Integrative Structure Validation Report

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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	9A0H
PDB-Dev ID	PDBDEV_00000053
Structure Title	Integrative model of Nup116 knockout (at 37C) yeast nuclear pore complex
Structure Authors	Vasileios Rantos; Matteo Allegretti; Christian E. Zimmerli; Florian Wilfling; Paolo Ronchi; Herman K.H. Fung; Chia-Wei Lee; Wim Hagen; Beata Turonova; Kai Karius; Mandy Boermel; Xiaojie Zhang; Christoph Mueller; Yannick Schwab; Julia Mahamid; Boris Pfander; Martin Beck; Jan Kosinski

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

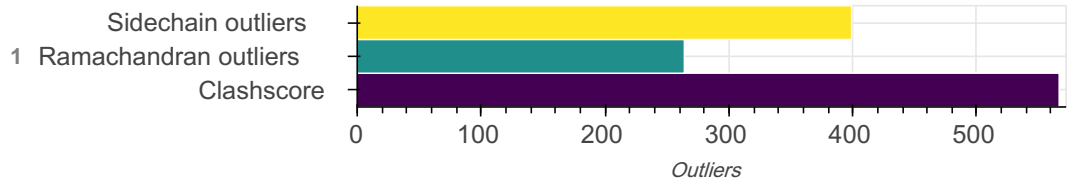
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 10 subunits in each model. A total of 7 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 10 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	Nic96	A1	A1	839
1	2	2	Nup188	B1	B1	1655
1	3	3	Nup157	D1	D1	1391
1	4	4	Nup133	K1	K1	1157
1	5	5	Nup84	L1	L1	726
1	6	6	Nup145c	M1	M1	712
1	7	7	Sec13	N1	N1	297
1	8	8	Seh1	O1	O1	349
1	9	9	Nup85	P1	P1	744
1	10	10	Nup120	R1	R1	1037

Datasets used for modeling

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	EMDB	EMD-10661
2	3DEM volume	File	10.5281/zenodo.3820319
3	3DEM volume	File	10.5281/zenodo.3820319
4	Integrative model	PDB-Dev	PDBDEV_00000051
5	Integrative model	PDB-Dev	PDBDEV_00000051
6	Other	File	https://doi.org/10.1038/nsmb1194
7	Other	File	https://doi.org/10.1038/nature26003

Representation

This entry has only one representation and includes 0 rigid bodies and 10 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A1	-	1-839
B1	-	1-1655
D1	-	1-1391
K1	-	1-1157
L1	-	1-726
M1	-	1-712
N1	-	1-297
O1	-	1-349
P1	-	1-744
R1	-	1-1037

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Monte Carlo simulated annealing optimization for NR Y-complex and IR asymmetric unit (outer nuclear copy)	Monte Carlo simulated annealing optimization of multiple rigid bodies with IMP	None	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	2.9.0	integrative model building	https://integrativemodeling.org

Data quality

3DEM volume

Validation for this section is under development.

