

# Integrative Structure Validation Report

July 22, 2024 - 04:06 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            | 9A0F  |
| PDB-Dev ID        | PDBDEV_00000051   |
| Structure Title   | Integrative model of the wild type 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](mailto:pdb-dev@mail.wwpdb.org)*

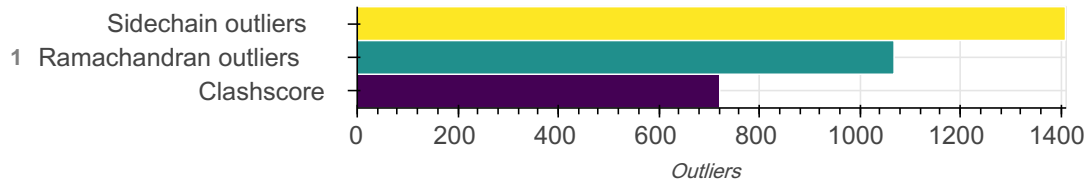
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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 46 subunits in each model. A total of 10 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 46 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          | Nup133       | K1       | K1              | 1157           |
| 1        | 2              | 1          | Nup133       | K2       | K2              | 1157           |
| 1        | 3              | 2          | Nup84        | L1       | L1              | 726            |
| 1        | 4              | 2          | Nup84        | L2       | L2              | 726            |
| 1        | 5              | 3          | Nup145c      | M1       | M1              | 712            |
| 1        | 6              | 3          | Nup145c      | M2       | M2              | 712            |
| 1        | 7              | 4          | Sec13        | N1       | N1              | 297            |
| 1        | 8              | 4          | Sec13        | N2       | N2              | 297            |
| 1        | 9              | 5          | Seh1         | O1       | O1              | 349            |
| 1        | 10             | 5          | Seh1         | O2       | O2              | 349            |
| 1        | 11             | 6          | Nup85        | P1       | P1              | 744            |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1        | 12             | 6          | Nup85        | P2       | P2              | 744            |
| 1        | 13             | 7          | Nup120       | R1       | R1              | 1037           |
| 1        | 14             | 7          | Nup120       | R2       | R2              | 1037           |
| 1        | 15             | 8          | Dyn2         | 91       | 91              | 92             |
| 1        | 16             | 8          | Dyn2         | 92       | 92              | 92             |
| 1        | 17             | 9          | Nup82        | W1       | W1              | 713            |
| 1        | 18             | 9          | Nup82        | W2       | W2              | 713            |
| 1        | 19             | 10         | Nup159       | V1       | V1              | 1460           |
| 1        | 20             | 10         | Nup159       | V2       | V2              | 1460           |
| 1        | 21             | 11         | Nsp1         | J1       | J1              | 823            |
| 1        | 22             | 11         | Nsp1         | J2       | J2              | 823            |
| 1        | 23             | 11         | Nsp1         | J3       | J3              | 823            |
| 1        | 24             | 11         | Nsp1         | J4       | J4              | 823            |
| 1        | 25             | 11         | Nsp1         | J5       | J5              | 823            |
| 1        | 26             | 11         | Nsp1         | J6       | J6              | 823            |
| 1        | 27             | 12         | Nic96        | A1       | A1              | 839            |
| 1        | 28             | 12         | Nic96        | A2       | A2              | 839            |
| 1        | 29             | 12         | Nic96        | A3       | A3              | 839            |
| 1        | 30             | 12         | Nic96        | A4       | A4              | 839            |
| 1        | 31             | 13         | Nup188       | B1       | B1              | 1655           |
| 1        | 32             | 13         | Nup188       | B2       | B2              | 1655           |
| 1        | 33             | 14         | Nup157       | D1       | D1              | 1391           |
| 1        | 34             | 14         | Nup157       | D2       | D2              | 1391           |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1        | 35             | 15         | Nup57        | H1       | H1              | 541            |
| 1        | 36             | 15         | Nup57        | H2       | H2              | 541            |
| 1        | 37             | 15         | Nup57        | H3       | H3              | 541            |
| 1        | 38             | 15         | Nup57        | H4       | H4              | 541            |
| 1        | 39             | 16         | Nup49        | I1       | I1              | 472            |
| 1        | 40             | 16         | Nup49        | I2       | I2              | 472            |
| 1        | 41             | 16         | Nup49        | I3       | I3              | 472            |
| 1        | 42             | 16         | Nup49        | I4       | I4              | 472            |
| 1        | 43             | 17         | Nup192       | C1       | C1              | 1683           |
| 1        | 44             | 17         | Nup192       | C2       | C2              | 1683           |
| 1        | 45             | 18         | Nup170       | d1       | d1              | 1502           |
| 1        | 46             | 18         | Nup170       | d2       | d2              | 1502           |

### Datasets used for modeling

There are 10 unique datasets used to build the models in this entry.

| ID | Dataset type       | Database name | Data access code       |
|----|--------------------|---------------|------------------------|
| 1  | 3DEM volume        | EMDB          | EMD-10198              |
| 2  | 3DEM volume        | File          | 10.5281/zenodo.3820319 |
| 3  | 3DEM volume        | File          | 10.5281/zenodo.3820319 |
| 4  | Experimental model | PDB           | 4XMM                   |
| 5  | Comparative model  | File          | 10.5281/zenodo.1194547 |
| 6  | Comparative model  | File          | 10.5281/zenodo.1194547 |

| ID | Dataset type      | Database name | Data access code  |
|----|-------------------|---------------|---|
| 7  | Integrative model | PDB-Dev       | PDBDEV_00000010   |
| 8  | Integrative model | PDB-Dev       | PDBDEV_00000010   |
| 9  | Integrative model | PDB-Dev       | PDBDEV_00000010   |
| 10 | Other             | File          | <a href="https://doi.org/10.1038/nsmb1194">https://doi.org/10.1038/nsmb1194</a> |

## Representation

*This entry has only one representation and includes 0 rigid bodies and 46 flexible units*

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--------------------|
| K1       | -            | 1-1157             |
| L1       | -            | 1-726              |
| M1       | -            | 1-712              |
| N1       | -            | 1-297              |
| O1       | -            | 1-349              |
| P1       | -            | 1-744              |
| R1       | -            | 1-1037             |
| 91       | -            | 1-92               |
| W1       | -            | 1-713              |
| V1       | -            | 1-1460             |
| J1       | -            | 1-823              |
| 92       | -            | 1-92               |
| W2       | -            | 1-713              |
| V2       | -            | 1-1460             |
| J2       | -            | 1-823              |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--------------------|
| A1       | -            | 1-839              |
| B1       | -            | 1-1655             |
| D1       | -            | 1-1391             |
| H1       | -            | 1-541              |
| I1       | -            | 1-472              |
| J3       | -            | 1-823              |
| A2       | -            | 1-839              |
| C1       | -            | 1-1683             |
| H2       | -            | 1-541              |
| I2       | -            | 1-472              |
| J4       | -            | 1-823              |
| d1       | -            | 1-1502             |
| A3       | -            | 1-839              |
| C2       | -            | 1-1683             |
| H3       | -            | 1-541              |
| I3       | -            | 1-472              |
| J5       | -            | 1-823              |
| d2       | -            | 1-1502             |
| A4       | -            | 1-839              |
| B2       | -            | 1-1655             |
| D2       | -            | 1-1391             |
| H4       | -            | 1-541              |
| I4       | -            | 1-472              |

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--------------|--------------------|
| J6       | -            | 1-823              |
| K2       | -            | 1-1157             |
| L2       | -            | 1-726              |
| M2       | -            | 1-712              |
| N2       | -            | 1-297              |
| O2       | -            | 1-349              |
| P2       | -            | 1-744              |
| R2       | -            | 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           | Systematic fitting of CR Y-complex, NR Y-complex, IR asymmetric unit and P-complex rigid bodies    | Systematic fitting to EM maps with Global search from UCSF Chimera             | None               | None                      | False                | False                |
| 2           | 1           | Monte Carlo simulated annealing optimization for CR Y-complex, NR Y-complex and IR asymmetric unit | Monte Carlo simulated annealing optimization of multiple rigid bodies with IMP | None               | None                      | False                | False                |

There are 2 software packages reported in this entry.

| ID | Software name                                       | Software version | Software classification       | Software location   |
|----|---|------------------|-------------------------------|---|
| 1  | <a href="#">Integrative Modeling Platform (IMP)</a> | 2.9.0            | integrative model building    | <a href="https://integrativemodeling.org">https://integrativemodeling.org</a>     |
| 2  | <a href="#">UCSF Chimera</a>                        | 1.14             | rigid body fitting to EM maps | <a href="https://www.cgl.ucsf.edu/chimera/">https://www.cgl.ucsf.edu/chimera/</a> |

## Data quality

### 3DEM volume

Validation for this section is under development.

## Model quality

For models with atomic structures, molprobability 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 10498 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             | 15.33           | 1                  |
| N-CA-CB           | 103.00             | 15.38           | 1                  |
| CA-N-CD           | 112.00             | 5.39            | 1                  |
| CA-N-CD           | 112.00             | 5.40            | 1                  |
| CA-N-CA-N-CA-N-CD | 112.00             | 10.68           | 1                  |
| CA-N-CD           | 112.00             | 10.74           | 1                  |
| CA-N-CD           | 112.00             | 17.93           | 1                  |



| Angle type                         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------------|--------------------|-----------------|--------------------|
| C-N-C-N-CA-C-CA-C-CA-C-CA-C-CA-C-N | 116.90             | 19.75           | 1                  |
| CA-C-N                             | 116.90             | 19.79           | 1                  |
| CA-N-CD                            | 112.00             | 21.54           | 1                  |
| CA-N-CD                            | 112.00             | 21.55           | 1                  |
| CA-N-CA-N-N-CA-CB                  | 103.00             | 172.85          | 1                  |
| N-CA-CB                            | 103.00             | 172.76          | 1                  |
| CA-C-CA-C-C-N-CA                   | 121.70             | 9.26            | 1                  |
| C-N-CA                             | 121.70             | 9.29            | 1                  |
| CA-N-CD                            | 112.00             | 24.89           | 1                  |
| CA-N-CD                            | 112.00             | 24.90           | 1                  |
| C-N-CA                             | 121.70             | 9.75            | 1                  |
| C-N-CA                             | 121.70             | 9.78            | 2                  |
| C-N-CA                             | 121.70             | 9.81            | 1                  |
| CA-C-CA-C-C-N-C-N-CA               | 121.70             | 12.14           | 1                  |
| C-N-C-N-CA                         | 121.70             | 12.22           | 1                  |
| CA-N-CD                            | 112.00             | 27.14           | 1                  |
| CA-N-CD                            | 112.00             | 27.16           | 1                  |
| CA-C-O                             | 120.80             | 18.19           | 1                  |
| CA-C-O                             | 120.80             | 18.20           | 1                  |
| CA-N-C-N-CA-N-C-N-C-N-CA           | 121.70             | 14.49           | 1                  |
| C-N-CA                             | 121.70             | 14.56           | 1                  |
| CA-N-CD                            | 112.00             | 28.82           | 1                  |

| Angle type                         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------------|--------------------|-----------------|--------------------|
| CA-N-CD                            | 112.00             | 28.83           | 1                  |
| C-N-CA                             | 121.70             | 15.33           | 1                  |
| C-N-CA                             | 121.70             | 15.44           | 1                  |
| C-N-CA                             | 121.70             | 15.50           | 1                  |
| C-N-C-N-CA-N-CD                    | 112.00             | 30.06           | 1                  |
| CA-N-CD                            | 112.00             | 30.09           | 1                  |
| C-N-CA                             | 121.70             | 16.85           | 1                  |
| C-N-CA                             | 121.70             | 16.87           | 1                  |
| CA-C-CA-C-N-CA-CB                  | 110.50             | 11.83           | 1                  |
| N-CA-CB                            | 110.50             | 11.83           | 1                  |
| C-N-C-N-C-N-CA                     | 121.70             | 17.83           | 1                  |
| C-N-CA                             | 121.70             | 17.83           | 1                  |
| CA-N-CD                            | 112.00             | 31.48           | 1                  |
| CA-N-CD                            | 112.00             | 31.51           | 1                  |
| CA-N-CA-N-N-CA-N-CA-C-N-C-N-C-N-CA | 121.70             | 19.95           | 1                  |
| C-N-CA                             | 121.70             | 19.98           | 1                  |
| C-N-CA-N-CA-N-C-N-CA               | 121.70             | 21.45           | 1                  |
| C-N-CA                             | 121.70             | 21.47           | 1                  |
| C-N-CA                             | 121.70             | 21.58           | 2                  |
| C-N-C-N-C-N-CA                     | 121.70             | 22.09           | 1                  |
| CA-C-O                             | 120.80             | 26.75           | 1                  |
| C-N-CA                             | 121.70             | 22.13           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-N-CA                 | 121.70             | 22.15           | 1                  |
| C-N-CA                 | 121.70             | 22.20           | 1                  |
| C-N-CA                 | 121.70             | 22.25           | 1                  |
| CA-C-C-N-CA            | 121.70             | 22.31           | 1                  |
| CA-C-C-N-C-N-CA        | 121.70             | 22.89           | 1                  |
| C-N-CA                 | 121.70             | 22.92           | 1                  |
| CA-C-N                 | 116.20             | 7.14            | 1                  |
| CA-C-N                 | 116.20             | 7.21            | 1                  |
| CA-N-CD                | 112.00             | 35.72           | 1                  |
| CA-C-CA-C-CA-C-O-C-N   | 123.00             | 36.39           | 1                  |
| O-C-N                  | 123.00             | 36.41           | 1                  |
| CA-C-N                 | 116.20             | 7.99            | 1                  |
| CA-C-N                 | 116.20             | 8.02            | 1                  |
| CA-N-CA-N-C-N-C-N-CA   | 121.70             | 24.68           | 1                  |
| C-N-C-N-C-N-CA         | 121.70             | 25.27           | 1                  |
| C-N-CA                 | 121.70             | 25.35           | 1                  |
| CA-N-CA-N-N-CA-CB      | 110.40             | 30.50           | 1                  |
| CA-C-O                 | 120.80             | 30.25           | 1                  |
| CA-C-CA-C-N            | 116.20             | 10.21           | 1                  |
| CA-C-N                 | 116.20             | 10.26           | 1                  |
| C-N-C-N-C-N-C-N-CA-C-N | 116.90             | 38.60           | 1                  |
| CA-C-N                 | 116.90             | 38.62           | 1                  |

| Angle type                         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                            | 110.10             | 11.06           | 1                  |
| C-CA-CB                            | 110.10             | 11.08           | 1                  |
| CA-C-O                             | 120.80             | 32.25           | 1                  |
| CA-N-CA-N-C-N-C-N-C-N-C-N-CA-C-N   | 116.90             | 39.31           | 1                  |
| CA-C-N                             | 116.90             | 39.33           | 1                  |
| C-N-CA                             | 121.70             | 28.73           | 1                  |
| C-N-CA                             | 121.70             | 28.81           | 2                  |
| C-N-CA                             | 121.70             | 28.82           | 1                  |
| C-N-CA                             | 121.70             | 29.00           | 1                  |
| C-N-CA                             | 121.70             | 29.01           | 1                  |
| C-N-CA                             | 121.70             | 29.02           | 1                  |
| C-N-CA                             | 121.70             | 29.08           | 1                  |
| C-N-CA                             | 121.70             | 29.11           | 1                  |
| CA-C-CA-C-CA-N-CA-N-CA-N-CD        | 112.00             | 40.59           | 1                  |
| CA-C-N                             | 116.20             | 14.22           | 1                  |
| C-N-CA                             | 121.70             | 30.14           | 1                  |
| C-N-CA                             | 121.70             | 30.15           | 1                  |
| CA-C-CA-C-C-N-C-N-N-CA-N-CA-C-N-CA | 121.70             | 30.49           | 1                  |
| C-N-CA                             | 121.70             | 30.50           | 1                  |
| N-CA-CB                            | 110.40             | 34.79           | 1                  |
| N-CA-CB                            | 110.40             | 34.80           | 1                  |
| C-N-C-N-C-N-C-N-CA-C-O             | 120.80             | 35.61           | 1                  |

| Angle type                               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-O                                   | 120.80             | 35.61           | 1                  |
| CA-C-O                                   | 120.80             | 35.66           | 1                  |
| CA-C-N                                   | 116.20             | 16.21           | 1                  |
| CA-C-O                                   | 120.80             | 35.92           | 1                  |
| CA-C-O                                   | 120.80             | 35.96           | 1                  |
| CA-C-CA-N-CA-N-CA-C-N                    | 116.20             | 17.37           | 1                  |
| CA-C-N                                   | 116.20             | 17.43           | 1                  |
| CA-C-CA-C-C-N-C-N-C-N-C-N-C-N-C-N-CA-C-N | 116.20             | 18.51           | 1                  |
| C-N-CA-C-N                               | 116.20             | 18.80           | 1                  |
| CA-C-N                                   | 116.20             | 18.81           | 1                  |
| CA-C-N                                   | 116.20             | 18.93           | 1                  |
| CA-C-N                                   | 116.20             | 18.97           | 1                  |
| C-N-CA                                   | 121.70             | 34.45           | 1                  |
| C-N-CA                                   | 121.70             | 34.50           | 1                  |
| O-C-C-CA-CB                              | 110.10             | 18.26           | 1                  |
| O-C-CA-C-N                               | 116.20             | 19.75           | 1                  |
| CA-C-N                                   | 116.20             | 19.79           | 1                  |
| C-N-C-N-CA                               | 121.70             | 34.98           | 1                  |
| C-N-C-N-C-N-CA                           | 121.70             | 35.34           | 1                  |
| C-N-CA                                   | 121.70             | 35.36           | 1                  |
| CA-C-CA-C-O                              | 120.80             | 39.41           | 1                  |
| CA-C-CA-C-O                              | 120.80             | 39.47           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| CA-C-N       | 116.20             | 20.59           | 1                  |
| CA-C-N       | 116.20             | 20.61           | 1                  |
| CA-C-N       | 116.20             | 20.96           | 1                  |
| CA-C-N       | 116.20             | 20.99           | 1                  |
| C-N-CA       | 121.70             | 36.24           | 1                  |
| C-N-CA       | 121.70             | 36.25           | 1                  |
| N-CA-CB      | 110.50             | 29.82           | 1                  |
| C-N-CA       | 121.70             | 36.31           | 1                  |
| N-CA-CB      | 110.50             | 29.91           | 1                  |
| C-N-CA       | 121.70             | 36.38           | 2                  |
| C-N-CA       | 121.70             | 36.42           | 1                  |
| C-N-CA       | 121.70             | 36.44           | 1                  |
| N-CA-CB      | 110.50             | 30.12           | 1                  |
| N-CA-CB      | 110.50             | 30.16           | 1                  |
| CA-C-C-N-CA  | 121.70             | 36.76           | 1                  |
| C-N-CA       | 121.70             | 36.78           | 1                  |
| C-N-CA       | 121.70             | 36.80           | 1                  |
| CA-C-C-N-CA  | 121.70             | 36.86           | 1                  |
| CA-N-CA-C-N  | 116.20             | 22.22           | 1                  |
| CA-N-CA-C-N  | 116.20             | 22.23           | 1                  |
| C-CA-CA-N-CD | 112.00             | 46.84           | 1                  |
| CA-N-CD      | 112.00             | 46.84           | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-N-C-N-N-CA-C-N-C-N-N-CA-C-N-CA | 121.70             | 39.24           | 1                  |
| C-N-C-N-CA                       | 121.70             | 39.27           | 1                  |
| C-N-C-CA-CB                      | 110.10             | 23.18           | 1                  |
| C-CA-CB                          | 110.10             | 23.18           | 1                  |
| CA-C-O                           | 120.80             | 43.07           | 2                  |
| C-N-CA                           | 121.70             | 39.39           | 1                  |
| C-N-CA                           | 121.70             | 39.41           | 1                  |
| CA-C-N                           | 116.20             | 24.82           | 1                  |
| CA-C-N                           | 116.20             | 24.83           | 1                  |
| CA-C-CA-C-CA-N-CD                | 112.00             | 48.86           | 1                  |
| CA-N-CD                          | 112.00             | 48.86           | 1                  |
| C-N-C-N-C-N-C-N-C-CA-C-N-CA      | 121.70             | 41.82           | 1                  |
| N-CA-CB                          | 110.40             | 43.84           | 1                  |
| N-CA-CB                          | 110.40             | 43.85           | 1                  |
| C-N-CA                           | 121.70             | 41.86           | 1                  |
| N-CA-N-CA-CA-C-O                 | 120.80             | 46.74           | 1                  |
| CA-C-O                           | 120.80             | 46.76           | 1                  |
| CA-C-CA-C-C-N-CA                 | 121.70             | 43.80           | 1                  |
| C-N-CA                           | 121.70             | 43.82           | 1                  |
| C-N-CA                           | 121.70             | 43.99           | 1                  |
| C-N-CA                           | 121.70             | 44.02           | 1                  |
| C-N-CA                           | 121.70             | 44.44           | 1                  |

| Angle type                               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-N-CA                                   | 121.70             | 44.47           | 1                  |
| C-N-CA                                   | 121.70             | 44.53           | 1                  |
| CA-C-CA-C-CA-N-O-C-CA-N-CA-C-CA-C-CA-C-N | 116.20             | 31.69           | 1                  |
| CA-C-N                                   | 116.20             | 31.69           | 1                  |
| N-CD-CG                                  | 103.20             | 166.05          | 1                  |
| C-N-CA                                   | 121.70             | 46.62           | 1                  |
| C-N-CA                                   | 121.70             | 46.63           | 1                  |
| N-CA-C-N-C-N-CA-C-N                      | 116.20             | 32.89           | 1                  |
| N-CD-CG                                  | 103.20             | 40.76           | 1                  |
| N-CD-CG                                  | 103.20             | 40.77           | 1                  |
| CA-C-N                                   | 116.20             | 32.98           | 1                  |
| CA-C-O                                   | 120.80             | 50.27           | 1                  |
| C-CA-CB                                  | 110.50             | 172.36          | 1                  |
| CA-C-CA-C-CA-C-CA-C-N                    | 116.20             | 34.05           | 1                  |
| CA-C-N                                   | 116.20             | 34.16           | 1                  |
| N-CA-N-CA-N-CA-N-CA-CA-C-N               | 116.20             | 34.65           | 1                  |
| CA-C-N                                   | 116.20             | 34.67           | 1                  |
| C-CA-CB                                  | 110.10             | 32.75           | 1                  |
| C-CA-CB                                  | 110.10             | 32.81           | 1                  |
| C-N-C-N-CA-C-O                           | 120.80             | 51.75           | 1                  |
| CA-C-O                                   | 120.80             | 51.75           | 1                  |
| C-N-C-N-N-CA-C                           | 112.10             | 10.82           | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 112.10             | 10.83           | 1                  |
| C-N-CA                | 121.70             | 48.92           | 1                  |
| CA-C-N                | 116.20             | 35.89           | 2                  |
| N-CA-N-CA-CB          | 110.50             | 42.34           | 1                  |
| N-CA-CB               | 110.50             | 42.35           | 1                  |
| CA-C-N                | 116.20             | 36.04           | 1                  |
| N-CA-CA-C-N           | 116.20             | 36.48           | 1                  |
| CA-C-O                | 120.80             | 53.04           | 1                  |
| CA-C-N                | 116.20             | 36.52           | 1                  |
| CA-C-O                | 120.80             | 53.08           | 1                  |
| CA-C-O                | 120.80             | 37.42           | 1                  |
| CA-C-O                | 120.80             | 37.46           | 1                  |
| C-N-CA                | 121.70             | 50.57           | 1                  |
| C-N-C-N-CA-C-C-N-CA   | 121.70             | 50.65           | 1                  |
| CA-C-C-N-CA           | 121.70             | 50.67           | 1                  |
| C-N-CA                | 121.70             | 50.67           | 1                  |
| CA-C-N                | 116.20             | 37.58           | 1                  |
| CA-C-CA-C-C-N-CA      | 121.70             | 51.09           | 1                  |
| C-N-CA                | 121.70             | 51.10           | 1                  |
| C-N-CA                | 121.70             | 51.23           | 1                  |
| C-N-CA                | 121.70             | 51.30           | 1                  |
| C-CA-CA-C-C-CA-N-CA-C | 111.00             | 1.74            | 1                  |

| Angle type  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| N-CA-C  | 111.00             | 1.76            | 1                  |
| CA-C-C-N-C-N-N-CA-N-CA-CA-C-CA-C-CA-C-CA-C-N-CA-C | 112.10             | 15.70           | 1                  |
| N-CA-C  | 112.10             | 15.71           | 1                  |
| CA-C-CA-C-CA-C-N                                  | 116.20             | 39.30           | 1                  |
| CA-C-N  | 116.20             | 39.31           | 1                  |
| CA-C-O  | 120.80             | 55.61           | 1                  |
| CA-C-O  | 120.80             | 55.66           | 1                  |
| CA-C-O  | 120.80             | 55.73           | 1                  |
| CA-C-O  | 120.80             | 55.74           | 1                  |
| N-CA-N-CA-CA-C-CA-C-O                             | 120.80             | 55.99           | 1                  |
| CA-C-O  | 120.80             | 56.01           | 1                  |
| CA-C-C-N-C-N-CA-C-O                               | 120.80             | 56.27           | 1                  |
| CA-C-O  | 120.80             | 56.27           | 1                  |
| CB-CG-OD1   | 120.80             | 44.97           | 1                  |
| CB-CG-OD1   | 120.80             | 45.05           | 1                  |
| N-CA-CB   | 110.50             | 46.41           | 1                  |
| CA-C-N  | 116.20             | 40.80           | 1                  |
| CA-N-CD   | 112.00             | 59.22           | 1                  |
| CA-C-N  | 116.20             | 40.84           | 1                  |
| N-CA-CB   | 110.50             | 46.49           | 1                  |
| N-CA-N-CA-N-CA-C                                  | 112.10             | 18.60           | 1                  |
| N-CA-C  | 112.10             | 18.63           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| N-CA-CB  | 103.00             | 144.07          | 1                  |
| N-CA-N-CA-N-CA-CB  | 103.00             | 143.98          | 1                  |
| C-N-CA-C-C-N-N-CA-C                                      | 111.00             | 6.85            | 1                  |
| N-CA-C   | 111.00             | 6.89            | 3                  |
| CA-C-CA-C-O  | 120.80             | 57.65           | 1                  |
| CA-C-O   | 120.80             | 57.65           | 1                  |
| CA-C-O   | 120.80             | 57.66           | 1                  |
| CA-C-O   | 120.80             | 57.67           | 1                  |
| C-N-CA   | 121.70             | 54.89           | 1                  |
| CA-C-O   | 120.80             | 42.95           | 1                  |
| C-N-CA   | 121.70             | 54.98           | 1                  |
| CA-C-O   | 120.80             | 42.97           | 1                  |
| CA-C-N-CA-N-CA-N-CA-C                                    | 111.00             | 7.74            | 1                  |
| N-CA-C   | 111.00             | 7.76            | 1                  |
| N-CA-C   | 111.00             | 7.80            | 1                  |
| N-CA-C   | 111.00             | 7.82            | 1                  |
| N-CA-N-CA-N-CA-C   | 111.00             | 8.09            | 1                  |
| CA-C-N-CA-C  | 111.00             | 8.11            | 1                  |
| CA-C-CA-C-CA-C-N-CA-CA-C-N-CA-CA-C-CA-C-N-CA-N-CA-N-CA-C | 111.00             | 8.48            | 1                  |
| N-CA-C   | 111.00             | 8.49            | 1                  |
| C-CA-C-N-CA  | 121.70             | 56.24           | 1                  |
| C-N-CA   | 121.70             | 56.31           | 1                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-C                               | 111.00             | 9.34            | 1                  |
| N-CA-C                               | 111.00             | 9.35            | 1                  |
| C-N-CA                               | 121.70             | 56.56           | 1                  |
| N-CA-C-N-CA                          | 121.70             | 56.64           | 1                  |
| N-CA-C                               | 111.00             | 9.94            | 1                  |
| N-CA-CB                              | 110.40             | 164.49          | 1                  |
| N-CA-CB                              | 110.40             | 164.48          | 1                  |
| CA-C-O                               | 120.80             | 59.53           | 1                  |
| CA-C-O                               | 120.80             | 59.60           | 1                  |
| N-CA-C                               | 111.00             | 10.41           | 1                  |
| N-CA-C                               | 111.00             | 10.53           | 1                  |
| N-CA-C                               | 111.00             | 10.54           | 1                  |
| N-CA-C                               | 111.00             | 10.58           | 2                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-C-N-CA | 121.70             | 57.32           | 1                  |
| N-CA-C                               | 111.00             | 10.87           | 1                  |
| N-CA-C                               | 111.00             | 10.89           | 1                  |
| CA-C-O                               | 120.80             | 60.04           | 1                  |
| CA-C-N                               | 116.20             | 44.75           | 1                  |
| CA-C-N                               | 116.20             | 44.76           | 1                  |
| CA-C-O                               | 120.80             | 60.09           | 1                  |
| N-CA-C                               | 111.00             | 11.02           | 2                  |
| C-N-CA                               | 121.70             | 57.43           | 1                  |

| Angle type  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| C-CA-CB   | 110.10             | 42.29           | 1                  |
| C-CA-CB   | 110.10             | 42.33           | 1                  |
| N-CA-N-CA-N-CA-CA-C-N                               | 116.20             | 44.87           | 1                  |
| CA-C-N  | 116.20             | 44.88           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-CA-C-O | 120.80             | 60.91           | 1                  |
| N-CA-CB   | 110.40             | 163.24          | 1                  |
| CA-C-N-CA-CB  | 110.40             | 163.22          | 1                  |
| N-CD-CA-C-O   | 120.80             | 61.00           | 1                  |
| N-CD-N-CA-CB  | 110.50             | 50.73           | 1                  |
| N-CA-CB   | 110.40             | 163.11          | 1                  |
| CA-C-CA-C-CA-C-N-CA-CA-C-N-CA-CA-C-N-CA-C           | 111.00             | 12.80           | 1                  |
| N-CA-C  | 111.00             | 12.81           | 2                  |
| N-CA-C  | 111.00             | 12.82           | 1                  |
| N-CA-CB   | 110.40             | 162.96          | 1                  |
| N-CA-CB   | 110.50             | 50.93           | 1                  |
| C-CA-N-CA-C   | 111.00             | 12.92           | 1                  |
| N-CA-C  | 111.00             | 12.94           | 1                  |
| C-CA-N-CA-C-N-N-CA-CB                               | 110.40             | 162.86          | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-C                          | 111.00             | 13.13           | 1                  |
| N-CA-C  | 111.00             | 13.13           | 2                  |
| N-CA-CB   | 110.40             | 162.83          | 1                  |
| N-CA-C  | 111.00             | 13.15           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-N                     | 116.20             | 46.36           | 1                  |
| CA-C-CA-C-N                | 116.20             | 46.40           | 1                  |
| CA-C-C-CA-N-CA-C           | 111.00             | 13.35           | 1                  |
| N-CA-C                     | 111.00             | 13.36           | 1                  |
| CA-C-N                     | 116.20             | 46.49           | 1                  |
| CA-C-N                     | 116.20             | 46.57           | 1                  |
| N-CA-C                     | 111.00             | 13.53           | 2                  |
| C-CA-CB                    | 110.10             | 43.97           | 2                  |
| CA-C-N                     | 116.20             | 46.69           | 1                  |
| N-CA-C                     | 111.00             | 13.76           | 1                  |
| N-CA-C                     | 111.00             | 13.77           | 2                  |
| N-CA-C                     | 111.00             | 13.78           | 1                  |
| CA-C-N                     | 116.20             | 46.86           | 1                  |
| CA-C-O                     | 120.80             | 61.87           | 1                  |
| CA-C-O                     | 120.80             | 61.89           | 1                  |
| N-CA-N-CA-C-N-CA           | 121.70             | 59.41           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-C | 111.00             | 14.37           | 1                  |
| C-CA-CB                    | 111.40             | 45.84           | 1                  |
| C-CA-CB                    | 111.40             | 45.88           | 1                  |
| N-CA-C                     | 111.00             | 14.48           | 1                  |
| N-CA-C                     | 111.00             | 14.49           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-C | 111.00             | 14.67           | 1                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CA-N-CD                    | 112.00             | 63.90           | 1                  |
| CA-N-CD                              | 112.00             | 63.94           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-C | 111.00             | 15.23           | 1                  |
| C-N-CA                               | 121.70             | 60.14           | 1                  |
| N-CA-C                               | 111.00             | 15.25           | 1                  |
| CA-C-CA-C-CA-C-N-CA-C                | 111.00             | 15.35           | 1                  |
| CA-C-N-CA-C                          | 111.00             | 15.36           | 1                  |
| N-CA-C                               | 111.00             | 15.37           | 2                  |
| C-CA-C-N-N-CA-C-N-C-CA-N-CA-CB       | 110.40             | 161.31          | 1                  |
| N-CA-C                               | 111.00             | 15.99           | 1                  |
| N-CA-C                               | 111.00             | 16.00           | 1                  |
| N-CA-N-CA-CB                         | 110.40             | 161.29          | 1                  |
| N-CA-N-CA-CB                         | 110.50             | 168.14          | 1                  |
| N-CA-C                               | 111.00             | 16.20           | 1                  |
| N-CA-C                               | 111.00             | 16.22           | 1                  |
| N-CA-N-CA-N-CA-CB                    | 110.50             | 167.93          | 1                  |
| CA-C-N                               | 116.20             | 48.68           | 1                  |
| N-CA-N-CD-CG                         | 103.20             | 153.82          | 1                  |
| N-CA-N-CA-C                          | 111.00             | 16.58           | 1                  |
| CA-C-N                               | 116.20             | 48.76           | 1                  |
| N-CA-CB                              | 110.50             | 167.81          | 1                  |
| N-CA-N-CA-N-CA-C                     | 111.00             | 16.88           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| N-CA-N-CA-C  | 111.00             | 16.89           | 1                  |
| C-N-C-N-CA-C-O                                     | 120.80             | 63.76           | 1                  |
| CA-C-O-C-N   | 123.00             | 69.34           | 1                  |
| CA-C-CA-C-O  | 120.80             | 63.79           | 1                  |
| C-CA-O-C-N   | 123.00             | 69.37           | 1                  |
| C-CA-N-CA-N-CA-N-CA-C                              | 111.00             | 17.29           | 1                  |
| N-CA-C   | 111.00             | 17.30           | 1                  |
| C-N-C-N-C-N-C-N-CA-C-N-CA-CB                       | 110.50             | 53.95           | 1                  |
| N-CA-C   | 111.00             | 17.89           | 1                  |
| N-CA-CB  | 110.50             | 53.97           | 1                  |
| N-CA-C   | 111.00             | 17.91           | 1                  |
| CA-C-N-CA-C  | 111.00             | 17.94           | 1                  |
| N-CA-C   | 111.00             | 17.94           | 1                  |
| N-CA-C   | 111.00             | 17.99           | 1                  |
| N-CA-C   | 111.00             | 18.03           | 1                  |
| N-CA-C   | 111.00             | 18.05           | 1                  |
| N-CA-C   | 111.00             | 18.06           | 1                  |
| N-CA-CA-C-N-CA-N-CA-N-CA-N-CA-CA-C-N-CA-N-CA-O-C-N | 123.00             | 70.13           | 1                  |
| N-CA-C   | 111.00             | 18.49           | 1                  |
| N-CA-C   | 111.00             | 18.50           | 1                  |
| N-CA-N-CA-N-CA-N-CA-CB                             | 103.00             | 139.32          | 1                  |
| N-CA-O-C-N   | 123.00             | 70.19           | 1                  |



| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-CB                     | 103.00             | 139.28          | 1                  |
| N-CA-N-CA-CA-C-O                      | 120.80             | 176.71          | 1                  |
| N-CA-C                                | 113.30             | 18.00           | 1                  |
| N-CA-C                                | 113.30             | 18.02           | 1                  |
| CA-C-O                                | 120.80             | 176.55          | 1                  |
| N-CA-CA-C-O                           | 120.80             | 65.06           | 1                  |
| N-CA-CA-C-O                           | 120.80             | 65.08           | 1                  |
| N-CA-N-CA-CA-C-O                      | 120.80             | 65.23           | 1                  |
| N-CA-C                                | 111.00             | 19.48           | 3                  |
| N-CA-C                                | 111.00             | 19.50           | 1                  |
| CA-C-O                                | 120.80             | 65.25           | 1                  |
| C-N-CA                                | 121.70             | 62.91           | 1                  |
| C-N-CA                                | 121.70             | 62.92           | 1                  |
| N-CA-N-CA-C                           | 112.10             | 30.53           | 1                  |
| N-CA-C                                | 111.00             | 19.67           | 1                  |
| C-N-CA                                | 121.70             | 63.02           | 1                  |
| N-CA-N-CA-N-CA-C-N-CA                 | 121.70             | 63.06           | 1                  |
| N-CA-C                                | 111.00             | 19.79           | 1                  |
| N-CA-C                                | 111.00             | 19.81           | 1                  |
| N-CA-N-CA-N-CD-N-CD-N-CA-C            | 111.00             | 20.74           | 1                  |
| N-CA-C                                | 111.00             | 20.74           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 170.87          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-CA-C-N-CA-CB | 110.50             | 164.75          | 1                  |
| N-CA-C                      | 111.00             | 21.65           | 1                  |
| N-CA-C                      | 111.00             | 21.66           | 1                  |
| CA-C-N-CA-C                 | 111.00             | 21.66           | 1                  |
| N-CA-C                      | 111.00             | 21.67           | 1                  |
| N-CA-N-CA-N-CA-CB           | 110.50             | 164.71          | 1                  |
| N-CA-C                      | 111.00             | 21.73           | 2                  |
| CA-C-N                      | 116.90             | 69.10           | 1                  |
| CA-C-N                      | 116.90             | 69.14           | 1                  |
| N-CA-C                      | 112.10             | 32.54           | 1                  |
| CA-C-CA-C-C-N-C-N-N-CA-CB   | 110.50             | 164.53          | 1                  |
| C-CA-N-CA-CB                | 110.50             | 164.48          | 1                  |
| N-CA-C                      | 111.00             | 22.14           | 1                  |
| C-CA-N-CA-C                 | 111.00             | 22.15           | 1                  |
| C-CA-CA-C-CA-C-N-CA-CB      | 111.50             | 57.64           | 1                  |
| C-CA-N-CA-C                 | 111.00             | 22.34           | 1                  |
| N-CA-CB                     | 110.50             | 164.33          | 1                  |
| N-CA-CB                     | 111.50             | 57.68           | 1                  |
| CA-C-N-CA-N-CA-N-CA-CB      | 110.50             | 56.78           | 1                  |
| N-CA-CB                     | 110.50             | 56.79           | 1                  |
| N-CA-C                      | 111.00             | 22.57           | 1                  |
| N-CA-C                      | 111.00             | 22.60           | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-C | 111.00             | 22.82           | 1                  |
| N-CA-C           | 111.00             | 22.82           | 2                  |
| N-CA-C           | 111.00             | 22.83           | 1                  |
| N-CA-CB          | 111.50             | 165.03          | 1                  |
| CA-C-N           | 116.20             | 53.25           | 1                  |
| N-CA-CB          | 111.50             | 164.97          | 1                  |
| N-CA-CA-C-N      | 116.20             | 53.30           | 1                  |
| CA-C-N           | 116.20             | 53.32           | 1                  |
| N-CA-CA-C-N      | 116.20             | 53.33           | 1                  |
| N-CA-C           | 111.00             | 23.00           | 2                  |
| C-N-CA-C-O       | 120.80             | 67.41           | 1                  |
| C-N-CA-C-O       | 120.80             | 67.45           | 1                  |
| N-CA-C           | 111.00             | 23.16           | 1                  |
| CA-C-CA-C-O      | 120.80             | 67.55           | 1                  |
| N-CA-N-CA-CA-C-O | 120.80             | 67.57           | 1                  |
| N-CA-CB          | 110.50             | 57.29           | 1                  |
| CA-C-N-CA-CB     | 110.50             | 163.62          | 1                  |
| N-CA-C           | 111.00             | 23.60           | 1                  |
| N-CA-C           | 111.00             | 23.62           | 1                  |
| N-CA-N-CA-N-CA-C | 111.00             | 23.80           | 1                  |
| N-CA-C           | 111.00             | 23.81           | 1                  |
| N-CA-C           | 111.00             | 23.83           | 2                  |

| Angle type                                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| N-CA-N-CA-CA-C-N-CA-CA-C-N-CA-N-CA-N-CA-N-CA-CB | 111.50             | 164.20          | 1                  |
| N-CA-CB   | 111.50             | 164.18          | 1                  |
| N-CA-C  | 111.00             | 24.26           | 1                  |
| N-CA-C  | 111.00             | 24.30           | 1                  |
| C-N-CA  | 121.70             | 66.05           | 1                  |
| CA-C-C-N-CA                                     | 121.70             | 66.07           | 1                  |
| C-CA-CB   | 110.10             | 168.82          | 1                  |
| N-CD-CG   | 103.20             | 149.51          | 1                  |
| N-CA-C  | 111.00             | 24.65           | 1                  |
| CA-N-CD   | 112.00             | 68.82           | 1                  |
| N-CD-CG   | 103.20             | 149.45          | 1                  |
| N-CA-C  | 111.00             | 24.70           | 1                  |
| C-CA-CB   | 110.10             | 51.55           | 1                  |
| N-CA-C  | 111.00             | 24.71           | 1                  |
| CA-N-CD   | 112.00             | 68.89           | 1                  |
| N-CA-C-CA-CB                                    | 110.10             | 51.63           | 1                  |
| N-CA-N-CA-C-CA-CB                               | 110.10             | 168.39          | 1                  |
| CA-C-C-CA-CB                                    | 110.10             | 168.36          | 1                  |
| CA-C-C-N-CA                                     | 121.70             | 66.62           | 1                  |
| C-N-CA  | 121.70             | 66.67           | 1                  |
| C-CA-CB   | 110.10             | 168.18          | 1                  |
| N-CA-C  | 111.00             | 25.44           | 2                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                     | 110.10             | 168.15          | 1                  |
| N-CA-C-CA-CB                | 110.10             | 168.10          | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 168.06          | 1                  |
| N-CA-N-CD-C-CA-N-CD-N-CD-CG | 103.20             | 57.56           | 1                  |
| CA-C-N-CA-C                 | 111.00             | 25.85           | 1                  |
| N-CD-CG                     | 103.20             | 57.60           | 1                  |
| C-CA-CA-C-C-N-CA            | 121.70             | 67.04           | 1                  |
| CA-C-N-CA-C                 | 111.00             | 26.08           | 1                  |
| N-CA-C                      | 111.00             | 26.10           | 1                  |
| N-CA-C                      | 111.00             | 26.11           | 1                  |
| N-CA-C                      | 111.00             | 26.12           | 1                  |
| CA-C-C-CA-C-CA-N-CA-C       | 112.10             | 36.65           | 1                  |
| CA-C-O                      | 120.80             | 69.49           | 1                  |
| CA-C-O                      | 120.80             | 69.52           | 1                  |
| N-CA-C                      | 112.10             | 36.72           | 1                  |
| CA-C-CA-C-O                 | 120.80             | 69.60           | 1                  |
| C-CA-CB                     | 110.10             | 167.21          | 1                  |
| N-CA-CB                     | 111.50             | 162.57          | 1                  |
| N-CA-C                      | 111.00             | 26.91           | 1                  |
| N-CA-C                      | 111.00             | 26.93           | 1                  |
| N-CA-CB                     | 111.50             | 162.54          | 1                  |
| CA-C-N-CA-C-CA-CB           | 110.10             | 167.10          | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-CB    | 110.50             | 59.66           | 1                  |
| N-CA-CB                             | 110.50             | 59.68           | 1                  |
| C-CA-CB                             | 110.10             | 53.40           | 1                  |
| N-CA-C                              | 111.00             | 27.53           | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-N-C-N-N-CA-CB | 110.50             | 60.02           | 1                  |
| CA-C-O                              | 120.80             | 171.26          | 1                  |
| N-CA-CB                             | 110.50             | 160.96          | 2                  |
| N-CA-C                              | 111.00             | 27.90           | 1                  |
| CA-C-O                              | 120.80             | 171.21          | 1                  |
| CA-C-CA-C-O                         | 120.80             | 171.20          | 1                  |
| N-CA-C                              | 111.00             | 27.99           | 1                  |
| N-CA-C                              | 111.00             | 28.01           | 1                  |
| C-N-C-N-N-CA-C                      | 111.00             | 28.10           | 1                  |
| CA-C-O                              | 120.80             | 171.12          | 1                  |
| N-CA-C                              | 111.00             | 28.12           | 1                  |
| C-CA-C-CA-C-CA-N-CA-C               | 111.00             | 28.37           | 1                  |
| N-CA-C                              | 111.00             | 28.39           | 1                  |
| N-CA-C                              | 111.00             | 28.40           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-C          | 111.00             | 28.50           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-C          | 111.00             | 28.57           | 1                  |
| N-CA-C                              | 111.00             | 28.59           | 1                  |
| N-CA-N-CA-C-CA-C-CA-CB              | 110.10             | 54.25           | 1                  |

| Angle type                                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| N-CA-N-CA-C-CA-N-CA-C                         | 111.00             | 28.77           | 1                  |
| N-CA-C  | 111.00             | 28.77           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-C-N-N-CA-CA-C-N | 116.20             | 57.72           | 1                  |
| N-CA-C-N-N-CA-CB                              | 110.50             | 160.16          | 1                  |
| CA-C-N  | 116.20             | 57.79           | 1                  |
| CA-C-CA-C-C-N-C-CA-CB                         | 110.10             | 54.74           | 1                  |
| N-CA-C  | 111.00             | 29.44           | 1                  |
| N-CA-C  | 111.00             | 29.46           | 1                  |
| C-CA-CB                                       | 110.10             | 54.77           | 1                  |
| C-N-C-CA-CB                                   | 109.10             | 45.05           | 1                  |
| C-CA-CB                                       | 109.10             | 45.10           | 1                  |
| N-CA-C  | 111.00             | 29.62           | 1                  |
| CA-C-N-CA-C                                   | 111.00             | 29.63           | 1                  |
| CA-C-CA-C-N-CA-C                              | 111.00             | 29.68           | 1                  |
| N-CA-C  | 111.00             | 29.70           | 1                  |
| C-CA-CB                                       | 109.10             | 45.26           | 1                  |
| N-CA-CB                                       | 111.50             | 160.79          | 1                  |
| C-CA-CB                                       | 109.10             | 45.32           | 1                  |
| CA-C-N-CA-CB                                  | 111.50             | 160.76          | 1                  |
| N-CA-CB                                       | 110.50             | 159.76          | 1                  |
| C-CA-CB                                       | 110.10             | 165.12          | 1                  |
| C-CA-CB                                       | 110.10             | 165.07          | 1                  |

| Angle type                                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-CA-CB  | 110.10             | 165.02          | 1                  |
| C-CA-CB  | 110.10             | 165.01          | 1                  |
| C-CA-CB  | 110.10             | 164.99          | 1                  |
| N-CD-CG  | 103.20             | 146.52          | 1                  |
| C-N-C-N-N-CA-N-CA-N-CA-N-CA-CA-C-O             | 120.80             | 71.96           | 1                  |
| CA-C-O   | 120.80             | 71.98           | 1                  |
| N-CA-CB  | 110.50             | 159.21          | 1                  |
| C-CA-N-CA-C                                    | 111.00             | 30.98           | 1                  |
| C-CA-N-CA-N-CA-C                               | 111.00             | 31.00           | 1                  |
| C-CA-N-CA-C                                    | 111.00             | 31.19           | 1                  |
| N-CA-C   | 111.00             | 31.20           | 1                  |
| N-CD-C-CA-N-CD-N-CA-N-CA-N-CA-N-CA-N-CD-N-CA-C | 111.00             | 31.41           | 1                  |
| N-CD-N-CA-C                                    | 111.00             | 31.42           | 1                  |
| C-N-C-N-CA-C-N-CA-N-CA-N-CA-C                  | 111.00             | 31.54           | 1                  |
| N-CA-C   | 111.00             | 31.56           | 1                  |
| CA-C-N-CA-CB                                   | 110.50             | 158.71          | 1                  |
| N-CA-C   | 113.30             | 31.09           | 1                  |
| N-CA-C   | 113.30             | 31.11           | 1                  |
| N-CA-N-CA-C                                    | 111.00             | 31.69           | 1                  |
| N-CA-N-CA-C                                    | 111.00             | 31.70           | 1                  |
| CA-C-N-CA-CB                                   | 110.50             | 62.39           | 1                  |
| CA-C-C-CA-CA-C-N                               | 116.20             | 59.63           | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-CB               | 110.50             | 62.43           | 1                  |
| CA-C-N-CA-C           | 111.00             | 31.87           | 1                  |
| CA-C-N                | 116.20             | 59.68           | 1                  |
| N-CA-C                | 111.00             | 31.88           | 2                  |
| N-CA-N-CA-C           | 111.00             | 31.90           | 1                  |
| CA-C-N                | 116.20             | 59.71           | 1                  |
| N-CA-CB               | 110.50             | 158.49          | 1                  |
| C-N-CA                | 121.70             | 70.90           | 1                  |
| CA-C-N                | 116.20             | 59.76           | 1                  |
| N-CA-N-CA-N-CA-C-N-CA | 121.70             | 70.97           | 1                  |
| N-CA-N-CA-N-CD-N-CA-C | 111.00             | 32.24           | 1                  |
| N-CA-C                | 111.00             | 32.24           | 1                  |
| CA-C-N                | 116.20             | 59.98           | 1                  |
| C-CA-CB               | 110.10             | 56.71           | 1                  |
| CA-C-N                | 116.20             | 60.01           | 1                  |
| CA-C-N-CD-C-CA-CB     | 110.10             | 56.76           | 1                  |
| N-CA-N-CA-C-CA-CB     | 110.50             | 68.41           | 1                  |
| C-CA-CB               | 110.50             | 68.42           | 1                  |
| C-CA-CB               | 110.10             | 163.28          | 1                  |
| N-CA-C                | 111.00             | 32.70           | 1                  |
| N-CA-C                | 111.00             | 32.71           | 1                  |
| CA-C-N-CA-CB          | 110.50             | 157.92          | 1                  |

| Angle type  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| O-C-N   | 123.00             | 78.38           | 1                  |
| CA-C-O-C-N  | 123.00             | 78.40           | 1                  |
| CA-C-N  | 116.20             | 60.49           | 1                  |
| CA-C-N  | 116.20             | 60.50           | 1                  |
| CA-C-N  | 116.20             | 60.51           | 1                  |
| CA-C-N  | 116.20             | 60.53           | 1                  |
| CA-C-CA-C-N   | 116.20             | 60.55           | 1                  |
| C-CA-C-CA-N-CA-C  | 111.00             | 33.11           | 1                  |
| N-CA-C  | 111.00             | 33.11           | 1                  |
| C-CA-CA-C-N   | 116.20             | 60.58           | 1                  |
| C-CA-N-CA-CB  | 111.50             | 158.76          | 1                  |
| CA-C-N-CA-C-N-N-CA-N-CA-C-N-CA-C-N-CA-CA-C-CA-C-N-CA-N-CA-N-CA-CA-C-O | 120.80             | 73.83           | 1                  |
| CA-C-O  | 120.80             | 73.84           | 1                  |
| CA-C-O  | 120.80             | 167.70          | 1                  |
| N-CA-C  | 111.00             | 33.78           | 1                  |
| CA-C-N-CA-C   | 111.00             | 33.80           | 1                  |
| CA-C-O  | 120.80             | 167.67          | 1                  |
| N-CA-C  | 111.00             | 33.97           | 1                  |
| N-CA-C  | 111.00             | 33.99           | 1                  |
| CA-C-N-CA-N-CA-CA-C-CA-C-C-CA-C-CA-N-CA-C                             | 111.00             | 34.09           | 1                  |
| N-CA-C  | 111.00             | 34.10           | 1                  |
| C-N-CA  | 121.70             | 72.28           | 1                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-C                               | 111.00             | 34.14           | 2                  |
| N-CA-C                               | 111.00             | 34.15           | 2                  |
| C-N-CA                               | 121.70             | 72.30           | 1                  |
| N-CA-N-CA-C                          | 111.00             | 34.23           | 1                  |
| N-CA-C                               | 111.00             | 34.26           | 1                  |
| N-CA-N-CA-N-CA-CA-C-CA-C-C-CA-CB     | 110.50             | 69.55           | 1                  |
| C-CA-CB                              | 110.50             | 69.56           | 1                  |
| N-CA-N-CA-C-CA-C-CA-N-CA-N-CA-N-CA-C | 111.00             | 34.91           | 1                  |
| N-CA-C                               | 111.00             | 34.97           | 1                  |
| N-CA-CB                              | 110.50             | 64.34           | 1                  |
| N-CA-C                               | 111.00             | 35.02           | 1                  |
| N-CA-N-CA-C                          | 111.00             | 35.05           | 1                  |
| N-CA-N-CD-CG                         | 103.20             | 62.52           | 1                  |
| CA-N-CD                              | 112.00             | 74.04           | 1                  |
| C-CA-CB                              | 110.10             | 161.57          | 1                  |
| CA-C-N                               | 116.20             | 62.03           | 1                  |
| CA-C-C-CA-CB                         | 110.10             | 161.54          | 1                  |
| N-CD-CG                              | 103.20             | 62.59           | 1                  |
| N-CA-CA-C-N-CA-C-CA-CB               | 110.10             | 58.75           | 1                  |
| C-CA-C-CA-CA-N-CD                    | 112.00             | 74.20           | 1                  |
| CA-C-C-CA-CB                         | 110.10             | 58.84           | 1                  |
| CA-C-O                               | 120.80             | 74.98           | 1                  |

| Angle type                                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-CA-C-CA-C-CA-C-N-CA-N-CA-C                  | 111.00             | 35.82           | 1                  |
| N-CA-N-CA-C                                      | 111.00             | 35.85           | 1                  |
| N-CA-C-CA-C-CA-C-CA-N-CA-N-CA-CB-CG1-N-CA-C-N-CA | 121.70             | 169.66          | 1                  |
| C-N-CA   | 121.70             | 73.75           | 1                  |
| C-CA-N-CA-C-N-CA                                 | 121.70             | 73.83           | 1                  |
| CB-CG1-N-CA-N-CA-CA-C-N                          | 116.90             | 77.02           | 1                  |
| N-CA-CA-C-N                                      | 116.90             | 77.02           | 1                  |
| N-CA-N-CA-C                                      | 111.00             | 36.61           | 1                  |
| N-CA-C   | 111.00             | 36.61           | 1                  |
| N-CA-C   | 111.00             | 36.66           | 1                  |
| C-CA-C-N-CA                                      | 121.70             | 169.42          | 1                  |
| C-CA-CA-C-CA-C-N-CA-C                            | 111.00             | 36.91           | 1                  |
| C-CA-CB  | 110.10             | 59.93           | 1                  |
| C-N-C-CA-CB                                      | 110.10             | 59.99           | 1                  |
| N-CA-C   | 113.30             | 36.83           | 2                  |
| C-N-N-CA-C                                       | 113.30             | 36.83           | 1                  |
| N-CA-C   | 113.30             | 36.84           | 1                  |
| N-CA-CB  | 110.50             | 65.70           | 1                  |
| N-CA-N-CA-N-CA-CB                                | 110.50             | 65.75           | 1                  |
| N-CA-C-N-C-CA-CB                                 | 110.10             | 60.12           | 1                  |
| N-CA-C-CA-CB                                     | 110.10             | 60.15           | 1                  |
| C-N-CA-C-O                                       | 120.80             | 165.41          | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| CA-C-O                    | 120.80             | 165.36          | 1                  |
| CA-C-N                    | 116.20             | 63.80           | 2                  |
| N-CA-CB                   | 110.40             | 71.12           | 2                  |
| CA-C-N                    | 116.20             | 63.84           | 1                  |
| CA-C-N                    | 116.20             | 63.87           | 1                  |
| C-N-CA                    | 121.70             | 74.61           | 1                  |
| C-CA-C-N-C-N-CA           | 121.70             | 74.62           | 1                  |
| C-CA-CA-N-CD              | 112.00             | 75.41           | 1                  |
| C-N-CA-N-CD               | 112.00             | 75.47           | 1                  |
| CA-N-CA-C-O               | 120.80             | 165.08          | 1                  |
| CA-N-CA-C-O               | 120.80             | 76.59           | 1                  |
| CA-C-O                    | 120.80             | 76.60           | 1                  |
| CA-C-O                    | 120.80             | 164.97          | 1                  |
| N-CA-N-CA-N-CA-N-CA-C     | 111.00             | 38.43           | 1                  |
| N-CA-N-CA-N-CA-C          | 111.00             | 38.49           | 1                  |
| N-CA-CA-C-N-CA-C-N-CA-C-O | 120.80             | 76.85           | 1                  |
| N-CA-CA-C-O               | 120.80             | 76.87           | 1                  |
| CA-C-O                    | 120.80             | 76.88           | 1                  |
| C-N-CA-C-C-CA-CA-C-O      | 120.80             | 76.91           | 1                  |
| C-N-CA                    | 121.70             | 75.24           | 1                  |
| C-CA-CB                   | 110.10             | 159.14          | 1                  |
| C-CA-CB                   | 110.10             | 159.13          | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB                          | 110.10             | 159.13          | 1                  |
| C-CA-C-CA-C-CA-C-N-CA                 | 121.70             | 75.32           | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 159.05          | 1                  |
| C-CA-C-N-CA                           | 121.70             | 75.34           | 1                  |
| C-CA-CB                               | 110.10             | 159.02          | 1                  |
| C-N-CA                                | 121.70             | 75.37           | 1                  |
| C-CA-CB                               | 110.10             | 158.96          | 1                  |
| C-CA-CB                               | 110.10             | 158.95          | 2                  |
| C-CA-CB                               | 110.10             | 158.94          | 1                  |
| C-CA-CB                               | 110.10             | 158.92          | 1                  |
| CA-C-N-CD-CG                          | 103.20             | 141.67          | 1                  |
| CA-C-N-CD-CG                          | 103.20             | 141.63          | 1                  |
| N-CA-C                                | 111.00             | 39.26           | 1                  |
| N-CA-N-CA-N-CA-CB                     | 110.50             | 66.98           | 1                  |
| N-CA-CB                               | 110.50             | 66.99           | 1                  |
| CA-C-O                                | 120.80             | 77.29           | 1                  |
| N-CA-C                                | 111.00             | 39.35           | 1                  |
| N-CA-CB                               | 110.50             | 153.98          | 1                  |
| CA-C-O                                | 120.80             | 77.35           | 1                  |
| N-CA-CB                               | 110.50             | 153.89          | 1                  |
| N-CA-N-CA-N-CA-C-CA-N-CA-N-CA-C-CA-CB | 110.10             | 61.75           | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 61.78           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-CA-CB  | 110.10             | 158.36          | 1                  |
| N-CA-C   | 111.00             | 39.89           | 1                  |
| N-CA-C   | 111.00             | 39.93           | 2                  |
| N-CA-C   | 111.00             | 39.94           | 1                  |
| N-CA-C-CA-CB   | 110.10             | 158.27          | 1                  |
| N-CA-C   | 111.00             | 40.05           | 1                  |
| N-CA-N-CA-N-CA-C-CA-C-CA-N-CA-C-CA-C-CA-N-CA-N-CA-C-N-CA | 121.70             | 76.25           | 1                  |
| C-CA-CB  | 110.50             | 72.62           | 1                  |
| N-CA-C-N-CA  | 121.70             | 76.28           | 1                  |
| C-N-CA   | 121.70             | 76.31           | 1                  |
| C-N-CA   | 121.70             | 76.35           | 1                  |
| C-N-CA   | 121.70             | 76.38           | 1                  |
| C-CA-CB  | 110.50             | 72.74           | 1                  |
| C-N-C-N-CA   | 121.70             | 76.41           | 1                  |
| C-N-C-N-CA   | 121.70             | 166.94          | 1                  |
| C-N-N-CA-CB  | 110.50             | 153.22          | 1                  |
| C-CA-N-CA-CB   | 110.50             | 153.20          | 1                  |
| CA-C-C-N-C-CA-C-N-CA                                     | 121.70             | 166.86          | 1                  |
| C-CA-CB  | 110.10             | 157.76          | 1                  |
| C-CA-CB  | 110.10             | 157.75          | 1                  |
| CA-C-N-CA-N-CA-C   | 112.10             | 49.52           | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-C-CA-N-CA-N-CA-N-CA-N-CA-CA-C-O | 120.80             | 78.47           | 1                  |

| Angle type                                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-O                                     | 120.80             | 78.48           | 1                  |
| N-CA-N-CA-C-CA-N-CD-CG                     | 103.20             | 65.99           | 1                  |
| N-CD-CG                                    | 103.20             | 65.99           | 1                  |
| CA-C-CA-C-C-CA-C-CA-CA-N-CA-N-CA-C-N-CA-CB | 110.50             | 68.54           | 1                  |
| N-CA-N-CA-CB                               | 103.00             | 130.13          | 1                  |
| N-CA-CB                                    | 103.00             | 130.11          | 1                  |
| C-N-CA-C-N-CA-C-N-N-CA-CB                  | 110.50             | 152.28          | 1                  |
| C-CA-C-CA-N-CA-N-CA-N-CA-CB                | 103.00             | 130.00          | 1                  |
| C-CA-CB                                    | 111.60             | 62.55           | 2                  |
| N-CA-CB                                    | 110.50             | 152.19          | 1                  |
| N-CA-CB                                    | 110.50             | 152.17          | 1                  |
| N-CA-CB                                    | 110.50             | 152.16          | 1                  |
| C-N-CA                                     | 121.70             | 77.61           | 1                  |
| N-CA-N-CA-N-CA-N-CA-CB                     | 103.00             | 129.91          | 1                  |
| C-N-CA                                     | 121.70             | 77.68           | 1                  |
| N-CA-C-CA-C-N-C-N-C-CA-CB                  | 110.10             | 63.79           | 1                  |
| N-CA-N-CA-C-CA-CB                          | 110.10             | 156.37          | 1                  |
| C-CA-CB                                    | 110.10             | 63.84           | 1                  |
| C-CA-CB                                    | 110.10             | 63.86           | 1                  |
| N-CA-CB                                    | 110.50             | 151.87          | 1                  |
| C-CA-CB                                    | 110.10             | 63.89           | 1                  |
| N-CA-CB                                    | 110.50             | 151.85          | 1                  |



| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-CB          | 110.50             | 151.84          | 2                  |
| C-CA-CB          | 110.10             | 156.28          | 1                  |
| N-CA-CB          | 110.50             | 69.20           | 1                  |
| N-CA-CB          | 111.50             | 152.80          | 1                  |
| N-CA-CB          | 110.50             | 151.79          | 1                  |
| N-CA-CB          | 110.50             | 151.78          | 1                  |
| N-CA-CB          | 110.50             | 69.23           | 1                  |
| N-CA-CB          | 111.50             | 152.75          | 1                  |
| N-CA-N-CA-CA-C-N | 116.20             | 67.89           | 1                  |
| CA-C-O           | 120.80             | 161.85          | 1                  |
| C-N-C-N-CA-C-N   | 116.20             | 67.94           | 1                  |
| CA-C-N           | 116.20             | 67.95           | 1                  |
| N-CA-CB          | 110.50             | 69.49           | 1                  |
| N-CA-CB          | 110.50             | 151.51          | 1                  |
| C-CA-CB          | 110.10             | 64.27           | 1                  |
| C-CA-CB          | 110.10             | 64.28           | 1                  |
| CA-C-N           | 116.20             | 67.99           | 1                  |
| CA-C-O           | 120.80             | 161.78          | 1                  |
| N-CA-CB          | 110.50             | 151.46          | 1                  |
| N-CA-CB          | 110.50             | 69.55           | 1                  |
| N-CA-CB          | 111.50             | 70.55           | 1                  |
| N-CA-C           | 111.00             | 43.55           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-C       | 111.00             | 43.56           | 1                  |
| N-CA-CA-C-N       | 116.20             | 68.08           | 1                  |
| N-CA-CA-C-N       | 116.20             | 68.09           | 1                  |
| CA-C-N            | 116.20             | 68.11           | 1                  |
| N-CA-CB           | 111.50             | 70.63           | 1                  |
| CA-C-N            | 116.20             | 68.17           | 1                  |
| CA-C-C-N-CA       | 121.70             | 78.52           | 1                  |
| N-CA-CB           | 110.50             | 69.73           | 1                  |
| CA-C-N-CA-CB      | 110.50             | 69.73           | 1                  |
| N-CA-N-CA-N-CA-CB | 110.50             | 69.78           | 1                  |
| N-CA-N-CA-CB      | 110.50             | 69.79           | 1                  |
| C-CA-CB           | 110.10             | 155.58          | 1                  |
| CA-C-N            | 116.20             | 68.33           | 1                  |
| C-CA-CB           | 110.10             | 155.57          | 1                  |
| N-CA-CB           | 110.50             | 69.81           | 1                  |
| CA-C-N            | 116.20             | 68.34           | 1                  |
| C-CA-CB           | 110.10             | 64.66           | 1                  |
| N-CA-CB           | 110.50             | 69.86           | 1                  |
| C-N-CA            | 121.70             | 78.70           | 1                  |
| C-N-CA            | 121.70             | 78.71           | 1                  |
| N-CA-N-CA-N-CA-C  | 111.00             | 44.25           | 1                  |
| N-CA-C            | 111.00             | 44.26           | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| CA-C-C-N-CA-C-C-N-CA-C-O            | 120.80             | 161.18          | 1                  |
| N-CA-CB                             | 103.00             | 129.10          | 1                  |
| N-CA-CB                             | 103.00             | 129.08          | 1                  |
| N-CA-N-CA-C-CA-CB                   | 111.60             | 158.98          | 1                  |
| N-CA-CB                             | 110.50             | 70.24           | 1                  |
| N-CA-N-CA-N-CA-CB                   | 110.50             | 70.28           | 1                  |
| CA-C-N                              | 116.20             | 68.88           | 1                  |
| N-CA-CB                             | 110.50             | 150.72          | 1                  |
| N-CA-CB                             | 110.50             | 70.28           | 1                  |
| CA-C-N                              | 116.20             | 68.89           | 1                  |
| CA-C-C-CA-CB                        | 111.60             | 158.87          | 1                  |
| CA-C-C-CA-CB                        | 110.10             | 65.21           | 1                  |
| N-CA-CB                             | 110.50             | 70.34           | 1                  |
| N-CA-N-CA-CB                        | 110.50             | 150.65          | 1                  |
| C-CA-CB                             | 110.10             | 65.25           | 1                  |
| C-N-CA-C-O                          | 120.80             | 160.91          | 1                  |
| N-CA-N-CA-N-CA-C-N-N-CA-C-CA-C-N-CA | 121.70             | 79.35           | 1                  |
| C-CA-N-CA-N-CA-C-N-CA               | 121.70             | 79.38           | 1                  |
| C-CA-CB                             | 110.50             | 75.24           | 1                  |
| C-CA-CB                             | 110.50             | 75.26           | 1                  |
| N-CA-N-CA-C-CA-CB                   | 110.10             | 154.71          | 1                  |
| C-CA-C-CA-C-CA-N-CA-C-CA-CB         | 110.10             | 154.60          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-CA-CB  | 111.60             | 158.38          | 1                  |
| N-CA-N-CA-C-CA-CB  | 111.60             | 158.37          | 1                  |
| C-CA-C-CA-C-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-C-CA-N-CA-C-CA-C-CA-CB | 111.40             | 67.31           | 1                  |
| C-CA-CB  | 111.40             | 67.31           | 1                  |
| N-CA-C   | 111.00             | 46.06           | 1                  |
| N-CA-C   | 111.00             | 46.08           | 1                  |
| CA-C-C-CA-CB   | 110.10             | 66.07           | 1                  |
| CA-C-N-CA-N-CA-C-CA-CB   | 110.10             | 154.11          | 1                  |
| C-CA-C-CA-CB   | 110.50             | 145.24          | 1                  |
| N-CA-CB  | 103.00             | 128.46          | 1                  |
| C-CA-C-CA-CB   | 110.10             | 66.13           | 1                  |
| C-CA-C-CA-CB   | 110.50             | 145.18          | 1                  |
| N-CA-C-CA-C-CA-C-CA-N-CA-CB  | 103.00             | 128.35          | 1                  |
| CA-C-O   | 120.80             | 159.94          | 1                  |
| N-CA-C-CA-CA-C-O   | 120.80             | 159.91          | 1                  |
| N-CA-CA-N-CA-N-C-CA-CB   | 110.50             | 76.04           | 1                  |
| N-CA-C-CA-CB   | 110.50             | 76.06           | 1                  |
| C-CA-CB  | 110.50             | 76.07           | 1                  |
| C-CA-N-CA-N-CA-C-CA-CB   | 110.50             | 76.10           | 1                  |
| CA-C-CA-C-C-CA-CB  | 110.50             | 144.87          | 1                  |
| C-CA-C-CA-CB   | 110.50             | 144.85          | 1                  |
| C-CA-C-CA-N-CA-N-CA-CB   | 103.00             | 128.16          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| N-CA-CB      | 103.00             | 128.15          | 1                  |
| N-CA-N-CA-C  | 111.00             | 47.14           | 1                  |
| C-CA-N-CA-C  | 111.00             | 47.19           | 1                  |
| N-CA-CB      | 103.00             | 128.06          | 1                  |
| C-CA-CB      | 110.10             | 66.88           | 1                  |
| N-CA-C       | 112.10             | 55.29           | 1                  |
| C-CA-CB      | 110.10             | 66.95           | 1                  |
| CA-C-N       | 116.20             | 161.51          | 1                  |
| N-CA-C-CA-CB | 110.10             | 67.23           | 1                  |
| C-CA-CB      | 110.10             | 67.24           | 1                  |
| CA-N-CD      | 112.00             | 80.43           | 1                  |
| CA-N-CD      | 112.00             | 80.44           | 1                  |
| C-N-CA       | 121.70             | 81.13           | 1                  |
| CA-N-CD      | 112.00             | 80.46           | 1                  |
| C-N-CA       | 121.70             | 81.15           | 1                  |
| C-CA-CB      | 110.10             | 152.88          | 1                  |
| C-CA-CB      | 110.10             | 152.87          | 1                  |
| CA-C-CA-N-CD | 112.00             | 80.50           | 1                  |
| C-CA-N-CA-C  | 111.00             | 48.04           | 1                  |
| C-CA-CB      | 110.10             | 67.38           | 1                  |
| N-CA-C       | 111.00             | 48.05           | 1                  |
| C-CA-CB      | 110.10             | 67.41           | 2                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| CA-C-N                               | 116.20             | 161.12          | 1                  |
| C-N-N-CA-C                           | 112.10             | 55.96           | 1                  |
| C-CA-N-CA-C                          | 112.10             | 55.97           | 1                  |
| C-N-N-CA-C                           | 111.00             | 48.21           | 1                  |
| CA-C-N-CA-C                          | 111.00             | 48.24           | 1                  |
| N-CA-N-CA-C-CA-C-CA-N-CA-CA-C-O      | 120.80             | 82.76           | 1                  |
| N-CA-N-CA-C-CA-C-CA-CA-C-O           | 120.80             | 82.78           | 1                  |
| C-CA-CB                              | 111.40             | 68.93           | 1                  |
| C-CA-CB                              | 110.10             | 152.57          | 1                  |
| N-CA-C                               | 111.00             | 48.42           | 2                  |
| C-CA-CB                              | 111.40             | 69.01           | 1                  |
| CA-C-CA-N-CD                         | 112.00             | 80.77           | 1                  |
| C-CA-C-CA-CA-C-O                     | 120.80             | 82.92           | 1                  |
| N-CA-CA-N-CD                         | 112.00             | 80.81           | 1                  |
| CA-C-C-CA-N-CA-CA-C-O                | 120.80             | 82.97           | 1                  |
| N-CA-N-CD-CG                         | 103.20             | 69.83           | 1                  |
| C-N-N-CD-CG                          | 103.20             | 69.86           | 1                  |
| C-CA-CB                              | 110.10             | 152.31          | 1                  |
| N-CA-C-CA-C-CA-CB                    | 110.10             | 152.26          | 1                  |
| CA-C-N-CA-N-CA-CA-C-N-CA-N-CA-N-CA-C | 111.00             | 49.04           | 1                  |
| N-CA-C                               | 111.00             | 49.04           | 1                  |
| N-CA-CB                              | 103.00             | 127.34          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| CA-C-O       | 120.80             | 83.19           | 1                  |
| CA-C-CA-C-O  | 120.80             | 83.25           | 1                  |
| N-CA-CB      | 110.50             | 148.03          | 1                  |
| N-CA-CA-C-O  | 120.80             | 158.25          | 1                  |
| N-CA-CB      | 110.50             | 147.95          | 1                  |
| C-CA-CA-C-N  | 116.20             | 72.18           | 1                  |
| N-CA-CB      | 110.50             | 147.91          | 1                  |
| CA-C-O       | 120.80             | 158.21          | 1                  |
| CA-C-O       | 120.80             | 83.44           | 1                  |
| C-CA-N-CA-CB | 111.50             | 74.15           | 1                  |
| N-CA-CB      | 111.50             | 74.16           | 1                  |
| CA-C-O       | 120.80             | 83.46           | 1                  |
| N-CA-CB      | 110.50             | 147.83          | 1                  |
| N-CA-C       | 111.00             | 49.58           | 1                  |
| N-CA-C       | 111.00             | 49.59           | 1                  |
| N-CA-C       | 111.00             | 49.60           | 2                  |
| C-CA-CB      | 110.10             | 68.47           | 1                  |
| N-CD-CG      | 103.20             | 70.34           | 1                  |
| N-CA-CB      | 103.00             | 127.10          | 1                  |
| C-CA-CA-C-N  | 116.20             | 72.42           | 1                  |
| C-CA-CB      | 110.10             | 68.52           | 1                  |
| CA-C-N       | 116.20             | 72.43           | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-N                    | 116.20             | 72.44           | 1                  |
| C-CA-CA-C-N                    | 116.20             | 72.48           | 1                  |
| C-CA-N-CD-CG                   | 103.20             | 70.44           | 1                  |
| C-CA-CB                        | 110.10             | 68.64           | 1                  |
| CA-C-O                         | 120.80             | 157.84          | 1                  |
| C-CA-N-CA-N-CA-C-CA-C-N-CA     | 121.70             | 82.58           | 1                  |
| C-N-CA                         | 121.70             | 82.59           | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-N-N-CA-C | 111.00             | 50.33           | 1                  |
| N-CA-C                         | 111.00             | 50.38           | 1                  |
| C-CA-C-CA-C-CA-CB              | 110.10             | 151.13          | 1                  |
| C-CA-CB                        | 110.10             | 151.12          | 1                  |
| C-CA-N-CA-CB                   | 110.50             | 73.85           | 1                  |
| N-CA-CB                        | 110.50             | 73.85           | 1                  |
| C-CA-C-CA-CB                   | 110.10             | 69.25           | 1                  |
| CA-C-O                         | 120.80             | 84.26           | 1                  |
| CA-C-O                         | 120.80             | 84.28           | 1                  |
| C-CA-CB                        | 110.10             | 69.30           | 1                  |
| N-CA-N-CA-CB                   | 110.50             | 74.01           | 1                  |
| N-CA-N-CA-C-CA-CB              | 110.10             | 150.85          | 1                  |
| N-CA-N-CA-CB                   | 110.50             | 74.06           | 1                  |
| CA-N-CD                        | 112.00             | 82.01           | 1                  |
| CA-C-CA-C-O                    | 120.80             | 157.20          | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 150.78          | 1                  |
| CA-N-CD               | 112.00             | 82.03           | 1                  |
| N-CA-CA-C-O           | 120.80             | 157.19          | 1                  |
| N-CA-C                | 111.00             | 51.07           | 1                  |
| N-CA-C                | 111.00             | 51.08           | 1                  |
| N-CA-N-CA-N-CA-CA-C-N | 116.90             | 84.85           | 1                  |
| C-CA-C-CA-CA-C-CA-C-N | 116.90             | 84.93           | 1                  |
| N-CA-CA-C-C-CA-CB     | 111.40             | 70.94           | 1                  |
| N-CA-C-CA-CB          | 111.40             | 70.97           | 1                  |
| N-CA-CB               | 111.50             | 147.66          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 69.72           | 1                  |
| N-CA-CB               | 111.50             | 147.62          | 1                  |
| C-N-CA                | 121.70             | 159.93          | 1                  |
| C-CA-CB               | 110.10             | 69.75           | 1                  |
| N-CA-C                | 112.10             | 59.04           | 2                  |
| C-N-CA                | 121.70             | 159.90          | 1                  |
| C-CA-CB               | 110.10             | 69.80           | 1                  |
| C-CA-CB               | 110.10             | 69.81           | 1                  |
| CA-C-O                | 120.80             | 84.79           | 1                  |
| C-CA-CB               | 110.10             | 69.89           | 1                  |
| C-CA-CA-C-O           | 120.80             | 156.74          | 1                  |
| CA-C-O                | 120.80             | 156.71          | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| CA-C-N                                | 116.20             | 158.40          | 1                  |
| CA-C-O                                | 120.80             | 84.93           | 1                  |
| N-CA-CA-C-N                           | 116.20             | 158.35          | 1                  |
| N-CA-C                                | 111.00             | 52.00           | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 70.08           | 1                  |
| N-CA-C                                | 111.00             | 52.05           | 1                  |
| N-CA-CA-C-O                           | 120.80             | 156.58          | 1                  |
| N-CA-N-CA-C-CA-CB                     | 110.10             | 70.19           | 1                  |
| CA-C-O                                | 120.80             | 156.50          | 1                  |
| N-CA-CB                               | 111.50             | 147.19          | 1                  |
| C-CA-CB                               | 110.10             | 70.22           | 1                  |
| N-CA-CB                               | 111.50             | 147.17          | 1                  |
| N-CA-C-N-N-CA-CB                      | 111.50             | 75.92           | 1                  |
| CA-C-N-CA-CB                          | 111.50             | 75.93           | 1                  |
| C-CA-CA-C-C-N-C-CA-C-CA-CB            | 111.60             | 69.85           | 1                  |
| N-CA-CA-N-CA-N-N-CA-CA-C-N            | 116.20             | 74.55           | 1                  |
| C-CA-CA-C-N                           | 116.20             | 74.58           | 1                  |
| C-CA-CA-N-N-CA-CB                     | 110.50             | 145.83          | 1                  |
| N-CA-N-CA-N-CA-CB                     | 110.50             | 145.82          | 1                  |
| CA-N-N-CA-CA-C-N-CA-CB                | 110.50             | 145.76          | 1                  |
| C-CA-CA-N-C-CA-CA-C-N-CA-N-CA-C-CA-CB | 110.10             | 149.45          | 1                  |
| N-CA-CB                               | 110.50             | 145.70          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                          | 110.10             | 149.43          | 1                  |
| C-CA-CB                          | 110.10             | 149.40          | 1                  |
| CA-N-N-CA-C                      | 111.00             | 53.09           | 1                  |
| C-CA-CB                          | 110.10             | 149.33          | 1                  |
| C-CA-CB                          | 110.10             | 70.87           | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-CA-C-CA-CB | 110.10             | 70.96           | 1                  |
| N-CA-C-CA-N-CA-CA-C-CA-C-CA-C-N  | 116.20             | 157.26          | 1                  |
| CA-C-N                           | 116.20             | 157.25          | 1                  |
| CA-C-O                           | 120.80             | 85.91           | 1                  |
| CA-C-N-CA-CA-C-O-C-N             | 123.00             | 90.20           | 1                  |
| N-CA-N-CA-N-CA-CB                | 110.50             | 75.68           | 1                  |
| N-CA-N-CA-N-CA-N-CA-CA-C-O       | 120.80             | 86.03           | 1                  |
| C-N-N-CA-O-C-N                   | 123.00             | 90.29           | 1                  |
| N-CA-C                           | 111.00             | 53.77           | 1                  |
| N-CA-C                           | 111.00             | 53.78           | 1                  |
| C-N-N-CA-CB                      | 110.50             | 75.78           | 1                  |
| C-CA-CB                          | 111.40             | 72.64           | 1                  |
| N-CA-CB                          | 110.50             | 75.82           | 1                  |
| N-CA-CB                          | 110.50             | 75.83           | 1                  |
| C-CA-C-CA-N-CA-C-CA-CA-C-N       | 116.20             | 75.53           | 1                  |
| C-CA-N-CA-CA-C-O                 | 120.80             | 155.31          | 1                  |
| C-CA-CB                          | 110.10             | 71.58           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| N-CA-C   | 111.00             | 54.28           | 1                  |
| CA-C-O   | 120.80             | 155.23          | 1                  |
| C-CA-C-CA-N-CA-C   | 111.00             | 54.30           | 1                  |
| C-CA-C-CA-CB   | 110.10             | 71.67           | 1                  |
| C-CA-CA-C-O  | 119.00             | 58.36           | 1                  |
| C-CA-N-CA-CA-C-N-CA-CA-C-C-CA-C-CA-N-CA-N-CA-C-CA-C-CA-CA-C-CA-C-C-CA-CA-C-N-CA-N-CA-CA-C-N-CA-C-CA-N-CA-C-CA-CB | 110.10             | 72.01           | 1                  |
| N-CA-C   | 111.00             | 54.87           | 1                  |
| CA-C-CA-C-N-CA-C   | 111.00             | 54.91           | 1                  |
| N-CA-C-CA-CB   | 110.10             | 72.10           | 1                  |
| N-CA-N-CA-CA-C-O   | 120.80             | 154.75          | 1                  |
| N-CA-CA-C-O  | 120.80             | 86.90           | 1                  |
| C-N-CA   | 121.70             | 85.82           | 2                  |
| CA-C-N   | 116.20             | 76.34           | 1                  |
| CA-C-N   | 116.20             | 76.36           | 2                  |
| C-N-CA-C-O   | 120.80             | 86.97           | 1                  |
| CA-C-O   | 120.80             | 154.63          | 1                  |
| CA-C-N   | 116.20             | 76.40           | 1                  |
| CA-C-C-CA-N-CA-C   | 111.00             | 55.33           | 1                  |
| N-CA-C   | 111.00             | 55.35           | 1                  |
| CA-C-O   | 120.80             | 154.59          | 1                  |
| CA-C-CA-C-O  | 120.80             | 154.58          | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-N-CA-C-N-C-N-N-CA-CB         | 110.50             | 144.19          | 1                  |
| N-CA-N-CA-CA-C-N                      | 116.20             | 155.77          | 1                  |
| C-N-N-CA-N-CA-CA-C-N                  | 116.20             | 155.72          | 1                  |
| N-CA-N-CA-N-CA-C-N-N-CA-CB            | 110.50             | 76.96           | 1                  |
| CA-C-CA-C-N-CA-C                      | 111.00             | 55.81           | 1                  |
| N-CA-C                                | 111.00             | 55.82           | 1                  |
| N-CA-C                                | 111.00             | 55.83           | 1                  |
| N-CA-CB                               | 110.50             | 77.01           | 1                  |
| C-CA-N-CA-C                           | 111.00             | 55.87           | 1                  |
| C-CA-CA-C-C-CA-C-CA-CB                | 111.40             | 148.79          | 1                  |
| C-CA-C-CA-C-CA-CA-C-C-CA-CA-C-C-CA-CB | 111.40             | 148.73          | 1                  |
| C-CA-N-CA-N-CA-C-CA-CB                | 110.10             | 72.81           | 1                  |
| C-CA-CB                               | 110.10             | 72.82           | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 147.34          | 1                  |
| CA-C-C-N-CA                           | 121.70             | 156.94          | 1                  |
| C-N-C-N-C-N-CA                        | 121.70             | 156.91          | 1                  |
| C-CA-CB                               | 110.10             | 147.26          | 2                  |
| N-CA-C-CA-C-CA-C-CA-CB                | 110.10             | 147.20          | 1                  |
| N-CA-N-CA-C                           | 111.00             | 56.39           | 1                  |
| N-CA-N-CA-C                           | 111.00             | 56.41           | 1                  |
| N-CA-N-CA-N-CA-C-CA-CB                | 110.10             | 147.12          | 1                  |
| CA-C-N-CA-CB                          | 110.50             | 143.55          | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| O-C-CA-C-C-CA-CA-C-N-CA-CB      | 110.40             | 139.50          | 1                  |
| O-C-N-CA-CB                     | 110.40             | 139.49          | 1                  |
| N-CA-CB                         | 110.50             | 143.47          | 1                  |
| C-CA-CA-C-N                     | 116.90             | 145.98          | 1                  |
| N-CA-C                          | 111.00             | 56.74           | 2                  |
| N-CA-C                          | 111.00             | 56.75           | 1                  |
| CA-C-N-CA-C                     | 111.00             | 56.78           | 1                  |
| C-CA-CB                         | 110.10             | 146.85          | 1                  |
| C-CA-CB                         | 110.10             | 146.83          | 1                  |
| CA-C-N                          | 116.20             | 154.86          | 1                  |
| CA-C-O                          | 120.80             | 87.95           | 1                  |
| CA-C-N                          | 116.90             | 145.88          | 1                  |
| N-CA-C                          | 111.00             | 56.92           | 1                  |
| N-CA-C                          | 111.00             | 56.93           | 1                  |
| CA-C-N                          | 116.20             | 154.80          | 1                  |
| C-CA-CB                         | 110.10             | 146.76          | 1                  |
| N-CA-C                          | 111.00             | 56.99           | 1                  |
| C-CA-CB                         | 110.10             | 146.73          | 1                  |
| N-CA-N-CA-N-CA-N-CA-N-CA-CA-C-N | 116.20             | 77.72           | 1                  |
| N-CA-CB                         | 110.50             | 143.21          | 1                  |
| N-CA-N-CA-N-CA-N-CA-CA-C-N      | 116.20             | 77.76           | 1                  |
| C-CA-CB                         | 110.10             | 73.59           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-CB               | 110.50             | 143.15          | 1                  |
| N-CA-C                | 111.00             | 57.24           | 1                  |
| CA-N-CD               | 112.00             | 85.13           | 1                  |
| C-CA-CB               | 110.10             | 73.65           | 1                  |
| N-CA-C                | 111.00             | 57.30           | 1                  |
| N-CA-C                | 111.00             | 57.31           | 1                  |
| N-CA-C                | 111.00             | 57.32           | 1                  |
| N-CA-C                | 111.00             | 57.34           | 1                  |
| CA-C-O                | 120.80             | 88.28           | 1                  |
| N-CA-C                | 113.30             | 168.77          | 1                  |
| N-CA-N-CA-CA-C-O      | 120.80             | 88.31           | 1                  |
| C-N-N-CA-N-CA-C       | 111.00             | 57.55           | 1                  |
| CA-N-CD               | 112.00             | 85.28           | 1                  |
| CA-C-N                | 116.20             | 154.37          | 1                  |
| N-CA-C                | 113.30             | 168.64          | 1                  |
| C-N-C-CA-CB           | 111.60             | 73.44           | 1                  |
| N-CA-CA-C-N-CA-N-CA-C | 111.00             | 57.63           | 1                  |
| CA-C-O                | 120.80             | 153.19          | 1                  |
| CA-C-N                | 116.20             | 154.30          | 1                  |
| CA-C-N-CA-N-CA-N-CA-C | 112.10             | 159.63          | 1                  |
| N-CA-CA-C-O           | 120.80             | 153.12          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 73.99           | 1                  |

| Angle type                                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-CD-NE-N-CA-C                              | 112.10             | 159.60          | 1                  |
| N-CA-C-CA-CA-C-O                               | 120.80             | 88.55           | 1                  |
| CA-C-C-CA-CB                                   | 110.10             | 74.07           | 1                  |
| N-CA-N-CA-N-CA-C-CA-C-CA-C-CA-N-CA-N-CA-CA-C-O | 120.80             | 88.61           | 1                  |
| CD-NE-C-CA-C-CA-CB                             | 110.10             | 146.00          | 1                  |
| N-CA-C   | 111.00             | 163.87          | 1                  |
| N-CA-C   | 111.00             | 163.81          | 1                  |
| C-CA-CB  | 110.10             | 145.91          | 1                  |
| N-CA-C-CA-CB                                   | 110.10             | 145.90          | 1                  |
| C-CA-C-CA-CB                                   | 110.10             | 145.89          | 1                  |
| N-CA-C   | 111.00             | 58.27           | 1                  |
| N-CA-N-CA-CA-C-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-C | 111.00             | 58.34           | 1                  |
| C-N-CA   | 121.70             | 87.87           | 2                  |
| CA-C-N-CA-CB                                   | 110.50             | 142.40          | 1                  |
| N-CA-CB  | 110.50             | 142.40          | 1                  |
| N-CA-CB  | 110.50             | 78.61           | 1                  |
| N-CA-CB  | 110.50             | 142.38          | 1                  |
| C-CA-CB  | 109.10             | 67.84           | 1                  |
| C-CA-CB  | 110.10             | 74.51           | 1                  |
| N-CA-CB  | 110.50             | 142.34          | 1                  |
| C-CA-CB  | 110.10             | 74.54           | 1                  |
| C-CA-CB  | 110.50             | 82.45           | 1                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                | 110.50             | 78.72           | 1                  |
| CA-C-C-CA-CB           | 110.50             | 82.50           | 1                  |
| CA-C-C-N-N-CA-CB       | 110.50             | 142.22          | 1                  |
| C-N-C-N-N-CA-CB        | 110.50             | 142.20          | 1                  |
| C-N-CA                 | 121.70             | 88.14           | 1                  |
| C-N-CA                 | 121.70             | 88.16           | 1                  |
| N-CA-CB                | 110.50             | 142.15          | 2                  |
| C-N-C-CA-C-CA-C-N-CA   | 121.70             | 88.23           | 1                  |
| N-CA-C-CA-CB           | 110.10             | 145.41          | 1                  |
| N-CA-N-CA-CB           | 110.50             | 142.05          | 1                  |
| N-CA-CB                | 110.50             | 78.97           | 1                  |
| C-CA-N-CA-CB           | 110.50             | 142.01          | 1                  |
| C-CA-CA-C-N            | 116.90             | 89.11           | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB | 110.50             | 141.96          | 1                  |
| N-CA-CB                | 110.50             | 79.05           | 1                  |
| C-CA-CB                | 110.10             | 74.96           | 1                  |
| N-CA-CB                | 110.50             | 141.94          | 2                  |
| C-CA-CB                | 110.10             | 74.97           | 1                  |
| N-CA-CB                | 110.50             | 141.93          | 1                  |
| C-CA-CB                | 110.10             | 74.99           | 1                  |
| CA-C-C-CA-C-CA-CB      | 110.10             | 75.01           | 1                  |
| CA-C-N                 | 116.90             | 89.21           | 1                  |

| Angle type                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA-C-C-CA-C-N-CA-C-N | 116.90             | 89.24           | 1                  |
| C-CA-C-N-N-CA-CB              | 110.50             | 141.84          | 1                  |
| N-CA-CB                       | 110.50             | 141.84          | 1                  |
| C-CA-N-CA-C                   | 111.00             | 59.40           | 1                  |
| C-CA-C-N-C-CA-N-CA-C          | 111.00             | 59.42           | 1                  |
| CA-C-N                        | 116.90             | 89.28           | 1                  |
| N-CA-C                        | 111.00             | 59.47           | 1                  |
| N-CA-CB                       | 110.50             | 79.28           | 1                  |
| N-CA-CB                       | 110.50             | 79.32           | 1                  |
| CA-C-CA-C-CA-N-CD             | 112.00             | 86.33           | 1                  |
| C-CA-N-CA-CB                  | 110.50             | 141.66          | 1                  |
| C-CA-CB                       | 110.10             | 75.29           | 1                  |
| C-CA-N-CA-CB                  | 110.50             | 141.63          | 1                  |
| N-CA-N-CA-C                   | 111.00             | 59.77           | 1                  |
| N-CA-CB                       | 111.50             | 142.61          | 1                  |
| N-CA-C                        | 111.00             | 59.80           | 1                  |
| N-CA-N-CA-CB                  | 111.50             | 142.56          | 1                  |
| C-CA-N-CA-C                   | 111.00             | 162.08          | 1                  |
| C-N-CA                        | 121.70             | 88.88           | 1                  |
| CA-C-O                        | 120.80             | 151.79          | 1                  |
| N-CA-CB                       | 110.50             | 141.48          | 1                  |
| N-CA-C                        | 111.00             | 162.03          | 1                  |

| Angle type  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| N-CA-CB   | 111.50             | 142.48          | 1                  |
| N-CA-N-CA-CB  | 111.50             | 142.44          | 1                  |
| N-CA-N-CA-N-CA-C  | 111.00             | 60.07           | 1                  |
| CA-C-O  | 120.80             | 151.72          | 1                  |
| N-CA-CA-C-N-CA-N-CA-N-CA-C-N-CA                           | 121.70             | 88.99           | 1                  |
| N-CA-N-CA-C   | 111.00             | 60.12           | 1                  |
| N-CA-CA-C-N-CA-N-CA-CA-C-N-CA-CA-C-CA-C-N-CA-N-CA-C-CA-CB | 110.10             | 75.66           | 1                  |
| CA-C-CA-C-N-CA-CB   | 110.50             | 141.30          | 1                  |
| CA-C-O  | 120.80             | 151.60          | 2                  |
| N-CA-C  | 111.00             | 60.27           | 1                  |
| N-CA-C  | 111.00             | 60.28           | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-CA-CA-C-N                           | 116.20             | 80.07           | 1                  |
| CA-C-N  | 116.20             | 152.30          | 1                  |
| CA-C-N  | 116.20             | 152.29          | 1                  |
| N-CA-CA-C-CA-C-C-CA-CB                                    | 110.10             | 144.36          | 1                  |
| CA-N-CD   | 112.00             | 86.76           | 1                  |
| CA-C-N  | 116.20             | 80.14           | 1                  |
| C-CA-CB   | 110.10             | 144.36          | 1                  |
| CA-C-CA-C-N-CA-N-CA-N-CA-N-CA-N-CA-N-CA-CB                | 110.50             | 141.05          | 1                  |
| N-CA-CB   | 110.50             | 141.02          | 1                  |
| C-N-N-CA-N-CA-N-CA-C                                      | 113.30             | 61.28           | 1                  |
| N-CA-C  | 113.30             | 61.28           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                     | 111.60             | 147.44          | 1                  |
| C-N-CA                      | 121.70             | 89.46           | 1                  |
| CA-C-CA-C-C-CA-CB           | 111.60             | 147.41          | 1                  |
| CA-C-C-CA-CB                | 110.10             | 144.08          | 1                  |
| CA-C-N-CA-CB                | 110.50             | 80.13           | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 144.00          | 1                  |
| CA-C-N-CA-N-CA-CB           | 110.50             | 80.18           | 1                  |
| N-CA-CB                     | 110.50             | 80.20           | 1                  |
| N-CA-C                      | 111.00             | 61.10           | 1                  |
| N-CA-C                      | 111.00             | 61.12           | 1                  |
| CA-C-N-CA-C                 | 111.00             | 61.19           | 1                  |
| N-CA-C                      | 111.00             | 61.20           | 1                  |
| C-CA-CB                     | 110.10             | 76.32           | 1                  |
| C-CA-CB                     | 110.50             | 83.85           | 1                  |
| C-CA-CB                     | 110.50             | 83.87           | 1                  |
| N-CA-N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 143.77          | 1                  |
| C-CA-CB                     | 110.10             | 143.75          | 1                  |
| CA-C-O                      | 120.80             | 90.69           | 1                  |
| C-CA-CB                     | 110.10             | 76.49           | 1                  |
| CA-C-CA-C-C-CA-CB           | 110.10             | 76.52           | 1                  |
| C-CA-N-CA-C                 | 111.00             | 61.52           | 1                  |
| N-CA-C                      | 111.00             | 61.55           | 1                  |

| Angle type  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| CA-C-CA-C-O   | 120.80             | 90.79           | 1                  |
| C-N-CA  | 121.70             | 89.95           | 1                  |
| C-CA-CB   | 110.10             | 143.61          | 2                  |
| CA-C-C-CA-CB  | 110.10             | 143.59          | 1                  |
| CA-C-O  | 120.80             | 90.85           | 1                  |
| N-CA-CB   | 110.50             | 140.45          | 1                  |
| CA-C-O  | 120.80             | 90.86           | 1                  |
| N-CA-CB   | 110.50             | 140.44          | 1                  |
| N-CA-CB   | 110.50             | 140.43          | 1                  |
| C-CA-C-CA-CB  | 110.10             | 143.53          | 1                  |
| C-CA-CB   | 110.10             | 143.52          | 1                  |
| C-CA-N-CA-CB  | 110.50             | 140.39          | 1                  |
| N-CD-C-CA-C-CA-CB   | 110.10             | 143.49          | 1                  |
| N-CA-N-CA-C-N-CA  | 121.70             | 90.09           | 1                  |
| N-CD-N-CA-N-CA-C-CA-N-CA-N-CA-C-CA-N-CA-CA-C-N-CA-CA-C-N-CA-CA-C-N-CA-CA-C-C-N-CA | 121.70             | 153.09          | 1                  |
| CA-C-C-CA-CB  | 111.60             | 76.76           | 1                  |
| CA-C-C-CA-CB  | 111.60             | 76.79           | 1                  |
| O-C-N   | 123.00             | 95.15           | 1                  |
| N-CA-CB   | 110.50             | 80.92           | 1                  |
| C-N-CA  | 121.70             | 153.00          | 1                  |
| N-CA-CA-C-N-CA-N-CA-CA-C-CA-C-N-CA-C-CA-O-C-N                                     | 123.00             | 95.21           | 1                  |
| C-CA-CB   | 110.10             | 77.11           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.10             | 77.13           | 1                  |
| CA-C-N-CA-N-CA-C           | 111.00             | 62.45           | 1                  |
| C-CA-N-CA-CB               | 111.50             | 82.03           | 1                  |
| C-CA-CB                    | 110.10             | 77.16           | 1                  |
| C-CA-C-CA-CB               | 110.10             | 77.17           | 1                  |
| CA-C-N-CA-C                | 111.00             | 62.49           | 1                  |
| CA-C-N-CA-N-CA-C-CA-CA-C-O | 120.80             | 150.20          | 1                  |
| N-CA-CA-C-C-CA-N-CA-C      | 111.00             | 62.60           | 1                  |
| N-CA-CB                    | 103.00             | 122.01          | 1                  |
| N-CA-CB                    | 111.50             | 82.12           | 1                  |
| N-CA-C                     | 111.00             | 62.61           | 1                  |
| N-CA-C-N-C-CA-N-CA-CB      | 110.50             | 81.14           | 1                  |
| CA-C-C-CA-CB               | 110.10             | 77.31           | 1                  |
| C-CA-CB                    | 110.10             | 77.31           | 1                  |
| N-CD-CA-C-O                | 120.80             | 150.11          | 1                  |
| N-CA-C                     | 111.00             | 62.72           | 1                  |
| N-CD-CA-C-N-CA-C           | 111.00             | 159.25          | 1                  |
| N-CA-N-CA-CB               | 110.50             | 81.21           | 1                  |
| N-CA-C                     | 111.00             | 159.22          | 1                  |
| C-CA-CB                    | 110.10             | 77.38           | 1                  |
| C-CA-CB                    | 110.10             | 77.39           | 1                  |
| CA-C-C-N-N-CA-C            | 111.00             | 62.89           | 1                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-O         | 120.80             | 91.59           | 1                  |
| N-CA-C              | 111.00             | 62.90           | 1                  |
| N-CA-CB             | 103.00             | 121.89          | 1                  |
| CA-C-N-CA-C         | 111.00             | 62.93           | 1                  |
| CA-C-O              | 120.80             | 91.62           | 1                  |
| C-CA-CB             | 110.10             | 77.49           | 1                  |
| N-CA-C              | 111.00             | 62.95           | 1                  |
| N-CA-C              | 111.00             | 62.97           | 2                  |
| CA-C-C-CA-CB        | 110.10             | 77.54           | 1                  |
| N-CA-C              | 111.00             | 63.03           | 2                  |
| C-N-C-N-N-CA-C-N-CD | 125.00             | 55.02           | 1                  |
| N-CA-C-N-CD         | 125.00             | 55.08           | 1                  |
| CA-C-N              | 116.20             | 150.28          | 1                  |
| N-CA-CA-C-CA-C-O    | 120.80             | 91.88           | 1                  |
| C-CA-CA-C-N         | 116.20             | 150.21          | 1                  |
| C-CA-C-CA-C-CA-CB   | 110.50             | 135.98          | 1                  |
| N-CA-C              | 111.00             | 158.56          | 1                  |
| C-N-C-CA-C-N-C-N-CD | 125.00             | 55.46           | 1                  |
| C-CA-CB             | 110.10             | 142.32          | 1                  |
| C-CA-CB             | 110.10             | 142.31          | 1                  |
| N-CA-CB             | 110.50             | 139.32          | 1                  |
| CA-C-N-CA-C-N-CD    | 125.00             | 55.56           | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                               | 110.10             | 77.94           | 1                  |
| CA-C-N                                | 116.20             | 82.36           | 1                  |
| N-CA-C                                | 111.00             | 158.37          | 1                  |
| N-CA-CB                               | 110.40             | 85.02           | 1                  |
| C-CA-CB                               | 109.10             | 146.32          | 1                  |
| C-N-N-CA-N-CA-CB                      | 110.50             | 139.24          | 1                  |
| CA-C-N-CA-CB                          | 110.40             | 85.04           | 1                  |
| CA-C-C-CA-CB                          | 110.50             | 135.85          | 1                  |
| C-CA-CB                               | 110.10             | 78.02           | 1                  |
| C-N-CA                                | 121.70             | 152.09          | 1                  |
| CA-C-N-CA-C                           | 111.00             | 63.74           | 1                  |
| CA-C-CA-C-N                           | 116.20             | 82.46           | 1                  |
| C-CA-CB                               | 109.10             | 146.21          | 1                  |
| CA-C-N-CA-C                           | 111.00             | 63.82           | 1                  |
| N-CA-C-N-CA                           | 121.70             | 152.01          | 1                  |
| CA-C-N-CA-C                           | 111.00             | 158.07          | 1                  |
| N-CA-N-CD-N-CA-N-CA-N-CA-N-CD-C-CA-CB | 110.10             | 141.98          | 1                  |
| CA-C-O                                | 120.80             | 149.33          | 1                  |
| N-CA-C-N-N-CA-C                       | 111.00             | 157.93          | 1                  |
| C-N-N-CA-N-CA-C                       | 111.00             | 64.08           | 1                  |
| N-CA-C                                | 111.00             | 64.08           | 1                  |
| N-CA-CB                               | 110.50             | 82.02           | 1                  |



| Angle type                                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| CA-C-N  | 116.20             | 149.71          | 1                  |
| CA-C-N-CA-CB                                  | 110.50             | 82.03           | 1                  |
| N-CA-N-CA-C                                   | 111.00             | 64.13           | 1                  |
| N-CA-C  | 111.00             | 64.14           | 1                  |
| N-CA-CB                                       | 110.50             | 82.05           | 1                  |
| CA-C-N  | 116.20             | 149.66          | 1                  |
| C-N-N-CA-CB                                   | 110.50             | 82.07           | 1                  |
| N-CA-N-CA-N-CA-CA-C-N-CA-CA-C-C-N-N-CA-C-N-CA | 121.70             | 91.69           | 1                  |
| N-CA-C  | 111.00             | 64.32           | 1                  |
| CA-C-O  | 120.80             | 92.46           | 1                  |
| CA-C-CA-C-O                                   | 120.80             | 149.13          | 1                  |
| CA-C-O  | 120.80             | 149.13          | 1                  |
| CA-N-CD                                       | 112.00             | 88.68           | 1                  |
| N-CA-C  | 111.00             | 64.36           | 1                  |
| CA-N-CD                                       | 112.00             | 88.69           | 1                  |
| CA-C-O  | 120.80             | 92.51           | 1                  |
| CA-C-O  | 120.80             | 92.52           | 1                  |
| CA-C-CA-N-CD                                  | 112.00             | 88.72           | 1                  |
| N-CA-CA-C-N-CA-CB                             | 110.50             | 138.74          | 1                  |
| CA-C-CA-C-CA-N-CD                             | 112.00             | 88.74           | 1                  |
| C-N-CD  | 125.00             | 56.90           | 1                  |
| C-N-CD  | 125.00             | 56.91           | 1                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| C-CA-CB             | 110.10             | 78.55           | 3                  |
| N-CA-CB             | 110.50             | 138.73          | 1                  |
| C-N-CD              | 125.00             | 56.93           | 1                  |
| N-CA-C              | 111.00             | 64.52           | 1                  |
| CA-C-N-CA-C         | 111.00             | 64.54           | 1                  |
| N-CA-CA-C-N         | 116.20             | 149.38          | 1                  |
| C-CA-CB             | 110.10             | 78.59           | 1                  |
| CA-C-N              | 116.20             | 83.04           | 1                  |
| C-N-N-CA-CA-C-N     | 116.20             | 83.05           | 1                  |
| C-N-CA              | 121.70             | 91.87           | 1                  |
| CA-C-C-CA-CB        | 110.10             | 141.57          | 1                  |
| C-N-CA-C-O          | 120.80             | 148.96          | 1                  |
| N-CA-CB             | 103.00             | 121.22          | 1                  |
| N-CA-N-CA-CA-C-N    | 116.20             | 149.28          | 1                  |
| C-N-C-N-C-CA-N-CA-C | 111.00             | 64.71           | 1                  |
| N-CA-C-N-CA         | 121.70             | 91.95           | 1                  |
| N-CA-CB             | 103.00             | 121.18          | 1                  |
| C-CA-N-CA-N-CA-CB   | 103.00             | 121.16          | 1                  |
| N-CA-C              | 111.00             | 64.77           | 1                  |
| N-CA-CB             | 103.00             | 121.15          | 1                  |
| C-CA-CB             | 110.10             | 141.44          | 1                  |
| CA-C-C-CA-CB        | 110.10             | 141.43          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-C-N-CA            | 121.70             | 92.08           | 1                  |
| C-CA-CB                | 111.40             | 80.15           | 1                  |
| N-CA-N-CA-C-CA-CB      | 110.10             | 141.34          | 1                  |
| C-N-CA                 | 121.70             | 92.12           | 1                  |
| C-CA-CB                | 111.40             | 80.19           | 1                  |
| CA-C-C-CA-CB           | 110.10             | 141.27          | 1                  |
| C-CA-CB                | 111.40             | 80.23           | 1                  |
| C-CA-CB                | 110.10             | 141.26          | 2                  |
| CA-C-C-CA-CB           | 111.40             | 80.25           | 1                  |
| C-CA-C-CA-CA-C-C-CA-CB | 110.10             | 141.19          | 1                  |
| N-CA-C-CA-N-CA-C       | 111.00             | 65.22           | 1                  |
| C-N-CA                 | 121.70             | 92.27           | 1                  |
| C-N-CA                 | 121.70             | 92.28           | 1                  |
| C-CA-CB                | 110.10             | 141.15          | 1                  |
| C-CA-N-CA-C            | 111.00             | 65.26           | 1                  |
| CA-C-N-CA-C-CA-CB      | 110.10             | 79.13           | 1                  |
| CA-C-O                 | 120.80             | 148.51          | 1                  |
| N-CA-CB                | 111.50             | 83.81           | 1                  |
| CA-C-O                 | 120.80             | 93.13           | 2                  |
| N-CA-CB                | 111.50             | 83.83           | 2                  |
| N-CA-C                 | 111.00             | 65.43           | 1                  |
| CA-C-N-CA-CB           | 111.50             | 83.86           | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-C-CA-CB                   | 110.10             | 140.97          | 1                  |
| N-CA-CA-C-N-CA-CA-N-CD              | 112.00             | 89.27           | 1                  |
| N-CA-C                              | 111.00             | 65.54           | 1                  |
| CA-C-CA-C-O                         | 120.80             | 148.39          | 1                  |
| CA-N-CD                             | 112.00             | 89.28           | 1                  |
| C-CA-CB                             | 110.10             | 140.93          | 1                  |
| C-CA-C-N-CA-C-CA-C-N                | 116.20             | 148.62          | 1                  |
| N-CA-CA-C-N                         | 116.20             | 148.61          | 1                  |
| C-CA-C-N-N-CA-N-CA-N-CA-N-CA-N-CA-C | 111.00             | 65.70           | 1                  |
| CA-C-CA-C-N-CD-CG                   | 103.20             | 78.95           | 1                  |
| N-CA-N-CA-C-CA-CB                   | 110.10             | 79.44           | 1                  |
| N-CA-C-CA-CB                        | 110.10             | 79.49           | 1                  |
| C-CA-N-CA-CB                        | 110.50             | 137.86          | 1                  |
| C-CA-C-CA-CB                        | 110.10             | 140.66          | 1                  |
| C-CA-N-CA-CB                        | 110.50             | 137.82          | 1                  |
| N-CA-C                              | 111.00             | 155.97          | 1                  |
| N-CA-CB                             | 110.50             | 137.79          | 2                  |
| N-CA-C                              | 111.00             | 155.94          | 1                  |
| N-CA-C                              | 111.00             | 155.93          | 1                  |
| C-CA-CB                             | 110.10             | 79.62           | 1                  |
| C-CA-CB                             | 110.10             | 140.58          | 1                  |
| N-CA-C                              | 111.00             | 155.92          | 1                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-C                               | 111.00             | 66.09           | 1                  |
| C-CA-N-CA-CB                         | 110.50             | 137.75          | 1                  |
| N-CA-C                               | 111.00             | 66.12           | 1                  |
| C-CA-CB                              | 110.10             | 79.66           | 1                  |
| C-CA-CB                              | 110.10             | 79.67           | 1                  |
| C-CA-CB                              | 110.10             | 79.69           | 3                  |
| C-CA-CB                              | 110.10             | 79.70           | 2                  |
| C-CA-N-CA-N-CA-C-CA-N-CA-CA-C-C-N-CA | 121.70             | 150.44          | 1                  |
| C-CA-C-CA-CB                         | 110.10             | 140.43          | 1                  |
| N-CA-C-CA-N-CA-N-CA-C-CA-CB          | 110.10             | 140.39          | 1                  |
| C-CA-C-CA-C-CA-CA-C-O                | 119.00             | 71.25           | 1                  |
| N-CA-C                               | 111.00             | 155.56          | 1                  |
| C-N-CA                               | 121.70             | 150.34          | 1                  |
| N-CA-C                               | 111.00             | 155.55          | 1                  |
| C-CA-C-CA-CB                         | 110.10             | 79.88           | 1                  |
| CA-C-N-CA-CB                         | 111.50             | 138.51          | 1                  |
| N-CA-N-CA-C-CA-CB                    | 110.10             | 79.94           | 1                  |
| C-CA-CB                              | 110.10             | 79.96           | 1                  |
| N-CA-CB                              | 103.00             | 120.45          | 1                  |
| C-CA-CA-C-C-CA-CB                    | 110.10             | 79.99           | 1                  |
| CA-N-CD                              | 112.00             | 89.82           | 1                  |
| CA-N-CA-N-N-CA-CB                    | 110.50             | 137.43          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                 | 110.10             | 80.02           | 2                  |
| C-CA-N-CD-N-CA-C-CA-CB  | 110.10             | 80.05           | 1                  |
| C-N-CA                  | 121.70             | 150.17          | 1                  |
| C-N-C-CA-N-CA-CB-CG-ND2 | 116.40             | 92.69           | 1                  |
| CA-C-O                  | 120.80             | 93.93           | 1                  |
| N-CA-CB                 | 111.50             | 138.37          | 1                  |
| CA-N-CD                 | 112.00             | 89.88           | 1                  |
| N-CA-C                  | 111.00             | 66.76           | 1                  |
| C-CA-C-N-CA             | 121.70             | 150.13          | 1                  |
| C-N-N-CA-C              | 111.00             | 66.83           | 1                  |
| C-CA-N-CA-C-N-CA        | 121.70             | 150.09          | 1                  |
| N-CA-CA-C-N             | 116.20             | 147.74          | 1                  |
| N-CD-C-N-CD             | 125.00             | 60.37           | 1                  |
| C-CA-CB                 | 110.10             | 140.05          | 1                  |
| N-CA-N-CA-CA-C-N        | 116.20             | 147.72          | 1                  |
| N-CA-C-CA-N-CA-N-CA-CB  | 111.50             | 138.28          | 1                  |
| N-CA-N-CA-CB            | 103.00             | 120.33          | 1                  |
| C-CA-CA-C-N             | 116.20             | 84.69           | 1                  |
| CB-CG-ND2               | 116.40             | 92.78           | 1                  |
| N-CA-N-CA-N-CA-CA-C-N   | 116.20             | 84.72           | 1                  |
| CA-C-O                  | 120.80             | 94.05           | 1                  |
| C-CA-C-CA-CB            | 110.10             | 139.99          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-C-N                | 116.20             | 84.75           | 1                  |
| N-CA-C                | 111.00             | 66.99           | 1                  |
| C-N-CA                | 121.70             | 149.99          | 1                  |
| N-CA-C                | 111.00             | 67.00           | 1                  |
| CA-C-N                | 116.20             | 84.79           | 1                  |
| C-N-C-CA-CB           | 110.10             | 80.29           | 1                  |
| CA-C-N                | 116.20             | 147.55          | 1                  |
| CA-C-N                | 116.20             | 147.54          | 1                  |
| C-CA-CB               | 110.10             | 139.86          | 1                  |
| C-N-C-CA-C-CA-C-CA-CB | 110.10             | 80.39           | 1                  |
| N-CA-N-CA-C           | 111.00             | 67.27           | 1                  |
| N-CA-C                | 111.00             | 67.27           | 1                  |
| N-CA-C                | 111.00             | 67.29           | 1                  |
| C-CA-CB               | 110.10             | 139.74          | 1                  |
| N-CA-C                | 111.00             | 67.32           | 1                  |
| C-CA-CB               | 110.10             | 139.71          | 1                  |
| N-CA-CA-C-O           | 120.80             | 94.34           | 1                  |
| C-CA-CB               | 110.10             | 139.67          | 1                  |
| N-CA-CB               | 110.50             | 136.93          | 1                  |
| CA-C-N                | 116.90             | 93.60           | 1                  |
| CA-C-O                | 120.80             | 94.39           | 1                  |
| N-CA-CB               | 110.50             | 84.10           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-O            | 120.80             | 94.40           | 1                  |
| N-CA-CB           | 110.50             | 136.88          | 1                  |
| CA-C-N            | 116.20             | 85.19           | 1                  |
| C-CA-CB           | 110.50             | 87.24           | 1                  |
| C-CA-CB           | 110.50             | 87.25           | 1                  |
| CA-C-C-CA-CB      | 110.10             | 80.66           | 1                  |
| CA-C-O            | 120.80             | 94.47           | 1                  |
| CA-C-N            | 116.90             | 93.67           | 1                  |
| CA-C-O            | 120.80             | 147.12          | 1                  |
| CA-C-O            | 120.80             | 94.48           | 1                  |
| C-CA-CB           | 110.50             | 87.28           | 1                  |
| C-CA-CB           | 110.10             | 80.70           | 1                  |
| N-CA-CA-C-C-CA-CB | 110.50             | 87.30           | 1                  |
| N-CA-C            | 111.00             | 67.70           | 1                  |
| C-CA-CB           | 110.10             | 139.48          | 1                  |
| N-CA-C-CA-CB      | 110.10             | 139.47          | 1                  |
| CD-NE-CZ          | 124.40             | 146.03          | 1                  |
| N-CA-C            | 113.30             | 158.11          | 1                  |
| N-CA-CA-C-O       | 120.80             | 147.06          | 1                  |
| C-N-CA            | 121.70             | 93.90           | 1                  |
| N-CA-CB           | 111.50             | 85.25           | 2                  |
| C-CA-CB           | 111.40             | 82.06           | 1                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-N-CA                 | 121.70             | 93.92           | 1                  |
| N-CA-CB                | 111.50             | 85.27           | 2                  |
| CA-C-O                 | 120.80             | 147.03          | 1                  |
| C-CA-CB                | 111.40             | 82.09           | 1                  |
| N-CA-CB                | 103.00             | 119.97          | 1                  |
| N-CA-CB                | 111.50             | 85.28           | 1                  |
| N-CA-CB                | 110.50             | 136.71          | 1                  |
| N-CA-C                 | 113.30             | 158.01          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 136.70          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 85.31           | 1                  |
| N-CA-CB                | 110.50             | 136.67          | 1                  |
| C-CA-C-CA-C-CA-CB      | 111.40             | 82.20           | 1                  |
| C-CA-N-CA-C            | 111.00             | 67.98           | 1                  |
| CA-C-O                 | 120.80             | 146.91          | 1                  |
| N-CA-C                 | 111.00             | 68.00           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 139.26          | 1                  |
| N-CA-CD-NE-CZ          | 124.40             | 145.88          | 1                  |
| N-CA-N-CA-CB           | 110.50             | 136.58          | 1                  |
| C-CA-CB                | 110.50             | 87.49           | 1                  |
| N-CA-N-CA-CA-C-C-CA-CB | 110.10             | 139.22          | 1                  |
| C-CA-CB                | 110.10             | 139.21          | 2                  |
| N-CA-N-CA-CB           | 110.50             | 136.52          | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| C-N-N-CA-N-CA-C-CA-C-CA-N-CA-CB | 103.00             | 119.81          | 1                  |
| N-CA-C-CA-C-CA-CB               | 110.50             | 87.59           | 1                  |
| C-N-CA                          | 121.70             | 149.19          | 1                  |
| C-CA-CA-C-N-CA-CB               | 103.00             | 119.79          | 1                  |
| N-CA-N-CA-C-CA-C-N-CA           | 121.70             | 149.16          | 1                  |
| C-CA-CB                         | 110.10             | 81.12           | 1                  |
| C-CA-C-N-C-CA-N-CA-CB           | 111.50             | 85.61           | 1                  |
| CA-C-N                          | 116.90             | 94.05           | 1                  |
| OD1-CG-ND2                      | 122.60             | 137.83          | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 81.18           | 1                  |
| N-CA-C                          | 111.00             | 153.60          | 1                  |
| N-CA-CA-C-N                     | 116.90             | 94.09           | 1                  |
| N-CA-CB                         | 111.50             | 85.65           | 1                  |
| N-CA-C                          | 111.00             | 68.43           | 1                  |
| N-CA-C                          | 111.00             | 68.45           | 2                  |
| N-CA-CB                         | 110.50             | 136.33          | 1                  |
| CA-C-N                          | 116.90             | 94.12           | 1                  |
| N-CA-C                          | 111.00             | 68.47           | 1                  |
| N-CA-CB                         | 110.50             | 136.31          | 1                  |
| N-CA-N-CA-CB                    | 110.50             | 136.29          | 1                  |
| CA-C-N                          | 116.20             | 85.87           | 1                  |
| C-CA-CB                         | 110.10             | 138.91          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-C       | 111.00             | 153.45          | 1                  |
| C-CA-CB           | 110.10             | 138.90          | 1                  |
| N-CA-CA-C-CA-C-N  | 116.20             | 85.89           | 1                  |
| N-CA-CB           | 110.50             | 136.26          | 1                  |
| CA-C-N            | 116.90             | 94.17           | 1                  |
| N-CA-N-CA-C       | 111.00             | 153.41          | 1                  |
| N-CA-CB           | 110.50             | 136.25          | 1                  |
| N-CA-CA-C-C-CA-CB | 110.10             | 81.34           | 1                  |
| N-CA-N-CA-CB      | 110.50             | 136.22          | 1                  |
| C-CA-CB           | 110.10             | 138.83          | 1                  |
| CA-C-N            | 116.20             | 85.95           | 1                  |
| N-CA-C            | 111.00             | 153.34          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 81.38           | 1                  |
| CA-C-N-CA-N-CA-C  | 111.00             | 153.31          | 1                  |
| CA-C-N            | 116.20             | 85.99           | 1                  |
| CA-C-C-CA-C-CA-CB | 110.10             | 138.78          | 1                  |
| C-N-N-CA-C        | 111.00             | 153.25          | 1                  |
| CA-C-O            | 119.00             | 73.74           | 1                  |
| N-CA-CB           | 110.50             | 84.85           | 1                  |
| C-N-N-CA-CB       | 110.50             | 84.86           | 1                  |
| CA-C-N-CA-C       | 111.00             | 153.23          | 1                  |
| N-CA-CA-C-O       | 119.00             | 73.77           | 1                  |

| Angle type                               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| N-CA-N-CA-C                              | 111.00             | 153.20          | 1                  |
| N-CA-C                                   | 111.00             | 153.19          | 1                  |
| C-CA-CB                                  | 110.50             | 87.90           | 1                  |
| CA-C-N-CA-C                              | 111.00             | 153.17          | 1                  |
| C-N-CA                                   | 121.70             | 94.59           | 1                  |
| N-CA-C                                   | 111.00             | 153.16          | 1                  |
| C-CA-OD1-CG-ND2                          | 122.60             | 137.65          | 1                  |
| CA-C-C-N-CA                              | 121.70             | 94.61           | 1                  |
| C-CA-CB                                  | 110.50             | 87.93           | 1                  |
| N-CA-C                                   | 111.00             | 153.13          | 1                  |
| N-CA-N-CA-N-CA-N-CD-C-N-C-N-N-CA-C-CA-CB | 110.10             | 81.59           | 1                  |
| N-CD-CA-C-CA-N-CD                        | 112.00             | 91.01           | 1                  |
| CA-C-C-N-CA                              | 121.70             | 94.73           | 1                  |
| C-N-C-CA-CB                              | 110.10             | 81.64           | 1                  |
| N-CA-CB                                  | 110.50             | 135.96          | 1                  |
| N-CA-CB                                  | 103.00             | 119.47          | 1                  |
| CA-C-C-N-N-CA-CB                         | 110.50             | 135.94          | 1                  |
| C-N-CA                                   | 121.70             | 94.77           | 1                  |
| CA-N-CD                                  | 112.00             | 91.06           | 1                  |
| C-CA-CB                                  | 110.10             | 138.52          | 1                  |
| C-CA-CB                                  | 110.10             | 138.51          | 1                  |
| N-CA-CB                                  | 110.50             | 85.08           | 1                  |

| Angle type                                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-O                                     | 120.80             | 95.39           | 2                  |
| N-CA-CB                                    | 110.50             | 135.90          | 1                  |
| CA-C-N-CA-CB                               | 110.50             | 135.89          | 1                  |
| CA-C-N-CA-CB                               | 110.50             | 85.12           | 1                  |
| N-CA-CA-C-N                                | 116.20             | 146.04          | 1                  |
| CA-C-N                                     | 116.20             | 146.02          | 1                  |
| N-CA-CB                                    | 110.50             | 135.84          | 1                  |
| N-CA-N-CA-C-CA-CB                          | 110.10             | 138.41          | 1                  |
| N-CA-CB                                    | 103.00             | 119.39          | 1                  |
| C-CA-C-CA-N-CA-CA-C-C-CA-C-CA-N-CA-C-CA-CB | 110.10             | 81.83           | 1                  |
| N-CA-C-CA-CB                               | 110.10             | 138.36          | 1                  |
| C-CA-CB                                    | 110.10             | 138.36          | 1                  |
| C-CA-CB                                    | 110.10             | 81.84           | 1                  |
| CA-C-N-CA-CB                               | 110.40             | 132.70          | 1                  |
| CA-C-N-CA-CB                               | 110.40             | 132.69          | 1                  |
| CA-C-C-CA-CB                               | 110.10             | 81.88           | 1                  |
| N-CA-N-CA-C                                | 112.10             | 149.21          | 1                  |
| C-CA-CB                                    | 110.10             | 81.92           | 1                  |
| N-CA-C-CA-N-CA-C                           | 112.10             | 149.16          | 1                  |
| C-CA-CB                                    | 110.10             | 138.26          | 1                  |
| N-CA-C                                     | 112.10             | 149.15          | 1                  |
| C-N-CA                                     | 121.70             | 95.02           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-N                     | 116.20             | 86.56           | 1                  |
| N-CA-C                     | 112.10             | 149.14          | 1                  |
| C-CA-CB                    | 110.10             | 81.95           | 1                  |
| C-CA-CB                    | 110.10             | 81.96           | 1                  |
| CA-C-O                     | 120.80             | 95.63           | 1                  |
| C-N-CA                     | 121.70             | 95.05           | 1                  |
| C-CA-CB                    | 110.10             | 81.98           | 2                  |
| N-CA-CB                    | 110.50             | 85.35           | 1                  |
| C-CA-CB                    | 110.10             | 82.00           | 2                  |
| C-CA-CB                    | 110.10             | 138.20          | 1                  |
| CA-C-O                     | 120.80             | 95.66           | 1                  |
| C-CA-CB                    | 110.10             | 82.02           | 1                  |
| C-CA-CB                    | 110.10             | 138.18          | 1                  |
| CA-C-C-CA-CB               | 110.10             | 138.17          | 1                  |
| CA-C-N                     | 116.20             | 86.66           | 1                  |
| N-CA-C-CA-C-CA-N-CA-CA-C-N | 116.20             | 86.71           | 1                  |
| CA-C-N                     | 116.20             | 86.71           | 2                  |
| CA-C-N                     | 116.20             | 86.72           | 1                  |
| N-CA-CB                    | 110.50             | 85.46           | 1                  |
| C-CA-CA-C-N-CA-N-CA-C-N-CA | 121.70             | 95.22           | 1                  |
| C-CA-CB                    | 111.40             | 83.45           | 1                  |
| C-CA-C-N-CA                | 121.70             | 95.24           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-O                 | 120.80             | 95.81           | 1                  |
| C-CA-N-CA-N-CA-N-CA-C  | 111.00             | 152.14          | 1                  |
| CA-C-O                 | 120.80             | 95.83           | 1                  |
| C-CA-N-CA-N-CA-CB      | 110.50             | 85.55           | 1                  |
| N-CA-C                 | 111.00             | 152.09          | 1                  |
| N-CA-N-CA-CA-C-O       | 120.80             | 95.86           | 1                  |
| CA-C-O                 | 120.80             | 95.87           | 1                  |
| C-CA-CB                | 109.10             | 141.36          | 1                  |
| N-CA-C                 | 111.00             | 152.06          | 1                  |
| C-CA-C-N-CA            | 121.70             | 95.31           | 1                  |
| C-CA-C-CA-C-CA-C-CA-CB | 109.10             | 141.32          | 1                  |
| N-CA-CA-C-N            | 116.20             | 86.92           | 1                  |
| N-CA-CA-C-N            | 116.20             | 86.95           | 1                  |
| N-CA-C                 | 111.00             | 151.96          | 1                  |
| CA-C-CA-C-N            | 116.20             | 86.95           | 1                  |
| C-CA-C-CA-C-N-CA       | 121.70             | 95.38           | 1                  |
| N-CA-N-CA-C            | 111.00             | 70.06           | 1                  |
| CA-C-N-CA-C            | 111.00             | 70.08           | 1                  |
| N-CA-C                 | 111.00             | 70.08           | 1                  |
| CA-C-N                 | 116.20             | 86.98           | 1                  |
| C-CA-CA-C-C-CA-N-CA-C  | 111.00             | 70.15           | 1                  |
| N-CA-CB                | 110.50             | 135.28          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-CA-C-C-N-CA       | 121.70             | 95.46           | 1                  |
| CA-C-CA-C-CA-C-C-N-CA  | 121.70             | 147.92          | 1                  |
| CA-C-CA-C-C-CA-CB      | 110.50             | 88.67           | 1                  |
| C-N-CA                 | 121.70             | 147.89          | 1                  |
| CA-C-C-N-CA            | 121.70             | 95.52           | 1                  |
| N-CA-CB                | 110.50             | 135.23          | 1                  |
| C-N-CA                 | 121.70             | 147.88          | 1                  |
| CA-C-C-CA-C-CA-CB      | 110.10             | 137.70          | 1                  |
| CA-C-N-CA-C-CA-CB      | 110.10             | 137.69          | 1                  |
| CA-C-C-N-CA            | 121.70             | 147.81          | 1                  |
| C-N-CA                 | 121.70             | 147.79          | 1                  |
| N-CA-CB                | 110.50             | 135.13          | 1                  |
| C-CA-C-N-CA            | 121.70             | 147.78          | 1                  |
| C-CA-C-CA-C-CA-CB      | 109.10             | 77.25           | 1                  |
| N-CA-CB                | 110.50             | 135.11          | 1                  |
| C-CA-CB                | 110.50             | 88.79           | 1                  |
| C-CA-N-CA-CA-C-N-CA-C  | 111.00             | 70.52           | 1                  |
| C-CA-N-CA-N-CA-C-CA-CB | 110.10             | 82.65           | 1                  |
| N-CA-C                 | 111.00             | 70.56           | 1                  |
| C-CA-CB                | 110.10             | 82.66           | 1                  |
| N-CA-C-CA-N-CA-C-CA-CB | 110.10             | 82.68           | 1                  |
| C-CA-N-CA-CB           | 110.50             | 86.00           | 1                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB           | 110.50             | 134.98          | 1                  |
| CA-N-N-CA-CA-C-C-N-CA  | 121.70             | 147.59          | 1                  |
| N-CA-CB                | 110.50             | 86.06           | 1                  |
| N-CA-C-CA-C-CA-C-CA-CB | 110.10             | 82.80           | 1                  |
| C-CA-C-CA-N-CA-CB      | 110.50             | 86.08           | 1                  |
| N-CA-CB                | 110.50             | 134.91          | 1                  |
| C-CA-CB                | 110.10             | 82.82           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 82.82           | 1                  |
| C-N-CA                 | 121.70             | 147.54          | 1                  |
| CA-C-O                 | 120.80             | 145.19          | 1                  |
| N-CA-CA-C-CA-C-O       | 120.80             | 145.18          | 1                  |
| C-CA-CA-C-O            | 120.80             | 145.17          | 1                  |
| CA-C-O                 | 120.80             | 145.17          | 1                  |
| CA-C-O                 | 120.80             | 145.16          | 1                  |
| N-CA-CA-N-N-CA-C       | 111.00             | 70.88           | 1                  |
| CA-C-C-CA-CB           | 110.10             | 82.88           | 1                  |
| C-CA-CB                | 110.10             | 82.88           | 1                  |
| N-CA-C                 | 111.00             | 70.91           | 1                  |
| C-CA-CB                | 110.10             | 137.30          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 137.29          | 1                  |
| N-CA-N-CA-CB           | 110.50             | 86.20           | 1                  |
| C-N-CA                 | 121.70             | 147.42          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-C-O                | 120.80             | 145.10          | 1                  |
| CA-C-O                | 120.80             | 145.09          | 1                  |
| CA-C-O                | 120.80             | 145.08          | 1                  |
| N-CA-CB               | 110.50             | 86.22           | 1                  |
| N-CA-CB               | 110.50             | 86.23           | 1                  |
| CA-C-N-CA-N-CA-C-N-CA | 121.70             | 147.35          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 83.03           | 1                  |
| CA-C-O                | 120.80             | 96.58           | 1                  |
| CA-C-O                | 120.80             | 96.59           | 1                  |
| C-CA-N-CA-CB          | 110.50             | 86.30           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 83.06           | 1                  |
| N-CA-N-CA-CB          | 110.50             | 86.33           | 1                  |
| N-CA-N-CA-N-CA-CB     | 110.50             | 86.37           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 137.06          | 1                  |
| C-CA-CB               | 110.10             | 137.05          | 1                  |
| C-N-CA                | 121.70             | 147.20          | 1                  |
| N-CA-CB               | 110.50             | 86.42           | 1                  |
| C-CA-CB               | 111.60             | 83.28           | 1                  |
| CA-C-C-CA-CB          | 111.60             | 83.29           | 1                  |
| N-CA-CB               | 110.50             | 134.54          | 1                  |
| CA-C-N                | 116.20             | 87.92           | 1                  |
| N-CA-CB               | 110.50             | 134.53          | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| C-N-CA                              | 121.70             | 147.14          | 2                  |
| C-CA-CB                             | 111.60             | 139.87          | 1                  |
| C-N-CA                              | 121.70             | 147.13          | 1                  |
| C-CA-CB                             | 111.40             | 84.56           | 1                  |
| C-CA-C-N-CA                         | 121.70             | 147.11          | 1                  |
| C-CA-C-CA-N-CA-C-CA-C-CA-CB         | 111.60             | 139.81          | 1                  |
| C-N-CA                              | 121.70             | 147.08          | 1                  |
| C-CA-CA-C-O                         | 120.80             | 96.86           | 1                  |
| CA-C-O                              | 120.80             | 144.73          | 1                  |
| CA-C-C-CA-CA-C-CA-C-O               | 120.80             | 144.70          | 1                  |
| CA-C-C-N-CA-C-C-CA-N-CA-C-N-C-CA-CB | 110.10             | 136.71          | 1                  |
| N-CA-C-CA-CA-C-O                    | 120.80             | 97.00           | 1                  |
| C-CA-CB                             | 110.10             | 136.69          | 2                  |
| C-CA-CB                             | 110.10             | 136.68          | 1                  |
| C-N-CA                              | 121.70             | 96.52           | 1                  |
| CA-C-CA-C-CA-C-O                    | 120.80             | 97.07           | 1                  |
| C-CA-CA-C-O                         | 120.80             | 97.09           | 1                  |
| N-CA-CB                             | 110.50             | 86.80           | 1                  |
| C-N-CA                              | 121.70             | 96.61           | 1                  |
| C-CA-C-CA-CB                        | 110.10             | 83.63           | 1                  |
| CA-C-O                              | 120.80             | 97.12           | 1                  |
| N-CA-CB                             | 111.50             | 135.17          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-O                      | 120.80             | 97.14           | 1                  |
| N-CA-CB                     | 111.50             | 135.15          | 1                  |
| CA-C-CA-C-N-CA-CB           | 110.50             | 86.86           | 1                  |
| C-CA-CA-C-N-CA-CB           | 111.50             | 135.11          | 1                  |
| CA-C-CA-C-O                 | 120.80             | 97.20           | 1                  |
| C-N-C-CA-C-N-C-CA-CB        | 110.10             | 136.46          | 1                  |
| C-CA-CB                     | 110.10             | 136.45          | 1                  |
| CA-C-CA-N-CA-C-C-CA-N-CA-CB | 111.50             | 135.04          | 1                  |
| CA-N-N-CA-CB                | 110.50             | 86.97           | 1                  |
| CA-C-O                      | 120.80             | 97.29           | 1                  |
| C-CA-CB                     | 110.10             | 136.38          | 1                  |
| C-N-N-CA-CB                 | 110.50             | 86.99           | 1                  |
| CA-C-C-CA-CB                | 110.10             | 136.37          | 1                  |
| N-CA-C-CA-C-CA-CB           | 111.60             | 83.96           | 1                  |
| C-CA-CB                     | 110.10             | 136.35          | 1                  |
| C-N-C-CA-CB                 | 110.10             | 136.35          | 1                  |
| CA-C-C-CA-CB                | 110.50             | 89.78           | 1                  |
| N-CA-C                      | 111.00             | 72.33           | 2                  |
| N-CA-C                      | 111.00             | 72.34           | 1                  |
| C-CA-CB                     | 111.60             | 83.99           | 1                  |
| C-CA-CB                     | 110.50             | 89.79           | 1                  |
| C-CA-N-CA-C                 | 111.00             | 72.36           | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CB                    | 110.50             | 87.05           | 1                  |
| CA-C-C-CA-N-CA-CB               | 110.50             | 87.08           | 1                  |
| N-CA-CB                         | 110.50             | 87.09           | 1                  |
| C-CA-CB                         | 110.10             | 83.95           | 1                  |
| C-CA-C-CA-C-CA-C-CA-CB          | 110.10             | 83.97           | 1                  |
| N-CA-C-CA-N-CA-C                | 111.00             | 72.50           | 1                  |
| N-CA-N-CA-N-CA-C                | 111.00             | 72.52           | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 136.20          | 1                  |
| CA-C-C-CA-C-CA-C-N-CA           | 121.70             | 96.99           | 1                  |
| N-CA-C-N-CA                     | 121.70             | 96.99           | 1                  |
| CA-C-N                          | 116.20             | 88.76           | 1                  |
| C-CA-N-CA-CA-C-C-CA-CB          | 110.10             | 136.16          | 1                  |
| N-CA-N-CA-CB                    | 110.50             | 133.80          | 1                  |
| C-CA-N-CA-CA-C-C-CA-CA-C-O      | 120.80             | 144.05          | 1                  |
| C-CA-N-CA-CB                    | 110.50             | 133.74          | 1                  |
| C-CA-CB                         | 111.40             | 85.43           | 1                  |
| N-CA-N-CA-CB                    | 110.50             | 87.28           | 1                  |
| CA-C-O                          | 120.80             | 144.00          | 1                  |
| C-CA-C-CA-CB                    | 111.40             | 85.48           | 1                  |
| N-CA-CA-C-O                     | 120.80             | 97.64           | 1                  |
| N-CA-C-CA-C-CA-N-CA-C-CA-C-N-CA | 121.70             | 146.16          | 1                  |
| C-CA-N-CA-CA-C-N-CA-CB          | 110.50             | 87.41           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-N-CA-C-N-CA      | 121.70             | 146.13          | 1                  |
| CA-C-O                     | 120.80             | 97.73           | 1                  |
| N-CA-C                     | 111.00             | 148.99          | 1                  |
| C-CA-N-CA-N-CA-C-CA-N-CA-C | 111.00             | 148.97          | 1                  |
| C-CA-CB                    | 111.40             | 85.63           | 1                  |
| N-CA-C-CA-CB               | 110.10             | 84.34           | 1                  |
| C-CA-CB                    | 111.40             | 85.66           | 1                  |
| N-CA-C                     | 112.10             | 78.24           | 1                  |
| C-CA-CB                    | 110.10             | 135.83          | 1                  |
| N-CA-C                     | 112.10             | 78.26           | 1                  |
| C-CA-CB                    | 110.10             | 135.82          | 1                  |
| N-CA-CB                    | 110.50             | 87.50           | 1                  |
| C-CA-CB                    | 110.10             | 84.39           | 1                  |
| C-CA-CB                    | 111.60             | 84.55           | 1                  |
| C-CA-N-CA-CB               | 110.50             | 87.51           | 1                  |
| C-CA-CB                    | 110.10             | 135.78          | 1                  |
| C-CA-CB                    | 110.10             | 84.43           | 1                  |
| C-CA-CB                    | 110.10             | 84.44           | 3                  |
| C-CA-CB                    | 111.60             | 84.60           | 1                  |
| C-CA-C-N-CA                | 121.70             | 97.45           | 1                  |
| N-CA-CB                    | 110.50             | 133.40          | 1                  |
| N-CD-CG                    | 103.20             | 123.41          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-C-CA-CB      | 110.10             | 135.67          | 1                  |
| C-CA-CB                | 110.10             | 135.67          | 1                  |
| N-CD-CG                | 103.20             | 123.38          | 1                  |
| C-CA-CB                | 110.10             | 135.66          | 2                  |
| N-CA-C-CA-C-CA-CB      | 110.10             | 135.64          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 87.67           | 2                  |
| N-CA-CB                | 111.50             | 134.31          | 2                  |
| CA-C-O                 | 120.80             | 98.00           | 2                  |
| N-CA-CB                | 111.50             | 134.30          | 1                  |
| CA-C-N-CA-CA-C-C-CA-CB | 110.10             | 84.62           | 1                  |
| C-N-CA                 | 121.70             | 97.57           | 1                  |
| N-CA-CB                | 111.50             | 134.29          | 2                  |
| CA-C-C-CA-CB           | 110.10             | 84.64           | 1                  |
| N-CA-CB                | 110.50             | 133.27          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 87.75           | 1                  |
| N-CA-C-N-CA            | 122.60             | 55.72           | 1                  |
| C-N-CA                 | 122.60             | 55.76           | 1                  |
| C-N-CD                 | 125.00             | 70.21           | 1                  |
| N-CA-CB                | 111.50             | 134.22          | 1                  |
| C-N-CD                 | 125.00             | 70.22           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 84.78           | 1                  |
| O-C-N                  | 123.00             | 101.68          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                     | 110.10             | 84.79           | 1                  |
| CA-C-N                      | 116.20             | 142.83          | 1                  |
| C-CA-CA-C-C-N-CA            | 121.70             | 97.74           | 1                  |
| C-N-CA                      | 121.70             | 97.74           | 1                  |
| C-N-CA                      | 121.70             | 97.75           | 2                  |
| C-CA-CB                     | 110.10             | 84.82           | 1                  |
| C-CA-CB                     | 110.10             | 84.83           | 1                  |
| C-CA-N-CA-N-CA-C-CA-C-CA-CB | 110.10             | 135.35          | 1                  |
| C-CA-CB                     | 110.10             | 135.35          | 1                  |
| N-CA-CA-C-N                 | 116.20             | 142.77          | 1                  |
| N-CA-CB                     | 110.50             | 87.91           | 1                  |
| CA-C-O                      | 120.80             | 98.23           | 1                  |
| O-C-N                       | 123.00             | 101.77          | 1                  |
| CA-C-O                      | 120.80             | 98.24           | 2                  |
| O-C-CA-C-CA-C-C-N-CA        | 121.70             | 145.56          | 1                  |
| C-N-CA                      | 121.70             | 145.55          | 1                  |
| CA-C-CA-C-O                 | 120.80             | 98.28           | 1                  |
| C-CA-CB                     | 110.10             | 84.94           | 1                  |
| O-C-C-N-CA                  | 121.70             | 145.53          | 1                  |
| O-C-N                       | 123.00             | 101.83          | 1                  |
| C-N-CA                      | 121.70             | 145.52          | 2                  |
| O-C-O-C-N                   | 123.00             | 101.84          | 2                  |



| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| C-CA-CB             | 110.10             | 84.97           | 1                  |
| C-N-CA              | 121.70             | 145.51          | 1                  |
| N-CA-C              | 111.00             | 73.97           | 1                  |
| O-C-N               | 123.00             | 101.84          | 1                  |
| O-C-C-CA-CB         | 110.10             | 84.99           | 1                  |
| O-C-N               | 123.00             | 101.86          | 1                  |
| O-C-N-CA-C          | 111.00             | 74.01           | 1                  |
| O-C-C-N-O-C-N       | 123.00             | 101.86          | 1                  |
| C-CA-CB             | 110.10             | 85.00           | 1                  |
| O-C-N               | 123.00             | 101.87          | 2                  |
| C-CA-C-CA-CB        | 109.10             | 138.14          | 1                  |
| O-C-O-C-N           | 123.00             | 101.88          | 1                  |
| O-C-N               | 123.00             | 101.88          | 1                  |
| C-CA-C-CA-O-C-N     | 123.00             | 101.90          | 1                  |
| O-C-O-C-CA-C-O      | 120.80             | 98.38           | 1                  |
| O-C-O-C-O-C-N       | 123.00             | 101.91          | 1                  |
| CA-C-O              | 120.80             | 98.39           | 1                  |
| N-CA-C              | 111.00             | 147.91          | 1                  |
| C-CA-O-C-O-C-CA-C-O | 120.80             | 98.41           | 1                  |
| C-CA-CB             | 110.10             | 135.13          | 1                  |
| C-CA-CB             | 109.10             | 138.08          | 1                  |
| O-C-N               | 123.00             | 101.93          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-O-C-O-C-O-C-CA-C-O                                | 120.80             | 98.41           | 1                  |
| O-C-O-C-N  | 123.00             | 101.94          | 1                  |
| N-CA-O-C-O-C-O-C-C-CA-CB                               | 110.10             | 85.10           | 1                  |
| N-CA-C   | 111.00             | 147.83          | 1                  |
| N-CA-CB  | 110.50             | 132.86          | 1                  |
| C-N-C-CA-O-C-O-C-C-CA-C-CA-CB                          | 110.10             | 135.07          | 1                  |
| C-CA-C-CA-CB   | 110.10             | 135.06          | 1                  |
| C-CA-CB  | 110.10             | 85.14           | 1                  |
| CA-C-O   | 120.80             | 98.47           | 1                  |
| N-CA-C-CA-CB   | 110.10             | 85.15           | 1                  |
| C-CA-C-N-O-C-N-CA-N-CA-N-CA-C-CA-CA-C-C-N-C-CA-C-CA-CB | 110.10             | 135.01          | 1                  |
| N-CA-CB  | 110.50             | 88.22           | 1                  |
| C-CA-CB  | 110.10             | 85.20           | 1                  |
| N-CA-C   | 111.00             | 147.69          | 1                  |
| N-CD-C-CA-CB   | 110.10             | 85.21           | 1                  |
| N-CA-CB  | 110.50             | 132.76          | 1                  |
| C-CA-N-CA-CA-C-O                                       | 120.80             | 98.55           | 1                  |
| C-CA-N-CA-C-CA-N-CA-C-N-C-CA-CB                        | 110.10             | 85.25           | 1                  |
| C-CA-CB  | 110.10             | 85.25           | 1                  |
| C-CA-C-CA-N-CD-N-CA-C                                  | 111.00             | 147.59          | 1                  |
| C-CA-C-CA-C-N-CA                                       | 121.70             | 145.21          | 1                  |
| C-CA-N-CA-C  | 111.00             | 74.44           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-O                 | 119.00             | 79.84           | 1                  |
| C-N-N-CA-C             | 111.00             | 74.46           | 1                  |
| N-CA-C-N-C-CA-CB       | 110.10             | 134.88          | 1                  |
| CA-C-O                 | 119.00             | 79.88           | 1                  |
| C-CA-CB                | 110.10             | 85.32           | 1                  |
| C-CA-CB                | 110.10             | 134.87          | 1                  |
| N-CA-C-CA-C-CA-C-CA-CB | 110.10             | 134.84          | 1                  |
| N-CA-CB                | 110.50             | 132.61          | 1                  |
| N-CA-CB                | 110.50             | 88.39           | 1                  |
| C-CA-C-N-CA            | 121.70             | 145.10          | 1                  |
| C-N-C-CA-CB            | 110.10             | 134.80          | 1                  |
| C-CA-CB                | 110.10             | 134.80          | 1                  |
| C-CA-C-CA-C-CA-CB      | 110.10             | 134.79          | 1                  |
| CA-C-N-CA-CB           | 110.50             | 132.58          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 134.78          | 1                  |
| N-CA-N-CA-C-CA-CB      | 110.10             | 134.77          | 1                  |
| N-CA-C                 | 111.00             | 74.65           | 1                  |
| CA-C-O                 | 120.80             | 98.73           | 1                  |
| CA-C-N-CA-CB           | 110.50             | 132.55          | 1                  |
| C-CA-CB                | 110.10             | 134.75          | 1                  |
| CA-C-N-CA-C            | 111.00             | 74.68           | 1                  |
| C-CA-CB                | 110.10             | 134.73          | 2                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-O        | 120.80             | 142.83          | 1                  |
| N-CA-N-CA-C-CA-CB | 110.10             | 134.71          | 1                  |
| N-CA-CB           | 110.50             | 132.52          | 1                  |
| C-CA-CB           | 110.10             | 134.70          | 1                  |
| C-N-CA            | 121.70             | 144.99          | 2                  |
| N-CA-CB           | 103.00             | 117.23          | 1                  |
| CA-C-O            | 120.80             | 98.81           | 1                  |
| C-CA-C-CA-C-N-CA  | 121.70             | 98.43           | 1                  |
| CA-C-O            | 120.80             | 142.78          | 2                  |
| C-CA-N-CA-C-CA-CB | 110.10             | 134.65          | 1                  |
| C-N-N-CA-CB       | 110.50             | 132.46          | 1                  |
| N-CA-N-CA-CA-C-O  | 120.80             | 98.85           | 1                  |
| C-CA-CA-C-O       | 120.80             | 142.74          | 1                  |
| N-CA-CB           | 110.50             | 132.44          | 1                  |
| CA-C-O            | 120.80             | 98.87           | 1                  |
| N-CA-CB           | 110.50             | 88.57           | 1                  |
| C-CA-CB           | 110.10             | 134.60          | 2                  |
| N-CA-C-CA-CB      | 110.10             | 134.60          | 1                  |
| C-CA-CB           | 110.10             | 134.59          | 1                  |
| CA-C-O            | 120.80             | 142.71          | 1                  |
| C-CA-CB           | 111.40             | 86.92           | 1                  |
| N-CA-C            | 112.10             | 144.31          | 2                  |

| Angle type                              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| N-CA-CB                                 | 110.50             | 88.60           | 1                  |
| C-N-CA                                  | 121.70             | 144.88          | 1                  |
| C-CA-CB                                 | 111.40             | 86.94           | 1                  |
| C-CA-CB                                 | 110.10             | 134.56          | 1                  |
| N-CA-C-CA-CB                            | 110.10             | 134.56          | 1                  |
| C-CA-CB                                 | 110.10             | 134.55          | 1                  |
| N-CA-CA-C-C-CA-CB                       | 110.10             | 134.54          | 1                  |
| CA-C-N-CA-C-N-CA                        | 121.70             | 98.55           | 1                  |
| CA-C-N-CA-CB                            | 103.00             | 117.14          | 1                  |
| C-CA-CA-C-N                             | 116.20             | 90.49           | 1                  |
| N-CA-CB                                 | 110.50             | 132.35          | 1                  |
| N-CA-N-CA-C-N-CA                        | 121.70             | 144.83          | 1                  |
| CA-C-N                                  | 116.20             | 141.89          | 2                  |
| N-CA-N-CA-C-CA-CB                       | 110.10             | 134.50          | 1                  |
| N-CA-N-CA-CB                            | 111.50             | 89.69           | 1                  |
| N-CA-CB                                 | 110.50             | 132.30          | 1                  |
| CA-C-N-CA-CB                            | 110.50             | 88.71           | 1                  |
| N-CA-CA-C-O                             | 120.80             | 99.02           | 1                  |
| N-CA-C-N-N-CA-N-CA-N-CA-C-CA-C-N-CA-C-O | 120.80             | 142.53          | 1                  |
| CA-C-N                                  | 116.20             | 90.64           | 1                  |
| N-CA-CB                                 | 110.50             | 132.23          | 1                  |
| C-N-CA-C-O                              | 120.80             | 99.08           | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| CA-C-O                          | 120.80             | 99.09           | 1                  |
| C-CA-CB                         | 110.10             | 134.35          | 1                  |
| CA-C-C-CA-CB                    | 110.10             | 85.85           | 1                  |
| C-CA-CB                         | 110.10             | 85.86           | 1                  |
| N-CA-CB                         | 110.50             | 132.18          | 1                  |
| C-CA-CB                         | 110.10             | 134.32          | 1                  |
| N-CA-CB                         | 110.40             | 91.28           | 1                  |
| N-CA-C-N-N-CA-N-CA-C-N-C-CA-CB  | 110.50             | 91.42           | 1                  |
| N-CA-CB                         | 110.40             | 91.32           | 1                  |
| CA-C-O                          | 120.80             | 99.17           | 1                  |
| C-CA-CB                         | 110.10             | 134.27          | 1                  |
| C-CA-CB                         | 110.10             | 134.26          | 1                  |
| C-N-N-CA-N-CA-C-CA-N-CA-C-CA-CB | 110.50             | 91.44           | 1                  |
| CA-C-N-CA-C-CA-CA-C-O           | 120.80             | 99.22           | 1                  |
| N-CA-CB                         | 103.00             | 116.95          | 1                  |
| CA-C-N                          | 116.20             | 90.83           | 1                  |
| N-CA-CA-C-N-CA-CA-C-C-CA-CB     | 110.10             | 86.01           | 1                  |
| C-CA-CA-C-N-CA-C                | 111.00             | 75.50           | 1                  |
| C-CA-CB                         | 110.10             | 134.19          | 1                  |
| CA-C-N                          | 116.20             | 90.85           | 1                  |
| C-CA-CB                         | 111.60             | 86.25           | 1                  |
| CA-C-C-CA-CB                    | 110.10             | 86.03           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CA-C-O      | 120.80             | 99.27           | 1                  |
| CA-C-CA-C-O           | 120.80             | 99.27           | 1                  |
| C-CA-CB               | 111.60             | 86.28           | 1                  |
| CA-C-CA-C-C-CA-CB     | 110.10             | 134.15          | 1                  |
| CA-C-CA-C-N-CA-C      | 111.00             | 75.57           | 1                  |
| CA-C-O                | 120.80             | 99.29           | 1                  |
| CA-C-N-CA-N-CA-C-N-CA | 121.70             | 98.94           | 1                  |
| N-CA-N-CA-C-CA-N-CA-C | 111.00             | 146.40          | 1                  |
| N-CA-C                | 111.00             | 75.62           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 86.09           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 86.10           | 1                  |
| C-CA-CB               | 110.10             | 86.10           | 1                  |
| CA-C-O                | 120.80             | 142.27          | 1                  |
| C-CA-CB               | 111.60             | 86.34           | 1                  |
| N-CA-C                | 111.00             | 75.63           | 1                  |
| CA-C-O                | 120.80             | 99.33           | 1                  |
| CA-C-C-N-CA           | 121.70             | 98.97           | 1                  |
| C-N-CA                | 121.70             | 98.97           | 2                  |
| CA-C-C-N-CA           | 121.70             | 98.98           | 1                  |
| N-CA-C                | 111.00             | 146.34          | 1                  |
| C-N-N-CA-CB           | 111.50             | 132.95          | 1                  |
| C-N-CA                | 121.70             | 144.40          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB                | 111.60             | 86.38           | 1                  |
| C-N-CA                      | 121.70             | 99.00           | 1                  |
| N-CA-CA-C-C-N-N-CA-CB       | 110.50             | 131.92          | 1                  |
| C-CA-CB                     | 110.10             | 86.17           | 2                  |
| CA-C-C-N-CA                 | 121.70             | 99.03           | 1                  |
| CA-C-O                      | 120.80             | 99.39           | 1                  |
| C-CA-C-CA-CB                | 110.10             | 86.18           | 1                  |
| C-N-CA                      | 121.70             | 144.36          | 1                  |
| CA-C-CA-C-O                 | 120.80             | 99.41           | 1                  |
| C-N-CA                      | 121.70             | 99.06           | 1                  |
| CA-C-O                      | 120.80             | 99.42           | 1                  |
| C-N-CA-C-O                  | 120.80             | 142.16          | 1                  |
| C-N-CA                      | 121.70             | 99.09           | 1                  |
| C-CA-CB                     | 110.10             | 133.96          | 1                  |
| N-CA-CB                     | 111.50             | 132.85          | 1                  |
| N-CA-CB                     | 110.50             | 131.84          | 1                  |
| N-CA-CB                     | 103.00             | 116.81          | 1                  |
| C-N-CA                      | 121.70             | 99.10           | 1                  |
| CA-C-CA-C-CA-C-C-CA-CB      | 110.10             | 133.92          | 1                  |
| C-N-C-N-C-CA-CB             | 110.10             | 133.91          | 1                  |
| N-CA-CB                     | 110.50             | 89.20           | 1                  |
| N-CA-C-CA-CA-C-C-CA-C-CA-CB | 110.10             | 133.87          | 1                  |



| Angle type                        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-N-CA-CB                  | 110.50             | 89.26           | 1                  |
| C-N-CA                            | 121.70             | 144.19          | 1                  |
| C-CA-CB                           | 110.10             | 133.83          | 1                  |
| CA-C-N-CA-CB                      | 110.50             | 131.73          | 1                  |
| N-CA-N-CA-C                       | 111.00             | 145.97          | 1                  |
| C-N-CA                            | 121.70             | 144.17          | 1                  |
| C-CA-N-CA-N-CA-C-CA-CB            | 110.10             | 133.78          | 1                  |
| CA-C-N-CA-C                       | 111.00             | 76.11           | 1                  |
| C-CA-CB                           | 110.10             | 133.77          | 1                  |
| N-CA-C                            | 111.00             | 76.12           | 1                  |
| N-CA-CB                           | 110.50             | 131.67          | 1                  |
| C-CA-N-CA-CB                      | 110.40             | 129.08          | 1                  |
| N-CA-C-CA-C-CA-C-CA-C-CA-C-CA-C-N | 116.20             | 141.07          | 1                  |
| N-CA-N-CA-N-CA-CB                 | 110.40             | 129.05          | 1                  |
| C-CA-CB                           | 110.10             | 133.71          | 1                  |
| C-N-N-CA-CB                       | 111.50             | 90.38           | 1                  |
| C-CA-N-CA-N-CA-C-N-CA-C-N         | 116.20             | 91.37           | 1                  |
| C-CA-CB                           | 110.10             | 86.52           | 2                  |
| N-CA-CB                           | 111.50             | 90.40           | 1                  |
| C-CA-C-CA-CB                      | 110.10             | 86.53           | 1                  |
| N-CA-CB                           | 111.50             | 90.41           | 1                  |
| N-CA-CB                           | 111.50             | 90.42           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.10             | 86.54           | 1                  |
| CA-CB-CG                   | 112.60             | 125.00          | 1                  |
| N-CA-N-CA-C-CA-CB          | 110.10             | 133.65          | 1                  |
| CA-C-N                     | 116.20             | 91.42           | 1                  |
| C-CA-CB                    | 110.10             | 86.57           | 1                  |
| CA-C-N                     | 116.90             | 98.33           | 1                  |
| CA-C-N                     | 116.20             | 140.96          | 1                  |
| C-N-CA-C-O                 | 120.80             | 141.84          | 1                  |
| N-CA-N-CA-N-CA-C-CA-N-CA-C | 111.00             | 145.60          | 1                  |
| C-CA-CB                    | 110.10             | 86.62           | 1                  |
| C-CA-CB                    | 110.10             | 86.64           | 2                  |
| CA-C-C-CA-N-CA-C-N-CA      | 121.70             | 99.49           | 1                  |
| CA-C-N-CA-CA-C-C-CA-CB     | 110.10             | 86.66           | 1                  |
| N-CA-C                     | 111.00             | 145.54          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 133.53          | 1                  |
| N-CA-C                     | 113.30             | 149.06          | 1                  |
| C-CA-CB                    | 110.10             | 86.68           | 1                  |
| CA-C-N                     | 116.90             | 98.41           | 1                  |
| N-CA-C                     | 113.30             | 149.05          | 1                  |
| C-CA-N-CA-C-CA-CA-CB-CG    | 112.60             | 124.92          | 1                  |
| C-CA-CB                    | 110.10             | 133.50          | 1                  |
| CA-C-N                     | 116.20             | 140.83          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-N-CA                     | 121.70             | 99.54           | 1                  |
| C-CA-CA-C-O                | 120.80             | 141.72          | 1                  |
| CA-C-O                     | 120.80             | 99.88           | 1                  |
| C-CA-CB                    | 110.10             | 86.72           | 1                  |
| C-CA-CA-C-N                | 116.20             | 140.80          | 1                  |
| C-CA-CA-C-O                | 120.80             | 99.89           | 1                  |
| N-CA-C                     | 111.00             | 76.58           | 1                  |
| C-CA-CB                    | 110.10             | 86.75           | 1                  |
| C-CA-N-CD-CG               | 103.20             | 84.77           | 1                  |
| N-CD-CG                    | 103.20             | 84.78           | 1                  |
| C-CA-C-CA-CB               | 110.10             | 133.42          | 1                  |
| CA-C-O                     | 120.80             | 99.94           | 1                  |
| CA-C-N-CA-C                | 111.00             | 76.64           | 1                  |
| N-CA-C                     | 111.00             | 76.65           | 1                  |
| CA-C-CA-C-C-CA-O-C-N-CA-CB | 111.50             | 132.34          | 1                  |
| C-CA-CB                    | 110.10             | 133.38          | 1                  |
| O-C-C-CA-CB                | 110.10             | 133.36          | 1                  |
| N-CA-CB                    | 110.40             | 128.76          | 1                  |
| CA-C-O                     | 120.80             | 99.99           | 1                  |
| C-CA-CB                    | 110.10             | 86.85           | 1                  |
| C-CA-CB                    | 110.10             | 133.35          | 2                  |
| N-CA-CB                    | 103.00             | 116.46          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| C-CA-CB      | 110.10             | 86.86           | 1                  |
| N-CA-N-CA-C  | 111.00             | 76.76           | 1                  |
| N-CA-CB      | 110.50             | 89.72           | 1                  |
| C-CA-CB      | 110.10             | 133.33          | 1                  |
| CA-C-O       | 120.80             | 100.03          | 1                  |
| C-CA-N-CA-C  | 111.00             | 76.79           | 1                  |
| N-CA-C       | 111.00             | 145.20          | 1                  |
| N-CA-CB      | 110.40             | 128.72          | 1                  |
| C-CA-CB      | 110.10             | 86.90           | 2                  |
| C-CA-C-CA-CB | 110.10             | 133.29          | 1                  |
| N-CA-CB      | 111.50             | 132.25          | 1                  |
| C-CA-CB      | 110.10             | 86.92           | 1                  |
| N-CA-C       | 111.00             | 145.16          | 1                  |
| N-CA-CB      | 110.50             | 131.24          | 1                  |
| N-CA-C       | 111.00             | 76.86           | 1                  |
| N-CA-CA-N-CD | 112.00             | 94.93           | 1                  |
| N-CA-CB      | 110.50             | 89.77           | 1                  |
| C-CA-CB      | 110.10             | 133.26          | 1                  |
| C-CA-CB      | 110.10             | 133.25          | 1                  |
| CA-N-CD      | 112.00             | 94.94           | 1                  |
| C-CA-CB      | 110.10             | 133.24          | 1                  |
| CA-C-N       | 116.20             | 91.84           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-N                | 116.20             | 91.85           | 1                  |
| C-CA-CB                    | 110.10             | 133.23          | 1                  |
| CA-C-N                     | 116.20             | 91.85           | 1                  |
| C-N-CA-C-N                 | 116.20             | 91.86           | 1                  |
| N-CA-CB                    | 103.00             | 116.39          | 1                  |
| CA-N-C-CA-CA-N-C-CA-CB     | 110.10             | 87.00           | 1                  |
| C-CA-CB                    | 110.10             | 133.20          | 2                  |
| C-CA-N-CA-C                | 111.00             | 145.01          | 1                  |
| N-CA-C                     | 111.00             | 145.01          | 1                  |
| N-CA-CB                    | 110.50             | 131.14          | 1                  |
| C-N-N-CA-CB                | 110.50             | 131.13          | 1                  |
| C-CA-N-CA-C                | 111.00             | 144.93          | 1                  |
| N-CA-C-CA-C-CA-CB          | 110.10             | 87.08           | 1                  |
| N-CA-CA-C-C-N-CA           | 121.70             | 143.49          | 1                  |
| N-CA-N-CA-C-CA-CA-C-C-N-CA | 121.70             | 143.47          | 1                  |
| N-CA-N-CA-N-CA-C           | 111.00             | 77.16           | 1                  |
| C-CA-CB                    | 109.10             | 82.52           | 2                  |
| N-CA-CB                    | 110.50             | 89.96           | 1                  |
| N-CA-CB                    | 110.50             | 131.04          | 1                  |
| CA-C-N                     | 116.20             | 92.05           | 1                  |
| N-CA-CB                    | 110.50             | 89.98           | 1                  |
| N-CA-CA-C-N                | 116.20             | 92.06           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-N-CA                      | 121.70             | 99.97           | 1                  |
| N-CA-C                      | 111.00             | 144.80          | 1                  |
| N-CA-CB                     | 110.50             | 131.02          | 1                  |
| C-CA-CA-C-C-CA-CB           | 110.10             | 133.03          | 1                  |
| CA-C-N-CA-C                 | 111.00             | 77.22           | 1                  |
| C-CA-C-CA-C-CA-CB           | 110.10             | 87.18           | 1                  |
| C-CA-CA-C-C-CA-N-CA-N-CA-CB | 111.50             | 131.99          | 1                  |
| C-CA-CB                     | 111.60             | 87.50           | 1                  |
| N-CA-C                      | 111.00             | 77.26           | 1                  |
| C-CA-N-CA-CB                | 110.50             | 130.98          | 1                  |
| C-CA-CB                     | 110.10             | 87.21           | 1                  |
| C-CA-N-CA-C                 | 111.00             | 77.28           | 1                  |
| N-CA-CB                     | 110.50             | 90.03           | 2                  |
| C-N-CA                      | 121.70             | 100.03          | 1                  |
| N-CA-CB                     | 110.50             | 130.96          | 1                  |
| C-CA-CB                     | 111.60             | 87.53           | 1                  |
| CA-C-C-CA-CB                | 110.10             | 132.97          | 1                  |
| N-CA-C                      | 111.00             | 77.31           | 1                  |
| N-CA-CB                     | 111.50             | 131.95          | 1                  |
| C-CA-CB                     | 110.10             | 132.96          | 1                  |
| C-CA-CA-C-O                 | 120.80             | 141.24          | 1                  |
| N-CA-C-N-CA                 | 121.70             | 100.06          | 1                  |

| Angle type                               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-CA-CB                                  | 111.60             | 87.56           | 1                  |
| C-CA-N-CA-C-CA-CB                        | 110.10             | 132.94          | 1                  |
| C-CA-N-CA-CB                             | 110.50             | 90.07           | 1                  |
| N-CA-C                                   | 111.00             | 77.36           | 1                  |
| C-N-N-CA-CB                              | 110.50             | 90.08           | 1                  |
| C-N-CA                                   | 121.70             | 100.08          | 1                  |
| C-CA-C-N-N-CA-C-CA-CB                    | 110.10             | 132.91          | 1                  |
| CA-C-C-CA-N-CA-N-CA-CB                   | 110.50             | 90.10           | 1                  |
| N-CA-N-CA-CA-C-O                         | 120.80             | 100.41          | 1                  |
| C-CA-C-CA-CB                             | 111.60             | 87.62           | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB                   | 110.50             | 90.12           | 1                  |
| CA-C-O                                   | 120.80             | 100.42          | 1                  |
| C-CA-C-CA-CB                             | 110.10             | 132.87          | 1                  |
| N-CA-CB                                  | 110.50             | 90.13           | 1                  |
| CA-C-N                                   | 116.20             | 140.16          | 1                  |
| N-CA-C-CA-N-CA-CA-C-O                    | 120.80             | 141.15          | 1                  |
| C-CA-CA-C-N                              | 116.20             | 140.13          | 1                  |
| N-CA-CA-C-N-CA-C-CA-CA-C-C-N-C-N-N-CA-CB | 110.50             | 90.20           | 1                  |
| N-CA-N-CA-CA-C-N                         | 116.20             | 140.08          | 1                  |
| C-CA-C-CA-C-CA-CB                        | 110.10             | 87.42           | 1                  |
| CA-C-N-CA-CB                             | 111.50             | 131.78          | 1                  |
| CA-C-C-CA-C-CA-N-CA-CB                   | 110.50             | 90.23           | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA-C-N                | 116.20             | 140.03          | 1                  |
| CA-C-N                         | 116.20             | 140.01          | 1                  |
| N-CA-CB                        | 111.50             | 131.73          | 1                  |
| CA-C-C-N-N-CA-N-CA-C-N-C-CA-CB | 110.10             | 132.68          | 1                  |
| C-CA-CB                        | 110.10             | 87.52           | 3                  |
| C-CA-CB                        | 110.10             | 132.68          | 1                  |
| C-N-C-CA-CB                    | 110.10             | 87.53           | 1                  |
| N-CA-CB                        | 110.50             | 90.31           | 1                  |
| C-N-C-N-CA                     | 121.70             | 143.07          | 1                  |
| N-CA-C                         | 111.00             | 144.24          | 1                  |
| C-N-N-CA-C                     | 111.00             | 144.23          | 1                  |
| N-CA-C-CA-C-N-CA               | 121.70             | 143.06          | 1                  |
| C-CA-C-N-C-CA-N-CA-CB          | 110.40             | 128.18          | 1                  |
| N-CA-C                         | 111.00             | 144.19          | 1                  |
| C-CA-C-N-CA                    | 121.70             | 143.02          | 1                  |
| CA-N-CD                        | 112.00             | 95.42           | 1                  |
| N-CA-CB                        | 110.40             | 128.16          | 1                  |
| C-CA-N-CA-C-CA-N-CA-C          | 111.00             | 144.11          | 1                  |
| C-N-CA                         | 121.70             | 142.98          | 1                  |
| N-CA-C                         | 111.00             | 144.09          | 1                  |
| C-CA-N-CA-CA-C-O               | 120.80             | 100.71          | 1                  |
| C-CA-N-CA-C                    | 111.00             | 77.93           | 1                  |



| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-C                      | 111.00             | 77.93           | 1                  |
| C-CA-C-CA-CB                | 110.10             | 87.68           | 1                  |
| C-CA-CA-C-O                 | 120.80             | 100.74          | 1                  |
| C-CA-C-CA-CA-N-CD           | 112.00             | 95.49           | 1                  |
| C-CA-C-CA-CB                | 110.10             | 87.71           | 1                  |
| N-CA-C                      | 111.00             | 143.99          | 1                  |
| N-CA-CB                     | 110.50             | 90.47           | 1                  |
| CA-C-O                      | 120.80             | 140.83          | 1                  |
| N-CA-C                      | 111.00             | 143.98          | 1                  |
| N-CA-C                      | 111.00             | 78.02           | 1                  |
| CA-C-O                      | 120.80             | 100.78          | 1                  |
| N-CA-C-N-CA                 | 121.70             | 100.51          | 1                  |
| C-N-N-CA-CB                 | 110.50             | 90.49           | 1                  |
| N-CA-N-CA-CB                | 110.50             | 90.49           | 1                  |
| N-CA-C                      | 111.00             | 78.06           | 1                  |
| N-CA-C-CA-C-CA-N-CA-C-CA-CB | 110.10             | 132.43          | 1                  |
| CA-C-O                      | 120.80             | 100.82          | 1                  |
| CA-C-C-N-CA                 | 121.70             | 142.85          | 1                  |
| N-CA-C-CA-C-CA-CB           | 110.10             | 87.81           | 1                  |
| CA-C-O                      | 120.80             | 145.44          | 1                  |
| N-CA-CA-C-N                 | 116.20             | 139.66          | 1                  |
| CA-C-C-N-CA                 | 121.70             | 142.81          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| CA-C-O                           | 120.80             | 100.87          | 1                  |
| CA-C-O                           | 120.80             | 145.42          | 1                  |
| N-CA-C-CA-CB                     | 110.10             | 132.36          | 1                  |
| C-CA-N-CA-C-CA-C-CA-C-CA-C-CA-CB | 110.10             | 87.87           | 1                  |
| CA-C-N-CA-CA-C-O                 | 120.80             | 100.92          | 1                  |
| C-CA-CA-C-O                      | 120.80             | 100.93          | 1                  |
| CA-C-O                           | 120.80             | 100.93          | 1                  |
| C-CA-C-N-CA                      | 121.70             | 142.73          | 1                  |
| CA-C-N                           | 116.20             | 92.84           | 1                  |
| C-CA-C-CA-CB                     | 110.10             | 132.28          | 1                  |
| C-N-CA                           | 121.70             | 142.72          | 1                  |
| C-CA-CB                          | 110.10             | 132.28          | 1                  |
| N-CA-CB                          | 110.50             | 130.35          | 1                  |
| CA-C-N                           | 116.20             | 139.55          | 1                  |
| C-N-CA                           | 121.70             | 142.71          | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB           | 110.50             | 130.31          | 1                  |
| CA-C-N                           | 116.20             | 92.90           | 1                  |
| CA-C-O                           | 120.80             | 100.99          | 1                  |
| CA-C-N-CA-C-N-CA                 | 121.70             | 142.65          | 1                  |
| CA-C-O                           | 120.80             | 96.39           | 1                  |
| CA-C-O                           | 120.80             | 101.04          | 1                  |
| N-CA-C                           | 111.00             | 78.47           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CA-C-C-CA-CB | 110.50             | 127.92          | 1                  |
| CA-C-N                 | 116.20             | 92.98           | 1                  |
| CA-C-N                 | 116.20             | 92.99           | 1                  |
| N-CA-N-CA-C            | 111.00             | 143.48          | 1                  |
| N-CA-C                 | 111.00             | 78.53           | 1                  |
| C-CA-CB                | 110.10             | 132.13          | 1                  |
| N-CA-N-CA-C            | 111.00             | 143.44          | 1                  |
| C-CA-CB                | 110.10             | 132.11          | 1                  |
| CA-C-N-CA-CA-C-O       | 120.80             | 96.49           | 1                  |
| C-CA-CB                | 110.10             | 132.09          | 1                  |
| N-CA-C                 | 111.00             | 78.60           | 1                  |
| C-CA-CB                | 110.10             | 132.08          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 132.08          | 1                  |
| N-CA-C                 | 111.00             | 78.61           | 1                  |
| C-CA-CB                | 110.10             | 132.07          | 1                  |
| C-CA-C-CA-C-CA-CB      | 110.50             | 127.83          | 1                  |
| CA-C-CA-C-N-CA-C-CA-CB | 110.10             | 132.04          | 1                  |
| N-CA-CB                | 110.40             | 93.09           | 2                  |
| C-CA-CB                | 110.10             | 132.02          | 1                  |
| N-CA-C-CA-C-N-C-CA-CB  | 110.10             | 88.19           | 1                  |
| N-CA-C-CA-CB           | 110.10             | 132.01          | 1                  |
| C-N-CA                 | 121.70             | 142.45          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-N-C-CA-CB                 | 110.10             | 88.20           | 1                  |
| C-CA-CA-C-N-CA-CA-C-C-CA-CB | 110.10             | 131.97          | 1                  |
| C-CA-CB                     | 110.10             | 88.23           | 1                  |
| C-CA-CB                     | 110.10             | 131.95          | 1                  |
| CA-C-N-CA-C-CA-CB           | 110.10             | 88.30           | 1                  |
| C-CA-CB                     | 110.10             | 131.90          | 1                  |
| C-CA-CB                     | 110.10             | 88.31           | 1                  |
| C-CA-CB                     | 110.10             | 131.89          | 1                  |
| C-N-CA                      | 121.70             | 101.06          | 1                  |
| CA-C-C-CA-CB                | 110.10             | 131.87          | 1                  |
| CA-C-O                      | 120.80             | 101.32          | 1                  |
| C-N-CA                      | 121.70             | 101.10          | 1                  |
| CA-C-C-CA-C-CA-CB           | 110.10             | 88.37           | 1                  |
| CA-C-O                      | 120.80             | 140.24          | 1                  |
| CA-C-CA-C-C-CA-CA-C-O       | 120.80             | 101.38          | 1                  |
| C-CA-CB                     | 110.10             | 88.40           | 1                  |
| C-CA-C-CA-N-CA-CA-C-O       | 120.80             | 101.40          | 1                  |
| N-CA-CA-C-O                 | 120.80             | 101.41          | 1                  |
| C-CA-CB                     | 110.10             | 131.77          | 1                  |
| C-CA-CA-C-O                 | 120.80             | 140.18          | 1                  |
| C-CA-N-CA-C                 | 111.00             | 142.88          | 1                  |
| C-CA-CB                     | 110.10             | 88.47           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 111.00             | 79.12           | 1                  |
| C-CA-CB               | 110.10             | 131.73          | 1                  |
| C-N-CA                | 121.70             | 142.18          | 1                  |
| N-CA-C                | 111.00             | 142.85          | 1                  |
| C-CA-CB               | 110.10             | 88.49           | 1                  |
| N-CA-C                | 111.00             | 142.82          | 1                  |
| N-CA-C-CA-CB          | 110.10             | 88.51           | 1                  |
| C-CA-CB               | 110.10             | 88.51           | 1                  |
| CA-C-N                | 116.20             | 138.92          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 88.52           | 1                  |
| C-CA-CB               | 110.10             | 88.52           | 1                  |
| N-CA-C                | 111.00             | 142.80          | 1                  |
| N-CA-N-CA-C           | 111.00             | 79.22           | 1                  |
| C-N-CA                | 121.70             | 142.13          | 1                  |
| N-CA-N-CA-CB          | 111.50             | 130.78          | 1                  |
| N-CA-CA-C-N           | 116.20             | 138.88          | 1                  |
| N-CA-N-CA-CB          | 111.50             | 130.76          | 1                  |
| CA-C-CA-C-O           | 120.80             | 101.55          | 1                  |
| C-N-CA                | 121.70             | 101.33          | 1                  |
| C-N-CA                | 121.70             | 142.07          | 1                  |
| N-CA-C-CA-CB          | 110.10             | 88.61           | 1                  |
| N-CA-N-CA-N-CA-C-N-CA | 121.70             | 101.37          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-O                 | 120.80             | 101.60          | 1                  |
| N-CA-N-CA-CA-C-O       | 120.80             | 139.99          | 1                  |
| C-CA-C-N-C-CA-C-N-CA   | 121.70             | 101.40          | 1                  |
| C-N-CA                 | 121.70             | 101.40          | 1                  |
| N-CA-C                 | 111.00             | 142.56          | 1                  |
| C-N-N-CA-C-CA-CB       | 111.60             | 89.07           | 1                  |
| C-N-N-CA-C             | 111.00             | 142.54          | 1                  |
| N-CA-N-CA-C-CA-CA-C-O  | 120.80             | 101.67          | 1                  |
| C-CA-CB                | 110.10             | 88.73           | 1                  |
| C-CA-CB                | 110.10             | 131.47          | 1                  |
| N-CA-C                 | 111.00             | 142.48          | 1                  |
| CA-C-O                 | 120.80             | 101.69          | 1                  |
| C-N-N-CA-C-N-N-CA-CB   | 110.50             | 91.40           | 1                  |
| N-CA-C-CA-CB           | 110.10             | 131.44          | 1                  |
| CA-C-N                 | 116.20             | 138.66          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 131.42          | 1                  |
| C-N-C-N-CA             | 121.70             | 141.90          | 1                  |
| C-CA-CB                | 111.60             | 89.16           | 1                  |
| C-CA-CB                | 110.10             | 88.79           | 2                  |
| C-CA-C-CA-CB           | 110.10             | 88.79           | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB | 110.50             | 129.56          | 1                  |
| C-CA-CB                | 111.60             | 89.18           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                | 110.50             | 91.44           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 131.40          | 1                  |
| C-CA-C-CA-N-CA-CB      | 110.50             | 129.53          | 1                  |
| C-CA-CB                | 110.10             | 131.37          | 1                  |
| C-CA-C-CA-C-CA-CB      | 110.10             | 88.85           | 1                  |
| CA-C-N                 | 116.20             | 138.57          | 1                  |
| CA-C-C-N-CA            | 121.70             | 141.83          | 1                  |
| N-CA-CB                | 110.50             | 129.50          | 1                  |
| C-CA-CA-C-C-N-CA       | 121.70             | 141.81          | 1                  |
| C-N-C-CA-CB            | 110.10             | 88.87           | 1                  |
| C-CA-CB                | 110.10             | 88.87           | 1                  |
| CA-N-CD                | 112.00             | 96.36           | 1                  |
| CA-C-N-CA-CB           | 110.50             | 129.48          | 1                  |
| N-CA-C-CA-CA-C-C-CA-CB | 110.10             | 88.89           | 1                  |
| C-CA-CB                | 111.60             | 89.27           | 1                  |
| N-CA-C                 | 111.00             | 142.25          | 1                  |
| CA-C-C-N-CA            | 121.70             | 141.77          | 1                  |
| C-N-CA-C-CA-C-O        | 120.80             | 101.85          | 1                  |
| CA-C-O                 | 120.80             | 101.85          | 1                  |
| CA-C-CA-C-N-CA-CB      | 103.00             | 90.74           | 1                  |
| N-CA-N-CA-CB           | 103.00             | 90.74           | 1                  |
| C-CA-CB                | 110.10             | 131.27          | 1                  |

| Angle type                                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB                              | 110.50             | 129.44          | 1                  |
| C-CA-N-CA-C-CA-CB                         | 110.10             | 131.25          | 1                  |
| C-N-CA                                    | 121.70             | 141.73          | 2                  |
| C-CA-CB                                   | 110.10             | 131.24          | 1                  |
| CA-N-CD                                   | 112.00             | 96.43           | 1                  |
| C-CA-CA-C-N-CA-CA-C-N-CA-CA-C-O           | 120.80             | 101.91          | 1                  |
| N-CA-CA-C-N-CA-CA-C-N                     | 116.20             | 93.99           | 1                  |
| N-CA-C-CA-CB                              | 110.10             | 131.20          | 1                  |
| CA-C-O                                    | 120.80             | 101.92          | 1                  |
| C-CA-CA-C-C-CA-CB                         | 110.10             | 131.19          | 1                  |
| N-CA-C-N-CA-C-N                           | 116.20             | 94.01           | 1                  |
| CA-C-O                                    | 120.80             | 101.94          | 1                  |
| N-CA-C                                    | 111.00             | 79.94           | 1                  |
| CA-C-C-CA-N-CA-CA-C-O                     | 120.80             | 101.94          | 1                  |
| CA-C-O                                    | 120.80             | 139.66          | 1                  |
| CA-C-O                                    | 120.80             | 101.95          | 1                  |
| C-N-C-CA-CB                               | 110.10             | 131.16          | 1                  |
| C-CA-N-CA-CB                              | 110.50             | 129.32          | 1                  |
| CA-C-O                                    | 120.80             | 139.62          | 1                  |
| N-CA-N-CA-C-CA-C-CA-CB                    | 110.10             | 131.12          | 1                  |
| N-CA-CB                                   | 110.50             | 91.69           | 1                  |
| C-CA-N-CA-N-CA-C-CA-C-CA-C-CA-N-CA-C-N-CA | 121.70             | 141.59          | 1                  |



| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| N-CA-CB              | 110.50             | 129.28          | 1                  |
| C-N-C-N-N-CA-C-CA-CB | 110.10             | 89.11           | 1                  |
| CA-C-O               | 120.80             | 102.03          | 1                  |
| C-CA-C-N-CA          | 121.70             | 141.57          | 1                  |
| N-CA-CB              | 111.50             | 130.27          | 1                  |
| C-CA-CB              | 109.10             | 84.82           | 1                  |
| C-CA-CB              | 110.10             | 89.13           | 1                  |
| N-CA-C-CA-CB         | 110.10             | 89.13           | 1                  |
| N-CA-C-N-CA-C-N      | 116.20             | 94.14           | 1                  |
| CA-C-O               | 120.80             | 139.55          | 1                  |
| CA-C-O               | 120.80             | 102.06          | 1                  |
| C-CA-CB              | 110.10             | 89.16           | 1                  |
| C-N-C-CA-C-CA-CB     | 110.10             | 89.18           | 1                  |
| C-N-CA               | 121.70             | 141.52          | 1                  |
| C-CA-CB              | 110.10             | 89.18           | 1                  |
| CA-C-O               | 120.80             | 102.09          | 1                  |
| C-N-C-CA-CB          | 110.10             | 89.19           | 1                  |
| C-CA-CB              | 110.10             | 89.20           | 1                  |
| N-CA-CB              | 111.50             | 130.20          | 1                  |
| CA-C-O               | 120.80             | 139.50          | 1                  |
| C-CA-N-CA-C          | 111.00             | 141.80          | 1                  |
| C-CA-CB              | 110.10             | 89.21           | 2                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-N-CA-C-CA-C-CA-C-N-C-N-CA | 121.70             | 141.48          | 1                  |
| C-CA-CB                             | 110.10             | 89.22           | 1                  |
| CA-C-N                              | 116.20             | 94.23           | 1                  |
| N-CA-C                              | 111.00             | 141.76          | 1                  |
| N-CA-CB                             | 111.50             | 130.17          | 1                  |
| C-CA-CA-C-O                         | 120.80             | 139.46          | 1                  |
| N-CA-C                              | 111.00             | 141.74          | 1                  |
| C-CA-CB                             | 109.10             | 84.95           | 1                  |
| C-CA-CB                             | 109.10             | 133.24          | 1                  |
| C-CA-CB                             | 110.10             | 89.25           | 1                  |
| C-CA-C-CA-CB                        | 110.10             | 89.27           | 1                  |
| N-CA-C-CA-CB                        | 109.10             | 133.21          | 1                  |
| N-CA-C                              | 111.00             | 141.68          | 1                  |
| N-CA-C                              | 111.00             | 80.33           | 1                  |
| C-CA-CB                             | 110.10             | 89.29           | 1                  |
| N-CD-C-CA-C-N-C-CA-C-CA-CB          | 109.10             | 85.02           | 1                  |
| N-CA-C                              | 111.00             | 80.37           | 1                  |
| C-N-NE-CZ-C-N-CA                    | 121.70             | 102.02          | 1                  |
| C-CA-C-N-C-N-CA                     | 121.70             | 141.37          | 1                  |
| C-CA-N-CA-CB                        | 110.50             | 129.07          | 1                  |
| C-CA-N-CD-NE-CZ-N-CA-CB             | 103.00             | 115.01          | 1                  |
| C-CA-CB                             | 109.10             | 133.12          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-CB-CG              | 113.80             | 102.88          | 1                  |
| N-CA-CB               | 110.50             | 129.05          | 1                  |
| C-CA-CB               | 110.10             | 89.37           | 1                  |
| N-CA-N-CA-C           | 111.00             | 141.54          | 1                  |
| C-CA-CB               | 110.10             | 130.82          | 3                  |
| C-CA-CB               | 109.10             | 133.09          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 130.82          | 1                  |
| C-CA-CB               | 110.10             | 89.38           | 1                  |
| C-CA-CB               | 110.10             | 89.39           | 1                  |
| N-CA-C-N-CA           | 121.70             | 102.10          | 1                  |
| N-CA-CB               | 103.00             | 114.98          | 1                  |
| C-N-N-CA-C            | 111.00             | 141.48          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 89.43           | 1                  |
| N-CA-N-CA-C-N-C-CA-CB | 110.10             | 130.76          | 1                  |
| N-CA-CB               | 111.50             | 93.01           | 1                  |
| C-CA-CB               | 109.10             | 85.18           | 1                  |
| C-N-C-CA-C-CA-CB      | 110.10             | 130.75          | 1                  |
| N-CA-C                | 111.00             | 80.57           | 1                  |
| C-CA-N-CA-C           | 111.00             | 80.58           | 1                  |
| C-CA-CB               | 110.10             | 89.46           | 1                  |
| N-CA-CB               | 111.50             | 93.04           | 1                  |
| C-CA-CB               | 111.40             | 90.76           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-N-C-CA-CB            | 110.10             | 130.73          | 1                  |
| N-CA-CB                | 110.50             | 128.95          | 1                  |
| CA-C-C-CA-CB           | 110.10             | 89.48           | 1                  |
| N-CA-CB                | 111.50             | 93.06           | 1                  |
| N-CA-CA-CB-CG          | 113.80             | 102.95          | 1                  |
| C-CA-CB                | 110.10             | 89.50           | 1                  |
| C-CA-CA-C-C-CA-CB      | 109.10             | 85.27           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 130.67          | 1                  |
| C-CA-N-CA-N-CA-N-CA-CB | 111.50             | 93.10           | 1                  |
| N-CA-CB                | 110.50             | 128.90          | 1                  |
| N-CA-C                 | 111.00             | 141.30          | 1                  |
| N-CA-N-CA-C            | 111.00             | 141.28          | 1                  |
| N-CA-C-CA-C-CA-CB      | 109.10             | 85.33           | 1                  |
| N-CA-CA-C-N            | 116.20             | 137.79          | 1                  |
| CA-C-O                 | 120.80             | 139.15          | 2                  |
| C-CA-C-CA-C-CA-CA-C-O  | 119.00             | 151.35          | 1                  |
| CA-C-O                 | 120.80             | 139.13          | 2                  |
| C-CA-CB                | 109.10             | 85.38           | 1                  |
| N-CA-CB                | 110.50             | 128.82          | 1                  |
| C-CA-N-CA-N-CA-CB      | 110.50             | 128.82          | 1                  |
| C-CA-C-CA-CB           | 111.40             | 90.94           | 1                  |
| N-CA-CB                | 111.50             | 129.81          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 109.10             | 85.41           | 1                  |
| N-CA-CB               | 111.50             | 129.80          | 1                  |
| C-N-N-CA-CB           | 110.50             | 128.79          | 1                  |
| CA-C-N                | 116.20             | 137.71          | 1                  |
| C-N-CA                | 121.70             | 141.05          | 1                  |
| C-CA-CB               | 110.10             | 130.52          | 1                  |
| C-CA-N-CA-C-CA-CB     | 111.40             | 90.99           | 1                  |
| C-CA-CB               | 109.10             | 85.47           | 1                  |
| C-N-C-CA-N-CA-CB      | 111.50             | 129.75          | 1                  |
| C-CA-CB               | 111.40             | 91.00           | 1                  |
| CA-C-C-N-N-CA-C-CA-CB | 110.10             | 130.49          | 1                  |
| C-CA-CB               | 110.10             | 89.71           | 1                  |
| C-N-C-CA-CB           | 110.10             | 89.72           | 1                  |
| C-N-N-CA-CB           | 111.50             | 129.74          | 1                  |
| C-CA-CB               | 110.10             | 130.47          | 1                  |
| N-CA-CB               | 110.50             | 128.73          | 1                  |
| C-N-CA                | 121.70             | 141.00          | 1                  |
| C-CA-CB               | 110.10             | 89.73           | 1                  |
| N-CA-CB               | 111.50             | 129.72          | 2                  |
| C-CA-C-CA-CB          | 109.10             | 85.52           | 1                  |
| C-CA-CB               | 111.40             | 91.03           | 1                  |
| N-CA-C-N-N-CA-C-N-CD  | 125.00             | 168.93          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                | 111.50             | 129.71          | 4                  |
| N-CA-CB                | 110.50             | 128.71          | 2                  |
| C-CA-C-CA-N-CA-N-CA-CB | 110.50             | 128.70          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 129.70          | 1                  |
| C-N-CA                 | 121.70             | 140.96          | 1                  |
| C-N-CD                 | 125.00             | 168.88          | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB | 111.50             | 129.69          | 1                  |
| C-N-C-CA-CB            | 109.10             | 85.57           | 1                  |
| C-CA-CB                | 109.10             | 85.57           | 1                  |
| C-N-C-N-CA             | 121.70             | 140.95          | 1                  |
| N-CA-C-CA-N-CA-CB      | 110.50             | 128.67          | 1                  |
| C-CA-CB                | 109.10             | 85.59           | 1                  |
| N-CA-CB                | 111.50             | 129.67          | 2                  |
| C-N-CA                 | 121.70             | 140.93          | 2                  |
| N-CA-N-CA-CB           | 111.50             | 129.66          | 1                  |
| C-N-CA                 | 121.70             | 140.92          | 1                  |
| C-CA-C-CA-C-N-C-CA-CB  | 110.10             | 130.38          | 1                  |
| C-CA-CB                | 110.10             | 89.82           | 1                  |
| N-CA-CB                | 111.50             | 129.64          | 1                  |
| C-N-C-CA-C-CA-CB       | 110.10             | 130.37          | 1                  |
| C-CA-CB                | 110.10             | 89.84           | 1                  |
| N-CA-CB                | 110.50             | 128.63          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                          | 110.10             | 130.36          | 2                  |
| CA-C-C-CA-CB                     | 110.10             | 89.84           | 1                  |
| C-CA-C-CA-N-CA-CB                | 110.50             | 128.61          | 1                  |
| N-CA-CB                          | 110.50             | 128.60          | 1                  |
| C-CA-CB                          | 110.10             | 130.33          | 1                  |
| C-CA-C-CA-C-CA-C-CA-CA-N-C-N-CA  | 121.70             | 140.85          | 1                  |
| C-CA-C-CA-N-CA-C-CA-N-CA-N-CA-CB | 110.50             | 128.57          | 1                  |
| C-N-CA                           | 121.70             | 140.83          | 1                  |
| C-CA-CB                          | 110.10             | 130.30          | 1                  |
| C-CA-C-CA-CB                     | 110.10             | 130.29          | 1                  |
| N-CA-O-C-C-N-CA                  | 121.70             | 140.82          | 1                  |
| C-CA-CB                          | 110.10             | 130.29          | 1                  |
| C-CA-CB                          | 110.10             | 130.28          | 1                  |
| C-CA-C-CA-CB                     | 110.10             | 89.93           | 1                  |
| N-CA-CB                          | 110.50             | 128.54          | 1                  |
| C-CA-CB                          | 110.10             | 89.94           | 1                  |
| C-N-CA                           | 121.70             | 140.80          | 1                  |
| N-CA-N-CA-C-N-CA                 | 121.70             | 140.78          | 1                  |
| C-CA-C-CA-C-CA-C-CA-CA-N-C-CA-CB | 110.10             | 89.98           | 1                  |
| C-N-CA                           | 121.70             | 102.64          | 1                  |
| C-N-C-N-CA                       | 121.70             | 140.75          | 1                  |
| C-CA-N-CA-C-CA-C-N-CA            | 121.70             | 102.65          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-C-CA-C-CA-CB           | 110.10             | 90.01           | 1                  |
| N-CA-CA-C-N-CA-CB                | 111.50             | 129.47          | 1                  |
| C-N-CA                           | 121.70             | 102.67          | 1                  |
| O-C-C-N-CA                       | 121.70             | 102.68          | 1                  |
| C-CA-N-CA-C-CA-CB                | 110.10             | 130.17          | 1                  |
| CA-C-N                           | 116.20             | 137.32          | 1                  |
| C-CA-CB                          | 110.10             | 90.05           | 1                  |
| N-CA-C                           | 111.00             | 81.46           | 1                  |
| N-CA-N-CA-C-N-N-CA-C             | 111.00             | 140.53          | 1                  |
| C-CA-CB                          | 110.10             | 130.14          | 1                  |
| CA-C-N                           | 116.20             | 137.28          | 1                  |
| C-CA-N-CA-CB                     | 103.00             | 114.59          | 1                  |
| C-CA-CB                          | 110.10             | 90.08           | 1                  |
| CA-C-C-CA-CB                     | 110.10             | 130.12          | 1                  |
| N-CA-C                           | 111.00             | 81.51           | 1                  |
| C-CA-N-CA-CA-C-C-N-CA            | 121.70             | 102.75          | 1                  |
| CA-C-N-CA-C-CA-N-CA-C            | 111.00             | 81.54           | 1                  |
| CA-C-N-CA-C                      | 111.00             | 81.55           | 1                  |
| N-CA-C                           | 111.00             | 140.45          | 1                  |
| CA-C-C-CA-C-CA-N-CA-C            | 111.00             | 81.58           | 1                  |
| CA-C-N-CA-N-CA-C-CA-C-CA-C-CA-CB | 110.10             | 130.05          | 1                  |
| N-CA-C                           | 111.00             | 81.60           | 2                  |



| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-N-CA-C            | 111.00             | 81.62           | 1                  |
| C-CA-N-CA-C-CA-C-N-CA       | 121.70             | 140.58          | 1                  |
| C-CA-CA-C-O                 | 120.80             | 102.97          | 1                  |
| C-N-CA                      | 121.70             | 102.82          | 1                  |
| C-CA-C-CA-CA-C-C-CA-CA-C-N  | 116.20             | 137.16          | 1                  |
| N-CA-C-CA-CB                | 110.10             | 130.02          | 1                  |
| CA-C-N                      | 116.20             | 95.24           | 1                  |
| C-CA-CB                     | 110.10             | 90.20           | 1                  |
| C-CA-C-CA-C-CA-CB           | 110.10             | 129.99          | 1                  |
| CA-C-N                      | 116.20             | 137.14          | 1                  |
| C-CA-N-CA-C-CA-CB           | 110.10             | 129.98          | 1                  |
| C-CA-CB                     | 110.10             | 129.98          | 1                  |
| N-CA-CB                     | 103.00             | 114.51          | 1                  |
| C-CA-CB                     | 111.60             | 90.68           | 1                  |
| N-CA-C                      | 111.00             | 140.28          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 90.23           | 1                  |
| CA-C-N-CA-N-CA-CA-C-O       | 120.80             | 103.05          | 1                  |
| N-CA-N-CA-CA-C-N-CA-C-CA-CB | 110.10             | 129.92          | 1                  |
| C-CA-N-CA-C                 | 111.00             | 140.19          | 1                  |
| C-CA-CB                     | 110.10             | 129.90          | 1                  |
| C-CA-C-CA-C-CA-C-CA-CB      | 110.10             | 129.90          | 1                  |
| C-CA-CB                     | 110.10             | 90.31           | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| C-N-N-CA-CA-C-O           | 120.80             | 103.09          | 1                  |
| C-CA-CB                   | 111.60             | 90.77           | 1                  |
| C-CA-CB                   | 110.10             | 129.88          | 1                  |
| C-CA-CB                   | 110.10             | 129.87          | 1                  |
| N-CA-C                    | 111.00             | 81.87           | 1                  |
| CA-C-O                    | 120.80             | 138.48          | 1                  |
| N-CA-CB                   | 110.40             | 126.00          | 1                  |
| N-CA-C-CA-C-CA-CB         | 110.10             | 129.84          | 1                  |
| N-CA-C-CA-CB              | 110.10             | 90.37           | 1                  |
| C-CA-N-CA-C               | 111.00             | 81.93           | 1                  |
| C-CA-CB                   | 110.10             | 129.82          | 1                  |
| C-CA-C-N-CA-C-C-CA-N-CA-C | 111.00             | 140.05          | 1                  |
| N-CA-CB                   | 110.50             | 92.87           | 1                  |
| N-CA-C                    | 111.00             | 140.04          | 1                  |
| C-CA-CB                   | 110.10             | 129.81          | 1                  |
| C-CA-C-CA-C-CA-CB         | 110.10             | 129.79          | 1                  |
| CA-C-O                    | 120.80             | 138.42          | 2                  |
| CA-C-O                    | 120.80             | 138.41          | 1                  |
| C-CA-CB                   | 110.10             | 129.78          | 1                  |
| CA-C-C-CA-CB              | 110.10             | 129.78          | 1                  |
| N-CA-CB                   | 110.50             | 92.89           | 1                  |
| CA-C-C-N-CA               | 121.70             | 140.34          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CA-C-C-CA-CB | 110.10             | 129.77          | 1                  |
| C-CA-CB                | 110.10             | 129.76          | 1                  |
| N-CA-CB                | 110.40             | 125.92          | 1                  |
| C-CA-N-CA-C-CA-CA-C-O  | 120.80             | 103.23          | 1                  |
| C-CA-CB                | 110.10             | 129.74          | 1                  |
| C-CA-CB                | 110.10             | 90.46           | 1                  |
| N-CA-C-CA-CB           | 110.10             | 129.73          | 1                  |
| C-CA-C-N-C-CA-C-CA-CB  | 110.10             | 129.71          | 1                  |
| C-CA-CB                | 110.10             | 129.71          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 129.70          | 1                  |
| C-CA-C-N-CA            | 121.70             | 140.25          | 1                  |
| C-CA-CB                | 110.10             | 129.68          | 1                  |
| C-N-C-CA-CB            | 110.10             | 129.67          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 129.66          | 1                  |
| C-N-C-CA-CB            | 110.10             | 129.65          | 1                  |
| CA-C-O                 | 120.80             | 138.29          | 1                  |
| N-CA-CB                | 110.50             | 127.99          | 1                  |
| C-CA-C-CA-C-CA-CB      | 110.10             | 90.56           | 1                  |
| CA-C-C-CA-CB           | 110.10             | 129.64          | 1                  |
| N-CA-C-CA-C-CA-CB      | 110.10             | 129.63          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 129.63          | 1                  |
| N-CA-CA-C-O            | 120.80             | 138.27          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-CB          | 110.50             | 127.97          | 1                  |
| CA-C-O           | 120.80             | 103.33          | 1                  |
| C-CA-CB          | 110.10             | 129.62          | 1                  |
| C-CA-C-CA-CB     | 110.10             | 129.62          | 1                  |
| C-CA-C-CA-CB     | 111.40             | 130.91          | 1                  |
| C-CA-CB          | 110.10             | 129.61          | 4                  |
| CA-C-O           | 120.80             | 138.26          | 1                  |
| C-CA-CB          | 110.10             | 90.59           | 1                  |
| C-N-CA           | 121.70             | 103.22          | 1                  |
| CA-C-O           | 120.80             | 138.24          | 1                  |
| C-CA-CB          | 110.10             | 129.59          | 2                  |
| CA-C-C-N-N-CA-CB | 110.40             | 125.78          | 1                  |
| C-CA-CB          | 110.10             | 129.58          | 1                  |
| C-CA-CB          | 110.10             | 129.57          | 1                  |
| C-CA-CB          | 110.10             | 129.56          | 2                  |
| N-CA-C           | 111.00             | 82.32           | 1                  |
| C-CA-C-CA-CB     | 110.10             | 90.64           | 1                  |
| C-CA-CB          | 110.50             | 125.86          | 1                  |
| C-CA-CB          | 110.10             | 129.55          | 2                  |
| C-CA-CB          | 110.10             | 90.66           | 1                  |
| C-N-N-CA-C       | 111.00             | 82.36           | 1                  |
| N-CA-CA-C-O      | 120.80             | 103.41          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                        | 110.40             | 125.74          | 1                  |
| C-CA-CB                        | 111.40             | 130.83          | 1                  |
| C-CA-CB                        | 110.10             | 129.53          | 1                  |
| C-CA-CB                        | 110.50             | 125.83          | 1                  |
| CA-C-C-CA-CB                   | 110.10             | 129.50          | 1                  |
| C-CA-CB                        | 110.50             | 125.82          | 1                  |
| N-CA-C-CA-CB                   | 110.10             | 90.71           | 1                  |
| CA-C-O                         | 120.80             | 103.45          | 1                  |
| C-N-CA                         | 121.70             | 103.33          | 1                  |
| C-CA-N-CA-CB                   | 111.50             | 128.85          | 1                  |
| N-CA-CB                        | 111.50             | 94.16           | 1                  |
| N-CA-C-CA-C-CA-C-CA-CB         | 111.60             | 91.20           | 1                  |
| C-CA-CB                        | 110.10             | 90.73           | 1                  |
| N-CA-CB                        | 111.50             | 94.17           | 1                  |
| C-CA-CB                        | 110.10             | 129.47          | 1                  |
| C-N-N-CA-C                     | 111.00             | 139.54          | 1                  |
| CA-C-O                         | 120.80             | 103.48          | 1                  |
| C-CA-CB                        | 110.10             | 90.74           | 1                  |
| CA-C-C-CA-CB                   | 110.50             | 125.78          | 1                  |
| N-CA-CA-C-O                    | 120.80             | 103.49          | 1                  |
| C-CA-CB                        | 110.10             | 90.75           | 1                  |
| N-CA-C-CA-N-CA-C-CA-C-N-N-CA-C | 111.00             | 139.47          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-N-N-CA-C-CA-CB                 | 110.10             | 90.78           | 1                  |
| C-CA-CA-C-C-CA-CB                | 110.10             | 129.40          | 1                  |
| C-CA-C-N-C-CA-C-CA-CB            | 110.10             | 90.81           | 1                  |
| C-CA-CB                          | 111.40             | 92.11           | 1                  |
| C-N-CA                           | 121.70             | 139.97          | 1                  |
| C-CA-CB                          | 110.10             | 90.82           | 1                  |
| N-CA-CA-C-C-CA-N-CA-CA-C-C-CA-CB | 110.10             | 129.37          | 1                  |
| C-CA-CB                          | 111.60             | 91.31           | 1                  |
| C-CA-CB                          | 110.10             | 129.37          | 1                  |
| C-CA-C-CA-CB                     | 110.10             | 90.84           | 1                  |
| N-CA-C                           | 111.00             | 82.62           | 1                  |
| C-CA-CB                          | 110.10             | 129.36          | 1                  |
| N-CA-N-CA-C                      | 111.00             | 82.62           | 1                  |
| C-CA-CB                          | 110.10             | 90.85           | 1                  |
| C-CA-CB                          | 110.10             | 129.35          | 1                  |
| N-CA-C-CA-CB                     | 110.10             | 129.35          | 1                  |
| N-CA-CB                          | 110.50             | 127.72          | 1                  |
| N-CA-C-CA-CB                     | 110.10             | 90.86           | 1                  |
| C-CA-CB                          | 110.10             | 129.33          | 1                  |
| N-CA-C                           | 111.00             | 82.66           | 1                  |
| C-CA-C-CA-C-CA-CB                | 110.10             | 129.32          | 1                  |
| C-N-C-CA-CA-C-N                  | 116.20             | 95.97           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.50             | 125.67          | 1                  |
| C-N-C-CA-C-CA-CB           | 110.10             | 90.90           | 1                  |
| C-CA-CB                    | 110.50             | 125.65          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 90.91           | 1                  |
| CA-C-O                     | 120.80             | 137.97          | 1                  |
| N-CA-N-CA-N-CA-CB          | 110.50             | 93.34           | 1                  |
| N-CA-C                     | 111.00             | 139.26          | 1                  |
| C-CA-C-CA-CA-C-N           | 116.20             | 96.02           | 1                  |
| C-CA-C-CA-CB               | 110.10             | 90.93           | 1                  |
| N-CA-C-CA-CB               | 110.10             | 129.26          | 1                  |
| C-CA-CB                    | 110.10             | 129.26          | 1                  |
| C-N-CD                     | 125.00             | 83.66           | 1                  |
| C-N-CA                     | 121.70             | 139.85          | 1                  |
| C-CA-CB                    | 110.10             | 90.95           | 1                  |
| N-CA-C                     | 111.00             | 82.77           | 1                  |
| N-CA-C                     | 111.00             | 82.78           | 1                  |
| N-CA-C-N-C-CA-N-CA-C-CA-CB | 110.10             | 129.24          | 1                  |
| CA-N-CD                    | 112.00             | 97.90           | 2                  |
| N-CA-N-CA-CB               | 110.50             | 127.62          | 1                  |
| C-CA-CB                    | 110.50             | 125.60          | 2                  |
| C-N-CD                     | 125.00             | 83.72           | 1                  |
| N-CA-C                     | 111.00             | 139.19          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-C           | 111.00             | 82.81           | 1                  |
| C-N-C-CA-CB      | 110.10             | 129.22          | 1                  |
| N-CA-N-CA-CB     | 103.00             | 114.07          | 1                  |
| C-N-C-CA-CA-N-CD | 112.00             | 97.92           | 1                  |
| C-N-C-CA-CB      | 110.10             | 129.21          | 1                  |
| C-CA-N-CA-CB     | 110.50             | 93.41           | 1                  |
| C-CA-CB          | 110.10             | 91.01           | 1                  |
| C-N-CA           | 121.70             | 139.79          | 1                  |
| C-N-N-CD-C-CA-CB | 110.10             | 129.19          | 1                  |
| CA-C-N-CA-C      | 111.00             | 82.88           | 1                  |
| C-CA-CB          | 110.10             | 129.18          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 129.18          | 1                  |
| N-CA-CB          | 110.50             | 93.43           | 1                  |
| N-CA-CB          | 103.00             | 114.04          | 1                  |
| N-CA-C           | 111.00             | 139.11          | 1                  |
| C-CA-CB          | 110.10             | 129.17          | 1                  |
| C-N-N-CA-C-CA-CB | 110.10             | 129.17          | 1                  |
| N-CA-C           | 111.00             | 82.90           | 1                  |
| CA-N-CD          | 112.00             | 97.95           | 1                  |
| N-CA-CB          | 111.50             | 94.44           | 1                  |
| N-CA-CA-C-O      | 120.80             | 137.85          | 1                  |
| C-CA-CB          | 110.10             | 91.05           | 1                  |



| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                             | 110.10             | 129.15          | 1                  |
| C-CA-C-CA-N-CA-C-CA-CB              | 110.10             | 91.07           | 1                  |
| N-CA-C                              | 111.00             | 139.04          | 1                  |
| CA-C-O                              | 119.00             | 88.97           | 1                  |
| CA-C-N-CD-C-CA-N-CA-C-N-C-CA-C-N-CA | 121.70             | 139.71          | 1                  |
| CA-C-O                              | 119.00             | 88.99           | 1                  |
| C-CA-CB                             | 110.50             | 125.50          | 1                  |
| N-CA-CB                             | 103.00             | 114.00          | 1                  |
| N-CA-CA-C-C-N-N-CA-C-N-CA           | 121.70             | 103.70          | 1                  |
| CA-C-C-CA-CB                        | 110.10             | 91.11           | 1                  |
| C-N-CA                              | 121.70             | 139.69          | 1                  |
| C-N-N-CA-C                          | 111.00             | 138.98          | 1                  |
| N-CA-C                              | 111.00             | 138.98          | 1                  |
| C-N-N-CA-CB                         | 110.50             | 93.52           | 1                  |
| C-CA-CB                             | 110.50             | 125.48          | 1                  |
| N-CA-C-N-CA                         | 121.70             | 139.67          | 1                  |
| C-CA-N-CA-CB                        | 103.00             | 113.98          | 1                  |
| N-CA-CB                             | 111.50             | 94.54           | 1                  |
| C-N-C-N-CA                          | 121.70             | 139.65          | 1                  |
| C-N-C-CA-C-N-CA                     | 121.70             | 103.76          | 1                  |
| N-CA-N-CA-CB                        | 110.50             | 93.57           | 1                  |
| N-CA-C-N-CA                         | 121.70             | 139.63          | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| OE1-CD-NE2                      | 122.60             | 112.64          | 1                  |
| CA-C-C-CA-N-CA-CB               | 110.50             | 93.58           | 1                  |
| CA-C-CA-C-C-CA-C-CA-N-CA-CA-C-N | 116.20             | 136.06          | 1                  |
| C-CA-CA-CB-N-CA-CB              | 110.50             | 93.62           | 1                  |
| N-CA-CB                         | 110.50             | 127.38          | 1                  |
| C-CA-CB                         | 109.10             | 130.94          | 1                  |
| N-CA-CA-C-N                     | 116.20             | 136.05          | 1                  |
| N-CA-CB                         | 103.00             | 113.92          | 1                  |
| N-CA-CB                         | 110.50             | 127.37          | 1                  |
| CA-C-C-CA-CA-C-N-CA-C           | 111.00             | 83.22           | 1                  |
| N-CA-C                          | 111.00             | 83.22           | 1                  |
| CA-C-CA-C-N                     | 116.20             | 136.04          | 1                  |
| N-CA-CB                         | 110.50             | 93.64           | 1                  |
| N-CA-CB                         | 110.50             | 127.36          | 1                  |
| N-CA-CB                         | 103.00             | 113.91          | 1                  |
| CA-C-C-CA-CA-C-CA-C-N-CA-CA-C-O | 120.80             | 137.63          | 1                  |
| C-CA-CB                         | 111.40             | 92.59           | 1                  |
| C-CA-N-CA-C                     | 111.00             | 83.29           | 1                  |
| C-CA-C-CA-CB                    | 111.40             | 92.60           | 1                  |
| CA-C-CA-C-CA-C-O                | 120.80             | 137.62          | 1                  |
| CA-CB-N-CA-CB                   | 110.50             | 127.31          | 1                  |
| C-CA-N-CA-CB                    | 110.50             | 127.31          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| N-CA-C-CA-N-CA-CB  | 110.50             | 127.31          | 1                  |
| CA-C-C-CA-CB   | 109.10             | 130.85          | 1                  |
| C-CA-N-CA-C  | 111.00             | 138.68          | 1                  |
| CA-C-CA-C-O  | 120.80             | 137.60          | 1                  |
| C-CA-CB  | 110.50             | 125.32          | 1                  |
| C-N-CA-C-CA-C-N  | 116.20             | 96.45           | 1                  |
| N-CA-CB  | 110.50             | 127.28          | 1                  |
| CA-C-N   | 116.20             | 135.94          | 1                  |
| C-N-C-N-N-CA-C   | 111.00             | 83.37           | 1                  |
| C-CA-CA-C-N-CA-C-CA-C-CA-C-N-C-N-N-CA-C-CA-C-N-C-CA-C-N-N-CA-C | 111.00             | 138.57          | 1                  |
| CA-C-N   | 116.20             | 96.51           | 1                  |
| C-CA-C-CA-N-CA-CB  | 110.50             | 127.22          | 1                  |
| OE1-CD-NE2   | 122.60             | 112.76          | 1                  |
| CA-C-O   | 120.80             | 137.52          | 1                  |
| C-CA-CB  | 110.10             | 128.79          | 1                  |
| N-CA-N-CA-C-N-N-CA-CB  | 111.50             | 128.20          | 1                  |
| C-CA-CB  | 110.50             | 125.24          | 2                  |
| C-CA-N-CA-CB   | 111.50             | 128.19          | 1                  |
| C-N-CA-C-N-CA-CB   | 110.50             | 127.19          | 1                  |
| C-N-C-CA-C-CA-CB   | 110.50             | 125.22          | 1                  |
| C-CA-N-CA-CB   | 110.50             | 127.18          | 1                  |
| C-CA-CB  | 110.50             | 125.22          | 2                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                             | 110.50             | 127.18          | 1                  |
| C-CA-CB                             | 110.10             | 128.73          | 1                  |
| C-N-CA                              | 121.70             | 104.05          | 1                  |
| N-CA-CB                             | 110.50             | 127.16          | 1                  |
| C-CA-CB                             | 110.10             | 128.72          | 1                  |
| N-CA-CB                             | 110.50             | 93.85           | 1                  |
| N-CA-C-N-CA                         | 121.70             | 104.08          | 1                  |
| C-CA-C-CA-C-CA-CB                   | 110.50             | 125.18          | 1                  |
| C-CA-N-CA-C                         | 111.00             | 83.61           | 1                  |
| N-CA-C-CA-N-CA-C-CA-N-CA-CB         | 110.50             | 127.12          | 1                  |
| C-N-CD                              | 125.00             | 165.08          | 1                  |
| C-CA-CB                             | 110.10             | 128.67          | 1                  |
| N-CA-CB                             | 110.50             | 93.89           | 1                  |
| N-CA-C                              | 111.00             | 83.65           | 1                  |
| C-CA-C-CA-C-N-CD                    | 125.00             | 165.04          | 1                  |
| C-CA-CB                             | 110.50             | 125.15          | 1                  |
| C-N-C-CA-N-CA-N-CA-C-CA-C-CA-C-N-CD | 125.00             | 165.00          | 1                  |
| N-CA-N-CA-CB                        | 110.50             | 127.08          | 1                  |
| C-CA-CB                             | 110.10             | 128.63          | 2                  |
| CA-C-N                              | 116.20             | 135.69          | 1                  |
| C-CA-CB                             | 110.50             | 125.12          | 1                  |
| C-CA-CB                             | 111.40             | 129.91          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-N-CA                | 121.70             | 104.17          | 1                  |
| C-CA-CB               | 110.50             | 125.11          | 1                  |
| C-CA-CA-C-N           | 116.20             | 135.67          | 1                  |
| C-CA-CB               | 110.50             | 125.09          | 1                  |
| N-CA-C                | 111.00             | 138.24          | 1                  |
| C-CA-CB               | 111.40             | 129.88          | 1                  |
| C-CA-CB               | 110.10             | 128.58          | 1                  |
| C-N-CD                | 125.00             | 164.88          | 1                  |
| C-CA-CB               | 110.10             | 128.57          | 2                  |
| C-CA-N-CA-C           | 111.00             | 83.78           | 1                  |
| C-CA-CB               | 110.50             | 125.08          | 1                  |
| C-CA-CB               | 110.10             | 128.56          | 1                  |
| N-CA-C                | 111.00             | 138.20          | 1                  |
| C-CA-CB               | 110.10             | 128.55          | 1                  |
| C-CA-CB               | 111.40             | 129.84          | 1                  |
| C-CA-N-CA-CB          | 111.50             | 128.00          | 1                  |
| N-CA-N-CA-C           | 111.00             | 138.17          | 1                  |
| N-CA-C                | 111.00             | 138.17          | 1                  |
| C-CA-CB               | 110.10             | 128.53          | 1                  |
| C-CA-N-CA-C           | 111.00             | 83.85           | 1                  |
| C-CA-CB               | 110.10             | 91.68           | 1                  |
| N-CA-C-CA-C-CA-CA-C-O | 120.80             | 137.27          | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                               | 110.10             | 128.51          | 2                  |
| C-CA-CB                               | 110.10             | 91.69           | 1                  |
| CA-C-N                                | 116.20             | 96.82           | 1                  |
| C-CA-CB                               | 110.10             | 91.70           | 1                  |
| CA-C-O                                | 120.80             | 137.26          | 1                  |
| C-CA-C-CA-N-CA-C-CA-CB                | 110.10             | 91.71           | 1                  |
| C-CA-CA-C-N                           | 116.20             | 96.84           | 1                  |
| CA-C-C-CA-CB                          | 110.10             | 91.71           | 1                  |
| C-CA-CB                               | 110.10             | 91.72           | 1                  |
| C-CA-N-CA-CA-C-N                      | 116.20             | 96.85           | 1                  |
| C-CA-CB                               | 110.10             | 128.48          | 1                  |
| CA-C-N-CA-C-CA-N-CA-C-CA-N-CA-C-CA-CB | 110.10             | 91.74           | 1                  |
| N-CA-CA-C-N                           | 116.20             | 96.88           | 2                  |
| C-CA-CB                               | 110.10             | 91.75           | 1                  |
| CA-C-N                                | 116.20             | 96.88           | 1                  |
| C-CA-CB                               | 110.10             | 128.45          | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 128.44          | 1                  |
| C-N-CA-C-O                            | 120.80             | 104.39          | 1                  |
| N-CA-CA-C-N                           | 116.20             | 96.90           | 1                  |
| CA-C-O                                | 120.80             | 104.39          | 1                  |
| C-CA-CB                               | 110.10             | 128.43          | 1                  |
| CA-C-O                                | 120.80             | 104.40          | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-C-CA-CB                     | 110.10             | 128.42          | 1                  |
| CA-C-C-CA-C-N-CA-C-N                  | 116.20             | 96.92           | 1                  |
| C-CA-N-CA-C-CA-CB                     | 110.10             | 128.41          | 1                  |
| CA-C-N                                | 116.20             | 96.93           | 1                  |
| C-CA-N-CA-CA-C-C-CA-N-CA-CA-C-N       | 116.20             | 96.94           | 1                  |
| CA-C-C-CA-N-CA-N-CA-C-CA-N-CA-C-CA-CB | 110.10             | 128.39          | 1                  |
| CA-C-CA-C-N                           | 116.20             | 96.96           | 1                  |
| CA-C-N                                | 116.20             | 135.44          | 1                  |
| C-CA-C-CA-CA-C-CA-C-O                 | 120.80             | 104.45          | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 128.36          | 1                  |
| C-CA-CB                               | 110.10             | 128.36          | 1                  |
| N-CA-N-CA-C-CA-CA-C-C-CA-CB           | 110.10             | 128.35          | 1                  |
| C-CA-N-CA-CB                          | 110.50             | 126.83          | 1                  |
| N-CA-CB                               | 110.50             | 126.82          | 2                  |
| N-CA-CB                               | 110.50             | 94.18           | 1                  |
| C-CA-CB                               | 110.10             | 128.34          | 1                  |
| CA-C-N                                | 116.20             | 97.00           | 1                  |
| CA-C-C-CA-CB                          | 110.10             | 128.33          | 1                  |
| N-CA-C                                | 111.00             | 84.13           | 1                  |
| N-CA-CA-C-C-CA-CA-C-C-CA-CB           | 110.10             | 128.32          | 1                  |
| CA-C-C-CA-CA-C-N                      | 116.20             | 97.03           | 1                  |
| C-CA-CB                               | 110.10             | 91.89           | 1                  |

| Angle type      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------|--------------------|-----------------|--------------------|
| C-N-CA          | 121.70             | 138.95          | 1                  |
| N-CA-CB         | 110.50             | 94.21           | 1                  |
| C-N-CA          | 121.70             | 104.45          | 1                  |
| N-CA-CB         | 110.50             | 126.79          | 1                  |
| N-CA-CB         | 110.50             | 126.78          | 1                  |
| C-CA-CB         | 111.60             | 130.75          | 1                  |
| C-CA-CB         | 110.10             | 91.91           | 1                  |
| C-N-CA-C-N-CA-C | 111.00             | 84.21           | 1                  |
| C-N-CA          | 121.70             | 104.48          | 1                  |
| C-CA-CB         | 111.60             | 130.73          | 1                  |
| CA-C-N-CA-C     | 111.00             | 137.79          | 1                  |
| CA-C-N          | 116.20             | 135.33          | 1                  |
| C-CA-CB         | 110.10             | 91.93           | 1                  |
| C-CA-CB         | 110.10             | 128.27          | 1                  |
| C-N-CA          | 121.70             | 104.49          | 1                  |
| N-CA-CB         | 110.50             | 94.25           | 1                  |
| N-CA-C          | 111.00             | 137.76          | 1                  |
| C-CA-CB         | 110.10             | 91.94           | 1                  |
| CA-C-O          | 120.80             | 137.04          | 1                  |
| C-N-CA          | 121.70             | 138.89          | 1                  |
| CA-C-N          | 116.20             | 97.10           | 1                  |
| N-CA-CB         | 110.50             | 94.26           | 1                  |



| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| N-CA-C       | 111.00             | 84.26           | 1                  |
| C-CA-CB      | 110.10             | 91.96           | 1                  |
| C-CA-CB      | 110.10             | 91.97           | 2                  |
| N-CA-C       | 111.00             | 137.72          | 1                  |
| CA-C-O       | 120.80             | 137.02          | 1                  |
| C-N-CA       | 121.70             | 104.53          | 2                  |
| C-CA-CB      | 111.60             | 130.68          | 1                  |
| C-CA-CB      | 111.60             | 92.53           | 1                  |
| C-CA-CB      | 111.60             | 130.66          | 1                  |
| C-N-CA       | 121.70             | 138.85          | 1                  |
| C-CA-CB      | 110.10             | 91.99           | 1                  |
| C-CA-CB      | 110.10             | 92.00           | 1                  |
| N-CA-N-CA-CB | 110.50             | 94.30           | 1                  |
| CA-C-O       | 120.80             | 137.00          | 1                  |
| C-CA-C-CA-CB | 111.60             | 130.64          | 1                  |
| C-N-CA       | 121.70             | 138.84          | 1                  |
| C-N-CA       | 121.70             | 104.57          | 1                  |
| N-CA-CA-C-O  | 120.80             | 104.62          | 1                  |
| C-N-C-CA-CB  | 111.60             | 92.57           | 1                  |
| C-CA-CB      | 110.10             | 128.18          | 1                  |
| C-CA-CB      | 111.60             | 130.63          | 1                  |
| N-CA-CB      | 110.40             | 124.67          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-C           | 111.00             | 137.64          | 1                  |
| C-CA-C-CA-C-N-CA | 121.70             | 138.82          | 1                  |
| C-CA-CB          | 110.10             | 92.03           | 1                  |
| C-CA-N-CA-C      | 111.00             | 137.62          | 1                  |
| N-CA-CB          | 110.50             | 94.34           | 1                  |
| C-N-CA           | 121.70             | 138.81          | 1                  |
| N-CA-CA-C-O      | 120.80             | 104.65          | 1                  |
| N-CA-C           | 111.00             | 137.60          | 1                  |
| CA-CB-N-CA-C     | 111.00             | 137.60          | 1                  |
| C-N-CA           | 121.70             | 138.80          | 1                  |
| N-CA-CB          | 110.40             | 124.64          | 1                  |
| N-CA-C           | 111.00             | 84.43           | 1                  |
| C-N-CA           | 121.70             | 138.78          | 1                  |
| N-CA-CA-N-CD     | 112.00             | 98.72           | 1                  |
| C-N-C-N-CA       | 121.70             | 138.78          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 128.12          | 1                  |
| N-CA-C           | 111.00             | 137.55          | 1                  |
| N-CA-N-CA-CA-C-O | 120.80             | 104.69          | 1                  |
| C-N-CA           | 121.70             | 138.76          | 1                  |
| N-CA-C-N-CA      | 121.70             | 138.75          | 1                  |
| CA-CB-CA-C-O     | 120.80             | 136.89          | 1                  |
| OD1-CG-ND2       | 122.60             | 132.06          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-C-CA-C-N-CA | 121.70             | 138.72          | 1                  |
| C-CA-CB               | 110.10             | 128.07          | 1                  |
| C-CA-CB               | 110.10             | 128.06          | 1                  |
| CA-N-CD               | 112.00             | 98.76           | 1                  |
| C-N-CA                | 121.70             | 138.71          | 2                  |
| N-CA-C                | 111.00             | 84.54           | 2                  |
| CA-C-O                | 120.80             | 104.74          | 1                  |
| C-CA-CB               | 110.10             | 92.15           | 1                  |
| C-N-CA                | 121.70             | 138.70          | 1                  |
| C-N-CA                | 121.70             | 104.70          | 1                  |
| N-CA-C-N-CA           | 121.70             | 104.70          | 1                  |
| C-N-CD                | 125.00             | 163.69          | 1                  |
| C-N-CA                | 121.70             | 138.68          | 2                  |
| OD1-CG-ND2            | 122.60             | 132.03          | 1                  |
| N-CA-CA-C-N           | 116.20             | 97.34           | 1                  |
| CA-C-N                | 116.20             | 97.34           | 1                  |
| C-N-CA                | 121.70             | 138.67          | 1                  |
| C-CA-CB               | 110.10             | 128.01          | 1                  |
| C-N-C-N-CD            | 125.00             | 163.64          | 1                  |
| CA-C-N                | 116.20             | 97.35           | 1                  |
| C-N-CA                | 121.70             | 138.66          | 1                  |
| N-CA-C-N-CA           | 121.70             | 138.65          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-O            | 120.80             | 104.80          | 1                  |
| C-N-CA            | 121.70             | 138.64          | 2                  |
| C-CA-N-CA-CB      | 110.50             | 126.50          | 1                  |
| C-CA-CB           | 110.10             | 127.97          | 1                  |
| CA-C-O            | 120.80             | 104.81          | 1                  |
| N-CA-CB           | 110.50             | 126.49          | 1                  |
| C-CA-CB           | 110.10             | 127.96          | 1                  |
| C-CA-N-CA-CB      | 111.50             | 95.52           | 1                  |
| C-CA-CB           | 110.10             | 127.95          | 1                  |
| C-N-C-CA-CB       | 110.10             | 127.95          | 1                  |
| N-CA-CB           | 110.50             | 94.53           | 1                  |
| C-CA-C-N-CA       | 121.70             | 138.60          | 1                  |
| CA-C-C-CA-CB      | 110.10             | 92.26           | 1                  |
| C-N-CA            | 121.70             | 138.60          | 1                  |
| CA-C-O            | 120.80             | 104.84          | 1                  |
| N-CA-CA-C-O       | 120.80             | 104.85          | 1                  |
| N-CA-CB           | 110.50             | 126.45          | 1                  |
| C-CA-CB           | 110.10             | 127.92          | 1                  |
| N-CA-CB           | 111.50             | 95.56           | 1                  |
| C-CA-C-CA-CB      | 110.10             | 127.91          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 92.30           | 1                  |
| CA-C-C-CA-N-CA-CB | 111.50             | 95.57           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB               | 111.50             | 95.58           | 1                  |
| C-N-CA                     | 121.70             | 138.56          | 1                  |
| C-CA-C-CA-CB               | 110.10             | 127.89          | 1                  |
| C-CA-CB                    | 110.10             | 127.89          | 1                  |
| NH1-CZ-NH2                 | 119.30             | 131.47          | 1                  |
| C-CA-CB                    | 110.10             | 92.31           | 1                  |
| C-CA-N-CA-C                | 111.00             | 137.21          | 1                  |
| CA-C-N                     | 116.20             | 134.92          | 1                  |
| N-CA-CB                    | 110.50             | 126.41          | 1                  |
| C-CA-C-N-CA                | 121.70             | 138.54          | 1                  |
| C-CA-CB                    | 110.10             | 92.32           | 1                  |
| C-CA-CA-C-N                | 116.20             | 97.49           | 1                  |
| N-CA-C                     | 111.00             | 84.81           | 2                  |
| CA-CB-C-CA-CB              | 110.10             | 92.33           | 1                  |
| CA-N-C-N-CA                | 121.70             | 138.53          | 1                  |
| N-CA-N-CA-CA-C-C-CA-CB     | 110.10             | 127.86          | 1                  |
| C-CA-CB                    | 110.10             | 92.34           | 1                  |
| C-CA-N-CA-N-CA-CA-C-CA-C-O | 120.80             | 104.92          | 1                  |
| C-CA-CB                    | 110.10             | 127.85          | 1                  |
| CA-CB-CG                   | 112.60             | 121.94          | 1                  |
| CA-C-N                     | 116.20             | 97.52           | 1                  |
| C-CA-CB                    | 110.10             | 92.35           | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-N-N-CA-C        | 111.00             | 137.15          | 1                  |
| C-CA-C-N-CA             | 121.70             | 138.51          | 1                  |
| C-CA-CB                 | 110.10             | 127.84          | 2                  |
| C-CA-NH1-CZ-NH2         | 119.30             | 131.43          | 1                  |
| C-N-CA                  | 121.70             | 138.50          | 1                  |
| C-CA-CA-C-N             | 116.20             | 97.53           | 1                  |
| CA-C-C-CA-C-CA-N-CA-CB  | 110.50             | 94.64           | 1                  |
| CA-C-N                  | 116.20             | 134.86          | 1                  |
| C-N-C-CA-C-CA-CB        | 109.10             | 129.62          | 1                  |
| CA-C-O                  | 120.80             | 104.95          | 1                  |
| N-CA-CB                 | 110.50             | 126.35          | 2                  |
| C-CA-CA-CB-N-CA-CB      | 110.40             | 124.38          | 1                  |
| C-CA-CB                 | 110.10             | 127.80          | 1                  |
| CA-C-O                  | 120.80             | 104.96          | 1                  |
| C-CA-C-CA-CA-C-CA-CB-CG | 112.60             | 121.91          | 1                  |
| C-CA-C-CA-CB            | 110.10             | 92.40           | 1                  |
| C-CA-CB                 | 110.10             | 92.41           | 1                  |
| CA-C-C-CA-CA-C-CA-C-O   | 120.80             | 104.97          | 1                  |
| C-N-CA                  | 121.70             | 138.46          | 1                  |
| C-CA-CA-C-O             | 120.80             | 104.98          | 1                  |
| CA-CB-N-CA-CB           | 111.50             | 95.68           | 1                  |
| C-CA-CB                 | 109.10             | 88.63           | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| C-CA-CB          | 110.10             | 127.78          | 1                  |
| C-N-C-CA-C-CA-CB | 110.10             | 127.78          | 1                  |
| C-CA-CB          | 110.10             | 127.77          | 1                  |
| C-CA-CB          | 109.10             | 88.64           | 1                  |
| CA-C-O           | 120.80             | 105.00          | 1                  |
| C-CA-C-CA-CB     | 111.60             | 130.19          | 1                  |
| C-CA-CB          | 109.10             | 88.65           | 1                  |
| C-N-C-CA-CB      | 110.10             | 127.76          | 1                  |
| C-CA-CB          | 110.10             | 127.76          | 2                  |
| C-CA-C-CA-CB     | 110.10             | 127.75          | 1                  |
| C-CA-CB          | 110.10             | 127.75          | 2                  |
| C-CA-C-N-CD      | 125.00             | 163.09          | 1                  |
| N-CA-CB          | 110.50             | 126.29          | 1                  |
| N-CA-N-CA-CB     | 111.50             | 95.71           | 1                  |
| CA-C-N           | 116.20             | 97.62           | 1                  |
| C-CA-CB          | 109.10             | 88.67           | 1                  |
| N-CA-C-CA-CB     | 110.10             | 92.46           | 1                  |
| C-N-CD           | 125.00             | 163.05          | 1                  |
| C-N-CA           | 121.70             | 138.40          | 1                  |
| C-CA-CB          | 110.10             | 92.47           | 2                  |
| C-CA-CB          | 110.50             | 96.58           | 1                  |
| C-N-CA-C-C-CA-CB | 109.10             | 129.50          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                | 110.10             | 127.72          | 1                  |
| C-CA-CB                | 111.60             | 130.14          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 126.26          | 1                  |
| C-N-N-CA-C-CA-CB       | 110.10             | 92.49           | 1                  |
| C-CA-CA-CB-N-CA-CB     | 110.50             | 126.26          | 1                  |
| N-CA-CB                | 110.50             | 126.26          | 1                  |
| C-CA-CB                | 110.10             | 92.49           | 3                  |
| N-CA-CB                | 111.50             | 95.75           | 1                  |
| C-CA-CB                | 110.50             | 96.60           | 1                  |
| C-N-C-CA-C-CA-CB       | 110.10             | 127.70          | 1                  |
| CA-C-O                 | 120.80             | 105.06          | 1                  |
| N-CA-CB                | 110.50             | 94.76           | 3                  |
| C-CA-C-CA-CB           | 110.10             | 92.51           | 1                  |
| N-CA-CB                | 111.50             | 95.77           | 1                  |
| N-CA-CB                | 110.50             | 94.77           | 1                  |
| CA-C-C-CA-CB           | 110.50             | 96.62           | 1                  |
| C-CA-CA-C-N-CA-CB      | 111.50             | 95.77           | 1                  |
| CA-C-O                 | 120.80             | 105.08          | 1                  |
| C-CA-CB                | 110.50             | 124.37          | 2                  |
| C-CA-CB                | 110.10             | 127.67          | 1                  |
| N-CA-CB                | 111.50             | 95.78           | 1                  |
| C-CA-CA-C-C-CA-N-CA-CB | 110.50             | 94.79           | 1                  |



| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| C-CA-CB              | 109.10             | 129.43          | 1                  |
| N-CA-CB              | 110.50             | 94.79           | 1                  |
| C-N-CA-C-C-CA-C-N-CA | 121.70             | 138.32          | 1                  |
| C-CA-CB              | 110.10             | 127.64          | 1                  |
| N-CA-CB              | 110.50             | 94.81           | 1                  |
| C-CA-CB              | 110.50             | 96.66           | 1                  |
| CA-C-N               | 116.20             | 134.66          | 1                  |
| C-N-CA               | 121.70             | 138.31          | 1                  |
| CA-C-O               | 120.80             | 136.49          | 1                  |
| N-CA-C-N-CA          | 121.70             | 138.30          | 1                  |
| C-CA-C-N-CA          | 121.70             | 138.30          | 1                  |
| N-CA-CA-C-O          | 120.80             | 105.13          | 1                  |
| C-CA-CB              | 110.50             | 124.32          | 2                  |
| CA-C-N               | 116.20             | 134.62          | 1                  |
| C-CA-CB              | 110.10             | 127.60          | 2                  |
| C-N-CA               | 121.70             | 138.28          | 1                  |
| C-CA-CB              | 109.10             | 129.36          | 1                  |
| C-CA-CB              | 110.10             | 92.61           | 1                  |
| N-CA-C               | 113.30             | 139.99          | 1                  |
| CA-C-O               | 120.80             | 105.16          | 1                  |
| N-CA-CA-C-N-CA-C     | 113.30             | 139.98          | 1                  |
| CA-C-O               | 120.80             | 136.43          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB      | 110.10             | 127.57          | 1                  |
| C-CA-CB           | 110.10             | 127.57          | 1                  |
| N-CA-C            | 113.30             | 139.96          | 1                  |
| C-CA-CB           | 110.10             | 127.56          | 1                  |
| C-CA-N-CA-C       | 111.00             | 85.27           | 1                  |
| N-CA-CB           | 110.50             | 126.11          | 1                  |
| N-CA-CB           | 111.50             | 127.11          | 1                  |
| C-CA-CB           | 110.10             | 127.54          | 1                  |
| CA-C-O            | 120.80             | 105.19          | 1                  |
| C-N-C-CA-CB       | 110.10             | 92.66           | 1                  |
| C-CA-N-CA-CA-N-CD | 112.00             | 99.15           | 1                  |
| N-CA-CB           | 110.50             | 126.10          | 1                  |
| CA-N-CD           | 112.00             | 99.16           | 1                  |
| N-CA-CB           | 110.50             | 126.09          | 1                  |
| C-CA-N-CA-C       | 113.30             | 139.89          | 1                  |
| N-CA-CB           | 110.50             | 94.91           | 1                  |
| N-CA-C-CA-N-CA-CB | 111.50             | 95.92           | 1                  |
| CA-C-O            | 120.80             | 136.38          | 1                  |
| C-CA-CB           | 110.10             | 127.51          | 1                  |
| C-CA-CB           | 110.10             | 92.69           | 1                  |
| C-CA-C-CA-C-CA-CB | 111.60             | 93.28           | 1                  |
| CA-C-N            | 116.20             | 134.52          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                        | 110.10             | 92.70           | 1                  |
| C-CA-CB                        | 110.10             | 127.50          | 1                  |
| CA-C-N                         | 116.20             | 134.51          | 1                  |
| C-CA-CB                        | 110.10             | 92.71           | 1                  |
| C-CA-CB                        | 110.10             | 127.49          | 1                  |
| N-CA-N-CA-CB                   | 111.50             | 95.94           | 1                  |
| C-CA-CB                        | 111.60             | 93.30           | 1                  |
| N-CA-CB                        | 103.00             | 113.06          | 1                  |
| N-CA-C-CA-CB                   | 110.10             | 127.48          | 1                  |
| C-CA-CB                        | 110.10             | 127.48          | 1                  |
| C-CA-N-CA-CB                   | 110.40             | 124.11          | 1                  |
| C-N-C-CA-CB                    | 110.10             | 127.47          | 1                  |
| N-CA-CB                        | 110.50             | 94.96           | 1                  |
| C-N-CA-C-N                     | 116.20             | 134.47          | 1                  |
| C-CA-CB                        | 110.10             | 127.46          | 1                  |
| CA-C-N                         | 116.20             | 134.47          | 1                  |
| N-CA-C-CA-CB                   | 110.10             | 92.75           | 1                  |
| N-CA-CB                        | 110.50             | 126.02          | 1                  |
| C-CA-CB                        | 110.10             | 92.76           | 1                  |
| N-CA-CB                        | 110.50             | 94.98           | 1                  |
| C-CA-C-N-N-CA-C-N-C-CA-C-CA-CB | 110.10             | 92.78           | 1                  |
| C-CA-CB                        | 110.10             | 127.42          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| CA-C-O           | 120.80             | 105.30          | 1                  |
| N-CA-C           | 111.00             | 136.52          | 1                  |
| C-CA-CB          | 110.10             | 92.78           | 1                  |
| CA-C-N           | 116.20             | 134.42          | 1                  |
| C-CA-CB          | 110.10             | 127.41          | 1                  |
| C-CA-N-CA-C      | 111.00             | 85.50           | 1                  |
| N-CA-C           | 111.00             | 136.50          | 1                  |
| N-CA-CB          | 103.00             | 113.02          | 1                  |
| C-CA-C-CA-CB     | 110.10             | 127.40          | 1                  |
| N-CA-C           | 113.30             | 139.70          | 1                  |
| C-CA-N-CA-C      | 111.00             | 136.49          | 1                  |
| CA-C-O           | 120.80             | 136.27          | 1                  |
| N-CA-CB          | 110.40             | 124.05          | 1                  |
| C-N-C-CA-CB      | 110.10             | 127.39          | 1                  |
| C-CA-N-CA-CA-C-O | 120.80             | 105.34          | 1                  |
| N-CA-CB          | 111.50             | 126.96          | 1                  |
| C-CA-CA-C-O      | 120.80             | 136.26          | 1                  |
| C-N-N-CA-C       | 111.00             | 85.54           | 1                  |
| C-N-N-CA-CB      | 111.50             | 126.95          | 1                  |
| N-CA-C           | 111.00             | 85.55           | 1                  |
| N-CA-C           | 113.30             | 139.65          | 1                  |
| CA-N-CD          | 112.00             | 99.28           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 127.36          | 1                  |
| C-CA-CB                | 110.10             | 127.35          | 3                  |
| CA-C-CA-C-N-CA-CB      | 103.00             | 112.99          | 1                  |
| N-CA-C-CA-C-N-N-CA-C   | 113.30             | 139.61          | 1                  |
| C-CA-CB                | 110.10             | 127.34          | 1                  |
| C-N-N-CA-C             | 113.30             | 139.58          | 1                  |
| N-CA-C-CA-N-CA-CB      | 111.50             | 126.91          | 1                  |
| N-CA-C                 | 111.00             | 136.38          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 127.31          | 1                  |
| C-N-CA-N-CD            | 112.00             | 99.32           | 1                  |
| C-N-CA                 | 121.70             | 138.00          | 1                  |
| N-CA-CB                | 110.50             | 125.89          | 1                  |
| N-CA-CB                | 103.00             | 112.96          | 1                  |
| N-CA-C                 | 111.00             | 85.68           | 1                  |
| C-CA-CB                | 110.10             | 127.28          | 2                  |
| CA-C-C-N-C-N-CA        | 121.70             | 105.44          | 1                  |
| C-CA-CB                | 110.10             | 127.26          | 1                  |
| N-CA-C                 | 111.00             | 136.29          | 1                  |
| C-CA-N-CA-C-N-CA       | 121.70             | 137.95          | 1                  |
| C-CA-CB                | 110.10             | 127.25          | 2                  |
| C-N-CA                 | 121.70             | 137.95          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 96.16           | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| CA-C-CA-C-N      | 116.20             | 134.25          | 1                  |
| N-CA-N-CA-C      | 111.00             | 85.74           | 1                  |
| C-CA-C-CA-CB     | 110.10             | 92.96           | 1                  |
| N-CA-CA-CB-CG    | 113.80             | 104.78          | 1                  |
| N-CA-CB          | 111.50             | 126.83          | 1                  |
| C-N-C-CA-N-CA-CB | 111.50             | 96.18           | 1                  |
| N-CA-N-CA-C      | 111.00             | 85.76           | 1                  |
| N-CA-C           | 111.00             | 136.23          | 1                  |
| CA-C-CA-C-O      | 120.80             | 105.48          | 1                  |
| C-CA-CB          | 110.10             | 92.98           | 1                  |
| N-CA-C           | 111.00             | 85.78           | 1                  |
| C-CA-CB          | 110.10             | 92.99           | 1                  |
| C-N-CA           | 121.70             | 105.49          | 1                  |
| N-CA-CB          | 103.00             | 112.90          | 1                  |
| N-CA-CB          | 111.50             | 96.19           | 1                  |
| N-CA-CB          | 110.50             | 95.20           | 1                  |
| C-CA-N-CA-N-CA-C | 111.00             | 136.20          | 1                  |
| C-N-CA           | 121.70             | 105.50          | 1                  |
| N-CA-C           | 111.00             | 136.19          | 1                  |
| N-CA-CB          | 110.50             | 125.80          | 1                  |
| C-CA-CB          | 110.10             | 93.00           | 1                  |
| C-N-N-CA-CB      | 111.50             | 96.21           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-C                 | 111.00             | 85.81           | 1                  |
| CA-CB-CG               | 113.80             | 104.80          | 1                  |
| N-CA-CB                | 111.50             | 126.79          | 1                  |
| CA-C-O                 | 120.80             | 105.51          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 127.19          | 1                  |
| C-CA-CB                | 110.10             | 93.01           | 1                  |
| C-CA-CB                | 110.50             | 123.99          | 1                  |
| C-N-N-CA-CB            | 110.50             | 95.22           | 1                  |
| CA-C-N                 | 116.20             | 98.23           | 1                  |
| N-CA-CB                | 103.00             | 112.88          | 1                  |
| C-CA-CB                | 109.10             | 128.87          | 1                  |
| C-CA-C-N-CA            | 121.70             | 105.53          | 1                  |
| C-N-CA                 | 121.70             | 137.87          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 95.23           | 1                  |
| C-CA-CB                | 110.50             | 123.97          | 1                  |
| CA-C-C-CA-C-CA-C-CA-CB | 110.10             | 93.05           | 1                  |
| C-CA-C-N-C-CA-CB       | 110.10             | 127.15          | 1                  |
| N-CA-CB                | 110.50             | 95.25           | 1                  |
| CA-C-C-N-C-N-CA        | 121.70             | 105.57          | 1                  |
| CA-C-CA-C-C-CA-N-CA-CB | 110.50             | 95.27           | 1                  |
| C-CA-C-N-N-CA-CB       | 110.50             | 95.28           | 1                  |
| C-CA-N-CA-CB           | 110.50             | 95.29           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA            | 121.70             | 105.60          | 1                  |
| C-CA-CB                | 110.10             | 127.09          | 1                  |
| N-CA-CB                | 110.50             | 95.30           | 1                  |
| CA-C-O                 | 120.80             | 105.61          | 1                  |
| CA-C-CA-C-N            | 116.20             | 98.33           | 1                  |
| C-CA-CB                | 110.10             | 93.13           | 1                  |
| N-CA-CB                | 110.50             | 95.31           | 1                  |
| C-CA-CB                | 110.10             | 127.07          | 1                  |
| C-N-CA                 | 121.70             | 105.63          | 1                  |
| C-CA-CB                | 109.10             | 128.74          | 1                  |
| C-N-CA                 | 121.70             | 137.77          | 1                  |
| N-CA-C-CA-N-CA-C-CA-CB | 111.60             | 93.75           | 1                  |
| C-CA-CB                | 110.50             | 123.88          | 1                  |
| C-CA-CB                | 110.50             | 123.87          | 1                  |
| CA-C-O                 | 120.80             | 105.64          | 1                  |
| C-CA-C-N-CA            | 121.70             | 105.66          | 1                  |
| C-CA-CB                | 110.10             | 93.18           | 1                  |
| CA-C-O                 | 120.80             | 135.94          | 1                  |
| C-CA-CB                | 110.10             | 127.02          | 1                  |
| C-CA-CB                | 111.60             | 93.80           | 1                  |
| N-CA-CB                | 110.50             | 95.37           | 2                  |
| C-CA-CB                | 110.10             | 127.01          | 2                  |



| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                          | 110.10             | 127.00          | 1                  |
| CA-C-C-CA-C-CA-C-N-CA            | 121.70             | 137.70          | 1                  |
| C-CA-N-CA-C-N-N-CA-C-CA-CB       | 110.10             | 126.97          | 1                  |
| N-CA-C                           | 111.00             | 135.85          | 1                  |
| N-CA-CB                          | 110.50             | 125.58          | 1                  |
| N-CA-C-N-CA                      | 121.70             | 137.67          | 1                  |
| CA-C-C-CA-CB                     | 110.10             | 126.95          | 1                  |
| N-CA-CB                          | 111.50             | 126.58          | 1                  |
| C-N-CA                           | 121.70             | 137.66          | 1                  |
| N-CA-C                           | 111.00             | 135.83          | 1                  |
| C-CA-CB                          | 110.10             | 126.95          | 1                  |
| C-CA-CB                          | 110.10             | 126.94          | 1                  |
| N-CA-CB                          | 110.50             | 95.43           | 1                  |
| CA-C-O                           | 120.80             | 135.87          | 2                  |
| C-CA-CB                          | 110.10             | 93.27           | 1                  |
| N-CA-C-CA-CB                     | 110.10             | 126.93          | 1                  |
| C-CA-CB                          | 110.50             | 123.78          | 1                  |
| C-CA-N-CA-CB                     | 110.50             | 125.55          | 1                  |
| N-CA-CB                          | 110.50             | 95.45           | 1                  |
| C-CA-CB                          | 110.10             | 126.92          | 1                  |
| N-CA-C-N-CA-CB-CA-C-CA-C-C-CA-CB | 110.10             | 126.90          | 1                  |
| C-CA-CB                          | 110.10             | 93.30           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB                | 110.10             | 93.30           | 1                  |
| C-CA-CB                     | 110.10             | 93.31           | 1                  |
| C-CA-C-CA-CB                | 111.40             | 128.19          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 93.31           | 1                  |
| C-CA-C-CA-CB                | 110.10             | 126.89          | 1                  |
| C-CA-CB                     | 110.10             | 126.88          | 2                  |
| C-CA-CB                     | 110.10             | 93.33           | 1                  |
| C-CA-CB                     | 110.10             | 126.87          | 1                  |
| C-N-CA                      | 121.70             | 105.82          | 1                  |
| C-CA-CB                     | 111.40             | 128.16          | 1                  |
| CA-CB-C-CA-CB               | 111.60             | 93.96           | 1                  |
| N-CA-CA-C-CA-C-N-CA-CB      | 111.50             | 126.48          | 1                  |
| C-CA-CB                     | 110.10             | 126.84          | 1                  |
| C-CA-CB                     | 110.10             | 126.83          | 1                  |
| C-CA-C-CA-C-CA-C-CA-C-CA-CB | 110.50             | 123.70          | 1                  |
| C-CA-CB                     | 110.10             | 126.82          | 2                  |
| C-CA-C-CA-CA-CB-CG          | 113.80             | 105.01          | 1                  |
| C-CA-CB                     | 110.10             | 93.39           | 1                  |
| N-CA-CB                     | 110.50             | 125.45          | 1                  |
| CA-C-C-CA-CB                | 111.40             | 128.10          | 1                  |
| C-CA-CB                     | 110.10             | 93.40           | 1                  |
| CA-C-N                      | 116.20             | 98.63           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| C-N-CA       | 121.70             | 137.51          | 1                  |
| N-CA-CB      | 111.50             | 126.43          | 2                  |
| C-CA-CB      | 110.10             | 126.78          | 1                  |
| C-N-CA       | 121.70             | 105.90          | 1                  |
| C-CA-CB      | 111.40             | 128.08          | 1                  |
| CA-C-C-CA-CB | 110.10             | 126.77          | 1                  |
| C-CA-CB      | 110.10             | 126.76          | 2                  |
| N-CA-CB      | 110.50             | 125.41          | 1                  |
| C-N-CA       | 121.70             | 137.49          | 1                  |
| C-N-CA       | 121.70             | 105.92          | 2                  |
| C-CA-CB      | 111.60             | 94.07           | 1                  |
| C-CA-CB      | 109.10             | 128.38          | 1                  |
| C-CA-C-N-CA  | 121.70             | 137.47          | 1                  |
| CA-C-N-CA-C  | 111.00             | 135.53          | 1                  |
| CA-C-N       | 116.20             | 98.69           | 1                  |
| C-CA-CB      | 110.10             | 126.73          | 1                  |
| N-CA-CB      | 111.50             | 96.62           | 1                  |
| CA-C-N-CA-C  | 111.00             | 135.49          | 1                  |
| N-CA-C-N-CA  | 121.70             | 105.96          | 1                  |
| C-CA-C-CA-CB | 110.10             | 126.72          | 1                  |
| N-CA-CB      | 111.50             | 96.64           | 1                  |
| C-N-CA       | 121.70             | 105.96          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| C-CA-CB              | 110.10             | 126.71          | 1                  |
| N-CA-C-CA-CB         | 110.10             | 126.71          | 1                  |
| CA-CB-CG             | 113.80             | 105.06          | 1                  |
| N-CA-C-CA-CB         | 110.10             | 126.70          | 1                  |
| C-CA-CB              | 110.10             | 126.70          | 1                  |
| C-N-N-CA-N-CA-CA-C-N | 116.20             | 133.66          | 1                  |
| C-N-CA               | 121.70             | 137.42          | 2                  |
| C-CA-CB              | 109.10             | 128.31          | 1                  |
| CA-C-O               | 120.80             | 105.96          | 1                  |
| CA-C-CA-C-C-CA-CB    | 110.10             | 126.68          | 1                  |
| CA-C-C-CA-CB         | 110.10             | 126.68          | 1                  |
| CA-C-C-CA-CB         | 110.10             | 93.52           | 1                  |
| N-CA-N-CA-CB         | 103.00             | 93.40           | 1                  |
| C-CA-CB              | 110.10             | 126.67          | 1                  |
| C-CA-CB              | 109.10             | 128.29          | 2                  |
| CA-C-CA-C-C-CA-CB    | 110.10             | 126.66          | 1                  |
| C-N-CA               | 121.70             | 106.01          | 1                  |
| C-CA-CB              | 110.10             | 126.66          | 2                  |
| CA-C-N               | 116.20             | 133.63          | 1                  |
| C-CA-CB              | 111.40             | 94.85           | 1                  |
| C-N-CA               | 121.70             | 137.38          | 1                  |
| CA-C-C-CA-CB         | 110.10             | 126.65          | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB                    | 110.10             | 126.64          | 1                  |
| CA-C-C-CA-CB                    | 110.10             | 126.64          | 1                  |
| C-CA-CB                         | 110.10             | 126.64          | 2                  |
| C-CA-CB                         | 111.40             | 94.87           | 1                  |
| N-CA-C-CA-CA-C-C-CA-CA-C-C-N-CA | 121.70             | 106.05          | 1                  |
| C-CA-CB                         | 111.40             | 94.88           | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 126.62          | 1                  |
| CA-C-O                          | 120.80             | 135.58          | 1                  |
| C-CA-C-CA-C-CA-CB               | 110.10             | 126.61          | 1                  |
| CA-C-O                          | 120.80             | 135.57          | 1                  |
| C-CA-CB                         | 110.10             | 93.59           | 2                  |
| C-CA-CB                         | 109.10             | 128.21          | 1                  |
| CA-C-N-CA-CA-C-N-CA-CB          | 111.50             | 96.73           | 1                  |
| C-N-C-CA-N-CA-C-CA-C-CA-C-CA-CB | 109.10             | 128.20          | 1                  |
| CA-C-C-CA-CB                    | 110.10             | 126.59          | 1                  |
| CA-C-O                          | 120.80             | 135.55          | 1                  |
| N-CA-C-N-CA                     | 121.70             | 137.31          | 1                  |
| C-CA-CA-C-CA-C-O                | 120.80             | 135.54          | 1                  |
| CA-C-CA-C-O                     | 120.80             | 135.53          | 1                  |
| C-CA-CB                         | 110.50             | 123.50          | 1                  |
| C-CA-CB                         | 110.10             | 93.64           | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 126.56          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 111.40             | 94.95           | 1                  |
| C-CA-CB               | 110.10             | 126.55          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 93.65           | 1                  |
| N-CA-C                | 111.00             | 86.76           | 1                  |
| C-CA-C-CA-CB          | 110.10             | 126.55          | 1                  |
| C-CA-CA-C-N-CA-C-N-CA | 121.70             | 106.12          | 1                  |
| C-CA-CB               | 110.10             | 126.54          | 2                  |
| C-CA-N-CA-C           | 111.00             | 135.23          | 1                  |
| C-CA-CB               | 110.50             | 123.48          | 1                  |
| N-CA-CB               | 103.00             | 93.48           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 126.53          | 1                  |
| N-CA-C-CA-CB          | 110.10             | 126.52          | 1                  |
| N-CA-C                | 111.00             | 86.80           | 1                  |
| C-N-N-CA-C            | 111.00             | 86.80           | 1                  |
| C-N-CA                | 121.70             | 106.15          | 2                  |
| N-CA-CB               | 111.50             | 96.81           | 1                  |
| N-CA-C                | 111.00             | 135.19          | 1                  |
| CA-C-O                | 120.80             | 135.49          | 1                  |
| N-CA-C                | 111.00             | 86.82           | 1                  |
| C-CA-CB               | 110.10             | 93.69           | 1                  |
| C-CA-N-CA-CB          | 110.40             | 123.35          | 1                  |
| C-CA-CB               | 110.50             | 123.45          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-O             | 120.80             | 135.48          | 1                  |
| C-CA-C-N-NH1-CZ-C-CA-CB | 110.10             | 126.49          | 1                  |
| CA-C-N                  | 116.20             | 133.45          | 1                  |
| C-CA-CB                 | 110.50             | 123.44          | 1                  |
| N-CA-CB                 | 110.40             | 123.34          | 1                  |
| C-CA-CB                 | 110.10             | 126.48          | 1                  |
| C-CA-C-CA-C-CA-CA-C-O   | 120.80             | 135.45          | 1                  |
| C-CA-N-CA-CB            | 111.50             | 96.85           | 1                  |
| NH1-CZ-N-CA-C-N-CA      | 121.70             | 137.20          | 1                  |
| N-CA-CB                 | 110.50             | 125.14          | 1                  |
| C-CA-C-CA-CB            | 110.10             | 126.45          | 1                  |
| C-N-CA-C-N              | 116.20             | 98.99           | 1                  |
| N-CA-CB                 | 110.50             | 125.13          | 1                  |
| C-CA-C-CA-CB            | 110.10             | 93.76           | 1                  |
| N-CA-C-CA-CA-C-N        | 116.20             | 99.01           | 1                  |
| C-CA-CB                 | 110.10             | 93.78           | 1                  |
| CA-C-C-CA-CB            | 110.10             | 126.42          | 1                  |
| N-CA-C-CA-CB            | 110.10             | 93.78           | 1                  |
| CA-C-O                  | 120.80             | 102.77          | 1                  |
| N-CA-C                  | 111.00             | 86.96           | 1                  |
| C-CA-CB                 | 110.10             | 126.41          | 1                  |
| N-CA-CB                 | 110.50             | 95.91           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB | 110.10             | 126.41          | 1                  |
| N-CA-C       | 111.00             | 135.03          | 1                  |
| C-CA-CB      | 110.10             | 126.40          | 1                  |
| C-CA-N-CA-C  | 111.00             | 86.98           | 1                  |
| CA-C-O       | 120.80             | 135.38          | 1                  |
| C-CA-CB      | 110.10             | 126.39          | 1                  |
| C-CA-CA-C-O  | 120.80             | 102.80          | 1                  |
| N-CA-C       | 111.00             | 87.01           | 1                  |
| C-CA-CB      | 110.10             | 126.38          | 1                  |
| N-CA-CB      | 111.50             | 96.93           | 1                  |
| CA-C-N-CA-C  | 111.00             | 87.03           | 1                  |
| CA-C-O       | 120.80             | 135.35          | 1                  |
| C-CA-C-CA-CB | 110.10             | 93.85           | 1                  |
| CA-C-CA-C-O  | 120.80             | 106.26          | 1                  |
| C-CA-CB      | 110.10             | 126.35          | 1                  |
| N-CA-C       | 111.00             | 87.06           | 1                  |
| CA-C-CA-C-N  | 116.20             | 133.30          | 1                  |
| N-CA-CB      | 110.50             | 125.03          | 1                  |
| CA-C-N       | 116.20             | 133.29          | 1                  |
| C-CA-CB      | 110.10             | 126.33          | 1                  |
| CA-C-O       | 120.80             | 106.28          | 1                  |
| CA-C-O       | 120.80             | 135.32          | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 93.87           | 1                  |
| N-CA-CB               | 110.50             | 125.02          | 1                  |
| C-N-CA                | 121.70             | 137.07          | 2                  |
| N-CA-CA-N-CD          | 112.00             | 100.05          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 93.88           | 1                  |
| CA-C-N                | 116.20             | 133.27          | 2                  |
| C-N-CA-C-O            | 120.80             | 135.31          | 1                  |
| C-N-CA                | 121.70             | 137.06          | 1                  |
| C-CA-CB               | 110.10             | 93.89           | 1                  |
| CA-C-N                | 116.20             | 99.14           | 1                  |
| CA-C-N                | 116.20             | 133.26          | 1                  |
| CA-C-CA-C-C-CA-C-N-CA | 121.70             | 137.05          | 1                  |
| N-CA-CA-C-O           | 120.80             | 135.29          | 1                  |
| CA-C-O                | 120.80             | 135.29          | 1                  |
| N-CA-C                | 111.00             | 87.13           | 1                  |
| C-CA-C-CA-CB          | 110.10             | 126.29          | 1                  |
| CA-C-CA-C-CA-N-CD     | 112.00             | 100.07          | 1                  |
| C-CA-C-CA-C-CA-N-CA-C | 111.00             | 87.18           | 1                  |
| CA-C-C-CA-CB          | 110.10             | 93.94           | 1                  |
| N-CA-C                | 111.00             | 87.18           | 1                  |
| C-CA-CA-C-C-CA-CB     | 111.60             | 94.60           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 93.95           | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| C-CA-CB              | 110.10             | 126.25          | 1                  |
| N-CA-CB              | 110.50             | 124.94          | 1                  |
| C-CA-CB              | 110.10             | 93.96           | 1                  |
| C-CA-C-CA-C-CA-C-C-O | 120.80             | 106.36          | 1                  |
| N-CA-C               | 111.00             | 87.23           | 1                  |
| N-CA-C-CA-C-CA-CB    | 111.60             | 94.62           | 1                  |
| C-CA-CA-C-C-CA-CB    | 110.10             | 93.98           | 1                  |
| N-CA-C               | 111.00             | 87.24           | 1                  |
| C-CA-CB              | 110.10             | 93.98           | 1                  |
| CA-C-N               | 116.20             | 133.16          | 1                  |
| CA-C-N-CA-C-CA-CB    | 110.10             | 126.21          | 1                  |
| C-CA-CB              | 110.10             | 93.99           | 1                  |
| CA-C-C-CA-CB         | 110.50             | 123.21          | 1                  |
| C-CA-CB              | 110.10             | 126.20          | 1                  |
| CA-C-O               | 120.80             | 106.40          | 1                  |
| CA-C-N               | 116.20             | 99.26           | 1                  |
| N-CA-C-CA-CB         | 110.10             | 94.01           | 1                  |
| N-CA-CB              | 110.50             | 96.10           | 1                  |
| C-CA-CB              | 110.10             | 126.19          | 1                  |
| C-CA-CB              | 110.10             | 94.01           | 1                  |
| N-CA-CB              | 110.50             | 96.11           | 1                  |
| C-CA-CA-C-N          | 116.20             | 133.13          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-N-CA-C            | 111.00             | 87.31           | 1                  |
| C-CA-C-CA-C-CA-C-CA-CB      | 110.10             | 94.03           | 1                  |
| C-CA-CB                     | 110.10             | 126.17          | 1                  |
| N-CA-N-CA-CB                | 110.50             | 124.88          | 1                  |
| C-CA-C-CA-CA-C-N-CA-C-CA-CB | 110.50             | 97.83           | 1                  |
| C-CA-C-CA-C-CA-CB           | 111.60             | 94.71           | 1                  |
| C-CA-C-CA-CB                | 110.50             | 123.16          | 2                  |
| CA-C-C-CA-CB                | 110.50             | 97.84           | 1                  |
| CA-CB-CG                    | 113.90             | 98.71           | 1                  |
| O-C-N                       | 123.00             | 136.50          | 1                  |
| C-CA-CB                     | 110.50             | 123.16          | 1                  |
| CA-N-N-CA-C-CA-CB           | 110.10             | 126.13          | 1                  |
| CA-C-O                      | 120.80             | 106.46          | 1                  |
| N-CA-CB                     | 110.50             | 124.84          | 1                  |
| O-C-N                       | 123.00             | 136.49          | 1                  |
| N-CA-C-CA-CB                | 110.10             | 126.12          | 1                  |
| C-CA-O-C-N                  | 123.00             | 136.48          | 1                  |
| C-CA-N-CA-C-CA-CB           | 110.10             | 126.10          | 1                  |
| CA-C-C-CA-CB                | 110.10             | 126.10          | 1                  |
| CA-CB-CG                    | 113.90             | 98.75           | 1                  |
| C-CA-C-CA-CB                | 111.60             | 94.77           | 1                  |
| O-C-N                       | 123.00             | 136.46          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-O            | 120.80             | 106.50          | 1                  |
| N-CA-C-N-CD            | 125.00             | 159.48          | 1                  |
| CA-CB-CG               | 112.60             | 104.19          | 1                  |
| CA-C-O                 | 120.80             | 106.50          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 126.08          | 1                  |
| CA-C-C-CA-C-CA-C-CA-CB | 110.10             | 126.07          | 1                  |
| C-CA-CB                | 110.10             | 126.07          | 1                  |
| CA-C-O                 | 120.80             | 106.51          | 1                  |
| N-CA-CB                | 111.50             | 125.79          | 1                  |
| C-CA-N-CA-C-CA-CB      | 110.10             | 126.06          | 1                  |
| C-CA-C-CA-CA-C-O       | 120.80             | 106.53          | 1                  |
| C-N-CA                 | 121.70             | 136.81          | 1                  |
| C-CA-CB                | 110.10             | 94.15           | 1                  |
| C-N-CD                 | 125.00             | 159.41          | 1                  |
| N-CA-CA-C-O            | 120.80             | 106.54          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 94.16           | 1                  |
| CA-N-N-CA-CB           | 110.50             | 124.76          | 1                  |
| C-CA-CB                | 110.10             | 126.03          | 2                  |
| N-CA-N-CA-C-CA-C-CA-CB | 110.10             | 94.17           | 1                  |
| C-CA-CB                | 110.10             | 94.17           | 1                  |
| CA-N-N-CA-N-CA-C-N-CA  | 121.70             | 136.78          | 1                  |
| CA-C-C-CA-CB           | 110.10             | 126.02          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                    | 111.50             | 97.26           | 1                  |
| C-CA-CB                    | 110.10             | 126.01          | 1                  |
| C-CA-N-CA-CA-C-N           | 116.20             | 132.94          | 1                  |
| C-N-CA                     | 121.70             | 136.76          | 1                  |
| C-CA-C-CA-CB               | 110.10             | 126.00          | 1                  |
| N-CA-CB                    | 111.50             | 125.72          | 1                  |
| C-CA-CB                    | 110.10             | 94.21           | 1                  |
| CA-C-N                     | 116.20             | 132.93          | 1                  |
| CA-C-N                     | 116.20             | 99.47           | 1                  |
| C-CA-CB                    | 110.10             | 125.99          | 3                  |
| CA-CB-CG                   | 112.60             | 104.24          | 1                  |
| C-CA-CA-C-N                | 116.20             | 99.48           | 1                  |
| CA-C-N                     | 116.20             | 132.92          | 1                  |
| C-CA-CB                    | 110.10             | 94.22           | 2                  |
| N-CA-CB                    | 110.50             | 124.70          | 1                  |
| N-CA-C                     | 111.00             | 87.62           | 1                  |
| C-CA-N-CA-CB               | 110.50             | 124.69          | 1                  |
| CA-C-N                     | 116.20             | 132.89          | 1                  |
| CA-C-C-CA-CB               | 110.10             | 125.95          | 1                  |
| C-CA-CB                    | 109.10             | 90.74           | 1                  |
| N-CA-C-CA-CB               | 110.10             | 125.95          | 1                  |
| C-CA-CA-C-CA-C-CA-C-C-N-CA | 121.70             | 106.69          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-CB-C-CA-CB               | 110.10             | 125.94          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 94.26           | 1                  |
| N-CA-CB                     | 110.40             | 97.90           | 1                  |
| N-CA-C                      | 111.00             | 87.67           | 1                  |
| CA-N-C-N-CA                 | 121.70             | 106.70          | 1                  |
| CA-C-C-CA-CA-C-N            | 116.20             | 132.86          | 1                  |
| C-CA-C-CA-N-CA-N-CA-CB      | 111.50             | 97.34           | 1                  |
| C-CA-CB                     | 110.10             | 94.28           | 1                  |
| CA-C-N                      | 116.20             | 132.85          | 1                  |
| N-CA-N-CA-C-CA-C-CA-C-CA-CB | 110.10             | 94.29           | 1                  |
| N-CA-CB                     | 111.50             | 125.64          | 2                  |
| C-CA-C-CA-CB                | 110.10             | 94.29           | 1                  |
| C-CA-CB                     | 110.10             | 94.29           | 1                  |
| C-CA-CB                     | 109.10             | 90.80           | 1                  |
| CA-CB-CG                    | 112.60             | 120.92          | 1                  |
| N-CA-C                      | 111.00             | 87.71           | 1                  |
| N-CA-CB                     | 110.40             | 97.92           | 1                  |
| C-CA-CB                     | 110.10             | 94.30           | 1                  |
| C-CA-N-CA-CB                | 110.50             | 96.37           | 1                  |
| N-CA-CB                     | 110.50             | 96.37           | 2                  |
| CA-C-O                      | 120.80             | 106.67          | 1                  |
| N-CA-C                      | 111.00             | 87.73           | 3                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-N-CA                      | 121.70             | 136.66          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 125.89          | 1                  |
| N-CA-CA-CB-CG               | 112.60             | 120.91          | 1                  |
| N-CA-CB                     | 110.50             | 96.38           | 1                  |
| N-CA-C-CA-C-CA-CB           | 110.10             | 94.32           | 1                  |
| C-CA-C-CA-CA-C-C-CA-N-CA-CB | 110.50             | 124.61          | 1                  |
| C-CA-CB                     | 110.10             | 125.86          | 2                  |
| N-CA-CB                     | 110.50             | 96.40           | 1                  |
| C-CA-C-CA-CB                | 110.50             | 122.94          | 1                  |
| C-CA-C-CA-CB                | 110.50             | 122.93          | 1                  |
| C-CA-CB                     | 110.10             | 125.84          | 4                  |
| CA-C-O                      | 120.80             | 106.71          | 1                  |
| N-CA-C                      | 111.00             | 87.80           | 1                  |
| C-CA-N-CA-C                 | 111.00             | 87.80           | 1                  |
| C-CA-C-CA-C-CA-CB           | 110.10             | 125.83          | 1                  |
| C-N-N-CA-C-CA-C-CA-CB       | 110.10             | 94.38           | 1                  |
| C-CA-CB                     | 110.10             | 94.38           | 1                  |
| C-CA-CB                     | 111.60             | 128.15          | 1                  |
| C-CA-CB                     | 110.10             | 125.82          | 1                  |
| N-CA-C                      | 111.00             | 87.84           | 1                  |
| C-CA-CB                     | 110.10             | 94.39           | 2                  |
| N-CA-C-CA-CB                | 110.10             | 94.39           | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-N-CA             | 121.70             | 136.58          | 2                  |
| N-CA-C             | 111.00             | 87.86           | 1                  |
| C-CA-CB            | 110.10             | 125.80          | 2                  |
| C-CA-CB            | 111.60             | 128.13          | 1                  |
| C-CA-CB            | 110.10             | 94.40           | 1                  |
| C-CA-CB            | 110.50             | 122.89          | 1                  |
| C-N-C-CA-CB        | 110.10             | 94.40           | 1                  |
| C-CA-CA-C-C-CA-CB  | 110.10             | 125.79          | 1                  |
| CA-CB-CG           | 113.80             | 105.55          | 1                  |
| N-CA-C-CA-CB       | 110.10             | 94.42           | 1                  |
| N-CA-CA-CB-CG      | 112.60             | 120.85          | 1                  |
| C-CA-N-CA-CA-C-N   | 116.20             | 132.70          | 1                  |
| C-N-CA             | 121.70             | 136.54          | 1                  |
| CA-CB-C-CA-C-CA-CB | 110.10             | 125.77          | 1                  |
| CA-CB-CG           | 112.60             | 120.84          | 1                  |
| N-CA-C             | 111.00             | 87.92           | 2                  |
| C-CA-CB            | 110.50             | 122.86          | 1                  |
| C-CA-C-CA-CB       | 110.10             | 94.45           | 1                  |
| CA-CB-CG           | 113.80             | 105.56          | 1                  |
| C-CA-C-CA-CB       | 110.50             | 98.14           | 1                  |
| C-N-CA             | 121.70             | 136.53          | 1                  |
| N-CA-N-CA-C-CA-CB  | 110.10             | 125.75          | 1                  |



| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 125.74          | 2                  |
| C-CA-CB           | 110.10             | 94.46           | 1                  |
| C-N-C-CA-CB       | 110.10             | 125.74          | 1                  |
| C-N-CA            | 121.70             | 136.52          | 1                  |
| C-CA-CA-C-O       | 120.80             | 134.79          | 1                  |
| N-CA-CB           | 110.50             | 96.51           | 1                  |
| C-N-C-N-CA        | 121.70             | 106.89          | 1                  |
| C-N-CA            | 121.70             | 106.89          | 2                  |
| N-CA-CA-C-O       | 120.80             | 134.79          | 1                  |
| C-CA-CB           | 110.10             | 94.47           | 1                  |
| C-N-N-CA-CB       | 110.40             | 122.74          | 1                  |
| N-CA-CB           | 110.50             | 124.48          | 1                  |
| C-CA-CB           | 111.40             | 127.03          | 1                  |
| N-CA-CB           | 110.40             | 98.07           | 1                  |
| C-CA-C-N-CA       | 121.70             | 106.90          | 1                  |
| C-CA-CA-C-C-CA-CB | 109.10             | 91.02           | 1                  |
| C-CA-C-N-CA       | 121.70             | 136.49          | 1                  |
| CA-C-CA-C-N-CA-CB | 110.50             | 96.54           | 1                  |
| CA-CB-N-CA-N-CA-C | 111.00             | 88.00           | 1                  |
| CA-C-O            | 120.80             | 134.76          | 1                  |
| C-N-CA-C-N        | 116.20             | 99.78           | 1                  |
| CA-C-N            | 116.20             | 132.62          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-O                 | 120.80             | 134.75          | 1                  |
| C-CA-CB                | 110.50             | 122.81          | 1                  |
| C-CA-CB                | 110.10             | 94.51           | 1                  |
| C-N-N-CA-CB            | 110.50             | 96.56           | 1                  |
| N-CA-C                 | 111.00             | 133.96          | 1                  |
| CA-C-N                 | 116.20             | 99.80           | 1                  |
| N-CA-C                 | 111.00             | 88.04           | 1                  |
| N-CA-C-CA-CB           | 110.10             | 125.68          | 1                  |
| CA-C-O                 | 120.80             | 134.74          | 1                  |
| C-N-CA-C-C-CA-CB       | 110.50             | 98.21           | 1                  |
| CA-C-O                 | 120.80             | 106.87          | 1                  |
| N-CA-N-CA-N-CA-C-CA-CB | 110.50             | 98.21           | 1                  |
| C-CA-CB                | 110.50             | 122.79          | 1                  |
| C-CA-CB                | 110.10             | 125.66          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 125.66          | 1                  |
| CA-C-CA-C-O            | 120.80             | 106.88          | 1                  |
| N-CA-CB                | 110.40             | 122.68          | 1                  |
| C-CA-CB                | 111.40             | 126.95          | 1                  |
| C-CA-CB                | 110.50             | 122.78          | 1                  |
| N-CA-C                 | 111.00             | 88.08           | 1                  |
| N-CA-CB                | 111.50             | 125.41          | 1                  |
| C-N-CA-C-N             | 116.20             | 132.57          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| C-CA-CB              | 110.50             | 122.77          | 1                  |
| C-N-N-CA-CA-C-N-CA-C | 111.00             | 88.09           | 1                  |
| C-N-CA               | 121.70             | 136.42          | 2                  |
| C-CA-CB              | 110.10             | 125.64          | 1                  |
| N-CA-CA-C-O          | 120.80             | 106.90          | 1                  |
| CA-C-N-CA-CB         | 111.50             | 125.40          | 1                  |
| CA-C-CA-C-N          | 116.20             | 99.85           | 1                  |
| C-CA-CB              | 109.10             | 91.12           | 1                  |
| CA-C-O               | 120.80             | 106.90          | 1                  |
| C-CA-CB              | 110.10             | 125.63          | 1                  |
| CA-CB-CG             | 113.80             | 105.63          | 1                  |
| CA-C-O               | 120.80             | 106.91          | 1                  |
| C-CA-CB              | 110.10             | 125.62          | 1                  |
| CA-C-CA-C-N          | 116.20             | 99.87           | 1                  |
| N-CA-C               | 111.00             | 88.14           | 1                  |
| C-N-CA-C-O           | 120.80             | 106.93          | 1                  |
| C-CA-CB              | 110.50             | 122.74          | 1                  |
| C-CA-CB              | 110.10             | 94.60           | 1                  |
| C-N-CA               | 121.70             | 136.38          | 1                  |
| CA-C-N               | 116.20             | 132.50          | 1                  |
| C-CA-C-CA-CB         | 110.10             | 125.58          | 1                  |
| N-CA-C               | 111.00             | 88.18           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-O                      | 120.80             | 106.95          | 1                  |
| N-CA-C                      | 111.00             | 88.19           | 1                  |
| N-CA-C                      | 111.00             | 133.81          | 1                  |
| CA-C-O                      | 120.80             | 134.64          | 1                  |
| N-CA-CA-CB-C-CA-CB          | 110.10             | 125.57          | 1                  |
| C-CA-CB                     | 110.10             | 94.63           | 1                  |
| N-CA-C                      | 111.00             | 133.79          | 1                  |
| CA-C-CA-C-CA-C-O            | 120.80             | 106.96          | 1                  |
| N-CA-C-N-CA                 | 121.70             | 136.35          | 1                  |
| C-CA-N-CA-N-CA-N-CA-N-CA-CB | 111.50             | 125.33          | 1                  |
| CA-C-CA-C-CA-CB-CG          | 113.80             | 121.93          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 125.55          | 1                  |
| CA-C-O                      | 120.80             | 106.98          | 1                  |
| CA-C-CA-C-O                 | 120.80             | 106.98          | 1                  |
| C-CA-CB                     | 110.50             | 122.69          | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB      | 110.40             | 98.22           | 1                  |
| C-N-CA                      | 121.70             | 136.32          | 1                  |
| CA-C-CA-C-O                 | 120.80             | 134.61          | 1                  |
| C-CA-CB                     | 110.10             | 125.53          | 1                  |
| CA-C-O                      | 120.80             | 107.00          | 1                  |
| N-CA-C-CA-CB                | 110.10             | 94.68           | 1                  |
| C-N-CA-C-C-CA-CB            | 110.10             | 94.68           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-CA-CB-C-N-CA | 121.70             | 136.31          | 1                  |
| C-CA-CB           | 110.10             | 94.68           | 1                  |
| N-CA-C            | 111.00             | 88.29           | 1                  |
| C-CA-CB           | 110.10             | 125.51          | 1                  |
| N-CA-C            | 111.00             | 133.70          | 1                  |
| C-CA-CB           | 110.10             | 94.70           | 2                  |
| N-CA-CB           | 110.50             | 96.72           | 1                  |
| C-CA-CB           | 110.50             | 98.34           | 1                  |
| C-N-N-CA-C-CA-CB  | 110.10             | 125.49          | 1                  |
| CA-C-C-CA-CB      | 110.50             | 98.35           | 1                  |
| CA-C-N-CA-C       | 111.00             | 88.33           | 1                  |
| N-CA-C            | 111.00             | 133.66          | 1                  |
| C-CA-CB           | 110.50             | 122.64          | 1                  |
| C-CA-CB           | 110.10             | 125.48          | 2                  |
| CA-C-O            | 120.80             | 107.04          | 1                  |
| C-CA-CB           | 110.10             | 125.47          | 1                  |
| N-CA-C            | 111.00             | 133.65          | 1                  |
| C-CA-CB           | 110.10             | 125.46          | 3                  |
| N-CA-CB           | 111.50             | 125.25          | 1                  |
| N-CA-C-CA-CB      | 110.10             | 94.74           | 1                  |
| C-N-CA            | 121.70             | 136.25          | 1                  |
| C-CA-CB           | 109.10             | 91.32           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 110.50             | 124.24          | 1                  |
| CA-C-N            | 116.20             | 100.04          | 1                  |
| N-CA-C            | 111.00             | 88.38           | 1                  |
| C-CA-CB           | 110.10             | 94.75           | 1                  |
| C-CA-CB           | 111.40             | 96.05           | 1                  |
| N-CA-CB           | 110.40             | 122.51          | 1                  |
| N-CA-C-CA-N-CA-C  | 111.00             | 133.61          | 1                  |
| C-CA-CB           | 110.10             | 125.44          | 1                  |
| N-CA-N-CA-CB      | 110.50             | 124.22          | 1                  |
| N-CA-C            | 111.00             | 133.60          | 1                  |
| C-CA-CB           | 110.10             | 94.76           | 1                  |
| CA-C-O            | 120.80             | 107.08          | 1                  |
| N-CA-C            | 111.00             | 88.40           | 1                  |
| C-CA-CB           | 111.40             | 96.06           | 1                  |
| C-CA-CB           | 110.10             | 94.77           | 2                  |
| C-CA-CB           | 110.50             | 98.40           | 1                  |
| C-CA-CB           | 110.10             | 125.43          | 1                  |
| C-CA-C-CA-C-CA-CB | 109.10             | 91.36           | 1                  |
| C-CA-C-CA-CB      | 110.10             | 94.78           | 1                  |
| C-CA-CA-C-CA-C-O  | 120.80             | 134.50          | 1                  |
| CA-C-O            | 120.80             | 134.50          | 1                  |
| C-CA-CB           | 109.10             | 91.37           | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| C-CA-CB      | 111.40             | 96.09           | 2                  |
| CA-C-C-N-CA  | 121.70             | 107.19          | 1                  |
| C-CA-CB      | 110.10             | 125.41          | 2                  |
| C-N-CA       | 121.70             | 107.20          | 1                  |
| N-CA-C-CA-CB | 110.10             | 94.80           | 1                  |
| CA-C-C-CA-CB | 110.10             | 94.80           | 1                  |
| C-CA-C-CA-CB | 110.10             | 125.39          | 1                  |
| CA-C-O       | 120.80             | 134.48          | 1                  |
| C-CA-CB      | 110.10             | 94.81           | 1                  |
| CA-C-CA-N-CD | 112.00             | 123.27          | 1                  |
| N-CA-CB      | 110.40             | 122.47          | 1                  |
| C-CA-N-CA-CB | 110.50             | 96.82           | 1                  |
| C-CA-N-CA-C  | 111.00             | 88.48           | 1                  |
| C-CA-C-CA-CB | 110.10             | 125.38          | 1                  |
| CA-C-C-CA-CB | 110.10             | 125.38          | 1                  |
| C-CA-CB      | 110.10             | 125.38          | 1                  |
| N-CA-C       | 111.00             | 133.52          | 1                  |
| C-CA-CB      | 109.10             | 91.41           | 1                  |
| N-CA-C-CA-CB | 110.10             | 125.38          | 1                  |
| C-CA-CB      | 111.40             | 96.12           | 1                  |
| CA-C-N       | 116.20             | 132.28          | 1                  |
| CA-C-O       | 120.80             | 134.47          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-N-CD                    | 112.00             | 123.25          | 1                  |
| CA-C-C-CA-CA-CB-N-CA-C     | 111.00             | 88.50           | 1                  |
| C-N-CA                     | 121.70             | 136.17          | 1                  |
| C-CA-CB                    | 110.10             | 125.37          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 125.37          | 1                  |
| C-CA-CB                    | 111.40             | 96.14           | 1                  |
| C-CA-CB                    | 110.10             | 94.84           | 1                  |
| N-CA-C                     | 111.00             | 133.48          | 1                  |
| C-CA-C-CA-CA-CB-CA-C-O     | 120.80             | 134.44          | 1                  |
| C-CA-CB                    | 110.50             | 122.54          | 1                  |
| C-CA-CB                    | 110.10             | 125.34          | 2                  |
| CA-CB-CG                   | 113.80             | 121.82          | 1                  |
| N-CA-CB                    | 111.50             | 125.13          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 125.33          | 1                  |
| C-CA-C-CA-C-CA-C-CA-C-N-CA | 121.70             | 136.13          | 1                  |
| C-N-CA                     | 121.70             | 107.28          | 1                  |
| CA-C-O                     | 120.80             | 107.18          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 94.88           | 1                  |
| N-CA-C                     | 111.00             | 133.43          | 1                  |
| CA-C-O                     | 120.80             | 134.41          | 1                  |
| CA-C-C-CA-CB               | 110.10             | 125.31          | 1                  |
| C-CA-CB                    | 110.10             | 94.89           | 1                  |



| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-N-CA             | 121.70             | 136.11          | 1                  |
| N-CA-C-CA-CA-C-O   | 120.80             | 134.41          | 1                  |
| N-CA-N-CA-C        | 111.00             | 133.41          | 1                  |
| C-N-CA             | 121.70             | 136.10          | 1                  |
| N-CA-C             | 111.00             | 88.60           | 1                  |
| C-CA-CB            | 110.10             | 125.30          | 5                  |
| N-CA-C-CA-CB       | 110.10             | 94.90           | 1                  |
| C-CA-CB            | 110.10             | 94.91           | 2                  |
| CA-C-O             | 120.80             | 134.39          | 1                  |
| N-CA-C             | 111.00             | 88.61           | 1                  |
| C-N-CA             | 121.70             | 136.09          | 1                  |
| N-CA-C             | 111.00             | 133.38          | 1                  |
| CA-C-N-CA-CB       | 111.50             | 125.09          | 1                  |
| C-CA-CB            | 110.10             | 125.28          | 2                  |
| N-CA-C             | 111.00             | 133.37          | 1                  |
| C-CA-C-CA-CB       | 110.10             | 125.28          | 1                  |
| CA-C-O             | 120.80             | 134.38          | 1                  |
| N-CA-CA-CB-C-CA-CB | 110.50             | 122.48          | 1                  |
| C-CA-CB            | 110.10             | 125.27          | 2                  |
| N-CA-C             | 111.00             | 88.64           | 1                  |
| C-N-CA-C-O         | 120.80             | 134.38          | 1                  |
| C-CA-CB            | 110.10             | 94.93           | 2                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-O            | 120.80             | 134.37          | 1                  |
| N-CA-C            | 111.00             | 88.65           | 1                  |
| C-CA-CB           | 110.10             | 125.26          | 2                  |
| N-CA-C-CA-CB      | 110.10             | 125.26          | 1                  |
| C-CA-CA-CB-CG     | 113.80             | 105.82          | 1                  |
| N-CA-C            | 111.00             | 133.34          | 2                  |
| C-CA-CB           | 110.50             | 122.47          | 1                  |
| CA-CB-CG          | 113.80             | 105.82          | 1                  |
| C-CA-CB           | 110.10             | 125.25          | 2                  |
| CA-CB-CG          | 113.80             | 105.83          | 1                  |
| C-N-CA            | 121.70             | 107.35          | 2                  |
| N-CA-C            | 111.00             | 133.32          | 1                  |
| N-CA-C-CA-C-CA-CB | 110.10             | 94.96           | 1                  |
| N-CA-C            | 111.00             | 88.69           | 1                  |
| CA-C-N            | 116.20             | 132.14          | 1                  |
| CA-CB-N-CA-N-CA-C | 111.00             | 88.70           | 1                  |
| C-CA-CA-N-CA-C-O  | 120.80             | 134.34          | 1                  |
| CA-C-O            | 120.80             | 107.26          | 1                  |
| CA-C-O            | 120.80             | 134.34          | 1                  |
| C-CA-CB           | 110.10             | 125.23          | 2                  |
| C-N-CA            | 121.70             | 107.37          | 1                  |
| C-CA-CB           | 110.10             | 94.98           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-O                 | 120.80             | 107.27          | 1                  |
| C-CA-N-CA-C                 | 113.30             | 90.22           | 1                  |
| C-N-C-CA-CB                 | 110.10             | 125.22          | 1                  |
| N-CA-CB                     | 110.50             | 124.02          | 1                  |
| C-N-CA                      | 121.70             | 107.38          | 1                  |
| CA-C-N                      | 116.20             | 100.29          | 1                  |
| C-N-N-CA-C-N-CA             | 121.70             | 136.01          | 1                  |
| C-CA-CB                     | 110.10             | 95.00           | 1                  |
| C-CA-CB                     | 110.10             | 125.20          | 1                  |
| C-CA-C-N-CA                 | 121.70             | 136.00          | 1                  |
| C-CA-CB                     | 110.10             | 95.01           | 1                  |
| C-CA-C-CA-N-CA-C-CA-C-CA-CB | 111.40             | 96.31           | 1                  |
| C-CA-CA-C-O                 | 120.80             | 107.31          | 1                  |
| CA-C-N                      | 116.20             | 100.33          | 1                  |
| C-CA-N-CA-CA-C-N            | 116.20             | 100.33          | 1                  |
| C-CA-C-N-CA                 | 121.70             | 107.42          | 1                  |
| N-CA-C-N-C-CA-CB            | 110.10             | 125.17          | 1                  |
| C-CA-CB                     | 110.10             | 125.17          | 2                  |
| CA-C-O                      | 120.80             | 134.28          | 1                  |
| N-CA-CB                     | 110.50             | 97.02           | 1                  |
| C-N-CA                      | 121.70             | 135.97          | 1                  |
| C-N-N-CA-C                  | 113.30             | 90.31           | 1                  |

| Angle type      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB    | 110.10             | 125.16          | 1                  |
| C-CA-CB         | 110.10             | 125.16          | 1                  |
| N-CA-C-CA-CB    | 110.10             | 125.16          | 1                  |
| C-CA-CB         | 110.10             | 125.15          | 1                  |
| C-CA-CB         | 110.10             | 95.05           | 1                  |
| C-CA-CA-C-O     | 120.80             | 134.27          | 1                  |
| N-CA-C-N-CA-C-N | 116.20             | 100.36          | 1                  |
| CA-C-C-CA-CB    | 110.10             | 125.14          | 1                  |
| C-N-CA          | 121.70             | 135.95          | 1                  |
| CA-C-O          | 120.80             | 107.34          | 1                  |
| N-CA-CA-C-N     | 116.20             | 100.37          | 1                  |
| N-CA-CA-C-O     | 120.80             | 107.35          | 1                  |
| N-CA-CB         | 111.50             | 124.95          | 1                  |
| C-CA-C-CA-CB    | 111.40             | 96.37           | 1                  |
| CA-C-N          | 116.20             | 132.02          | 1                  |
| N-CA-C          | 111.00             | 133.15          | 1                  |
| C-CA-CB         | 110.10             | 125.13          | 1                  |
| C-CA-N-CA-CB    | 110.50             | 123.94          | 1                  |
| N-CA-C          | 111.00             | 133.14          | 1                  |
| CA-C-N          | 116.20             | 100.39          | 2                  |
| CA-C-O          | 120.80             | 107.36          | 1                  |
| N-CA-CB         | 110.50             | 123.94          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 125.12          | 1                  |
| N-CA-C                | 111.00             | 133.13          | 1                  |
| C-N-N-CA-N-CA-C-CA-CB | 110.10             | 125.10          | 1                  |
| C-CA-CB               | 110.10             | 125.10          | 1                  |
| N-CA-C                | 111.00             | 133.11          | 1                  |
| C-CA-CB               | 110.10             | 95.10           | 1                  |
| N-CA-CB               | 110.50             | 97.08           | 1                  |
| C-N-CA                | 121.70             | 107.50          | 1                  |
| N-CA-C                | 111.00             | 88.91           | 1                  |
| N-CA-N-CA-N-CA-C      | 111.00             | 88.91           | 1                  |
| N-CA-CB               | 110.50             | 97.09           | 1                  |
| C-N-C-CA-CB           | 110.10             | 125.09          | 1                  |
| C-N-CA                | 121.70             | 135.90          | 1                  |
| N-CA-CB               | 111.50             | 124.91          | 1                  |
| C-CA-CB               | 110.10             | 125.09          | 1                  |
| N-CA-C                | 111.00             | 133.08          | 1                  |
| C-CA-CB               | 110.10             | 125.08          | 2                  |
| N-CA-CB               | 110.50             | 123.90          | 1                  |
| C-CA-C-N-CA           | 121.70             | 135.89          | 1                  |
| N-CA-CA-CB-CG         | 113.80             | 105.92          | 1                  |
| CA-C-N                | 116.20             | 131.97          | 1                  |
| N-CA-C                | 111.00             | 88.93           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                | 110.10             | 95.12           | 1                  |
| N-CA-C                 | 111.00             | 133.07          | 1                  |
| CA-C-N                 | 116.90             | 105.08          | 1                  |
| C-N-CA                 | 121.70             | 135.88          | 1                  |
| N-CA-C                 | 111.00             | 133.06          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 125.07          | 1                  |
| CA-C-O                 | 120.80             | 107.41          | 1                  |
| N-CA-C                 | 111.00             | 88.94           | 1                  |
| N-CA-CB                | 110.50             | 123.89          | 1                  |
| CA-C-N                 | 116.20             | 131.95          | 1                  |
| N-CA-C-N-CA            | 121.70             | 135.87          | 1                  |
| N-CA-C                 | 111.00             | 88.95           | 1                  |
| N-CA-N-CA-N-CA-N-CA-CB | 111.50             | 124.88          | 1                  |
| N-CA-C-N-CA            | 121.70             | 107.54          | 1                  |
| C-N-C-N-N-CA-C         | 111.00             | 88.98           | 1                  |
| CA-C-N                 | 116.20             | 131.93          | 1                  |
| N-CA-CB                | 110.50             | 123.87          | 1                  |
| C-CA-CB                | 110.10             | 125.04          | 2                  |
| C-N-CA                 | 121.70             | 107.55          | 1                  |
| CA-C-O                 | 120.80             | 134.16          | 1                  |
| CA-C-O                 | 120.80             | 107.44          | 1                  |
| N-CA-C                 | 111.00             | 89.00           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                | 110.10             | 125.03          | 1                  |
| CA-C-N                 | 116.20             | 100.49          | 1                  |
| N-CA-CA-C-N            | 116.20             | 100.49          | 1                  |
| C-CA-C-CA-C-CA-CB      | 110.10             | 125.02          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 125.02          | 1                  |
| CA-C-N                 | 116.20             | 131.90          | 1                  |
| CA-C-N                 | 116.20             | 100.50          | 1                  |
| N-CA-N-CA-C            | 111.00             | 89.02           | 1                  |
| CA-C-N                 | 116.90             | 105.13          | 1                  |
| C-N-C-CA-N-CA-CB       | 110.50             | 97.16           | 1                  |
| CA-C-CA-C-C-CA-N-CA-CB | 110.50             | 123.84          | 1                  |
| C-N-C-N-CA             | 121.70             | 135.82          | 1                  |
| CA-C-O                 | 120.80             | 134.13          | 1                  |
| CA-C-N                 | 116.20             | 131.89          | 1                  |
| N-CA-CB                | 111.50             | 124.83          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 97.17           | 1                  |
| C-CA-CB                | 110.10             | 125.00          | 1                  |
| C-CA-CB                | 110.10             | 124.99          | 1                  |
| C-N-N-CA-N-CA-CB       | 110.50             | 123.82          | 1                  |
| C-CA-CB                | 110.50             | 98.75           | 1                  |
| CA-C-N-CA-CB           | 111.50             | 124.82          | 1                  |
| C-N-C-CA-C-CA-CB       | 110.10             | 95.23           | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-C-CA-CA-C-C-CA-C-N-CA | 121.70             | 135.78          | 1                  |
| CA-CB-C-CA-C-CA-N-CA-C-N-CA     | 121.70             | 135.77          | 1                  |
| C-CA-CB                         | 110.10             | 124.95          | 1                  |
| C-CA-CB                         | 110.10             | 95.25           | 1                  |
| C-CA-N-CA-C-CA-N-CA-CB          | 111.50             | 124.78          | 1                  |
| N-CA-C-CA-N-CA-CB               | 110.50             | 123.78          | 1                  |
| C-CA-N-CA-CB                    | 110.50             | 123.78          | 1                  |
| C-CA-N-CA-C-N-CA                | 121.70             | 107.65          | 1                  |
| C-N-CA                          | 121.70             | 107.65          | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 124.93          | 1                  |
| N-CA-CB                         | 110.50             | 123.77          | 1                  |
| N-CA-C                          | 111.00             | 132.85          | 1                  |
| C-CA-CB                         | 111.60             | 127.20          | 1                  |
| C-CA-CB                         | 111.60             | 96.00           | 1                  |
| C-CA-CB                         | 110.10             | 95.28           | 1                  |
| C-CA-N-CA-CA-C-O                | 120.80             | 107.54          | 1                  |
| C-N-N-CA-C                      | 111.00             | 132.84          | 1                  |
| N-CA-N-CA-C-CA-CB               | 111.60             | 96.01           | 1                  |
| N-CA-CA-C-N                     | 116.20             | 131.79          | 1                  |
| C-CA-CB                         | 110.10             | 124.91          | 1                  |
| C-CA-N-CA-C-CA-CB               | 111.60             | 127.18          | 1                  |
| N-CA-C                          | 111.00             | 132.82          | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CB          | 110.50             | 123.74          | 1                  |
| C-CA-C-CA-CB          | 111.60             | 96.02           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 95.30           | 1                  |
| N-CA-CB               | 110.50             | 123.74          | 1                  |
| N-CA-C                | 111.00             | 132.80          | 1                  |
| C-CA-CB               | 110.10             | 95.31           | 1                  |
| N-CA-CA-C-O           | 120.80             | 107.57          | 1                  |
| N-CA-CB               | 111.50             | 124.73          | 1                  |
| C-CA-CB               | 111.40             | 126.18          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 124.88          | 1                  |
| CA-CB-CG              | 113.80             | 106.03          | 1                  |
| C-CA-C-N-C-N-CA-CB-CG | 113.80             | 106.03          | 1                  |
| N-CA-CA-C-N           | 116.20             | 100.66          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 124.86          | 1                  |
| C-CA-C-N-C-CA-CB      | 110.10             | 95.34           | 1                  |
| N-CA-C                | 111.00             | 132.74          | 1                  |
| CA-C-N                | 116.20             | 100.67          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 124.85          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 95.35           | 1                  |
| CA-CB-C-CA-C-CA-CB    | 110.10             | 124.84          | 1                  |
| CA-C-CA-C-N           | 116.20             | 100.69          | 1                  |
| C-CA-CB               | 110.10             | 95.36           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-N           | 116.20             | 100.69          | 1                  |
| C-CA-CA-C-N           | 116.90             | 105.27          | 1                  |
| C-N-CA-C-O            | 120.80             | 133.98          | 1                  |
| C-CA-CA-C-CA-C-N      | 116.20             | 100.70          | 1                  |
| N-CA-CA-C-C-CA-CA-C-N | 116.20             | 100.71          | 1                  |
| C-CA-C-CA-N-CA-CB     | 110.50             | 123.66          | 1                  |
| C-CA-CB               | 111.40             | 126.11          | 1                  |
| C-CA-CB               | 110.10             | 124.81          | 2                  |
| C-N-CA                | 121.70             | 135.63          | 1                  |
| CA-C-N                | 116.90             | 105.29          | 1                  |
| N-CA-CB               | 110.50             | 123.65          | 1                  |
| C-N-N-CA-CB           | 110.50             | 123.65          | 1                  |
| C-CA-CB               | 110.10             | 124.80          | 1                  |
| C-CA-CB               | 110.10             | 95.40           | 1                  |
| CA-C-O                | 120.80             | 107.65          | 1                  |
| C-CA-C-CA-CA-C-N      | 116.20             | 100.73          | 1                  |
| C-CA-N-CA-C-CA-CB     | 110.10             | 95.42           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 95.42           | 1                  |
| C-CA-CB               | 110.10             | 124.78          | 1                  |
| CA-C-N-CA-CA-C-O      | 120.80             | 107.67          | 1                  |
| C-CA-C-CA-N-CA-CA-C-N | 116.20             | 100.76          | 1                  |
| N-CA-CB               | 110.50             | 123.63          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 111.00             | 132.62          | 1                  |
| C-CA-N-CA-C           | 111.00             | 89.39           | 1                  |
| C-CA-CB               | 110.10             | 95.44           | 1                  |
| N-CA-CB               | 110.50             | 97.39           | 1                  |
| N-CA-C-CA-C-N-CA      | 121.70             | 107.82          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 124.75          | 1                  |
| N-CA-CB               | 111.50             | 98.39           | 1                  |
| C-CA-CB               | 111.60             | 96.18           | 1                  |
| N-CA-CB               | 110.50             | 97.40           | 1                  |
| CA-C-N                | 116.20             | 100.79          | 1                  |
| C-CA-C-CA-C-CA-C-N-CA | 121.70             | 135.57          | 1                  |
| C-CA-CB               | 109.10             | 126.05          | 1                  |
| CA-C-O                | 120.80             | 133.90          | 1                  |
| N-CA-CB               | 110.50             | 123.60          | 1                  |
| N-CA-CB               | 110.50             | 97.41           | 2                  |
| N-CA-C                | 111.00             | 132.56          | 1                  |
| C-CA-CB               | 109.10             | 126.03          | 1                  |
| N-CA-C                | 112.10             | 92.86           | 1                  |
| C-CA-CB               | 110.10             | 124.72          | 2                  |
| N-CA-N-CA-CB          | 111.50             | 124.58          | 1                  |
| CA-C-N                | 116.20             | 100.81          | 1                  |
| C-CA-CB               | 111.60             | 96.21           | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                         | 111.50             | 124.58          | 1                  |
| C-N-CA-C-C-N-CA                 | 121.70             | 107.85          | 1                  |
| N-CA-CB                         | 111.50             | 124.57          | 3                  |
| C-CA-CB                         | 110.10             | 124.71          | 1                  |
| N-CA-C-N-C-CA-C-CA-C-CA-C-CA-CB | 109.10             | 126.00          | 1                  |
| N-CA-CB                         | 111.50             | 124.56          | 1                  |
| N-CA-C-CA-N-CA-C-CA-N-CA-CB     | 111.50             | 98.45           | 1                  |
| C-CA-CB                         | 109.10             | 125.99          | 1                  |
| N-CA-CB                         | 111.50             | 124.55          | 1                  |
| C-CA-CB                         | 110.10             | 124.68          | 1                  |
| C-CA-C-CA-N-CA-C                | 111.00             | 132.48          | 1                  |
| N-CA-C                          | 111.00             | 132.47          | 1                  |
| C-N-CA-C-O                      | 120.80             | 133.84          | 1                  |
| N-CA-C                          | 112.10             | 92.94           | 1                  |
| C-CA-CB                         | 110.10             | 95.54           | 2                  |
| N-CA-CB                         | 111.50             | 98.47           | 1                  |
| CA-C-O                          | 120.80             | 133.83          | 1                  |
| N-CA-CB                         | 111.50             | 124.53          | 1                  |
| C-CA-CA-C-O                     | 120.80             | 133.82          | 1                  |
| C-CA-N-CA-C-CA-CB               | 110.10             | 124.65          | 1                  |
| C-CA-CB                         | 110.10             | 95.55           | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 95.55           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                     | 111.60             | 126.91          | 1                  |
| CA-C-O                      | 120.80             | 133.81          | 1                  |
| C-CA-CB                     | 110.10             | 95.56           | 1                  |
| CA-C-N-CA-C                 | 111.00             | 132.41          | 1                  |
| C-N-C-CA-N-CA-C             | 111.00             | 132.40          | 1                  |
| CA-C-CA-C-N                 | 116.90             | 105.44          | 1                  |
| C-CA-CB                     | 110.10             | 124.62          | 1                  |
| C-CA-CB                     | 110.10             | 124.61          | 1                  |
| N-CA-C-CA-C-CA-CB           | 110.10             | 95.59           | 1                  |
| C-CA-CB                     | 111.60             | 126.87          | 1                  |
| CA-C-CA-C-N                 | 116.20             | 100.94          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 124.60          | 1                  |
| C-CA-CB                     | 111.60             | 126.86          | 1                  |
| CA-C-C-N-C-CA-CA-C-C-CA-CB  | 110.10             | 124.59          | 1                  |
| CA-C-CA-C-N-CA-N-CA-N-CA-CB | 110.50             | 97.54           | 1                  |
| CA-C-O                      | 120.80             | 133.76          | 1                  |
| CA-C-C-CA-N-CD-CG           | 103.20             | 91.77           | 1                  |
| C-CA-CB                     | 110.10             | 124.58          | 1                  |
| N-CA-C                      | 111.00             | 89.66           | 1                  |
| C-N-CA                      | 121.70             | 135.42          | 1                  |
| C-CA-CA-N-CD                | 112.00             | 101.33          | 1                  |
| C-CA-CB                     | 110.10             | 124.57          | 4                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                  | 110.10             | 95.63           | 1                  |
| C-N-CA                   | 121.70             | 135.41          | 1                  |
| CA-C-N                   | 116.90             | 105.48          | 1                  |
| N-CA-CB                  | 110.50             | 97.55           | 1                  |
| N-CA-C                   | 111.00             | 132.32          | 2                  |
| N-CA-N-CA-C-N-C-N-C-N-CA | 121.70             | 135.40          | 1                  |
| N-CA-CB                  | 111.50             | 98.56           | 1                  |
| N-CA-C                   | 111.00             | 89.69           | 1                  |
| N-CA-CA-C-N-CD-CG        | 103.20             | 91.78           | 1                  |
| C-CA-C-CA-CB             | 110.10             | 124.56          | 1                  |
| C-CA-C-CA-CA-C-C-CA-CB   | 110.10             | 124.55          | 1                  |
| C-CA-CB                  | 111.60             | 126.81          | 1                  |
| C-N-CA                   | 121.70             | 108.01          | 1                  |
| N-CA-C                   | 111.00             | 89.71           | 1                  |
| N-CA-CA-C-O              | 120.80             | 107.87          | 1                  |
| C-CA-N-CA-CB             | 110.50             | 97.58           | 1                  |
| C-CA-N-CA-CB             | 110.50             | 123.42          | 1                  |
| N-CA-C                   | 111.00             | 132.27          | 1                  |
| N-CA-CB                  | 110.50             | 123.41          | 2                  |
| CA-C-N                   | 116.20             | 101.01          | 1                  |
| C-N-CA                   | 121.70             | 108.03          | 1                  |
| N-CA-CA-C-N-CA-CB        | 110.50             | 97.59           | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| N-CD-CG              | 103.20             | 91.81           | 1                  |
| C-CA-CB              | 110.10             | 95.68           | 1                  |
| C-N-CA               | 121.70             | 108.04          | 2                  |
| N-CD-CG              | 103.20             | 91.82           | 1                  |
| N-CA-CB              | 110.50             | 123.40          | 1                  |
| C-CA-CB              | 110.10             | 124.52          | 1                  |
| CA-C-O               | 120.80             | 107.90          | 1                  |
| C-CA-CB              | 110.50             | 121.88          | 1                  |
| N-CA-CB              | 110.40             | 121.77          | 1                  |
| C-N-CA               | 121.70             | 108.05          | 1                  |
| C-CA-CB              | 110.10             | 95.69           | 2                  |
| CA-C-CA-C-N          | 116.90             | 105.53          | 1                  |
| N-CA-CB              | 110.50             | 123.39          | 1                  |
| C-N-CA               | 121.70             | 108.06          | 1                  |
| C-CA-CB              | 110.10             | 95.70           | 2                  |
| CA-C-N               | 116.90             | 105.53          | 1                  |
| N-CA-CB              | 110.50             | 123.38          | 2                  |
| C-N-N-CA-C-CA-C-N-CA | 121.70             | 135.33          | 1                  |
| CA-C-CA-C-N-CA-C     | 111.00             | 89.80           | 1                  |
| C-CA-CA-C-CA-C-O     | 120.80             | 107.93          | 1                  |
| C-CA-CB              | 111.60             | 126.74          | 1                  |
| CA-C-C-CA-CB         | 110.10             | 95.72           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 124.48          | 1                  |
| CA-C-CA-C-O           | 120.80             | 133.66          | 1                  |
| C-N-CA                | 121.70             | 108.08          | 1                  |
| C-CA-N-CA-C           | 111.00             | 89.82           | 1                  |
| C-CA-CB               | 110.10             | 95.73           | 2                  |
| CA-C-O                | 120.80             | 107.94          | 1                  |
| N-CA-N-CA-N-CA-CB     | 110.50             | 123.35          | 1                  |
| CA-C-C-N-CA           | 121.70             | 108.10          | 1                  |
| C-CA-CB               | 110.10             | 124.46          | 2                  |
| CA-C-C-N-CA-C-C-CA-CB | 110.50             | 121.83          | 1                  |
| C-N-CA                | 121.70             | 108.10          | 1                  |
| N-CA-CB               | 111.50             | 124.34          | 1                  |
| C-CA-N-CA-CB          | 110.40             | 121.73          | 1                  |
| C-CA-C-CA-C-CA-CB     | 110.10             | 124.44          | 1                  |
| C-CA-CB               | 110.10             | 124.44          | 1                  |
| C-CA-CB               | 111.60             | 96.50           | 1                  |
| CA-C-C-CA-CB          | 111.60             | 96.51           | 1                  |
| C-CA-CB               | 110.10             | 95.76           | 1                  |
| N-CA-CB               | 111.50             | 98.67           | 1                  |
| CA-C-O                | 120.80             | 107.97          | 2                  |
| C-N-CA                | 121.70             | 108.12          | 1                  |
| N-CA-CB               | 111.50             | 124.33          | 1                  |



| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.50             | 121.82          | 1                  |
| CA-C-C-CA-CB      | 110.10             | 124.43          | 1                  |
| C-N-CA            | 121.70             | 135.28          | 1                  |
| N-CA-CB           | 110.50             | 123.32          | 1                  |
| C-CA-C-CA-CB      | 109.10             | 125.69          | 1                  |
| C-N-CA            | 121.70             | 108.13          | 1                  |
| N-CA-C            | 111.00             | 132.11          | 1                  |
| C-CA-C-N-C-N-CA   | 121.70             | 135.27          | 1                  |
| C-CA-CB           | 111.60             | 126.68          | 1                  |
| N-CA-N-CA-N-CA-CB | 111.50             | 98.69           | 1                  |
| C-N-N-CA-CA-N-CD  | 112.00             | 101.45          | 1                  |
| CA-C-O            | 120.80             | 133.61          | 1                  |
| CA-C-N            | 116.20             | 101.13          | 1                  |
| CA-N-CD           | 112.00             | 101.45          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 95.79           | 1                  |
| N-CA-CA-C-C-CA-CB | 110.10             | 124.40          | 1                  |
| C-N-CA            | 121.70             | 135.25          | 1                  |
| CA-C-O            | 120.80             | 108.00          | 1                  |
| C-CA-CB           | 110.50             | 121.79          | 1                  |
| CA-C-C-N-CA       | 121.70             | 135.25          | 1                  |
| N-CA-C-CA-CB      | 111.60             | 96.55           | 1                  |
| C-CA-CB           | 110.10             | 95.80           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-N            | 116.20             | 101.15          | 1                  |
| CA-C-O            | 120.80             | 108.01          | 1                  |
| CA-N-CD           | 112.00             | 101.47          | 2                  |
| N-CA-CB           | 110.50             | 123.29          | 2                  |
| N-CA-C            | 111.00             | 132.07          | 1                  |
| N-CA-C            | 113.30             | 91.49           | 1                  |
| N-CA-CB           | 111.50             | 124.29          | 1                  |
| C-CA-CB           | 110.10             | 124.39          | 1                  |
| CA-CB-CG          | 112.60             | 120.12          | 1                  |
| CA-C-O            | 120.80             | 133.58          | 1                  |
| CA-C-CA-N-N-CA-CB | 111.50             | 124.28          | 1                  |
| C-CA-N-CA-CB      | 110.50             | 123.28          | 1                  |
| C-CA-CB           | 110.50             | 121.77          | 1                  |
| C-CA-CB           | 110.10             | 124.38          | 1                  |
| N-CA-C-CA-CB      | 111.60             | 96.57           | 1                  |
| N-CA-C            | 111.00             | 89.96           | 1                  |
| C-CA-CB           | 110.10             | 124.37          | 1                  |
| N-CA-C            | 112.10             | 130.88          | 1                  |
| C-CA-CB           | 110.10             | 95.83           | 1                  |
| N-CA-CB           | 103.00             | 111.26          | 1                  |
| CA-C-N-CA-C       | 111.00             | 89.97           | 1                  |
| N-CA-C-CA-CB      | 110.10             | 95.84           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.10             | 124.36          | 1                  |
| C-N-C-N-CA                 | 121.70             | 108.19          | 1                  |
| C-CA-N-CA-O-C-N-CA-C-CA-CB | 110.10             | 124.35          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 95.85           | 1                  |
| C-CA-CB                    | 109.10             | 125.59          | 1                  |
| CA-C-CA-CB-N-CA-CB         | 110.50             | 97.76           | 1                  |
| N-CA-C                     | 113.30             | 91.56           | 1                  |
| C-CA-CB                    | 110.10             | 124.34          | 1                  |
| N-CA-CB                    | 111.50             | 124.24          | 1                  |
| N-CA-C                     | 113.30             | 91.57           | 2                  |
| N-CA-C-CA-CB               | 109.10             | 92.61           | 1                  |
| C-N-CA                     | 121.70             | 108.21          | 2                  |
| CA-N-CD                    | 112.00             | 101.51          | 1                  |
| N-CA-C                     | 112.10             | 130.83          | 1                  |
| N-CA-CB                    | 110.50             | 97.76           | 1                  |
| C-CA-C-CA-C-N-N-CA-C-N-CA  | 121.70             | 135.18          | 1                  |
| N-CA-CB                    | 110.50             | 97.77           | 1                  |
| C-CA-CB                    | 109.10             | 125.57          | 1                  |
| N-CA-C                     | 113.30             | 91.59           | 1                  |
| N-CA-C-N-CA                | 121.70             | 108.23          | 1                  |
| C-CA-CB                    | 110.10             | 124.32          | 1                  |
| C-N-CA                     | 121.70             | 108.23          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.50             | 121.72          | 1                  |
| C-CA-CB               | 109.10             | 125.56          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 124.31          | 1                  |
| C-N-N-CA-CB           | 103.00             | 111.23          | 1                  |
| C-CA-CB               | 110.10             | 124.31          | 1                  |
| C-CA-CB               | 109.10             | 92.65           | 1                  |
| N-CA-CB               | 110.50             | 97.79           | 3                  |
| C-CA-CB               | 110.10             | 95.89           | 1                  |
| C-N-C-CA-CB           | 110.10             | 124.31          | 1                  |
| CA-C-O                | 120.80             | 133.51          | 1                  |
| C-N-CA                | 121.70             | 108.25          | 2                  |
| CA-CB-CG              | 112.60             | 105.13          | 1                  |
| C-CA-CB               | 110.10             | 124.30          | 1                  |
| N-CA-C                | 113.30             | 91.63           | 1                  |
| C-CA-N-CA-CA-N-C-N-CA | 121.70             | 108.25          | 1                  |
| N-CA-C                | 112.10             | 93.43           | 1                  |
| C-CA-C-CA-CB          | 110.10             | 95.91           | 1                  |
| N-CA-CB               | 111.50             | 98.81           | 1                  |
| C-CA-CB               | 111.60             | 96.67           | 1                  |
| C-CA-C-CA-N-CA-CB     | 111.50             | 124.19          | 1                  |
| CA-C-N                | 116.20             | 131.13          | 1                  |
| O-C-C-CA-CB           | 110.10             | 124.28          | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| CA-C-N             | 116.20             | 101.28          | 1                  |
| C-CA-CB            | 110.10             | 124.27          | 1                  |
| C-CA-CB            | 111.60             | 126.52          | 1                  |
| C-CA-CB            | 109.10             | 125.51          | 1                  |
| N-CA-CB            | 110.50             | 97.82           | 2                  |
| C-N-CA             | 121.70             | 108.28          | 1                  |
| C-N-CA             | 121.70             | 135.12          | 1                  |
| CA-CB-N-CA-N-CA-CB | 110.50             | 97.83           | 1                  |
| N-CA-CB            | 110.50             | 123.17          | 1                  |
| N-CA-C-CA-C-CA-CB  | 110.10             | 95.94           | 1                  |
| C-N-CA             | 121.70             | 135.11          | 1                  |
| C-CA-CA-C-N        | 116.20             | 131.10          | 1                  |
| C-CA-CB            | 110.10             | 124.25          | 2                  |
| CA-C-O             | 120.80             | 108.14          | 1                  |
| N-CA-C             | 111.00             | 90.14           | 1                  |
| C-N-CA             | 121.70             | 108.29          | 1                  |
| C-CA-CB            | 110.10             | 95.95           | 2                  |
| C-CA-CB            | 109.10             | 125.49          | 1                  |
| CA-N-CD            | 112.00             | 101.57          | 1                  |
| N-CA-C-N-CA        | 121.70             | 108.29          | 1                  |
| N-CA-CB            | 110.50             | 97.84           | 1                  |
| C-N-CD             | 125.00             | 94.47           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-O            | 120.80             | 133.46          | 1                  |
| N-CA-C            | 111.00             | 90.15           | 1                  |
| C-CA-C-CA-CB      | 110.10             | 95.95           | 1                  |
| N-CA-C-CA-CB      | 111.60             | 126.49          | 1                  |
| CA-C-O            | 120.80             | 108.15          | 1                  |
| CA-C-N            | 116.20             | 101.31          | 1                  |
| C-CA-CB           | 110.10             | 95.96           | 1                  |
| C-CA-C-CA-CB      | 110.10             | 95.96           | 1                  |
| N-CA-C            | 112.10             | 93.50           | 1                  |
| CA-CB-CG          | 112.60             | 105.16          | 1                  |
| CA-N-N-CA-CB      | 110.50             | 123.15          | 1                  |
| C-CA-CB           | 110.10             | 124.23          | 1                  |
| C-CA-CB           | 111.40             | 97.27           | 1                  |
| CA-CB-N-CA-CB     | 110.50             | 123.14          | 1                  |
| N-CA-CA-CB-CG     | 112.60             | 120.03          | 1                  |
| C-CA-CB           | 110.10             | 95.98           | 2                  |
| C-N-CA            | 121.70             | 108.32          | 1                  |
| N-CA-C-CA-C-CA-CB | 110.10             | 124.22          | 1                  |
| C-CA-CB           | 110.10             | 124.22          | 2                  |
| C-CA-C-CA-C-CA-CB | 110.10             | 95.99           | 1                  |
| C-N-C-CA-CB       | 110.10             | 95.99           | 1                  |
| N-CA-CB           | 110.50             | 123.13          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-C                 | 111.00             | 90.20           | 1                  |
| CA-CB-C-CA-CB          | 110.10             | 124.21          | 1                  |
| N-CA-CA-N-C-CA-N-CA-CB | 110.50             | 97.88           | 1                  |
| C-N-CD                 | 125.00             | 94.56           | 1                  |
| C-CA-CB                | 110.10             | 124.21          | 1                  |
| N-CA-CB                | 110.50             | 97.88           | 1                  |
| N-CA-C                 | 111.00             | 131.78          | 2                  |
| C-CA-CB                | 110.10             | 124.20          | 1                  |
| C-CA-C-N-CA            | 121.70             | 108.34          | 1                  |
| CA-C-O                 | 120.80             | 133.41          | 2                  |
| CA-CB-CA-C-O           | 120.80             | 108.19          | 1                  |
| CA-CB-CG               | 113.80             | 106.38          | 1                  |
| C-CA-CB                | 110.10             | 96.00           | 1                  |
| C-CA-CA-N-CD           | 112.00             | 101.61          | 1                  |
| C-CA-N-CA-C            | 111.00             | 90.23           | 1                  |
| C-N-CA                 | 121.70             | 108.35          | 1                  |
| C-N-CA                 | 121.70             | 135.05          | 2                  |
| N-CA-CB                | 110.50             | 123.11          | 1                  |
| N-CA-CB                | 110.50             | 97.89           | 1                  |
| C-CA-CB                | 110.10             | 124.19          | 1                  |
| C-CA-CB                | 111.40             | 125.49          | 1                  |
| C-CA-CB                | 110.10             | 124.18          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-O                 | 120.80             | 108.20          | 2                  |
| C-N-C-CA-N-CA-CB       | 110.50             | 123.10          | 1                  |
| C-CA-CB                | 111.40             | 97.32           | 1                  |
| C-CA-C-N-CA            | 121.70             | 108.36          | 1                  |
| CA-CB-CA-C-N-CA-C      | 111.00             | 131.74          | 1                  |
| C-N-CA                 | 121.70             | 108.37          | 1                  |
| C-N-C-N-CA             | 121.70             | 108.37          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 124.17          | 1                  |
| C-CA-CB                | 111.60             | 96.79           | 1                  |
| C-CA-CB                | 110.10             | 96.03           | 1                  |
| CA-C-O                 | 120.80             | 108.22          | 1                  |
| C-CA-CA-CB-CG          | 112.60             | 120.00          | 1                  |
| CA-C-O                 | 120.80             | 133.38          | 1                  |
| CA-C-C-CA-CB           | 111.40             | 97.34           | 1                  |
| C-CA-C-CA-N-CA-C-CA-CB | 110.10             | 96.04           | 1                  |
| C-CA-CA-CB-CG          | 113.80             | 106.40          | 1                  |
| C-N-CA                 | 121.70             | 108.39          | 1                  |
| CA-C-O                 | 120.80             | 108.23          | 1                  |
| C-CA-C-N-CA            | 121.70             | 108.39          | 1                  |
| N-CA-CB                | 110.50             | 97.93           | 1                  |
| C-N-C-N-CA             | 121.70             | 135.01          | 1                  |
| C-CA-CB                | 110.10             | 124.15          | 2                  |



| Angle type                                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-N-CD  | 112.00             | 101.65          | 1                  |
| C-CA-N-CA-CB                                   | 111.50             | 98.93           | 1                  |
| C-N-N-CA-N-CA-C-CA-C-N-C-CA-CA-CB-C-CA-C-CA-CB | 111.40             | 125.43          | 1                  |
| CA-C-C-CA-CB                                   | 110.10             | 96.07           | 1                  |
| C-N-CA   | 121.70             | 108.41          | 1                  |
| N-CA-N-CA-CB                                   | 110.50             | 123.05          | 1                  |
| C-CA-N-CA-CB                                   | 110.50             | 97.95           | 1                  |
| N-CA-CB  | 110.50             | 97.95           | 1                  |
| C-CA-C-N-CA-C-N                                | 116.20             | 130.96          | 1                  |
| C-CA-CB  | 110.10             | 96.08           | 1                  |
| C-N-N-CA-C                                     | 111.00             | 131.65          | 1                  |
| C-N-CA   | 121.70             | 108.42          | 1                  |
| C-N-CA   | 121.70             | 134.98          | 1                  |
| CA-C-O   | 120.80             | 108.26          | 1                  |
| C-CA-CB  | 110.10             | 124.11          | 2                  |
| N-CA-C   | 111.00             | 131.65          | 1                  |
| C-CA-CB  | 111.40             | 97.39           | 1                  |
| C-CA-CA-C-O                                    | 120.80             | 108.27          | 1                  |
| N-CA-CB  | 110.50             | 97.97           | 1                  |
| CA-C-C-CA-CB                                   | 110.10             | 124.10          | 1                  |
| C-CA-CB  | 110.10             | 96.10           | 1                  |
| C-CA-C-CA-N-CD-CG                              | 103.20             | 92.15           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                     | 110.50             | 97.98           | 1                  |
| C-N-CA                      | 121.70             | 108.44          | 1                  |
| N-CA-C                      | 111.00             | 131.62          | 1                  |
| C-CA-CB                     | 110.10             | 124.09          | 1                  |
| C-CA-CA-CB-CA-N-CD          | 112.00             | 101.69          | 1                  |
| N-CA-CB                     | 110.50             | 123.02          | 1                  |
| C-CA-CB                     | 110.10             | 96.11           | 1                  |
| CA-C-N-CA-CB                | 110.50             | 123.01          | 1                  |
| C-CA-CB                     | 110.10             | 124.08          | 2                  |
| C-CA-CB                     | 110.10             | 96.12           | 1                  |
| C-CA-CA-C-N-CA-NE-CZ-NH2    | 119.20             | 112.58          | 1                  |
| CA-CB-CG                    | 112.60             | 119.95          | 1                  |
| N-CA-CB                     | 110.50             | 123.00          | 1                  |
| N-CD-CG                     | 103.20             | 92.18           | 1                  |
| CA-C-C-CA-C-CA-C-CA-C-CA-CB | 110.10             | 124.06          | 1                  |
| N-CA-N-CA-CB                | 110.50             | 122.98          | 1                  |
| CA-C-N                      | 116.20             | 130.88          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 124.04          | 1                  |
| C-CA-C-N-CA                 | 121.70             | 108.49          | 1                  |
| C-CA-CB                     | 110.10             | 124.04          | 1                  |
| C-N-CA                      | 121.70             | 108.50          | 1                  |
| C-N-CA                      | 121.70             | 134.90          | 2                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB          | 110.50             | 121.50          | 1                  |
| C-CA-CB               | 110.10             | 96.17           | 1                  |
| C-CA-C-N-CA           | 121.70             | 108.51          | 1                  |
| N-CA-CB               | 103.00             | 111.06          | 1                  |
| C-N-C-CA-CB           | 110.10             | 96.18           | 1                  |
| C-N-N-CA-CB           | 110.50             | 98.04           | 1                  |
| C-CA-CB               | 110.10             | 124.02          | 1                  |
| N-CA-CB               | 110.50             | 122.95          | 1                  |
| CA-C-N                | 116.20             | 130.85          | 1                  |
| C-CA-C-CA-C-CA-CA-C-O | 120.80             | 108.36          | 1                  |
| CA-C-N                | 116.20             | 130.84          | 1                  |
| CD-NE-CZ              | 124.40             | 134.64          | 1                  |
| N-CA-CB               | 103.00             | 111.05          | 1                  |
| C-N-N-CA-CA-C-O       | 120.80             | 108.36          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 124.00          | 1                  |
| N-CA-CD-NE-CZ         | 124.40             | 134.64          | 1                  |
| C-CA-CB               | 110.10             | 96.21           | 3                  |
| N-CA-CA-C-N           | 116.20             | 130.82          | 1                  |
| N-CA-CB               | 103.00             | 111.04          | 1                  |
| N-CA-CB               | 111.50             | 99.08           | 1                  |
| C-CA-N-CA-C           | 111.00             | 131.46          | 1                  |
| N-CA-C                | 112.10             | 93.83           | 1                  |

| Angle type                         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-C-CA-C-CA-C-CA-C-N-CA-CB | 103.00             | 111.03          | 1                  |
| C-N-C-CA-N-CA-N-CA-C-N-CA          | 121.70             | 134.84          | 1                  |
| C-CA-CB                            | 110.10             | 123.96          | 1                  |
| C-CA-CB                            | 110.50             | 121.44          | 1                  |
| CA-C-N                             | 116.20             | 101.61          | 1                  |
| CD-NE-CZ                           | 124.40             | 134.61          | 2                  |
| C-N-C-CA-CB                        | 110.10             | 123.96          | 1                  |
| C-N-CA                             | 121.70             | 134.83          | 1                  |
| CA-C-CA-C-N                        | 116.20             | 101.61          | 1                  |
| N-CA-CB                            | 110.50             | 98.10           | 1                  |
| C-CA-CB                            | 110.10             | 123.95          | 1                  |
| N-CA-C                             | 111.00             | 90.59           | 1                  |
| CA-C-N                             | 116.20             | 130.78          | 1                  |
| C-N-C-N-CA-C-CD-NE-CZ              | 124.40             | 134.60          | 1                  |
| CD-NE-CZ                           | 124.40             | 134.60          | 1                  |
| N-CA-C                             | 111.00             | 90.60           | 1                  |
| C-CA-CB                            | 110.10             | 123.94          | 1                  |
| C-CA-C-CA-CA-C-O                   | 120.80             | 108.42          | 1                  |
| N-CA-CB                            | 110.50             | 98.12           | 1                  |
| C-CA-C-CA-C-N-C-CA-CB              | 111.60             | 97.04           | 1                  |
| C-CA-N-CA-CB                       | 111.50             | 99.13           | 1                  |
| C-CA-CB                            | 110.10             | 123.92          | 2                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-CB               | 111.60             | 97.05           | 1                  |
| C-N-CA                     | 121.70             | 134.79          | 1                  |
| N-CA-CA-C-N                | 116.20             | 130.74          | 1                  |
| C-CA-CB                    | 110.10             | 96.29           | 1                  |
| C-CA-C-CA-CB               | 110.10             | 123.91          | 1                  |
| C-N-CA                     | 121.70             | 134.78          | 1                  |
| CA-C-N                     | 116.20             | 101.66          | 1                  |
| N-CA-CB                    | 111.50             | 99.14           | 2                  |
| N-CA-C                     | 111.00             | 131.35          | 1                  |
| N-CA-C                     | 112.10             | 93.93           | 1                  |
| CA-C-C-N-CA                | 121.70             | 108.62          | 1                  |
| CA-C-C-CA-CB               | 110.10             | 96.30           | 1                  |
| C-N-CA-C-N                 | 116.20             | 130.73          | 1                  |
| N-CA-CB                    | 110.50             | 98.15           | 1                  |
| N-CD-CG                    | 103.20             | 92.30           | 1                  |
| C-CA-C-CA-N-CA-CA-C-N      | 116.20             | 101.67          | 1                  |
| CA-C-CA-C-N-CA-N-CA-CA-C-N | 116.20             | 101.68          | 1                  |
| N-CA-C-CA-C-CA-C-CA-CB     | 111.60             | 97.09           | 1                  |
| C-CA-CB                    | 110.10             | 96.31           | 1                  |
| CA-CB-CG                   | 113.80             | 106.55          | 1                  |
| C-CA-CB                    | 110.10             | 123.88          | 2                  |
| C-CA-CA-C-N                | 116.20             | 130.70          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                | 111.50             | 99.18           | 1                  |
| N-CA-C-N-CA            | 121.70             | 108.65          | 1                  |
| CA-C-O                 | 120.80             | 108.48          | 1                  |
| N-CA-CA-C-N-CA-CB      | 110.50             | 122.82          | 1                  |
| C-CA-CB                | 110.10             | 123.86          | 1                  |
| C-N-CA                 | 121.70             | 108.66          | 1                  |
| N-CA-C-CA-CB           | 109.10             | 125.03          | 1                  |
| N-CA-N-CA-N-CA-N-CA-CB | 110.50             | 98.19           | 1                  |
| N-CA-CB                | 111.50             | 99.19           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 123.85          | 1                  |
| CA-C-N                 | 116.20             | 101.72          | 1                  |
| C-CA-CA-C-N-CD-CG      | 103.20             | 92.34           | 1                  |
| N-CA-CB                | 110.50             | 98.20           | 1                  |
| N-CA-CB                | 111.50             | 99.20           | 1                  |
| C-CA-CB                | 111.60             | 97.13           | 1                  |
| C-CA-CB                | 111.40             | 97.65           | 1                  |
| N-CA-CB                | 110.50             | 122.80          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 123.84          | 1                  |
| N-CA-C-N-CA            | 121.70             | 134.72          | 2                  |
| N-CA-CB                | 111.50             | 123.79          | 1                  |
| C-CA-CB                | 111.40             | 125.14          | 1                  |
| N-CA-CB                | 110.50             | 98.21           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CA-C-C-CA-CB | 110.10             | 123.83          | 1                  |
| CA-C-O                 | 120.80             | 108.52          | 2                  |
| C-N-CA                 | 121.70             | 108.69          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 99.22           | 1                  |
| C-CA-CB                | 111.40             | 97.67           | 1                  |
| N-CA-CB                | 110.50             | 98.22           | 1                  |
| CA-C-CA-C-O            | 120.80             | 108.52          | 1                  |
| N-CA-N-CA-NE-CZ-NH2    | 119.20             | 112.70          | 1                  |
| CA-C-N                 | 116.20             | 101.76          | 1                  |
| N-CA-CB                | 110.50             | 122.78          | 1                  |
| C-N-CA                 | 121.70             | 108.70          | 1                  |
| C-CA-C-N-CA            | 121.70             | 134.70          | 1                  |
| N-CA-CB                | 110.50             | 98.23           | 1                  |
| N-CA-C-CA-CB           | 109.10             | 124.98          | 1                  |
| N-CA-C-CA-CA-C-N       | 116.20             | 101.77          | 1                  |
| C-N-CA                 | 121.70             | 134.69          | 1                  |
| N-CA-N-CA-CB           | 111.50             | 123.77          | 1                  |
| CA-C-N                 | 116.20             | 101.77          | 2                  |
| C-N-CA                 | 121.70             | 108.71          | 1                  |
| N-CA-C-CA-N-CA-CB      | 111.50             | 123.76          | 1                  |
| C-CA-CB                | 110.10             | 123.80          | 1                  |
| CA-C-N                 | 116.20             | 130.62          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-O             | 120.80             | 108.54          | 1                  |
| C-CA-CB                | 111.40             | 97.70           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 123.80          | 1                  |
| C-N-CA                 | 121.70             | 108.72          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 123.80          | 1                  |
| N-CA-C                 | 112.10             | 94.08           | 1                  |
| N-CA-C-CA-CB           | 109.10             | 93.24           | 1                  |
| N-CA-N-CA-C-CA-CB      | 110.10             | 123.79          | 1                  |
| CA-C-O                 | 120.80             | 108.55          | 1                  |
| C-CA-CB                | 109.10             | 124.95          | 2                  |
| N-CA-C                 | 111.00             | 131.17          | 1                  |
| CA-C-N-CA-N-CA-N-CA-CB | 110.50             | 122.75          | 1                  |
| N-CA-CB                | 110.50             | 98.26           | 2                  |
| CA-C-O                 | 120.80             | 108.56          | 1                  |
| CA-C-O                 | 120.80             | 133.04          | 1                  |
| C-N-CA                 | 121.70             | 134.66          | 1                  |
| CA-C-N-CA-C            | 111.00             | 131.16          | 1                  |
| N-CA-CB                | 111.50             | 99.26           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 96.43           | 1                  |
| N-CA-CB                | 111.50             | 99.27           | 2                  |
| C-CA-N-CA-CB           | 111.50             | 99.27           | 1                  |
| C-CA-CB                | 110.10             | 123.77          | 1                  |



| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-CB          | 110.50             | 122.73          | 1                  |
| CA-C-N           | 116.20             | 130.59          | 1                  |
| N-CA-C           | 112.10             | 94.12           | 1                  |
| C-CA-C-CA-CA-C-O | 120.80             | 133.03          | 1                  |
| N-CA-CB          | 111.50             | 123.73          | 1                  |
| N-CA-CA-C-O      | 120.80             | 135.90          | 1                  |
| C-CA-CB          | 109.10             | 124.92          | 2                  |
| C-CA-CB          | 110.10             | 123.76          | 2                  |
| C-CA-CB          | 110.10             | 96.44           | 2                  |
| N-CA-C-CA-CB     | 110.10             | 123.75          | 1                  |
| N-CA-C-CA-CB     | 111.40             | 125.05          | 1                  |
| CA-C-O           | 120.80             | 108.59          | 1                  |
| N-CA-CB          | 111.50             | 99.29           | 1                  |
| C-CA-CB          | 109.10             | 93.30           | 1                  |
| C-CA-N-CA-CB     | 111.50             | 123.71          | 1                  |
| C-CA-CB          | 110.10             | 123.74          | 1                  |
| CA-C-N           | 116.20             | 101.84          | 1                  |
| C-CA-CB          | 111.40             | 97.76           | 1                  |
| C-N-CA           | 121.70             | 134.62          | 1                  |
| CA-C-C-CA-CB     | 109.10             | 124.88          | 1                  |
| N-CA-CA-C-O      | 120.80             | 108.61          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 96.48           | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB     | 110.10             | 123.72          | 1                  |
| C-N-CA           | 121.70             | 108.80          | 1                  |
| C-CA-CB          | 110.10             | 123.71          | 1                  |
| N-CA-CB          | 111.50             | 123.68          | 1                  |
| C-N-CA           | 121.70             | 108.81          | 1                  |
| CA-C-N           | 116.20             | 101.88          | 1                  |
| C-CA-CB          | 110.50             | 121.24          | 1                  |
| CA-CB-OG1        | 109.60             | 98.86           | 1                  |
| CA-C-O           | 120.80             | 105.77          | 1                  |
| C-CA-CB          | 109.10             | 124.85          | 1                  |
| C-CA-C-CA-CA-C-O | 120.80             | 132.96          | 1                  |
| N-CA-CB          | 110.50             | 98.34           | 1                  |
| C-CA-CB          | 110.10             | 96.51           | 2                  |
| CA-C-O           | 120.80             | 135.81          | 1                  |
| CA-CB-CG         | 113.80             | 106.65          | 1                  |
| CA-C-N           | 116.20             | 101.90          | 1                  |
| CA-C-O           | 120.80             | 132.95          | 1                  |
| CA-C-N           | 116.20             | 130.50          | 1                  |
| N-CA-CB          | 110.50             | 98.35           | 1                  |
| N-CA-C-CA-CB     | 110.10             | 123.68          | 1                  |
| N-CA-CB          | 110.50             | 122.64          | 1                  |
| N-CA-C-CA-C-N-CA | 121.70             | 134.56          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB      | 110.50             | 122.64          | 1                  |
| C-CA-C-CA-CA-C-O  | 120.80             | 132.93          | 1                  |
| N-CA-C            | 111.00             | 91.02           | 1                  |
| N-CA-CB           | 103.00             | 110.85          | 1                  |
| N-CA-CB           | 111.50             | 99.37           | 1                  |
| C-CA-CA-C-N       | 116.20             | 101.93          | 1                  |
| C-CA-CB           | 110.10             | 123.65          | 1                  |
| N-CA-C-CA-CB      | 110.10             | 123.65          | 1                  |
| C-CA-CB           | 111.60             | 97.34           | 1                  |
| C-CA-N-CA-CB      | 111.50             | 99.38           | 2                  |
| CA-C-N            | 116.20             | 101.94          | 1                  |
| N-CA-CA-C-O       | 120.80             | 108.69          | 1                  |
| N-CA-CB           | 110.50             | 98.39           | 1                  |
| C-CA-N-CA-C-CA-CB | 110.10             | 123.64          | 1                  |
| CA-C-O            | 120.80             | 135.76          | 1                  |
| N-CA-CB           | 110.50             | 122.61          | 1                  |
| C-CA-N-CA-C       | 111.00             | 91.06           | 1                  |
| C-CA-CB           | 110.10             | 123.63          | 1                  |
| C-N-CA            | 121.70             | 134.52          | 1                  |
| C-CA-CB           | 110.50             | 99.82           | 3                  |
| N-CA-CB           | 110.50             | 122.60          | 1                  |
| N-CA-CB           | 110.50             | 98.40           | 2                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                 | 111.50             | 123.60          | 1                  |
| C-CA-CB                 | 110.10             | 123.62          | 1                  |
| C-N-CA                  | 121.70             | 134.50          | 1                  |
| CA-CB-OG1               | 109.60             | 98.93           | 1                  |
| N-CA-CB                 | 110.50             | 122.59          | 1                  |
| C-CA-C-N-CA             | 121.70             | 134.49          | 1                  |
| N-CA-CB                 | 110.50             | 122.58          | 2                  |
| C-CA-CB                 | 110.10             | 96.60           | 1                  |
| C-CA-CB                 | 111.60             | 97.39           | 1                  |
| N-CA-CB                 | 111.50             | 123.58          | 1                  |
| CA-C-CA-C-CA-C-O        | 120.80             | 105.89          | 1                  |
| N-CA-N-CA-CB            | 110.50             | 122.57          | 1                  |
| C-CA-CA-CB-C-CA-C-CA-CB | 110.10             | 123.58          | 1                  |
| N-CA-CB                 | 111.50             | 99.44           | 1                  |
| CA-C-O                  | 120.80             | 132.86          | 1                  |
| N-CA-CB                 | 110.50             | 122.56          | 1                  |
| NE-CZ-NH2               | 119.20             | 112.81          | 1                  |
| N-CA-C-CA-C-CA-C-CA-CB  | 110.50             | 99.86           | 1                  |
| N-CA-CB                 | 111.50             | 123.56          | 1                  |
| C-CA-CB                 | 110.10             | 123.57          | 1                  |
| CA-CB-N-CA-N-CA-CB      | 111.50             | 123.55          | 1                  |
| N-CA-CB                 | 111.50             | 99.45           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-C-CA-CB     | 110.10             | 96.64           | 1                  |
| C-CA-CB               | 110.10             | 123.56          | 1                  |
| C-N-CA                | 122.60             | 158.02          | 1                  |
| N-CA-CA-C-N-CA-CB     | 110.50             | 98.46           | 2                  |
| N-CA-CB               | 111.50             | 123.54          | 1                  |
| C-CA-CB               | 110.50             | 121.12          | 1                  |
| C-N-CA                | 122.60             | 157.98          | 1                  |
| CA-C-O                | 120.80             | 132.83          | 1                  |
| C-CA-CB               | 110.10             | 123.54          | 2                  |
| C-CA-CB               | 110.10             | 96.66           | 3                  |
| C-N-CA                | 121.70             | 134.43          | 1                  |
| N-CA-C-CA-CB          | 110.10             | 123.54          | 1                  |
| C-CA-N-CA-C-N-N-CA-CB | 110.50             | 98.48           | 1                  |
| N-CA-C-CA-CB          | 110.10             | 123.53          | 1                  |
| CA-C-O                | 120.80             | 132.82          | 1                  |
| C-CA-CB               | 110.10             | 123.53          | 1                  |
| C-CA-CB               | 110.10             | 123.52          | 3                  |
| N-CA-CA-CB-CG         | 113.80             | 106.74          | 1                  |
| C-N-C-N-CA            | 121.70             | 134.41          | 1                  |
| N-CA-C-CA-CB          | 110.10             | 123.52          | 1                  |
| N-CA-CB               | 110.50             | 122.50          | 1                  |
| C-CA-CA-CB-C-N-CA     | 121.70             | 134.41          | 1                  |

| Angle type                             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-N                                 | 116.20             | 102.08          | 1                  |
| CA-C-C-CA-N-CA-CB                      | 110.50             | 98.50           | 1                  |
| C-CA-N-CA-CA-C-N-CA-CA-CB-CA-CB-C-N-CA | 121.70             | 134.40          | 1                  |
| C-CA-CB                                | 110.10             | 123.50          | 3                  |
| CA-CB-CG                               | 113.80             | 106.75          | 1                  |
| C-N-CA                                 | 121.70             | 134.39          | 1                  |
| CA-CB-C-CA-CA-CB-C-N-CA                | 121.70             | 134.39          | 1                  |
| C-CA-CB                                | 110.10             | 96.70           | 1                  |
| C-N-C-CA-CB                            | 110.10             | 96.70           | 1                  |
| N-CA-CB                                | 110.50             | 98.51           | 1                  |
| CA-CB-C-CA-CB                          | 110.10             | 123.49          | 1                  |
| CA-CB-C-N-C-CA-CB                      | 110.10             | 96.71           | 1                  |
| CA-C-O                                 | 120.80             | 108.82          | 2                  |
| N-CA-CB                                | 110.50             | 122.48          | 1                  |
| N-CA-CB                                | 110.50             | 98.53           | 2                  |
| C-CA-N-CA-CB                           | 110.50             | 122.47          | 1                  |
| N-CA-C-CA-C-CA-CB                      | 110.10             | 123.48          | 1                  |
| C-CA-C-N-CA                            | 121.70             | 134.37          | 1                  |
| C-CA-CB                                | 110.10             | 123.47          | 1                  |
| C-N-CA                                 | 121.70             | 109.03          | 1                  |
| CA-CB-C-CA-N-CA-CA-C-N-CA-CB           | 111.50             | 123.46          | 1                  |
| C-CA-CB                                | 109.10             | 93.63           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-CB-C-CA-CB         | 110.10             | 96.74           | 1                  |
| CA-C-N                     | 116.20             | 102.14          | 1                  |
| C-CA-CB                    | 111.60             | 125.66          | 1                  |
| C-CA-CB                    | 110.10             | 123.46          | 1                  |
| C-CA-C-N-CA                | 121.70             | 134.35          | 1                  |
| CA-C-O                     | 120.80             | 108.85          | 1                  |
| N-CA-CB                    | 110.50             | 98.56           | 1                  |
| C-CA-N-CA-CA-C-O           | 120.80             | 108.86          | 1                  |
| C-CA-CB                    | 110.10             | 123.44          | 1                  |
| N-CA-C-CA-CA-C-O           | 120.80             | 108.87          | 1                  |
| C-N-CA                     | 121.70             | 134.33          | 1                  |
| C-CA-CB                    | 109.10             | 93.66           | 1                  |
| C-N-CA                     | 121.70             | 134.32          | 1                  |
| C-CA-CB                    | 111.60             | 125.63          | 1                  |
| N-CA-CB                    | 110.50             | 98.58           | 1                  |
| CA-C-CA-C-N-CA-CA-C-C-N-CA | 122.60             | 87.56           | 1                  |
| C-N-C-N-CA                 | 121.70             | 109.09          | 1                  |
| C-CA-C-CA-CB               | 110.10             | 96.79           | 1                  |
| CA-C-O                     | 120.80             | 108.89          | 1                  |
| N-CA-CA-C-O                | 120.80             | 108.89          | 1                  |
| C-N-CD                     | 125.00             | 153.72          | 1                  |
| N-CA-CB                    | 111.50             | 99.59           | 1                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-CA-N-N-CA-C-N-CD      | 125.00             | 153.70          | 1                  |
| N-CA-CB                              | 110.50             | 98.60           | 1                  |
| CA-C-N                               | 116.20             | 130.20          | 1                  |
| CA-C-O                               | 120.80             | 108.90          | 1                  |
| N-CA-CA-C-N                          | 116.20             | 130.19          | 1                  |
| C-CA-CB                              | 109.10             | 93.71           | 1                  |
| CA-C-N-CA-CB                         | 110.50             | 98.61           | 1                  |
| N-CA-CA-C-C-CA-N-CA-CA-N-N-CA-CA-C-N | 116.20             | 102.22          | 1                  |
| CA-C-N-CA-N-CA-CB                    | 111.50             | 99.62           | 1                  |
| C-CA-CB                              | 110.10             | 96.83           | 1                  |
| CA-C-O                               | 120.80             | 108.92          | 1                  |
| C-N-CA                               | 122.60             | 87.67           | 1                  |
| C-CA-CB                              | 111.60             | 97.63           | 1                  |
| N-CA-CA-C-O                          | 120.80             | 108.93          | 1                  |
| N-CA-N-CA-C                          | 111.00             | 130.55          | 1                  |
| N-CA-CB                              | 110.50             | 98.63           | 1                  |
| NE-CZ-NH2                            | 119.20             | 112.92          | 1                  |
| C-N-CA                               | 121.70             | 109.13          | 1                  |
| N-CA-CB                              | 111.50             | 99.63           | 1                  |
| CA-CB-CA-C-O                         | 121.00             | 100.06          | 1                  |
| C-N-CA                               | 121.70             | 134.26          | 1                  |
| N-CA-N-CA-CB                         | 103.00             | 110.68          | 1                  |



| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| CA-C-O                    | 120.80             | 108.94          | 1                  |
| C-CA-CB                   | 110.10             | 123.36          | 1                  |
| C-CA-CB                   | 110.10             | 123.35          | 1                  |
| CA-C-C-N-CA               | 121.70             | 134.25          | 1                  |
| CA-C-O                    | 121.00             | 100.08          | 1                  |
| C-CA-CB                   | 111.60             | 125.55          | 1                  |
| CA-CB-CA-CB-CG            | 113.80             | 106.83          | 2                  |
| C-CA-CB                   | 110.10             | 96.85           | 1                  |
| N-CA-N-CA-CB              | 110.50             | 98.65           | 1                  |
| CA-C-O                    | 120.80             | 108.95          | 1                  |
| N-CA-C                    | 111.00             | 130.51          | 1                  |
| C-N-CA                    | 121.70             | 109.16          | 1                  |
| C-CA-CB                   | 110.10             | 123.34          | 1                  |
| C-CA-CB                   | 110.10             | 96.87           | 1                  |
| C-CA-CB                   | 110.10             | 123.33          | 2                  |
| N-CA-CA-C-O               | 121.00             | 100.11          | 1                  |
| N-CA-C                    | 111.00             | 130.49          | 1                  |
| CA-CB-C-CA-C-CA-CB        | 110.10             | 96.88           | 1                  |
| CA-C-O                    | 121.00             | 100.12          | 1                  |
| C-N-CA                    | 121.70             | 134.23          | 1                  |
| C-CA-CB                   | 110.10             | 123.32          | 1                  |
| N-CA-C-CA-C-CA-C-N-CA-C-N | 116.20             | 102.29          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 123.31          | 1                  |
| C-CA-C-CA-C-N-CA  | 121.70             | 134.21          | 1                  |
| N-CA-CB           | 103.00             | 110.65          | 1                  |
| C-CA-CB           | 111.40             | 98.19           | 1                  |
| C-CA-CB           | 111.60             | 125.50          | 1                  |
| C-CA-C-CA-CB      | 109.10             | 93.81           | 1                  |
| C-N-CA            | 121.70             | 109.19          | 1                  |
| CA-CB-CG          | 113.80             | 106.85          | 1                  |
| C-CA-CA-C-N       | 116.20             | 102.31          | 1                  |
| N-CA-C            | 111.00             | 130.45          | 1                  |
| CA-C-O            | 120.80             | 108.99          | 1                  |
| C-N-CA            | 122.60             | 157.32          | 1                  |
| N-CA-C            | 111.00             | 130.44          | 1                  |
| N-CA-C-CA-CB      | 109.10             | 93.83           | 1                  |
| C-CA-N-CA-CB      | 111.50             | 99.70           | 1                  |
| N-CA-CB           | 103.00             | 110.63          | 1                  |
| N-CA-N-CA-CB      | 103.00             | 110.63          | 1                  |
| N-CA-C-CA-C-CA-CB | 110.10             | 96.92           | 1                  |
| C-N-CA            | 122.60             | 157.28          | 1                  |
| C-CA-CB           | 110.10             | 123.28          | 1                  |
| C-N-CA-C-O        | 120.80             | 109.01          | 1                  |
| C-CA-CA-C-N-CA-CB | 111.50             | 99.71           | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                        | 111.60             | 97.73           | 1                  |
| CA-C-O                         | 120.80             | 109.01          | 1                  |
| C-CA-CB                        | 110.10             | 123.27          | 2                  |
| C-CA-C-CA-CA-CB-CG             | 113.80             | 106.87          | 1                  |
| CA-C-O                         | 120.80             | 109.02          | 1                  |
| N-CA-CB                        | 103.00             | 110.62          | 1                  |
| N-CA-C-CA-CB                   | 111.40             | 98.23           | 1                  |
| N-CA-C-CA-C-N-N-CA-C-CA-CA-C-N | 116.20             | 102.35          | 1                  |
| C-CA-CB                        | 110.10             | 123.26          | 1                  |
| N-CD-C-CA-CB                   | 110.10             | 96.95           | 1                  |
| N-CA-CB                        | 110.50             | 98.73           | 1                  |
| N-CA-CB                        | 110.50             | 122.27          | 1                  |
| C-CA-C-CA-CB                   | 111.40             | 98.25           | 1                  |
| C-CA-CB                        | 111.40             | 98.26           | 1                  |
| C-N-CA                         | 121.70             | 109.25          | 1                  |
| C-CA-CB                        | 110.10             | 96.96           | 1                  |
| C-CA-N-CA-C-CA-CB              | 110.10             | 96.96           | 1                  |
| N-CA-C                         | 111.00             | 130.37          | 1                  |
| C-CA-N-CA-C-N-CA               | 121.70             | 134.14          | 1                  |
| N-CA-CB                        | 110.50             | 122.25          | 1                  |
| C-CA-CB                        | 110.10             | 123.23          | 2                  |
| C-N-CA                         | 121.70             | 109.26          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-C           | 111.00             | 130.35          | 1                  |
| CA-C-C-CA-C-N-N-CA-CB | 110.50             | 122.25          | 1                  |
| CA-CB-CA-C-O          | 120.80             | 109.06          | 1                  |
| C-CA-CB               | 110.10             | 96.97           | 1                  |
| C-N-CA                | 121.70             | 134.13          | 1                  |
| C-CA-CB               | 109.10             | 124.30          | 1                  |
| C-CA-CB               | 110.10             | 123.22          | 1                  |
| N-CA-CB               | 111.50             | 99.76           | 1                  |
| C-CA-CB               | 110.10             | 96.99           | 2                  |
| CA-C-O                | 120.80             | 109.07          | 1                  |
| C-CA-CB               | 110.10             | 123.21          | 1                  |
| CA-CB-CG              | 113.80             | 106.90          | 1                  |
| CA-C-C-N-CA           | 121.70             | 134.11          | 1                  |
| N-CA-CB               | 103.00             | 110.58          | 1                  |
| N-CD-N-CA-CB          | 110.50             | 122.22          | 1                  |
| C-CA-CB               | 110.10             | 97.00           | 2                  |
| C-CA-N-CA-C           | 111.00             | 130.30          | 1                  |
| C-CA-CB               | 110.10             | 123.19          | 1                  |
| C-CA-C-N-CA-C-N       | 116.20             | 102.43          | 1                  |
| C-CA-CB               | 110.10             | 123.18          | 1                  |
| N-CA-C-CA-CB          | 109.10             | 124.25          | 1                  |
| C-N-CA                | 122.60             | 88.18           | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-CB-CG              | 113.80             | 106.92          | 1                  |
| N-CA-CB                    | 103.00             | 110.57          | 1                  |
| N-CA-CB                    | 110.50             | 122.20          | 2                  |
| CA-C-C-N-C-CA-C-CA-CA-C-O  | 120.80             | 109.11          | 1                  |
| C-CA-C-N-N-CA-CB           | 103.00             | 110.56          | 1                  |
| CA-C-N-CA-CB               | 110.50             | 98.81           | 1                  |
| N-CA-C                     | 111.00             | 91.75           | 1                  |
| C-CA-N-CA-C-CA-C-CA-N-CA-C | 111.00             | 91.76           | 1                  |
| C-CA-CB                    | 110.10             | 123.15          | 2                  |
| C-CA-CB                    | 110.50             | 100.20          | 1                  |
| C-N-CA                     | 121.70             | 134.06          | 1                  |
| C-CA-N-CA-C                | 111.00             | 130.23          | 1                  |
| N-CA-C                     | 111.00             | 130.23          | 1                  |
| C-CA-CA-C-CA-C-N           | 116.20             | 129.93          | 1                  |
| C-N-CA                     | 121.70             | 109.34          | 1                  |
| C-CA-CB                    | 111.60             | 97.87           | 1                  |
| C-CA-CB                    | 110.10             | 123.14          | 2                  |
| N-CA-CB                    | 110.50             | 122.17          | 1                  |
| C-N-CA                     | 121.70             | 109.35          | 1                  |
| N-CA-N-CA-C                | 111.00             | 91.79           | 1                  |
| C-CA-N-CA-CB               | 110.50             | 122.16          | 1                  |
| C-N-CA                     | 122.60             | 88.30           | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB                     | 103.00             | 110.55          | 1                  |
| C-N-C-CA-CB                      | 111.40             | 98.37           | 1                  |
| C-N-CA-C-CA-C-N                  | 116.20             | 129.91          | 1                  |
| CA-C-O                           | 120.80             | 109.15          | 1                  |
| C-CA-CB                          | 110.10             | 123.12          | 2                  |
| C-CA-CB                          | 111.40             | 98.38           | 1                  |
| N-CA-C-N-CA                      | 121.70             | 109.36          | 1                  |
| N-CA-C                           | 111.00             | 91.81           | 1                  |
| C-CA-N-CA-C                      | 111.00             | 91.82           | 1                  |
| N-CA-CA-C-N-CA-CB                | 110.50             | 98.86           | 1                  |
| N-CA-C                           | 111.00             | 91.82           | 1                  |
| CA-C-C-CA-CB                     | 110.10             | 123.11          | 1                  |
| N-CA-C                           | 111.00             | 91.83           | 1                  |
| C-CA-CB                          | 110.10             | 123.10          | 1                  |
| C-CA-CB                          | 110.10             | 97.10           | 1                  |
| C-N-CA                           | 121.70             | 134.02          | 1                  |
| C-CA-CB                          | 111.60             | 97.91           | 1                  |
| C-CA-C-CA-C-CA-C-CA-N-CA-C-CA-CB | 111.60             | 97.92           | 1                  |
| CA-C-O                           | 120.80             | 132.43          | 1                  |
| CA-C-O                           | 120.80             | 109.17          | 1                  |
| N-CA-C                           | 111.00             | 91.85           | 1                  |
| CA-C-C-CA-C-N-CA                 | 121.70             | 134.01          | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                         | 110.10             | 123.09          | 1                  |
| C-CA-CB                         | 110.10             | 97.11           | 1                  |
| C-N-CA                          | 121.70             | 134.00          | 1                  |
| N-CA-CB                         | 110.50             | 98.88           | 1                  |
| C-CA-C-CA-C-CA-C-CA-CB          | 110.10             | 123.09          | 1                  |
| CA-C-C-CA-CB                    | 111.60             | 97.94           | 1                  |
| C-CA-CB                         | 110.10             | 123.08          | 2                  |
| N-CA-CB                         | 103.00             | 110.51          | 1                  |
| C-N-CA                          | 121.70             | 109.41          | 1                  |
| N-CA-CB                         | 110.50             | 122.11          | 1                  |
| C-CA-C-CA-N-CA-CA-C-C-CA-C-N-CA | 121.70             | 109.42          | 1                  |
| C-CA-CB                         | 110.10             | 97.14           | 1                  |
| N-CA-N-CA-CB                    | 110.40             | 100.17          | 1                  |
| C-CA-CB                         | 111.60             | 97.96           | 1                  |
| CA-C-O                          | 120.80             | 132.40          | 1                  |
| C-CA-CA-C-C-CA-CB               | 110.10             | 123.05          | 1                  |
| C-CA-C-N-N-CA-CB                | 111.50             | 123.09          | 1                  |
| N-CA-CB                         | 110.40             | 100.18          | 1                  |
| N-CA-CA-C-C-N-CA                | 121.70             | 133.96          | 1                  |
| N-CA-N-CA-CB                    | 110.50             | 122.08          | 1                  |
| C-CA-CB                         | 110.10             | 123.04          | 3                  |
| C-CA-N-CA-C-CA-C-CA-CB          | 110.10             | 97.16           | 1                  |

| Angle type                         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                            | 110.50             | 98.93           | 1                  |
| C-CA-CB                            | 111.60             | 97.99           | 1                  |
| N-CA-N-CA-C-CA-C-CA-CB             | 110.50             | 100.29          | 1                  |
| N-CA-C-N-C-N-C-CA-N-CA-C-N-C-CA-CB | 110.10             | 123.03          | 1                  |
| C-CA-CG-CD-NE2                     | 116.40             | 126.60          | 1                  |
| N-CA-C                             | 111.00             | 91.96           | 1                  |
| C-CA-CB                            | 110.10             | 123.02          | 2                  |
| C-CA-CB                            | 110.10             | 97.18           | 1                  |
| N-CA-CA-C-N-CA-N-CA-C              | 111.00             | 91.97           | 1                  |
| CA-C-N-CA-N-CA-CB                  | 110.50             | 98.95           | 1                  |
| N-CA-CB                            | 111.50             | 123.05          | 1                  |
| C-N-CA                             | 121.70             | 109.47          | 1                  |
| C-CA-C-N-CA                        | 121.70             | 109.47          | 1                  |
| N-CA-CB                            | 111.50             | 99.95           | 1                  |
| C-CA-CB                            | 110.10             | 97.19           | 1                  |
| C-N-CA-C-O                         | 120.80             | 109.26          | 1                  |
| C-CA-C-CA-CB                       | 110.10             | 97.20           | 1                  |
| CA-C-O                             | 120.80             | 109.26          | 1                  |
| C-CA-CB                            | 110.10             | 122.99          | 1                  |
| C-CA-N-CA-C-CA-C-N-CA              | 121.70             | 109.49          | 1                  |
| C-N-CA-C-C-CA-CB                   | 110.10             | 122.98          | 1                  |
| C-CA-C-N-C-CA-CB                   | 110.10             | 97.22           | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB          | 110.40             | 100.24          | 1                  |
| N-CA-CB               | 110.50             | 122.02          | 2                  |
| C-CA-N-CA-N-CA-C      | 111.00             | 92.03           | 1                  |
| C-CA-N-CA-CB          | 110.50             | 98.99           | 1                  |
| N-CA-CB               | 103.00             | 110.45          | 2                  |
| N-CA-CB               | 111.50             | 99.99           | 1                  |
| C-CA-C-CA-CB          | 109.10             | 123.99          | 1                  |
| C-N-CA                | 121.70             | 133.89          | 1                  |
| C-CA-CB               | 110.10             | 122.96          | 1                  |
| C-CA-CB               | 109.10             | 123.99          | 1                  |
| C-CA-N-CA-CB          | 110.50             | 122.00          | 1                  |
| N-CA-CA-C-CA-C-N-CA-C | 111.00             | 92.05           | 1                  |
| C-CA-CB               | 109.10             | 123.98          | 1                  |
| C-CA-CB               | 110.10             | 122.95          | 1                  |
| CA-C-O                | 120.80             | 132.30          | 1                  |
| C-CA-C-CA-CB          | 109.10             | 123.98          | 1                  |
| N-CA-CB               | 110.50             | 122.00          | 2                  |
| C-CA-C-CA-CB          | 110.10             | 122.95          | 1                  |
| C-N-CA                | 121.70             | 109.53          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 122.94          | 1                  |
| C-CA-CB               | 110.10             | 122.94          | 1                  |
| N-CA-C                | 113.30             | 132.89          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-O                     | 120.80             | 132.28          | 1                  |
| N-CA-N-CA-C-N-CA           | 121.70             | 109.55          | 1                  |
| N-CA-C                     | 111.00             | 92.10           | 2                  |
| C-CA-CB                    | 110.10             | 122.92          | 1                  |
| C-N-CA                     | 121.70             | 109.55          | 1                  |
| N-CA-C-CA-CA-CB-CG         | 112.60             | 119.35          | 1                  |
| C-CA-CB                    | 110.10             | 97.28           | 1                  |
| C-CA-CA-C-C-CA-CA-C-CA-C-N | 116.20             | 129.69          | 1                  |
| C-CA-CB                    | 110.10             | 97.29           | 1                  |
| N-CA-N-CA-CB               | 110.50             | 121.96          | 1                  |
| CD-NE-C-CA-CB              | 110.10             | 122.91          | 1                  |
| C-CA-CB                    | 110.10             | 122.91          | 1                  |
| CA-C-N                     | 116.20             | 129.68          | 1                  |
| N-CA-C                     | 113.30             | 132.85          | 1                  |
| CA-CB-CG                   | 113.80             | 107.06          | 1                  |
| C-CA-CB                    | 110.50             | 120.61          | 1                  |
| N-CA-C                     | 111.00             | 92.13           | 2                  |
| CA-C-O                     | 120.80             | 132.26          | 1                  |
| N-CA-C                     | 111.00             | 92.14           | 1                  |
| CA-C-C-CA-C-CA-C-CA-CB     | 110.10             | 97.31           | 1                  |
| C-N-CA                     | 121.70             | 133.82          | 1                  |
| N-CA-C                     | 111.00             | 92.15           | 1                  |

| Angle type                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB                  | 110.50             | 121.94          | 1                  |
| N-CA-CB                       | 110.40             | 100.30          | 1                  |
| CA-C-C-CA-C-CA-CA-CB-CG       | 112.60             | 119.33          | 1                  |
| N-CA-C                        | 111.00             | 92.16           | 2                  |
| C-CA-CB                       | 110.50             | 120.59          | 1                  |
| C-N-CA-C-C-CA-C-CA-C-CA-CB    | 110.10             | 97.32           | 1                  |
| N-CA-N-CA-C-CA-CB             | 111.40             | 124.18          | 1                  |
| C-CA-CB                       | 111.40             | 124.18          | 1                  |
| C-CA-CA-C-O                   | 120.80             | 132.23          | 1                  |
| C-N-C-CA-C-CA-CB              | 110.50             | 120.58          | 1                  |
| C-CA-CB                       | 109.10             | 94.31           | 1                  |
| N-CA-CA-C-C-CA-CD-NE-CD-NE-CZ | 124.40             | 133.81          | 1                  |
| CA-C-CA-C-O                   | 120.80             | 132.22          | 1                  |
| C-CA-CB                       | 110.10             | 97.33           | 1                  |
| C-CA-CB                       | 110.10             | 122.87          | 1                  |
| N-CA-CB                       | 110.50             | 121.92          | 1                  |
| C-CA-CB                       | 110.10             | 97.34           | 1                  |
| C-CA-CA-CB-CG                 | 113.80             | 107.08          | 1                  |
| N-CA-N-CA-CB                  | 110.50             | 99.08           | 1                  |
| C-N-CA                        | 121.70             | 133.79          | 1                  |
| C-CA-CB                       | 110.50             | 120.57          | 1                  |
| N-CA-N-CA-CB                  | 110.50             | 121.91          | 2                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                | 110.50             | 121.91          | 1                  |
| N-CA-C                 | 111.00             | 92.20           | 1                  |
| CA-C-O                 | 120.80             | 132.21          | 1                  |
| C-CA-CB                | 109.10             | 94.33           | 1                  |
| N-CA-CA-C-C-CA-N-CA-CB | 110.50             | 121.91          | 1                  |
| CA-C-O                 | 120.80             | 132.20          | 1                  |
| C-CA-CB                | 110.10             | 97.35           | 1                  |
| C-CA-CA-C-O            | 120.80             | 132.20          | 1                  |
| CA-C-C-CA-CB           | 110.10             | 122.84          | 1                  |
| CA-C-N                 | 116.20             | 129.61          | 1                  |
| N-CA-CA-C-O            | 120.80             | 132.20          | 1                  |
| C-CA-CB                | 110.10             | 97.36           | 1                  |
| N-CA-CB                | 110.50             | 99.10           | 1                  |
| CA-C-N-CA-N-CA-N-CA-CB | 110.50             | 121.89          | 1                  |
| C-CA-CB                | 110.10             | 97.37           | 1                  |
| C-CA-CB                | 109.10             | 94.36           | 1                  |
| C-CA-N-CA-CA-C-C-CA-CB | 110.10             | 97.37           | 1                  |
| C-N-C-N-CA             | 121.70             | 109.64          | 1                  |
| CA-C-N                 | 116.20             | 129.59          | 1                  |
| CA-C-C-N-C-CA-CB       | 110.10             | 122.82          | 1                  |
| C-CA-N-CA-C            | 111.00             | 92.26           | 1                  |
| N-CA-C-N-C-CA-CB       | 111.40             | 124.12          | 1                  |

| Angle type                        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB                      | 111.40             | 124.12          | 1                  |
| C-CA-CB                           | 110.10             | 122.82          | 1                  |
| C-N-C-N-CA-C-C-N-C-CA-CB          | 110.10             | 97.39           | 1                  |
| CA-C-N                            | 116.20             | 129.58          | 1                  |
| CA-C-N-CA-CB                      | 110.50             | 121.87          | 1                  |
| N-CA-CA-C-C-N-CA                  | 121.70             | 133.74          | 1                  |
| C-N-C-CA-CB                       | 109.10             | 94.39           | 1                  |
| C-CA-C-CA-C-N-CA-C-N-CA-CG-CD-NE2 | 116.40             | 126.42          | 1                  |
| N-CA-N-CA-CA-C-N-CA-CB            | 110.50             | 99.14           | 1                  |
| CA-C-N-CA-C-CA-CB                 | 110.10             | 97.41           | 1                  |
| N-CA-C-CA-C-CA-CB                 | 110.10             | 97.41           | 1                  |
| C-CA-CB                           | 109.10             | 94.41           | 1                  |
| N-CA-CA-C-O                       | 120.80             | 132.15          | 1                  |
| C-CA-CB                           | 110.10             | 97.41           | 1                  |
| CA-C-CA-C-N                       | 116.20             | 129.55          | 1                  |
| N-CA-C-CA-CB                      | 110.10             | 122.78          | 1                  |
| C-CA-CB                           | 110.10             | 122.78          | 1                  |
| N-CA-CB                           | 110.50             | 121.85          | 1                  |
| CA-C-O                            | 120.80             | 132.15          | 1                  |
| C-N-C-CA-CB                       | 111.40             | 124.08          | 1                  |
| CA-C-N                            | 116.20             | 129.55          | 1                  |
| N-CA-C-CA-N-CA-N-CA-C             | 111.00             | 92.32           | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-O                 | 120.80             | 132.14          | 1                  |
| N-CA-CB                     | 110.50             | 99.16           | 1                  |
| C-N-CA                      | 121.70             | 133.70          | 1                  |
| C-CA-CB                     | 110.10             | 97.43           | 2                  |
| C-N-CA                      | 121.70             | 109.70          | 1                  |
| CA-C-N                      | 116.20             | 129.54          | 1                  |
| C-CA-CB                     | 110.50             | 120.50          | 1                  |
| CA-C-N                      | 116.20             | 129.53          | 2                  |
| CA-C-O                      | 120.80             | 132.13          | 1                  |
| C-CA-C-CA-CA-C-C-CA-C-CA-CB | 109.10             | 94.44           | 1                  |
| C-CA-CB                     | 110.10             | 122.76          | 2                  |
| C-CA-CB                     | 110.10             | 97.44           | 2                  |
| C-N-C-CA-CB                 | 111.40             | 124.06          | 1                  |
| CA-CB-N-CA-C-CA-CB          | 110.10             | 97.45           | 1                  |
| N-CA-C                      | 111.00             | 129.65          | 1                  |
| N-CA-CB                     | 110.50             | 99.18           | 1                  |
| N-CA-CA-C-O                 | 120.80             | 109.48          | 1                  |
| C-CA-CB                     | 111.40             | 124.05          | 2                  |
| C-CA-C-N-C-CA-N-CA-C        | 111.00             | 92.36           | 1                  |
| C-CA-C-CA-CB                | 110.50             | 120.48          | 1                  |
| C-CA-CB                     | 110.10             | 122.74          | 1                  |
| C-CA-CA-C-CA-C-O            | 120.80             | 109.49          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| CA-C-N                         | 116.90             | 126.88          | 1                  |
| C-CA-CB                        | 110.50             | 120.47          | 2                  |
| N-CA-N-CA-C-N-C-N-C-CA-C-CA-CB | 110.10             | 122.73          | 1                  |
| CD-NE-CZ                       | 124.40             | 133.71          | 1                  |
| CA-C-N                         | 116.90             | 126.87          | 1                  |
| CA-C-C-CA-CB                   | 110.10             | 97.47           | 1                  |
| C-N-N-CA-C-CA-N-CA-CA-C-C-N-CA | 121.70             | 133.66          | 1                  |
| N-CA-CB                        | 110.50             | 99.21           | 1                  |
| N-CA-C                         | 111.00             | 129.60          | 1                  |
| N-CA-N-CA-CB                   | 110.50             | 121.79          | 1                  |
| C-CA-CB                        | 110.10             | 97.48           | 1                  |
| CA-C-O                         | 119.00             | 138.92          | 2                  |
| N-CA-CB                        | 110.50             | 121.79          | 1                  |
| CA-C-CA-C-O                    | 119.00             | 138.92          | 1                  |
| N-CA-C                         | 111.00             | 92.41           | 1                  |
| N-CA-C-CA-N-CA-C-CA-CB         | 110.10             | 122.71          | 1                  |
| CA-C-C-CA-CA-C-N               | 116.20             | 129.47          | 1                  |
| C-CA-CB                        | 110.10             | 122.71          | 1                  |
| N-CA-C                         | 111.00             | 92.42           | 1                  |
| C-CA-CB                        | 110.50             | 120.45          | 1                  |
| CA-C-N                         | 116.20             | 102.93          | 1                  |
| N-CA-C-N-CA                    | 121.70             | 133.64          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB               | 110.50             | 121.77          | 1                  |
| C-CA-CB                    | 110.10             | 122.70          | 2                  |
| N-CA-C                     | 111.00             | 92.43           | 1                  |
| N-CA-CB                    | 110.50             | 121.77          | 1                  |
| N-CA-CA-C-O                | 119.00             | 138.89          | 1                  |
| N-CA-N-CA-N-CA-N-CA-CA-C-N | 116.20             | 129.45          | 1                  |
| C-N-C-CA-CB                | 110.10             | 122.69          | 1                  |
| N-CA-CB                    | 110.50             | 121.76          | 2                  |
| CA-CB-CG                   | 113.80             | 107.18          | 2                  |
| C-CA-CB                    | 110.10             | 122.68          | 1                  |
| N-CA-N-CA-CB               | 110.50             | 99.24           | 1                  |
| C-CA-CB                    | 110.50             | 120.43          | 2                  |
| CA-C-O                     | 120.80             | 132.05          | 1                  |
| C-CA-C-CA-CA-CB-C-CA-CB    | 110.10             | 122.67          | 1                  |
| C-CA-CB                    | 110.10             | 122.67          | 1                  |
| C-N-N-CA-CB                | 110.50             | 99.25           | 1                  |
| C-CA-CB                    | 110.50             | 120.42          | 1                  |
| C-N-C-CA-N-CA-CB           | 110.50             | 99.26           | 1                  |
| C-CA-CB                    | 110.50             | 120.41          | 1                  |
| N-CA-CB                    | 110.50             | 121.74          | 1                  |
| ND1-CG-CD2                 | 106.10             | 112.71          | 1                  |
| CA-C-N-CA-C                | 111.00             | 92.50           | 1                  |



| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB            | 110.10             | 122.65          | 1                  |
| C-CA-CB                 | 109.10             | 94.57           | 1                  |
| N-CA-N-CA-N-CA-CA-CB-CG | 112.60             | 106.00          | 1                  |
| C-CA-CB                 | 110.10             | 122.65          | 1                  |
| C-N-CA                  | 121.70             | 109.81          | 1                  |
| N-CA-C                  | 111.00             | 92.51           | 1                  |
| C-CA-CB                 | 110.10             | 122.64          | 3                  |
| C-N-C-CA-CB             | 110.10             | 97.56           | 1                  |
| NE-CZ-NH1               | 121.50             | 128.10          | 1                  |
| N-CA-C                  | 111.00             | 92.53           | 1                  |
| C-CA-CB                 | 110.10             | 97.57           | 1                  |
| N-CA-CB                 | 110.50             | 121.71          | 1                  |
| C-CA-CB                 | 110.10             | 122.63          | 1                  |
| N-CA-N-CA-CB            | 110.50             | 121.71          | 1                  |
| CA-C-O                  | 120.80             | 132.01          | 1                  |
| C-N-N-CA-N-CA-C         | 111.00             | 129.45          | 1                  |
| ND1-CG-CD2              | 106.10             | 112.69          | 1                  |
| CA-C-O                  | 120.80             | 132.00          | 1                  |
| C-CA-C-N-N-CA-CB        | 110.50             | 121.70          | 1                  |
| N-CA-CB                 | 110.50             | 121.70          | 1                  |
| C-CA-CB                 | 110.50             | 120.38          | 1                  |
| CA-C-C-N-CA-C-N         | 116.20             | 103.03          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.10             | 122.61          | 1                  |
| C-N-C-CA-CB                | 110.50             | 120.37          | 1                  |
| C-CA-C-CA-CA-CB-CG         | 112.60             | 106.02          | 1                  |
| C-CA-CB                    | 111.40             | 98.90           | 1                  |
| C-N-CA                     | 121.70             | 109.86          | 1                  |
| CA-CB-CA-CB-CG             | 112.60             | 119.18          | 1                  |
| C-CA-CB                    | 110.10             | 122.60          | 1                  |
| C-CA-C-CA-CB               | 110.10             | 122.60          | 1                  |
| CA-C-N                     | 116.20             | 129.35          | 2                  |
| N-CA-CB                    | 110.50             | 99.32           | 1                  |
| N-CA-N-CA-N-CA-CB          | 103.00             | 110.23          | 1                  |
| N-CA-CB                    | 110.50             | 121.68          | 1                  |
| C-CA-CB                    | 110.10             | 122.59          | 1                  |
| CA-C-O                     | 120.80             | 109.63          | 1                  |
| N-CA-CA-C-N                | 116.20             | 103.06          | 1                  |
| C-CA-C-CA-C-CA-C-CA-CA-C-N | 116.20             | 103.07          | 1                  |
| CA-C-N-CA-CA-C-O           | 120.80             | 131.96          | 1                  |
| C-CA-C-N-CA                | 121.70             | 133.51          | 1                  |
| N-CA-CB                    | 110.50             | 99.34           | 1                  |
| N-CA-CB                    | 110.50             | 121.66          | 1                  |
| CA-C-O                     | 120.80             | 131.96          | 1                  |
| C-CA-N-CA-C-CA-CB          | 110.50             | 120.34          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 111.00             | 129.36          | 1                  |
| C-CA-CA-C-N           | 116.20             | 103.09          | 1                  |
| C-CA-CB               | 110.10             | 97.64           | 1                  |
| C-CA-C-CA-CB          | 110.10             | 122.55          | 1                  |
| C-CA-CB               | 110.50             | 120.33          | 1                  |
| N-CA-CB               | 110.40             | 100.57          | 1                  |
| CA-C-N                | 116.20             | 103.10          | 1                  |
| C-N-C-CA-N-CA-CB      | 110.50             | 99.37           | 1                  |
| CA-CB-CG              | 113.80             | 107.25          | 1                  |
| C-CA-CB               | 111.40             | 98.96           | 1                  |
| C-CA-CA-C-C-CA-CA-C-O | 120.80             | 131.92          | 1                  |
| CA-C-N                | 116.20             | 103.12          | 1                  |
| CA-C-O                | 120.80             | 109.68          | 1                  |
| N-CA-C                | 111.00             | 129.32          | 1                  |
| N-CA-C-CA-CA-C-N      | 116.20             | 103.12          | 1                  |
| N-CA-CA-CB-CG         | 112.60             | 119.14          | 1                  |
| N-CA-CA-C-C-CA-CB     | 110.10             | 122.52          | 1                  |
| N-CA-CB               | 103.00             | 110.19          | 1                  |
| C-CA-CB               | 110.50             | 120.30          | 1                  |
| CA-CB-CG              | 113.80             | 107.27          | 1                  |
| C-CA-C-N-CA           | 121.70             | 133.46          | 1                  |
| C-CA-N-CA-C           | 111.00             | 129.29          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-C-CA-N-CA-CB     | 110.50             | 99.40           | 1                  |
| C-N-C-N-CA                 | 121.70             | 109.95          | 1                  |
| N-CA-C                     | 111.00             | 129.27          | 1                  |
| C-CA-C-CA-N-CA-C           | 111.00             | 129.27          | 1                  |
| CA-C-O                     | 120.80             | 131.89          | 1                  |
| C-CA-CA-C-C-CA-N-CA-C      | 111.00             | 129.26          | 1                  |
| N-CA-C                     | 111.00             | 129.26          | 1                  |
| CA-C-CB-CG1-CD1            | 113.80             | 100.11          | 1                  |
| N-CA-CB                    | 103.00             | 110.17          | 1                  |
| N-CA-N-CA-C                | 111.00             | 129.25          | 1                  |
| C-CA-N-CA-CB               | 110.50             | 121.57          | 1                  |
| N-CA-CA-C-O                | 120.80             | 109.73          | 1                  |
| C-CA-CB                    | 110.50             | 100.73          | 1                  |
| C-N-N-CA-N-CA-C            | 111.00             | 129.23          | 1                  |
| C-CA-CB                    | 110.10             | 122.47          | 2                  |
| C-CA-CB                    | 110.50             | 120.27          | 1                  |
| C-N-C-CA-C-CA-N-CA-C-N-CA  | 121.70             | 133.41          | 1                  |
| NE-CZ-NH1                  | 121.50             | 128.01          | 1                  |
| N-CA-CB                    | 110.50             | 99.44           | 1                  |
| C-N-N-CA-C-CA-N-CA-C-CA-CB | 110.10             | 97.75           | 1                  |
| C-CA-CA-C-N                | 116.20             | 103.20          | 1                  |
| N-CA-CA-C-N                | 116.20             | 103.20          | 1                  |

| Angle type                        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-CA-C-O                  | 120.80             | 131.84          | 1                  |
| CA-C-C-CA-CB                      | 110.10             | 97.76           | 1                  |
| CA-C-N                            | 116.20             | 103.21          | 1                  |
| N-CA-CB                           | 110.40             | 100.66          | 1                  |
| C-CA-CB                           | 110.10             | 122.44          | 1                  |
| N-CA-C                            | 111.00             | 129.18          | 1                  |
| C-CA-CB                           | 110.10             | 97.76           | 1                  |
| CA-C-O                            | 120.80             | 109.76          | 1                  |
| N-CA-CB                           | 110.50             | 99.47           | 2                  |
| N-CA-C-CA-CB                      | 111.60             | 98.62           | 1                  |
| C-CA-CB                           | 110.10             | 97.77           | 1                  |
| CA-C-CA-C-N-CA-CB                 | 110.50             | 121.53          | 1                  |
| C-N-CA                            | 121.70             | 110.02          | 1                  |
| C-CA-CB                           | 110.10             | 122.43          | 1                  |
| C-CA-CB                           | 110.10             | 97.78           | 2                  |
| CA-C-N                            | 116.20             | 103.23          | 1                  |
| C-N-C-N-C-CA-N-CA-CA-C-C-N-C-N-CA | 121.70             | 110.03          | 1                  |
| N-CA-C                            | 111.00             | 92.84           | 1                  |
| CA-C-CA-C-N-CA-CB                 | 110.40             | 100.68          | 1                  |
| N-CA-C                            | 111.00             | 129.15          | 2                  |
| CB-CG1-CD1                        | 113.80             | 100.19          | 1                  |
| N-CA-N-CA-CA-C-N                  | 116.20             | 103.24          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-C-N-N-CA-CB | 110.50             | 121.51          | 1                  |
| CA-C-O                | 120.80             | 131.81          | 1                  |
| CA-C-C-N-CA           | 121.70             | 110.04          | 1                  |
| C-CA-CB               | 110.10             | 122.41          | 1                  |
| N-CA-C                | 111.00             | 129.13          | 1                  |
| C-CA-CB               | 109.10             | 123.34          | 1                  |
| CA-C-C-CA-C-CA-CB     | 110.10             | 122.40          | 1                  |
| N-CA-N-CA-C           | 111.00             | 92.87           | 1                  |
| C-CA-CB               | 110.10             | 122.40          | 2                  |
| C-CA-CB               | 110.10             | 97.80           | 1                  |
| C-N-CA                | 121.70             | 133.35          | 2                  |
| CA-C-N                | 116.20             | 103.25          | 1                  |
| CA-C-O                | 120.80             | 131.80          | 1                  |
| CA-C-O                | 120.80             | 109.80          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 122.39          | 1                  |
| CA-C-N                | 116.20             | 103.26          | 1                  |
| C-CA-CB               | 110.10             | 122.39          | 1                  |
| C-N-C-CA-CB           | 110.10             | 97.81           | 1                  |
| C-CA-CB               | 110.50             | 120.20          | 1                  |
| CB-CG1-C-N-C-N-C-N-CA | 121.70             | 133.33          | 1                  |
| N-CA-C-N-CA           | 121.70             | 110.07          | 1                  |
| N-CA-CB               | 103.00             | 110.11          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 97.83           | 1                  |
| C-CA-CB           | 110.10             | 122.37          | 1                  |
| CA-C-O            | 120.80             | 109.82          | 1                  |
| N-CA-C-CA-CB      | 111.60             | 98.69           | 1                  |
| CA-C-N            | 116.20             | 103.29          | 1                  |
| N-CA-N-CA-CB      | 111.50             | 122.47          | 1                  |
| C-N-CA            | 121.70             | 133.32          | 1                  |
| CA-C-O            | 120.80             | 109.83          | 1                  |
| N-CA-CB           | 103.00             | 110.10          | 1                  |
| C-CA-C-N-C-CA-CB  | 109.10             | 123.29          | 1                  |
| C-CA-CB           | 110.10             | 122.36          | 1                  |
| C-N-C-CA-CB       | 109.10             | 94.91           | 1                  |
| C-CA-C-CA-C-CA-CB | 109.10             | 123.29          | 1                  |
| C-CA-CB           | 110.50             | 100.83          | 1                  |
| N-CA-N-CA-CB      | 111.50             | 122.46          | 1                  |
| C-CA-CB           | 110.10             | 122.34          | 1                  |
| CA-C-CA-C-O       | 120.80             | 109.85          | 1                  |
| C-CA-C-CA-CB      | 109.10             | 94.93           | 1                  |
| C-CA-CB           | 110.50             | 120.16          | 1                  |
| CB-CG1-C-N-CA     | 121.70             | 133.29          | 1                  |
| N-CA-C            | 111.00             | 92.97           | 1                  |
| N-CA-N-CA-CB      | 103.00             | 110.08          | 1                  |

| Angle type                   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                      | 110.50             | 99.56           | 2                  |
| N-CA-C-CA-CB                 | 110.50             | 100.84          | 1                  |
| C-CA-C-CA-C-CA-N-CA-CA-CB-CG | 113.80             | 107.37          | 1                  |
| N-CA-CB                      | 110.50             | 121.44          | 1                  |
| C-N-CA                       | 121.70             | 110.12          | 1                  |
| CA-C-N                       | 116.20             | 103.34          | 2                  |
| C-CA-CB                      | 110.10             | 122.32          | 2                  |
| CA-C-O                       | 120.80             | 131.73          | 1                  |
| C-CA-CA-C-O                  | 119.00             | 99.71           | 1                  |
| N-CA-CB                      | 110.50             | 121.43          | 1                  |
| C-CA-CB                      | 110.50             | 100.86          | 2                  |
| C-CA-CB                      | 110.10             | 97.89           | 1                  |
| N-CA-CA-C-C-CA-N-CA-CB       | 110.50             | 121.42          | 1                  |
| CA-C-N                       | 116.20             | 103.35          | 2                  |
| CA-C-O                       | 120.80             | 131.72          | 1                  |
| C-N-CA                       | 121.70             | 133.26          | 1                  |
| CA-C-N-CA-C-N-CA             | 121.70             | 133.26          | 1                  |
| C-CA-CB                      | 110.10             | 122.30          | 2                  |
| C-N-CA                       | 121.70             | 110.14          | 1                  |
| C-N-CA                       | 121.70             | 110.15          | 3                  |
| CA-CB-CG                     | 113.80             | 107.38          | 1                  |
| CA-C-O                       | 119.00             | 99.75           | 1                  |



| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB       | 110.50             | 120.13          | 1                  |
| C-CA-CB            | 110.10             | 97.91           | 1                  |
| N-CA-CB            | 110.50             | 99.59           | 1                  |
| N-CA-CB            | 110.50             | 121.41          | 1                  |
| C-N-CA-C-O         | 120.80             | 109.89          | 1                  |
| N-CA-CB            | 110.50             | 121.40          | 1                  |
| C-N-CA             | 121.70             | 110.16          | 1                  |
| CA-C-N-CA-CA-CB-CG | 113.80             | 107.39          | 1                  |
| C-CA-CB            | 110.10             | 122.28          | 1                  |
| C-CA-C-CA-CB       | 110.50             | 100.89          | 1                  |
| C-CA-CB            | 110.10             | 97.93           | 1                  |
| C-CA-CB            | 109.10             | 123.19          | 1                  |
| C-CA-N-CA-C        | 111.00             | 93.07           | 1                  |
| C-CA-CB            | 111.40             | 99.23           | 1                  |
| C-CA-CB            | 110.10             | 97.94           | 1                  |
| N-CA-C             | 111.00             | 93.08           | 1                  |
| C-CA-N-CA-CB       | 110.40             | 100.80          | 1                  |
| CA-C-O             | 120.80             | 131.68          | 1                  |
| CA-CB-CG           | 113.80             | 107.40          | 1                  |
| C-CA-C-CA-CA-C-N   | 116.20             | 103.41          | 1                  |
| C-CA-CB            | 110.10             | 97.95           | 4                  |
| N-CA-C-CA-C-CA-CB  | 110.50             | 100.91          | 1                  |

| Angle type                             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-O                                 | 120.80             | 131.67          | 1                  |
| CA-CB-CG                               | 113.80             | 107.41          | 1                  |
| C-CA-CB                                | 110.10             | 122.24          | 1                  |
| C-CA-C-CA-CA-C-C-CA-CB                 | 110.10             | 97.96           | 1                  |
| C-CA-CB                                | 110.10             | 97.96           | 1                  |
| N-CA-C                                 | 111.00             | 93.11           | 1                  |
| C-N-CA                                 | 121.70             | 110.20          | 1                  |
| N-CA-CB                                | 110.50             | 121.36          | 1                  |
| C-CA-CB                                | 110.10             | 97.97           | 1                  |
| C-CA-C-CA-C-N-CA                       | 121.70             | 110.21          | 1                  |
| C-N-CA                                 | 121.70             | 110.21          | 1                  |
| C-CA-CB                                | 110.10             | 122.23          | 1                  |
| C-N-CA-C-O                             | 119.00             | 99.85           | 1                  |
| C-CA-N-CA-C                            | 111.00             | 128.87          | 1                  |
| C-CA-C-N-C-N-CA                        | 121.70             | 110.22          | 1                  |
| C-CA-CB                                | 110.10             | 122.22          | 1                  |
| C-CA-CB                                | 110.10             | 97.98           | 1                  |
| C-CA-C-CA-C-CA-C-CA-CA-CB-CA-C-N-CA-CB | 110.50             | 99.66           | 1                  |
| CA-C-CA-C-N                            | 116.20             | 103.45          | 1                  |
| N-CA-CB                                | 111.50             | 122.33          | 1                  |
| N-CA-CB                                | 110.50             | 121.33          | 2                  |
| C-CA-CB                                | 110.10             | 98.00           | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB       | 110.50             | 99.67           | 1                  |
| C-N-CA             | 121.70             | 133.16          | 2                  |
| CA-N-CD            | 112.00             | 103.09          | 1                  |
| C-CA-C-CA-CB       | 110.10             | 98.00           | 1                  |
| CA-C-O             | 119.00             | 99.90           | 1                  |
| N-CA-C-CA-CB       | 110.10             | 98.00           | 1                  |
| C-CA-C-CA-CA-CB-CG | 112.60             | 118.96          | 1                  |
| C-CA-CB            | 110.10             | 98.01           | 1                  |
| N-CA-CB            | 110.50             | 121.32          | 1                  |
| C-CA-CB            | 110.50             | 100.96          | 1                  |
| C-CA-CB            | 111.40             | 99.31           | 1                  |
| N-CA-C             | 111.00             | 128.81          | 1                  |
| CA-C-C-CA-CB       | 110.10             | 98.02           | 1                  |
| CA-C-CA-CB-C-CA-CB | 110.10             | 122.18          | 1                  |
| C-CA-ND1-CG-CD2    | 106.10             | 112.46          | 1                  |
| C-CA-C-CA-CB       | 110.10             | 122.18          | 1                  |
| C-N-CA             | 121.70             | 133.14          | 1                  |
| N-CA-C             | 111.00             | 128.79          | 1                  |
| CA-C-CA-N-CD       | 112.00             | 103.10          | 1                  |
| C-CA-C-N-CA        | 121.70             | 110.26          | 1                  |
| CA-C-N             | 116.20             | 103.50          | 1                  |
| N-CA-C             | 111.00             | 128.78          | 2                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| C-N-CA                                | 121.70             | 110.27          | 1                  |
| C-CA-CB                               | 111.40             | 99.34           | 1                  |
| C-CA-C-CA-C-CA-N-CA-C-N-CA            | 121.70             | 133.12          | 1                  |
| C-N-CA                                | 121.70             | 133.12          | 1                  |
| CA-CB-N-CA-CB                         | 111.50             | 122.28          | 1                  |
| C-CA-CB                               | 110.10             | 122.15          | 1                  |
| CA-CB-N-CA-CB                         | 110.50             | 121.28          | 1                  |
| C-CA-N-CA-CB                          | 110.50             | 121.28          | 1                  |
| N-CA-C-CA-C-CA-CB                     | 110.10             | 122.14          | 1                  |
| C-CA-C-N-CA                           | 121.70             | 133.11          | 1                  |
| N-CA-C-CA-CA-CB-N-CA-C-CA-CB          | 111.40             | 99.37           | 1                  |
| CA-C-O                                | 120.80             | 131.57          | 1                  |
| N-CA-CB                               | 110.50             | 121.27          | 1                  |
| C-CA-C-N-CA                           | 121.70             | 133.10          | 1                  |
| N-CA-N-CA-CA-C-N-CA-CA-C-CA-C-N-CA-CB | 110.50             | 99.74           | 1                  |
| CA-CB-C-N-CA                          | 121.70             | 133.09          | 1                  |
| C-CA-CB                               | 110.10             | 122.12          | 1                  |
| C-CA-C-CA-C-N-CA                      | 121.70             | 110.31          | 1                  |
| C-CA-CB                               | 110.10             | 98.08           | 2                  |
| N-CA-C                                | 111.00             | 128.71          | 1                  |
| N-CA-CB                               | 110.50             | 99.75           | 1                  |
| C-CA-CA-C-C-N-CA                      | 121.70             | 133.08          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 98.09           | 3                  |
| C-N-CA            | 121.70             | 110.32          | 1                  |
| C-CA-CB           | 110.10             | 122.11          | 2                  |
| C-CA-CA-N-CD      | 112.00             | 103.15          | 1                  |
| N-CA-C-N-CA       | 121.70             | 110.33          | 1                  |
| N-CA-C            | 111.00             | 128.69          | 1                  |
| C-CA-CB           | 110.10             | 98.10           | 3                  |
| C-N-CA            | 121.70             | 110.33          | 1                  |
| C-CA-CB           | 110.10             | 122.10          | 2                  |
| C-N-CA            | 121.70             | 133.07          | 2                  |
| N-CA-C-CA-CB      | 110.10             | 122.09          | 1                  |
| CA-CB-CG          | 113.80             | 107.49          | 1                  |
| C-N-CA            | 121.70             | 133.06          | 1                  |
| N-CA-C            | 111.00             | 128.67          | 1                  |
| C-CA-N-CA-C-CA-CB | 110.10             | 122.08          | 1                  |
| N-CA-C-CA-CB      | 110.10             | 122.08          | 1                  |
| CA-CB-C-N-CA      | 121.70             | 110.35          | 1                  |
| C-CA-CB           | 110.10             | 122.08          | 1                  |
| N-CA-CB           | 110.50             | 121.22          | 1                  |
| C-CA-CB           | 110.10             | 98.12           | 1                  |
| CA-CB-CG          | 112.60             | 106.30          | 1                  |
| CA-N-CD           | 112.00             | 103.17          | 1                  |

| Angle type                   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB                 | 110.50             | 121.22          | 1                  |
| C-N-CD                       | 125.00             | 99.16           | 1                  |
| CA-C-N                       | 116.20             | 128.81          | 1                  |
| N-CA-CA-C-CA-CB-CG           | 113.80             | 107.50          | 1                  |
| C-CA-CB                      | 110.10             | 122.07          | 2                  |
| C-CA-C-CA-CB                 | 110.10             | 98.13           | 1                  |
| CA-CB-N-CA-N-CA-C-CA-C-CA-CB | 110.10             | 122.07          | 1                  |
| N-CA-N-CA-CB                 | 110.50             | 121.21          | 1                  |
| C-CA-C-CA-CB                 | 110.10             | 122.06          | 1                  |
| N-CA-C                       | 111.00             | 93.37           | 2                  |
| C-N-CD                       | 125.00             | 99.20           | 1                  |
| N-CA-C-CA-C-N-CA             | 121.70             | 133.03          | 1                  |
| C-CA-CB                      | 110.10             | 122.06          | 1                  |
| C-CA-N-CA-CB                 | 110.50             | 121.19          | 1                  |
| N-CA-CA-C-N                  | 116.20             | 103.62          | 1                  |
| CA-C-N                       | 116.20             | 103.63          | 1                  |
| N-CA-CB                      | 110.50             | 121.19          | 2                  |
| C-N-CA                       | 121.70             | 133.02          | 1                  |
| C-CA-N-CA-CB                 | 103.00             | 96.09           | 1                  |
| C-CA-C-CA-CB                 | 110.10             | 98.16           | 1                  |
| CA-C-N                       | 116.20             | 128.77          | 1                  |
| N-CA-CB                      | 110.50             | 121.18          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-CB-CG              | 113.80             | 107.52          | 3                  |
| N-CA-C                | 111.00             | 93.40           | 1                  |
| C-CA-CB               | 110.10             | 98.16           | 2                  |
| N-CA-CB               | 110.50             | 99.82           | 1                  |
| C-N-CA                | 121.70             | 133.01          | 1                  |
| N-CA-N-CA-C           | 111.00             | 93.41           | 1                  |
| C-CA-C-CA-C-CA-CA-C-O | 120.80             | 131.48          | 1                  |
| C-CA-CB               | 110.10             | 122.03          | 1                  |
| N-CA-N-CA-CB          | 110.50             | 121.17          | 1                  |
| N-CA-CA-C-C-CA-CB     | 110.10             | 98.17           | 1                  |
| CA-C-O                | 120.80             | 131.47          | 1                  |
| C-CA-CB               | 110.10             | 98.18           | 1                  |
| C-CA-C-CA-CB          | 110.10             | 98.18           | 1                  |
| CA-CB-CG              | 112.60             | 118.87          | 1                  |
| C-N-CA                | 121.70             | 110.41          | 1                  |
| CA-C-N                | 116.20             | 103.65          | 1                  |
| CA-CB-CG              | 113.80             | 107.53          | 1                  |
| CA-C-C-N-CA           | 121.70             | 110.41          | 1                  |
| N-CA-CB               | 110.50             | 99.84           | 1                  |
| CA-C-C-CA-N-CA-N-CA-C | 111.00             | 93.44           | 1                  |
| C-CA-CB               | 110.10             | 122.01          | 3                  |
| N-CA-C                | 111.00             | 93.44           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-C-CA-CB | 109.10             | 95.31           | 1                  |
| C-CA-CB           | 110.10             | 98.19           | 1                  |
| N-CA-C-N-CA       | 121.70             | 132.98          | 1                  |
| CA-CB-C-CA-CB     | 110.10             | 98.20           | 1                  |
| CA-CB-CG          | 113.80             | 107.54          | 1                  |
| N-CA-CB           | 110.50             | 99.85           | 1                  |
| C-N-CA            | 121.70             | 132.97          | 3                  |
| C-N-C-CA-CB       | 109.10             | 95.32           | 1                  |
| C-CA-CB           | 110.50             | 101.11          | 2                  |
| CA-C-N-CA-CB      | 110.50             | 99.86           | 1                  |
| N-CA-CB           | 110.50             | 121.14          | 1                  |
| C-CA-CB           | 110.10             | 98.21           | 2                  |
| C-CA-C-CA-C-CA-CB | 110.50             | 119.89          | 1                  |
| CA-C-O            | 120.80             | 131.44          | 1                  |
| N-CA-C            | 111.00             | 93.48           | 1                  |
| N-CA-CB           | 110.50             | 99.87           | 1                  |
| CA-C-O            | 120.80             | 110.17          | 2                  |
| N-CA-C-CA-CB      | 110.10             | 121.98          | 1                  |
| N-CA-C            | 111.00             | 128.50          | 2                  |
| CA-C-N-CA-C       | 111.00             | 93.50           | 1                  |
| C-N-CA            | 121.70             | 132.95          | 1                  |
| C-CA-CA-C-N       | 116.20             | 103.70          | 1                  |



| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                  | 110.10             | 98.23           | 1                  |
| C-CA-N-CA-CB             | 110.50             | 99.88           | 1                  |
| C-CA-CB                  | 110.10             | 121.97          | 1                  |
| N-CA-C-N-CA-CB-CG        | 113.80             | 107.55          | 1                  |
| C-CA-CA-CB-N-CA-N-CA-CB  | 110.50             | 121.11          | 1                  |
| CA-CB-CG                 | 113.80             | 107.56          | 1                  |
| C-N-CA                   | 121.70             | 132.93          | 3                  |
| N-CA-CB                  | 110.50             | 121.11          | 1                  |
| C-N-C-CA-CB              | 110.10             | 121.96          | 1                  |
| CA-C-N                   | 116.20             | 103.72          | 1                  |
| CA-C-C-N-CA              | 121.70             | 110.47          | 1                  |
| N-CA-C-N-N-CA-CB         | 111.50             | 122.10          | 1                  |
| C-CA-C-N-CA              | 121.70             | 110.47          | 1                  |
| CA-C-CA-CB-CG            | 114.10             | 101.63          | 1                  |
| C-CA-CB                  | 110.10             | 121.95          | 1                  |
| N-CA-C                   | 111.00             | 128.46          | 2                  |
| N-CA-N-CA-CB             | 103.00             | 96.14           | 1                  |
| C-CA-CB                  | 110.10             | 121.94          | 1                  |
| N-CA-CB                  | 110.50             | 99.91           | 3                  |
| N-CA-C                   | 111.00             | 93.55           | 1                  |
| CA-C-CA-CB-CA-CB-C-CA-CB | 110.10             | 98.27           | 1                  |
| C-CA-CB                  | 110.10             | 121.93          | 2                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 98.27           | 1                  |
| CA-C-N-CA-CB      | 110.50             | 99.91           | 1                  |
| C-N-CA            | 121.70             | 132.91          | 1                  |
| N-CA-CA-CB-CG     | 113.80             | 107.57          | 1                  |
| C-N-CA            | 121.70             | 110.49          | 1                  |
| C-N-CA            | 121.70             | 110.50          | 1                  |
| CA-CB-CA-CB-CG    | 113.80             | 107.58          | 1                  |
| N-CA-C            | 111.00             | 93.58           | 1                  |
| CA-C-N-CA-C       | 111.00             | 93.58           | 1                  |
| N-CA-N-CA-CB      | 111.50             | 122.07          | 1                  |
| CA-C-C-N-CA       | 121.70             | 132.89          | 1                  |
| N-CA-N-CA-N-CA-CB | 110.50             | 99.93           | 1                  |
| N-CA-C            | 111.00             | 93.59           | 1                  |
| N-CA-CB           | 110.50             | 99.93           | 1                  |
| CA-CB-CG          | 113.80             | 107.59          | 2                  |
| CA-CB-CG          | 114.10             | 101.67          | 1                  |
| C-CA-CB           | 111.60             | 124.03          | 1                  |
| CG-CD-NE2         | 116.40             | 125.72          | 1                  |
| CA-CB-N-CA-CB     | 110.50             | 99.94           | 1                  |
| CA-CB-C-N-CA      | 121.70             | 110.52          | 1                  |
| C-N-CA            | 121.70             | 132.88          | 1                  |
| N-CA-CA-CB-CG     | 113.80             | 107.59          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                | 112.60             | 106.39          | 1                  |
| C-N-N-CA-CB             | 110.50             | 121.06          | 1                  |
| C-CA-N-CA-CB            | 110.50             | 121.05          | 1                  |
| CA-C-N                  | 116.20             | 128.61          | 1                  |
| CG-CD-NE2               | 116.40             | 125.71          | 1                  |
| N-CA-C                  | 111.00             | 128.38          | 1                  |
| O-C-N                   | 123.00             | 132.93          | 1                  |
| C-CA-CA-C-O             | 120.80             | 110.25          | 1                  |
| CA-CB-N-CA-C            | 111.00             | 128.37          | 1                  |
| C-CA-CB                 | 111.60             | 124.00          | 1                  |
| CA-CB-CG                | 113.80             | 107.60          | 1                  |
| N-CA-CB                 | 110.50             | 121.04          | 1                  |
| N-CA-C-CA-CA-C-O        | 120.80             | 110.26          | 1                  |
| N-CA-CB                 | 111.50             | 100.96          | 1                  |
| CA-C-N                  | 116.20             | 103.80          | 1                  |
| CA-C-CA-C-C-CA-CA-CB-CG | 113.80             | 107.60          | 1                  |
| C-N-CA                  | 121.70             | 110.55          | 1                  |
| CA-CB-N-CA-CB           | 111.50             | 122.03          | 1                  |
| C-CA-CA-CB-CG           | 113.80             | 107.61          | 1                  |
| N-CA-N-CA-C             | 111.00             | 128.34          | 1                  |
| N-CA-N-CA-CB            | 110.50             | 121.02          | 1                  |
| C-CA-CB                 | 110.10             | 98.34           | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA            | 121.70             | 110.57          | 1                  |
| CA-C-N-CA-CB           | 110.50             | 99.99           | 1                  |
| N-CA-C-CA-C-CA-C-N-CA  | 121.70             | 110.57          | 1                  |
| N-CA-C-N-CA            | 121.70             | 110.58          | 1                  |
| C-CA-C-N-N-CA-C        | 111.00             | 93.70           | 1                  |
| CA-N-C-CA-N-CA-C       | 111.00             | 128.29          | 1                  |
| C-CA-CB                | 110.10             | 121.83          | 1                  |
| CA-C-N                 | 116.20             | 128.55          | 1                  |
| CA-C-O                 | 120.80             | 131.30          | 1                  |
| CA-CB-CG               | 113.80             | 107.63          | 2                  |
| N-CA-C                 | 111.00             | 93.72           | 1                  |
| N-CA-CB                | 110.50             | 120.99          | 1                  |
| C-CA-CB                | 110.10             | 98.37           | 1                  |
| CA-C-C-CA-CB           | 110.10             | 98.38           | 1                  |
| C-N-CA                 | 121.70             | 110.59          | 1                  |
| CA-N-N-CA-C            | 111.00             | 93.73           | 1                  |
| CA-C-N                 | 116.20             | 128.54          | 1                  |
| N-CA-CB                | 110.50             | 120.98          | 1                  |
| N-CA-C                 | 111.00             | 93.73           | 1                  |
| C-CA-C-CA-CB           | 111.60             | 123.93          | 1                  |
| CA-CB-N-CA-CB          | 110.50             | 100.02          | 1                  |
| CA-C-C-CA-C-CA-C-CA-CB | 111.60             | 123.93          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.10             | 121.81          | 1                  |
| C-CA-CB                    | 111.40             | 99.69           | 2                  |
| C-CA-C-N-CA                | 121.70             | 132.79          | 1                  |
| N-CA-C-CA-N-CA-C           | 111.00             | 93.76           | 1                  |
| N-CA-N-CA-C-CA-CB          | 111.40             | 123.10          | 1                  |
| N-CA-N-CA-N-CA-CB          | 110.50             | 120.97          | 1                  |
| C-N-CA                     | 121.70             | 132.78          | 1                  |
| CA-CB-CG                   | 112.60             | 106.44          | 1                  |
| CA-C-N                     | 116.20             | 103.89          | 2                  |
| N-CA-C-N-CA                | 121.70             | 110.63          | 2                  |
| C-CA-CB                    | 111.40             | 99.71           | 1                  |
| C-CA-C-CA-CA-C-CA-C-N      | 116.20             | 103.90          | 1                  |
| N-CA-CB                    | 110.50             | 120.95          | 1                  |
| N-CA-C                     | 111.00             | 93.78           | 1                  |
| N-CA-C-CA-CB               | 111.40             | 99.72           | 1                  |
| CA-CB-CG                   | 113.80             | 107.65          | 1                  |
| CA-C-O                     | 120.80             | 110.35          | 1                  |
| CA-C-N-CA-CB               | 111.50             | 121.95          | 1                  |
| N-CA-CA-N-CD               | 112.00             | 103.40          | 1                  |
| N-CA-C-N-C-CA-N-CA-C-CA-CB | 110.10             | 98.43           | 1                  |
| N-CA-CA-CB-CG              | 113.80             | 107.66          | 1                  |
| CA-C-N                     | 116.20             | 103.92          | 1                  |

| Angle type                        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-O                       | 120.80             | 131.24          | 1                  |
| C-N-CA                            | 121.70             | 132.75          | 1                  |
| C-CA-CA-C-N                       | 116.20             | 128.48          | 1                  |
| CA-CB-CG                          | 112.60             | 106.46          | 1                  |
| C-CA-CB                           | 110.10             | 121.76          | 1                  |
| N-CA-CB                           | 110.50             | 100.07          | 1                  |
| C-N-CA                            | 121.70             | 110.66          | 1                  |
| N-CA-C                            | 111.00             | 93.82           | 1                  |
| C-CA-CB                           | 110.50             | 119.70          | 1                  |
| N-CA-CB                           | 111.50             | 121.93          | 1                  |
| N-CA-CA-C-C-CA-CB                 | 110.10             | 121.75          | 1                  |
| N-CA-C                            | 111.00             | 128.17          | 1                  |
| C-CA-CB                           | 111.40             | 123.05          | 1                  |
| N-CA-CA-C-C-CA-CA-C-C-CA-CD-NE-CZ | 124.40             | 132.98          | 1                  |
| CA-C-N                            | 116.20             | 103.95          | 2                  |
| C-N-CA                            | 121.70             | 110.67          | 2                  |
| N-CA-CB                           | 110.50             | 120.91          | 1                  |
| CA-C-CA-C-O                       | 120.80             | 131.21          | 1                  |
| C-CA-N-CA-CB                      | 111.50             | 121.91          | 1                  |
| CA-C-N                            | 116.20             | 128.44          | 1                  |
| C-CA-CB                           | 110.10             | 121.73          | 1                  |
| CA-CB-N-CA-CA-C-CA-C-C-CA-C-CA-CB | 110.10             | 98.48           | 1                  |

| Angle type                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                       | 110.40             | 101.23          | 1                  |
| C-CA-CB                       | 110.10             | 121.72          | 1                  |
| N-CA-CB                       | 111.50             | 121.89          | 1                  |
| N-CA-C                        | 111.00             | 93.88           | 1                  |
| CA-N-CD                       | 112.00             | 103.44          | 1                  |
| N-CA-N-CA-C                   | 111.00             | 93.89           | 1                  |
| CA-C-C-N-CA                   | 121.70             | 110.70          | 1                  |
| N-CA-N-CA-C-N-CA              | 121.70             | 110.70          | 1                  |
| N-CA-C-N-CA                   | 121.70             | 110.71          | 1                  |
| C-CA-CB                       | 110.10             | 121.70          | 1                  |
| OD1-CG-ND2                    | 122.60             | 116.49          | 1                  |
| CA-C-N                        | 116.20             | 128.41          | 1                  |
| N-CA-CA-C-N                   | 116.20             | 103.99          | 1                  |
| CA-C-O                        | 120.80             | 131.18          | 2                  |
| CA-C-O                        | 120.80             | 110.42          | 1                  |
| N-CA-C                        | 111.00             | 128.09          | 1                  |
| C-CA-C-CA-C-N-C-CA-C-N-CA-C-N | 116.20             | 128.40          | 1                  |
| N-CA-CB                       | 110.50             | 100.13          | 1                  |
| N-CA-C                        | 112.10             | 96.85           | 1                  |
| CA-C-O                        | 120.80             | 110.43          | 1                  |
| N-CA-C                        | 111.00             | 128.08          | 1                  |
| CA-C-CA-CB-CG                 | 113.80             | 107.70          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                     | 110.10             | 98.51           | 1                  |
| C-N-CA                      | 121.70             | 110.72          | 1                  |
| C-CA-N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 98.52           | 1                  |
| N-CA-C                      | 111.00             | 128.07          | 1                  |
| C-CA-CB                     | 110.10             | 98.52           | 1                  |
| CA-C-N-CA-CB                | 110.40             | 101.26          | 1                  |
| N-CA-CB                     | 110.50             | 120.86          | 1                  |
| O-C-N                       | 123.00             | 132.75          | 1                  |
| C-CA-CB                     | 110.10             | 121.68          | 1                  |
| CA-C-O                      | 120.80             | 131.16          | 1                  |
| OD1-CG-N-CA-C               | 111.00             | 128.06          | 1                  |
| C-N-CA                      | 121.70             | 132.66          | 1                  |
| N-CA-CB                     | 110.50             | 100.14          | 1                  |
| CA-C-N                      | 116.20             | 128.38          | 1                  |
| C-CA-CB                     | 110.10             | 121.67          | 1                  |
| N-CA-C                      | 111.00             | 93.95           | 1                  |
| C-CA-CB                     | 110.10             | 98.53           | 1                  |
| OD1-CG-ND2                  | 122.60             | 116.51          | 1                  |
| CA-C-C-CA-CB                | 110.10             | 98.53           | 1                  |
| CA-C-N                      | 116.20             | 128.37          | 2                  |
| N-CA-C                      | 112.10             | 96.89           | 1                  |
| C-CA-CB                     | 110.10             | 98.54           | 1                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-N-CA                 | 121.70             | 110.75          | 1                  |
| N-CA-OD1-CG-ND2        | 122.60             | 116.52          | 1                  |
| CA-C-N-CA-N-CA-C-CA-CB | 110.10             | 121.65          | 1                  |
| CA-C-N-CA-CA-C-N-CA-C  | 111.00             | 128.02          | 1                  |
| C-CA-CB                | 110.10             | 121.65          | 2                  |
| N-CA-N-CA-C-CA-CA-C-N  | 116.20             | 128.35          | 1                  |
| CA-C-N                 | 116.20             | 128.35          | 1                  |
| C-CA-CB                | 109.10             | 95.73           | 1                  |
| C-CA-CB                | 110.10             | 98.56           | 1                  |
| C-CA-CB                | 110.10             | 121.64          | 2                  |
| N-CA-N-CA-CB           | 110.50             | 100.18          | 1                  |
| CA-C-CA-C-O            | 120.80             | 131.12          | 1                  |
| N-CA-CB                | 110.50             | 100.18          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 98.57           | 1                  |
| N-CA-CA-C-O            | 120.80             | 110.48          | 1                  |
| CA-CB-CA-C-N           | 116.20             | 104.07          | 1                  |
| C-CA-CB                | 110.10             | 121.63          | 1                  |
| N-CA-C                 | 111.00             | 94.01           | 1                  |
| N-CA-CB                | 110.50             | 100.19          | 1                  |
| CA-C-O                 | 120.80             | 110.49          | 1                  |
| C-N-CA-C-C-N-N-CA-CB   | 110.50             | 100.19          | 1                  |
| C-CA-CB                | 110.10             | 121.62          | 1                  |

| Angle type                             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-N-CA                                 | 121.70             | 132.61          | 1                  |
| C-CA-CB                                | 110.10             | 121.61          | 2                  |
| N-CA-C                                 | 111.00             | 94.03           | 1                  |
| C-CA-CB                                | 110.50             | 101.41          | 1                  |
| CA-C-O                                 | 120.80             | 110.50          | 1                  |
| N-CA-CA-C-C-CA-CB                      | 110.10             | 121.61          | 1                  |
| C-CA-C-CA-C-CA-C-N-CA                  | 121.70             | 110.80          | 1                  |
| OD1-CG-ND2                             | 122.60             | 116.54          | 1                  |
| C-CA-N-CA-C                            | 111.00             | 94.05           | 1                  |
| N-CA-C-CA-CB                           | 110.10             | 98.60           | 1                  |
| CA-CB-N-CA-CA-C-N-CA-C-CA-N-CA-C-CA-CB | 110.10             | 98.60           | 1                  |
| N-CA-C                                 | 111.00             | 94.06           | 1                  |
| C-CA-CB                                | 110.10             | 98.60           | 1                  |
| C-CA-CB                                | 110.10             | 121.59          | 1                  |
| N-CA-CB                                | 110.50             | 100.22          | 1                  |
| C-CA-C-CA-CA-C-C-CA-C-CA-N-CA-C-CA-CB  | 110.10             | 121.59          | 1                  |
| CA-C-N                                 | 116.20             | 128.29          | 1                  |
| C-CA-CB                                | 109.10             | 95.80           | 1                  |
| C-CA-C-CA-CB                           | 110.10             | 121.59          | 1                  |
| C-N-N-CA-CA-C-O                        | 120.80             | 110.53          | 1                  |
| C-CA-CB                                | 110.10             | 121.58          | 3                  |
| N-CA-N-CA-C                            | 111.00             | 94.08           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 98.62           | 1                  |
| CA-C-N-CA-C           | 111.00             | 94.09           | 1                  |
| C-CA-C-CA-CB          | 110.50             | 101.44          | 1                  |
| C-CA-CB               | 110.50             | 101.44          | 1                  |
| N-CA-CB               | 110.50             | 120.76          | 2                  |
| C-CA-CA-CB-CG         | 113.80             | 107.76          | 1                  |
| C-N-CA                | 121.70             | 110.84          | 1                  |
| CA-CB-CG              | 113.80             | 107.77          | 1                  |
| CA-C-N                | 116.20             | 104.13          | 1                  |
| C-CA-CB               | 110.10             | 121.56          | 1                  |
| N-CA-CA-C-N           | 116.20             | 104.14          | 1                  |
| C-CA-CA-C-O           | 120.80             | 131.05          | 1                  |
| CA-C-N                | 116.20             | 128.26          | 1                  |
| C-CA-CA-C-N           | 116.90             | 125.94          | 1                  |
| C-CA-CB               | 110.10             | 121.55          | 1                  |
| CD-NE-CZ              | 124.40             | 132.84          | 1                  |
| C-CA-CB               | 110.10             | 98.65           | 1                  |
| N-CA-CB               | 110.50             | 100.26          | 1                  |
| C-CA-CB               | 110.10             | 121.54          | 2                  |
| N-CA-C                | 111.00             | 94.13           | 1                  |
| C-N-CA                | 121.70             | 132.54          | 1                  |
| C-CA-C-CA-CA-C-CA-C-N | 116.20             | 128.24          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-C-CA-C-CA-CB     | 110.50             | 101.48          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 98.67           | 1                  |
| C-CA-C-CA-CB               | 111.60             | 99.57           | 1                  |
| C-CA-C-N-CA                | 121.70             | 132.53          | 1                  |
| CA-C-CA-C-CA-CB-CG         | 112.60             | 106.59          | 1                  |
| N-CA-CA-C-N                | 116.20             | 128.23          | 1                  |
| N-CA-N-CA-C-CA-CB          | 110.10             | 121.52          | 1                  |
| C-CA-CB                    | 111.40             | 122.82          | 1                  |
| CA-C-O                     | 120.80             | 131.02          | 2                  |
| N-CA-C                     | 111.00             | 127.83          | 1                  |
| C-CA-CB                    | 110.10             | 121.52          | 1                  |
| N-CA-CA-C-N-CA-C-CA-CB     | 110.10             | 121.51          | 1                  |
| C-N-CA                     | 121.70             | 132.51          | 1                  |
| CA-C-O                     | 120.80             | 131.00          | 1                  |
| C-CA-CA-C-C-CA-C-CA-C-N-CA | 121.70             | 132.50          | 1                  |
| N-CA-CB                    | 110.50             | 100.30          | 1                  |
| C-CA-CA-C-O                | 120.80             | 110.60          | 1                  |
| C-CA-CB                    | 110.10             | 121.50          | 1                  |
| C-CA-C-N-CA                | 121.70             | 132.50          | 1                  |
| OD1-CG-C-CA-CB             | 110.10             | 121.49          | 1                  |
| CA-CB-C-CA-C-CA-CB         | 110.10             | 121.49          | 1                  |
| C-CA-CB                    | 110.10             | 121.49          | 2                  |

| Angle type                                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| CA-C-N  | 116.20             | 104.21          | 1                  |
| C-CA-C-CA-CB                                    | 110.10             | 98.72           | 1                  |
| C-N-CA  | 121.70             | 110.92          | 1                  |
| N-CA-CB   | 110.50             | 120.68          | 1                  |
| CA-C-C-CA-CA-C-N-CA-CA-C-C-CA-C-CA-CA-C-C-CA-CB | 110.10             | 98.73           | 1                  |
| CA-C-N-CA-C-CA-CB                               | 110.10             | 121.47          | 1                  |
| N-CA-C  | 111.00             | 127.75          | 1                  |
| N-CA-C  | 111.00             | 94.25           | 1                  |
| C-CA-CA-C-CA-C-O                                | 120.80             | 130.97          | 1                  |
| C-CA-C-N-CA                                     | 121.70             | 132.46          | 1                  |
| C-CA-CB   | 110.10             | 98.74           | 1                  |
| N-CA-C  | 112.10             | 127.05          | 1                  |
| C-N-CA  | 121.70             | 132.46          | 2                  |
| CA-C-O  | 120.80             | 110.64          | 1                  |
| N-CA-C-CA-CB                                    | 111.40             | 122.75          | 1                  |
| N-CA-CB   | 110.50             | 120.66          | 1                  |
| C-CA-CB   | 111.40             | 122.75          | 1                  |
| C-CA-C-CA-CB                                    | 110.10             | 121.45          | 1                  |
| C-N-CA  | 121.70             | 132.45          | 1                  |
| CA-CB-C-CA-CB                                   | 110.10             | 98.76           | 1                  |
| N-CA-CB   | 110.50             | 100.35          | 1                  |
| CA-CB-CG  | 112.60             | 106.63          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-C                      | 111.00             | 127.71          | 1                  |
| C-N-CA                      | 121.70             | 132.44          | 1                  |
| CA-C-N                      | 116.20             | 104.27          | 1                  |
| CA-C-C-N-CA                 | 121.70             | 110.96          | 1                  |
| CA-CB-CA-C-C-N-CA           | 121.70             | 132.44          | 1                  |
| C-CA-C-CA-C-CA-N-CA-C       | 111.00             | 94.30           | 1                  |
| CA-C-C-CA-N-CA-N-CA-N-CA-CB | 110.50             | 120.63          | 1                  |
| N-CA-C                      | 111.00             | 94.33           | 2                  |
| CA-C-N                      | 116.90             | 125.83          | 1                  |
| N-CA-C-N-CA                 | 121.70             | 110.99          | 1                  |
| N-CA-N-CA-C-N-CA            | 121.70             | 110.99          | 1                  |
| C-CA-CB                     | 110.50             | 119.42          | 1                  |
| C-N-CA                      | 121.70             | 132.41          | 1                  |
| C-CA-CB                     | 110.10             | 121.40          | 1                  |
| C-CA-CB                     | 111.60             | 99.71           | 1                  |
| N-CA-N-CA-C                 | 111.00             | 94.35           | 1                  |
| C-CA-CB                     | 110.50             | 101.58          | 1                  |
| CA-C-N                      | 116.20             | 128.09          | 1                  |
| N-CA-C                      | 112.10             | 126.96          | 1                  |
| C-CA-CB                     | 111.40             | 122.69          | 1                  |
| C-CA-N-CA-C-CA-CB           | 110.10             | 98.81           | 1                  |
| N-CA-N-CA-CB                | 111.50             | 101.40          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| N-CA-C                      | 111.00             | 127.63          | 1                  |
| N-CA-CB                     | 111.50             | 121.60          | 1                  |
| N-CA-CB                     | 110.50             | 120.59          | 1                  |
| CA-C-N                      | 116.20             | 104.32          | 1                  |
| C-N-N-CA-CB                 | 110.50             | 120.59          | 1                  |
| C-N-CA-C-C-CA-CB            | 110.10             | 98.82           | 1                  |
| C-CA-CB                     | 110.10             | 98.82           | 1                  |
| C-CA-N-CA-C-N-C-N-CA        | 121.70             | 111.02          | 1                  |
| N-CA-CB                     | 110.50             | 100.41          | 1                  |
| C-N-CA                      | 121.70             | 132.38          | 1                  |
| CA-C-N                      | 116.20             | 104.33          | 1                  |
| N-CA-C                      | 111.00             | 94.39           | 1                  |
| C-CA-N-CA-CB                | 111.50             | 121.58          | 1                  |
| C-CA-CB                     | 110.50             | 119.40          | 1                  |
| CA-C-N                      | 116.20             | 128.06          | 1                  |
| C-CA-C-CA-CA-C-O            | 120.80             | 130.88          | 1                  |
| CA-C-O                      | 120.80             | 130.88          | 2                  |
| N-CA-C-CA-CB                | 110.10             | 121.36          | 1                  |
| C-CA-C-CA-N-CA-N-CA-N-CA-CB | 111.50             | 121.57          | 1                  |
| CA-C-N-CA-C-N-CA            | 121.70             | 132.36          | 1                  |
| N-CA-CA-C-C-CA-N-CA-C       | 111.00             | 127.58          | 1                  |
| N-CA-CB                     | 111.50             | 121.56          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                       | 113.80             | 107.88          | 1                  |
| C-N-CA-C-CA-C-CA-C-N           | 116.20             | 104.37          | 1                  |
| C-CA-CA-C-N                    | 116.90             | 125.77          | 1                  |
| CA-C-N                         | 116.20             | 104.37          | 1                  |
| N-CA-CB                        | 110.50             | 100.45          | 1                  |
| C-CA-CB                        | 110.10             | 121.33          | 1                  |
| CA-C-N                         | 116.20             | 104.38          | 1                  |
| C-N-CA                         | 121.70             | 132.34          | 1                  |
| CA-C-CA-C-O                    | 120.80             | 130.85          | 1                  |
| N-CA-N-CA-CA-C-C-N-N-CA-CA-C-O | 120.80             | 110.75          | 1                  |
| CA-C-C-N-N-CA-CB               | 110.50             | 120.54          | 1                  |
| N-CA-CA-C-N-CA-CA-C-N-CA-CB    | 110.50             | 100.46          | 1                  |
| CA-C-O                         | 120.80             | 130.84          | 1                  |
| CA-CB-CG                       | 112.60             | 106.69          | 1                  |
| N-CA-CB                        | 110.50             | 120.54          | 1                  |
| N-CA-CA-CB-CG                  | 112.60             | 106.70          | 1                  |
| N-CA-CB                        | 110.50             | 100.47          | 1                  |
| N-CA-CB                        | 110.50             | 120.53          | 1                  |
| N-CA-N-CA-CB                   | 111.50             | 121.53          | 1                  |
| CA-C-O                         | 120.80             | 130.83          | 2                  |
| CA-CB-CG                       | 112.60             | 106.70          | 1                  |
| C-CA-CB                        | 110.10             | 98.89           | 1                  |



| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB              | 110.50             | 101.65          | 1                  |
| N-CA-N-CA-CB              | 110.50             | 100.48          | 1                  |
| N-CA-CB                   | 110.50             | 120.52          | 2                  |
| C-CA-N-CA-CB              | 111.50             | 121.52          | 1                  |
| CA-C-N-CA-C-CA-C-N-CA-C-N | 116.90             | 108.06          | 1                  |
| N-CA-CB                   | 110.50             | 100.48          | 1                  |
| N-CA-C                    | 111.00             | 94.50           | 1                  |
| CA-C-O                    | 120.80             | 130.82          | 1                  |
| CA-C-C-CA-CA-C-N          | 116.20             | 127.98          | 1                  |
| C-N-CA                    | 121.70             | 132.30          | 2                  |
| N-CA-CB                   | 110.50             | 120.51          | 1                  |
| N-CA-CB                   | 111.50             | 121.51          | 1                  |
| N-CA-C-CA-CB              | 110.10             | 98.92           | 1                  |
| CA-C-CA-C-N-CA-CB         | 110.50             | 100.50          | 1                  |
| CA-CB-CG                  | 113.80             | 107.92          | 1                  |
| C-N-CA-C-O                | 120.80             | 110.80          | 1                  |
| C-CA-CA-C-N-CA-C          | 111.00             | 94.53           | 1                  |
| N-CA-CB                   | 110.50             | 120.49          | 2                  |
| CA-C-N                    | 116.20             | 127.96          | 1                  |
| CA-C-C-CA-CB              | 110.10             | 98.93           | 1                  |
| C-CA-N-CA-CB              | 110.50             | 120.49          | 1                  |
| C-CA-CB                   | 110.10             | 98.94           | 2                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-O                     | 120.80             | 130.79          | 1                  |
| N-CA-C-CA-C-N-CA           | 121.70             | 132.27          | 1                  |
| C-CA-C-CA-C-CA-CA-C-N      | 116.20             | 104.46          | 1                  |
| CA-C-CA-C-C-N-CA           | 121.70             | 132.27          | 1                  |
| N-CA-CB                    | 110.50             | 100.52          | 1                  |
| N-CA-C-N-C-CA-C-CA-N-CA-CB | 110.50             | 120.47          | 1                  |
| C-CA-CB                    | 111.60             | 99.87           | 2                  |
| C-CA-N-CA-C-N-C-N-N-CA-CB  | 110.50             | 120.47          | 1                  |
| N-CA-CB                    | 111.50             | 121.47          | 1                  |
| CA-C-N                     | 116.20             | 127.93          | 1                  |
| N-CA-CA-C-CA-C-N           | 116.20             | 104.47          | 1                  |
| CA-C-O                     | 120.80             | 130.77          | 1                  |
| N-CA-N-CA-C                | 111.00             | 94.59           | 1                  |
| C-CA-C-CA-CB               | 110.10             | 98.97           | 1                  |
| C-CA-CB                    | 110.10             | 98.97           | 1                  |
| CA-C-N                     | 116.20             | 104.48          | 1                  |
| CA-C-O                     | 120.80             | 130.76          | 2                  |
| N-CA-C-N-CA                | 121.70             | 132.24          | 2                  |
| CA-CB-CG                   | 113.80             | 119.66          | 1                  |
| CA-CB-CG                   | 113.80             | 107.94          | 1                  |
| N-CA-CB                    | 110.50             | 120.46          | 1                  |
| C-CA-CA-C-N-CA-CB          | 110.50             | 100.55          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB            | 110.50             | 100.55          | 1                  |
| CA-CB-N-CA-C-CA-C-CA-CB | 110.10             | 98.98           | 1                  |
| C-CA-N-CA-CB            | 110.50             | 120.45          | 1                  |
| C-CA-N-CA-CB            | 110.50             | 100.55          | 1                  |
| C-CA-CB                 | 110.10             | 98.98           | 1                  |
| N-CA-CA-C-N             | 116.20             | 104.50          | 1                  |
| C-CA-N-CA-C-CA-CB       | 110.10             | 98.98           | 1                  |
| C-N-CA                  | 121.70             | 132.23          | 1                  |
| CA-C-N-CA-C             | 111.00             | 127.38          | 1                  |
| N-CA-N-CA-C             | 111.00             | 127.38          | 1                  |
| CA-C-N                  | 116.20             | 127.90          | 1                  |
| CA-C-N-CA-C             | 111.00             | 94.63           | 1                  |
| CA-C-N                  | 116.20             | 127.89          | 1                  |
| N-CA-CB                 | 110.50             | 120.44          | 1                  |
| C-N-CA                  | 121.70             | 132.22          | 1                  |
| C-CA-C-N-CA             | 121.70             | 132.22          | 1                  |
| C-CA-C-CA-CA-C-CA-C-O   | 120.80             | 130.73          | 1                  |
| CA-CB-CG                | 113.80             | 119.64          | 1                  |
| C-CA-N-CA-N-CA-N-CA-CB  | 110.50             | 100.57          | 1                  |
| CA-C-N                  | 116.90             | 108.14          | 2                  |
| N-CA-C                  | 111.00             | 94.65           | 1                  |
| C-CA-CB                 | 110.10             | 99.00           | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-C-CA-CA-CB-CG | 112.60             | 106.76          | 1                  |
| N-CA-CB                 | 110.50             | 120.42          | 1                  |
| C-CA-C-CA-N-CA-C-CA-CB  | 110.10             | 99.01           | 1                  |
| C-CA-CB                 | 109.10             | 96.26           | 1                  |
| N-CD-CG                 | 103.20             | 94.45           | 1                  |
| CA-C-C-N-CA             | 121.70             | 132.20          | 1                  |
| CA-CB-CG                | 113.80             | 119.63          | 1                  |
| CA-C-C-CA-CB            | 109.10             | 121.93          | 1                  |
| CA-CB-CG                | 113.80             | 107.97          | 1                  |
| C-CA-C-N-C-CA-CB        | 110.10             | 99.02           | 1                  |
| CA-C-O                  | 120.80             | 110.89          | 1                  |
| N-CA-CB                 | 103.00             | 109.41          | 1                  |
| N-CA-CB                 | 110.50             | 100.59          | 2                  |
| C-CA-CB                 | 109.10             | 96.28           | 1                  |
| N-CA-CB                 | 110.50             | 120.41          | 1                  |
| N-CA-C                  | 111.00             | 94.68           | 2                  |
| C-CA-CB                 | 110.10             | 99.03           | 2                  |
| CA-CB-CG                | 112.60             | 106.77          | 1                  |
| N-CA-CB                 | 111.50             | 121.41          | 1                  |
| C-N-N-CA-C              | 111.00             | 94.69           | 1                  |
| C-CA-N-CA-CB            | 110.40             | 119.14          | 1                  |
| CA-C-C-CA-N-CA-CB       | 110.50             | 120.40          | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                  | 110.10             | 121.17          | 1                  |
| C-CA-CB                  | 109.10             | 121.91          | 1                  |
| C-CA-C-N-CA              | 121.70             | 132.18          | 1                  |
| C-CA-CB                  | 110.50             | 119.23          | 1                  |
| OD1-CG-ND2               | 122.60             | 116.78          | 1                  |
| C-CA-C-CA-C-N-C-N-C-N-CA | 121.70             | 132.17          | 1                  |
| CA-C-O                   | 120.80             | 130.69          | 1                  |
| CA-CB-CA-CB-CG           | 112.60             | 106.78          | 1                  |
| N-CA-N-CA-CB             | 111.50             | 121.39          | 1                  |
| C-CA-C-CA-C-CA-C-N-CA    | 121.70             | 132.17          | 1                  |
| N-CA-C-N-CA              | 121.70             | 132.17          | 1                  |
| N-CA-C                   | 111.00             | 94.72           | 1                  |
| C-CA-C-CA-CB             | 110.10             | 99.05           | 1                  |
| C-CA-CB                  | 110.10             | 99.05           | 1                  |
| C-CA-N-CA-CA-C-C-CA-CB   | 110.10             | 121.14          | 1                  |
| C-CA-CB                  | 110.10             | 121.14          | 1                  |
| C-N-CA                   | 121.70             | 111.24          | 1                  |
| CA-C-O                   | 120.80             | 110.92          | 1                  |
| CA-C-C-CA-CA-CB-CG       | 113.80             | 107.99          | 1                  |
| C-CA-CB                  | 110.10             | 99.06           | 1                  |
| C-CA-CA-CB-CG            | 113.80             | 119.61          | 1                  |
| N-CA-C                   | 111.00             | 94.74           | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| C-N-CA-CB-CG                    | 112.60             | 106.79          | 1                  |
| N-CA-C-CA-CB                    | 109.10             | 121.88          | 1                  |
| N-CA-CB                         | 111.50             | 121.37          | 1                  |
| CA-C-C-CA-C-CA-C-CA-N-CA-CA-C-N | 116.90             | 108.19          | 1                  |
| C-N-C-N-N-CA-C                  | 112.10             | 97.59           | 1                  |
| C-CA-CB                         | 110.10             | 121.13          | 1                  |
| CA-CB-CG                        | 112.60             | 106.80          | 1                  |
| CA-C-O                          | 120.80             | 130.66          | 1                  |
| C-N-CA                          | 121.70             | 111.26          | 1                  |
| C-CA-C-N-CA-C-O                 | 120.80             | 110.94          | 1                  |
| N-CA-CB                         | 111.50             | 121.36          | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 99.08           | 1                  |
| N-CA-C-N-CA                     | 121.70             | 132.14          | 1                  |
| C-N-CA                          | 121.70             | 132.14          | 2                  |
| CA-N-CD                         | 112.00             | 103.88          | 1                  |
| C-CA-N-CA-CA-C-O                | 120.80             | 130.65          | 1                  |
| CA-C-O                          | 120.80             | 110.95          | 1                  |
| CA-N-CD                         | 112.00             | 103.89          | 1                  |
| N-CA-C                          | 112.10             | 97.62           | 1                  |
| C-N-CA                          | 121.70             | 132.13          | 1                  |
| C-CA-CB                         | 109.10             | 121.85          | 1                  |
| C-CA-CB                         | 110.10             | 99.09           | 3                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 111.00             | 94.78           | 1                  |
| N-CA-CB               | 110.50             | 120.35          | 1                  |
| C-CA-CB               | 109.10             | 96.36           | 1                  |
| C-CA-C-CA-CB          | 109.10             | 121.84          | 1                  |
| C-CA-CB               | 110.10             | 99.10           | 1                  |
| CA-CB-N-CA-C-CA-CB    | 110.10             | 99.10           | 1                  |
| CA-C-CA-C-O           | 120.80             | 130.64          | 1                  |
| N-CA-CB               | 111.50             | 101.66          | 1                  |
| CA-C-N                | 116.20             | 127.78          | 1                  |
| CA-C-C-N-CA           | 121.70             | 111.28          | 1                  |
| CA-C-O                | 120.80             | 110.96          | 1                  |
| CA-CB-CG              | 113.80             | 119.59          | 1                  |
| C-CA-CB               | 111.60             | 123.17          | 1                  |
| CA-CB-CG              | 113.80             | 108.01          | 1                  |
| C-CA-CB               | 111.60             | 100.03          | 2                  |
| CA-C-N                | 116.20             | 104.63          | 2                  |
| CA-C-O                | 120.80             | 130.63          | 2                  |
| CA-C-C-CA-CB          | 109.10             | 96.37           | 1                  |
| C-N-N-CA-N-CA-C-CA-CB | 111.60             | 100.03          | 1                  |
| CA-CB-C-CA-CB         | 110.10             | 99.11           | 1                  |
| N-CA-CA-CB-CG         | 112.60             | 106.82          | 1                  |
| C-CA-CB               | 109.10             | 96.38           | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| C-CA-CB          | 110.10             | 121.08          | 1                  |
| C-CA-C-CA-CA-C-O | 120.80             | 110.97          | 1                  |
| C-N-CA           | 121.70             | 111.29          | 1                  |
| C-N-C-CA-CB      | 110.50             | 119.17          | 1                  |
| N-CA-C-CA-CB     | 109.10             | 96.38           | 1                  |
| C-CA-C-CA-CB     | 110.10             | 99.12           | 1                  |
| C-N-C-CA-CB      | 109.10             | 121.81          | 1                  |
| N-CA-CA-CB-CG    | 113.80             | 119.58          | 1                  |
| C-CA-C-CA-CB     | 110.10             | 121.07          | 1                  |
| N-CA-C           | 111.00             | 94.83           | 1                  |
| N-CA-CA-CB-CG    | 113.80             | 108.03          | 1                  |
| CA-C-CA-C-O      | 120.80             | 130.62          | 1                  |
| N-CA-CB          | 110.50             | 100.69          | 1                  |
| C-CA-CB          | 110.10             | 121.07          | 1                  |
| N-CA-CB          | 110.50             | 120.31          | 1                  |
| C-CA-CB          | 110.10             | 99.13           | 1                  |
| C-CA-CA-CB-CG    | 113.80             | 119.57          | 1                  |
| C-CA-CB          | 111.60             | 123.14          | 1                  |
| CA-C-O           | 120.80             | 110.99          | 1                  |
| C-N-CA           | 121.70             | 111.31          | 1                  |
| C-N-C-CA-CA-C-N  | 116.20             | 104.66          | 1                  |
| C-CA-CA-C-N      | 116.20             | 104.66          | 1                  |



| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 121.06          | 1                  |
| CA-C-N                | 116.20             | 127.74          | 2                  |
| OD1-CG-C-CA-CB        | 110.10             | 99.14           | 1                  |
| N-CA-CB               | 111.50             | 101.69          | 1                  |
| N-CA-C                | 111.00             | 94.85           | 1                  |
| N-CA-C-N-N-CA-C-CA-CB | 111.60             | 100.06          | 1                  |
| N-CA-C                | 111.00             | 127.15          | 1                  |
| C-CA-N-CA-C-CA-CB     | 110.10             | 121.06          | 1                  |
| CA-C-O                | 120.80             | 111.00          | 2                  |
| C-CA-CB               | 111.40             | 122.36          | 1                  |
| N-CA-CB               | 110.50             | 100.70          | 1                  |
| N-CA-N-CA-C-CA-CB     | 110.10             | 99.15           | 1                  |
| N-CA-C                | 111.00             | 94.86           | 2                  |
| C-CA-CB               | 111.40             | 122.35          | 1                  |
| C-N-N-CA-C            | 111.00             | 94.87           | 1                  |
| CA-C-N                | 116.20             | 127.72          | 1                  |
| CA-CB-CG              | 112.60             | 106.84          | 1                  |
| N-CA-C                | 111.00             | 94.87           | 1                  |
| N-CA-C                | 111.00             | 94.88           | 2                  |
| CA-CB-CG              | 113.80             | 119.56          | 1                  |
| C-CA-CB               | 110.10             | 99.16           | 1                  |
| C-N-CA                | 121.70             | 111.34          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-CB-CA-CB-CA-C-O | 120.80             | 130.58          | 1                  |
| N-CA-C-CA-CB            | 110.10             | 99.16           | 1                  |
| N-CA-C-N-N-CD-CG        | 103.20             | 94.57           | 1                  |
| C-CA-CB                 | 110.10             | 99.17           | 1                  |
| N-CA-C                  | 111.00             | 94.89           | 1                  |
| C-CA-CB                 | 110.10             | 121.03          | 1                  |
| N-CA-C-CA-CB            | 110.50             | 119.13          | 1                  |
| N-CA-CB                 | 111.50             | 121.28          | 1                  |
| CA-C-N                  | 116.20             | 104.70          | 1                  |
| OD1-CG-C-CA-CB          | 110.10             | 99.17           | 1                  |
| CA-C-CA-C-C-CA-CB       | 110.10             | 99.18           | 1                  |
| C-CA-CB                 | 110.10             | 99.18           | 2                  |
| N-CA-C-CA-N-CA-C        | 111.00             | 94.91           | 1                  |
| CA-C-O                  | 120.80             | 111.03          | 1                  |
| N-CA-C                  | 111.00             | 94.91           | 1                  |
| C-N-N-CA-C              | 111.00             | 127.09          | 1                  |
| CA-C-N                  | 116.20             | 127.69          | 1                  |
| N-CA-N-CA-CB            | 110.50             | 120.27          | 1                  |
| CA-C-O                  | 120.80             | 130.57          | 1                  |
| CA-C-CA-C-N             | 116.20             | 104.71          | 1                  |
| C-N-C-CA-CB             | 110.10             | 121.01          | 1                  |
| C-CA-CA-C-CA-C-O        | 120.80             | 111.04          | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                  | 110.50             | 120.26          | 1                  |
| C-CA-CB                  | 110.10             | 99.19           | 1                  |
| C-CA-CB                  | 110.10             | 121.01          | 1                  |
| N-CA-C                   | 111.00             | 94.93           | 2                  |
| N-CA-C-N-CA              | 121.70             | 132.03          | 1                  |
| CA-CB-CG                 | 113.80             | 108.06          | 1                  |
| C-CA-CB                  | 110.10             | 121.00          | 3                  |
| C-N-CA                   | 121.70             | 132.03          | 1                  |
| N-CA-CB                  | 110.50             | 120.25          | 2                  |
| C-CA-C-CA-CB             | 110.10             | 121.00          | 1                  |
| CA-CB-CG                 | 112.60             | 106.86          | 2                  |
| CA-C-N                   | 116.20             | 127.67          | 1                  |
| CA-C-O                   | 120.80             | 130.55          | 1                  |
| C-CA-CB                  | 111.60             | 100.13          | 1                  |
| N-CA-C-CA-CB             | 110.10             | 99.21           | 1                  |
| C-CA-CB                  | 110.10             | 120.99          | 1                  |
| C-N-CA                   | 121.70             | 132.02          | 1                  |
| N-CA-CB                  | 110.50             | 120.24          | 1                  |
| CA-CB-C-N-CA             | 121.70             | 111.39          | 1                  |
| C-CA-CB                  | 110.10             | 99.21           | 1                  |
| C-CA-CA-C-C-N-C-N-CA-C-O | 120.80             | 111.07          | 1                  |
| C-N-CA                   | 121.70             | 132.01          | 1                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-C                               | 111.00             | 127.03          | 1                  |
| CA-C-O                               | 120.80             | 130.53          | 1                  |
| N-CA-CA-CB-C-N-CA                    | 121.70             | 132.00          | 1                  |
| C-CA-C-N-CA-C-O                      | 120.80             | 111.07          | 1                  |
| CA-C-CA-C-O                          | 120.80             | 130.53          | 1                  |
| C-CA-CB                              | 110.10             | 120.97          | 1                  |
| C-CA-CB                              | 110.10             | 99.23           | 3                  |
| N-CA-CB                              | 110.50             | 120.23          | 1                  |
| N-CA-C                               | 111.00             | 94.98           | 1                  |
| C-N-N-CA-C                           | 111.00             | 94.98           | 1                  |
| CA-CB-N-CA-C                         | 111.00             | 127.02          | 1                  |
| N-CA-C-N-CA                          | 121.70             | 132.00          | 1                  |
| C-CA-C-CA-C-CA-CA-C-C-N-N-CA-C-CA-CB | 110.10             | 99.23           | 1                  |
| CA-CB-CG                             | 112.60             | 106.88          | 1                  |
| C-CA-CA-CB-CA-C-N-CA-C               | 111.00             | 127.01          | 1                  |
| C-CA-CB                              | 110.10             | 99.24           | 1                  |
| C-CA-C-CA-C-N-CA-C-O                 | 120.80             | 130.52          | 1                  |
| N-CA-CA-C-O                          | 120.80             | 130.52          | 1                  |
| C-N-C-CA-CA-C-C-CA-CB                | 110.10             | 120.95          | 1                  |
| N-CA-CB                              | 111.50             | 121.21          | 1                  |
| N-CA-C                               | 111.00             | 127.00          | 1                  |
| C-CA-CB                              | 110.50             | 119.07          | 1                  |

| Angle type                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------|--------------------|-----------------|--------------------|
| CD-NE-CZ                      | 124.40             | 116.40          | 1                  |
| CA-CB-C-N-CA                  | 121.70             | 131.98          | 1                  |
| CA-C-C-CA-CB                  | 110.10             | 99.25           | 1                  |
| N-CA-CB                       | 110.50             | 120.21          | 1                  |
| C-CA-CB                       | 110.10             | 99.25           | 1                  |
| C-N-CA                        | 121.70             | 131.98          | 1                  |
| CA-C-O                        | 120.80             | 130.50          | 1                  |
| C-CA-CB                       | 110.10             | 120.95          | 1                  |
| N-CA-C                        | 111.00             | 126.98          | 1                  |
| C-CA-N-CA-OD1-CG-ND2          | 122.60             | 116.89          | 1                  |
| OD1-CG-CA-CB-CG               | 113.80             | 119.51          | 1                  |
| N-CA-CA-C-C-N-CA              | 121.70             | 131.97          | 1                  |
| CA-CB-CG                      | 112.60             | 106.90          | 2                  |
| N-CA-CB                       | 110.50             | 120.20          | 1                  |
| CA-C-O                        | 120.80             | 111.10          | 1                  |
| C-CA-C-CA-C-CA-CB             | 110.10             | 120.93          | 1                  |
| C-CA-C-CA-C-N-CA              | 121.70             | 131.96          | 1                  |
| C-CA-CA-C-O                   | 120.80             | 130.49          | 1                  |
| N-CA-C                        | 111.00             | 95.04           | 1                  |
| CA-CB-C-CA-CB                 | 110.10             | 99.27           | 1                  |
| C-CA-CB                       | 111.60             | 100.20          | 1                  |
| CA-CB-C-CA-N-CA-N-CA-CA-CB-CG | 112.60             | 106.90          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-C-O                | 120.80             | 111.11          | 1                  |
| C-CA-C-N-C-N-CA       | 121.70             | 131.96          | 1                  |
| CA-CB-N-CA-CB         | 110.50             | 120.18          | 1                  |
| N-CA-CB               | 110.50             | 120.18          | 1                  |
| CA-CB-CG              | 112.60             | 106.91          | 2                  |
| CA-C-O                | 120.80             | 111.12          | 1                  |
| CA-C-C-CA-C-CA-C-N-CA | 121.70             | 131.94          | 1                  |
| N-CA-C                | 111.00             | 95.07           | 3                  |
| CA-CB-CG              | 112.60             | 118.29          | 1                  |
| C-N-CA                | 121.70             | 131.94          | 1                  |
| N-CA-C                | 111.00             | 126.93          | 1                  |
| C-CA-C-CA-C-N-CA      | 121.70             | 131.94          | 1                  |
| CA-C-O                | 120.80             | 130.47          | 1                  |
| CA-CB-C-N-CA          | 121.70             | 131.94          | 1                  |
| C-CA-CB               | 110.10             | 99.30           | 1                  |
| CA-C-CA-CB-N-CA-CB    | 110.50             | 120.17          | 1                  |
| N-CA-C                | 111.00             | 95.08           | 1                  |
| C-CA-CB               | 110.10             | 120.90          | 1                  |
| CA-CB-CG              | 112.60             | 106.92          | 2                  |
| C-CA-C-N-CA-C-O       | 120.80             | 130.46          | 1                  |
| N-CA-CB               | 110.50             | 120.16          | 2                  |
| C-CA-CA-C-N           | 116.20             | 104.83          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-C            | 111.00             | 95.09           | 1                  |
| CA-C-O                 | 120.80             | 130.46          | 1                  |
| C-N-C-CA-CB            | 110.10             | 99.30           | 1                  |
| C-N-CA                 | 121.70             | 131.93          | 1                  |
| C-N-CA                 | 121.70             | 131.92          | 1                  |
| CA-C-N-CA-C            | 111.00             | 95.10           | 1                  |
| N-CA-C                 | 111.00             | 126.90          | 2                  |
| CA-C-O                 | 120.80             | 130.45          | 1                  |
| C-CA-CB                | 110.10             | 99.31           | 1                  |
| CA-CB-C-CA-C-N-CA      | 121.70             | 111.48          | 1                  |
| OD1-CG-CA-C-C-N-C-N-CA | 121.70             | 111.49          | 1                  |
| N-CA-N-CA-C            | 111.00             | 95.12           | 1                  |
| N-CA-C                 | 111.00             | 95.12           | 1                  |
| C-CA-CA-CB-CG          | 113.80             | 108.13          | 1                  |
| CD-NE-CZ               | 124.40             | 116.46          | 1                  |
| C-N-CA                 | 121.70             | 131.91          | 2                  |
| C-CA-N-CA-N-CA-CB      | 110.50             | 120.14          | 1                  |
| C-N-C-CA-CB            | 110.10             | 120.87          | 1                  |
| CA-C-O                 | 120.80             | 130.44          | 1                  |
| C-CA-CA-C-N-CA-CB      | 110.50             | 100.86          | 1                  |
| N-CA-C                 | 111.00             | 95.13           | 1                  |
| C-CA-C-CA-CB           | 110.10             | 99.33           | 2                  |

| Angle type                                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-CA-CB                                    | 110.10             | 99.33           | 1                  |
| C-CA-N-CA-C-CA-CA-C-C-CA-CB                | 111.60             | 100.27          | 1                  |
| C-CA-N-CA-C-CA-CB                          | 110.10             | 99.34           | 1                  |
| C-CA-CB                                    | 110.50             | 119.00          | 1                  |
| CA-C-N                                     | 116.20             | 127.53          | 1                  |
| C-CA-CB                                    | 110.10             | 120.86          | 1                  |
| N-CA-C-CA-N-CA-C                           | 111.00             | 95.15           | 1                  |
| CA-C-N                                     | 116.20             | 127.52          | 1                  |
| CA-CB-CG                                   | 112.60             | 106.94          | 1                  |
| NE-CZ-NH1                                  | 121.50             | 115.84          | 1                  |
| C-N-CA                                     | 121.70             | 131.89          | 1                  |
| N-CA-C-N-CA                                | 121.70             | 131.89          | 1                  |
| C-CA-C-CA-N-CA-C                           | 111.00             | 95.15           | 1                  |
| C-CA-C-N-C-CA-CB                           | 110.10             | 120.85          | 1                  |
| C-CA-CB                                    | 110.10             | 120.85          | 2                  |
| C-N-C-N-CA                                 | 121.70             | 131.89          | 1                  |
| C-CA-CB                                    | 110.10             | 99.35           | 1                  |
| CA-CB-CG                                   | 113.80             | 119.46          | 1                  |
| C-CA-C-CA-OD1-CG-C-CA-C-N-N-CA-C-N-N-CA-CB | 110.50             | 100.89          | 1                  |
| N-CA-C                                     | 111.00             | 95.17           | 1                  |
| C-CA-CA-C-O                                | 120.80             | 111.19          | 1                  |
| CA-C-C-CA-CB                               | 110.10             | 99.36           | 1                  |



| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                         | 110.50             | 100.89          | 1                  |
| N-CA-CB                         | 110.50             | 120.11          | 1                  |
| CA-C-O                          | 120.80             | 130.41          | 1                  |
| CA-C-C-N-CA-C-N-CA-CA-C-N-CA-C  | 111.00             | 126.82          | 1                  |
| C-CA-N-CA-N-CA-CB               | 110.50             | 120.11          | 1                  |
| C-CA-CA-C-CA-CB-CG              | 112.60             | 106.95          | 1                  |
| CA-CB-CG                        | 112.60             | 106.95          | 1                  |
| CA-CB-CG                        | 113.80             | 108.15          | 1                  |
| N-CA-C                          | 111.00             | 95.19           | 1                  |
| CA-C-O                          | 120.80             | 111.20          | 2                  |
| C-CA-CB                         | 109.10             | 121.52          | 1                  |
| C-CA-CB                         | 110.10             | 120.83          | 1                  |
| C-CA-CB                         | 110.10             | 120.82          | 1                  |
| N-CA-C-CA-CB                    | 110.10             | 120.82          | 1                  |
| CA-C-O                          | 120.80             | 130.39          | 1                  |
| N-CA-CB                         | 110.50             | 120.09          | 1                  |
| C-N-CA                          | 121.70             | 111.54          | 1                  |
| N-CA-C-CA-C-CA-N-CA-C-CA-N-CA-C | 111.00             | 95.21           | 1                  |
| C-CA-CB                         | 111.40             | 100.68          | 1                  |
| CA-C-C-N-CA                     | 121.70             | 111.55          | 1                  |
| C-CA-CB                         | 111.40             | 100.69          | 1                  |
| C-CA-CA-C-O                     | 120.80             | 111.21          | 1                  |

| Angle type      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-O     | 120.80             | 111.22          | 1                  |
| N-CA-CB         | 110.50             | 120.08          | 1                  |
| CA-C-CA-C-O     | 120.80             | 111.22          | 1                  |
| C-CA-CB         | 109.10             | 121.50          | 1                  |
| N-CA-C          | 111.00             | 126.78          | 1                  |
| CA-C-C-N-CA     | 121.70             | 131.84          | 1                  |
| C-N-C-CA-CA-C-O | 120.80             | 111.22          | 1                  |
| N-CA-C          | 111.00             | 126.77          | 1                  |
| C-N-CA          | 121.70             | 131.84          | 1                  |
| CA-N-CD         | 112.00             | 104.11          | 1                  |
| CA-C-CA-CB-CG   | 112.60             | 106.97          | 1                  |
| OD1-CG-C-N-CA   | 121.70             | 131.84          | 1                  |
| CA-C-CA-C-O     | 120.80             | 111.23          | 1                  |
| C-N-CA          | 121.70             | 131.83          | 1                  |
| OD1-CG-C-CA-CB  | 110.10             | 99.40           | 1                  |
| CA-CB-CG        | 113.80             | 119.43          | 1                  |
| C-N-C-CA-N-CA-C | 111.00             | 126.76          | 1                  |
| C-CA-CB         | 110.10             | 99.41           | 3                  |
| CA-C-O          | 120.80             | 111.23          | 1                  |
| N-CA-CB         | 111.50             | 101.93          | 1                  |
| N-CA-CB         | 110.50             | 120.07          | 1                  |
| C-CA-C-N-CA     | 121.70             | 111.58          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                | 110.10             | 120.79          | 2                  |
| CA-C-N                 | 116.20             | 127.45          | 1                  |
| C-CA-C-N-C-N-CA        | 121.70             | 111.58          | 1                  |
| C-CA-CB                | 110.50             | 118.93          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 101.95          | 1                  |
| CA-C-O                 | 120.80             | 130.35          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 120.78          | 1                  |
| CA-C-N                 | 116.20             | 127.44          | 1                  |
| CA-CB-CA-CB-N-CA-C     | 111.00             | 95.27           | 1                  |
| C-N-CA                 | 121.70             | 111.59          | 1                  |
| C-CA-CB                | 109.10             | 121.46          | 1                  |
| CA-CB-CG               | 112.60             | 106.98          | 1                  |
| C-CA-CB                | 110.10             | 99.43           | 1                  |
| C-CA-C-CA-C-CA-N-CA-CB | 110.50             | 120.05          | 1                  |
| C-CA-N-CA-N-CA-CB      | 110.50             | 120.05          | 1                  |
| C-N-CA                 | 121.70             | 131.80          | 1                  |
| CA-C-CB-CG1-N-CA-C     | 111.00             | 126.72          | 1                  |
| C-CA-CA-C-C-CA-CB      | 110.10             | 120.76          | 1                  |
| C-CA-N-CA-C-CA-C-CA-CB | 111.60             | 100.38          | 1                  |
| CA-C-N-CA-C            | 111.00             | 126.70          | 1                  |
| CA-C-C-CA-CB           | 109.10             | 121.44          | 1                  |
| C-CA-CB                | 110.10             | 120.75          | 2                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-N-CA                  | 121.70             | 111.61          | 2                  |
| CA-C-O                  | 120.80             | 130.33          | 1                  |
| CA-CB-CG                | 113.80             | 108.19          | 1                  |
| N-CA-CA-C-CA-C-O        | 120.80             | 111.27          | 1                  |
| CA-C-N-CA-CB            | 110.50             | 120.02          | 1                  |
| C-CA-C-N-CA             | 121.70             | 111.62          | 1                  |
| C-N-C-CA-CA-C-O         | 120.80             | 111.28          | 1                  |
| CA-C-O                  | 120.80             | 111.28          | 1                  |
| N-CA-C-CA-C-N-CA        | 121.70             | 131.78          | 1                  |
| C-N-CA                  | 121.70             | 111.62          | 1                  |
| N-CA-CB                 | 110.50             | 100.99          | 1                  |
| N-CA-C                  | 113.30             | 97.07           | 1                  |
| N-CA-C-CA-CA-C-N        | 116.20             | 105.01          | 1                  |
| N-CA-C-CA-N-CA-CA-CB-CG | 112.60             | 118.19          | 1                  |
| C-CA-N-CA-CB            | 111.50             | 101.99          | 1                  |
| C-N-CA                  | 121.70             | 111.63          | 1                  |
| C-N-CA                  | 121.70             | 131.77          | 1                  |
| C-CA-N-CA-C             | 111.00             | 126.66          | 1                  |
| CA-C-N-CA-CA-C-O        | 120.80             | 130.30          | 1                  |
| C-N-CA                  | 121.70             | 111.64          | 1                  |
| C-CA-CB                 | 110.10             | 99.48           | 1                  |
| C-CA-CB                 | 109.10             | 121.39          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| NE-CZ-NH1               | 121.50             | 115.91          | 1                  |
| C-CA-CB                 | 110.10             | 120.71          | 4                  |
| C-CA-N-CA-CB            | 111.50             | 102.00          | 1                  |
| CA-C-O                  | 120.80             | 111.31          | 1                  |
| C-CA-N-CA-C             | 111.00             | 126.64          | 1                  |
| C-CA-N-CA-CB            | 110.50             | 119.99          | 1                  |
| C-CA-C-N-CA             | 121.70             | 111.65          | 1                  |
| CB-CG1-N-CA-CB          | 110.50             | 119.99          | 1                  |
| OD1-CG-CA-C-N           | 116.20             | 127.36          | 1                  |
| C-CA-CB                 | 111.60             | 100.44          | 1                  |
| CA-C-O                  | 120.80             | 130.29          | 1                  |
| N-CA-CA-C-CA-C-CA-CB-CG | 113.80             | 108.22          | 1                  |
| N-CA-C                  | 111.00             | 95.38           | 1                  |
| CA-C-N                  | 116.20             | 105.04          | 1                  |
| N-CA-CA-C-N             | 116.20             | 127.36          | 1                  |
| N-CA-C                  | 113.30             | 97.12           | 1                  |
| CA-CB-CG                | 112.60             | 107.02          | 1                  |
| CA-C-O                  | 120.80             | 111.32          | 2                  |
| C-CA-C-CA-CB            | 110.10             | 120.70          | 1                  |
| CA-C-N-CA-C-N-CA        | 121.70             | 131.73          | 1                  |
| C-CA-CA-C-N             | 116.20             | 127.35          | 1                  |
| C-CA-CB                 | 110.50             | 118.86          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-N-CA            | 121.70             | 131.73          | 1                  |
| N-CA-C-CA-CB      | 110.10             | 120.69          | 1                  |
| N-CA-CB           | 110.50             | 119.97          | 2                  |
| N-CA-N-CA-CB      | 110.50             | 119.97          | 2                  |
| N-CA-C-CA-CB      | 110.10             | 120.68          | 1                  |
| CA-N-CD           | 112.00             | 104.20          | 1                  |
| CA-C-O            | 120.80             | 111.33          | 1                  |
| N-CA-C            | 111.00             | 95.40           | 1                  |
| C-CA-CB           | 110.10             | 120.68          | 1                  |
| CA-C-N            | 116.20             | 127.34          | 1                  |
| C-CA-CB           | 110.10             | 99.52           | 2                  |
| N-CA-C            | 111.00             | 95.41           | 1                  |
| CA-C-C-CA-CB      | 111.60             | 100.47          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 120.68          | 1                  |
| C-N-CA            | 121.70             | 131.72          | 1                  |
| N-CA-CB           | 110.50             | 119.96          | 1                  |
| C-CA-CB           | 110.10             | 120.67          | 1                  |
| C-CA-C-N-CA       | 121.70             | 111.69          | 2                  |
| N-CA-CB           | 111.50             | 102.04          | 1                  |
| CA-CB-CA-C-O      | 120.80             | 111.34          | 1                  |
| N-CA-C-CA-C-CA-CB | 110.10             | 99.53           | 1                  |
| C-N-CA-C-N        | 116.20             | 105.08          | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CB              | 110.50             | 119.95          | 1                  |
| N-CA-CB                   | 111.50             | 120.95          | 1                  |
| N-CA-N-CA-C-N-N-CA-N-CA-C | 111.00             | 126.56          | 1                  |
| N-CA-CB                   | 110.50             | 119.95          | 2                  |
| C-N-CA                    | 121.70             | 131.70          | 1                  |
| CA-C-C-CA-CB              | 110.10             | 99.54           | 1                  |
| N-CA-CB                   | 110.50             | 101.06          | 1                  |
| C-CA-CB                   | 110.10             | 120.66          | 1                  |
| N-CA-N-CA-C               | 112.10             | 98.21           | 1                  |
| C-CA-CB                   | 110.10             | 120.65          | 2                  |
| C-CA-CA-CB-CG             | 113.80             | 108.25          | 1                  |
| N-CA-C-CA-CB              | 110.10             | 120.65          | 1                  |
| C-CA-C-CA-CB              | 110.10             | 120.65          | 1                  |
| C-N-CA                    | 121.70             | 131.69          | 2                  |
| C-N-CA                    | 121.70             | 111.71          | 1                  |
| C-CA-CB                   | 110.10             | 99.56           | 1                  |
| CA-C-C-CA-CB              | 110.10             | 99.56           | 1                  |
| N-CA-C                    | 111.00             | 95.46           | 1                  |
| CA-C-N                    | 116.20             | 127.30          | 1                  |
| N-CA-C                    | 112.10             | 98.23           | 1                  |
| N-CA-CB                   | 110.50             | 119.93          | 1                  |
| N-CA-C-CA-CB              | 110.10             | 120.64          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| CA-C-O       | 120.80             | 130.23          | 1                  |
| CA-C-O       | 120.80             | 111.37          | 1                  |
| CA-C-N       | 116.20             | 127.29          | 1                  |
| N-CA-CA-C-O  | 120.80             | 111.38          | 1                  |
| C-N-CA-C-O   | 120.80             | 130.22          | 1                  |
| C-CA-CB      | 110.10             | 120.63          | 1                  |
| N-CA-CB      | 111.50             | 102.08          | 2                  |
| N-CA-C       | 111.00             | 95.48           | 1                  |
| C-CA-CB      | 110.10             | 99.57           | 1                  |
| C-N-C-N-CA   | 121.70             | 131.67          | 1                  |
| CA-C-C-CA-CB | 110.10             | 99.57           | 1                  |
| C-CA-CB      | 111.60             | 122.68          | 2                  |
| CA-CB-CG     | 112.60             | 107.06          | 1                  |
| CA-C-C-CA-CB | 110.10             | 120.62          | 1                  |
| C-CA-C-CA-CB | 110.10             | 120.62          | 1                  |
| C-CA-C-N-CA  | 121.70             | 131.67          | 1                  |
| N-CA-N-CA-CB | 110.50             | 101.09          | 1                  |
| N-CA-CA-C-O  | 120.80             | 111.39          | 1                  |
| CA-CB-CG     | 112.60             | 107.07          | 1                  |
| C-CA-CB      | 110.10             | 120.61          | 1                  |
| CA-C-C-CA-CB | 110.10             | 120.61          | 1                  |
| CA-C-C-N-CA  | 121.70             | 131.65          | 1                  |



| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB      | 110.10             | 120.61          | 1                  |
| C-N-CA            | 121.70             | 131.65          | 1                  |
| C-CA-C-CA-CA-C-N  | 116.20             | 127.26          | 1                  |
| CA-CB-N-CA-CB     | 110.50             | 101.10          | 1                  |
| C-N-C-CA-CA-C-N   | 116.20             | 127.25          | 1                  |
| C-CA-CB           | 110.50             | 102.21          | 1                  |
| N-CA-C-N-CA       | 121.70             | 131.64          | 1                  |
| N-CA-C            | 111.00             | 95.54           | 1                  |
| C-CA-C-CA-C-CA-CB | 110.10             | 120.59          | 1                  |
| CA-C-N            | 116.20             | 127.24          | 1                  |
| C-CA-CB           | 110.10             | 120.59          | 1                  |
| CA-C-O            | 120.80             | 111.42          | 2                  |
| C-CA-CB           | 110.10             | 99.61           | 1                  |
| N-CA-CA-C-N       | 116.20             | 127.24          | 1                  |
| C-CA-CB           | 110.10             | 99.62           | 2                  |
| CA-C-O            | 120.80             | 130.18          | 1                  |
| CA-CB-CG          | 112.60             | 107.08          | 1                  |
| C-CA-CB           | 110.10             | 120.58          | 1                  |
| C-N-C-CA-CB       | 110.10             | 120.58          | 1                  |
| C-CA-C-CA-CB      | 111.60             | 122.63          | 1                  |
| N-CA-C            | 111.00             | 95.56           | 1                  |
| N-CA-C            | 111.00             | 126.44          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                 | 110.50             | 101.13          | 2                  |
| N-CA-CA-C-O             | 120.80             | 130.17          | 1                  |
| C-CA-CA-C-O             | 120.80             | 111.43          | 2                  |
| C-CA-CB                 | 110.10             | 99.63           | 1                  |
| C-N-CA-CB-CG            | 113.80             | 108.29          | 1                  |
| C-CA-CB                 | 110.10             | 120.57          | 3                  |
| C-N-N-CA-CB             | 111.50             | 120.87          | 1                  |
| N-CA-CB                 | 111.50             | 120.86          | 1                  |
| N-CA-C-N-N-CA-C         | 111.00             | 95.58           | 1                  |
| C-CA-N-CA-CB            | 110.50             | 119.86          | 1                  |
| C-CA-CB                 | 110.10             | 120.56          | 2                  |
| C-CA-CA-C-N             | 116.20             | 127.21          | 2                  |
| N-CA-C-N-C-CA-CB        | 110.10             | 120.56          | 1                  |
| CA-C-C-N-C-CA-CB        | 110.10             | 99.64           | 1                  |
| N-CA-C-CA-C-CA-CA-CB-CG | 113.80             | 108.30          | 1                  |
| N-CA-C                  | 111.00             | 126.41          | 1                  |
| C-CA-CB                 | 110.10             | 120.55          | 3                  |
| N-CA-CB                 | 110.50             | 101.15          | 1                  |
| CA-C-O                  | 120.80             | 111.45          | 1                  |
| CA-C-N                  | 116.20             | 105.20          | 1                  |
| C-N-N-CA-C              | 111.00             | 95.60           | 1                  |
| N-CA-C-CA-CB            | 110.10             | 99.65           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 103.00             | 109.05          | 1                  |
| C-CA-CB           | 111.40             | 100.95          | 1                  |
| N-CA-CB           | 111.50             | 102.15          | 1                  |
| C-CA-N-CA-CB      | 110.50             | 101.15          | 1                  |
| N-CA-C            | 111.00             | 95.61           | 1                  |
| C-CA-CB           | 110.10             | 99.66           | 3                  |
| N-CA-N-CA-CB      | 103.00             | 109.05          | 1                  |
| CA-CB-CG          | 112.60             | 107.10          | 1                  |
| C-N-CA            | 121.70             | 131.59          | 2                  |
| N-CA-N-CA-C       | 111.00             | 126.39          | 1                  |
| C-CA-CA-C-N-CA-CB | 110.50             | 101.16          | 1                  |
| CA-C-N            | 116.20             | 105.21          | 1                  |
| N-CA-C            | 111.00             | 95.62           | 1                  |
| C-CA-CB           | 111.60             | 122.58          | 1                  |
| N-CA-N-CA-C       | 111.00             | 126.38          | 1                  |
| C-CA-CB           | 110.10             | 99.67           | 1                  |
| N-CA-C            | 111.00             | 126.37          | 1                  |
| CA-C-O            | 120.80             | 111.47          | 1                  |
| CA-C-N            | 116.20             | 105.22          | 2                  |
| C-N-N-CA-C        | 111.00             | 126.37          | 1                  |
| C-CA-CB           | 110.10             | 120.53          | 3                  |
| N-CA-C            | 111.00             | 95.64           | 2                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-CB-C-CA-N-CA-CB     | 111.50             | 120.83          | 1                  |
| C-CA-CB                | 110.10             | 99.68           | 1                  |
| C-N-N-CA-CB            | 111.50             | 102.17          | 1                  |
| N-CA-CA-CB-C-CA-CA-C-O | 120.80             | 111.48          | 1                  |
| C-CA-CA-CB-CG2         | 110.50             | 101.18          | 1                  |
| CA-CB-CG               | 113.80             | 108.32          | 1                  |
| C-N-CA                 | 121.70             | 111.83          | 1                  |
| C-CA-N-CA-C-N-N-CA-CB  | 110.50             | 119.82          | 1                  |
| CA-CB-C-N-N-CA-CB      | 110.50             | 119.82          | 1                  |
| C-CA-N-CA-C            | 111.00             | 95.66           | 1                  |
| C-CA-CB                | 110.10             | 99.69           | 1                  |
| N-CA-C                 | 111.00             | 126.34          | 1                  |
| N-CA-C                 | 111.00             | 95.66           | 1                  |
| C-CA-CB                | 110.10             | 120.51          | 1                  |
| N-CA-CA-C-O            | 120.80             | 111.49          | 1                  |
| N-CA-CB                | 110.50             | 119.81          | 2                  |
| C-CA-CB                | 111.60             | 100.65          | 1                  |
| C-CA-CA-C-N            | 116.20             | 127.15          | 1                  |
| CA-CB-CG               | 112.60             | 107.12          | 1                  |
| N-CA-C-N-CA            | 121.70             | 111.84          | 1                  |
| C-CA-C-N-CA            | 121.70             | 111.84          | 1                  |
| CA-CB-CG               | 112.60             | 107.13          | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-O        | 120.80             | 111.49          | 1                  |
| N-CA-CB            | 111.50             | 102.19          | 1                  |
| C-N-C-CA-C-N-CA    | 121.70             | 131.55          | 1                  |
| C-CA-CB            | 110.10             | 120.50          | 2                  |
| C-CA-CB            | 110.10             | 99.70           | 2                  |
| C-N-CA             | 121.70             | 131.55          | 2                  |
| C-N-CA             | 121.70             | 111.85          | 2                  |
| CA-C-O             | 120.80             | 111.50          | 1                  |
| CA-CB-CG           | 113.80             | 108.33          | 1                  |
| CA-CB-CG2          | 110.50             | 101.20          | 1                  |
| C-CA-N-CA-N-CA-CB  | 111.50             | 120.80          | 1                  |
| N-CA-N-CA-CA-CB-CG | 112.60             | 107.13          | 1                  |
| CA-C-O             | 120.80             | 130.10          | 1                  |
| C-CA-CA-CB-C-CA-CB | 110.10             | 120.49          | 1                  |
| C-CA-CA-C-O        | 120.80             | 111.51          | 1                  |
| C-CA-CA-CB-CG      | 112.60             | 107.14          | 1                  |
| C-CA-CB            | 110.10             | 120.48          | 3                  |
| OD1-CG-ND2         | 122.60             | 117.14          | 1                  |
| N-CA-C-CA-C-CA-CB  | 110.10             | 99.72           | 1                  |
| CA-C-CA-C-N        | 116.20             | 127.12          | 1                  |
| C-CA-N-CA-CB       | 110.50             | 119.78          | 1                  |
| C-N-CA             | 121.70             | 111.87          | 1                  |

