-CB-HB2	122.14	110.00	1
CA-N-HN	126.15	114.00	1
C-CA-HA	96.85	109.00	2
CA-CB-HB1	121.15	109.00	1
CA-CB-HB3	121.15	109.00	1
C-N-HN	112.15	124.30	3
HB1-CB-HB2	97.85	110.00	1
N-CD-HD1	121.15	109.00	1
CG1-CB-HB	95.85	108.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE-CD-HD1	120.15	108.00	1
CG-CB-HB1	120.15	108.00	1
CB-OG1-HG1	97.84	110.00	1
C-CA-HA	96.84	109.00	2
CB-CG1-HG13	121.16	109.00	1
CA-N-HN	126.16	114.00	2
HD21-CD2-HD22	97.84	110.00	1
CA-CB-HB2	121.16	109.00	1
HB1-CB-HB2	97.84	110.00	2
C-N-HN	112.14	124.30	1
CD-CG-HG1	120.16	108.00	1
CB-CA-HA	121.16	109.00	1
CG-CB-HB2	122.16	110.00	1
CA-CB-HB1	96.84	109.00	1
CD-NE-HE	130.06	117.90	1
HG21-CG2-HG22	97.84	110.00	1
CG-CB-HB2	120.16	108.00	1
HG1-CG-HG2	97.83	110.00	1
CD-CG-HG1	120.17	108.00	1
HA1-CA-HA2	121.17	109.00	1
CB-CG-HG2	121.17	109.00	1
HZ2-NZ-HZ3	96.83	109.00	1
CB-CA-HA	96.83	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB2	96.83	109.00	2
N-CA-HA	97.83	110.00	1
C-N-HN	112.13	124.30	3
CZ-OH-HH	97.83	110.00	1
CA-N-HN	126.17	114.00	1
HD1-CD-HD3	97.83	110.00	1
HD1-CD-HD2	97.83	110.00	1
CG-CB-HB1	97.83	110.00	1
HD2-CD-HD3	97.83	110.00	1
C-CA-HA1	96.83	109.00	1
CD-CG-HG2	120.17	108.00	1
CG-CB-HB2	122.17	110.00	1
C-N-HN	112.12	124.30	2
CG-CD2-HD21	121.18	109.00	1
HD21-ND2-HD22	132.18	120.00	1
CA-N-HN	126.18	114.00	1
HB1-CB-HB2	97.82	110.00	1
C-CA-HA	96.82	109.00	1
HG21-CG2-HG22	97.82	110.00	1
HG1-CG-HG2	97.82	110.00	1
CG-CD-HD2	121.19	109.00	1
HE21-NE2-HE22	132.19	120.00	1
C-N-HN	112.11	124.30	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	122.19	110.00	1
HB1-CB-HB2	97.81	110.00	2
HG11-CG1-HG13	97.81	110.00	1
CD-CG-HG2	97.81	110.00	1
HG22-CG2-HG23	97.81	110.00	1
CB-CA-HA	96.81	109.00	1
HD1-CD-HD2	97.81	110.00	1
HB1-CB-HB3	97.81	110.00	1
CA-CB-HB2	96.81	109.00	2
CA-CB-HB	96.81	109.00	1
HD1-CD-HD3	97.81	110.00	2
CG-CD1-HD13	121.19	109.00	1
HA1-CA-HA2	121.19	109.00	1
CB-CG-HG2	121.19	109.00	1
CB-CG-HG1	121.19	109.00	1
CG-CB-HB1	95.80	108.00	1
HG1-CG-HG2	97.80	110.00	1
HZ2-NZ-HZ3	96.80	109.00	1
HB1-CB-HB2	97.80	110.00	2
HD1-CD-HD2	97.80	110.00	1
CA-CB-HB2	121.20	109.00	1
CG2-CB-HB	120.20	108.00	1
HA1-CA-HA2	121.20	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CD-HD2	121.20	109.00	1
CA-N-HN	126.20	114.00	1
CD-NE2-HE21	107.80	120.00	1
C-N-HN	112.09	124.30	1
HB1-CB-HB2	97.79	110.00	4
HB2-CB-HB3	97.79	110.00	1
CB-CA-HA	96.79	109.00	1
HA1-CA-HA2	121.21	109.00	1
HG11-CG1-HG12	97.79	110.00	1
HD21-ND2-HD22	107.79	120.00	1
CD-CG-HG2	95.79	108.00	1
C-CA-HA	96.79	109.00	1
HG1-CG-HG2	97.79	110.00	1
CD-CG-HG2	120.21	108.00	1
CB-CG2-HG22	121.22	109.00	1
CD-CE-HE1	121.22	109.00	1
CB-CG-HG2	121.22	109.00	2
C-N-HN	112.08	124.30	3
CA-CB-HB	121.22	109.00	1
CG1-CB-HB	95.78	108.00	1
HZ1-NZ-HZ3	96.78	109.00	1
CG-CB-HB1	95.78	108.00	1
HE21-NE2-HE22	107.78	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD12-CD1-HD13	97.78	110.00	1
CZ-NE-HE	105.68	117.90	1
CA-CB-HB1	121.22	109.00	2
CA-N-HN	126.22	114.00	1
N-CA-HA2	122.22	110.00	1
CB-CG1-HG12	121.22	109.00	1
HB2-CB-HB3	122.22	110.00	1
CD-CG-HG1	95.78	108.00	1
HG1-CG-HG2	97.77	110.00	2
HD1-CD-HD2	97.77	110.00	2
CA-CB-HB1	121.23	109.00	1
HB1-CB-HB2	97.77	110.00	3
CB-CA-HA	121.23	109.00	1
CB-CA-HA	96.77	109.00	1
CD-CG-HG1	97.77	110.00	1
HD11-CD1-HD12	97.77	110.00	1
SG-CB-HB2	120.23	108.00	1
C-CA-HA	96.77	109.00	1
HD22-CD2-HD23	97.77	110.00	1
CB-CG2-HG23	121.23	109.00	1
CB-CG2-HG23	121.24	109.00	1
CB-CA-HA	96.76	109.00	1
CA-N-HN	126.24	114.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	112.06	124.30	1
HZ1-NZ-HZ3	96.76	109.00	1
CG-CD-HD1	96.76	109.00	1
CG-CD-HD2	121.24	109.00	1
HB1-CB-HB2	97.76	110.00	1
HG21-CG2-HG22	96.75	109.00	1
C-N-HN	112.05	124.30	2
HG11-CG1-HG12	97.75	110.00	1
CB-CG1-HG12	121.25	109.00	1
HG21-CG2-HG22	97.75	110.00	1
CA-CB-HB1	96.75	109.00	1
C-CA-HA1	96.75	109.00	1
CB-CG2-HG21	121.26	109.00	1
C-CA-HA	96.74	109.00	2
CD-NE2-HE21	107.74	120.00	1
C-N-HN	112.04	124.30	1
C-N-HN	112.03	124.30	5
HD1-CD-HD3	97.73	110.00	1
CE2-CD2-HD2	107.38	119.65	1
HG1-CG-HG2	97.73	110.00	1
HG21-CG2-HG22	97.73	110.00	1
CA-N-HN	126.27	114.00	2
HD22-CD2-HD23	122.27	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CB-HB2	120.28	108.00	1
CG2-CB-HB	120.28	108.00	1
CG-CD1-HD13	121.28	109.00	1
C-N-HN	112.02	124.30	1
CB-CA-HA	121.28	109.00	1
HD22-CD2-HD23	97.72	110.00	1
HD1-CD-HD2	97.72	110.00	1
CA-CB-HB1	121.28	109.00	1
HD11-CD1-HD12	97.72	110.00	1
HE21-NE2-HE22	132.28	120.00	1
HG11-CG1-HG13	122.29	110.00	1
N-CA-HA	97.71	110.00	2
CG-CB-HB2	120.29	108.00	1
CA-CB-HB2	96.71	109.00	1
HG1-CG-HG2	97.71	110.00	1
C-N-HN	112.01	124.30	3
CB-CG2-HG23	121.29	109.00	1
CB-CA-HA	121.29	109.00	1
HG11-CG1-HG12	97.71	110.00	1
OG1-CB-HB	96.71	109.00	1
CA-CB-HB1	96.70	109.00	2
HD1-CD-HD2	97.70	110.00	1
HB1-CB-HB3	97.70	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	112.00	124.30	4
CA-N-HN	101.70	114.00	1
HG1-CG-HG2	97.70	110.00	2
HH21-NH2-HH22	107.69	120.00	1
CB-CG-HG1	121.31	109.00	1
CB-CA-HA	96.69	109.00	1
HD1-CD-HD2	97.69	110.00	2
HG11-CG1-HG12	97.69	110.00	2
CG-CD2-HD21	121.31	109.00	1
CA-CB-HB2	96.69	109.00	1
HH11-NH1-HH12	107.69	120.00	1
C-N-HN	111.99	124.30	2
CB-CG2-HG23	121.31	109.00	2
HA1-CA-HA2	121.31	109.00	1
CA-CB-HB1	121.31	109.00	1
N-CA-HA2	97.69	110.00	1
HD21-ND2-HD22	107.68	120.00	1
HG11-CG1-HG12	97.68	110.00	1
HD1-CD-HD2	97.68	110.00	1
CB-CG-HG2	121.32	109.00	1
C-N-HN	111.98	124.30	2
CG-CD2-HD22	121.32	109.00	1
CE-NZ-HZ2	122.32	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD2-CD-HD3	97.68	110.00	1
HG21-CG2-HG22	122.32	110.00	1
CA-CB-HB1	121.32	109.00	1
N-CA-HA	97.68	110.00	2
CB-CA-HA	96.68	109.00	1
C-N-HN	111.97	124.30	4
N-CA-HA	97.67	110.00	1
HD1-CD-HD2	97.67	110.00	2
HG11-CG1-HG12	97.67	110.00	1
HD1-CD-HD3	97.67	110.00	1
CB-CG-HG	96.67	109.00	1
HB1-CB-HB2	97.67	110.00	2
CA-N-HN	126.33	114.00	2
CB-CA-HA	96.67	109.00	1
CA-CB-HB2	121.33	109.00	1
CB-CG-HG1	121.33	109.00	1
CB-CG-HG2	96.67	109.00	1
N-CA-HA	97.66	110.00	1
HB1-CB-HB2	97.66	110.00	1
CG-CD-HD1	121.34	109.00	1
C-N-HN	111.96	124.30	1
CB-CG-HG2	96.66	109.00	1
HA1-CA-HA2	121.34	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	96.66	109.00	1
CD-NE2-HE21	132.34	120.00	1
HB2-CB-HB3	97.65	110.00	1
HB1-CB-HB3	97.65	110.00	1
C-N-HN	111.95	124.30	1
HB1-CB-HB2	97.65	110.00	1
CB-CG2-HG22	121.35	109.00	1
C-CA-HA	96.65	109.00	1
C-CA-HA2	96.65	109.00	1
HG22-CG2-HG23	97.65	110.00	1
HD21-CD2-HD23	97.65	110.00	1
CG2-CB-HB	120.35	108.00	1
CB-CG2-HG21	121.35	109.00	1
HG1-CG-HG2	97.65	110.00	1
CG-CB-HB1	120.35	108.00	1
HG21-CG2-HG23	96.64	109.00	1
CB-SG-HG1	88.41	109.00	1
C-CA-HA	96.64	109.00	1
CA-CB-HB2	96.64	109.00	1
CA-CB-HB1	121.36	109.00	1
HD21-ND2-HD22	107.64	120.00	1
CA-N-HN	126.36	114.00	2
HD21-CD2-HD23	97.64	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-HA1	97.64	110.00	1
CB-CG2-HG23	121.36	109.00	1
HB1-CB-HB2	97.64	110.00	1
C-N-HN	111.93	124.30	3
N-CA-HA	97.63	110.00	2
CA-CB-HB2	121.37	109.00	1
HD11-CD1-HD13	122.37	110.00	1
CZ-OH-HH	97.63	110.00	1
CA-CB-HB2	96.63	109.00	1
HG12-CG1-HG13	122.37	110.00	1
C-CA-HA	96.63	109.00	1
C-N-HN	111.92	124.30	2
CA-N-HN	126.38	114.00	1
CB-CA-HA	96.62	109.00	1
CA-CB-HB1	96.62	109.00	1
CB-CG1-HG11	121.38	109.00	1
HB1-CB-HB2	97.62	110.00	2
HG22-CG2-HG23	122.38	110.00	1
CB-CG1-HG12	96.61	109.00	1
C-N-HN	111.91	124.30	3
CB-CA-HA	96.61	109.00	1
HD1-CD-HD2	97.61	110.00	1
HB1-CB-HB2	97.61	110.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CD-HD3	121.39	109.00	1
C-CA-HA2	121.39	109.00	1
HG12-CG1-HG13	97.61	110.00	1
C-CA-HA	96.61	109.00	2
HD2-CD-HD3	97.61	110.00	1
CG-CD1-HD13	121.39	109.00	1
C-N-HN	111.90	124.30	3
HG12-CG1-HG13	97.60	110.00	1
C-CA-HA	96.60	109.00	1
HD21-CD2-HD23	97.60	110.00	1
HB1-CB-HB2	122.40	110.00	1
N-CA-HA	97.60	110.00	1
CA-CB-HB1	121.40	109.00	1
CG-CD-HD1	121.40	109.00	1
HB1-CB-HB2	97.60	110.00	3
CZ-NH2-HH21	107.60	120.00	1
CD-CG-HG2	120.40	108.00	1
HG22-CG2-HG23	97.60	110.00	1
HB1-CB-HB3	97.60	110.00	1
HG21-CG2-HG23	97.60	110.00	1
HD2-CD-HD3	97.59	110.00	1
CE-NZ-HZ3	122.41	110.00	1
HB1-CB-HB2	97.59	110.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD21-CD2-HD23	97.59	110.00	1
OG1-CB-HB	96.59	109.00	1
CG-CB-HB1	120.41	108.00	1
C-N-HN	111.89	124.30	1
HD21-CD2-HD22	97.59	110.00	1
C-CA-HA	96.59	109.00	1
CA-CB-HB2	121.41	109.00	1
CE-CD-HD2	120.41	108.00	1
HH11-NH1-HH12	107.58	120.00	1
CB-CG1-HG12	121.42	109.00	1
N-CA-HA	97.58	110.00	2
HG22-CG2-HG23	97.58	110.00	2
C-N-HN	111.88	124.30	1
HB1-CB-HB2	97.58	110.00	1
CB-CG-HG2	96.58	109.00	1
CG2-CB-HB	95.58	108.00	1
CB-CA-HA	121.42	109.00	1
HD22-CD2-HD23	97.57	110.00	1
HD1-CD-HD2	97.57	110.00	1
N-CA-HA	122.43	110.00	1
HB1-CB-HB2	97.57	110.00	1
HG21-CG2-HG22	97.57	110.00	1
C-N-HN	111.87	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD1-HD11	121.43	109.00	1
HE21-NE2-HE22	132.43	120.00	1
HA1-CA-HA2	121.43	109.00	1
CB-CG2-HG21	96.57	109.00	1
CA-N-HN	126.43	114.00	1
C-N-HN	111.86	124.30	1
CG-ND2-HD21	107.56	120.00	1
C-CA-HA	96.56	109.00	1
HZ1-NZ-HZ2	121.44	109.00	1
HD11-CD1-HD12	97.56	110.00	1
HB1-CB-HB2	97.56	110.00	2
CA-CB-HB1	96.56	109.00	1
CG-CD-HD1	121.44	109.00	1
CZ-NE-HE	105.46	117.90	1
HG1-CG-HG2	97.56	110.00	1
CG-CB-HB1	120.44	108.00	1
CB-CG2-HG22	122.44	110.00	1
CB-CA-HA	121.44	109.00	1
C-N-HN	111.85	124.30	2
HG21-CG2-HG22	97.55	110.00	1
HA1-CA-HA2	121.45	109.00	2
CB-CA-HA	96.55	109.00	1
CG-CD-HD1	121.45	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-CG-HG1	95.55	108.00	1
CB-CG-HG1	96.55	109.00	1
HZ1-NZ-HZ2	96.55	109.00	1
HG1-CG-HG2	97.54	110.00	1
HG21-CG2-HG22	97.54	110.00	1
HD1-CD-HD3	122.46	110.00	1
C-CA-HA	96.54	109.00	1
HG22-CG2-HG23	96.53	109.00	1
HG1-CG-HG2	97.53	110.00	2
CA-CB-HB1	96.53	109.00	1
HH11-NH1-HH12	107.53	120.00	1
HA1-CA-HA2	121.47	109.00	1
HG21-CG2-HG23	122.47	110.00	1
CA-CB-HB1	121.47	109.00	1
CE-NZ-HZ1	122.47	110.00	1
C-N-HN	111.83	124.30	2
HD1-CD-HD2	97.53	110.00	1
HG11-CG1-HG13	97.53	110.00	1
HD1-CD-HD2	122.48	110.00	1
CB-CA-HA	121.48	109.00	1
CG-CD1-HD13	121.48	109.00	1
HG21-CG2-HG23	97.52	110.00	1
C-N-HN	111.82	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB1	96.52	109.00	2
CA-CB-HB1	121.48	109.00	1
CG-CD1-HD12	121.48	109.00	1
CA-N-HN	126.49	114.00	2
C-CA-HA	96.51	109.00	1
HD1-CD-HD2	97.51	110.00	1
CG-ND2-HD21	107.51	120.00	1
C-N-HN	111.81	124.30	1
HG1-CG-HG2	122.49	110.00	1
CG1-CD-HD1	121.49	109.00	1
CB-CG-HG1	96.51	109.00	1
HB1-CB-HB2	122.49	110.00	1
CA-N-HN	126.50	114.00	1
CG-CD1-HD12	121.50	109.00	1
C-N-HN	111.80	124.30	1
CB-CA-HA	96.50	109.00	2
HB1-CB-HB2	97.50	110.00	2
C-CA-HA	96.50	109.00	1
HD21-CD2-HD22	97.50	110.00	1
HG1-CG-HG2	97.50	110.00	1
HA1-CA-HA2	121.50	109.00	1
CA-CB-HB2	96.50	109.00	1
HD1-CD-HD2	122.50	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CB-HB2	120.50	108.00	1
HD11-CD1-HD13	97.50	110.00	1
HD21-CD2-HD22	97.49	110.00	1
HZ2-NZ-HZ3	96.49	109.00	1
CD-CG1-HG11	120.51	108.00	1
HG22-CG2-HG23	97.48	110.00	1
CG-CD-HD1	121.52	109.00	1
CA-CB-HB1	96.48	109.00	1
CD1-CG-HG	95.48	108.00	1
CE-NZ-HZ1	122.52	110.00	1
CD-CG1-HG11	120.52	108.00	1
CG-CD2-HD21	121.52	109.00	1
HG21-CG2-HG22	97.48	110.00	2
HB1-CB-HB3	97.48	110.00	1
HB1-CB-HB2	97.48	110.00	2
C-CA-HA	96.48	109.00	1
CD-CG1-HG11	95.48	108.00	1
C-N-HN	111.78	124.30	1
OG-CB-HB2	96.47	109.00	1
HG22-CG2-HG23	97.47	110.00	1
N-CA-HA1	97.47	110.00	1
HD11-CD1-HD12	97.47	110.00	1
CA-CB-HB2	96.47	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	111.77	124.30	1
C-CA-HA	96.47	109.00	1
HD11-CD1-HD13	97.47	110.00	1
HB1-CB-HB2	97.47	110.00	1
C-N-HN	111.76	124.30	1
CB-CG-HG2	121.54	109.00	1
C-CA-HA	96.46	109.00	1
N-CD-HD2	121.54	109.00	1
CD-NE2-HE21	107.46	120.00	1
HG22-CG2-HG23	96.46	109.00	1
CD-CG1-HG11	120.54	108.00	1
HB1-CB-HB2	97.46	110.00	1
HG1-CG-HG2	97.45	110.00	1
CG-CD2-HD2	138.95	126.40	1
HB1-CB-HB2	97.45	110.00	1
C-N-HN	111.75	124.30	3
HG21-CG2-HG23	97.45	110.00	1
HG21-CG2-HG22	97.45	110.00	1
HG11-CG1-HG12	97.45	110.00	1
HB1-CB-HB2	122.55	110.00	1
N-CA-HA	97.45	110.00	1
CB-OG1-HG1	97.44	110.00	1
HE1-CE-HE2	122.56	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB1	121.56	109.00	1
CA-CB-HB2	121.56	109.00	1
CA-N-HN	126.56	114.00	1
C-N-HN	111.74	124.30	1
HD1-CD-HD2	97.44	110.00	1
HD11-CD1-HD12	97.44	110.00	1
CB-CG-HG1	121.56	109.00	1
C-N-HN	111.73	124.30	2
C-CA-HA	96.44	109.00	1
CB-CG2-HG21	121.57	109.00	1
CA-CB-HB2	121.57	109.00	1
N-CA-HA	97.43	110.00	1
CD-CE-HE1	121.57	109.00	1
HG11-CG1-HG13	97.43	110.00	1
HB1-CB-HB2	97.43	110.00	1
CB-CG-HG1	121.57	109.00	1
CA-N-HN	126.57	114.00	1
CG-CB-HB2	95.43	108.00	1
NE-CD-HD2	120.58	108.00	1
CE-CD-HD1	120.58	108.00	1
C-N-HN	111.72	124.30	2
HG12-CG1-HG13	122.58	110.00	1
HB1-CB-HB2	97.42	110.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-HG	96.42	109.00	1
CE-NZ-HZ1	122.58	110.00	1
CA-CB-HB1	96.42	109.00	1
HD22-CD2-HD23	97.42	110.00	1
HD12-CD1-HD13	97.42	110.00	1
CG-CD1-HD12	121.58	109.00	1
C-CA-HA1	96.42	109.00	1
CB-CG2-HG22	96.42	109.00	1
CB-CG2-HG21	121.58	109.00	1
HG22-CG2-HG23	122.58	110.00	1
CB-OG1-HG1	97.41	110.00	1
C-N-HN	111.71	124.30	3
C-CA-HA	96.41	109.00	1
CB-CG-HG1	121.59	109.00	1
HG11-CG1-HG12	97.41	110.00	1
C-CA-HA1	96.41	109.00	1
HG21-CG2-HG22	97.41	110.00	1
CG2-CB-HB	96.41	109.00	1
C-N-HN	111.70	124.30	3
CG-CD1-HD11	121.60	109.00	1
CD-CG-HG2	97.40	110.00	1
CB-CA-HA	96.40	109.00	1
HG11-CG1-HG12	97.40	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-OG1-HG1	97.40	110.00	1
HB1-CB-HB3	97.40	110.00	1
N-CA-HA	97.40	110.00	1
C-CA-HA	96.40	109.00	1
CA-CB-HB1	121.60	109.00	1
CB-CG-HG2	121.61	109.00	1
C-N-HN	111.69	124.30	1
HB1-CB-HB2	97.39	110.00	1
C-CA-HA	96.39	109.00	2
CB-CG2-HG22	121.61	109.00	1
CA-CB-HB	121.61	109.00	1
C-N-HN	111.68	124.30	3
CA-CB-HB2	96.38	109.00	1
N-CA-HA	97.38	110.00	1
HG11-CG1-HG12	97.38	110.00	1
HB2-CB-HB3	97.38	110.00	1
C-CA-HA	96.38	109.00	1
CA-CB-HB2	121.63	109.00	1
HZ1-NZ-HZ2	96.37	109.00	1
HD21-CD2-HD22	97.37	110.00	1
C-CA-HA	96.37	109.00	1
CB-CG-HG2	121.63	109.00	1
C-N-HN	111.67	124.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-HN	126.64	114.00	2
CE2-CD2-HD2	132.04	119.40	1
CZ-NE-HE	105.26	117.90	1
CB-CG-HG2	121.64	109.00	2
CA-CB-HB2	96.36	109.00	2
HZ1-NZ-HZ3	96.36	109.00	1
CB-CG-HG1	121.64	109.00	1
HG22-CG2-HG23	97.36	110.00	1
CG-CD2-HD21	121.64	109.00	1
HB1-CB-HB2	97.36	110.00	1
C-CA-HA	96.36	109.00	1
HG21-CG2-HG22	97.36	110.00	1
C-N-HN	111.65	124.30	1
CG1-CD-HD3	121.65	109.00	1
C-CA-HA	96.35	109.00	1
HG21-CG2-HG22	97.35	110.00	1
CG-CD2-HD21	121.65	109.00	1
HB2-CB-HB3	97.35	110.00	1
CB-OG1-HG1	97.35	110.00	1
CA-N-HN	126.65	114.00	2
HD1-CD-HD2	97.35	110.00	1
HB1-CB-HB2	97.35	110.00	1
CB-CG2-HG23	121.65	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG21-CG2-HG23	97.35	110.00	1
HG21-CG2-HG22	122.66	110.00	1
C-N-HN	111.64	124.30	2
HG11-CG1-HG13	122.66	110.00	1
HG21-CG2-HG22	96.34	109.00	1
CG1-CD-HD2	121.66	109.00	1
CA-CB-HB1	96.34	109.00	1
HH21-NH2-HH22	132.66	120.00	1
HG1-CG-HG2	97.34	110.00	1
HG22-CG2-HG23	97.34	110.00	1
CA-CB-HB3	96.34	109.00	1
CG-CD2-HD22	121.66	109.00	1
C-CA-HA	96.33	109.00	2
CA-CB-HB2	121.67	109.00	1
HD21-CD2-HD23	97.33	110.00	1
N-CA-HA	97.33	110.00	1
HG11-CG1-HG12	97.33	110.00	1
HG21-CG2-HG23	97.33	110.00	2
CD-CG-HG2	122.67	110.00	1
CG-CB-HB1	120.67	108.00	1
CA-CB-HB1	96.33	109.00	1
CG1-CD-HD1	121.68	109.00	1
CB-SG-HG1	87.87	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-HA	97.32	110.00	1
C-N-HN	111.62	124.30	3
C-CA-HA	96.32	109.00	3
CA-CB-HB1	96.32	109.00	1
HG1-CG-HG2	97.32	110.00	1
C-CA-HA	96.31	109.00	3
HB1-CB-HB2	97.31	110.00	1
HG22-CG2-HG23	97.31	110.00	1
C-N-HN	111.61	124.30	3
HG1-CG-HG2	97.31	110.00	2
HG1-CG-HG2	97.30	110.00	1
C-N-HN	111.60	124.30	2
HG11-CG1-HG12	97.30	110.00	1
N-CA-HA2	122.70	110.00	1
CA-CB-HB1	96.30	109.00	1
C-CA-HA	96.30	109.00	1
HD1-CD-HD3	97.30	110.00	1
HB1-CB-HB2	97.30	110.00	1
CB-CA-HA	96.30	109.00	1
HG21-CG2-HG22	97.30	110.00	1
CG-CD-HD1	121.71	109.00	1
CB-CG1-HG13	96.29	109.00	1
C-N-HN	111.59	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG22-CG2-HG23	122.71	110.00	1
C-CA-HA	121.71	109.00	1
C-CA-HA1	96.29	109.00	1
HG21-CG2-HG23	97.29	110.00	1
C-CA-HA	96.29	109.00	1
CB-CG2-HG22	122.72	110.00	1
CB-CG-HG1	96.28	109.00	1
C-CA-HA	96.28	109.00	1
HB1-CB-HB2	97.28	110.00	3
CD-CG-HG2	97.28	110.00	1
CD2-CG-HG	95.28	108.00	1
HD12-CD1-HD13	122.72	110.00	1
CG-CD1-HD12	121.72	109.00	1
HG11-CG1-HG12	97.28	110.00	1
CA-N-HN	126.72	114.00	1
CB-CG-HG1	121.72	109.00	1
C-N-HN	111.57	124.30	3
CA-CB-HB2	96.27	109.00	1
HE21-NE2-HE22	132.73	120.00	1
HN1-N-HN2	115.89	103.16	1
HG22-CG2-HG23	96.27	109.00	1
CG1-CD-HD1	121.73	109.00	1
C-N-HN	111.56	124.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	97.27	110.00	1
CA-N-HN	126.73	114.00	1
C-CA-HA	96.26	109.00	2
CB-CG-HG2	121.74	109.00	1
HG1-CG-HG2	97.26	110.00	2
HD21-ND2-HD22	107.26	120.00	1
CG1-CD-HD3	121.74	109.00	1
HG11-CG1-HG12	97.26	110.00	1
CB-CG-HG1	121.74	109.00	1
N-CA-HA	97.26	110.00	1
CD-CG-HG1	120.75	108.00	1
C-N-HN	111.55	124.30	1
C-CA-HA	96.25	109.00	1
CB-CG1-HG11	121.75	109.00	1
HZ1-NZ-HZ3	96.25	109.00	1
CG-CB-HB2	120.75	108.00	1
CB-CA-HA	121.75	109.00	1
CE-CD-HD2	95.25	108.00	1
C-N-HN	111.54	124.30	3
CA-N-HN	101.24	114.00	1
CB-CG-HG2	121.76	109.00	1
HD2-CD-HD3	97.24	110.00	1
HG11-CG1-HG13	97.24	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD12-CD1-HD13	97.24	110.00	1
C-N-HN	111.53	124.30	3
HB1-CB-HB2	97.23	110.00	1
CA-N-HN	126.77	114.00	1
CB-CA-HA	96.23	109.00	1
CG-CD2-HD2	132.42	119.65	1
CA-CB-HB3	121.77	109.00	1
CB-CG1-HG11	121.78	109.00	1
HG22-CG2-HG23	122.78	110.00	1
CB-CG2-HG21	121.78	109.00	1
C-CA-HA	96.22	109.00	3
HG21-CG2-HG22	97.22	110.00	1
HD1-CD-HD2	97.22	110.00	1
CE-NZ-HZ1	122.78	110.00	1
C-N-HN	111.51	124.30	4
HB1-CB-HB2	97.21	110.00	1
N-CA-HA	97.21	110.00	1
CB-OG1-HG1	97.21	110.00	1
CB-CG2-HG21	121.79	109.00	1
C-CA-HA	96.21	109.00	1
CA-CB-HB	96.21	109.00	1
CG-CD2-HD22	121.79	109.00	1
C-N-HN	111.50	124.30	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	96.20	109.00	1
HD11-CD1-HD12	97.20	110.00	1
HD1-CD-HD2	122.80	110.00	1
CG-CB-HB2	120.80	108.00	1
HA1-CA-HA2	121.80	109.00	1
HD22-CD2-HD23	122.80	110.00	1
CB-CG1-HG11	121.80	109.00	1
CA-CB-HB1	96.20	109.00	1
CB-CG2-HG21	121.80	109.00	1
CB-CA-HA	96.19	109.00	3
HD1-CD-HD2	97.19	110.00	1
CG-CB-HB1	95.19	108.00	1
HD21-CD2-HD23	122.81	110.00	1
HA1-CA-HA2	121.81	109.00	1
HD12-CD1-HD13	97.19	110.00	1
CA-N-HN	126.81	114.00	1
C-N-HN	111.49	124.30	1
HD1-CD-HD2	97.18	110.00	1
N-CA-HA1	97.18	110.00	1
HA1-CA-HA2	121.82	109.00	1
HB1-CB-HB2	97.18	110.00	1
HG21-CG2-HG22	97.18	110.00	1
C-CA-HA	96.18	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-CG-HG1	95.18	108.00	1
C-N-HN	111.48	124.30	2
CD-CG-HG2	120.82	108.00	1
HN1-N-HN2	115.98	103.16	1
CB-CA-HA	96.17	109.00	1
HG21-CG2-HG23	97.17	110.00	1
HG11-CG1-HG12	97.17	110.00	1
HD11-CD1-HD12	97.17	110.00	1
HB1-CB-HB2	97.17	110.00	1
HD11-CD1-HD13	97.17	110.00	1
C-N-HN	111.47	124.30	1
C-CA-HA	96.16	109.00	1
HA1-CA-HA2	121.84	109.00	1
CA-CB-HB1	121.84	109.00	1
CB-CA-HA	96.16	109.00	2
HB1-CB-HB2	97.16	110.00	1
CB-CA-HA	121.84	109.00	1
HG11-CG1-HG12	97.16	110.00	1
CB-CG-HG1	96.16	109.00	1
C-N-HN	111.45	124.30	2
N-CA-HA	97.15	110.00	1
HA1-CA-HA2	121.85	109.00	1
HB1-CB-HB2	97.15	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
NE2-CD2-HD2	113.55	126.40	1
HG21-CG2-HG23	97.15	110.00	1
HG12-CG1-HG13	97.15	110.00	1
HE1-CE-HE2	97.15	110.00	1
CA-CB-HB2	121.85	109.00	1
CG1-CB-HB	96.14	109.00	1
CE-NZ-HZ2	97.14	110.00	1
C-N-HN	111.44	124.30	4
HD22-CD2-HD23	97.14	110.00	1
CE-CD-HD2	120.86	108.00	1
HB1-CB-HB2	97.14	110.00	2
CB-CG1-HG12	121.86	109.00	1
CG-CB-HB1	95.14	108.00	1
HB1-CB-HB2	122.86	110.00	1
CA-CB-HB1	96.14	109.00	1
CG-CB-HB2	120.86	108.00	1
CA-CB-HB2	121.87	109.00	1
CG-CD1-HD13	121.87	109.00	1
HD1-CD-HD2	97.13	110.00	1
CB-CG-HG1	121.88	109.00	1
C-N-HN	111.42	124.30	3
C-CA-HA2	96.12	109.00	1
HD22-CD2-HD23	97.12	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-CE-HE2	121.88	109.00	1
CB-OG1-HG1	97.12	110.00	1
HB1-CB-HB2	97.12	110.00	2
N-CA-HA	97.12	110.00	1
CA-N-HN	126.88	114.00	1
CE-NZ-HZ3	122.88	110.00	1
C-N-HN	111.41	124.30	2
CB-CG2-HG22	121.89	109.00	1
HB1-CB-HB2	97.11	110.00	1
CA-N-HN	126.89	114.00	1
CB-CG1-HG11	121.89	109.00	1
C-N-HN	111.40	124.30	5
HH11-NH1-HH12	107.10	120.00	1
HB1-CB-HB2	97.10	110.00	1
C-N-HN	111.39	124.30	1
CD-CE-HE1	121.91	109.00	1
HB1-CB-HB2	97.09	110.00	1
CB-CG2-HG22	121.91	109.00	1
N-CA-HA	122.91	110.00	1
CA-CB-HB2	121.91	109.00	1
HD11-CD1-HD13	97.09	110.00	1
CB-CG2-HG23	122.92	110.00	1
CA-CB-HB2	96.08	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	111.38	124.30	4
HZ1-NZ-HZ2	96.08	109.00	1
CA-N-HN	126.92	114.00	1
CB-OG1-HG1	97.08	110.00	1
N-CA-HA	97.08	110.00	1
HB1-CB-HB2	97.08	110.00	1
C-N-HN	111.37	124.30	2
HD21-CD2-HD23	97.07	110.00	1
CA-N-HN	126.93	114.00	1
HB1-CB-HB2	97.07	110.00	1
CB-CA-HA	96.07	109.00	1
CG1-CD-HD2	121.93	109.00	1
HD11-CD1-HD12	97.07	110.00	1
HB2-CB-HB3	97.06	110.00	1
CG-ND1-HD1	138.29	125.35	1
CA-CB-HB1	96.06	109.00	1
CA-N-HN	126.94	114.00	1
HG1-CG-HG2	97.06	110.00	1
N-CA-HA	97.06	110.00	2
C-N-HN	111.36	124.30	1
HB1-CB-HB2	97.06	110.00	2
CB-CA-HA	96.06	109.00	1
C-CA-HA	96.06	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	97.05	110.00	1
CB-CG1-HG13	121.95	109.00	1
CA-CB-HB1	121.96	109.00	1
CB-CG1-HG13	121.96	109.00	1
C-CA-HA1	96.04	109.00	1
CD-CE-HE1	121.96	109.00	1
HD21-CD2-HD22	97.04	110.00	1
HG21-CG2-HG23	97.04	110.00	1
CG-CB-HB1	95.04	108.00	1
CD2-CE2-HE2	107.03	120.00	1
N-CA-HA1	97.03	110.00	1
CA-CB-HB1	121.97	109.00	1
CA-N-HN	126.97	114.00	1
HD11-CD1-HD12	97.03	110.00	1
CD-CG-HG2	97.03	110.00	1
C-N-HN	111.33	124.30	1
HG11-CG1-HG13	97.03	110.00	1
CG-CD2-HD22	121.97	109.00	1
CG-ND2-HD21	132.98	120.00	1
CG2-CB-HB	95.02	108.00	1
N-CA-HA2	97.02	110.00	1
CB-CG1-HG13	121.98	109.00	1
HG21-CG2-HG22	97.02	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	97.02	110.00	1
HD21-ND2-HD22	132.98	120.00	1
H1-N-H3	96.49	109.47	1
N-CA-HA	97.02	110.00	1
HG1-CG-HG2	97.02	110.00	1
CB-CG2-HG22	121.98	109.00	1
C-CA-HA	96.02	109.00	1
CB-CA-HA	96.01	109.00	1
C-N-HN	111.31	124.30	2
CD-CG-HG1	95.01	108.00	1
HB1-CB-HB2	97.01	110.00	1
CG1-CD-HD2	121.99	109.00	1
CD-CE-HE2	121.99	109.00	1
CB-CG-HG1	122.00	109.00	1
CD2-CE2-HE2	107.00	120.00	1
CA-CB-HB2	122.00	109.00	1
HH11-NH1-HH12	107.00	120.00	1
CA-CB-HB2	122.01	109.00	1
HD21-CD2-HD23	123.01	110.00	1
HG1-CG-HG2	96.99	110.00	1
HD11-CD1-HD12	96.99	110.00	1
CA-CB-HB1	122.01	109.00	1
CG-CB-HB1	123.01	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
OG-CB-HB2	122.01	109.00	1
CG-CD1-HD11	122.02	109.00	1
CA-N-HN	127.02	114.00	1
C-N-HN	111.28	124.30	1
HD11-CD1-HD12	96.98	110.00	1
CB-CG-HG2	122.03	109.00	1
CA-N-HN	127.03	114.00	1
CZ-NH2-HH21	106.97	120.00	1
HB2-CB-HB3	96.97	110.00	1
CB-CG2-HG21	122.03	109.00	1
HB1-CB-HB2	123.03	110.00	1
C-N-HN	111.27	124.30	3
CA-CB-HB1	95.96	109.00	1
CD-NE2-HE22	106.96	120.00	1
HD12-CD1-HD13	123.04	110.00	1
HB2-CB-HB3	96.96	110.00	1
HB1-CB-HB2	96.96	110.00	1
CG-CD1-HD13	122.04	109.00	1
C-CA-HA1	95.96	109.00	1
HH21-NH2-HH22	106.96	120.00	1
C-N-HN	111.25	124.30	2
N-CA-HA2	96.95	110.00	1
HG1-CG-HG2	96.95	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CA-HA	122.05	109.00	1
HG21-CG2-HG22	96.94	110.00	2
CA-N-HN	127.06	114.00	1
CE-CD-HD2	94.94	108.00	1
C-CA-HA1	95.94	109.00	1
HA1-CA-HA2	122.06	109.00	1
CZ-NH1-HH11	106.94	120.00	1
CA-CB-HB1	122.06	109.00	1
HB1-CB-HB2	96.94	110.00	1
HD1-CD-HD2	123.06	110.00	1
HG1-CG-HG2	96.94	110.00	1
CB-CG-HG2	122.06	109.00	1
C-N-HN	111.24	124.30	1
CB-CA-HA	95.93	109.00	2
CB-CA-HA	122.07	109.00	1
C-CA-HA	95.93	109.00	1
C-N-HN	111.23	124.30	1
CG-ND2-HD21	106.93	120.00	1
CG1-CD-HD2	122.08	109.00	1
HG1-CG-HG2	96.92	110.00	1
HG21-CG2-HG23	95.92	109.00	1
CA-CB-HB1	122.08	109.00	1
N-CD-HD1	95.92	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	111.22	124.30	2
CB-CG1-HG12	122.08	109.00	1
HG21-CG2-HG23	96.92	110.00	1
CG1-CB-HB	121.09	108.00	1
CA-CB-HB2	95.91	109.00	1
HG22-CG2-HG23	96.91	110.00	1
HB1-CB-HB2	96.91	110.00	2
CA-CB-HB1	95.91	109.00	1
HD11-CD1-HD12	96.90	110.00	1
CD-CE-HE2	122.10	109.00	1
CB-CA-HA	122.10	109.00	1
CB-CG2-HG21	122.10	109.00	1
CA-N-HN	127.10	114.00	1
CB-CA-HA	95.90	109.00	1
HG21-CG2-HG23	96.90	110.00	1
CG1-CB-HB	94.90	108.00	1
CB-OG1-HG1	96.90	110.00	1
CD-CE-HE1	122.10	109.00	1
HE1-CE-HE2	96.90	110.00	1
HH21-NH2-HH22	133.10	120.00	1
HA1-CA-HA2	122.11	109.00	1
HE21-NE2-HE22	133.11	120.00	1
N-CA-HA	96.89	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CA-HA	122.11	109.00	2
CA-N-HN	100.89	114.00	1
HG11-CG1-HG12	96.89	110.00	1
CB-CA-HA	95.89	109.00	1
CB-CA-HA	122.12	109.00	1
C-N-HN	111.18	124.30	2
CA-CB-HB1	122.12	109.00	1
CD-CG-HG2	123.12	110.00	1
N-CA-HA	96.88	110.00	1
CG-CD2-HD22	122.12	109.00	1
CB-CG2-HG22	122.12	109.00	1
C-N-HN	111.17	124.30	2
C-CA-HA	95.87	109.00	1
CA-CB-HB1	95.87	109.00	1
C-N-HN	111.16	124.30	2
CE-CD-HD2	121.14	108.00	1
CA-CB-HB1	95.86	109.00	1
C-CA-HA1	95.86	109.00	1
HG21-CG2-HG23	96.86	110.00	1
CB-CG-HG1	122.14	109.00	1
HB1-CB-HB2	123.14	110.00	1
HB1-CB-HB2	96.86	110.00	1
HG11-CG1-HG12	123.14	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE-NZ-HZ2	123.14	110.00	1
C-N-HN	111.15	124.30	2
HE21-NE2-HE22	133.15	120.00	1
C-CA-HA	95.85	109.00	1
HD2-CD-HD3	96.85	110.00	1
HG1-CG-HG2	123.15	110.00	1
HG21-CG2-HG23	123.15	110.00	1
CB-CG-HG2	122.15	109.00	1
HG1-CG-HG2	96.85	110.00	1
CG-CD-HD2	122.16	109.00	1
CB-CA-HA	95.84	109.00	1
CA-N-HN	127.17	114.00	1
CE-CD-HD2	121.17	108.00	1
HB1-CB-HB2	96.83	110.00	1
HZ2-NZ-HZ3	95.83	109.00	1
HD1-CD-HD2	96.83	110.00	1
HD2-CD-HD3	96.83	110.00	1
HN1-N-HN2	116.33	103.16	1
HG11-CG1-HG13	96.82	110.00	1
C-N-HN	111.12	124.30	1
CD2-CG-HG	121.18	108.00	1
HG1-CG-HG2	96.82	110.00	1
HB2-CB-HB3	96.82	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG11-CG1-HG12	96.82	110.00	1
CG-CB-HB1	121.18	108.00	1
HD21-CD2-HD22	96.82	110.00	1
CE-CD-HD1	121.18	108.00	1
C-CA-HA	95.81	109.00	1
CB-CA-HA	122.19	109.00	1
CA-N-HN	127.19	114.00	1
HA1-CA-HA2	122.19	109.00	1
HG21-CG2-HG23	96.81	110.00	1
CB-CG-HG2	122.19	109.00	1
HD22-CD2-HD23	96.81	110.00	1
CA-CB-HB3	122.20	109.00	1
CG-CD1-HD13	122.20	109.00	1
N-CA-HA	96.80	110.00	1
CA-CB-HB2	122.20	109.00	1
HG21-CG2-HG23	95.80	109.00	1
C-N-HN	111.10	124.30	1
HB1-CB-HB2	96.80	110.00	1
HB1-CB-HB2	96.79	110.00	1
CG-CB-HB1	94.79	108.00	1
CA-CB-HB1	95.79	109.00	1
C-CA-HA	95.79	109.00	4
CB-CA-HA	95.79	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CA-HA	122.21	109.00	1
C-N-HN	111.09	124.30	1
N-CA-HA1	96.78	110.00	1
CA-CB-HB1	122.22	109.00	2
CG-CD2-HD23	122.22	109.00	1
CA-N-HN	127.22	114.00	1
CB-CA-HA	95.78	109.00	1
CA-CB-HB3	95.78	109.00	1
CD-CG-HG2	123.22	110.00	1
CB-CG-HG2	122.22	109.00	1
HD12-CD1-HD13	96.78	110.00	1
C-CA-HA	95.77	109.00	1
HG1-CG-HG2	96.77	110.00	1
HB1-CB-HB2	96.77	110.00	1
HB1-CB-HB2	123.23	110.00	1
C-N-HN	111.07	124.30	1
HG12-CG1-HG13	123.24	110.00	1
CG-CD2-HD21	122.24	109.00	1
C-N-HN	111.06	124.30	2
CB-CA-HA	95.76	109.00	1
HB1-CB-HB2	96.76	110.00	2
HG1-CG-HG2	96.76	110.00	1
HB2-CB-HB3	96.76	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CA-HA	122.24	109.00	1
CB-CA-HA	95.75	109.00	1
HB1-CB-HB2	96.75	110.00	1
C-N-HN	111.05	124.30	1
HA1-CA-HA2	122.25	109.00	1
HD11-CD1-HD13	96.75	110.00	1
CB-CG-HG1	122.25	109.00	1
CA-CB-HB3	122.25	109.00	1
HB1-CB-HB2	96.74	110.00	2
CB-CG-HG1	122.26	109.00	1
N-CA-HA	96.73	110.00	2
HA1-CA-HA2	122.27	109.00	1
CE-NZ-HZ1	123.27	110.00	1
HG11-CG1-HG13	96.73	110.00	1
CB-CG-HG1	122.27	109.00	1
HD1-CD-HD3	96.72	110.00	1
HG21-CG2-HG22	123.28	110.00	1
CB-CG2-HG23	122.28	109.00	1
HA1-CA-HA2	122.28	109.00	1
HG1-CG-HG2	96.72	110.00	1
CA-N-HN	127.28	114.00	1
C-N-HN	111.02	124.30	1
CB-CG2-HG23	122.29	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB1	122.29	109.00	1
C-N-HN	111.01	124.30	2
CA-CB-HB2	95.71	109.00	1
HB1-CB-HB2	96.71	110.00	1
CB-CG2-HG21	122.29	109.00	1
CA-CB-HB2	122.29	109.00	1
CG-CB-HB1	94.70	108.00	1
CE-NZ-HZ2	123.30	110.00	1
C-CA-HA	95.69	109.00	2
CA-N-HN	127.31	114.00	1
C-N-HN	110.99	124.30	1
HD2-CD-HD3	96.69	110.00	1
HG1-CG-HG2	96.69	110.00	1
N-CA-HA	96.69	110.00	1
CD-CE-HE2	122.31	109.00	1
CB-CG2-HG22	122.32	109.00	1
C-N-HN	110.98	124.30	5
C-CA-HA	95.68	109.00	1
HD12-CD1-HD13	96.68	110.00	1
HZ1-NZ-HZ2	95.68	109.00	1
HB1-CB-HB2	96.68	110.00	2
CB-CA-HA	95.68	109.00	1
CA-CB-HB2	122.32	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-HG2	122.32	109.00	1
CA-CB-HB2	95.67	109.00	2
CZ-NH2-HH21	106.67	120.00	1
CG-CB-HB2	121.33	108.00	1
HB1-CB-HB2	96.67	110.00	1
CB-CA-HA	122.33	109.00	1
CB-CG-HG2	122.33	109.00	1
C-CA-HA1	95.67	109.00	1
HA1-CA-HA2	122.33	109.00	2
CD-CG-HG2	121.33	108.00	1
HG22-CG2-HG23	96.67	110.00	1
C-N-HN	110.96	124.30	3
HD21-CD2-HD22	96.66	110.00	1
CB-CG1-HG12	95.66	109.00	1
HD21-CD2-HD23	96.66	110.00	1
CB-CA-HA	122.34	109.00	1
HB1-CB-HB2	96.66	110.00	1
HB1-CB-HB2	96.65	110.00	1
CB-CG2-HG22	122.35	109.00	1
N-CA-HA2	123.35	110.00	1
HH21-NH2-HH22	106.65	120.00	1
HG21-CG2-HG22	96.65	110.00	1
C-N-HN	110.95	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HD11-CD1-HD13	123.36	110.00	1
C-N-HN	110.94	124.30	3
CB-CG-HG2	122.36	109.00	1
CG2-CB-HB	95.64	109.00	1
CA-CB-HB3	95.64	109.00	1
CG-CB-HB1	121.36	108.00	1
CG-CD1-HD12	122.36	109.00	1
CA-N-HN	127.36	114.00	1
HB1-CB-HB2	96.63	110.00	1
CB-CG1-HG12	122.37	109.00	1
HD21-CD2-HD22	96.63	110.00	1
HG12-CG1-HG13	96.63	110.00	1
CB-CG2-HG22	122.37	109.00	1
CG-CB-HB2	94.63	108.00	1
CZ-CE2-HE2	133.57	120.20	1
HG21-CG2-HG23	96.63	110.00	1
CB-CA-HA	122.37	109.00	1