Model quality

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

Standard geometry: bond outliers

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

There are 2033 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
N-CA-CB	103.00	15.36	1
CA-N-CD	112.00	5.42	1
CA-N-C-N-CA-C-CA-C-N	116.90	19.77	1
CA-C-CA-N-C-N-CA	121.70	14.49	1
C-N-CA	121.70	15.46	1
C-N-CA-N-CD	112.00	30.07	1
C-N-CA	121.70	16.84	1
N-CA-CB	110.50	11.86	1
C-N-C-N-CA	121.70	17.83	1
CA-N-CD	112.00	31.52	1
C-N-C-N-CA	121.70	19.96	1
CA-N-C-N-C-N-CA	121.70	22.29	1
C-N-CA	121.70	22.91	1
CA-C-N	116.20	7.17	1
O-C-N	123.00	36.40	1
CA-N-C-N-CA	121.70	25.31	1
CA-N-CA-C-N	116.20	10.26	1
C-N-C-CA-CB	110.10	11.09	1
C-N-C-N-C-N-CA	121.70	29.03	1
CA-C-N-CA-N-CA-CB	110.40	34.78	1
C-N-CA-C-O	120.80	35.98	1
CA-C-C-N-C-N-CA	121.70	34.50	1
CA-C-N	116.20	19.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-C-N-CA	121.70	35.34	1
CA-C-O	120.80	39.38	1
CA-C-N	116.20	20.95	1
C-N-CA	121.70	36.20	1
C-N-CA	121.70	36.26	1
N-CA-CB	110.50	29.88	1
C-N-CA	121.70	36.37	1
CA-C-CA-N-CD	112.00	46.83	1
C-N-C-N-C-N-C-N-CA	121.70	39.36	1
CA-C-O	120.80	43.09	1
CA-C-N	116.20	24.86	1
C-N-N-CA-CA-C-O	120.80	46.68	1
C-N-CA	121.70	43.97	1
C-N-CA	121.70	44.47	1
CA-N-CA-C-CA-C-N-CD-CG	103.20	40.74	1
CA-C-N	116.20	32.95	1
CA-C-CA-C-N	116.20	34.22	1
N-CA-CA-C-N	116.20	34.53	1
CA-C-O	120.80	51.67	1
CA-C-O	120.80	37.49	1
C-N-C-N-CA	121.70	51.13	1
N-CA-C	111.00	1.76	1
C-N-CA-C-CA-C-N	116.20	39.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	56.00	1
CA-C-C-N-CA-C-O	120.80	56.30	1
CB-CG-OD1	120.80	45.08	1
CA-C-N	116.20	40.82	1
N-CA-N-CA-C	112.10	18.62	1
C-N-CA	121.70	54.63	1
CA-C-N-CA-C	111.00	6.86	1
N-CA-C	111.00	6.89	1
N-CA-C	111.00	7.75	1
N-CA-N-CA-C	111.00	8.11	1
CA-C-CA-C-N-CA-C	111.00	8.48	1
C-N-CA	121.70	56.26	1
N-CA-C	111.00	9.34	1
C-N-CA	121.70	56.62	1
CA-C-O	120.80	59.53	1
N-CA-C	111.00	10.58	1
N-CA-N-CA-C-N-CA	121.70	57.33	1
N-CA-C	111.00	10.88	1
CA-C-O	120.80	60.03	1
CA-C-N	116.20	44.73	1
CA-C-N	116.20	44.87	1
N-CA-N-CA-CA-C-O	120.80	60.90	1
N-CD-N-CA-CB	110.50	50.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	163.06	1
N-CA-N-CA-C	111.00	12.93	1
C-CA-N-CA-N-CA-C	111.00	13.12	1
N-CA-C	111.00	13.12	1
CA-C-N	116.20	46.30	1
CA-C-C-CA-CB	110.10	43.99	1
CA-C-O	120.80	61.85	1
N-CA-C-CA-CB	111.40	45.90	1
N-CA-CA-N-CD	112.00	63.89	1
N-CA-N-CA-C	111.00	15.24	1
CA-C-CA-C-C-CA-C-N-N-CA-CB	110.40	161.34	1
N-CA-N-CA-C	111.00	16.21	1
N-CA-CB	110.50	168.01	1
N-CA-CA-C-N	116.20	48.77	1
N-CA-C-N-CA-C-O	120.80	63.79	1
N-CA-C	111.00	17.29	1
CA-C-N-CA-CB	110.50	54.01	1
N-CA-C	111.00	18.05	1
N-CA-CA-C-N-CA-N-CA-CB	103.00	139.34	1
N-CA-C	111.00	18.49	1
O-C-N	123.00	70.18	1
N-CA-N-CA-N-CA-C	113.30	18.02	1
CA-C-O	120.80	65.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-N-CA-CA-C-O	120.80	65.21	1
N-CA-C	111.00	19.47	1
N-CA-C	111.00	19.48	1
N-CA-N-CA-N-CD-N-CA-C	111.00	20.74	1
N-CA-N-CA-CA-C-N-CA-C	111.00	21.72	1
CA-C-N	116.90	69.14	1
C-CA-N-CA-C	111.00	22.17	1
N-CA-CB	111.50	57.68	1
N-CA-N-CA-CB	111.50	165.02	1
N-CA-N-CA-C	111.00	23.00	1
CA-C-N	116.20	53.35	1
C-N-CA-C-N-CA-C	111.00	23.61	1
N-CA-N-CA-N-CA-CA-C-N-CA-N-CA-C	111.00	24.26	1
C-N-CA	121.70	66.09	1
C-CA-CB	110.10	51.59	1
N-CA-CA-C-N-CA-N-CA-N-CD-CG	103.20	57.61	1
N-CA-C	111.00	26.11	1
CA-C-CA-C-O	120.80	69.39	1
N-CA-C	112.10	36.67	1
C-CA-CB	110.10	167.27	1
N-CA-CB	111.50	162.55	1
N-CA-N-CA-N-CA-CB	110.50	160.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	28.00	1
C-N-N-CA-C	111.00	28.10	1
C-CA-N-CA-C	111.00	28.39	1
N-CA-N-CA-N-CA-N-CA-N-CA-C	111.00	28.61	1
N-CA-N-CA-N-CA-N-CA-CA-C-N-CA-C	111.00	29.46	1
N-CA-C	111.00	29.63	1
C-N-N-CA-CA-C-O	120.80	71.98	1
N-CA-C	111.00	31.22	1
C-CA-N-CA-N-CD-N-CA-CA-C-N-CA-N-CA-N-CA-C	111.00	31.70	1
N-CA-CB	110.50	158.56	1
N-CA-N-CA-C	111.00	32.25	1
CA-C-N	116.20	60.01	1
N-CA-C	111.00	32.71	1
O-C-N	123.00	78.37	1
CA-C-CA-C-N	116.20	60.49	1
CA-C-N-CA-C-CA-N-CA-C-N-CA-C-O	120.80	73.77	1
N-CA-CA-C-O	120.80	167.71	1
CA-C-C-CA-C-N-CA	121.70	72.31	1
N-CA-C	111.00	34.24	1
CA-C-C-CA-CB	110.50	69.58	1
C-CA-N-CA-N-CA-N-CA-C-CA-CB	110.10	161.64	1
N-CA-CA-C-C-CA-CB	110.10	58.79	1
N-CA-C	111.00	35.82	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CA-C-N	116.90	76.96	1
CB-CG1-N-CA-C-N-CA	121.70	73.81	1
C-N-CA	121.70	169.52	1
C-CA-N-CA-C	111.00	36.83	1
CA-C-N-CA-C-N-C-CA-CB	110.10	60.09	1
N-CA-CA-C-O	120.80	165.34	1
C-N-CA	121.70	74.58	1
C-CA-CA-N-CD	112.00	75.38	1
CA-N-CA-C-O	120.80	76.60	1
CA-C-O	120.80	76.83	1
CA-C-O	120.80	76.85	1
N-CA-C-N-C-N-CA	121.70	75.33	1
C-CA-C-CA-CB	110.10	158.84	1
N-CA-C	111.00	39.28	1
N-CA-CA-C-O	120.80	77.38	1
N-CA-C-CA-C-CA-CB	110.10	61.80	1
N-CA-C	111.00	39.89	1
N-CA-C	111.00	39.96	1
C-CA-CB	110.10	158.30	1
N-CA-N-CA-C-CA-CB	110.50	72.71	1
C-N-CA	121.70	76.43	1
C-N-C-CA-C-CA-CB	110.10	157.76	1
N-CA-C-N-CA	121.70	166.78	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CA-C-O	120.80	78.41	1
C-CA-CA-C-N-CD-CG	103.20	66.01	1
C-N-C-CA-N-CA-CB	103.00	130.02	1
N-CA-C-CA-CB	111.60	62.59	1
C-N-CA	121.70	77.65	1
N-CA-N-CA-N-CA-CB	110.50	151.90	1
N-CA-CB	110.50	151.85	1
C-CA-CB	110.10	156.27	1
N-CA-CB	111.50	152.80	1
N-CA-CB	110.50	69.26	1
N-CA-N-CA-CB	110.50	69.44	1
C-N-N-CA-N-CA-C	111.00	43.54	1
CA-C-N	116.20	68.08	1
N-CA-CB	111.50	70.66	1
CA-C-N	116.20	68.35	1
C-N-CA	121.70	78.73	1
N-CA-N-CA-C	111.00	44.27	1
CA-C-C-N-N-CA-N-CA-CA-C-N	116.20	68.90	1
CA-C-N-CA-CB	110.50	150.67	1
C-CA-CB	110.10	65.21	1
C-N-C-N-CA	121.70	79.40	1
C-CA-C-CA-CB	110.10	154.72	1
N-CA-C-CA-C-CA-CB	111.60	158.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	163.64	1
N-CA-N-CA-C-CA-C-CA-CB	111.40	67.37	1
CA-C-C-CA-C-CA-CB	110.50	145.22	1
C-CA-C-CA-N-CA-CB	103.00	128.38	1
N-CA-CA-C-O	120.80	159.89	1
C-CA-C-CA-CB	110.50	76.11	1
C-CA-N-CA-N-CA-C	111.00	47.17	1
CA-N-CD	112.00	80.46	1
C-N-CA	121.70	81.22	1
C-CA-N-CA-C	111.00	48.04	1
N-CA-C	112.10	55.90	1
CA-C-N-CA-C	111.00	48.25	1
CA-C-O	120.80	82.76	1
N-CA-C-CA-C-CA-CA-C-O	120.80	82.95	1
N-CA-C-CA-CB	110.10	152.27	1
N-CA-N-CA-C	111.00	49.04	1
CA-C-O	120.80	83.18	1
N-CA-CB	110.50	147.97	1
CA-C-O	120.80	158.25	1
CA-C-O	120.80	83.46	1
N-CA-CB	111.50	74.20	1
C-CA-C-CA-CA-C-N	116.20	72.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CD-CG	103.20	70.41	1
N-CA-C-N-CA	121.70	82.59	1
N-CA-C	111.00	50.38	1
C-CA-C-CA-CB	110.10	69.25	1
CA-C-O	120.80	84.32	1
CA-N-CD	112.00	81.98	1
C-CA-CB	110.10	150.83	1
CA-C-O	120.80	157.23	1
N-CA-N-CA-N-CA-C	111.00	51.16	1
N-CA-CB	111.50	147.71	1
N-CA-C-N-CA	121.70	159.94	1
N-CA-C	112.10	59.08	1
N-CA-C	111.00	52.00	1
C-CA-CA-C-N	116.20	158.33	1
N-CA-N-CA-CB	111.50	147.20	1
C-CA-CB	110.10	70.22	1
CA-C-N	116.20	74.54	1
CA-N-N-CA-N-CA-CB	110.50	145.79	1
CA-N-CA-C-C-CA-CB	110.10	149.46	1
C-CA-CB	110.10	70.91	1
N-CA-CA-C-CA-C-N	116.20	157.19	1
N-CA-O-C-N	123.00	90.25	1
N-CA-C	111.00	53.78	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-N-CA-C-CA-N-CA-C	111.00	54.30	1
C-CA-C-CA-N-CA-N-CA-CA-C-C-CA-N-CA-CA-C-C-N-CA	121.70	85.79	1
C-N-CA-C-O	120.80	154.47	1
N-CA-CA-C-N	116.20	155.78	1
N-CA-N-CA-C-N-CA-C-CA-C-C-CA-CB	111.40	148.75	1
C-CA-N-CA-C-N-C-N-C-CA-CB	110.10	147.24	1
C-CA-CB	110.10	147.22	1
N-CA-N-CA-CA-C-N	116.90	145.95	1
N-CA-CB	110.50	143.42	1
CA-C-N	116.20	154.87	1
N-CA-C	111.00	56.91	1
C-CA-CB	110.10	146.76	2
N-CA-CA-C-N	116.20	77.76	1
N-CA-C	111.00	57.31	1
N-CA-N-CA-C	113.30	168.74	1
CA-C-N	116.20	154.37	1
CA-C-C-N-N-CA-N-CA-C	111.00	57.61	1
N-CA-CA-C-O	120.80	153.11	1
C-CA-CB	110.10	74.04	1
CA-C-N-CA-N-CA-CA-C-O	120.80	88.61	1
N-CA-N-CA-C	111.00	58.27	1
N-CA-N-CA-CA-C-C-N-CA	121.70	87.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	78.65	1
CA-C-C-N-C-N-N-CA-CB	110.50	142.14	1
C-CA-N-CA-CB	110.50	142.05	1
C-CA-CA-C-CA-C-N	116.90	89.14	1
N-CA-CB	110.50	79.05	1
N-CA-CB	110.50	141.86	1
C-CA-N-CA-C	111.00	59.37	1
C-CA-N-CA-CB	110.50	79.29	1
C-CA-CA-C-N-CA-CB	110.50	141.60	1
N-CA-N-CA-C	111.00	59.82	1
N-CA-C	111.00	162.10	1
N-CA-CA-C-O	120.80	151.72	1
N-CA-CB	110.50	141.40	1
CA-C-O	120.80	151.69	1
CA-C-N-CA-C	111.00	60.20	1
CA-C-CA-C-N	116.20	80.07	1
N-CA-CA-C-N	116.20	152.26	1
C-CA-CB	110.10	144.34	1
CA-C-C-CA-CB	111.60	147.50	1
N-CA-CB	110.50	80.14	1
N-CA-N-CA-CA-C-N-CA-C-CA-CB	110.50	83.90	1
C-CA-CB	110.10	76.49	1
CA-C-O	120.80	90.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CA-C-O	120.80	90.82	1
C-N-CA	121.70	90.02	1
N-CD-N-CA-C-CA-CA-C-N-CA-C-CA-C-N-CA	121.70	153.10	1
CA-C-C-CA-CB	111.60	76.74	1
CA-C-CA-C-O-C-N	123.00	95.24	1
N-CA-N-CA-N-CA-C-CA-N-CA-C-N-N-CA-C	111.00	62.83	1
CA-C-C-CA-CB	110.10	77.45	1
N-CA-C	111.00	62.96	1
N-CA-C	111.00	62.98	1
C-N-C-N-CD	125.00	55.08	1
C-CA-C-N-CD	125.00	55.43	1
C-CA-CB	110.10	77.90	1
N-CA-C	111.00	158.43	1
CA-C-N-CA-CB	110.40	85.05	1
C-CA-CB	109.10	146.27	1
CA-C-N-CA-C	111.00	63.82	1
N-CD-C-N-CA	121.70	152.01	1
N-CA-N-CA-C	111.00	64.02	1
CA-C-N	116.20	149.69	1
N-CA-C	111.00	64.17	1
N-CA-CA-C-O	120.80	92.47	1
C-N-CA-N-CD	112.00	88.71	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	64.53	1
CA-C-C-CA-CB	110.10	78.60	1
C-N-CA	121.70	91.86	1
N-CA-N-CA-C-CA-N-CA-C	111.00	64.73	1
N-CA-N-CA-CB	103.00	121.12	1
N-CA-C-CA-CA-C-C-CA-CB	110.10	141.19	1
N-CA-C-N-CA	121.70	92.30	1
CA-C-O	120.80	93.11	1
CA-N-CD	112.00	89.28	1
C-CA-CB	110.10	140.94	1
N-CA-C-CA-CB	110.10	79.46	1
C-CA-N-CA-CB	110.50	137.79	1
N-CA-C	111.00	66.10	1
N-CA-CB	110.50	137.73	1
C-CA-CB	110.10	79.68	1
C-CA-C-CA-CB	110.10	140.42	1
N-CA-C-CA-N-CA-C	111.00	155.55	1
C-CA-CA-C-CA-N-CD	112.00	89.81	1
C-CA-N-CD-N-CA-CB	110.50	137.35	1
C-CA-CB	110.10	80.09	1
C-N-N-CA-CB	103.00	120.36	1
N-CA-N-CA-CA-C-O	120.80	94.04	1
CB-CG-ND2	116.40	92.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	84.72	1
C-CA-CB	110.10	140.00	1
C-N-CA	121.70	150.02	1
C-CA-CA-C-N	116.20	147.52	1
N-CA-C	111.00	67.24	1
N-CA-C	111.00	67.27	1
C-CA-CB	110.10	139.77	1
CA-C-O	120.80	94.40	1
CA-C-O	120.80	147.14	1
C-CA-CB	110.10	139.50	1
C-CA-CB	110.50	87.29	1
C-CA-CB	111.40	82.06	1
C-N-CA	121.70	93.95	1
N-CA-CB	111.50	85.30	1
CA-C-O	120.80	146.98	1
C-CA-N-CA-C	111.00	67.97	1
N-CA-C-CA-CB	110.10	139.24	1
N-CA-CA-C-C-CA-CB	110.50	87.55	1
C-CA-OD1-CG-ND2	122.60	137.87	1
C-CA-CB	110.10	81.12	1
N-CA-CB	111.50	85.59	1
C-CA-CA-C-N	116.20	85.85	1
CA-C-N	116.90	94.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CA-C-N	116.20	85.96	1
N-CA-CB	110.50	136.19	1
N-CA-CA-C-C-CA-CB	110.50	87.89	1
C-N-CA	121.70	94.57	1
CA-C-O	119.00	73.80	1
CA-C-N-CA-C-N-N-CD-C-CA-CB	110.10	138.57	1
N-CA-CA-C-O	120.80	95.34	1
CA-N-CD	112.00	91.05	1
C-N-CA	121.70	94.77	1
C-N-N-CA-CB	110.50	85.12	1
N-CA-CB	103.00	119.42	1
N-CA-C-CA-CB	110.10	81.86	1
N-CA-CB	110.40	132.66	1
C-CA-N-CA-C	112.10	149.15	1
N-CA-C-CA-CA-C-CA-C-O	120.80	95.81	1
C-CA-C-CA-CB	109.10	141.37	1
C-N-CA	121.70	95.30	1
N-CA-CA-C-O	120.80	95.89	1
CA-C-CA-C-N	116.20	86.94	1
C-CA-N-CA-C	111.00	70.11	1
C-CA-N-CA-CA-C-C-CA-CA-C-C-CA-CB	110.10	137.65	1
C-N-CA	121.70	147.78	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-N-CA-N-CA-C	111.00	70.52	1
C-CA-C-CA-N-CA-C-CA-CB	110.10	82.70	1
N-CA-CB	110.50	134.97	1
CA-N-N-CA-CB	110.50	86.08	1
C-CA-CB	110.10	82.83	1
N-CA-N-CA-N-CA-C	111.00	70.88	1
CA-C-O	120.80	145.15	1
CA-C-O	120.80	145.13	1
CA-C-O	120.80	96.55	1
C-CA-CB	110.10	83.01	1
C-CA-N-CA-CB	110.50	86.35	1
C-CA-CB	110.10	137.02	1
C-CA-CB	111.60	139.83	1
C-CA-CA-C-O	120.80	144.75	1
CA-C-C-N-C-N-CA	121.70	96.53	1
CA-C-C-CA-N-CA-N-CA-CB	111.50	135.23	1
CA-C-C-CA-CB	110.10	136.45	1
C-N-C-CA-C-CA-C-CA-CB	110.10	136.37	1
CA-C-N-CA-CB	110.50	87.02	1
N-CA-C	111.00	72.33	1
N-CA-C	111.00	72.36	1
C-CA-C-CA-CA-C-N-CA-N-CA-CA-C-C-CA-CB	110.10	84.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-CA-N-CA-C-CA-CA-C-O	120.80	144.01	1
N-CA-CB	110.50	87.35	1
N-CA-CA-C-CA-C-N-CA-C-CA-C-N-CA	121.70	146.11	1
N-CA-CB	110.50	87.47	1
N-CA-C	112.10	78.25	1
N-CD-CG	103.20	123.46	1
C-CA-CB	111.60	84.61	1
C-CA-CB	110.10	135.70	1
CA-C-O	120.80	97.91	1
C-CA-CB	110.10	135.64	1
C-CA-N-CA-CB	110.50	87.70	1
N-CA-C-CA-CB	110.10	84.63	1
CA-C-N-CA-CB	111.50	134.26	1
C-N-CA	122.60	55.75	1
N-CA-CB	110.50	87.82	1
C-N-CA	121.70	97.73	1
CA-C-N	116.20	142.82	1
C-CA-CB	110.10	84.83	1
C-CA-N-CA-CA-C-O-C-N	123.00	101.76	1
C-CA-CB	110.10	135.32	1
O-C-C-N-CA	121.70	145.54	1
CA-C-CA-C-O	120.80	98.29	1
C-CA-CB	110.10	84.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	101.84	1
O-C-O-C-O-C-O-C-O-C-N	123.00	101.90	1
C-CA-CB	110.10	135.15	1
O-C-N	123.00	101.92	1
C-CA-CB	109.10	138.06	1
N-CA-C	111.00	147.84	1
O-C-CA-C-O	120.80	98.44	1
C-CA-CB	110.10	85.13	1
N-CA-C-N-CA-C-N-CA-N-CA-C	111.00	147.66	1
C-CA-C-CA-N-CA-C	111.00	74.42	1
C-CA-C-CA-N-CA-C	111.00	74.64	1
C-CA-N-CA-CB	110.50	132.57	1
C-CA-CB	110.10	134.76	1
C-N-C-N-CA	121.70	145.03	1
N-CA-N-CA-CB	103.00	117.25	1
C-CA-CB	110.10	134.70	1
C-CA-N-CA-N-CA-C	112.10	144.31	1
CA-C-C-N-CA	121.70	144.85	1
CA-C-N	116.20	141.92	1
C-N-CA	121.70	98.56	1
N-CA-CA-C-O	120.80	142.62	1
C-CA-CB	110.10	134.46	1
C-N-N-CA-C-N-CA-C-N-CA-CB	110.50	132.21	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	90.74	1
C-CA-CB	110.10	134.27	1
CA-C-O	120.80	99.19	1
CA-C-O	120.80	99.20	1
N-CA-CB	110.40	91.34	1
C-CA-N-CA-CA-C-O	120.80	99.26	1
C-CA-CB	110.10	134.17	1
CA-C-C-CA-CB	110.10	86.04	1
N-CA-N-CA-CB	111.50	132.99	1
CA-C-N-CA-C-CA-CB	110.10	86.12	1
CA-C-O	120.80	142.24	1
N-CA-C-N-CA	121.70	99.06	1
CA-C-O	120.80	99.42	1
C-CA-CB	110.10	133.96	1
CA-C-N-CA-C-N-CA-C-N-CA-CB	110.50	131.80	1
C-CA-CA-C-C-CA-CB	110.10	133.82	1
C-CA-C-N-N-CA-C	111.00	76.12	1
CA-C-N	116.20	141.03	1
C-CA-C-CA-CB	110.10	86.54	1
N-CA-N-CA-CA-C-N	116.20	91.42	1
N-CA-C	111.00	145.62	1
CA-CB-CG	112.60	124.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-C-CA-CB	110.10	86.67	1
C-CA-CB	110.10	133.52	1
C-CA-CB	110.10	86.69	1
C-N-CA	121.70	99.53	1
CA-C-O	120.80	141.71	1
CA-C-N	116.20	140.78	1
C-CA-N-CA-CB	110.40	128.76	1
N-CA-CB	111.50	132.28	1
N-CA-C	111.00	76.80	1
C-CA-CB	110.10	86.89	1
C-CA-CB	110.10	133.30	1
N-CA-CB	110.50	89.78	1
CA-N-C-CA-CB	110.10	86.97	1
CA-C-N	116.20	91.91	1
C-N-C-CA-CA-C-N-CA-C	111.00	144.93	1
C-CA-CB	110.10	87.08	1
N-CA-CB	111.50	132.03	1
N-CA-C	111.00	77.19	1
N-CA-CB	110.50	131.02	1
N-CA-C	111.00	77.24	1
CA-C-CA-C-N	116.20	92.10	1
N-CA-CB	110.50	130.98	1
C-CA-N-CA-CB	110.50	90.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	100.03	1
C-CA-CB	110.10	132.97	1
C-CA-N-CA-C	111.00	77.30	1
N-CA-C-CA-CA-C-O	120.80	141.22	1
C-CA-CB	110.10	132.91	1
C-CA-N-CA-N-CA-CB	110.50	90.13	1
CA-C-O	120.80	100.44	1
N-CA-CA-C-N	116.20	140.11	1
N-CA-CB	110.50	90.18	1
CA-C-C-CA-CB	110.10	87.46	1
C-CA-CA-C-N	116.20	140.03	1
C-CA-C-N-C-N-CA	121.70	143.09	1
N-CA-C-N-CA	121.70	143.08	1
C-N-CA-N-CD	112.00	95.40	1
C-CA-CA-C-O	120.80	100.66	1
N-CA-C	111.00	144.17	1
C-CA-N-CA-CB	110.40	128.14	1
N-CA-C-N-C-CA-C-CA-CB	110.10	87.73	1
N-CA-C-CA-CA-C-O	120.80	100.86	1
N-CA-C-CA-C-N-CA	121.70	142.79	1
CA-C-N	116.20	139.62	1
C-CA-CA-C-O	120.80	145.37	1
C-CA-CB	110.10	132.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	100.94	1
N-CA-CA-C-N	116.20	92.87	1
C-CA-N-CA-CA-C-N	116.20	92.93	1
CA-C-N-CA-C	111.00	143.46	1
N-CA-C	111.00	78.58	1
CA-C-C-CA-CB	110.10	88.21	1
CA-C-C-N-CA-C-CA-C-O	120.80	101.36	1
C-CA-CB	110.10	88.38	1
C-CA-C-CA-N-CA-C	111.00	79.12	1
C-N-CA	121.70	142.18	1
CA-C-N-CA-N-CA-C-CA-CB	110.10	88.56	1
CA-C-N	116.20	138.87	1
N-CA-C-CA-N-CA-C	111.00	142.58	1
N-CA-C-N-CA	121.70	101.45	1
C-CA-CB	111.60	89.13	1
CA-C-N	116.20	138.65	1
C-CA-C-CA-C-CA-CB	110.10	88.81	1
N-CA-CB	110.50	91.47	1
N-CA-CB	110.50	129.53	1
C-CA-CA-C-CA-C-N-CA-N-CA-N-CA-C-CA-C-N-CA	121.70	141.74	1
C-CA-CB	110.10	131.22	1
CA-C-O	120.80	101.91	1
CA-C-CA-C-N	116.20	94.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	101.95	1
C-CA-C-CA-C-N-N-CA-N-CA-CB	110.50	129.32	1
C-N-CA	121.70	141.63	1
N-CA-N-CA-N-CA-C-CA-CB	110.10	89.13	1
C-CA-CB	110.10	89.16	1
C-CA-C-CA-N-CA-C	111.00	141.76	1
N-CA-CB	103.00	115.06	1
C-N-C-CA-N-CA-C	111.00	80.39	1
N-CA-CB	110.50	129.08	1
C-N-CA	121.70	102.03	1
C-CA-N-CA-C	111.00	141.47	1
CA-CB-CG	113.80	102.92	1
C-CA-CB	110.10	130.77	1
N-CA-C	111.00	80.59	1
C-CA-CB	110.10	130.73	1
C-CA-CB	109.10	85.21	1
C-CA-C-CA-CB	110.10	89.48	1
C-N-C-CA-C-CA-N-CA-C-N-CA	121.70	141.09	1
N-CA-CB	111.50	129.81	1
C-N-C-CA-CB	109.10	85.49	1
N-CA-CB	110.50	128.74	1
C-CA-N-CA-C-N-CA	121.70	140.99	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-CA-C-CA-CA-C-C-CA-CA-N-C-N-CD	125.00	168.86	1
N-CA-CB	110.50	128.66	1
N-CA-CB	111.50	129.66	1
C-CA-C-CA-C-CA-CB	110.10	130.36	1
N-CA-C-CA-CB	110.10	130.33	1
N-CA-C-N-CA	121.70	140.81	1
N-CA-CB	110.50	128.54	1
C-CA-CB	110.10	89.96	1
N-CA-C-CA-N-CA-CB	103.00	114.65	1
CA-C-N	116.20	137.37	1
C-CA-N-CA-N-CA-C	111.00	81.46	1
CA-C-N-CA-C-N-CA	121.70	102.73	1
C-CA-CB	110.10	130.12	1
C-N-N-CA-C	111.00	81.52	1
C-N-CA	121.70	102.75	1
C-CA-CB	110.10	130.09	1
C-CA-N-CA-N-CA-C	111.00	140.40	1
CA-C-CA-C-N	116.20	137.18	1
N-CA-C-CA-CB	110.10	130.03	1
C-CA-N-CA-N-CA-N-CA-C-CA-N-CA-N-CA-C	111.00	81.87	1
C-CA-CA-C-CA-C-O	120.80	138.45	1
N-CA-C	111.00	140.04	1
C-CA-CB	110.10	129.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	92.90	1
C-CA-CB	110.10	129.77	1
C-CA-C-N-CA	121.70	140.30	1
N-CA-C-N-C-CA-CB	110.10	90.48	1
C-N-CA-C-O	120.80	138.31	1
CA-C-CA-C-O	120.80	103.30	1
N-CA-CB	111.50	94.08	1
CA-C-C-CA-CB	110.10	129.55	1
C-CA-CB	110.50	125.82	1
C-CA-CB	111.60	91.22	1
N-CA-C	111.00	139.49	1
N-CA-C-N-N-CA-C-N-CA	121.70	139.94	1
C-CA-C-CA-C-CA-CB	110.10	90.87	1
C-CA-CB	110.10	90.88	2
CA-C-O	120.80	137.98	1
CA-C-N	116.20	96.02	1
C-CA-C-N-N-CA-C	111.00	82.77	1
CA-C-N-CA-CB	110.50	127.62	1
N-CA-CA-N-CD	112.00	97.92	1
C-CA-CB	110.10	129.21	1
N-CA-C	111.00	82.85	1
N-CA-C	111.00	139.15	1
C-N-C-N-CA	121.70	139.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-CA-C-CA-CB	110.50	125.51	1
CA-C-O	119.00	88.99	1
C-N-CA	121.70	139.67	1
N-CA-CB	110.50	93.56	1
C-N-CA	121.70	139.63	1
C-CA-CA-C-CA-C-C-CA-CA-C-O	120.80	137.65	1
C-CA-CA-C-N-CA-CB	110.50	127.32	1
N-CA-CB	103.00	113.88	1
CA-C-N	116.20	135.98	1
CA-CB-N-CA-CB	110.50	127.29	1
N-CA-N-CA-C	111.00	138.59	1
CA-C-C-CA-N-CA-CB	110.50	127.19	1
C-CA-C-N-N-CA-CB	110.50	93.83	1
C-CA-C-CA-N-CA-C-CA-C-CA-C-N-CA	121.70	104.12	1
CA-C-N	116.20	135.74	1
N-CA-C	111.00	83.65	1
C-N-CD	125.00	165.00	1
C-CA-CB	110.50	125.12	1
C-CA-CB	111.40	129.88	1
C-CA-CB	110.10	128.56	1
N-CA-C-CA-N-CA-C	111.00	138.14	1
C-CA-CB	110.10	91.68	1
CA-C-O	120.80	104.33	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-CA-CB	110.10	91.72	1
C-CA-N-CA-N-CA-C-CA-CB	110.10	128.43	1
N-CA-N-CA-CB	110.50	126.89	1
CA-C-CA-C-O	120.80	104.41	1
N-CA-CB	110.50	94.12	1
N-CA-N-CA-C-CA-N-CA-CB	110.50	94.17	1
C-CA-N-CA-C-CA-CA-C-N-CA-CB	110.50	126.80	1
CA-C-N	116.20	135.37	1
CA-C-CA-C-C-CA-CB	110.10	128.30	1
C-N-CA	121.70	138.94	1
C-CA-CB	110.10	91.91	1
CA-C-CA-C-N	116.20	97.05	1
CA-C-O	120.80	137.07	1
C-CA-CB	110.10	91.93	1
C-CA-C-CA-CB	110.10	92.01	1
N-CA-N-CA-C	111.00	137.58	1
N-CA-CB	110.40	124.63	1
N-CA-C	111.00	84.45	1
CA-CB-OD1-CG-ND2	122.60	132.08	1
C-CA-N-CA-C	111.00	84.50	1
C-N-CA	121.70	138.73	1
C-N-CA	121.70	104.67	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-N-CA	121.70	138.70	1
C-N-CA	121.70	138.68	1
N-CA-C-N-CD	125.00	163.62	1
C-CA-N-CA-CB	110.50	126.48	1
C-CA-CB	110.10	127.95	1
C-N-CA	121.70	138.59	1
N-CA-CB	111.50	95.56	1
CA-C-O	120.80	104.87	1
C-CA-CB	110.10	92.29	1
N-CA-C	111.00	84.78	1
CA-C-N	116.20	97.50	1
C-CA-CB	110.10	127.84	1
C-CA-CA-C-O	120.80	104.93	1
C-CA-N-CA-CB	110.50	126.37	1
C-CA-C-N-CA	121.70	138.50	1
C-CA-CB	110.10	127.83	1
CA-C-N-CA-C	111.00	137.11	1
C-CA-C-CA-C-CA-CB	110.10	127.79	1
C-CA-C-CA-CB	110.10	92.42	1
CA-C-O	120.80	104.99	1
C-CA-CB	109.10	129.56	1
N-CA-CB	111.50	95.69	1
N-CA-CB	110.50	94.70	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	95.71	1
N-CA-C-N-CD	125.00	163.06	1
N-CA-CB	110.50	94.72	1
CA-C-O	120.80	105.02	1
CA-C-C-CA-CB	110.50	96.58	1
C-CA-C-CA-CB	110.10	92.48	1
C-CA-CB	110.10	92.49	1
C-CA-C-N-CA-C-O	120.80	136.53	1