CB-CG2-HG22	122.38	109.00	1
HB1-CB-HB2	96.62	110.00	1
HG11-CG1-HG12	96.62	110.00	1
CB-CA-HA	95.62	109.00	1
HG22-CG2-HG23	96.62	110.00	1
HG1-CG-HG2	96.62	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG21-CG2-HG23	96.62	110.00	1
CB-CG-HG2	122.39	109.00	1
C-N-HN	110.91	124.30	1
N-CA-HA	96.61	110.00	1
HG22-CG2-HG23	96.61	110.00	1
CD2-CG-HG	121.39	108.00	1
CB-CA-HA	95.61	109.00	1
OG1-CB-HB	95.61	109.00	1
C-CA-HA	95.61	109.00	1
CG-CB-HB2	123.40	110.00	1
CB-CA-HA	122.40	109.00	1
C-N-HN	110.90	124.30	1
CG-CD1-HD12	122.40	109.00	1
CG-CB-HB1	121.41	108.00	1
CA-CB-HB1	95.59	109.00	1
HA1-CA-HA2	122.41	109.00	1
CA-CB-HB2	122.41	109.00	1
C-N-HN	110.89	124.30	1
CZ-NH2-HH22	106.59	120.00	1
N-CA-HA	96.59	110.00	1
HG1-CG-HG2	96.59	110.00	1
CB-CA-HA	95.58	109.00	1
CG-CD2-HD22	122.42	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	110.88	124.30	2
CD-CG1-HG11	94.58	108.00	1
HG21-CG2-HG22	96.58	110.00	1
CA-CB-HB2	122.43	109.00	1
HG22-CG2-HG23	96.57	110.00	1
HD12-CD1-HD13	96.57	110.00	1
HB2-CB-HB3	96.57	110.00	1
HB1-CB-HB3	96.57	110.00	1
HB2-CB-HB3	96.56	110.00	1
C-CA-HA	95.56	109.00	2
N-CA-HA	96.56	110.00	1
HB1-CB-HB2	96.56	110.00	1
CD-CG-HG2	121.44	108.00	1
C-N-HN	110.86	124.30	1
HA1-CA-HA2	122.44	109.00	1
HE21-NE2-HE22	133.44	120.00	1
HB1-CB-HB2	96.55	110.00	1
HD21-CD2-HD23	96.55	110.00	1
C-N-HN	110.85	124.30	1
N-CD-HD2	122.46	109.00	1
CB-CA-HA	122.46	109.00	1
HB1-CB-HB2	96.54	110.00	1
CA-N-HN	127.46	114.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB2	122.46	109.00	1
C-CA-HA	95.54	109.00	1
HD12-CD1-HD13	96.54	110.00	1
CG-CD-HD1	122.46	109.00	1
CB-CG-HG2	122.47	109.00	1
HB2-CB-HB3	123.47	110.00	1
CZ-NH2-HH21	106.53	120.00	1
CD-CG-HG2	121.47	108.00	1
C-N-HN	110.83	124.30	1
CD-CG-HG2	123.47	110.00	1
C-N-HN	110.82	124.30	3
CA-CB-HB1	95.51	109.00	1
CB-CA-HA	95.51	109.00	1
CB-CG-HG1	122.49	109.00	1
C-CA-HA1	95.51	109.00	1
HG1-CG-HG2	96.51	110.00	1
C-N-HN	110.81	124.30	1
HB1-CB-HB2	96.51	110.00	1
N-CD-HD2	122.49	109.00	1
OG-CB-HB2	122.49	109.00	1
C-CA-HA	96.51	110.00	1
CG-CB-HB2	121.49	108.00	1
CG-CD1-HD11	122.49	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG1-HG11	95.50	109.00	1
C-N-HN	110.80	124.30	3
HG11-CG1-HG12	96.50	110.00	1
N-CA-HA	96.50	110.00	1
CB-CA-HA	95.50	109.00	1
HD1-CD-HD2	96.49	110.00	1
HG11-CG1-HG12	96.49	110.00	1
CG-CB-HB1	94.49	108.00	1
HG21-CG2-HG23	96.49	110.00	1
C-CA-HA	95.49	109.00	1
CE-NZ-HZ1	123.51	110.00	1
C-N-HN	110.79	124.30	2
HB1-CB-HB3	96.49	110.00	1
CB-CG1-HG12	122.51	109.00	1
CA-N-HN	127.51	114.00	1
HB1-CB-HB2	123.52	110.00	1
HZ1-NZ-HZ3	95.48	109.00	1
CA-CB-HB2	122.52	109.00	1
HA1-CA-HA2	122.52	109.00	1
HG1-CG-HG2	96.48	110.00	1
CD-CG-HG1	123.52	110.00	1
C-N-HN	110.77	124.30	1
HD1-CD-HD3	96.47	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG21-CG2-HG22	96.47	110.00	1
CE-CD-HD1	94.47	108.00	1
C-N-HN	110.76	124.30	3
CD-CG-HG1	121.54	108.00	1
HE1-CE-HE2	96.46	110.00	1
CA-CB-HB1	95.45	109.00	1
CG-CB-HB2	96.45	110.00	1
CB-CA-HA	95.45	109.00	1
HA1-CA-HA2	122.55	109.00	1
C-CA-HA	95.45	109.00	1
CA-CB-HB1	122.55	109.00	1
CA-N-HN	127.56	114.00	1
CA-CB-HB2	122.56	109.00	1
N-CA-HA	96.44	110.00	1
C-N-HN	110.73	124.30	3
CB-CG-HG2	122.57	109.00	1
HG21-CG2-HG23	122.58	109.00	1
HA1-CA-HA2	122.58	109.00	1
CB-CG2-HG23	122.58	109.00	1
HG11-CG1-HG12	96.42	110.00	1
C-N-HN	110.71	124.30	1
CG-CD1-HD11	122.59	109.00	1
HG11-CG1-HG12	96.41	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	96.41	110.00	2
CB-CA-HA	95.41	109.00	1
CG-CB-HB1	121.59	108.00	1
HB1-CB-HB3	96.40	110.00	1
HD21-CD2-HD22	96.40	110.00	1
HG12-CG1-HG13	123.60	110.00	1
C-N-HN	110.70	124.30	2
HZ1-NZ-HZ2	95.40	109.00	1
CA-CB-HB2	122.60	109.00	1
HD21-ND2-HD22	133.60	120.00	1
HG1-CG-HG2	96.39	110.00	1
C-N-HN	110.69	124.30	1
CA-CB-HB2	122.61	109.00	1
CB-CG2-HG23	122.61	109.00	1
CB-CA-HA	122.61	109.00	1
HN1-N-HN2	116.78	103.16	1
C-CA-HA	95.38	109.00	1
N-CA-HA1	96.38	110.00	1
HB1-CB-HB2	96.38	110.00	1
OG1-CB-HB	122.62	109.00	1
HB1-CB-HB2	96.37	110.00	2
C-N-HN	110.67	124.30	3
CA-CB-HB2	122.64	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG21-CG2-HG22	96.36	110.00	1
HB1-CB-HB2	96.36	110.00	1
CB-CG2-HG23	122.65	109.00	1
HD11-CD1-HD12	96.35	110.00	1
HD1-CD-HD2	96.35	110.00	1
CA-N-HN	127.66	114.00	1
CB-CA-HA	122.66	109.00	1
CG1-CD-HD3	122.66	109.00	1
N-CA-HA	96.34	110.00	1
CB-OG1-HG1	96.34	110.00	1
C-N-HN	110.63	124.30	3
CG-CD-HD2	95.33	109.00	1
HG1-CG-HG2	96.33	110.00	1
HD1-CD-HD2	96.33	110.00	1
C-N-HN	110.62	124.30	3
CA-CB-HB2	122.68	109.00	1
CA-N-HN	127.68	114.00	1
CB-CA-HA	122.68	109.00	1
CE-NZ-HZ1	123.69	110.00	1
CB-CG-HG1	122.69	109.00	1
CB-CG2-HG21	122.69	109.00	1
CA-CB-HB2	122.69	109.00	1
CB-CG1-HG11	122.69	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CB-HB2	121.69	108.00	1
CB-CG2-HG22	122.69	109.00	1
CB-CG2-HG23	122.69	109.00	1
C-N-HN	110.60	124.30	1
CB-CA-HA	95.30	109.00	1
HA1-CA-HA2	122.71	109.00	1
CG1-CD-HD1	122.71	109.00	1
CG-CD-HD1	95.29	109.00	1
CB-CG1-HG13	122.71	109.00	1
CA-CB-HB1	122.71	109.00	1
C-N-HN	110.58	124.30	1
HD21-CD2-HD22	96.28	110.00	1
HB1-CB-HB2	96.28	110.00	2
CA-N-HN	127.72	114.00	1
CA-CB-HB1	95.28	109.00	1
CG-CD1-HD11	122.72	109.00	1
HD1-CD-HD2	96.28	110.00	1
C-CA-HA	95.28	109.00	1
C-N-HN	110.57	124.30	2
HD21-CD2-HD23	96.27	110.00	1
HG1-CG-HG2	96.27	110.00	1
HB1-CB-HB2	96.27	110.00	1
CA-N-HN	127.74	114.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-CG-HG2	121.74	108.00	1
C-N-HN	110.56	124.30	2
CA-CB-HB2	122.74	109.00	1
HG11-CG1-HG12	96.26	110.00	1
HB1-CB-HB2	96.26	110.00	1
N-CA-HA2	96.25	110.00	1
HG11-CG1-HG12	96.25	110.00	1
HG12-CG1-HG13	96.25	110.00	1
HB1-CB-HB2	96.25	110.00	2
CE-NZ-HZ1	123.75	110.00	1
CA-CB-HB1	122.75	109.00	1
HD11-CD1-HD13	96.24	110.00	1
CB-CG1-HG12	122.76	109.00	1
CG-CB-HB1	94.24	108.00	1
C-CA-HA	95.24	109.00	1
HZ1-NZ-HZ3	122.76	109.00	1
C-N-HN	110.54	124.30	1
HG21-CG2-HG22	96.24	110.00	1
CB-CA-HA	95.24	109.00	1
HD21-CD2-HD23	96.24	110.00	1
CB-CA-HA	122.77	109.00	1
CA-CB-HB2	122.77	109.00	1
HG12-CG1-HG13	96.23	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HA1-CA-HA2	122.77	109.00	1
CG-ND2-HD22	133.78	120.00	1
C-N-HN	110.52	124.30	1
HD2-CD-HD3	96.22	110.00	1
CB-CG-HG1	122.78	109.00	1
CG-CB-HB2	121.78	108.00	1
C-CA-HA	95.22	109.00	1
HD1-CD-HD2	96.22	110.00	1
CA-CB-HB2	122.78	109.00	1
CE-NZ-HZ1	96.22	110.00	1
CB-CA-HA	95.22	109.00	1
HG12-CG1-HG13	96.22	110.00	1
CB-CG-HG2	95.21	109.00	1
N-CA-HA	96.21	110.00	1
HG11-CG1-HG13	96.21	110.00	1
HB1-CB-HB2	96.21	110.00	1
HZ1-NZ-HZ2	95.21	109.00	1
CB-CG2-HG23	122.79	109.00	1
CE2-CD2-HD2	105.60	119.40	1
HD1-CD-HD2	96.20	110.00	1
CD-CG-HG2	123.80	110.00	1
C-N-HN	110.50	124.30	2
CD1-CG-HG	94.20	108.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG2-HG22	122.80	109.00	1
HB1-CB-HB2	96.20	110.00	2
C-CA-HA	96.20	110.00	1
C-CA-HA	95.20	109.00	1
HB1-CB-HB2	96.19	110.00	2
HD2-CD-HD3	96.18	110.00	1
CD-CG-HG2	123.82	110.00	1
C-N-HN	110.48	124.30	1
C-N-HN	110.47	124.30	3
HG22-CG2-HG23	96.17	110.00	1
CB-CG-HG1	122.83	109.00	1
HD1-CD-HD2	96.17	110.00	1
CA-N-HN	127.83	114.00	1
C-N-HN	110.46	124.30	1
NE2-CD2-HD2	112.55	126.40	1
HB1-CB-HB2	96.15	110.00	1
HG21-CG2-HG23	96.15	110.00	1
HZ1-NZ-HZ2	95.15	109.00	1
HG1-CG-HG2	96.15	110.00	1
CG-CD-HD1	122.85	109.00	1
N-CA-HA	96.15	110.00	1
C-CA-HA	95.15	109.00	1
CG-CB-HB2	121.85	108.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CA-HA	122.85	109.00	1
HD1-CD-HD2	96.14	110.00	2
HE21-NE2-HE22	106.14	120.00	1
HG11-CG1-HG13	96.14	110.00	1
CG-CB-HB2	121.86	108.00	1
CB-CG1-HG13	122.86	109.00	1
CD-CE-HE2	122.86	109.00	1
HG11-CG1-HG12	96.14	110.00	1
HB1-CB-HB3	96.13	110.00	1
CB-CA-HA	95.13	109.00	1
CB-CG2-HG22	122.87	109.00	1
C-N-HN	110.43	124.30	1
CB-OG1-HG1	96.13	110.00	1
HG11-CG1-HG12	96.13	110.00	1
C-CA-HA	95.12	109.00	1
HZ2-NZ-HZ3	122.88	109.00	1
CD-CG-HG1	94.12	108.00	1
C-N-HN	110.42	124.30	1
C-N-HN	110.41	124.30	3
N-CA-HA	96.11	110.00	1
C-CA-HA	122.89	109.00	1
NE-CD-HD1	121.89	108.00	1
CG-CB-HB2	94.11	108.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	95.11	109.00	1
CG-CB-HB1	123.90	110.00	1
C-N-HN	110.40	124.30	1
C-CA-HA	95.10	109.00	1
HG22-CG2-HG23	96.10	110.00	1
CA-N-HN	127.90	114.00	1
HA1-CA-HA2	122.90	109.00	1
C-N-HN	110.39	124.30	1
HB1-CB-HB2	96.09	110.00	1
HG1-CG-HG2	96.09	110.00	1
HA1-CA-HA2	122.91	109.00	1
HA1-CA-HA2	122.92	109.00	1
CG-CB-HB1	96.08	110.00	1
CG1-CD-HD2	122.92	109.00	1
C-N-HN	110.38	124.30	1
C-CA-HA2	95.08	109.00	1
HD21-CD2-HD23	96.07	110.00	1
HH11-NH1-HH12	106.07	120.00	1
C-CA-HA	95.07	109.00	1
CB-SG-HG1	85.78	109.00	1
CE-NZ-HZ1	123.93	110.00	1
C-N-HN	110.36	124.30	2
CB-CG2-HG23	123.94	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-HA	96.05	110.00	1
C-CA-HA	95.05	109.00	2
CA-CB-HB1	122.95	109.00	2
C-N-HN	110.35	124.30	1
CA-N-HN	127.95	114.00	1
CB-CG1-HG13	122.95	109.00	1
HD1-CD-HD2	96.05	110.00	1
HG21-CG2-HG22	95.04	109.00	1
CA-N-HN	127.97	114.00	1
HB1-CB-HB2	96.03	110.00	1
CD-CG-HG2	121.97	108.00	1
C-N-HN	110.33	124.30	1
N-CA-HA	96.02	110.00	1
C-CA-HA	95.02	109.00	1
CA-CB-HB2	122.98	109.00	1
CD-CG-HG2	121.98	108.00	1
C-N-HN	110.31	124.30	2
HG11-CG1-HG12	96.01	110.00	1
HG1-CG-HG2	96.01	110.00	1
HA1-CA-HA2	122.99	109.00	1
CD-CG1-HG11	94.01	108.00	1
HB1-CB-HB2	96.00	110.00	1
HD12-CD1-HD13	96.00	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE-NZ-HZ3	124.00	110.00	1
HG11-CG1-HG13	95.99	110.00	1
C-N-HN	110.28	124.30	3
CB-CG1-HG11	94.98	109.00	1
HG11-CG1-HG12	124.02	110.00	1
C-N-HN	110.27	124.30	3
CE2-CD2-HD2	133.43	119.40	1
CA-CB-HB2	94.97	109.00	1
CA-CB-HB1	123.04	109.00	1
CB-CA-HA	94.96	109.00	1
CB-CG2-HG23	124.04	110.00	1
CB-CG2-HG21	123.05	109.00	1
HB1-CB-HB2	95.95	110.00	1
HB2-CB-HB3	95.95	110.00	1
HG22-CG2-HG23	95.95	110.00	1
CD-CE-HE1	123.06	109.00	1
HE1-CE-HE2	95.94	110.00	1
CD-CG-HG2	122.06	108.00	1
N-CA-HA	95.94	110.00	1
C-N-HN	110.23	124.30	2
CB-CG-HG1	123.07	109.00	1
HB1-CB-HB2	95.93	110.00	1
HG1-CG-HG2	95.93	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	94.93	109.00	1
CA-CB-HB1	94.93	109.00	1
CA-N-HN	128.07	114.00	1
HG11-CG1-HG12	95.92	110.00	1
C-CA-HA	94.92	109.00	2
CB-CA-HA	94.92	109.00	1
CG-CB-HB1	124.08	110.00	1
CG-CB-HB2	122.08	108.00	1
HB1-CB-HB2	95.91	110.00	1
CB-CG-HG1	123.09	109.00	1
HB1-CB-HB3	95.91	110.00	1
HA1-CA-HA2	123.09	109.00	1
C-N-HN	110.21	124.30	1
CG-CD2-HD23	123.09	109.00	1
HG1-CG-HG2	95.89	110.00	3
C-CA-HA	94.89	109.00	2
C-N-HN	110.19	124.30	1
HB1-CB-HB2	95.89	110.00	2
HG21-CG2-HG22	95.89	110.00	1
CB-CG2-HG22	123.11	109.00	1
C-N-HN	110.18	124.30	1
HD2-CD-HD3	95.88	110.00	1
CZ-NH2-HH21	105.88	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB2	123.13	109.00	1
HB2-CB-HB3	95.87	110.00	1
OG1-CB-HB	94.86	109.00	1
C-N-HN	110.16	124.30	1
C-CA-HA	94.85	109.00	1
CB-CA-HA	94.85	109.00	1
CB-CA-HA	94.84	109.00	1
HB1-CB-HB2	95.84	110.00	1
CE-CD-HD1	122.16	108.00	1
C-N-HN	110.14	124.30	1
NE-CD-HD1	122.16	108.00	1
C-N-HN	110.13	124.30	1
CG-CD1-HD12	123.17	109.00	1
CG-CD-HD1	123.18	109.00	1
HG22-CG2-HG23	95.82	110.00	1
CB-CA-HA	94.82	109.00	1
HA1-CA-HA2	123.18	109.00	1
HE1-CE-HE2	95.81	110.00	1
CB-CA-HA	123.19	109.00	1
CG1-CD-HD3	123.19	109.00	1
HG11-CG1-HG13	95.80	110.00	1
HG1-CG-HG2	124.20	110.00	1
C-N-HN	110.10	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG11-CG1-HG12	95.80	110.00	1
N-CD-HD2	123.20	109.00	1
CA-N-HN	105.79	120.00	1
HB1-CB-HB2	95.78	110.00	1
CB-CA-HA	94.78	109.00	2
CB-CA-HA	123.22	109.00	1
N-CA-HA	95.78	110.00	1
HD11-CD1-HD13	95.78	110.00	1
HZ1-NZ-HZ3	123.22	109.00	1
C-N-HN	110.08	124.30	2
HD12-CD1-HD13	95.77	110.00	1
HG21-CG2-HG23	95.77	110.00	1
CA-CB-HB2	123.23	109.00	1
CB-CG2-HG23	123.23	109.00	1
CA-N-HN	128.23	114.00	1
C-N-HN	110.06	124.30	3
HE1-CE-HE2	95.76	110.00	1
HB1-CB-HB2	95.76	110.00	1
HG22-CG2-HG23	95.75	110.00	1
CB-OG1-HG1	95.75	110.00	1
CB-CG-HG1	123.26	109.00	1
HD1-CD-HD2	95.74	110.00	1
HB1-CB-HB2	95.74	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	95.74	110.00	1
HZ1-NZ-HZ2	94.74	109.00	1
C-N-HN	110.03	124.30	1
HB1-CB-HB2	95.73	110.00	1
N-CA-HA	95.73	110.00	1
CZ-NH2-HH22	105.72	120.00	1
CD2-CE2-HE2	134.28	120.00	1
HE21-NE2-HE22	134.28	120.00	1
CE1-CZ-HZ	134.28	120.00	1
HG11-CG1-HG12	95.71	110.00	1
N-CA-HA2	95.71	110.00	1
HB1-CB-HB2	95.70	110.00	1
CG-ND2-HD21	105.69	120.00	1
HB1-CB-HB2	95.69	110.00	1
CA-CB-HB2	123.32	109.00	1
CB-CA-HA	123.32	109.00	1
C-CA-HA	94.68	109.00	1
CZ-NH2-HH21	105.68	120.00	1
CD-CG-HG1	124.33	110.00	1
CA-CB-HB1	123.33	109.00	1
CZ-NH2-HH22	105.67	120.00	1
CD-CE-HE1	123.34	109.00	1
C-N-HN	109.96	124.30	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-HD1	94.66	109.00	1
C-CA-HA	94.65	109.00	1
CZ-NH2-HH22	105.65	120.00	1
C-N-HN	109.95	124.30	1
HG1-CG-HG2	95.64	110.00	1
C-N-HN	109.94	124.30	3
HZ1-NZ-HZ3	94.64	109.00	1
HG21-CG2-HG23	95.63	110.00	2
HA1-CA-HA2	123.37	109.00	1
HN1-N-HN2	117.53	103.16	1
CA-N-HN	128.37	114.00	1
CG-CB-HB1	122.37	108.00	1
CE-NZ-HZ1	124.38	110.00	1
CG-CD2-HD23	123.38	109.00	1
C-N-HN	109.92	124.30	1
HD21-ND2-HD22	105.62	120.00	1
CG1-CB-HB	93.62	108.00	1
HD1-CD-HD2	95.61	110.00	1
HB1-CB-HB2	95.61	110.00	1
C-N-HN	109.91	124.30	2
HG1-CG-HG2	95.61	110.00	1
CA-CB-HB2	123.40	109.00	1
HG1-CG-HG2	95.60	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-OG1-HG1	95.60	110.00	1
C-N-HN	109.90	124.30	2
CZ-NH2-HH22	105.59	120.00	1
HG11-CG1-HG12	95.59	110.00	1
CD-NE2-HE21	105.59	120.00	1
CG-CD2-HD21	123.41	109.00	1
CB-CG1-HG12	123.41	109.00	1
CE-NZ-HZ3	95.59	110.00	1
HB1-CB-HB2	95.58	110.00	1
N-CA-HA	95.58	110.00	1
HB1-CB-HB3	95.57	110.00	1
C-N-HN	109.87	124.30	2
HD1-CD-HD3	95.57	110.00	1
N-CA-HA	95.56	110.00	1
H1-N-H3	95.02	109.47	1
HB1-CB-HB2	95.55	110.00	2
HA1-CA-HA2	123.45	109.00	1
C-CA-HA	94.55	109.00	1
HB1-CB-HB2	124.46	110.00	1
HB1-CB-HB2	95.54	110.00	3
CG-CB-HB1	124.46	110.00	1
CB-CA-HA	94.54	109.00	1
HB1-CB-HB2	95.53	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG1-CD-HD1	123.47	109.00	1
C-CA-HA	94.53	109.00	1
C-N-HN	109.83	124.30	1
CA-N-HN	128.48	114.00	1
HG22-CG2-HG23	95.52	110.00	1
N-CA-HA	95.52	110.00	1
CG-CD1-HD12	123.49	109.00	1
HG21-CG2-HG22	95.51	110.00	1
C-CA-HA	94.50	109.00	1
HB1-CB-HB2	95.50	110.00	1
C-N-HN	109.80	124.30	1
HG21-CG2-HG23	94.50	109.00	1
HG11-CG1-HG12	95.50	110.00	1
C-N-HN	109.79	124.30	2
C-CA-HA	94.49	109.00	1
CB-CA-HA	123.51	109.00	1
HD1-CD-HD2	95.48	110.00	1
CE-NZ-HZ2	124.52	110.00	1
HB1-CB-HB2	95.48	110.00	1
CG-CB-HB2	93.47	108.00	1
CD-NE2-HE21	105.47	120.00	1
HE2-CE-HE3	95.47	110.00	1
C-N-HN	109.77	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD-HD1	123.53	109.00	1
HG11-CG1-HG12	95.47	110.00	1
CE-NZ-HZ2	95.47	110.00	1
CA-CB-HB2	123.54	109.00	1
CA-CB-HB1	94.46	109.00	1
C-N-HN	109.75	124.30	2
CB-CG1-HG11	94.45	109.00	1
HD12-CD1-HD13	95.44	110.00	1
HB1-CB-HB2	95.44	110.00	1
CB-CA-HA	94.43	109.00	1
CE-CD-HD1	93.43	108.00	1
HG21-CG2-HG23	95.43	110.00	1
HD21-CD2-HD22	95.42	110.00	1
CB-CG1-HG12	123.58	109.00	1
NE2-CD2-HD2	111.82	126.40	1
HD21-CD2-HD23	95.42	110.00	1
C-CA-HA1	94.42	109.00	1
C-N-HN	109.72	124.30	2
CD1-CG-HG	93.41	108.00	1
C-N-HN	109.71	124.30	1
HB1-CB-HB2	95.41	110.00	1
CG1-CD-HD1	123.60	109.00	1
HA1-CA-HA2	123.60	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB1	123.60	109.00	1
N-CA-HA	95.40	110.00	1
CE-CD-HD1	93.40	108.00	1
CB-CG1-HG13	123.61	109.00	1
HB1-CB-HB2	95.39	110.00	1
C-N-HN	109.69	124.30	2
CB-CG-HG2	123.61	109.00	1
CB-CA-HA	94.38	109.00	1
N-CA-HA	95.37	110.00	1
HB1-CB-HB2	124.63	110.00	1
HG1-CG-HG2	95.36	110.00	1
HB1-CB-HB2	95.36	110.00	1
C-N-HN	109.65	124.30	1
HG21-CG2-HG22	95.35	110.00	1
HG11-CG1-HG12	95.35	110.00	2
C-N-HN	109.64	124.30	1
CE-NZ-HZ1	124.66	110.00	1
HG21-CG2-HG23	95.34	110.00	1
HH21-NH2-HH22	105.33	120.00	1
C-N-HN	109.62	124.30	1
HG1-CG-HG2	95.32	110.00	1
HB1-CB-HB2	95.32	110.00	2
OG-CB-HB2	123.68	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG22-CG2-HG23	94.31	109.00	1
HB1-CB-HB2	95.31	110.00	2
CE-CD-HD1	122.69	108.00	1
CD-CG-HG2	95.31	110.00	1
HB1-CB-HB3	95.31	110.00	1
HD1-CD-HD2	95.31	110.00	1
C-N-HN	109.59	124.30	1
HD21-ND2-HD22	134.72	120.00	1
N-CA-HA	95.28	110.00	1
HG1-CG-HG2	95.27	110.00	1
C-N-HN	109.57	124.30	1
CG-ND2-HD21	105.26	120.00	1
CB-CA-HA	94.26	109.00	1
C-N-HN	109.56	124.30	1
CG-CB-HB1	93.25	108.00	1
C-N-HN2	110.17	120.00	1
CB-CG2-HG22	124.75	110.00	1
CG-CB-HB2	122.75	108.00	1
CG-CB-HB2	93.25	108.00	1
C-N-HN	109.54	124.30	1
CB-CA-HA	94.22	109.00	1
C-CA-HA1	94.22	109.00	1
HH21-NH2-HH22	134.78	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	109.51	124.30	1
CD-CE-HE2	123.79	109.00	1
CA-CB-HB1	123.79	109.00	1
CB-CA-HA	94.20	109.00	2
CZ-OH-HH	95.20	110.00	1
C-CA-HA	94.19	109.00	2
N-CA-HA	95.19	110.00	2
HD22-CD2-HD23	95.18	110.00	1
CG-ND2-HD22	105.18	120.00	1
CB-CA-HA	123.82	109.00	1
CG2-CB-HB	94.17	109.00	1
N-CA-HA	95.17	110.00	2
CA-CB-HB2	123.83	109.00	1
HG1-CG-HG2	95.16	110.00	1
C-N-HN	109.46	124.30	3
CA-N-HN	128.84	114.00	1
HB1-CB-HB2	95.16	110.00	1
N-CA-HA	95.16	110.00	1
C-N-HN	109.45	124.30	2
CA-CB-HB2	94.13	109.00	1
HB1-CB-HB2	95.13	110.00	1
HB1-CB-HB2	95.12	110.00	1
HG1-CG-HG2	95.12	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	109.42	124.30	2
C-N-HN	109.41	124.30	1
HB1-CB-HB2	95.11	110.00	1
HG11-CG1-HG12	95.10	110.00	1
C-CA-HA	94.10	109.00	1
HD1-CD-HD3	95.10	110.00	1
CD-CG-HG1	122.92	108.00	1
HE1-CE-HE2	95.08	110.00	1
HA1-CA-HA2	123.93	109.00	1
HB1-CB-HB2	95.07	110.00	1
HA1-CA-HA2	123.94	109.00	2
CE-NZ-HZ3	95.06	110.00	1
CB-CG-HG1	123.94	109.00	1
HG22-CG2-HG23	94.06	109.00	1
CD-CG-HG2	122.94	108.00	1
HG11-CG1-HG12	95.05	110.00	2
CA-CB-HB1	94.05	109.00	1
HG22-CG2-HG23	123.95	109.00	1
HZ1-NZ-HZ2	94.04	109.00	1
CB-CG-HG	123.96	109.00	1
HD21-CD2-HD22	95.04	110.00	1
CB-CG1-HG13	123.97	109.00	1
HB1-CB-HB2	95.02	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB1	123.99	109.00	1
HG22-CG2-HG23	94.01	109.00	1
CA-N-HN	128.99	114.00	1
N-CA-HA	95.01	110.00	1
HG11-CG1-HG12	95.00	110.00	1
CG-CB-HB2	93.00	108.00	1
CE1-CD1-HD1	134.40	119.40	1
HG12-CG1-HG13	95.00	110.00	1
CZ-NH1-HH12	105.00	120.00	1
HB1-CB-HB2	95.00	110.00	1
HA1-CA-HA2	124.01	109.00	1
CA-CB-HB1	124.02	109.00	1
HG1-CG-HG2	94.98	110.00	1
HD1-CD-HD2	94.98	110.00	1
HA1-CA-HA2	124.03	109.00	1
HG21-CG2-HG22	94.97	110.00	1
CG-CB-HB1	125.03	110.00	1
CB-CA-HA	124.04	109.00	1
CB-CA-HA	93.96	109.00	1
CB-CA-HA	93.95	109.00	1
HA1-CA-HA2	124.06	109.00	1
C-N-HN	109.24	124.30	2
N-CA-HA	94.94	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-ND2-HD22	104.94	120.00	1
CA-N-HN	129.07	114.00	1
C-CA-HA	93.93	109.00	1
HB1-CB-HB2	94.92	110.00	1
C-CA-HA	93.92	109.00	1
C-CA-HA	93.91	109.00	2
CB-CG2-HG23	124.09	109.00	1
HD22-CD2-HD23	94.91	110.00	1
HE21-NE2-HE22	104.90	120.00	1
CB-CA-HA	93.88	109.00	1
N-CA-HA	94.88	110.00	1
CA-N-HN	129.12	114.00	1
C-N-HN2	109.92	120.00	1
HG21-CG2-HG22	94.88	110.00	1
CA-CB-HB1	93.88	109.00	1
CA-CB-HB2	124.13	109.00	1
CA-CB-HB1	124.13	109.00	1
HG21-CG2-HG22	94.86	110.00	1
CG-CB-HB2	94.84	110.00	1
HB1-CB-HB2	94.84	110.00	1
N-CA-HA	94.84	110.00	1
C-CA-HA	93.83	109.00	1
HE1-CE-HE2	94.83	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	109.12	124.30	1
N-CA-HA	94.82	110.00	1
CA-N-HN	129.18	114.00	1
CB-CA-HA	124.18	109.00	1
CG-CB-HB1	123.19	108.00	1
CG-CB-HB2	123.19	108.00	1
CB-CA-HA	93.81	109.00	1
CA-CB-HB1	124.20	109.00	1
CG1-CB-HB	93.80	109.00	1
CA-N-HN	129.21	114.00	1
HG11-CG1-HG12	94.79	110.00	1
C-CA-HA2	93.79	109.00	1
HD1-CD-HD2	94.78	110.00	1
C-N-HN	109.08	124.30	2
C-CA-HA	93.78	109.00	1
HG21-CG2-HG22	94.78	110.00	1
HG1-CG-HG2	94.77	110.00	1
HD1-CD-HD2	125.23	110.00	1
HD21-CD2-HD23	94.76	110.00	1
HG1-CG-HG2	94.76	110.00	2
CG-CD1-HD13	124.25	109.00	1
C-N-HN	109.05	124.30	1
HB1-CB-HB2	94.75	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-HB2	124.25	109.00	1
CB-OG1-HG1	94.74	110.00	1
HB1-CB-HB2	94.73	110.00	2
C-N-HN	109.03	124.30	1
HD1-CD-HD2	94.72	110.00	1
C-N-HN	109.01	124.30	2
HN1-N-HN2	118.46	103.16	1
HG11-CG1-HG13	94.70	110.00	1
CG-CB-HB2	123.31	108.00	1
NE2-CD2-HD2	111.09	126.40	1
CD1-CG-HG	92.68	108.00	1
CA-CB-HB2	93.67	109.00	1
HG12-CG1-HG13	94.66	110.00	1
C-CA-HA	93.66	109.00	1
HG1-CG-HG2	94.66	110.00	1
CB-CG2-HG21	125.34	110.00	1
CE-NZ-HZ1	125.35	110.00	1
HB1-CB-HB2	94.65	110.00	1
HD12-CD1-HD13	94.65	110.00	1
HD2-CD-HD3	94.65	110.00	1
C-N-HN	108.95	124.30	1
CB-CG-HG2	93.64	109.00	1
C-N-HN	108.93	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HG12-CG1-HG13	94.63	110.00	1
CA-CB-HB2	93.63	109.00	1
HD21-CD2-HD23	94.62	110.00	1
CA-CB-HB1	93.62	109.00	1
N-CA-HA	94.60	110.00	1
CB-CA-HA	93.60	109.00	1
CG1-CD-HD1	124.40	109.00	1
HG11-CG1-HG12	94.60	110.00	1
HG1-CG-HG2	94.59	110.00	1
CB-CG-HG1	124.41	109.00	1
HZ1-NZ-HZ2	93.58	109.00	1
C-N-HN	108.88	124.30	1
HG1-CG-HG2	94.57	110.00	1
HE1-CE-HE2	94.57	110.00	1
C-N-HN	108.87	124.30	1
C-N-HN	108.86	124.30	1
C-N-HN	108.85	124.30	2
HB2-CB-HB3	94.55	110.00	1
CB-CA-HA	93.53	109.00	1
HG12-CG1-HG13	94.53	110.00	1
CB-OG1-HG1	94.53	110.00	1
C-N-HN	108.82	124.30	2
C-CA-HA	93.51	109.00	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	108.80	124.30	2
HE21-NE2-HE22	104.48	120.00	1
CB-CG-HG1	124.52	109.00	1
HD1-CD-HD3	94.47	110.00	1
CG-CB-HB2	94.46	110.00	1
C-CA-HA	93.46	109.00	1
C-CA-HA	93.43	109.00	1
HN1-N-HN2	118.73	103.16	1
HB1-CB-HB2	94.42	110.00	1
CG-CB-HB2	125.58	110.00	1
HE1-CE-HE3	94.42	110.00	1
C-CA-HA	93.42	109.00	1
N-CA-HA	94.41	110.00	2
C-CA-HA	93.39	109.00	1
C-N-HN	108.69	124.30	1
N-CA-HA	94.38	110.00	1
C-N-HN	108.68	124.30	1
HN1-N-HN2	118.79	103.16	1
C-N-HN	108.66	124.30	1
CA-CB-HB1	124.65	109.00	1
HG21-CG2-HG23	94.34	110.00	1
C-CA-HA	93.34	109.00	1
HD2-CD-HD3	94.33	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	93.32	109.00	1
HD12-CD1-HD13	94.31	110.00	1
HG1-CG-HG2	94.31	110.00	1
HN1-N-HN2	118.85	103.16	1
CA-N-HN	129.69	114.00	1
C-N-HN	108.61	124.30	1
CG1-CD-HD2	124.69	109.00	1
HG1-CG-HG2	94.30	110.00	1
C-N-HN	108.60	124.30	1
N-CD-HD2	124.71	109.00	1
CB-CA-HA	93.28	109.00	1
CA-CB-HB1	93.27	109.00	1
CD-CG-HG2	125.73	110.00	1
C-CA-HA	93.27	109.00	1
HB1-CB-HB2	94.27	110.00	1
C-N-HN	108.56	124.30	1
HE21-NE2-HE22	135.74	120.00	1
N-CA-HA	94.26	110.00	1
CB-CG1-HG11	93.26	109.00	1
CB-CG-HG2	93.26	109.00	1
C-N-HN	108.54	124.30	1
HD12-CD1-HD13	94.23	110.00	1
N-CA-HA	94.23	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HA1-CA-HA2	124.78	109.00	1
CE-NZ-HZ2	94.22	110.00	1
HG21-CG2-HG23	94.22	110.00	1
C-N-HN	108.50	124.30	1
CB-CA-HA	93.20	109.00	1
CG-CB-HB1	92.20	108.00	1
HG21-CG2-HG23	94.20	110.00	1
C-CA-HA	93.19	109.00	1
CA-CB-HB2	124.83	109.00	1
C-CA-HA	93.16	109.00	1
HD1-CD-HD2	94.14	110.00	1
CG2-CB-HB	93.13	109.00	1
HN1-N-HN2	119.03	103.16	1
C-CA-HA	93.10	109.00	1
C-N-HN	108.40	124.30	1
HD12-CD1-HD13	94.10	110.00	1
CB-CG-HG1	124.92	109.00	1
CB-CA-HA	93.06	109.00	1
C-N-HN	108.35	124.30	1
CA-CB-HB1	93.05	109.00	1
C-CA-HA	93.05	109.00	1
C-N-HN	108.34	124.30	1
C-N-HN	108.33	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD-CG1-HG12	123.98	108.00	1
HD2-CD-HD3	94.02	110.00	1
C-N-HN	108.32	124.30	1
CB-CG1-HG13	124.98	109.00	1
C-CA-HA	93.02	109.00	1
HZ2-NZ-HZ3	93.02	109.00	1
CA-CB-HB1	124.98	109.00	1
HG12-CG1-HG13	94.01	110.00	1
C-N-HN	108.31	124.30	1
N-CA-HA	94.01	110.00	1
C-N-HN	108.30	124.30	1
C-N-HN	108.28	124.30	1
CB-CG2-HG23	125.03	109.00	1
HG1-CG-HG2	93.94	110.00	1
CG-CB-HB2	124.06	108.00	1
CD-CG-HG2	126.07	110.00	1
C-N-HN	108.22	124.30	3
C-N-HN1	109.27	120.00	1
HG11-CG1-HG12	93.91	110.00	1
CB-CG2-HG22	125.10	109.00	1
CB-CG2-HG23	125.10	109.00	1
C-N-HN	108.19	124.30	1
CD-NE2-HE22	103.89	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-HA	92.89	109.00	1
CB-CG-HG1	92.89	109.00	1
C-CA-HA2	92.88	109.00	1
HB1-CB-HB3	93.86	110.00	1
CB-CA-HA	125.14	109.00	1
HG21-CG2-HG23	93.85	110.00	1
C-N-HN	108.15	124.30	1
HG21-CG2-HG23	92.85	109.00	1
HG1-CG-HG2	126.15	110.00	1
N-CA-HA	93.82	110.00	1
C-N-HN	108.11	124.30	1
CA-CB-HB1	125.19	109.00	1
C-N-HN	108.10	124.30	1
HG1-CG-HG2	93.79	110.00	1
HB1-CB-HB2	93.77	110.00	1
C-CA-HA	92.77	109.00	1
HB1-CB-HB2	93.76	110.00	1
HG11-CG1-HG12	93.76	110.00	1
C-CA-HA	92.76	109.00	1
CG-CD1-HD12	125.24	109.00	1
HN1-N-HN2	119.40	103.16	1
CA-N-HN	130.24	114.00	1
HB1-CB-HB2	93.75	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	93.73	110.00	1
HA1-CA-HA2	125.27	109.00	1
CG-ND2-HD21	103.73	120.00	1
C-N-HN	108.01	124.30	2
HB1-CB-HB2	93.71	110.00	1
HN1-N-HN2	119.46	103.16	1
CA-N-H3	125.77	109.47	1
HN1-N-HN2	119.47	103.16	1
C-N-HN	107.97	124.30	1
HG1-CG-HG2	93.67	110.00	1
C-N-HN	107.96	124.30	1
HB1-CB-HB2	93.66	110.00	1
C-N-HN	107.94	124.30	1
HB1-CB-HB2	93.64	110.00	1
HG1-CG-HG2	93.62	110.00	1
HD22-CD2-HD23	93.59	110.00	1
CZ-NE-HE	101.48	117.90	1
C-N-HN	107.88	124.30	2
HD1-CD-HD2	93.56	110.00	1
HG1-CG-HG2	93.54	110.00	1
N-CA-HA	126.48	110.00	1
HB1-CB-HB3	93.51	110.00	1
HG1-CG-HG2	93.50	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CZ-NH2-HH22	103.49	120.00	1
CD-CG-HG1	126.52	110.00	1
C-N-HN	107.75	124.30	1
N-CA-HA	93.44	110.00	1
HE21-NE2-HE22	136.56	120.00	1
HG11-CG1-HG12	93.43	110.00	1
N-CA-HA	93.41	110.00	1
HG21-CG2-HG22	93.38	110.00	1
CG-CB-HB2	91.37	108.00	1
C-N-HN	107.67	124.30	1
HN1-N-HN2	119.81	103.16	1
C-N-HN	107.64	124.30	1
CA-CB-HB1	125.66	109.00	1
C-N-HN	107.63	124.30	1
C-N-HN	107.62	124.30	1
C-N-HN	107.53	124.30	1
CA-CB-HB1	125.77	109.00	1
HD2-CD-HD3	126.77	110.00	1
C-CA-HA	92.22	109.00	1
C-N-HN	107.49	124.30	1
C-N-HN	107.48	124.30	1
N-CA-HA	93.17	110.00	1
HB1-CB-HB2	93.17	110.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-HA	93.16	110.00	1
HG12-CG1-HG13	93.14	110.00	1
CB-SG-HG1	80.90	109.00	1
C-N-HN	107.42	124.30	1
HB1-CB-HB2	93.12	110.00	1
HD11-CD1-HD12	93.09	110.00	1
HD21-CD2-HD22	93.08	110.00	1
CA-N-HN	130.92	114.00	1
C-N-HN	107.37	124.30	1
HA1-CA-HA2	125.94	109.00	1
CA-CB-HB1	125.95	109.00	1
HD11-CD1-HD13	93.05	110.00	1
N-CA-HA	93.04	110.00	1
HE1-CE-HE2	93.03	110.00	1
CA-CB-HB2	92.02	109.00	1
CB-CG-HG1	125.99	109.00	1
HG21-CG2-HG22	92.99	110.00	1
HG22-CG2-HG23	92.99	110.00	1
CB-CA-HA	91.96	109.00	1
C-N-HN1	108.64	120.00	1
HB2-CB-HB3	92.95	110.00	1
C-N-HN	107.24	124.30	1
C-N-HN	107.22	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HN1-N-HN2	120.25	103.16	1
C-N-HN1	131.40	120.00	1
HG21-CG2-HG23	92.89	110.00	1
HG22-CG2-HG23	92.87	110.00	1
HN1-N-HN2	120.29	103.16	1
HB1-CB-HB2	92.87	110.00	1
C-CA-HA	91.83	109.00	1
HD21-ND2-HD22	137.21	120.00	1
HG1-CG-HG2	92.78	110.00	1
HB1-CB-HB2	92.77	110.00	1
CA-N-HN	131.26	114.00	1
CD-CG-HG1	125.28	108.00	1
N-CA-HA1	92.72	110.00	1
CB-CG-HG1	126.31	109.00	1
C-CA-HA	91.66	109.00	1
HB1-CB-HB2	92.65	110.00	1
HG11-CG1-HG13	127.38	110.00	1
HZ1-NZ-HZ3	91.62	109.00	1
HD11-CD1-HD12	92.61	110.00	1
CG-CB-HB2	92.60	110.00	1
CA-CB-HB1	126.41	109.00	1
HG11-CG1-HG12	92.57	110.00	1
HD21-ND2-HD22	102.57	120.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HN1-N-HN2	120.59	103.16	1
HG21-CG2-HG22	92.56	110.00	1
C-N-HN	106.85	124.30	1
C-CA-HA	91.52	109.00	1
CA-N-HN	131.53	114.00	1
HG11-CG1-HG12	92.47	110.00	1
HB1-CB-HB2	92.44	110.00	1
HB1-CB-HB2	92.40	110.00	1
C-N-HN	106.65	124.30	1
HG11-CG1-HG13	92.33	110.00	1
HG1-CG-HG2	92.33	110.00	1
HD21-ND2-HD22	137.68	120.00	1
HZ1-NZ-HZ2	91.30	109.00	1
CB-CG-HG1	91.30	109.00	1
C-CA-HA	91.26	109.00	1
C-N-HN	106.55	124.30	1
HG22-CG2-HG23	92.24	110.00	1
C-N-HN	106.54	124.30	1
HN1-N-HN2	120.96	103.16	1
C-N-HN	106.50	124.30	1
HH21-NH2-HH22	102.20	120.00	1
CE-NZ-HZ3	127.84	110.00	1
C-N-HN	106.44	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	92.13	110.00	1
C-N-HN	106.43	124.30	1
C-N-HN	106.31	124.30	1
HD1-CD-HD2	92.00	110.00	1
HN1-N-HN2	121.16	103.16	1
CD-CG-HG1	128.01	110.00	1
HB1-CB-HB2	91.98	110.00	1
CB-CG-HG2	127.04	109.00	1
HG11-CG1-HG13	91.95	110.00	1
CG-CD-HD1	127.06	109.00	1
HN1-N-HN2	121.23	103.16	1
C-N-HN	106.19	124.30	1
HG22-CG2-HG23	91.84	110.00	1
HN1-N-HN2	121.34	103.16	1
C-N-HN	106.11	124.30	1
HB2-CB-HB3	91.78	110.00	1
HN1-N-HN2	121.41	103.16	1
C-N-HN	106.04	124.30	1
HG22-CG2-HG23	91.70	110.00	1
HH11-NH1-HH12	101.69	120.00	1
CZ-NH1-HH12	101.59	120.00	1
HD12-CD1-HD13	91.56	110.00	1
C-N-HN	105.82	124.30	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-HN	105.81	124.30	1
HG21-CG2-HG22	91.50	110.00	1
HB1-CB-HB2	91.49	110.00	1
HG21-CG2-HG22	91.49	110.00	1
C-N-HN	105.78	124.30	1
CB-CA-HA	90.42	109.00	1
N-CA-HA	91.42	110.00	1
HG1-CG-HG2	91.25	110.00	1
C-N-HN	105.54	124.30	1
HD21-CD2-HD23	91.20	110.00	1
C-N-HN	105.42	124.30	1
HN1-N-HN2	122.13	103.16	1
CG-CD2-HD23	128.07	109.00	1
C-N-HN2	107.23	120.00	1
CB-CG1-HG13	128.22	109.00	1
HG11-CG1-HG13	90.74	110.00	1
C-CA-HA	89.53	109.00	1
N-CA-HA	90.46	110.00	1
HN1-N-HN2	122.76	103.16	1
C-CA-HA	89.11	109.00	1
C-N-HN	104.40	124.30	1
HB1-CB-HB2	90.00	110.00	1
HN1-N-HN2	123.31	103.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HB1-CB-HB2	89.81	110.00	1
CG-CB-HB2	128.23	108.00	1
C-N-HN	103.95	124.30	1
C-N-HN	103.70	124.30	1
HN1-N-HN2	123.78	103.16	1
HN1-N-HN2	124.01	103.16	1
HN1-N-HN2	124.08	103.16	1
HD21-ND2-HD22	141.29	120.00	1
HD22-CD2-HD23	88.63	110.00	1
C-N-HN	102.90	124.30	1
HN1-N-HN2	124.59	103.16	1
HN1-N-HN2	124.94	103.16	1
HN1-N-HN2	124.95	103.16	1
HN1-N-HN2	125.00	103.16	1
HN1-N-HN2	125.12	103.16	1
HN1-N-HN2	125.15	103.16	1
HN1-N-HN2	125.50	103.16	1
HN1-N-HN2	125.83	103.16	1
HB1-CB-HB2	86.80	110.00	1
HN1-N-HN2	126.59	103.16	1
C-N-HN	100.59	124.30	1
HN1-N-HN2	126.92	103.16	1
CB-CA-HA	84.11	109.00	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
HN1-N-HN2	128.18	103.16	1
HN1-N-HN2	129.46	103.16	1
HN1-N-HN2	129.62	103.16	1
HN1-N-HN2	130.25	103.16	1
HN1-N-HN2	130.69	103.16	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	0.95	175