C-N-CA	121.70	138.36	1
CA-C-C-CA-C-CA-CB	110.50	124.35	1
N-CA-CA-C-O	120.80	105.14	1
C-CA-CB	109.10	129.37	1
N-CA-C	113.30	139.96	1
C-CA-CB	110.10	127.54	1
C-CA-CB	111.60	93.26	1
C-CA-CB	110.10	127.52	1
C-CA-C-CA-N-CA-C-CA-C-N-C-CA-CB	110.10	92.76	1
N-CA-CB	110.50	94.99	1
C-CA-N-CA-C	111.00	136.51	1
C-CA-CB	110.10	127.39	1
CA-C-N	116.20	134.38	1
C-CA-N-CA-CA-C-O	120.80	105.38	1
C-N-C-N-C-N-CA	121.70	105.40	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	126.86	1
C-N-CA	121.70	137.96	1
N-CA-N-CA-CB	111.50	96.16	1
C-CA-CB	110.10	92.96	1
CA-CB-CG	113.80	104.78	1
C-CA-CA-C-O	120.80	105.48	1
C-N-N-CA-CB	111.50	96.20	1
C-CA-C-CA-C-N-N-CA-CB	110.50	95.28	1
CA-C-CA-C-N-CA-CB	110.50	95.30	1
C-CA-CB	110.50	123.90	1
CA-C-C-N-CA	121.70	105.63	1
C-CA-CB	110.10	93.16	1
C-CA-CB	109.10	128.71	1
C-CA-C-CA-CB	110.10	126.93	1
N-CA-C-CA-CB	111.40	128.18	1
C-CA-CB	110.10	126.88	1
N-CA-CB	110.50	95.49	1
C-N-CA	121.70	137.58	1
C-CA-C-CA-CB	110.10	93.41	1
CA-C-N	116.20	98.64	1
CA-C-C-CA-N-CA-CB	111.50	126.39	1
CA-CB-CG	113.80	105.05	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	105.95	1
C-N-CA	121.70	137.45	1
N-CA-CA-C-N	116.20	133.67	1
C-CA-CB	111.40	94.81	1
C-N-CA	121.70	137.41	1
C-CA-CB	110.10	126.69	1
N-CA-CB	103.00	93.40	1
N-CA-CA-C-C-CA-CB	110.10	93.54	1
N-CA-C	111.00	135.38	1
C-CA-CA-C-C-CA-C-CA-C-N-CA-C-C-CA-N-CA-CA-C-C-CA-CB	110.10	126.57	1
C-CA-N-CA-CB	110.40	123.39	1
CA-C-O	120.80	135.51	1
C-CA-N-CA-C	111.00	135.23	1
C-CA-CB	110.10	126.54	1
C-CA-CB	110.10	126.53	1
N-CA-CB	111.50	96.82	1
CA-C-O	120.80	135.47	1
N-CA-CB	110.50	125.16	1
N-CA-CA-C-CA-C-N	116.20	133.44	1
C-N-CA	121.70	106.21	1
C-CA-CB	110.50	123.41	1
C-CA-CB	110.10	126.44	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	86.94	1
CA-C-N	116.20	99.03	1
C-CA-CA-C-C-CA-CA-C-O	120.80	135.33	1
CA-C-N	116.20	133.28	1
C-CA-N-CA-C	111.00	87.12	1
C-CA-CB	110.10	126.28	1
C-N-CA	121.70	137.03	1
C-CA-C-CA-CB	110.10	93.93	1
C-CA-CB	110.10	93.94	1
CA-C-N	116.20	133.21	1
C-CA-CA-C-N-CA-N-CA-C-CA-CB	110.10	93.98	1
CA-C-N	116.20	133.17	1
CA-C-N-CA-C-CA-C-CA-CB	110.50	123.19	1
C-CA-CB	110.50	97.82	1
C-CA-N-CA-CA-C-C-CA-CB	110.10	126.12	1
C-CA-CB	110.10	94.09	1
CA-C-O	120.80	106.48	1
CA-N-N-CA-C-N-CA	121.70	136.82	1
C-CA-CB	110.10	126.05	1
C-CA-CB	110.10	94.16	1
N-CA-C-CA-C-CA-N-CA-CB	110.50	124.73	1
C-CA-CA-C-N-CA-CA-C-N-CA-CB	111.50	97.32	1
CA-CB-N-CA-CB	110.50	96.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	87.69	1
C-CA-CA-C-O	120.80	106.65	1
CA-C-N	116.20	132.85	1
C-CA-C-CA-CB	110.10	125.90	1
N-CA-CB	110.40	97.93	1
C-CA-C-CA-CB	111.60	128.21	1
C-CA-C-CA-CB	110.10	125.87	1
C-CA-N-CA-CB	110.50	96.40	1
N-CA-C	111.00	87.79	1
N-CA-C-CA-CB	109.10	90.88	1
CA-CB-CG	112.60	104.32	1
CA-C-O	120.80	134.87	1
C-CA-C-CA-CB	110.10	94.40	1
C-CA-CB	110.10	125.79	2
C-N-C-N-CA	121.70	136.56	1
C-CA-C-CA-CB	110.10	94.43	1
N-CA-CA-CB-CG	113.80	105.56	1
C-CA-CB	110.50	98.16	1
CA-C-N	116.20	99.74	1
C-CA-C-CA-CB	110.10	94.49	1
CA-C-O	120.80	134.76	1
CA-C-O	120.80	106.84	1
C-CA-N-CA-CA-CB-N-CA-C-N-CA	121.70	136.46	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-C-CA-C-N-CA	121.70	106.94	1
C-N-CA	121.70	106.94	1
C-CA-CB	110.10	125.68	1
N-CA-C	111.00	88.06	1
N-CA-CB	110.50	96.57	1
CA-C-C-N-N-CA-C-CA-CB	110.10	125.64	1
CA-C-O	120.80	106.91	1
C-N-CA	121.70	136.40	1
C-CA-CB	111.40	126.91	1
C-N-CA-C-C-CA-CB	110.10	94.61	1
C-N-CA	121.70	136.37	1
CA-C-O	120.80	106.94	1
C-CA-N-CA-N-CA-CB	111.50	125.34	1
N-CA-CA-C-CA-C-N-CA-CB	110.50	124.28	1
C-CA-CB	110.10	125.47	1
C-CA-C-CA-C-CA-CB	109.10	91.33	1
N-CA-C	111.00	88.40	1
N-CA-N-CA-CA-CB-C-N-CA	121.70	107.19	1
C-CA-CB	110.50	98.41	1
C-CA-C-N-CA	121.70	136.18	1
N-CA-C	111.00	133.53	1
N-CA-C-CA-CB	110.10	94.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-C-O	120.80	107.14	1
C-CA-C-CA-C-CA-C-CA-CB	110.10	125.34	1
C-CA-C-CA-CA-CB-CG	113.80	105.78	1
N-CA-C-CA-CB	110.10	125.32	1
C-CA-CB	110.10	94.89	1
CA-CB-CG	113.80	121.80	1
N-CA-C	111.00	133.37	1
C-CA-CB	110.10	94.92	1
C-CA-CB	110.10	125.27	1
CA-CB-N-CA-C	111.00	88.65	1
C-CA-N-CA-C	111.00	133.34	1
N-CA-C	111.00	88.68	1
CA-CB-CG	113.80	105.84	1
CA-CB-C-CA-CB	110.10	125.21	1
C-N-CA-C-N	116.20	132.10	1
N-CA-C	113.30	90.25	1
C-N-CA	121.70	136.01	1
CA-C-O	120.80	134.31	1
N-CA-CA-C-N	116.20	100.34	1
CA-C-O	120.80	134.28	2
C-CA-C-CA-N-CA-N-CA-C	111.00	133.16	1
C-N-CA	121.70	107.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-N-CA-C	111.00	133.12	1
C-CA-CB	110.10	125.10	1
C-CA-CB	110.10	125.08	2
N-CA-C	111.00	88.93	1
N-CA-N-CA-C	111.00	88.96	1
C-N-N-CA-CA-C-O	120.80	107.42	1
C-N-CA	121.70	135.84	1
N-CA-CB	111.50	124.85	1
C-CA-N-CA-C	111.00	89.01	1
N-CA-CB	110.50	123.84	1
CA-C-N	116.20	131.88	1
C-CA-CA-CB-CG	113.80	105.97	1
N-CA-N-CA-CB	110.50	123.80	1
C-N-CA	121.70	107.62	1
C-N-C-CA-N-CA-CA-C-N	116.20	100.59	1
N-CA-C	111.00	132.84	1
C-CA-CA-CB-N-CA-N-CA-C-CA-C-N-C-CA-C-CA-C-CA-CA-C-N	116.20	100.70	1
CA-C-C-CA-CB	110.10	95.38	1
CA-C-N	116.90	105.29	1
C-CA-CA-C-N	116.20	100.72	1
CA-C-N-CA-CB	110.50	123.66	1
N-CA-C	112.10	92.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-N-CA	121.70	107.78	1
C-CA-CB	110.10	124.78	1
CA-C-O	120.80	107.67	1
C-N-C-CA-C-CA-CB	109.10	126.06	1
N-CA-CB	111.50	124.60	1
N-CA-C	111.00	132.57	1
CA-C-O	120.80	133.89	1
N-CA-CB	110.50	123.59	1
N-CA-CB	111.50	124.59	1
C-CA-C-CA-N-CA-CB	110.50	97.43	1
CA-C-N	116.90	105.40	1
C-CA-CB	110.10	95.53	1
C-CA-C-CA-CB	111.60	126.90	1
C-N-N-CA-CA-C-N-CA-C-CA-N-CD-CG	103.20	91.75	1
N-CA-C	111.00	132.37	1
C-CA-CB	111.60	126.85	1
CA-C-C-N-C-CA-CB	110.10	124.58	1
CA-C-N	116.20	100.97	1
C-CA-C-CA-CB	110.10	124.56	1
N-CA-CB	110.50	97.58	1
C-CA-CB	110.10	95.67	1
CA-C-CA-C-N-CA-CA-C-O	120.80	107.90	1
C-CA-CB	110.10	95.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	124.51	1
N-CA-CB	110.50	97.61	1
N-CA-C-CA-CB	110.10	95.71	1
CA-C-O	120.80	107.93	1
C-CA-C-N-CA	121.70	108.10	1
C-CA-CB	111.60	126.71	1
N-CA-CB	111.50	124.35	1
CA-C-O	120.80	107.96	1
CA-C-O	120.80	107.97	1
CA-C-CA-N-CD	112.00	101.44	1
C-N-CA	121.70	108.12	1
N-CA-CB	111.50	98.69	1
O-C-CA-C-N	116.20	101.14	1
N-CA-C	111.00	132.08	1
C-CA-CB	111.60	96.55	1
N-CA-CB	110.40	121.67	1
C-CA-CB	110.10	95.83	1
N-CA-C	113.30	91.52	1
C-N-CA	121.70	108.19	1
N-CA-C-N-C-N-CA	121.70	108.19	1
N-CA-C	113.30	91.54	1
C-CA-CA-C-N	116.20	101.22	1
C-CA-CB	109.10	125.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-N-CA-CB	103.00	111.23	1
C-CA-CB	110.10	124.31	1
C-N-CA	121.70	108.24	1
C-CA-CB	110.10	95.90	1
C-CA-CB	109.10	92.66	1
CA-N-C-CA-CA-N-N-CA-C-N-CA	121.70	108.30	1
CA-C-N	116.20	131.09	1
N-CA-CB	110.50	123.15	1
C-N-N-CA-C	111.00	90.18	1
C-CA-CB	110.10	124.23	1
CA-C-O	120.80	133.44	1
C-CA-CB	110.10	124.22	1
C-CA-CB	111.60	126.46	1
C-CA-CB	110.10	95.98	1
C-N-CD	125.00	94.54	1
C-N-CA	121.70	108.34	1
C-CA-C-CA-N-CA-C	111.00	131.75	1
C-N-CA	121.70	135.04	1
N-CA-CB	110.50	123.09	1
C-CA-C-N-CA	121.70	108.38	1
CA-N-CD	112.00	101.65	1
N-CA-C-CA-CB	110.10	124.13	1
N-CA-CA-C-C-N-C-CA-CB	110.10	124.09	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-N-CA-C-CA-CA-C-N	116.20	130.90	1
N-CA-CB	110.50	98.02	1
C-CA-C-CA-CB	111.40	125.35	1
C-CA-CB	110.50	121.51	1
C-CA-CB	110.10	96.16	1
C-CA-CB	110.10	96.17	1
N-CA-CA-CB-CG	113.80	106.48	1
N-CA-CA-CB-CG	112.60	105.29	1
C-CA-CA-C-N	116.20	130.80	1
N-CA-C-CA-C-CA-CB	110.10	96.26	1
N-CA-C	112.10	93.91	1
C-CA-CB	110.10	123.92	1
C-CA-CB	110.10	123.91	1
C-N-C-N-CA	121.70	134.78	1
N-CA-C-CA-CB	109.10	125.08	1
C-CA-N-CA-C-N-CA	121.70	134.77	1
N-CA-CB	110.50	98.16	1
CA-C-CA-C-N-CA-CB	110.50	98.17	1
C-N-CA	121.70	108.65	1
C-CA-N-CA-CA-C-N-CA-CB	110.50	122.82	1
CA-C-N	116.20	101.71	1
N-CA-CB	110.50	122.82	1
CD-NE-CZ	124.40	134.54	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	111.50	99.20	2
N-CA-N-CA-N-CA-CA-C-O	120.80	108.52	1
C-N-N-CA-CB	111.50	123.78	1
N-CA-CB	111.50	99.23	1
N-CA-N-CA-CA-C-O	120.80	108.55	1
C-CA-CB	110.10	123.79	1
C-CA-CB	110.10	96.42	1
C-CA-CB	110.10	123.77	1
C-CA-CB	109.10	124.93	1
C-CA-N-CA-CB	111.50	123.73	1
C-CA-CB	111.40	97.74	1
CA-C-N	116.20	101.82	1
CA-C-O	120.80	135.87	1
C-CA-N-CA-CB	111.50	99.31	1
C-CA-CB	110.10	96.47	1
CA-C-O	120.80	108.61	1
N-CA-CB	110.50	98.33	1
C-CA-CA-CB-CG	113.80	106.64	1
C-CA-CB	110.10	123.68	1
CA-C-N	116.20	130.50	1
CA-C-O	120.80	132.95	1
C-CA-N-CA-CB	111.50	99.36	1
N-CA-CB	110.50	122.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	101.93	1
CA-C-O	120.80	132.93	1
C-CA-CB	110.50	99.82	1
N-CA-CB	111.50	123.60	1
CA-C-O	120.80	105.86	1
N-CA-CB	110.50	122.59	1
C-CA-CA-CB-C-CA-C-N-CA	121.70	134.47	1
N-CA-CB	110.50	122.55	2
N-CA-CB	111.50	123.55	1
C-CA-CB	110.50	99.87	1
C-CA-CB	110.10	123.56	1
C-N-CA	121.70	134.43	1
C-CA-CB	110.10	123.53	1
C-N-C-CA-CB	110.10	123.51	1
N-CA-N-CA-N-CA-CB	110.50	98.52	1
C-CA-CB	110.10	96.73	1
NE-CZ-NH2	119.20	112.87	1
C-CA-CB	110.10	123.46	1
CA-C-O	120.80	108.86	1
C-CA-N-CA-N-CA-CB	110.50	98.57	1
C-CA-CB	109.10	93.67	1
N-CA-C	111.00	91.37	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-C-N-CA	121.70	109.09	1
C-N-CA	121.70	134.31	1
CA-C-O	120.80	108.90	1
C-N-CD	125.00	153.70	1
CA-CB-C-N-CA	121.70	109.11	1
CA-CB-CA-CB-CG	113.80	106.82	1
CA-C-N	116.20	102.26	1
C-CA-N-CA-N-CA-C	111.00	130.51	1
N-CA-CB	110.50	98.66	1
N-CA-C-CA-CB	110.10	123.33	1
C-CA-N-CA-CB	111.50	99.68	1
C-CA-N-CA-CB	103.00	110.64	1
C-CA-N-CA-C	111.00	130.45	1
N-CA-CB	103.00	110.64	1
C-CA-CB	110.10	123.28	1
CA-CB-CG	113.80	106.87	1
C-CA-C-CA-N-CA-N-CA-CA-C-O	120.80	109.04	1
C-N-C-N-CA	121.70	134.13	1
C-CA-C-CA-N-CA-CB	110.50	122.22	1
C-N-C-CA-C-CA-CB	110.10	97.01	1
C-CA-CB	110.10	97.02	1
N-CA-CB	110.50	122.19	1
C-CA-CA-C-C-CA-C-N-CA	122.60	88.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N-CA-CB	103.00	110.55	1
N-CA-C	111.00	91.79	1
N-CA-C	111.00	130.21	1
N-CA-CB	110.50	98.84	1
C-CA-CB	110.50	100.23	1
N-CA-C	111.00	91.83	1
C-CA-CB	110.10	123.10	1
C-CA-CA-C-C-CA-CA-C-N	116.20	129.86	1
CA-CB-CG	112.60	119.43	1
N-CA-CA-C-N-CA-N-CA-CB	103.00	110.50	1
CA-CB-CG	113.80	106.99	1
C-CA-CB	110.10	123.04	1
C-N-C-CA-C-CA-CB	110.10	97.18	1
C-CA-N-CA-C-CA-C-CA-CB	109.10	124.02	1
CA-C-O	120.80	109.27	1
C-CA-N-CA-N-CA-C-CA-CB	110.10	122.96	1
N-CA-C	113.30	132.93	1
C-CA-CB	110.10	122.96	1
CA-CB-CG	113.80	107.04	1
N-CA-CB	110.50	122.00	1
CA-C-N-CA-N-CA-N-CA-C	111.00	92.10	1
C-CA-C-N-N-CA-CB	110.50	121.96	1
N-CA-C	111.00	92.13	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	132.25	1
CA-C-N-CA-CB	110.50	121.94	1
N-CA-C-CA-CB	110.10	122.87	1
N-CA-CB	110.50	121.93	1
N-CA-CA-C-O	120.80	132.22	1
C-CA-CB	111.40	124.15	1
C-N-CA	121.70	109.62	1
C-N-CA	121.70	133.77	1
CA-C-N	116.20	129.61	1
N-CA-N-CA-CB	110.50	121.90	1
N-CA-CB	110.50	121.87	1
C-CA-C-N-CA-C-N	116.20	129.57	1
C-CA-CB	110.10	122.80	1
CA-C-N-CA-N-CA-CA-C-O	120.80	132.15	1
C-CA-CA-CB-C-CA-CB	110.10	97.42	1
CA-C-N	116.20	129.55	1
CA-CB-CG	113.80	107.13	1
CA-C-C-N-C-N-CA-C-N	116.20	129.53	1
CA-C-N-CA-C-CA-CB	111.40	124.05	1
CD-NE-CZ	124.40	133.71	1
C-CA-CB	110.10	122.73	1
N-CA-C	111.00	92.39	1
N-CA-C-CA-CB	110.50	120.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	122.72	1
N-CA-CB	103.00	110.30	1
CA-C-O	119.00	138.89	1
N-CA-CB	110.50	121.77	1
N-CA-C-CA-CB	110.10	122.68	1
C-CA-CB	110.10	122.68	1
N-CA-CB	110.50	121.75	1
C-N-C-N-C-CA-CB	110.10	122.67	1
CA-C-N	116.20	102.98	1
N-CA-CB	110.50	99.27	1
C-CA-CB	109.10	94.56	1
CA-CB-CG	112.60	105.99	1
CA-C-O	120.80	132.03	1
C-CA-CB	110.10	122.63	1
C-CA-C-CA-CB	110.10	122.62	1
N-CA-CB	110.50	121.69	1
C-N-CA	121.70	133.54	1
N-CA-C-N-CA	121.70	133.53	1
N-CA-C-N-CA	121.70	133.52	1
N-CA-CB	110.50	99.34	1
C-CA-N-CA-N-CA-CB	110.50	99.34	1
C-CA-CB	110.50	120.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	103.09	1
CA-CB-CG	112.60	119.15	1
N-CA-CA-CB-CG	113.80	107.26	1
C-N-CA	121.70	133.46	1
C-CA-C-CA-CB	110.10	122.49	1
C-CA-C-CA-CB	110.10	97.72	1
C-CA-C-N-N-CA-C-CA-N-CA-C-N-CA	121.70	110.01	1
N-CA-C-CA-C-N-CA	121.70	110.03	1
C-N-CA	121.70	133.37	1
CA-C-O	120.80	131.81	1
CA-C-N	116.20	103.24	1
N-CA-C	111.00	92.87	1
CA-C-CA-C-CA-C-N	116.20	103.26	1
C-CA-CA-C-C-CA-CB	110.10	97.82	1
C-CA-CB	109.10	123.31	1
CA-CB-CG	113.80	107.35	1
N-CA-CB	110.40	100.72	1
C-CA-CB	110.10	122.36	1
C-CA-CB	109.10	94.91	1
N-CA-CB	111.50	122.45	1
CB-CG1-CA-C-N	116.20	103.32	1
CA-C-O	120.80	109.86	1
C-CA-CB	111.60	98.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	121.43	1
C-CA-N-CA-CB	103.00	110.07	1
C-CA-C-CA-C-CA-CB	110.10	97.91	1
N-CA-C	111.00	93.03	1
CA-C-CA-C-O	120.80	109.89	1
N-CA-C	111.00	93.05	1
C-CA-CA-CB-CG	113.80	107.39	1
C-CA-C-CA-CB	110.10	97.93	1
N-CA-N-CA-CB	110.50	99.62	1
C-CA-C-N-CA	121.70	110.19	1
CA-C-N-CA-C-N-CA	121.70	110.21	1
CA-N-CD	112.00	103.06	1
C-CA-C-CA-C-N-CA	121.70	133.18	1
C-N-CA	121.70	133.17	1
C-CA-CB	110.10	98.01	1
C-CA-C-N-C-CA-N-CA-CB	110.50	121.30	1
N-CA-C-CA-CB	110.50	100.98	1
N-CA-C	111.00	128.76	1
C-CA-CA-C-O	120.80	131.58	1
C-CA-N-CA-CB	110.50	121.27	1
C-CA-C-CA-N-CA-C	111.00	93.28	1
CA-CB-C-CA-CB	110.10	122.12	1
N-CA-CB	111.50	122.25	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	98.09	2
C-CA-C-CA-CB	110.10	122.10	1
CA-C-O	120.80	131.54	1
CA-C-N	116.20	103.57	1
N-CA-C-CA-CB	110.10	98.11	1
C-CA-CB	110.10	98.11	1
N-CA-CB	110.50	99.78	1
N-CA-C-CA-CB	110.10	122.08	1
C-N-CD	125.00	99.16	1
C-CA-CB	110.10	122.07	1
C-CA-CB	110.10	122.06	1
N-CA-CB	110.50	121.20	1
N-CA-CA-C-N-CA-C-N-CA	121.70	133.01	1
C-CA-N-CA-CB	110.50	121.17	1
C-CA-CB	109.10	95.29	1
N-CA-C	111.00	93.42	1
CA-CB-C-N-CA	121.70	132.99	1
C-N-C-CA-CB	110.10	121.99	1
CA-C-N-CA-C	111.00	128.51	1
N-CA-CA-C-N	116.20	128.70	1
CA-C-N	116.20	103.70	1
N-CA-C-CA-CB	110.10	98.24	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	121.95	1
N-CA-C	111.00	93.55	1
C-N-CA	121.70	110.49	1
N-CA-CA-CB-CG	114.10	101.67	1
CA-CB-CG	113.80	107.59	1
C-CA-CB	110.50	119.81	1
CA-CB-CG	112.60	118.80	1
C-N-CA	121.70	132.87	1
CA-C-C-CA-CB	110.10	121.87	1
CA-CB-CG	113.80	107.61	2
C-N-CA	121.70	110.56	1
C-CA-N-CA-N-CA-CB	110.50	121.00	1
CA-CB-CA-C-O	120.80	110.31	1
C-CA-CB	111.60	123.94	1
CA-C-N-CA-CB	110.50	120.98	1
CA-C-O	120.80	131.27	1
CA-N-N-CA-O-C-N	123.00	132.85	1
C-CA-C-CA-CB	110.10	98.42	1
CA-CB-CG	113.80	107.66	1
CA-CB-CG	112.60	106.46	1
C-CA-CB	111.40	123.07	1
N-CA-CB	111.50	121.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-N-CA-C	111.00	93.83	1
C-CA-CA-C-N	116.20	128.46	1
CA-CB-CG	112.60	106.49	1
C-N-CA	121.70	132.70	1
N-CA-C	111.00	128.10	1
N-CA-CA-C-N	116.20	103.99	1
CA-C-N-CA-CA-C-N-CA-C	111.00	93.94	1
CA-CB-CG	113.80	107.71	1
C-CA-CB	110.10	98.53	1
C-N-CA	121.70	110.74	1
CA-C-N	116.20	128.37	1
CA-C-O	120.80	110.46	1
CA-C-CA-CB-C-CA-C-CA-C-CA-CA-C-N-CA-CB	110.50	100.18	1
C-CA-CB	109.10	95.76	1
C-CA-CA-C-N	116.20	128.32	1
C-CA-CB	110.10	98.60	1
N-CA-C-N-CA-C-N	116.20	128.29	1
C-N-CA	121.70	132.58	1
OD1-CG-ND2	122.60	116.56	1
C-CA-CB	110.10	121.57	1
N-CA-N-CA-C	111.00	94.12	1
OD1-CG-ND2	122.60	116.57	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-CA-CB	110.10	121.54	1
C-CA-CB	111.60	99.56	1
N-CA-C-CA-C-CA-CA-C-N-CA-C-CA-C-CA-C-CA-CA-C-N	116.20	128.19	1
CA-C-N	116.20	104.21	1
C-CA-CB	110.10	121.48	1
CA-CB-C-CA-C-N-CA	121.70	110.93	1
C-CA-CB	111.40	122.77	1
CA-CB-CG	113.80	107.82	1
N-CA-C	112.10	127.04	1
CA-C-O	120.80	110.64	1
C-CA-CB	110.50	119.46	1
N-CA-C	111.00	94.28	1
N-CA-CA-C-N-CA-CB	110.50	120.64	1
CA-C-C-N-CA	121.70	132.43	1
N-CA-CB	110.50	100.37	1
N-CA-CA-C-N-CA-CB	110.50	120.62	1
CA-CB-CG	112.60	106.65	1
C-N-CA	121.70	132.40	1
CA-C-N-CA-N-CA-C	111.00	127.60	1
N-CA-CB	110.50	100.42	1
C-CA-CB	110.10	121.36	1
C-CA-CA-C-N	116.20	104.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-N-CA	121.70	132.35	1
N-CA-CB	111.50	121.56	1
C-CA-CA-CB-CG	112.60	106.69	1
N-CA-CB	111.50	121.54	1
CA-CB-CG	113.80	107.90	1
N-CA-C-N-CA-C-N-CA-CB	110.50	120.52	1
C-CA-C-N-CA-C-N	116.20	104.42	1
N-CA-N-CA-C	111.00	94.52	1
C-N-CA-CB-CG	112.60	106.72	1
C-N-CA	121.70	132.29	1
N-CA-CB	111.50	121.50	1
N-CA-CB	111.50	101.51	1
CA-C-O	120.80	130.79	1
N-CA-CB	110.50	120.49	1
C-N-CA	121.70	132.28	1
C-CA-CA-C-C-CA-C-CA-CA-C-C-CA-CA-C-O	120.80	130.75	1
C-CA-CB	111.60	99.89	1
C-N-CA	121.70	132.23	1
N-CA-CB	110.50	100.55	1
N-CA-CA-CB-C-N-C-N-CA-C-N-CA-CB	110.50	100.56	1
CA-C-N-CA-CB	110.50	120.43	1
N-CA-C-CA-CB	109.10	121.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CA-C-N	116.20	127.88	1
N-CA-C	111.00	127.34	1
N-CA-CA-CB-CG	113.80	107.97	1
C-CA-CA-C-N	116.20	104.54	1
CA-C-N	116.90	108.16	1
C-N-CA	121.70	132.18	1
CA-C-O	120.80	130.70	1
C-CA-N-CA-C-CA-C-N-C-N-CA	121.70	132.17	1
C-CA-C-N-CA-CB-CG	112.60	106.79	1
N-CA-CB	110.50	120.38	1
C-CA-CA-CB-CG	113.80	107.99	1
C-CA-CB	109.10	121.87	1
N-CA-C	111.00	94.75	1
C-CA-CA-C-O	120.80	130.67	1
CA-CB-CG	113.80	119.60	1
C-N-CA	121.70	111.26	1
C-N-N-CA-C-CA-CB	109.10	96.35	1
C-N-CA	121.70	132.13	1
N-CA-CB	111.50	121.35	1
CA-C-O	120.80	130.65	1
CA-C-N	116.20	127.78	1
CA-C-O	120.80	110.96	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C	111.00	94.80	1
C-CA-CB	110.10	121.09	1
CA-C-O	120.80	110.97	1
C-CA-CB	110.10	99.12	1
C-CA-CB	111.60	100.04	1
CA-CB-CG	113.80	108.02	1
C-CA-CB	110.10	121.08	1
C-CA-N-CA-C	111.00	94.83	1
C-CA-CA-C-N	116.20	127.75	1
CA-C-N	116.20	104.66	1
N-CA-C-CA-C-CA-CB	109.10	96.41	1
N-CA-CA-CB-CG	112.60	106.84	1
C-N-N-CA-C	111.00	94.89	1
C-CA-CA-CB-CG	112.60	106.85	1
CA-C-C-CA-N-CA-CA-CB-CG	113.80	119.54	1
C-CA-CB	110.10	121.00	1
N-CA-C	111.00	127.06	1
C-CA-CB	111.40	122.29	1
CA-C-O	120.80	111.05	1
C-CA-C-CA-CA-CB-CG	112.60	106.87	1
C-N-CA	121.70	132.02	1
C-N-C-CA-C-N-CA	121.70	131.99	1
CA-CB-CA-CB-CG	112.60	106.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	120.21	1
C-CA-CB	110.10	99.26	1
C-CA-CB	110.10	120.94	1
C-N-CD-NE-CZ	124.40	116.42	1
C-N-CA	121.70	111.44	1
C-CA-C-CA-CB	110.10	99.27	1
CA-C-CA-C-N-CA-C-CA-CB	110.10	99.28	1
C-CA-CA-C-O	120.80	130.48	1
CA-CB-CG	112.60	106.91	1
CA-CB-CG	113.80	108.11	1
C-N-C-CA-CA-CB-CG	112.60	106.91	1
C-CA-N-CA-CB	110.50	120.16	1
C-CA-C-N-CA-CB-C-CA-C-N-CA	121.70	131.91	1
C-N-CA	121.70	131.91	1
CA-C-C-CA-N-CA-C	111.00	95.13	1
CA-C-N	116.20	127.53	1
N-CA-CB	111.50	101.87	1
N-CA-CA-CB-CG	112.60	106.94	1
C-CA-CA-C-N-CA-N-CA-C-N-CA	121.70	131.87	1
C-N-C-N-CA	121.70	131.86	1
OD1-CG-C-N-CA	121.70	111.55	1
C-CA-C-N-CA-C-C-CA-CB	110.10	99.40	1
CA-CB-CG	112.60	106.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CA-CB-CA-C-O	120.80	111.24	1
CA-CB-CG	113.80	108.18	1
C-CA-CB	110.10	120.78	1
CA-C-C-CA-N-CA-CB	110.50	120.04	1
CA-C-CA-C-O	120.80	111.26	1
CA-CB-CG	113.80	108.19	1
C-CA-CB	109.10	121.44	1
N-CA-CB	111.50	101.97	1
CA-C-N	116.20	127.42	1
CA-C-O	120.80	111.27	1
N-CA-C-CA-C-CA-CB	110.10	120.75	1
CA-C-O	120.80	111.28	1
N-CA-C	111.00	95.32	1
N-CA-CB	110.50	120.02	1
C-CA-CB	110.10	99.47	1
C-CA-C-CA-CB	111.60	100.41	1
C-N-CA	121.70	111.63	1
CA-CB-CA-C-O	120.80	130.30	1
C-CA-N-CA-N-CA-C-CA-CA-CB-CG	112.60	107.02	1
C-CA-CB	110.10	99.51	1
C-CA-CB	110.10	120.69	1
CA-C-N	116.20	127.34	1
C-CA-C-CA-CB	110.10	120.67	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.71	1
N-CA-C	113.30	97.17	1
C-N-CA	121.70	111.69	1
C-CA-CA-C-O	120.80	130.24	1
C-CA-CB	110.10	120.65	1
CA-C-N-CA-C-CA-CB	110.10	120.63	1
C-N-N-CA-C-CA-CB	110.10	120.62	1
CA-C-C-CA-CB	110.10	120.61	1
C-CA-CB	110.10	120.60	1
N-CA-C	111.00	95.53	1
C-CA-C-CA-CB	110.10	120.60	1
CA-N-CA-CB-CG	112.60	107.08	1
N-CA-CA-C-N	116.20	127.23	1
N-CA-CB	110.50	101.12	1
CA-CB-CG	112.60	107.09	1
C-CA-CB	110.10	120.58	1
N-CA-C-N-N-CA-C	111.00	126.42	1
N-CA-C	111.00	95.58	1
N-CA-CB	111.50	120.86	1
C-CA-CB	111.60	122.60	1
CA-C-N	116.20	105.20	1
C-N-N-CA-C-CA-C-CA-CB	110.10	120.53	1
C-CA-C-CA-CA-CB-CG	112.60	107.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.20	127.17	1
C-CA-CA-CB-CG	112.60	107.12	1
C-N-C-N-CA	121.70	131.56	1
CA-CB-CG2	110.50	101.20	1
N-CA-C	111.00	126.31	1
C-N-C-N-CA-CB-CG	113.80	108.33	1
C-N-CA	121.70	131.53	1
N-CA-C	111.00	95.73	1
C-CA-CA-C-O	120.80	111.53	1
C-CA-N-CA-CA-CB-CG	112.60	107.15	1
C-CA-CB	110.10	99.75	1
C-CA-CB	110.10	120.45	1