All 175 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	I:28:GLN:HE21	I:31:HIS:CE1	0.657
1	BA:28:GLN:H	BA:31:HIS:CE1	0.656
1	KA:17:TYR:CE2	LA:22:LEU:HD23	0.620
1	ZA:183:ILE:HB	ZA:187:VAL:HG22	0.618
1	B:28:GLN:H	B:31:HIS:CE1	0.609
1	D:183:ILE:HG22	D:185:LYS:H	0.585
1	L:183:ILE:HG22	L:185:LYS:H	0.577
1	V:111:PHE:HB3	V:166:VAL:HG23	0.567
1	QA:65:ALA:HB2	RA:209:LYS:HE3	0.566
1	SA:24:ARG:O	SA:212:VAL:HG22	0.566
1	D:62:ARG:HE	D:119:ASP:CG	0.560
1	F:205:TYR:CE2	F:211:LEU:HD13	0.557

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	J:75:GLU:HG2	K:197:VAL:HG23	0.556
1	NA:67:ALA:H	OA:211:LEU:CD2	0.551
1	IA:62:ARG:HE	IA:119:ASP:CG	0.547
1	OA:28:GLN:H	OA:31:HIS:CE1	0.541
1	K:222:VAL:HG12	K:227:ILE:CD	0.538
1	AA:17:TYR:CD1	AA:216:LYS:HG3	0.536
1	FA:62:ARG:HE	FA:119:ASP:CG	0.535
1	SA:183:ILE:HG22	SA:185:LYS:H	0.535
1	C:62:ARG:HE	C:119:ASP:CG	0.532
1	UA:124:LEU:HD11	VA:32:LEU:HD23	0.531
1	JA:229:LEU:HD12	KA:140:PRO:HG2	0.526
1	NA:60:ILE:HG22	NA:62:ARG:HD2	0.517
1	L:87:LYS:HG3	M:186:VAL:HG21	0.510
1	F:67:ALA:H	G:211:LEU:HD21	0.508
1	KA:67:ALA:H	LA:211:LEU:HD21	0.508
1	V:50:ILE:HG23	V:133:ALA:HB1	0.507
1	M:119:ASP:CG	M:160:LYS:HZ3	0.502
1	GA:118:ALA:HB2	GA:159:ILE:HG22	0.500
1	M:231:ALA:HB3	N:36:GLN:HG3	0.499
1	KA:62:ARG:HE	KA:119:ASP:CG	0.498
1	SA:100:GLU:HB2	SA:177:GLN:HE21	0.498
1	K:113:PHE:CE1	K:213:PHE:CD2	0.497
1	M:7:PRO:HB3	M:73:LYS:HD3	0.497