C-CA-C-CA-C-N-CA	121.70	131.49	1
N-CA-C-CA-CB	110.10	99.78	1
CA-CB-CG	113.80	108.37	1
N-CA-CB	110.50	101.26	1
CA-C-C-CA-CB	110.10	99.79	1
N-CA-C-CA-CB	110.50	102.36	1
N-CA-CA-C-N	116.20	127.04	1
C-CA-CB	110.10	99.80	1
CA-C-CA-CB-N-CA-C	111.00	95.82	1
N-CA-CB	110.50	101.29	1
C-CA-C-CA-CB	111.60	122.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-CA-CB	110.10	99.81	1
C-N-CA	121.70	111.95	1
C-N-N-CA-CA-CB-CG	112.60	107.19	1
C-CA-CB	111.60	100.78	1
C-CA-CB	110.10	99.83	1
N-CA-C-CA-CB	109.10	120.98	1
C-N-CA	121.70	111.98	1
CA-CB-C-N-CA	121.70	111.99	1
CA-CB-CG	112.60	107.21	1
N-CA-C-N-C-CA-CB	110.10	99.86	1
C-CA-CA-CB-CG	112.60	107.21	1
C-N-CA	121.70	131.39	1
C-CA-CB	110.50	102.43	1
CA-C-N	116.20	105.44	1
N-CA-C-CA-CB	109.10	120.94	1
C-CA-C-CA-C-CA-CB	110.10	99.90	1
C-N-CA	121.70	131.35	1
C-N-CA	121.70	112.05	1
N-CA-C-N-CA	121.70	112.05	1
N-CA-N-CA-CB	110.50	119.60	1
CA-C-O	120.80	111.70	1
N-CA-C-CA-CB	110.10	120.26	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-C-N-CA-C	111.00	96.03	1
C-N-C-CA-CB	110.10	120.26	1
N-CA-N-CA-CB	110.50	101.42	1
CA-CB-C-N-N-CD-CG	103.20	95.19	1
CA-CB-CG	113.80	108.46	1
N-CA-CB	110.50	101.43	1
CA-C-C-CA-CA-CB-C-CA-N-CA-CB	111.50	102.45	1
C-CA-CA-CB-CG	112.60	107.28	1
C-CA-C-CA-C-N-CA	121.70	112.13	1
C-N-CA	121.70	131.26	1
N-CA-CB	110.50	119.52	1
N-CA-C-CA-CB	110.10	120.18	1
N-CA-CB	110.50	101.49	1
C-N-CA-C-O	120.80	111.79	1
C-N-N-CA-CB	110.50	101.49	1
CA-CB-CG	113.80	108.50	1
C-CA-N-CA-N-CA-CB	110.50	119.50	1
C-N-C-N-CA	121.70	131.23	1
CA-CB-CG	113.80	108.51	1
N-CA-C	111.00	125.81	1
CA-C-N	116.20	105.63	1
CA-C-N	116.20	126.76	1
CA-C-C-CA-C-CA-CB	110.10	100.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	131.20	1
C-CA-N-CA-CB	110.50	119.46	1
C-N-CA-CB-CG	112.60	107.34	1
C-CA-CB	110.10	100.11	1
C-CA-C-N-C-CA-CB	110.10	100.11	1
C-CA-C-CA-CB	110.10	120.08	1
C-CA-CB	110.10	120.07	1
CA-CB-CG	113.80	108.55	1
CA-C-O	120.80	111.88	1
C-N-CA	121.70	131.14	1
CA-CB-CG	113.80	108.56	1
C-CA-C-CA-CB	111.40	121.36	1
CA-C-C-CA-CA-CB-C-N-C-CA-CB	110.10	120.04	1
N-CA-C-CA-CA-C-CA-C-CA-CB-CG	112.60	107.38	1
N-CA-C	111.00	96.38	1
CA-C-N	116.20	105.76	1
CA-C-C-CA-C-CA-CA-CB-CG	112.60	107.38	1
CA-C-N-CA-C-N-CA	121.70	112.32	1
C-CA-CB	111.60	101.17	1
C-CA-C-N-CA	121.70	131.07	1
C-N-CA-C-N-CA-C-N-CA	121.70	112.34	1
C-CA-CB	110.10	100.23	1
C-CA-CB	110.10	119.97	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	112.35	1
C-CA-CB	110.10	119.96	1
C-N-CA	121.70	112.36	2
CA-C-CA-CB-C-N-CA	121.70	131.03	1
CA-CB-CG	113.80	108.62	1
C-N-CA-C-N	116.20	126.56	1
CA-C-O	120.80	129.60	1
C-CA-N-CA-CB	110.50	101.70	1
C-CA-C-N-CA-C-O	120.80	112.01	1
CA-C-O	120.80	112.01	1
CA-N-CD	112.00	104.77	1
CA-CB-CG	112.60	107.43	1
CA-CB-CG	112.60	107.44	1
N-CA-CB	110.50	101.72	1
CA-C-O	120.80	112.02	1
N-CA-C	111.00	125.45	1
NE-CZ-N-CA-N-CA-CB	103.00	108.68	1
C-N-N-CA-CB	111.50	102.73	1
N-CA-C-CA-C-CA-CA-N-N-CA-CB	110.50	119.25	1
C-CA-CB	110.50	118.22	1
C-CA-CB	110.10	119.87	1
N-CA-C	111.00	96.60	1
NE-CZ-NH1	121.50	126.64	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-C-CA-CB	110.10	100.34	1
C-CA-C-CA-C-CA-C-N-CA	121.70	130.93	1
CA-CB-N-CA-CB	110.50	101.79	1
CA-C-N-CA-CB	110.50	119.21	1
C-CA-C-CA-CA-C-N	116.20	126.44	1
C-N-CA	121.70	130.92	1
N-CA-CB	110.50	101.80	1
N-CA-C	111.00	96.67	1
C-CA-CB	110.10	119.82	1
N-CA-CB	110.50	119.20	1
CA-C-N-CA-CB	111.50	102.81	1
N-CA-CA-C-N-CA-C-CA-CB	110.10	100.40	1
C-CA-CB	110.10	119.79	2
N-CA-CB	110.50	101.83	1
N-CA-CB	111.50	102.83	1
CA-CB-CG	112.60	107.50	1
N-CA-CB	111.50	102.84	1
C-N-CA	121.70	112.53	1
C-CA-C-N-CA	121.70	112.54	1
C-N-CA	121.70	130.86	1
C-CA-C-CA-CA-CB-CG	113.80	108.72	1
C-CA-CB	110.10	119.76	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-C-CA-CA-CB-CG	112.60	107.52	1
CA-C-O	120.80	112.17	1
C-CA-C-N-CA	121.70	130.83	1
N-CA-N-CA-CB	110.50	101.88	1
N-CA-CB	110.50	119.12	1
C-CA-CA-C-O	120.80	112.18	1
CA-C-N	116.20	106.06	1
C-CA-CB	110.10	119.73	1
C-CA-C-N-CA-C-N	116.20	106.07	1
C-CA-CB	111.60	101.47	1
C-CA-CB	110.10	100.47	1
CA-C-CA-C-O	120.80	129.41	1
OE1-CD-OE2	122.90	135.05	1
N-CA-CA-C-O	120.80	129.40	1
C-N-CA	121.70	130.81	1
CA-C-N	116.90	109.32	1
CA-N-C-CA-C-CA-C-CA-CB	110.10	119.69	1
CA-C-O	120.80	129.38	1
CA-C-C-N-CA	121.70	112.62	1
N-CA-CB	111.50	120.08	1
C-CA-C-CA-N-CA-CA-C-O	120.80	129.36	1
N-CA-C-CA-N-CA-CB	110.50	119.06	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-N-CA-CB	110.50	101.94	1
C-CA-CB	109.10	120.17	1
C-N-N-CA-C-CA-CB	110.10	119.65	1
N-CA-CA-CB-CG	112.60	107.58	1
CA-C-N	116.20	126.24	1
CA-N-CD	112.00	104.97	1
CA-C-O	120.80	129.33	1
C-CA-C-CA-CB	110.10	119.63	1
C-CA-CB	110.50	102.98	1
CA-C-C-CA-CA-C-C-N-N-CA-N-CA-C	113.30	98.79	1
CA-C-O	120.80	129.30	1
CB-CG-N-CA-CA-C-N-CA-CA-C-N	116.20	126.18	1
C-N-N-CA-CB	110.50	102.02	1
CB-CG-CA-C-O	120.80	129.27	1
N-CA-CA-CB-CG	112.60	107.62	1
CA-CB-CG	112.60	107.62	1
C-N-CA-C-O	120.80	129.26	1
N-CA-C-N-C-CA-CB	111.40	101.95	1
C-CA-CB	110.10	119.55	1
N-CA-CB	110.50	118.95	1
C-CA-CB	110.10	119.54	1
CA-CB-CG	113.80	118.77	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-OE1-CD-NE2	122.60	127.57	1
CA-C-CA-C-CA-C-C-CA-N-CA-N-CA-C	111.00	124.87	1
C-CA-CB	110.10	119.50	1
CA-CB-CG	113.80	108.85	1
CA-C-N	116.20	106.31	1
CA-CB-CG	112.60	107.66	2
C-CA-CA-CB-CG	112.60	107.66	1
C-CA-C-CA-CB	110.10	119.48	1
C-N-CA	121.70	112.82	1
C-CA-CB	111.60	121.47	1
C-CA-CA-CB-N-CA-C	111.00	97.20	1
N-CA-CB	110.50	102.12	1
CA-C-CA-CB-CG	113.80	108.88	1
C-CA-C-N-CA	121.70	130.55	1
N-CA-C	111.00	124.76	1
N-CA-C	111.00	97.25	1
CA-C-C-CA-CB	110.10	119.43	1
CA-CB-CG2	110.50	118.84	1
N-CA-CA-C-CA-N-CD	112.00	118.86	1
N-CA-N-CA-N-CA-CA-C-O	120.80	129.12	1
CA-C-C-CA-CA-CB-CG	113.80	108.91	1
C-N-N-CA-C-CA-CB	110.10	100.81	1
C-CA-CA-C-N	116.20	106.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	100.83	1
C-CA-CB	111.60	101.84	1
C-CA-N-CA-C	111.00	124.65	1
C-CA-CB	110.10	119.36	1
CA-CB-CG	113.80	118.67	1
C-CA-CB	110.10	100.85	1
N-CA-CA-CB-CG2	110.50	118.78	1
C-N-C-CA-C-N-CA	121.70	130.46	1
N-CA-CB	103.00	108.35	1
N-CA-C-N-CA-CB-CG	112.60	107.74	1
C-CA-CA-C-O	120.80	112.55	1
C-CA-CB	110.10	100.88	1
CA-CB-CG	112.60	107.75	1
N-CA-C	111.00	124.58	1
N-CA-CB	111.50	103.25	1
N-CA-C-CA-N-CA-C-N-CA	121.70	130.42	1
N-CA-C	111.00	124.56	1
CA-CB-C-N-C-N-CA	121.70	112.99	1
C-N-CA-C-CA-C-CA-C-N-CA-CA-CB-CA-CB-CG	113.80	108.97	1
N-CA-C-CA-CB	110.10	100.93	1
CA-C-O	120.80	112.59	1
C-CA-CB	110.10	100.93	1
CA-C-N	116.20	125.85	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-C-N-CA	121.70	113.02	1
C-CA-N-CA-C-CA-CB	110.10	119.26	1
CA-C-N	116.20	106.56	1
CA-C-O	120.80	112.61	1
C-N-CA	121.70	113.03	1
N-CA-CA-C-O	120.80	112.62	1
CA-CB-CG	113.80	118.61	1
CA-C-C-CA-CB	110.10	119.24	1
C-CA-CB	110.10	100.96	2
C-N-CA	121.70	130.36	1
C-N-CA	121.70	130.35	1
C-CA-CA-N-CA-C-N-CA-C	111.00	124.43	1
N-CD-CG	103.20	96.01	1
N-CA-C-CA-CB	110.10	119.21	1
CA-CB-CA-CB-CG	112.60	107.81	1
CA-CB-CG	113.80	118.59	1
CA-CB-CG	112.60	107.81	1
CA-C-N	116.20	125.77	1
CA-C-CA-C-CA-C-C-CA-CB	110.10	119.19	1
C-CA-CA-CB-CG	113.90	105.29	1
N-CA-CB	110.50	118.63	1
N-CA-CB	111.50	119.62	1
CA-C-O	120.80	112.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-CA-CB	110.10	119.16	1
C-CA-N-CA-C	111.00	124.34	1
CA-CB-CG	112.60	107.84	1
C-CA-CB	110.10	101.05	1
C-N-CA-CB-C-CA-C-CA-CA-C-C-N-CA	121.70	130.25	1
N-CA-N-CA-N-CA-CB	111.50	103.43	1
CA-CB-CG	112.60	117.35	1
C-CA-CB	110.10	119.12	1
CA-C-O	120.80	128.87	1
CA-C-O	120.80	128.86	1
CA-C-CA-N-CD	112.00	105.37	1
C-CA-CA-CB-CG	112.60	107.87	1
CA-C-C-N-CA-C-C-N-CA	121.70	113.19	1
CA-CB-C-CA-C-CA-CB	110.10	119.08	1
C-N-CA-CB-CG1	110.40	118.43	1
C-CA-C-N-C-N-CA-C-N-CA-CB	110.50	118.52	1
C-N-CA-C-O	120.80	128.82	1
N-CA-CB	103.00	97.82	1
C-N-CA	121.70	130.18	1
N-CA-N-CA-CB	111.50	103.50	1
C-CA-O-C-N	123.00	115.47	1
N-CA-C	111.00	124.17	1
CA-C-N	116.20	106.79	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-C-C-N-N-CA-CB	110.50	102.51	1
C-N-C-CA-CB	110.10	119.02	1
C-CA-CB	109.10	119.43	1
N-CA-C-CA-CB	110.10	119.02	1
CA-CB-CG	113.80	109.10	1
C-CA-CA-C-N-CA-CA-C-O	120.80	112.82	1
CB-CG-CD	112.60	104.62	1
C-CA-CB	110.10	119.01	2
C-N-CA	121.70	130.14	1
N-CA-CA-C-O	120.80	128.77	1
CA-N-N-CA-N-CA-CA-CB-OG1	109.60	102.58	1
C-N-CA	122.60	99.20	1
C-CA-OE1-CD-N-CA-C	111.00	124.10	1
CA-CB-CG	112.60	107.92	2
C-CA-CB	111.40	102.51	1
C-CA-N-CA-C	111.00	124.09	1
CA-C-O	120.80	112.85	1
CA-C-N	116.20	106.86	1
CA-C-O	120.80	112.86	1
N-CA-CB	110.50	102.56	1
N-CA-C-CA-CB	110.10	118.96	1
C-N-CA	121.70	113.31	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-N-CA	121.70	113.31	1
C-N-CA-CB-C-N-N-CA-CB	110.50	118.41	1
CA-C-N	116.90	123.88	1
N-CA-C-CA-CB	110.10	101.26	1
N-CA-C	111.00	124.01	1
C-CA-N-CA-CB	110.50	118.39	1
C-CA-CB	109.10	98.89	1
N-CA-N-CA-CB	111.50	119.38	1
CA-CB-CG	112.60	107.96	1
CB-CG-CA-CB-CA-CB-CA-N-CD	112.00	105.52	1
CA-C-O	120.80	128.67	1
C-CA-CA-C-N	116.20	106.95	1
C-CA-CB	110.10	101.31	1
CA-C-O	120.80	128.66	1
N-CA-CB	111.50	119.35	1
N-CA-CB	110.50	102.65	1
N-CA-C	113.30	99.92	1
CA-C-O	120.80	112.95	1
N-CA-C-N-CA-C-N-CA-CB	111.50	119.33	1
CA-CB-CG	112.60	107.99	1
CB-CG-CD2	131.20	125.21	1
C-CA-CB	110.50	117.41	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-C-CA-CB	110.10	118.84	1
C-N-CA-C-C-CA-C-N-CA-CB-CA-CB-CG	112.60	108.00	1
C-N-N-CA-C	111.00	98.13	1
CA-C-O	120.80	112.99	1
CA-C-C-CA-N-CA-CB	110.50	118.30	1
C-CA-CA-CB-CG	113.80	109.22	1
N-CA-C-N-CA	121.70	113.45	1
CA-C-N	116.20	107.04	1
N-CA-C	111.00	123.82	1
C-CA-N-CA-CB	111.50	103.72	1
CA-C-N	116.20	107.05	1
CA-CB-CA-C-CA-CB-C-N-C-CA-C-N-CA	121.70	113.47	1
C-CA-CB	110.10	101.42	1
C-N-CA	121.70	113.49	1
CA-C-N-CA-C	111.00	98.23	1
C-N-C-CA-CB	110.10	118.76	1
CA-C-N	116.20	107.09	1
CA-CB-CG	112.60	108.05	2
CA-CB-CG	113.80	109.25	1
N-CA-CB	111.50	103.77	1
C-N-CA	121.70	113.51	1
C-CA-N-CA-C	111.00	123.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-CA	121.70	129.89	1
N-CA-CB	103.00	98.00	1
CA-C-C-CA-CB	110.10	101.47	1