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	KA:87:LYS:HG3	LA:186:VAL:HG21	0.495
1	OA:67:ALA:HA	PA:205:TYR:HB2	0.492
1	G:210:GLN:C	G:211:LEU:HD12	0.488
1	SA:27:ILE:HA	SA:31:HIS:CE1	0.487
1	GA:79:PHE:CZ	GA:103:TYR:HB3	0.485
1	IA:18:ASN:O	IA:214:GLY:HA2	0.485
1	GA:27:ILE:HB	GA:212:VAL:HG21	0.484
1	FA:66:ALA:HB3	FA:116:VAL:HG12	0.483
1	GA:124:LEU:HD11	HA:32:LEU:HD23	0.483
1	YA:62:ARG:HE	YA:119:ASP:CG	0.480
1	HA:124:LEU:HD11	IA:32:LEU:HD23	0.479
1	XA:157:GLN:HB3	XA:216:LYS:HB2	0.476
1	K:157:GLN:HE22	L:24:ARG:CZ	0.474
1	G:35:GLN:HA	G:39:THR:O	0.473
1	K:27:ILE:HB	K:212:VAL:HG21	0.473
1	DA:68:GLY:HA2	DA:116:VAL:HG21	0.473
1	AA:113:PHE:CE1	AA:213:PHE:CD2	0.471
1	MA:46:LEU:HD21	MA:126:VAL:HG13	0.471
1	WA:43:LEU:HD22	WA:141:VAL:HG11	0.471
1	GA:220:ILE:HA	GA:229:LEU:HD23	0.470
1	VA:118:ALA:HB2	VA:159:ILE:HG22	0.469
1	K:3:LEU:N	K:3:LEU:HD13	0.466
1	X:67:ALA:H	Y:211:LEU:HD21	0.466

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	U:6:ASP:CG	U:170:LYS:HZ1	0.464
1	JA:28:GLN:H	JA:31:HIS:CD2	0.464
1	F:184:GLN:CD	F:184:GLN:H	0.463
1	N:78:SER:HA	N:104:ASN:HA	0.463
1	S:24:ARG:HA	S:211:LEU:HD23	0.463
1	GA:205:TYR:CZ	GA:207:GLY:HA3	0.463
1	J:24:ARG:O	J:212:VAL:HG22	0.462
1	VA:71:GLY:HA2	WA:200:GLN:HE22	0.461
1	EA:184:GLN:CD	EA:184:GLN:H	0.460
1	J:205:TYR:CE2	J:211:LEU:HD13	0.459
1	BA:81:ILE:HA	CA:191:LEU:HB3	0.459
1	PA:33:LEU:HD12	PA:40:VAL:HG12	0.459
1	VA:18:ASN:HB2	VA:215:PHE:CE1	0.459
1	Y:23:PRO:HD2	Y:203:VAL:HG11	0.457
1	HA:124:LEU:HD13	IA:48:LYS:HB2	0.455
1	IA:109:VAL:HG23	IA:168:ALA:HB2	0.455
1	J:123:PRO:HG3	J:156:THR:HG21	0.454
1	B:29:PRO:HA	B:155:ILE:HG22	0.453
1	D:72:GLN:HB3	D:110:ARG:HA	0.453
1	X:67:ALA:H	Y:211:LEU:CD2	0.452
1	K:67:ALA:HA	L:205:TYR:CD1	0.450
1	UA:132:MET:HA	UA:132:MET:HE2	0.450
1	PA:113:PHE:CD1	PA:164:PHE:HB3	0.447