N-CA-C-CA-N-CA-CB	111.50	119.22	1
N-CA-CA-CB-CG	112.60	108.06	1
CA-C-O	120.80	128.52	1
C-N-CA	121.70	129.87	1
C-CA-CB	110.10	101.48	1
CA-C-N	116.20	125.27	1
CA-C-O	120.80	128.51	1
C-CA-CA-C-N	116.20	125.27	1
CD2-NE2-CE1	109.00	104.47	1
C-CA-CA-CB-CG	112.60	108.07	1
CA-CB-N-CA-CB	110.50	102.80	1
C-N-CA	121.70	129.85	1
C-N-CA-N-C-N-N-CA-CB	110.50	118.19	1
C-CA-C-CA-CA-C-CA-CB-CG	112.60	108.08	1
N-CA-C-N-CD2-NE2-CE1	109.00	104.48	1
C-N-CA	121.70	113.57	1
CA-C-O	120.80	128.48	1
C-CA-CA-C-N	116.20	107.17	1
CB-CG-CD	112.60	120.27	1
CA-CB-CA-C-O	120.80	128.47	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	101.53	1
N-CA-CB	111.50	119.16	1
N-CD-C-CA-N-CA-C	111.00	98.39	1
C-N-CA	121.70	113.59	1
N-CA-CB	110.40	117.15	1
C-CA-CD2-NE2-CE1	109.00	104.50	1
C-CA-CA-CB-CG	113.90	105.80	1
CD2-NE2-N-CA-CA-C-N-CA-N-CA-C	111.00	123.58	1
CA-CB-CG	113.80	109.31	1
CD2-NE2-CE1	109.00	104.51	2
N-CA-CA-C-O	120.80	128.43	1
C-N-CA	121.70	113.62	1
CG-CD2-C-N-CA-C-N	116.20	125.17	1
CA-CB-CG	112.60	108.11	1
CA-C-CD2-NE2-CA-C-O	120.80	113.18	1
CD2-NE2-CE1	109.00	104.52	3
C-N-CA	121.70	129.77	1
CD1-CG-CD2	110.80	100.95	1
CA-C-CD2-NE2-C-CA-CB	110.10	118.60	1
CD2-NE2-CE1	109.00	104.53	1
N-CA-N-CA-CB	110.50	102.90	1
C-N-CA	121.70	129.75	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-C-N-CA	121.70	129.75	1
N-CA-CA-C-CA-CB-CD2-NE2-CE1	109.00	104.53	1
C-CA-CB	110.10	118.59	2
N-CA-C-N-CA	121.70	113.66	1
CA-N-CD	112.00	105.75	1
CA-CB-OG	111.10	102.17	1
C-N-CA-C-N-CA-CB	110.50	118.09	1
CD2-NE2-CE1	109.00	104.54	1
CA-C-N	116.20	125.13	1
C-N-C-CA-CB	110.10	101.62	1
C-CA-C-CA-CA-CB-CG	112.60	108.14	1
C-CA-N-CA-CB	110.50	118.08	1
C-N-CA-CB-CG	113.80	109.34	1
C-CA-C-CA-CB	110.10	101.64	1
C-CA-C-CA-C-CA-CB	109.10	118.89	1
C-CA-CB	110.10	118.55	1
N-CA-N-CA-CB	111.50	103.94	1
C-CA-C-N-CA	121.70	129.70	1
C-CA-CB	110.10	118.54	1
CA-CB-CA-C-CA-C-N	116.20	107.32	1
CA-C-N-CA-C-CA-N-CA-CB	110.50	102.96	1
C-CA-C-N-C-CA-CB	110.10	101.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.50	118.03	1
C-N-N-CA-C	111.00	98.60	1
C-CA-CB	110.10	101.68	1
C-CA-CD2-NE2-CE1	109.00	104.57	1
C-CA-C-N-CA	121.70	113.74	1
C-N-CA	121.70	129.66	1
N-CA-N-CA-C-CA-CB	110.10	101.70	1
N-CA-CB	110.50	102.99	1
C-CA-C-CA-CB	109.10	118.82	1
C-CA-CB	110.10	118.49	1
C-N-N-CA-C	111.00	98.65	1
C-CA-CB	110.10	118.48	1
N-CA-C-N-CA	121.70	113.76	1
CA-C-N	116.20	125.02	1
C-N-C-N-CA	121.70	113.77	1
CD2-NE2-CE1	109.00	104.59	1
CA-C-CA-CB-CG	112.60	108.19	1
C-CA-CB	110.10	101.73	1
C-N-CA	121.70	113.77	1
N-CA-CB	110.50	103.02	1
C-CA-CB	110.10	101.74	1
CA-C-N-CA-CD2-NE2-CE1	109.00	104.60	1
N-CA-C	111.00	98.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-C-CA-C-CA-C-N	116.20	124.99	1
C-CA-CB	110.10	101.75	2
C-N-C-CA-CB	110.10	101.75	1
C-CA-CA-C-C-N-CA	121.70	113.80	1
C-CA-CB	110.50	117.09	1
CA-CB-CD2-NE2-CE1	109.00	104.61	1
CA-C-O	120.80	113.35	1
N-CA-CB	110.50	117.95	1
C-CA-CB	110.10	118.43	1
C-CA-CB	110.10	101.77	1
C-N-C-N-C-CA-CB	111.60	120.37	1
N-CA-CD2-NE2-CE1	109.00	104.62	1
CA-C-N	116.20	124.96	1
CD2-NE2-CE1	109.00	104.62	1
C-N-CA-CB-CG	112.60	108.23	1
N-CA-CA-CB-CA-C-CA-CB-C-CA-C-CA-C-N-CA	121.70	113.84	1
CA-CB-CG	112.60	108.24	2
C-N-CA	121.70	113.85	1
C-CA-C-CA-CB	109.10	118.70	1
C-CA-CB	110.10	118.39	1
C-N-CA	121.70	129.55	1
CA-C-N-CA-CA-CB-CG	113.80	109.44	1
C-CA-N-CA-CB	110.50	117.91	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
N-CA-CB	110.40	103.86	1
C-CA-N-CA-CB	111.50	104.10	1
N-CA-CB	103.00	107.79	1
C-N-CA	121.70	113.87	2
C-CA-CB	110.10	101.84	1
CA-C-O	120.80	113.41	1
C-CA-C-CA-N-CA-CB	111.50	104.12	1
N-CA-CB	110.50	103.12	1
CA-CB-CG	112.60	108.26	1
CA-C-N-CA-C	111.00	98.86	1
C-N-CA	121.70	113.89	1
CA-CB-N-CA-CB	111.50	104.13	1
C-N-CA-C-N	116.20	124.87	1
C-CA-N-CA-CB	110.50	103.13	1
N-CA-CB	110.50	117.86	1
CA-C-N	116.90	123.40	1
C-N-C-CA-CD2-NE2-C-CA-CB	110.10	101.88	1
CA-C-O	120.80	113.44	1
CA-C-N-CA-CA-C-O	120.80	128.15	1
CG-CD2-C-CA-C-CA-CD2-NE2-C-N-N-CA-C-CA-CB	110.10	101.89	1
C-CA-CA-C-N	116.20	124.84	1
C-CA-CB	110.10	101.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.60	121.81	1
CA-CB-CG	112.60	108.28	1
CA-C-N-CA-CA-C-CA-CB-N-CA-CD2-NE2-CE1	109.00	104.69	1
CA-CB-CG2	110.40	117.73	1
C-CA-C-CA-CB	110.10	101.91	1
N-CA-CB	111.50	104.18	1
CA-C-O	120.80	113.48	1
C-CA-CB	110.10	118.28	1
CA-C-N	116.90	123.36	1
N-CA-N-CA-C-N-C-N-N-CA-N-CA-N-CA-CB	111.50	118.81	1
C-CA-CB	110.10	118.27	1
N-CA-N-CA-C-CA-C-CA-CB	111.60	120.20	1
C-CA-CB	110.10	118.26	1
C-CA-CA-C-O	120.80	113.50	1
N-CD-CG	103.20	109.64	1
N-CA-C-N-CA	121.70	113.97	1
C-N-C-N-CA	121.70	129.43	1
N-CA-N-CA-N-CA-CB	110.40	103.97	1
N-CA-C	111.00	99.00	1
C-CA-CB	110.10	118.24	1
CA-CB-CG	112.60	108.31	1
N-CA-CA-CB-CA-CB-CG	112.60	108.32	1
CA-C-CA-N-CD	112.00	106.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-O	120.80	128.08	1
CA-C-N	116.20	124.76	1
CA-C-N-CA-CB	111.50	118.77	1
C-N-N-CA-CB	110.50	103.23	1
C-N-NE-CZ-N-CA-C	111.00	122.97	1
N-CA-CB	110.50	103.23	1
CA-C-O	120.80	113.53	1
C-CA-C-N-CA	121.70	129.39	1
CA-C-O	120.80	128.06	1
CB-CG-CA-C-CA-C-CA-CB-CG	113.80	109.53	1
C-CA-CB	111.40	103.29	1
N-CA-C	111.00	122.95	1
N-CA-CB	110.50	117.75	1
C-CA-CB	110.10	118.21	1
CD2-NE2-CE1	109.00	104.73	1
CA-C-C-N-CA-C-O	120.80	113.55	1
CA-C-O	120.80	128.04	1
CA-C-N	116.20	107.68	1
CA-CB-C-CA-CA-CB-CG	113.90	106.23	1
CA-C-C-N-C-N-N-CA-C	113.30	125.64	1
CA-C-O	120.80	128.03	1
C-CA-CB	110.10	102.02	1
CA-C-N	116.20	107.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	108.35	1
C-N-CA-C-N	116.20	107.71	1
CA-C-C-N-CA-C-C-CA-C-CA-C-CA-CB	110.10	118.16	1
CA-CB-CG	112.60	108.36	1
C-N-C-N-C-N-CA	121.70	114.08	1
CA-CB-CA-C-CA-CB-CG	114.10	105.63	1
C-N-C-CA-N-CA-CA-N-CD	112.00	106.07	1
C-CA-C-CA-N-CA-CB	110.50	117.69	1
C-CA-CA-C-O	120.80	127.99	1
CA-C-N	116.20	107.74	1
N-CA-C	111.00	99.16	1
C-CA-CB	110.10	102.07	2
C-N-C-N-CA	121.70	114.09	1
CB-CG-C-N-CA	121.70	129.30	1
CA-CB-OG1	109.60	103.26	1
N-CA-C-N-N-CA-CB	110.50	117.67	1
CA-C-N	116.20	107.76	1
CA-C-C-N-C-CA-CB	111.60	120.03	1
CA-CB-CG	112.60	108.39	1
C-CA-C-N-C-N-CA	121.70	114.12	1
C-N-CA	121.70	129.28	1
C-CA-CB	110.50	116.82	1
C-CA-CB	110.10	102.10	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-CA-CB	110.10	102.11	1
CA-C-O	120.80	113.65	1
C-N-CA	121.70	114.13	1
CA-CB-C-CA-CB	110.10	118.09	1
CA-C-N-CA-CB	110.50	103.36	1
CA-C-CA-CB-N-CA-C	111.00	99.24	1
C-N-CA	121.70	114.14	1
CA-CB-CG	113.90	106.35	1
CA-C-O	120.80	113.67	1
C-CA-CB	110.10	102.14	1
C-CA-CB	110.10	118.06	1
CD-NE-CZ	124.40	118.54	1
C-N-N-CA-CA-C-CA-CB-CG	113.80	109.62	1
CA-CB-CG	113.80	109.62	1
C-CA-C-N-CA	121.70	114.17	1
N-CA-C	111.00	99.29	1
N-CA-C-N-CA	121.70	114.18	1
N-CA-C	111.00	99.30	1
C-N-CB-CG-CD	112.60	105.50	2
C-CA-C-N-CA	121.70	114.18	1
N-CA-N-CA-C	112.10	101.66	1
CA-C-C-N-CB-CG-CD	112.60	105.50	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C-N-C-CA-CB	110.10	118.03	1
N-CA-CB	111.50	118.59	1
C-N-CA	121.70	129.21	1
N-CA-C-CA-CB	110.10	102.18	1
C-CA-CB	110.10	118.02	1
CA-CB-C-CA-CB	110.10	102.18	1
CA-CB-CG	112.60	108.43	1
CA-CB-N-CA-CB	110.50	103.42	1
C-CA-CA-C-O	120.80	113.72	1
C-CA-CB	111.40	119.31	1
C-CA-N-CA-CA-C-C-N-CA	121.70	114.22	1
CA-CB-CG	112.60	108.44	1
N-CA-C	111.00	99.36	1
CA-C-CA-CB-C-CA-CB	110.10	102.21	1
N-CA-CB	110.50	103.44	1
C-N-CA	121.70	129.17	1
C-CA-C-N-C-CA-CB	110.10	102.21	1
N-CA-C	111.00	99.38	1
C-N-C-CA-CB	110.10	102.22	1
C-N-CA-C-N	116.20	107.91	1
N-CA-C	111.00	99.39	1
N-CA-C	111.00	122.61	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-CA-C-N	116.20	124.49	1
C-CA-C-N-CA	122.60	143.32	1
C-CA-CB	110.10	102.23	1
CA-C-O	120.80	113.76	1
CA-C-CA-C-N	116.20	124.48	1
N-CA-C-CA-CB	109.10	118.21	1
C-N-C-CA-CB-CG-CD	112.60	105.56	1
C-CA-CA-C-C-N-N-CA-C	111.00	99.42	1
C-N-CA	121.70	129.14	1
C-N-CA-C-N-CA-CB	103.00	107.54	1
C-CA-CB	110.10	102.26	1
C-CA-C-CA-N-CA-CB	110.50	103.49	1
CA-CB-C-CA-CB	110.10	117.93	1
CA-C-N	116.20	107.96	1
C-CA-CB	110.10	117.93	1
C-CA-CB	111.40	103.57	1
CA-C-O	120.80	113.80	2
C-CA-CB	110.10	102.29	2
C-CA-CA-CB-CG	112.60	108.49	1
CA-CB-CG	112.60	108.49	1
CA-C-N-CA-CB	110.50	103.52	1
N-CA-CB	110.50	103.52	2
C-CA-CB	111.40	103.60	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-N-N-CA-CB	111.50	118.47	1
CA-C-O	120.80	127.76	1
CA-CB-CG	113.90	106.53	1
CA-C-N-CA-N-CA-C	111.00	122.46	1
C-CA-CB	110.10	102.33	1
N-CA-CB	111.50	104.55	2
CA-CB-CG	112.60	108.51	1
N-CA-C	111.00	99.55	1
C-CA-C-N-N-CA-CA-C-C-C-CA-CB	110.10	102.34	1
C-CA-CB	110.10	117.86	1
CB-CG-N-CA-CA-C-O	120.80	127.74	1
CA-C-CA-N-CD	112.00	106.29	1
C-N-CA	121.70	114.36	1
CA-C-N-CA-N-CA-C	111.00	99.59	1
C-CA-CB	110.10	117.85	1
OE1-CD-NE2	122.60	118.52	1
CA-C-C-N-CA	121.70	114.37	1
N-CA-C	111.00	122.40	1
N-CA-CA-CB-CA-CB-CG	112.60	108.53	1
C-CA-N-CA-C	111.00	122.39	1
N-CA-CA-CB-N-CA-CB	110.50	117.41	1
N-CA-C-CA-CB	110.10	117.83	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-ND1-CE1-NE2	108.40	112.47	1
C-N-CA	121.70	114.38	1
CA-CB-CA-C-O	120.80	127.71	1
CA-C-CA-C-N	116.20	124.32	1
ND1-CE1-C-N-CA-C-N-CA-C-N-N-CA-N-CA-C-N-CA	121.70	128.99	1
N-CA-CB-CG-CD	112.60	119.49	1
N-CA-C	111.00	99.66	1
C-N-N-CA-N-CA-CA-C-C-N-N-CA-C	111.00	122.33	1
C-N-CA	121.70	128.98	1
C-CA-CB	110.10	117.78	2
C-N-C-CA-N-CA-CB	111.50	104.64	1
CA-C-O	120.80	113.94	1
C-N-C-N-N-CA-CB	110.40	104.35	1
C-N-CA	121.70	114.44	1
CA-C-N	116.90	122.95	1
C-CA-CB	111.40	103.74	1
CA-C-O	120.80	113.95	1
CA-C-N	116.90	122.94	1
C-N-C-CA-CA-C-C-N-C-N-CA	121.70	114.45	1
C-N-CA	121.70	114.45	1
ND1-CE1-C-CA-CB	110.10	102.45	1
C-CA-CB	111.40	119.05	1
C-N-CA	121.70	128.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-C-CA-CB	110.10	102.46	1
C-N-CA	121.70	128.93	1
C-N-CA	121.70	114.47	1
C-CA-CB	110.10	102.47	1
N-CA-C	112.10	102.06	1
CA-CB-CG	112.60	108.59	1
C-N-C-N-C-N-CA-CB-C-N-CA	121.70	128.91	1
C-N-CA	121.70	128.91	1
CA-C-N-CA-CB	110.50	117.31	1
ND1-CE1-NE2	108.40	112.40	1
CA-CB-CG	112.60	108.60	1
CA-C-O	120.80	127.60	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	566.51	32256