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:111:PHE:HB3	A:166:VAL:HG23	0.445
1	OA:35:GLN:HB2	OA:40:VAL:HG22	0.445
1	L:28:GLN:HB2	L:31:HIS:CE1	0.444
1	Z:66:ALA:HB3	Z:116:VAL:HG12	0.444
1	CA:160:LYS:HB3	CA:212:VAL:HG12	0.444
1	NA:72:GLN:HB2	NA:109:VAL:O	0.444
1	TA:231:ALA:HB1	UA:41:GLU:HG3	0.444
1	T:124:LEU:HD21	U:142:LEU:HD21	0.442
1	VA:17:TYR:CD1	VA:216:LYS:HG3	0.441
1	MA:151:ARG:HH21	MA:219:GLU:CD	0.439
1	M:231:ALA:HB3	N:36:GLN:CG	0.438
1	HA:28:GLN:H	HA:31:HIS:CE1	0.438
1	VA:65:ALA:HB2	WA:209:LYS:HD3	0.437
1	JA:160:LYS:HA	JA:212:VAL:HA	0.436
1	LA:72:GLN:O	MA:199:SER:HB2	0.436
1	NA:27:ILE:HB	NA:212:VAL:HG21	0.436
1	NA:123:PRO:HG3	NA:156:THR:HG21	0.436
1	I:67:ALA:HA	J:205:TYR:CD1	0.435
1	K:28:GLN:HB2	K:31:HIS:CE1	0.435
1	W:32:LEU:HD13	W:46:LEU:HD13	0.435
1	M:8:ALA:HA	M:109:VAL:HG21	0.434
1	R:27:ILE:HB	R:212:VAL:HG11	0.434
1	BA:118:ALA:HB2	BA:159:ILE:HG22	0.433

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	TA:84:ASN:O	UA:187:VAL:HA	0.433
1	ZA:60:ILE:HG21	ZA:62:ARG:NE	0.433
1	I:28:GLN:NE2	I:31:HIS:CE1	0.432
1	DA:184:GLN:CD	DA:184:GLN:H	0.432
1	C:65:ALA:HB3	D:211:LEU:HD11	0.431
1	M:73:LYS:O	M:108:LYS:HA	0.431
1	OA:222:VAL:HG12	OA:227:ILE:CD	0.431
1	A:48:LYS:HB2	ZA:124:LEU:HD13	0.429
1	U:50:ILE:HG22	U:52:GLN:H	0.428
1	VA:122:GLU:OE2	WA:45:SER:N	0.427
1	O:124:LEU:HD11	P:32:LEU:HD23	0.426
1	P:111:PHE:CD1	P:111:PHE:N	0.426
1	VA:18:ASN:CB	VA:215:PHE:CE1	0.425
1	E:17:TYR:CE1	E:216:LYS:HG3	0.424
1	K:11:TYR:CE2	K:19:VAL:HG11	0.424
1	HA:86:LEU:HD23	HA:96:GLY:HA2	0.424
1	O:139:ASN:HA	O:140:PRO:HD2	0.423
1	T:29:PRO:O	T:30:LEU:HG	0.423
1	QA:122:GLU:HG2	RA:44:GLY:HA2	0.422
1	DA:124:LEU:HD11	EA:32:LEU:HD23	0.421
1	HA:42:TYR:CZ	HA:44:GLY:HA2	0.419
1	KA:28:GLN:HB3	KA:29:PRO:HD2	0.419
1	S:67:ALA:H	T:211:LEU:HD21	0.418