All 32256 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

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

Model ID	Analyzed	Favored	Allowed	Outliers
1	7081	6290	527	264

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	6268	5386	483	399

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A1	205	0.0LYS
1	A1	251	0.0GLU
1	A1	266	0.0LEU
1	A1	276	0.0THR
1	A1	359	0.0GLU
1	A1	668	0.0SER
1	A1	406	0.0GLN
1	A1	417	0.0THR
1	A1	431	0.0PHE
1	A1	480	0.0PRO
1	A1	481	0.0PHE
1	A1	483	0.0ARG
1	A1	494	0.0ASP
1	A1	795	0.0GLN
1	A1	563	0.0ASN
1	A1	564	0.0ILE
1	B1	25	0.0ARG
1	B1	58	0.0THR
1	B1	71	0.0PRO

Model ID	Chain	Residue ID	Residue type
1	B1	75	0.0GLN
1	B1	77	0.0PHE
1	B1	103	0.0PHE
1	B1	110	0.0ILE
1	B1	136	0.0SER
1	B1	156	0.0LEU
1	B1	165	0.0VAL
1	B1	182	0.0VAL
1	B1	186	0.0THR
1	B1	211	0.0GLN
1	B1	214	0.0TYR
1	B1	267	0.0SER
1	B1	269	0.0ASP
1	B1	270	0.0VAL
1	B1	290	0.0VAL
1	B1	292	0.0THR
1	B1	303	0.0PRO
1	B1	320	0.0PRO
1	B1	336	0.0LYS
1	B1	337	0.0LEU
1	B1	344	0.0LEU
1	B1	345	0.0PRO
1	B1	348	0.0ILE

Model ID	Chain	Residue ID	Residue type
1	B1	357	0.0ASP
1	B1	358	0.0THR
1	B1	359	0.0GLU
1	B1	374	0.0THR
1	B1	377	0.0SER
1	B1	378	0.0LEU
1	B1	380	0.0ASP
1	B1	389	0.0PRO
1	B1	396	0.0SER
1	B1	402	0.0PRO
1	B1	403	0.0PRO
1	B1	404	0.0ASN
1	B1	405	0.0CYS
1	B1	418	0.0LEU
1	B1	441	0.0LEU
1	B1	442	0.0LEU
1	B1	447	0.0ASP
1	B1	469	0.0ILE
1	B1	497	0.0ARG
1	B1	515	0.0PRO
1	B1	516	0.0ASN
1	B1	527	0.0LYS
1	B1	574	0.0LEU

Model ID	Chain	Residue ID	Residue type
1	B1	576	0.0ASN
1	B1	590	0.0LYS
1	B1	650	0.0THR
1	B1	653	0.0ASP
1	B1	654	0.0SER
1	B1	656	0.0ASP
1	B1	661	0.0THR
1	B1	675	0.0LYS
1	B1	676	0.0ILE
1	B1	680	0.0LYS
1	B1	691	0.0ASN
1	B1	707	0.0ASN
1	B1	715	0.0LEU
1	B1	730	0.0TYR
1	B1	731	0.0THR
1	B1	772	0.0LEU
1	B1	776	0.0LEU
1	B1	782	0.0PRO
1	B1	802	0.0SER
1	B1	815	0.0GLN
1	B1	829	0.0ASP
1	B1	847	0.0SER
1	B1	849	0.0PRO

Model ID	Chain	Residue ID	Residue type
1	B1	858	0.0GLU
1	B1	875	0.0LYS
1	B1	889	0.0ASP
1	B1	896	0.0LYS
1	B1	898	0.0GLU
1	B1	903	0.0ASP
1	B1	913	0.0LYS
1	B1	919	0.0VAL
1	B1	929	0.0SER
1	B1	934	0.0SER
1	B1	940	0.0LEU
1	B1	941	0.0ASN
1	B1	943	0.0THR
1	B1	948	0.0LEU
1	B1	949	0.0ASN
1	B1	957	0.0TYR
1	B1	960	0.0PRO
1	B1	971	0.0SER
1	B1	1018	0.0THR
1	B1	1023	0.0ASP
1	B1	1029	0.0VAL
1	B1	1061	0.0ILE
1	B1	1066	0.0ASN

Model ID	Chain	Residue ID	Residue type
1	B1	1077	0.0LEU
1	B1	1081	0.0PHE
1	B1	1096	0.0VAL
1	B1	1097	0.0ILE
1	B1	1119	0.0GLU
1	B1	1400	0.0PRO
1	B1	1170	0.0ILE
1	B1	1172	0.0ASP
1	B1	1173	0.0GLU
1	B1	1182	0.0THR
1	B1	1192	0.0PRO
1	B1	1224	0.0PHE
1	B1	1226	0.0PRO
1	B1	1507	0.0LEU
1	B1	1508	0.0SER
1	B1	1264	0.0LYS
1	B1	1530	0.0LYS
1	B1	1278	0.0LEU
1	B1	1303	0.0TYR
1	B1	1305	0.0HIS
1	B1	1306	0.0ASP
1	B1	1342	0.0LEU
1	B1	1652	0.0PHE

Model ID	Chain	Residue ID	Residue type
1	D1	101	0.0SER
1	D1	142	0.0ASP
1	D1	175	0.0ASN
1	D1	177	0.0ILE
1	D1	194	0.0VAL
1	D1	203	0.0LYS
1	D1	210	0.0ASN
1	D1	222	0.0GLN
1	D1	246	0.0LEU
1	D1	269	0.0SER
1	D1	278	0.0LYS
1	D1	343	0.0ILE
1	D1	349	0.0SER
1	D1	354	0.0PRO
1	D1	367	0.0HIS
1	D1	413	0.0THR
1	D1	431	0.0LYS
1	D1	504	0.0VAL
1	D1	511	0.0VAL
1	D1	539	0.0ILE
1	D1	541	0.0ILE
1	D1	550	0.0LEU
1	D1	569	0.0SER

Model ID	Chain	Residue ID	Residue type
1	D1	570	0.0THR
1	D1	602	0.0ASP
1	D1	614	0.0MET
1	D1	615	0.0TYR
1	D1	626	0.0LEU
1	D1	668	0.0LYS
1	D1	673	0.0ILE
1	D1	719	0.0PRO
1	D1	774	0.0ASP
1	D1	813	0.0SER
1	D1	820	0.0LEU
1	D1	829	0.0GLU
1	D1	830	0.0ILE
1	D1	845	0.0LEU
1	D1	854	0.0LEU
1	D1	863	0.0LEU
1	D1	866	0.0ARG
1	D1	991	0.0THR
1	D1	998	0.0THR
1	D1	1005	0.0VAL
1	D1	1299	0.0LYS
1	D1	1300	0.0SER
1	D1	1301	0.0SER

Model ID	Chain	Residue ID	Residue type
1	D1	1041	0.0HIS
1	D1	1081	0.0ARG
1	D1	1083	0.0SER
1	D1	1099	0.0THR
1	D1	1113	0.0LEU
1	D1	1114	0.0LYS
1	K1	58	0.0ILE
1	K1	106	0.0ILE
1	K1	165	0.0ASN
1	K1	182	0.0LYS
1	K1	225	0.0LYS
1	K1	239	0.0LEU
1	K1	281	0.0GLU
1	K1	363	0.0LYS
1	K1	411	0.0ILE
1	K1	416	0.0LYS
1	K1	430	0.0ILE
1	K1	472	0.0ILE
1	K1	529	0.0ILE
1	K1	531	0.0LYS
1	K1	565	0.0ILE
1	K1	581	0.0ASP
1	K1	589	0.0LYS

Model ID	Chain	Residue ID	Residue type
1	K1	632	0.0ILE
1	K1	633	0.0LEU
1	K1	678	0.0ILE
1	K1	682	0.0GLU
1	K1	687	0.0LEU
1	K1	714	0.0GLU
1	K1	793	0.0LEU
1	K1	802	0.0VAL
1	K1	814	0.0ASN
1	K1	849	0.0LYS
1	K1	856	0.0ILE
1	K1	858	0.0GLU
1	K1	865	0.0GLU
1	K1	939	0.0LYS
1	L1	7	0.0THR
1	L1	11	0.0ASP
1	L1	20	0.0GLN
1	L1	45	0.0ASP
1	L1	58	0.0GLU
1	L1	64	0.0LEU
1	L1	73	0.0ASN
1	L1	75	0.0ASP
1	L1	105	0.0GLN

Model ID	Chain	Residue ID	Residue type
1	L1	115	0.0GLU
1	L1	128	0.0THR
1	L1	153	0.0THR
1	L1	212	0.0THR
1	L1	224	0.0ILE
1	L1	255	0.0SER
1	L1	261	0.0GLN
1	L1	271	0.0SER
1	L1	285	0.0ILE
1	L1	330	0.0ILE
1	L1	344	0.0SER
1	L1	352	0.0MET
1	L1	380	0.0SER
1	L1	399	0.0LEU
1	L1	408	0.0ILE
1	L1	426	0.0ILE
1	L1	527	0.0ILE
1	M1	94	0.0LEU
1	M1	152	0.0ILE
1	M1	168	0.0SER
1	M1	179	0.0LEU
1	M1	188	0.0SER
1	M1	196	0.0LEU

Model ID	Chain	Residue ID	Residue type
1	M1	201	0.0LEU
1	M1	206	0.0THR
1	M1	209	0.0CYS
1	M1	211	0.0ILE
1	M1	215	0.0ILE
1	M1	228	0.0GLU
1	M1	230	0.0LEU
1	M1	231	0.0PHE
1	M1	260	0.0LEU
1	M1	262	0.0SER
1	M1	266	0.0SER
1	M1	268	0.0LEU
1	M1	272	0.0SER
1	M1	279	0.0ILE
1	M1	300	0.0ARG
1	M1	303	0.0THR
1	M1	316	0.0GLN
1	M1	324	0.0ARG
1	M1	325	0.0VAL
1	M1	327	0.0SER
1	M1	329	0.0GLU
1	M1	368	0.0ILE
1	M1	376	0.0ILE

Model ID	Chain	Residue ID	Residue type
1	M1	382	0.0SER
1	M1	384	0.0ASN
1	M1	390	0.0ARG
1	M1	391	0.0LEU
1	M1	399	0.0PHE
1	M1	407	0.0ARG
1	N1	15	0.0LYS
1	N1	36	0.0HIS
1	N1	39	0.0ILE
1	N1	40	0.0ASP
1	N1	132	0.0ILE
1	N1	206	0.0VAL
1	N1	208	0.0GLN
1	N1	210	0.0ARG
1	N1	256	0.0ASP
1	O1	61	0.0ILE
1	O1	80	0.0THR
1	O1	125	0.0LEU
1	O1	154	0.0MET
1	O1	168	0.0ASP
1	O1	183	0.0LEU
1	O1	226	0.0ARG
1	O1	313	0.0ASN

Model ID	Chain	Residue ID	Residue type
1	O1	314	0.0LEU
1	O1	295	0.0THR
1	P1	90	0.0ASN
1	P1	92	0.0THR
1	P1	184	0.0VAL
1	P1	214	0.0ASP
1	P1	225	0.0VAL
1	P1	269	0.0ILE
1	P1	329	0.0VAL
1	P1	332	0.0THR
1	P1	384	0.0ASP
1	P1	419	0.0LEU
1	P1	427	0.0THR
1	P1	456	0.0ILE
1	P1	470	0.0TYR
1	R1	103	0.0SER
1	R1	138	0.0VAL
1	R1	148	0.0GLN
1	R1	151	0.0VAL
1	R1	159	0.0LEU
1	R1	164	0.0LYS
1	R1	185	0.0THR
1	R1	235	0.0MET

Model ID	Chain	Residue ID	Residue type
1	R1	246	0.0PHE
1	R1	256	0.0LEU
1	R1	281	0.0VAL
1	R1	285	0.0THR
1	R1	299	0.0ILE
1	R1	312	0.0GLU
1	R1	341	0.0ASP
1	R1	375	0.0VAL
1	R1	379	0.0PHE
1	R1	399	0.0SER
1	R1	561	0.0GLN
1	R1	576	0.0ILE
1	R1	609	0.0VAL
1	R1	615	0.0THR
1	R1	634	0.0LEU
1	R1	661	0.0VAL
1	R1	674	0.0ASP

Fit of model to data used for modeling

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

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