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	BA:92:GLN:HB3	BA:93:PHE:H	0.418
1	P:183:ILE:HG22	P:184:GLN:N	0.417
1	T:109:VAL:HG23	T:168:ALA:HB2	0.417
1	D:160:LYS:HA	D:212:VAL:HA	0.416
1	H:86:LEU:HD23	H:96:GLY:HA2	0.416
1	KA:79:PHE:HB3	LA:193:VAL:HG13	0.416
1	PA:8:ALA:HA	PA:109:VAL:HG21	0.416
1	B:165:THR:HA	B:203:VAL:O	0.415
1	X:53:PRO:HA	X:54:PRO:HD3	0.415
1	WA:89:VAL:HG11	XA:185:LYS:HA	0.415
1	B:27:ILE:HA	B:31:HIS:CE1	0.414
1	F:62:ARG:HE	F:119:ASP:CG	0.414
1	Z:28:GLN:H	Z:31:HIS:CE1	0.414
1	IA:60:ILE:HG22	IA:62:ARG:HD2	0.414
1	BA:229:LEU:HD12	CA:140:PRO:HG2	0.413
1	SA:210:GLN:C	SA:211:LEU:HD12	0.412
1	RA:33:LEU:HD23	RA:42:TYR:HA	0.411
1	L:57:PRO:HA	L:58:PRO:HD3	0.410
1	M:124:LEU:HD21	N:142:LEU:HD21	0.410
1	IA:89:VAL:O	IA:89:VAL:HG12	0.410
1	D:120:SER:HB3	D:157:GLN:HE21	0.409
1	G:23:PRO:HA	G:212:VAL:O	0.409
1	R:147:LEU:HA	R:147:LEU:HD23	0.409

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	DA:23:PRO:HG3	DA:213:PHE:HA	0.408
1	TA:33:LEU:HD23	TA:42:TYR:HA	0.408
1	E:39:THR:HG22	E:41:GLU:HG2	0.407
1	F:57:PRO:HA	F:58:PRO:HD3	0.407
1	Y:178:LEU:HD23	Y:191:LEU:HD12	0.407
1	HA:89:VAL:HG13	IA:185:LYS:HD3	0.407
1	B:68:GLY:HA2	B:116:VAL:CG2	0.406
1	W:205:TYR:CE2	W:211:LEU:HD13	0.406
1	Y:160:LYS:HB3	Y:212:VAL:HG12	0.406
1	IA:87:LYS:HD2	JA:186:VAL:HG21	0.405
1	SA:87:LYS:HB2	TA:186:VAL:HB	0.405
1	G:24:ARG:O	G:212:VAL:HG22	0.404
1	M:160:LYS:HA	M:212:VAL:HA	0.404
1	X:130:LEU:HD11	X:227:ILE:HG21	0.404
1	OA:69:ILE:HG23	OA:113:PHE:HB2	0.404
1	OA:17:TYR:CE2	PA:22:LEU:HD23	0.404
1	TA:205:TYR:CZ	TA:207:GLY:HA3	0.404
1	X:143:LYS:HE2	X:147:LEU:HD21	0.403
1	EA:153:TYR:CD2	EA:219:GLU:HA	0.403
1	JA:75:GLU:HB3	KA:197:VAL:HG23	0.403
1	W:162:ASN:O	W:206:LYS:HA	0.402
1	I:17:TYR:CE1	I:216:LYS:HG3	0.401
1	S:124:LEU:HD13	T:48:LYS:HB2	0.400

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	V:11:TYR:CE1	V:12:LEU:HG	0.400
1	W:124:LEU:HA	W:124:LEU:HD23	0.400

Torsion angles: Protein backbone

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	11856	10576	958	322

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	9100	7887	800	413

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	3	LEU
1	A	7	PRO
1	A	19	VAL
1	A	57	PRO
1	A	104	ASN
1	A	165	THR
1	A	184	GLN
1	A	197	VAL
1	A	203	VAL
1	A	212	VAL
1	B	3	LEU

Model ID	Chain	Residue ID	Residue type
1	B	23	PRO
1	B	30	LEU
1	B	39	THR
1	B	54	PRO
1	B	135	VAL
1	B	186	VAL
1	B	230	PHE
1	C	3	LEU
1	C	28	GLN
1	C	35	GLN
1	C	47	GLU
1	C	158	VAL
1	C	186	VAL
1	D	3	LEU
1	D	76	ASN
1	D	90	LEU
1	D	108	LYS
1	D	109	VAL
1	D	154	VAL
1	D	158	VAL
1	D	203	VAL
1	D	212	VAL
1	E	3	LEU

Model ID	Chain	Residue ID	Residue type
1	E	23	PRO
1	E	88	SER
1	E	104	ASN
1	E	166	VAL
1	E	177	GLN
1	E	204	THR
1	E	212	VAL
1	F	3	LEU
1	F	30	LEU
1	F	53	PRO
1	F	58	PRO
1	F	104	ASN
1	F	191	LEU
1	F	197	VAL
1	F	204	THR
1	F	218	PHE
1	G	3	LEU
1	G	47	GLU
1	G	70	ASN
1	G	154	VAL
1	G	200	GLN
1	H	3	LEU
1	H	41	GLU

Model ID	Chain	Residue ID	Residue type
1	H	61	THR
1	H	158	VAL
1	H	179	ASP
1	H	218	PHE
1	I	3	LEU
1	I	49	LEU
1	I	186	VAL
1	I	192	LYS
1	I	208	GLU
1	I	212	VAL
1	I	222	VAL
1	J	3	LEU
1	J	14	ARG
1	J	19	VAL
1	J	49	LEU
1	J	121	VAL
1	J	158	VAL
1	J	184	GLN
1	K	3	LEU
1	K	39	THR
1	L	3	LEU
1	L	104	ASN
1	L	166	VAL

Model ID	Chain	Residue ID	Residue type
1	L	186	VAL
1	L	204	THR
1	L	218	PHE
1	M	3	LEU
1	M	19	VAL
1	M	77	LEU
1	M	108	LYS
1	M	114	SER
1	M	212	VAL
1	N	3	LEU
1	N	104	ASN
1	N	153	TYR
1	N	212	VAL
1	O	3	LEU
1	O	102	GLN
1	O	104	ASN
1	O	135	VAL
1	O	154	VAL
1	O	158	VAL
1	O	166	VAL
1	O	184	GLN
1	O	197	VAL
1	O	212	VAL

Model ID	Chain	Residue ID	Residue type
1	O	218	PHE
1	P	3	LEU
1	P	104	ASN
1	P	108	LYS
1	P	123	PRO
1	P	158	VAL
1	P	166	VAL
1	P	191	LEU
1	P	229	LEU
1	Q	3	LEU
1	Q	6	ASP
1	Q	23	PRO
1	Q	33	LEU
1	Q	58	PRO
1	Q	86	LEU
1	Q	186	VAL
1	Q	212	VAL
1	Q	228	THR
1	R	3	LEU
1	R	23	PRO
1	R	30	LEU
1	R	104	ASN
1	S	3	LEU

Model ID	Chain	Residue ID	Residue type
1	S	15	LEU
1	S	30	LEU
1	S	39	THR
1	S	58	PRO
1	S	158	VAL
1	S	178	LEU
1	S	184	GLN
1	S	187	VAL
1	S	212	VAL
1	S	222	VAL
1	T	3	LEU
1	T	70	ASN
1	T	104	ASN
1	T	121	VAL
1	T	149	ASN
1	T	158	VAL
1	T	177	GLN
1	T	185	LYS
1	T	212	VAL
1	T	218	PHE
1	U	3	LEU
1	U	53	PRO
1	U	135	VAL

Model ID	Chain	Residue ID	Residue type
1	U	184	GLN
1	U	191	LEU
1	U	212	VAL
1	V	3	LEU
1	V	104	ASN
1	V	208	GLU
1	V	211	LEU
1	V	212	VAL
1	W	3	LEU
1	W	23	PRO
1	W	30	LEU
1	W	39	THR
1	W	104	ASN
1	W	135	VAL
1	W	158	VAL
1	W	191	LEU
1	W	212	VAL
1	X	3	LEU
1	X	22	LEU
1	X	30	LEU
1	X	39	THR
1	X	57	PRO
1	X	107	ARG

Model ID	Chain	Residue ID	Residue type
1	X	135	VAL
1	X	181	PRO
1	Y	3	LEU
1	Y	70	ASN
1	Y	90	LEU
1	Y	123	PRO
1	Y	135	VAL
1	Y	158	VAL
1	Y	177	GLN
1	Y	208	GLU
1	Y	218	PHE
1	Y	230	PHE
1	Z	3	LEU
1	Z	39	THR
1	Z	56	GLU
1	Z	74	THR
1	Z	89	VAL
1	Z	104	ASN
1	Z	108	LYS
1	Z	212	VAL
1	AA	3	LEU
1	AA	30	LEU
1	AA	58	PRO

Model ID	Chain	Residue ID	Residue type
1	AA	76	ASN
1	AA	88	SER
1	AA	115	ASN
1	AA	228	THR
1	BA	3	LEU
1	BA	23	PRO
1	BA	35	GLN
1	BA	184	GLN
1	BA	191	LEU
1	BA	197	VAL
1	BA	228	THR
1	BA	230	PHE
1	CA	3	LEU
1	CA	156	THR
1	CA	166	VAL
1	CA	181	PRO
1	CA	184	GLN
1	CA	212	VAL
1	DA	3	LEU
1	DA	186	VAL
1	DA	191	LEU
1	DA	212	VAL
1	DA	222	VAL

Model ID	Chain	Residue ID	Residue type
1	EA	3	LEU
1	EA	47	GLU
1	EA	58	PRO
1	EA	166	VAL
1	EA	191	LEU
1	EA	204	THR
1	EA	208	GLU
1	EA	218	PHE
1	FA	3	LEU
1	FA	102	GLN
1	FA	184	GLN
1	FA	186	VAL
1	FA	200	GLN
1	FA	218	PHE
1	GA	3	LEU
1	GA	19	VAL
1	GA	23	PRO
1	GA	30	LEU
1	GA	58	PRO
1	GA	76	ASN
1	GA	104	ASN
1	GA	200	GLN
1	GA	203	VAL

Model ID	Chain	Residue ID	Residue type
1	GA	222	VAL
1	HA	3	LEU
1	HA	7	PRO
1	HA	39	THR
1	HA	58	PRO
1	HA	70	ASN
1	HA	104	ASN
1	HA	158	VAL
1	HA	166	VAL
1	HA	177	GLN
1	HA	184	GLN
1	HA	200	GLN
1	IA	3	LEU
1	IA	5	SER
1	IA	33	LEU
1	IA	35	GLN
1	IA	104	ASN
1	IA	121	VAL
1	IA	126	VAL
1	IA	181	PRO
1	IA	187	VAL
1	JA	3	LEU
1	JA	35	GLN

Model ID	Chain	Residue ID	Residue type
1	JA	115	ASN
1	JA	130	LEU
1	JA	165	THR
1	JA	166	VAL
1	JA	184	GLN
1	JA	186	VAL
1	JA	187	VAL
1	JA	209	LYS
1	KA	3	LEU
1	KA	24	ARG
1	KA	39	THR
1	KA	56	GLU
1	KA	121	VAL
1	KA	228	THR
1	KA	233	GLN
1	LA	3	LEU
1	LA	15	LEU
1	LA	30	LEU
1	LA	33	LEU
1	LA	89	VAL
1	LA	158	VAL
1	LA	186	VAL
1	LA	212	VAL

Model ID	Chain	Residue ID	Residue type
1	LA	218	PHE
1	MA	3	LEU
1	MA	19	VAL
1	MA	22	LEU
1	MA	39	THR
1	MA	57	PRO
1	MA	70	ASN
1	MA	108	LYS
1	MA	180	VAL
1	MA	190	LYS
1	MA	203	VAL
1	NA	3	LEU
1	NA	122	GLU
1	NA	135	VAL
1	NA	166	VAL
1	NA	190	LYS
1	NA	208	GLU
1	OA	1	SER
1	OA	3	LEU
1	OA	7	PRO
1	OA	14	ARG
1	OA	57	PRO
1	OA	104	ASN

Model ID	Chain	Residue ID	Residue type
1	OA	158	VAL
1	OA	191	LEU
1	OA	208	GLU
1	OA	211	LEU
1	OA	212	VAL
1	OA	228	THR
1	PA	3	LEU
1	PA	23	PRO
1	PA	25	GLU
1	PA	30	LEU
1	PA	52	GLN
1	PA	77	LEU
1	PA	104	ASN
1	PA	108	LYS
1	PA	111	PHE
1	PA	135	VAL
1	PA	161	SER
1	PA	186	VAL
1	PA	206	LYS
1	PA	218	PHE
1	QA	3	LEU
1	QA	42	TYR
1	QA	104	ASN

Model ID	Chain	Residue ID	Residue type
1	QA	184	GLN
1	RA	3	LEU
1	RA	7	PRO
1	RA	23	PRO
1	RA	104	ASN
1	RA	156	THR
1	RA	165	THR
1	RA	166	VAL
1	RA	200	GLN
1	RA	212	VAL
1	SA	3	LEU
1	SA	10	THR
1	SA	47	GLU
1	SA	166	VAL
1	SA	177	GLN
1	SA	186	VAL
1	SA	208	GLU
1	TA	3	LEU
1	TA	23	PRO
1	TA	58	PRO
1	TA	104	ASN
1	TA	158	VAL
1	TA	187	VAL

Model ID	Chain	Residue ID	Residue type
1	TA	191	LEU
1	TA	212	VAL
1	TA	228	THR
1	UA	3	LEU
1	UA	23	PRO
1	UA	30	LEU
1	UA	104	ASN
1	UA	158	VAL
1	UA	193	VAL
1	UA	212	VAL
1	UA	218	PHE
1	VA	3	LEU
1	VA	23	PRO
1	VA	47	GLU
1	VA	49	LEU
1	VA	88	SER
1	VA	104	ASN
1	VA	166	VAL
1	VA	186	VAL
1	VA	191	LEU
1	VA	206	LYS
1	WA	3	LEU
1	WA	24	ARG

Model ID	Chain	Residue ID	Residue type
1	WA	107	ARG
1	WA	112	GLU
1	WA	141	VAL
1	WA	156	THR
1	WA	158	VAL
1	WA	186	VAL
1	WA	191	LEU
1	WA	212	VAL
1	WA	218	PHE
1	WA	228	THR
1	XA	3	LEU
1	XA	6	ASP
1	XA	28	GLN
1	XA	76	ASN
1	XA	104	ASN
1	XA	122	GLU
1	XA	156	THR
1	XA	185	LYS
1	XA	212	VAL
1	YA	3	LEU
1	YA	70	ASN
1	YA	104	ASN
1	YA	110	ARG

Model ID	Chain	Residue ID	Residue type
1	YA	141	VAL
1	YA	154	VAL
1	YA	200	GLN
1	YA	205	TYR
1	YA	218	PHE
1	ZA	3	LEU
1	ZA	25	GLU
1	ZA	42	TYR
1	ZA	104	ASN
1	ZA	121	VAL
1	ZA	166	VAL

Fit of model to data used for modeling

Fit of model to data used for validation

Validation for this section is under development.

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