| Angle type                              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| C-CA-CB                                 | 110.10             | 99.73           | 1                  |
| C-CA-N-CA-CA-C-N                        | 116.20             | 127.12          | 1                  |
| CA-N-N-CA-C                             | 111.00             | 95.72           | 1                  |
| C-N-C-CA-C-N-CA                         | 121.70             | 131.52          | 1                  |
| C-CA-C-N-C-CA-N-CA-C-N-CA               | 121.70             | 111.89          | 1                  |
| N-CA-C-CA-C-CA-C-CA-C-CA-CB             | 110.10             | 120.46          | 1                  |
| CA-C-O                                  | 120.80             | 111.53          | 1                  |
| CA-CB-CG                                | 112.60             | 107.15          | 1                  |
| N-CA-CA-C-O                             | 120.80             | 130.06          | 1                  |
| C-N-CA                                  | 121.70             | 111.89          | 1                  |
| N-CA-C-CA-CA-C-N                        | 116.20             | 105.31          | 1                  |
| CA-N-C-CA-C-CA-CA-CB-CA-CB-N-CA-N-CA-CB | 110.50             | 101.25          | 1                  |
| CA-C-N                                  | 116.20             | 127.09          | 1                  |
| CA-CB-CG                                | 113.80             | 108.36          | 1                  |
| CA-C-CA-C-O                             | 120.80             | 111.55          | 1                  |
| N-CA-N-CA-CB                            | 111.50             | 120.75          | 1                  |
| C-CA-CB                                 | 110.10             | 99.76           | 1                  |
| C-CA-CB                                 | 110.10             | 120.44          | 1                  |
| C-CA-N-CA-CA-CB-CG                      | 112.60             | 107.16          | 1                  |
| C-N-CA                                  | 121.70             | 131.49          | 1                  |
| C-CA-CA-C-O                             | 120.80             | 130.04          | 1                  |
| C-N-N-CA-CA-C-O                         | 120.80             | 111.56          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-CB-C-N-N-CA-C-N-CA | 121.70             | 111.92          | 1                  |
| CA-C-O                     | 120.80             | 130.04          | 1                  |
| CA-C-N                     | 116.20             | 127.07          | 1                  |
| C-N-CA                     | 121.70             | 111.92          | 1                  |
| CA-C-N-CA-C-CA-CB          | 109.10             | 97.15           | 1                  |
| N-CA-C                     | 111.00             | 126.21          | 1                  |
| C-CA-CB                    | 110.10             | 99.78           | 2                  |
| C-CA-CB                    | 109.10             | 97.15           | 1                  |
| C-CA-N-CA-CB               | 110.50             | 119.73          | 1                  |
| N-CA-CB                    | 111.50             | 120.73          | 1                  |
| C-CA-N-CA-C-CA-CB          | 110.10             | 99.78           | 1                  |
| C-N-C-N-C-CA-N-CA-C        | 111.00             | 126.20          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 99.79           | 2                  |
| CA-C-N                     | 116.20             | 127.05          | 1                  |
| N-CA-CA-N-CD               | 112.00             | 104.40          | 1                  |
| C-CA-CB                    | 110.10             | 99.79           | 1                  |
| CA-C-N                     | 116.20             | 105.35          | 1                  |
| CA-CB-CG                   | 112.60             | 107.18          | 1                  |
| N-CA-N-CA-CA-CB-CG         | 112.60             | 107.18          | 1                  |
| CA-N-CD                    | 112.00             | 104.41          | 1                  |
| N-CA-C-N-CA                | 121.70             | 131.46          | 2                  |
| N-CA-CB                    | 110.50             | 119.72          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-N                  | 116.20             | 127.05          | 1                  |
| N-CA-CB                     | 110.50             | 101.28          | 2                  |
| CA-C-N                      | 116.20             | 127.04          | 1                  |
| C-CA-C-CA-CB                | 110.50             | 102.37          | 1                  |
| C-CA-CB                     | 110.10             | 120.40          | 1                  |
| CA-C-CA-C-O                 | 120.80             | 130.01          | 1                  |
| C-N-C-N-CA                  | 121.70             | 111.94          | 1                  |
| N-CA-CB                     | 111.50             | 102.29          | 1                  |
| C-CA-N-CA-C-CA-CB           | 110.10             | 99.81           | 1                  |
| C-CA-CB                     | 110.10             | 99.81           | 2                  |
| C-N-CA                      | 121.70             | 111.95          | 1                  |
| C-CA-CB                     | 110.10             | 120.39          | 1                  |
| CA-C-N                      | 116.20             | 127.03          | 1                  |
| CA-C-N                      | 116.20             | 105.37          | 1                  |
| C-CA-C-N-CA                 | 121.70             | 111.95          | 1                  |
| C-N-N-CA-CA-CB-N-CA-C-CA-CB | 111.60             | 100.77          | 1                  |
| C-CA-C-N-CA                 | 121.70             | 111.96          | 1                  |
| C-CA-N-CA-C-CA-C-CA-CB      | 110.10             | 99.82           | 1                  |
| CA-C-N                      | 116.20             | 127.02          | 1                  |
| C-CA-CB                     | 110.10             | 99.82           | 1                  |
| C-N-CA                      | 121.70             | 111.96          | 1                  |
| N-CA-C                      | 111.00             | 95.85           | 1                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-N                 | 116.20             | 105.38          | 1                  |
| C-CA-CB                | 110.50             | 102.39          | 1                  |
| N-CA-CA-C-O            | 120.80             | 129.99          | 1                  |
| N-CA-CB                | 111.50             | 102.31          | 1                  |
| N-CA-N-CA-N-CA-CB      | 110.50             | 101.31          | 1                  |
| C-CA-C-CA-C-CA-CB      | 110.50             | 102.39          | 1                  |
| C-CA-CB                | 110.10             | 99.83           | 2                  |
| N-CA-CA-C-N            | 116.20             | 105.39          | 1                  |
| C-CA-N-CA-CA-C-O       | 120.80             | 129.99          | 1                  |
| N-CA-CB                | 110.50             | 119.69          | 1                  |
| C-N-CA                 | 121.70             | 131.43          | 1                  |
| N-CA-CB                | 110.50             | 119.68          | 2                  |
| CA-CB-CG               | 112.60             | 107.20          | 1                  |
| C-CA-N-CA-C-CA-CB      | 110.10             | 99.84           | 1                  |
| C-CA-CB                | 110.10             | 99.84           | 3                  |
| C-N-CA                 | 121.70             | 111.98          | 1                  |
| CA-C-N                 | 116.20             | 127.00          | 1                  |
| CA-CB-C-N-CA           | 121.70             | 111.98          | 1                  |
| C-CA-CB                | 110.10             | 120.36          | 3                  |
| C-CA-C-CA-CB           | 110.10             | 120.36          | 1                  |
| C-N-N-CA-C-CA-CB       | 111.60             | 122.40          | 1                  |
| C-CA-CA-CB-C-CA-CA-C-N | 116.20             | 126.99          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-C-N                | 116.20             | 105.41          | 1                  |
| CA-C-N                | 116.20             | 126.99          | 1                  |
| C-N-CA                | 121.70             | 111.99          | 2                  |
| N-CA-N-CA-CB          | 110.50             | 101.33          | 1                  |
| N-CA-C                | 111.00             | 126.10          | 1                  |
| C-CA-CB               | 110.10             | 99.85           | 1                  |
| N-CA-C-N-CA           | 121.70             | 131.41          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 99.85           | 1                  |
| C-CA-CB               | 111.60             | 122.39          | 1                  |
| CA-C-O                | 120.80             | 111.63          | 1                  |
| CA-CB-C-CA-CB         | 111.60             | 122.39          | 1                  |
| C-CA-CB               | 110.10             | 120.35          | 1                  |
| CA-N-CA-CB-CA-CB-CG   | 112.60             | 107.21          | 1                  |
| N-CA-CB               | 110.50             | 119.67          | 1                  |
| C-CA-C-N-CA           | 121.70             | 131.40          | 1                  |
| C-N-CA                | 121.70             | 131.40          | 2                  |
| N-CA-CB               | 110.50             | 119.66          | 1                  |
| N-CA-N-CA-C-N-C-CA-CB | 110.50             | 102.42          | 1                  |
| OD1-CG-ND2            | 122.60             | 117.21          | 1                  |
| N-CA-C-CA-CB          | 110.50             | 102.42          | 1                  |
| C-N-CA                | 121.70             | 112.00          | 1                  |
| N-CA-C                | 111.00             | 126.08          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-O                      | 120.80             | 129.96          | 1                  |
| C-CA-CB                     | 110.10             | 99.87           | 1                  |
| CA-CB-CG                    | 113.80             | 108.41          | 1                  |
| N-CA-C-CA-CB                | 109.10             | 120.95          | 1                  |
| CA-C-C-CA-CA-C-N            | 116.20             | 126.96          | 1                  |
| CA-C-C-CA-CB                | 110.10             | 99.88           | 1                  |
| CA-C-N                      | 116.20             | 105.44          | 1                  |
| C-CA-CB                     | 110.10             | 120.32          | 2                  |
| CA-C-O                      | 120.80             | 111.65          | 1                  |
| N-CA-C-CA-CA-N-N-CA-C-CA-CB | 109.10             | 120.93          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 120.32          | 1                  |
| CA-C-N-CA-C-N-CA            | 121.70             | 131.38          | 1                  |
| C-N-CA                      | 121.70             | 131.38          | 2                  |
| CA-C-O                      | 120.80             | 111.66          | 2                  |
| N-CA-N-CA-CB                | 110.50             | 119.64          | 1                  |
| N-CA-CB                     | 110.50             | 119.64          | 1                  |
| C-N-CA                      | 121.70             | 112.02          | 1                  |
| CA-N-CD                     | 112.00             | 104.48          | 2                  |
| N-CA-CA-C-N-CA-CB           | 110.50             | 119.64          | 1                  |
| C-N-CA                      | 121.70             | 131.37          | 1                  |
| C-CA-CB                     | 110.10             | 99.89           | 1                  |
| N-CA-CB                     | 110.50             | 119.63          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-N-C-N-CA                  | 121.70             | 131.37          | 1                  |
| CA-CB-CG                    | 113.80             | 108.43          | 1                  |
| CA-CB-C-CA-CB               | 110.10             | 120.30          | 1                  |
| C-N-CA-CB-CA-CB-CG          | 112.60             | 107.23          | 1                  |
| C-CA-CB                     | 110.10             | 120.30          | 1                  |
| CA-C-N                      | 116.20             | 105.47          | 1                  |
| C-CA-CB                     | 110.10             | 99.90           | 1                  |
| N-CA-CB                     | 110.50             | 119.62          | 1                  |
| C-N-CA                      | 121.70             | 131.36          | 1                  |
| N-CA-CB                     | 111.50             | 120.62          | 1                  |
| N-CA-C                      | 111.00             | 95.98           | 1                  |
| C-CA-CB                     | 110.10             | 120.29          | 3                  |
| N-CA-N-CA-C-CA-CB           | 109.10             | 120.90          | 1                  |
| CA-CB-CG                    | 112.60             | 107.24          | 1                  |
| N-CA-CB                     | 110.50             | 101.38          | 1                  |
| C-CA-CB                     | 111.40             | 121.59          | 1                  |
| C-N-N-CA-C-CA-CB            | 110.10             | 120.29          | 1                  |
| C-N-CA                      | 121.70             | 112.05          | 1                  |
| C-CA-CB                     | 110.10             | 120.28          | 2                  |
| CA-C-N                      | 116.20             | 105.48          | 1                  |
| N-CA-N-CA-C-CA-C-CA-N-CA-CB | 110.50             | 119.61          | 1                  |
| CA-C-C-N-CA                 | 121.70             | 112.06          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 110.50             | 101.40          | 1                  |
| CA-C-C-CA-CB      | 109.10             | 120.88          | 1                  |
| CA-C-O            | 120.80             | 129.90          | 2                  |
| C-CA-CB           | 110.10             | 120.27          | 1                  |
| CA-CB-C-N-CA      | 121.70             | 112.06          | 1                  |
| N-CA-C-N-CA       | 121.70             | 131.33          | 1                  |
| C-CA-CB           | 110.10             | 99.93           | 1                  |
| C-CA-N-CA-CB      | 110.50             | 101.40          | 1                  |
| N-CA-C            | 111.00             | 125.99          | 1                  |
| CA-C-N            | 116.20             | 105.50          | 1                  |
| C-N-CA            | 121.70             | 131.33          | 1                  |
| CA-C-C-CA-CB      | 110.10             | 120.26          | 1                  |
| C-N-CA            | 121.70             | 112.07          | 2                  |
| C-CA-CB           | 110.10             | 120.26          | 2                  |
| N-CA-CA-C-O       | 120.80             | 111.71          | 1                  |
| N-CA-CA-C-CA-C-O  | 120.80             | 111.71          | 1                  |
| CA-C-O            | 120.80             | 111.71          | 1                  |
| N-CA-CB           | 110.50             | 101.41          | 1                  |
| N-CA-C-CA-C-N-CA  | 121.70             | 112.08          | 1                  |
| CA-C-CA-C-O       | 120.80             | 111.71          | 1                  |
| N-CA-CA-C-N-CA-CB | 110.50             | 119.59          | 1                  |
| N-CA-C            | 111.00             | 125.96          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-N-CA                 | 121.70             | 131.32          | 1                  |
| CA-C-N                 | 116.20             | 126.89          | 1                  |
| N-CA-C                 | 111.00             | 96.04           | 1                  |
| CA-C-CA-CB-CG          | 113.80             | 108.46          | 1                  |
| C-CA-CB                | 111.40             | 121.55          | 1                  |
| CA-C-N-CA-C            | 111.00             | 125.96          | 1                  |
| N-CA-CB                | 110.50             | 119.58          | 1                  |
| C-CA-C-N-N-CA-CB       | 110.50             | 101.42          | 1                  |
| N-CA-N-CA-CB           | 110.50             | 101.42          | 1                  |
| C-CA-CB                | 110.10             | 120.24          | 1                  |
| N-CA-C                 | 111.00             | 125.95          | 1                  |
| CA-C-C-N-CA            | 121.70             | 131.31          | 1                  |
| CA-C-CA-C-O            | 120.80             | 111.73          | 1                  |
| N-CA-CB                | 110.50             | 101.43          | 2                  |
| C-N-CA                 | 121.70             | 131.31          | 1                  |
| CA-CB-N-CA-CB          | 111.50             | 102.43          | 1                  |
| C-CA-CB                | 109.10             | 97.36           | 1                  |
| C-CA-CB                | 110.10             | 120.23          | 2                  |
| C-CA-CB                | 110.10             | 99.97           | 1                  |
| N-CA-CA-CB-CA-C-N      | 116.90             | 124.90          | 1                  |
| N-CA-N-CA-CA-C-C-CA-CB | 111.60             | 122.26          | 1                  |
| N-CD-CG                | 103.20             | 95.21           | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-C            | 111.00             | 96.08           | 1                  |
| C-CA-CB           | 111.60             | 122.26          | 1                  |
| N-CA-CB           | 110.50             | 119.56          | 1                  |
| C-N-CA            | 121.70             | 131.29          | 1                  |
| CA-C-N            | 116.90             | 124.89          | 1                  |
| N-CA-CB           | 110.50             | 101.44          | 1                  |
| CA-C-O            | 120.80             | 111.74          | 1                  |
| C-N-C-N-CD        | 125.00             | 103.16          | 1                  |
| C-N-CA            | 121.70             | 112.11          | 1                  |
| N-CA-C            | 111.00             | 125.92          | 1                  |
| C-CA-CB           | 110.10             | 120.22          | 1                  |
| C-N-C-N-CA        | 121.70             | 131.29          | 1                  |
| N-CA-CB           | 111.50             | 102.45          | 1                  |
| C-CA-CB           | 110.10             | 99.98           | 1                  |
| N-CA-CB           | 110.40             | 102.41          | 1                  |
| N-CA-CB           | 110.50             | 119.55          | 1                  |
| N-CA-C            | 111.00             | 96.09           | 1                  |
| C-N-CD            | 125.00             | 103.17          | 1                  |
| C-CA-CA-CB-C-N-CA | 121.70             | 131.28          | 1                  |
| C-CA-CB           | 111.60             | 122.24          | 1                  |
| CA-C-O            | 120.80             | 111.75          | 1                  |
| CA-C-CA-CB-CG     | 113.80             | 108.48          | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| N-CD-CG                  | 103.20             | 95.22           | 2                  |
| CA-CB-CG                 | 113.80             | 108.48          | 1                  |
| C-N-CD                   | 125.00             | 103.19          | 1                  |
| N-CA-CB                  | 110.50             | 119.54          | 1                  |
| C-N-CA-C-N               | 116.20             | 105.56          | 1                  |
| N-CA-CB                  | 110.50             | 101.46          | 1                  |
| C-N-CA-C-O               | 120.80             | 111.76          | 1                  |
| C-N-CA-CB-CG             | 112.60             | 107.28          | 1                  |
| N-CA-CA-C-N-CA-CB        | 110.50             | 119.54          | 1                  |
| C-N-CA                   | 121.70             | 131.27          | 1                  |
| CA-CB-CG                 | 113.80             | 108.49          | 2                  |
| N-CA-C                   | 111.00             | 96.12           | 1                  |
| C-N-CD                   | 125.00             | 103.21          | 1                  |
| C-CA-N-CA-CB             | 110.50             | 119.53          | 1                  |
| C-CA-C-N-CA              | 121.70             | 131.26          | 1                  |
| C-CA-C-N-CA              | 121.70             | 112.14          | 1                  |
| N-CA-C                   | 111.00             | 125.88          | 1                  |
| C-CA-N-CA-N-CA-CB        | 110.40             | 102.43          | 1                  |
| N-CA-C-CA-N-CA-CB        | 110.50             | 119.53          | 1                  |
| N-CD-CG                  | 103.20             | 95.23           | 1                  |
| C-CA-C-N-C-N-CA-C-CA-C-O | 120.80             | 111.78          | 1                  |
| C-CA-N-CA-N-CA-CB        | 110.50             | 119.52          | 1                  |



| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-N-N-CA-C-CA-CA-CB-CG  | 113.80             | 108.49          | 1                  |
| C-N-CA-CB-CG            | 112.60             | 107.29          | 1                  |
| C-N-CA                  | 121.70             | 112.15          | 2                  |
| CA-C-O                  | 120.80             | 111.78          | 1                  |
| C-N-C-N-CA              | 121.70             | 112.15          | 1                  |
| C-CA-C-CA-CB            | 110.10             | 120.18          | 1                  |
| C-CA-CB                 | 111.40             | 101.33          | 1                  |
| N-CA-CB                 | 110.50             | 119.51          | 1                  |
| C-CA-CA-C-N             | 116.20             | 105.60          | 1                  |
| C-CA-CB                 | 110.10             | 100.03          | 1                  |
| N-CA-C                  | 111.00             | 96.16           | 1                  |
| CA-CB-CG                | 113.80             | 108.50          | 1                  |
| C-CA-C-CA-CA-CB-C-CA-CB | 110.10             | 100.03          | 1                  |
| C-CA-N-CA-C-CA-CB       | 110.10             | 120.16          | 1                  |
| C-CA-N-CA-CB            | 110.40             | 118.34          | 1                  |
| CA-C-CA-C-N             | 116.20             | 105.61          | 1                  |
| N-CA-C                  | 111.00             | 125.83          | 1                  |
| C-CA-N-CA-CB            | 110.50             | 101.50          | 1                  |
| C-N-CA                  | 121.70             | 131.23          | 1                  |
| N-CA-CB                 | 103.00             | 108.82          | 2                  |
| N-CA-CB                 | 110.50             | 119.50          | 1                  |
| C-CA-CA-C-N-CA-CB       | 103.00             | 108.82          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-CA-C-N      | 116.20             | 126.78          | 1                  |
| N-CA-C                | 111.00             | 96.19           | 1                  |
| C-CA-CB               | 110.10             | 120.15          | 1                  |
| C-CA-C-N-C-CA-CB      | 110.10             | 100.05          | 1                  |
| N-CA-C-N-C-CA-CB      | 110.10             | 120.15          | 1                  |
| N-CA-C                | 111.00             | 96.20           | 1                  |
| C-CA-C-CA-CB          | 111.40             | 101.36          | 1                  |
| C-CA-CB               | 110.10             | 120.14          | 2                  |
| C-CA-C-N-CA-C-CA-C-N  | 116.20             | 105.63          | 1                  |
| C-CA-CB               | 111.40             | 121.44          | 1                  |
| CA-C-O                | 120.80             | 111.82          | 1                  |
| CA-C-O                | 120.80             | 129.78          | 1                  |
| N-CA-CB               | 110.50             | 119.48          | 1                  |
| N-CA-CA-C-N           | 116.20             | 126.76          | 1                  |
| N-CA-N-CA-C-N-C-CA-CB | 110.10             | 100.07          | 1                  |
| C-CA-CB               | 110.10             | 100.07          | 1                  |
| C-CA-CB               | 110.10             | 120.13          | 2                  |
| N-CA-C                | 111.00             | 125.78          | 2                  |
| N-CA-CB               | 110.50             | 119.47          | 2                  |
| C-CA-N-CA-CB          | 110.50             | 101.53          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 120.12          | 1                  |
| N-CA-CB               | 110.50             | 101.53          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 103.00             | 108.80          | 1                  |
| C-N-CA            | 121.70             | 131.19          | 1                  |
| N-CA-CB           | 110.50             | 101.54          | 2                  |
| C-CA-CB           | 110.10             | 120.12          | 2                  |
| N-CD-CG           | 103.20             | 95.29           | 1                  |
| C-CA-CB           | 110.10             | 100.09          | 3                  |
| C-N-N-CA-C        | 111.00             | 125.76          | 1                  |
| C-N-CA            | 121.70             | 112.21          | 1                  |
| C-N-CA            | 121.70             | 131.18          | 2                  |
| C-CA-C-N-CA       | 121.70             | 131.18          | 1                  |
| C-CA-CB           | 109.10             | 97.51           | 1                  |
| C-CA-CA-CB-CG     | 113.80             | 119.07          | 1                  |
| CA-C-N            | 116.20             | 126.73          | 2                  |
| CA-C-C-CA-CB      | 109.10             | 97.52           | 1                  |
| C-N-C-CA-CB       | 111.40             | 101.40          | 1                  |
| CA-C-N            | 116.20             | 105.67          | 1                  |
| NE-CZ-NH1         | 121.50             | 116.24          | 1                  |
| C-CA-CB           | 110.10             | 100.10          | 1                  |
| C-CA-CA-C-C-CA-CB | 111.60             | 101.08          | 1                  |
| CA-CB-CG          | 113.80             | 108.54          | 1                  |
| C-N-C-CA-CB       | 110.10             | 120.10          | 1                  |
| CA-C-C-CA-CB      | 110.10             | 120.09          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 110.50             | 119.44          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 120.09          | 1                  |
| C-N-CA            | 121.70             | 112.23          | 1                  |
| C-N-C-N-CA        | 121.70             | 131.16          | 1                  |
| C-CA-CB           | 110.10             | 100.11          | 1                  |
| C-CA-CB           | 110.10             | 120.09          | 2                  |
| C-CA-N-CD-CG      | 103.20             | 95.32           | 1                  |
| C-N-CA            | 121.70             | 112.24          | 2                  |
| C-CA-CB           | 111.40             | 121.38          | 1                  |
| C-CA-C-N-CA       | 121.70             | 112.24          | 1                  |
| C-CA-N-CA-C       | 111.00             | 96.29           | 1                  |
| C-N-C-CA-CB       | 110.10             | 100.12          | 1                  |
| C-CA-N-CA-N-CA-CB | 110.50             | 119.43          | 1                  |
| C-CA-CB           | 111.60             | 101.10          | 1                  |
| CA-C-O            | 120.80             | 111.87          | 1                  |
| C-CA-CB           | 110.10             | 120.07          | 3                  |
| C-CA-CB           | 110.10             | 100.13          | 1                  |
| C-N-CA            | 121.70             | 131.15          | 1                  |
| C-N-CA            | 121.70             | 112.25          | 1                  |
| C-N-CA-C-C-N-CA   | 121.70             | 131.15          | 1                  |
| CA-C-CA-C-N       | 116.20             | 105.71          | 1                  |
| C-N-C-CA-CB       | 110.10             | 100.13          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| C-CA-CB          | 109.10             | 97.56           | 1                  |
| N-CA-CB          | 110.50             | 119.42          | 2                  |
| C-N-C-CA-CB      | 110.10             | 120.06          | 1                  |
| CA-C-O           | 120.80             | 129.71          | 2                  |
| C-N-CA           | 121.70             | 112.26          | 1                  |
| CA-C-C-N-CA      | 121.70             | 131.14          | 1                  |
| C-N-CA           | 121.70             | 131.14          | 1                  |
| CA-CB-CG         | 112.60             | 107.36          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 100.14          | 1                  |
| C-CA-CB          | 110.10             | 120.06          | 2                  |
| C-CA-CB          | 110.10             | 100.14          | 2                  |
| C-N-CA           | 121.70             | 112.27          | 1                  |
| CA-C-O           | 120.80             | 111.89          | 1                  |
| N-CA-CA-C-C-N-CA | 121.70             | 112.27          | 1                  |
| C-CA-C-N-CA      | 121.70             | 112.27          | 1                  |
| C-CA-CB          | 110.10             | 100.15          | 1                  |
| CA-C-CA-C-O      | 120.80             | 111.90          | 1                  |
| C-CA-C-CA-CA-C-O | 120.80             | 111.90          | 1                  |
| C-N-CA           | 121.70             | 131.13          | 2                  |
| C-CA-C-CA-CB     | 110.10             | 100.15          | 1                  |
| CA-C-N           | 116.20             | 105.73          | 1                  |
| C-N-C-N-CA       | 121.70             | 112.28          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-C-N-CA       | 121.70             | 131.12          | 1                  |
| C-CA-CA-C-N       | 116.20             | 126.67          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 120.04          | 1                  |
| N-CA-CB           | 111.50             | 102.60          | 1                  |
| C-CA-CA-C-O       | 120.80             | 111.91          | 1                  |
| C-CA-C-N-CA       | 121.70             | 112.28          | 1                  |
| C-N-CA            | 121.70             | 131.11          | 1                  |
| C-N-CA            | 121.70             | 112.29          | 2                  |
| N-CA-C            | 111.00             | 125.64          | 1                  |
| C-CA-C-CA-C-CA-CB | 110.10             | 120.03          | 1                  |
| N-CA-C            | 111.00             | 96.36           | 1                  |
| C-CA-CB           | 110.10             | 120.03          | 1                  |
| C-CA-CB           | 111.60             | 101.15          | 3                  |
| CA-C-O            | 120.80             | 111.92          | 1                  |
| N-CA-C            | 111.00             | 96.37           | 1                  |
| C-N-C-CA-CB       | 111.40             | 101.47          | 1                  |
| C-CA-CB           | 110.10             | 120.02          | 4                  |
| N-CA-C            | 111.00             | 96.38           | 3                  |
| N-CA-N-CA-C       | 111.00             | 96.38           | 1                  |
| C-N-CA            | 121.70             | 131.10          | 1                  |
| C-CA-CB           | 110.50             | 118.33          | 1                  |
| N-CA-CB           | 110.50             | 101.62          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB | 110.10             | 120.02          | 1                  |
| N-CA-C       | 111.00             | 96.39           | 1                  |
| C-CA-C-CA-CB | 111.60             | 101.16          | 1                  |
| C-N-CA       | 121.70             | 112.31          | 3                  |
| CA-CB-CG     | 112.60             | 107.38          | 1                  |
| N-CA-C       | 111.00             | 125.61          | 1                  |
| C-CA-CB      | 111.40             | 121.31          | 1                  |
| CA-C-N       | 116.20             | 105.77          | 2                  |
| C-CA-CB      | 110.10             | 100.19          | 1                  |
| C-N-CA       | 121.70             | 131.09          | 2                  |
| CA-CB-CG     | 113.80             | 119.01          | 1                  |
| C-N-CA       | 121.70             | 131.08          | 3                  |
| N-CA-C       | 111.00             | 125.60          | 1                  |
| C-CA-CA-C-N  | 116.20             | 105.77          | 1                  |
| C-N-CA       | 121.70             | 112.32          | 4                  |
| CA-C-N       | 116.20             | 126.63          | 1                  |
| C-CA-CB      | 110.10             | 100.20          | 1                  |
| CA-CB-CG     | 112.60             | 107.39          | 2                  |
| CA-C-CA-C-N  | 116.20             | 105.78          | 1                  |
| N-CA-N-CA-C  | 111.00             | 125.59          | 1                  |
| N-CA-C       | 111.00             | 125.58          | 1                  |
| C-CA-CB      | 110.10             | 100.21          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-N-CA                     | 121.70             | 131.07          | 1                  |
| C-N-CA-C-O                 | 120.80             | 129.65          | 1                  |
| CA-C-O                     | 120.80             | 111.95          | 1                  |
| C-N-C-CA-CB                | 110.10             | 119.99          | 1                  |
| CA-C-C-CA-CA-C-O           | 120.80             | 111.95          | 1                  |
| CA-C-N                     | 116.20             | 126.61          | 1                  |
| C-N-C-N-CA                 | 121.70             | 112.33          | 1                  |
| CA-CB-CG                   | 112.60             | 107.40          | 1                  |
| CA-CB-C-CA-CB              | 110.10             | 119.98          | 2                  |
| CA-C-O                     | 120.80             | 111.96          | 1                  |
| C-N-CA                     | 121.70             | 131.06          | 1                  |
| C-N-C-N-N-CA-CB            | 110.50             | 101.66          | 1                  |
| CA-C-N                     | 116.20             | 105.80          | 1                  |
| CA-C-CA-C-C-CA-C-CA-CA-C-O | 120.80             | 129.64          | 1                  |
| N-CA-CB                    | 111.50             | 102.66          | 1                  |
| CA-CB-CA-C-O               | 120.80             | 111.97          | 1                  |
| CA-N-N-CA-C-CA-CB          | 111.40             | 121.27          | 1                  |
| C-CA-CB                    | 110.10             | 119.97          | 3                  |
| NE-CZ-C-N-CA               | 121.70             | 131.05          | 1                  |
| C-CA-CA-CB-CG              | 112.60             | 107.41          | 1                  |
| C-CA-CB                    | 110.10             | 100.23          | 2                  |
| C-CA-CA-C-C-CA-CB          | 110.10             | 100.23          | 1                  |



| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| C-N-CA                               | 121.70             | 131.04          | 2                  |
| C-N-CA                               | 121.70             | 112.36          | 2                  |
| CA-CB-CG                             | 112.60             | 107.41          | 1                  |
| C-CA-CB                              | 110.10             | 119.96          | 2                  |
| N-CA-CB                              | 110.50             | 101.68          | 1                  |
| CA-C-O                               | 120.80             | 111.98          | 2                  |
| C-CA-CA-C-O                          | 120.80             | 129.62          | 1                  |
| C-N-CA-C-O                           | 120.80             | 111.98          | 1                  |
| C-CA-CB                              | 109.10             | 120.51          | 1                  |
| N-CA-CB                              | 111.50             | 102.68          | 1                  |
| N-CA-C                               | 111.00             | 125.52          | 1                  |
| C-CA-CB                              | 110.10             | 100.25          | 1                  |
| C-CA-CB                              | 110.10             | 119.95          | 1                  |
| C-N-CA                               | 121.70             | 112.37          | 1                  |
| C-CA-CB                              | 110.50             | 118.28          | 1                  |
| N-CA-C-CA-N-CA-CB                    | 110.50             | 101.69          | 1                  |
| CA-C-C-CA-C-N-C-CA-C-CA-C-CA-C-CA-CB | 110.10             | 100.25          | 1                  |
| CA-C-C-CA-CB                         | 110.10             | 119.94          | 1                  |
| CA-C-O                               | 120.80             | 111.99          | 1                  |
| CA-C-C-N-CA                          | 121.70             | 112.37          | 1                  |
| CA-C-N                               | 116.20             | 105.84          | 1                  |
| N-CA-CB                              | 110.50             | 101.69          | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA               | 121.70             | 131.02          | 1                  |
| N-CA-N-CA-C               | 111.00             | 125.50          | 1                  |
| CA-C-C-CA-CA-C-N          | 116.90             | 109.13          | 1                  |
| CA-CB-C-N-CA              | 121.70             | 131.02          | 1                  |
| C-CA-CB                   | 110.10             | 119.94          | 1                  |
| CA-CB-CG                  | 112.60             | 107.42          | 1                  |
| C-N-C-CA-CB               | 110.10             | 100.26          | 1                  |
| C-CA-CB                   | 109.10             | 120.49          | 1                  |
| C-CA-C-CA-CB              | 110.10             | 100.27          | 1                  |
| C-N-CA-C-C-N-CA           | 121.70             | 112.39          | 1                  |
| C-N-CA                    | 121.70             | 112.39          | 2                  |
| C-CA-CB                   | 110.10             | 100.27          | 1                  |
| CA-C-C-CA-C-CA-C-N-CA-C-O | 120.80             | 112.01          | 1                  |
| CA-C-N                    | 116.90             | 109.14          | 1                  |
| C-CA-N-CA-CB              | 110.50             | 119.29          | 1                  |
| C-CA-N-CA-CB              | 110.50             | 101.71          | 1                  |
| CA-C-O                    | 120.80             | 112.01          | 1                  |
| C-CA-CB                   | 110.10             | 119.92          | 2                  |
| N-CA-CB                   | 103.00             | 108.69          | 1                  |
| NE-CZ-CA-C-N              | 116.20             | 126.54          | 1                  |
| CA-CB-CG                  | 112.60             | 107.43          | 1                  |
| CA-C-O                    | 120.80             | 129.59          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-N                     | 116.20             | 105.87          | 2                  |
| N-CA-CB                    | 110.50             | 101.72          | 1                  |
| C-N-CA                     | 121.70             | 130.99          | 1                  |
| CA-C-N                     | 116.20             | 105.88          | 2                  |
| C-N-CA                     | 121.70             | 112.41          | 1                  |
| C-CA-CB                    | 110.10             | 100.29          | 2                  |
| N-CA-C                     | 111.00             | 125.45          | 2                  |
| N-CA-CB                    | 110.50             | 101.73          | 1                  |
| C-CA-N-CA-CB               | 110.50             | 101.73          | 1                  |
| N-CA-C-CA-C-CA-N-CA-C-N-CA | 121.70             | 112.41          | 1                  |
| C-CA-CB                    | 110.10             | 100.30          | 2                  |
| C-N-N-CA-C                 | 111.00             | 125.45          | 1                  |
| C-N-C-CA-CB                | 110.10             | 100.30          | 1                  |
| CA-C-C-CA-C-CA-CB          | 110.10             | 119.90          | 1                  |
| N-CA-CB                    | 110.40             | 102.66          | 1                  |
| CA-C-O                     | 120.80             | 112.03          | 1                  |
| C-N-CA                     | 121.70             | 130.98          | 3                  |
| CA-C-C-N-CA                | 121.70             | 130.98          | 1                  |
| CA-C-O                     | 120.80             | 129.56          | 1                  |
| CA-C-CA-C-CA-C-N           | 116.20             | 105.89          | 1                  |
| N-CA-C                     | 111.00             | 96.57           | 1                  |
| C-CA-CB                    | 110.10             | 119.89          | 2                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| NE-CZ-NH1           | 121.50             | 126.65          | 1                  |
| CA-C-CA-C-CA-N-CD   | 112.00             | 104.79          | 1                  |
| CA-C-C-N-CA         | 121.70             | 130.97          | 1                  |
| N-CA-CB             | 111.50             | 120.25          | 1                  |
| C-N-CA              | 121.70             | 112.43          | 1                  |
| C-CA-CB             | 110.10             | 119.88          | 2                  |
| N-CA-CB             | 110.50             | 119.25          | 2                  |
| N-CA-CB             | 110.50             | 101.75          | 2                  |
| C-N-CA-CB-CG        | 113.80             | 108.65          | 1                  |
| C-N-CA              | 121.70             | 112.44          | 1                  |
| C-CA-CB             | 110.10             | 100.33          | 1                  |
| N-CA-CB             | 111.50             | 102.76          | 1                  |
| C-CA-C-CA-CB        | 110.10             | 119.87          | 1                  |
| C-N-C-CA-CB         | 110.10             | 100.33          | 1                  |
| CA-C-N              | 116.20             | 105.91          | 1                  |
| CA-CB-CG            | 112.60             | 107.46          | 1                  |
| N-CA-CB             | 110.50             | 119.24          | 1                  |
| N-CA-CA-C-O         | 120.80             | 129.54          | 1                  |
| CA-CB-CG            | 113.80             | 108.66          | 1                  |
| N-CA-CB             | 110.50             | 101.76          | 2                  |
| C-N-CA              | 121.70             | 112.45          | 1                  |
| CA-C-C-CA-NE-CZ-NH1 | 121.50             | 116.36          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-CA-C-C-CA-CB      | 110.10             | 119.86          | 2                  |
| N-CA-C                 | 111.00             | 96.62           | 1                  |
| C-N-CA                 | 121.70             | 130.95          | 1                  |
| N-CA-CA-CB-CG          | 112.60             | 107.46          | 1                  |
| N-CA-C                 | 111.00             | 125.38          | 2                  |
| C-N-C-N-CA             | 121.70             | 130.94          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 120.23          | 1                  |
| N-CA-N-CA-CB           | 110.50             | 119.23          | 1                  |
| C-CA-CB                | 110.10             | 100.35          | 1                  |
| N-CA-C                 | 111.00             | 125.37          | 1                  |
| C-N-CA                 | 121.70             | 130.94          | 1                  |
| N-CA-CB                | 110.50             | 119.23          | 1                  |
| N-CA-C-N-N-CA-CB       | 110.50             | 119.22          | 1                  |
| C-CA-N-CA-CA-C-C-CA-CB | 110.10             | 119.85          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 101.78          | 1                  |
| C-CA-C-N-CA            | 121.70             | 112.47          | 1                  |
| C-N-C-CA-C-N-CA        | 121.70             | 112.47          | 1                  |
| N-CA-N-CA-CB           | 111.50             | 120.21          | 1                  |
| C-N-CA-N-N-CA-C        | 111.00             | 96.65           | 1                  |
| C-CA-CB                | 110.10             | 119.84          | 2                  |
| C-CA-CA-C-O            | 120.80             | 129.51          | 1                  |
| CA-C-O                 | 120.80             | 112.09          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB           | 111.50             | 120.21          | 1                  |
| C-CA-C-N-C-CA-N-CA-CB  | 110.50             | 101.79          | 1                  |
| C-N-CA                 | 121.70             | 130.92          | 1                  |
| C-CA-CB                | 110.10             | 100.37          | 1                  |
| C-CA-CA-C-N            | 116.20             | 126.44          | 1                  |
| C-N-CA                 | 121.70             | 112.48          | 1                  |
| C-CA-CB                | 110.10             | 119.83          | 1                  |
| CA-CB-C-CA-CB          | 110.10             | 100.37          | 1                  |
| N-CA-CB                | 111.50             | 102.80          | 2                  |
| N-CA-CB                | 110.40             | 102.72          | 1                  |
| CA-C-N                 | 116.90             | 109.22          | 1                  |
| CA-C-CA-C-NE-CZ-NH1    | 121.50             | 126.62          | 1                  |
| C-N-N-CA-CB            | 103.00             | 97.37           | 1                  |
| C-CA-CB                | 110.10             | 119.82          | 2                  |
| CA-C-O                 | 120.80             | 112.10          | 1                  |
| CA-C-N-CA-C            | 111.00             | 125.33          | 1                  |
| CA-C-C-CA-CB           | 110.10             | 100.38          | 1                  |
| CA-C-C-N-CA            | 121.70             | 112.49          | 1                  |
| C-CA-CA-C-N-CA-CB      | 110.50             | 101.81          | 1                  |
| C-N-C-CA-NE-CZ-C-CA-CB | 110.10             | 119.81          | 1                  |
| CA-CB-CG               | 112.60             | 107.49          | 1                  |
| CA-CB-CG               | 113.80             | 118.91          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| CA-C-N            | 116.90             | 109.23          | 1                  |
| C-CA-CB-CG-CA-C-N | 116.20             | 105.98          | 1                  |
| CA-C-O            | 120.80             | 112.11          | 1                  |
| N-CA-CB           | 111.50             | 102.81          | 1                  |
| N-CA-C            | 111.00             | 96.69           | 1                  |
| N-CA-CB           | 103.00             | 108.62          | 1                  |
| CA-C-O            | 120.80             | 129.48          | 1                  |
| N-CA-CA-CB-CG     | 113.80             | 108.69          | 1                  |
| C-N-CA            | 121.70             | 112.51          | 2                  |
| CB-CG-N-CA-CB     | 110.50             | 101.82          | 1                  |
| C-CA-CA-N-CD      | 112.00             | 104.85          | 1                  |
| C-CA-N-CA-CB      | 103.00             | 97.38           | 1                  |
| N-CA-N-CA-CB      | 111.50             | 102.82          | 1                  |
| CA-C-O            | 120.80             | 112.12          | 1                  |
| C-CA-CB           | 110.10             | 100.40          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 100.40          | 1                  |
| N-CA-C-CA-N-CA-C  | 111.00             | 96.71           | 1                  |
| CA-C-N-CA-CB      | 111.50             | 102.83          | 1                  |
| CA-C-O            | 120.80             | 129.47          | 1                  |
| C-CA-CB           | 110.10             | 119.79          | 1                  |
| CA-CB-CA-C-N      | 116.20             | 106.00          | 1                  |
| N-CA-CB           | 111.50             | 102.83          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-N             | 116.20             | 126.40          | 1                  |
| C-CA-CB                 | 110.10             | 100.41          | 1                  |
| CA-C-C-N-CA             | 121.70             | 130.88          | 1                  |
| C-N-CA                  | 121.70             | 112.53          | 1                  |
| C-CA-N-CA-CB            | 103.00             | 97.39           | 1                  |
| CA-C-O                  | 120.80             | 112.14          | 1                  |
| C-N-N-CA-CB             | 110.50             | 101.84          | 1                  |
| C-N-CA                  | 121.70             | 130.87          | 1                  |
| C-CA-N-CA-CB            | 111.50             | 102.84          | 1                  |
| N-CA-CB                 | 110.50             | 101.84          | 2                  |
| N-CA-CB                 | 110.50             | 119.16          | 1                  |
| N-CA-CB                 | 111.50             | 102.84          | 1                  |
| N-CA-N-CA-NE-CZ-C-CA-CB | 110.10             | 100.42          | 1                  |
| C-CA-CB                 | 110.10             | 119.77          | 3                  |
| CA-C-NE-CZ-C-CA-CB      | 110.10             | 119.77          | 1                  |
| C-N-C-CA-N-CA-CB        | 110.50             | 119.15          | 1                  |
| CA-C-C-CA-CA-C-N        | 116.90             | 109.27          | 1                  |
| C-N-CA                  | 121.70             | 130.86          | 3                  |
| CA-C-C-CA-NE-CZ-C-CA-CB | 111.60             | 101.42          | 1                  |
| N-CA-CB                 | 110.50             | 119.15          | 1                  |
| N-CA-CA-C-O             | 120.80             | 129.45          | 1                  |
| CA-C-N                  | 116.20             | 106.02          | 1                  |



| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| CA-C-N                          | 116.20             | 126.38          | 1                  |
| N-CA-CB                         | 111.50             | 120.15          | 1                  |
| CA-C-O                          | 120.80             | 129.45          | 1                  |
| C-CA-CB                         | 110.10             | 119.76          | 2                  |
| CA-C-O                          | 120.80             | 112.16          | 1                  |
| CA-C-N-CA-C-CA-C-CA-N-CA-C-N-CA | 121.70             | 130.85          | 1                  |
| CA-C-CA-C-N-CA-CB               | 103.00             | 97.41           | 1                  |
| CA-C-CA-C-O                     | 120.80             | 112.16          | 1                  |
| CA-C-N                          | 116.90             | 109.28          | 1                  |
| C-CA-CA-C-N                     | 116.90             | 124.52          | 1                  |
| N-CA-CA-C-O                     | 120.80             | 112.17          | 1                  |
| C-CA-C-CA-C-N-CA                | 121.70             | 112.56          | 1                  |
| C-N-CA                          | 121.70             | 130.84          | 1                  |
| N-CA-C                          | 111.00             | 125.22          | 1                  |
| CA-C-O                          | 120.80             | 112.17          | 1                  |
| N-CA-C-CA-C-N-CA                | 121.70             | 130.84          | 1                  |
| CA-C-CA-C-C-N-CA                | 121.70             | 130.84          | 1                  |
| C-CA-CB                         | 110.10             | 119.74          | 2                  |
| C-CA-N-CA-CB                    | 110.50             | 101.87          | 1                  |
| CA-C-C-CA-CB                    | 111.60             | 101.45          | 1                  |
| C-N-CA                          | 121.70             | 112.57          | 1                  |
| CA-C-N                          | 116.20             | 106.06          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CA-C-O     | 120.80             | 112.18          | 1                  |
| CA-C-O               | 120.80             | 112.18          | 1                  |
| C-CA-CA-C-O          | 120.80             | 129.42          | 1                  |
| C-CA-CB              | 110.10             | 119.73          | 1                  |
| C-CA-C-CA-CB         | 110.10             | 100.47          | 1                  |
| C-CA-CB              | 110.10             | 100.47          | 1                  |
| N-CA-OE1-CD-OE2      | 122.90             | 135.06          | 1                  |
| N-CA-CB              | 111.50             | 102.89          | 1                  |
| CA-C-O               | 120.80             | 129.41          | 2                  |
| CA-CB-N-CA-C         | 111.00             | 96.81           | 1                  |
| C-CA-CA-C-N          | 116.90             | 109.30          | 1                  |
| C-N-CA               | 121.70             | 130.82          | 1                  |
| N-CA-CB              | 110.50             | 119.11          | 1                  |
| CA-CB-CA-C-C-N-CA    | 121.70             | 112.58          | 1                  |
| N-CA-CA-C-N          | 116.20             | 106.07          | 1                  |
| CA-C-N               | 116.20             | 106.07          | 1                  |
| C-N-C-N-N-CA-CB      | 110.50             | 119.11          | 1                  |
| CA-C-C-CA-C-N-C-N-CA | 121.70             | 130.81          | 1                  |
| N-CA-CB              | 110.50             | 101.90          | 2                  |
| C-CA-CB              | 110.10             | 119.72          | 1                  |
| C-CA-C-CA-N-CA-CB    | 110.50             | 119.10          | 1                  |
| CA-C-C-CA-CB         | 111.60             | 101.48          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                       | 113.80             | 118.86          | 1                  |
| C-N-N-CA-N-CA-CA-C-O           | 120.80             | 129.40          | 1                  |
| CA-C-N                         | 116.20             | 106.08          | 1                  |
| C-N-CA                         | 121.70             | 130.81          | 1                  |
| C-CA-CB                        | 110.10             | 100.49          | 1                  |
| C-CA-C-CA-CB                   | 110.10             | 100.49          | 1                  |
| C-N-C-CA-CA-C-N                | 116.20             | 126.31          | 1                  |
| CA-C-O                         | 120.80             | 129.40          | 1                  |
| C-N-CA                         | 121.70             | 130.80          | 1                  |
| CA-C-C-N-C-CA-CA-C-C-CA-C-N-CA | 121.70             | 130.80          | 1                  |
| CA-C-N                         | 116.20             | 106.09          | 1                  |
| N-CA-CB                        | 103.00             | 108.56          | 1                  |
| N-CA-C-CA-C-CA-CB              | 110.10             | 100.50          | 1                  |
| CA-C-N                         | 116.20             | 126.31          | 1                  |
| N-CA-N-CA-CA-C-N               | 116.20             | 106.10          | 1                  |
| CA-C-N-CA-C-N-CA-CB-CG         | 112.60             | 107.55          | 1                  |
| C-CA-CB                        | 110.10             | 100.50          | 1                  |
| C-CA-CB                        | 110.10             | 119.70          | 1                  |
| N-CA-CB                        | 110.50             | 119.09          | 1                  |
| C-CA-CB                        | 110.50             | 102.92          | 1                  |
| CA-CB-CG                       | 113.80             | 108.75          | 1                  |
| CA-C-C-CA-CB                   | 110.10             | 100.51          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB         | 110.10             | 119.69          | 1                  |
| CA-C-C-CA-CB         | 110.10             | 119.69          | 1                  |
| C-CA-CB              | 109.10             | 120.21          | 1                  |
| N-CA-C-CA-CB         | 111.60             | 101.50          | 1                  |
| N-CA-CB              | 111.50             | 120.08          | 1                  |
| C-N-CA               | 121.70             | 130.78          | 1                  |
| N-CA-CB              | 111.50             | 102.92          | 1                  |
| C-CA-CB              | 110.10             | 119.69          | 1                  |
| N-CA-C               | 111.00             | 125.13          | 2                  |
| C-CA-CA-C-O          | 120.80             | 129.38          | 1                  |
| CA-C-CA-C-N-CA-CB    | 110.50             | 101.92          | 1                  |
| CA-C-C-CA-CB         | 110.10             | 119.68          | 2                  |
| CA-C-N-CA-OE1-CD-NE2 | 122.60             | 127.64          | 1                  |
| C-CA-C-CA-N-CA-CB    | 111.50             | 102.93          | 1                  |
| N-CA-OE1-CD-OE2      | 122.90             | 135.00          | 1                  |
| CA-C-N               | 116.90             | 109.34          | 1                  |
| C-CA-CA-C-N          | 116.20             | 126.28          | 1                  |
| CA-CB-CG             | 112.60             | 107.56          | 2                  |
| C-CA-N-CA-C          | 111.00             | 96.89           | 1                  |
| N-CA-C-CA-CB         | 110.10             | 119.67          | 1                  |
| N-CA-N-CA-CB         | 110.50             | 119.07          | 1                  |
| C-CA-CB              | 111.40             | 101.83          | 1                  |

| Angle type                            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                               | 110.10             | 100.53          | 1                  |
| C-CA-N-CA-CA-C-C-CA-CA-C-N-CA-C-CA-CB | 109.10             | 120.18          | 1                  |
| C-CA-C-N-CA                           | 121.70             | 112.63          | 1                  |
| C-N-CA                                | 121.70             | 112.64          | 1                  |
| CA-CB-CG                              | 113.80             | 118.84          | 1                  |
| CA-CB-CG                              | 113.80             | 108.76          | 1                  |
| C-CA-C-CA-CB                          | 110.10             | 119.67          | 1                  |
| N-CA-CB                               | 110.50             | 101.94          | 2                  |
| CA-C-O                                | 120.80             | 129.36          | 2                  |
| C-CA-CB                               | 109.10             | 98.03           | 1                  |
| C-CA-CB                               | 109.10             | 120.17          | 1                  |
| C-CA-CB                               | 110.50             | 102.95          | 1                  |
| CA-C-N                                | 116.20             | 106.14          | 1                  |
| CA-C-CA-C-N                           | 116.20             | 126.26          | 1                  |
| CA-C-N                                | 116.20             | 126.26          | 1                  |
| C-CA-CB-CG-CA-C-O                     | 120.80             | 112.25          | 1                  |
| CA-C-C-CA-CB                          | 110.10             | 100.54          | 1                  |
| C-N-N-CA-C                            | 111.00             | 96.92           | 1                  |
| C-N-CA                                | 121.70             | 130.75          | 2                  |
| CB-CG-C-N-CA                          | 121.70             | 112.65          | 1                  |
| CA-C-O                                | 120.80             | 112.25          | 2                  |
| C-CA-CB                               | 111.60             | 101.54          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                    | 110.10             | 119.65          | 2                  |
| CA-C-O                     | 120.80             | 129.35          | 1                  |
| N-CA-C-N-C-CA-CB           | 111.60             | 101.54          | 1                  |
| C-N-C-CA-CB                | 111.60             | 101.55          | 1                  |
| C-N-CA-C-O                 | 120.80             | 129.35          | 1                  |
| C-CA-CB                    | 110.50             | 102.96          | 1                  |
| CA-C-N                     | 116.90             | 109.36          | 1                  |
| N-CA-C-N-CA                | 121.70             | 112.65          | 1                  |
| C-CA-CB                    | 110.10             | 100.55          | 1                  |
| N-CA-C-N-N-CA-N-CA-C-CA-CB | 110.10             | 119.65          | 1                  |
| N-CA-N-CA-CB               | 111.50             | 102.96          | 1                  |
| C-CA-CB                    | 109.10             | 120.15          | 1                  |
| C-N-N-CA-C-CA-CA-C-N       | 116.20             | 106.15          | 1                  |
| C-CA-N-CA-CB               | 110.50             | 101.96          | 1                  |
| C-N-CA-CB-CG               | 112.60             | 107.58          | 1                  |
| C-CA-CB                    | 110.10             | 119.64          | 1                  |
| CA-CB-CG                   | 113.80             | 108.78          | 1                  |
| C-CA-C-CA-CA-C-O           | 120.80             | 129.33          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 119.64          | 1                  |
| N-CA-C-N-CA                | 121.70             | 112.67          | 2                  |
| CA-C-O                     | 120.80             | 129.33          | 2                  |
| C-CA-CA-C-N                | 116.20             | 126.24          | 1                  |

| Angle type   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------|--------------------|-----------------|--------------------|
| C-N-N-CA-C   | 111.00             | 125.05          | 1                  |
| N-CA-C       | 111.00             | 125.05          | 1                  |
| N-CA-N-CA-CB | 110.50             | 101.97          | 1                  |
| N-CA-C       | 111.00             | 125.04          | 1                  |
| OE1-CD-NE2   | 122.60             | 127.62          | 1                  |
| N-CA-C-CA-CB | 110.10             | 119.63          | 1                  |
| C-N-CA       | 121.70             | 130.73          | 1                  |
| N-CA-CA-C-O  | 120.80             | 129.33          | 1                  |
| C-N-CA       | 121.70             | 112.67          | 2                  |
| C-CA-CB      | 109.10             | 98.07           | 1                  |
| CA-C-O       | 120.80             | 129.32          | 1                  |
| C-CA-CB      | 110.10             | 119.63          | 1                  |
| C-N-CA-C-N   | 116.20             | 106.17          | 1                  |
| CA-C-N-CA-CB | 110.50             | 119.02          | 1                  |
| CG-CD2-CE2   | 107.20             | 101.18          | 1                  |
| C-CA-CB      | 110.10             | 119.62          | 1                  |
| C-CA-CB      | 110.10             | 100.58          | 1                  |
| N-CA-CB      | 110.50             | 101.98          | 1                  |
| CA-N-C-CA-CB | 110.50             | 118.02          | 1                  |
| CA-C-N       | 116.20             | 106.18          | 1                  |
| C-N-CA       | 121.70             | 112.68          | 1                  |
| N-CA-C-CA-CB | 111.60             | 101.58          | 1                  |

| Angle type                   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------|--------------------|-----------------|--------------------|
| N-CA-C-N-C-CA-CB             | 110.10             | 119.62          | 1                  |
| C-CA-CB                      | 110.10             | 100.59          | 1                  |
| C-CA-CB                      | 110.10             | 119.61          | 1                  |
| CA-C-N-CA-C                  | 111.00             | 125.02          | 1                  |
| C-CA-CB                      | 111.60             | 101.59          | 1                  |
| CA-C-C-CA-CA-C-O             | 120.80             | 129.31          | 1                  |
| N-CA-C-CA-N-CA-N-CA-CA-CB-CG | 112.60             | 107.60          | 1                  |
| N-CA-CB                      | 110.50             | 119.01          | 1                  |
| C-N-CD                       | 125.00             | 104.49          | 1                  |
| CA-CB-CG                     | 112.60             | 107.60          | 4                  |
| N-CA-CA-C-CA-C-N-CA-CB       | 103.00             | 108.50          | 1                  |
| N-CA-C-CA-CB                 | 110.10             | 100.60          | 2                  |
| C-CA-CB                      | 110.10             | 119.60          | 2                  |
| C-CA-CB                      | 111.40             | 101.90          | 1                  |
| C-N-CA                       | 121.70             | 130.70          | 1                  |
| C-CA-CA-C-N                  | 116.90             | 109.40          | 1                  |
| OE1-CD-OE2                   | 122.90             | 134.90          | 1                  |
| C-N-CA                       | 121.70             | 112.70          | 1                  |
| CA-C-N                       | 116.20             | 126.20          | 1                  |
| CA-CB-CG                     | 113.80             | 108.80          | 1                  |
| N-CA-CA-C-C-N-C-CA-CB        | 109.10             | 98.11           | 1                  |
| OE1-CD-OE2                   | 122.90             | 134.89          | 1                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-CB-CG          | 112.60             | 107.61          | 1                  |
| C-N-CA                 | 121.70             | 112.71          | 1                  |
| CA-C-O                 | 120.80             | 129.29          | 1                  |
| N-CA-CB                | 110.50             | 102.01          | 1                  |
| C-N-CA                 | 121.70             | 130.69          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 100.61          | 1                  |
| CA-C-N                 | 116.20             | 126.19          | 1                  |
| C-CA-C-N-C-N-CA-N-CD   | 112.00             | 105.01          | 1                  |
| CB-CG-N-CA-CB          | 110.50             | 118.99          | 1                  |
| C-N-CA                 | 121.70             | 130.68          | 1                  |
| C-N-CD                 | 125.00             | 104.54          | 1                  |
| C-CA-CB                | 110.10             | 119.58          | 1                  |
| CA-C-CA-C-CA-CB-CG     | 113.80             | 108.81          | 1                  |
| N-CA-C-N-CA            | 121.70             | 130.68          | 1                  |
| C-N-CA-C-O             | 120.80             | 129.28          | 1                  |
| CA-C-N-CA-CA-C-O       | 120.80             | 112.32          | 1                  |
| N-CA-N-CA-C            | 111.00             | 124.96          | 1                  |
| N-CA-CB                | 110.50             | 102.03          | 1                  |
| C-CA-CB                | 110.10             | 119.57          | 1                  |
| N-CA-CA-C-N-CA-C-CA-CB | 110.10             | 119.57          | 1                  |
| CA-CB-CA-N-CA-C-N      | 116.20             | 126.17          | 1                  |
| C-CA-CB                | 110.10             | 100.63          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-C-O                 | 120.80             | 129.27          | 2                  |
| C-CA-CA-CB-CG          | 113.80             | 118.78          | 1                  |
| CA-CB-C-CA-N-CA-CA-C-O | 120.80             | 129.27          | 1                  |
| C-N-CA                 | 121.70             | 112.74          | 2                  |
| C-CA-C-CA-CB           | 109.10             | 120.06          | 1                  |
| CA-C-N                 | 116.20             | 106.24          | 1                  |
| C-CA-CB                | 110.10             | 119.56          | 2                  |
| C-CA-C-N-N-CA-CB       | 110.50             | 102.04          | 1                  |
| N-CA-CB                | 111.50             | 103.04          | 1                  |
| N-CA-CB                | 110.50             | 118.96          | 1                  |
| C-N-CD                 | 125.00             | 104.59          | 1                  |
| N-CA-CB                | 110.50             | 102.04          | 2                  |
| C-N-CA                 | 121.70             | 130.66          | 1                  |
| C-N-N-CA-CB            | 111.50             | 119.96          | 1                  |
| CA-C-CA-C-N            | 116.20             | 106.25          | 1                  |
| CA-C-N                 | 116.20             | 106.25          | 1                  |
| C-CA-CB                | 110.10             | 119.55          | 4                  |
| C-CA-C-N-CA            | 121.70             | 112.74          | 1                  |
| CA-CB-CG               | 112.60             | 107.62          | 1                  |
| C-CA-N-CA-CB           | 111.50             | 103.04          | 1                  |
| C-CA-C-N-CA            | 121.70             | 112.75          | 1                  |
| C-CA-CA-C-O            | 120.80             | 129.25          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 100.65          | 1                  |
| CA-C-N            | 116.20             | 126.14          | 1                  |
| CA-N-CD           | 112.00             | 105.04          | 1                  |
| C-CA-C-N-CD       | 125.00             | 104.62          | 1                  |
| CA-CB-CG          | 113.80             | 118.77          | 1                  |
| N-CA-CB           | 110.50             | 118.95          | 2                  |
| C-CA-CB           | 110.10             | 119.54          | 3                  |
| C-CA-N-CA-N-CA-C  | 111.00             | 124.91          | 1                  |
| CA-C-O            | 120.80             | 129.25          | 1                  |
| N-CA-C            | 111.00             | 97.09           | 1                  |
| CA-C-CA-C-C-N-CA  | 121.70             | 130.64          | 1                  |
| C-CA-CB           | 111.60             | 101.67          | 1                  |
| C-CA-CB           | 110.50             | 103.05          | 1                  |
| N-CA-CB           | 111.50             | 119.94          | 1                  |
| CA-CB-CG          | 113.80             | 108.83          | 1                  |
| C-N-CA            | 121.70             | 130.64          | 1                  |
| CA-C-O            | 120.80             | 129.24          | 1                  |
| C-N-C-CA-N-CA-C   | 113.30             | 127.69          | 1                  |
| CA-CB-N-CA-C-N-CA | 121.70             | 112.77          | 1                  |
| CA-CB-N-CA-CB     | 111.50             | 103.07          | 1                  |
| C-N-CA            | 121.70             | 130.63          | 1                  |
| CA-C-O            | 120.80             | 129.23          | 3                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| CA-C-N                   | 116.20             | 106.28          | 1                  |
| C-CA-C-N-C-N-C-CA-N-CA-C | 111.00             | 97.11           | 1                  |
| CA-C-C-CA-CB             | 110.10             | 119.52          | 1                  |
| C-CA-N-CA-CA-C-N         | 116.20             | 106.28          | 1                  |
| CA-C-CA-C-N-CA-C-N-CA    | 121.70             | 112.78          | 1                  |
| C-CA-CB                  | 110.10             | 119.52          | 3                  |
| CA-C-O                   | 120.80             | 112.37          | 1                  |
| CA-C-C-N-CA              | 121.70             | 130.62          | 1                  |
| N-CA-CB                  | 110.50             | 102.07          | 1                  |
| N-CA-C                   | 111.00             | 124.88          | 1                  |
| C-N-C-CA-CB              | 111.60             | 121.51          | 1                  |
| CA-CB-CG                 | 112.60             | 107.64          | 1                  |
| N-CA-CB                  | 110.50             | 118.92          | 1                  |
| C-CA-CB                  | 111.60             | 121.51          | 1                  |
| CA-C-N                   | 116.20             | 106.29          | 1                  |
| N-CA-C-N-CA              | 121.70             | 112.78          | 1                  |
| C-N-CA                   | 121.70             | 112.78          | 1                  |
| N-CA-CB                  | 111.50             | 119.92          | 1                  |
| C-N-CA                   | 121.70             | 130.62          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 119.51          | 1                  |
| C-N-CA                   | 121.70             | 130.61          | 1                  |
| N-CA-C                   | 112.10             | 99.72           | 2                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB           | 111.50             | 103.08          | 1                  |
| C-CA-CB                | 110.10             | 119.51          | 2                  |
| C-N-CA                 | 121.70             | 112.79          | 1                  |
| CA-C-O                 | 120.80             | 112.38          | 1                  |
| N-CA-CB                | 103.00             | 108.45          | 1                  |
| CA-C-N                 | 116.20             | 106.30          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 119.50          | 1                  |
| CB-CG-CB-CG-CA-C-N     | 116.20             | 106.30          | 1                  |
| N-CA-C                 | 111.00             | 97.15           | 1                  |
| N-CA-CA-C-N-CA-C       | 111.00             | 97.15           | 1                  |
| N-CA-CA-C-CA-CB-CG     | 112.60             | 107.65          | 1                  |
| CA-C-C-N-C-CA-CB       | 110.50             | 117.92          | 1                  |
| CA-C-N                 | 116.20             | 106.31          | 1                  |
| N-CA-C                 | 111.00             | 124.85          | 1                  |
| C-CA-C-CA-CA-CB-CG     | 113.80             | 118.74          | 1                  |
| N-CA-C                 | 111.00             | 97.16           | 1                  |
| N-CA-C-CA-CB           | 110.10             | 119.49          | 1                  |
| CA-C-N                 | 116.20             | 126.09          | 1                  |
| C-N-CA                 | 121.70             | 112.80          | 1                  |
| C-CA-CA-C-O            | 120.80             | 112.40          | 1                  |
| C-CA-CA-CB-CG          | 112.60             | 107.66          | 1                  |
| N-CA-C-CA-C-CA-C-CA-CB | 109.10             | 98.23           | 1                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| CA-C-O              | 120.80             | 129.20          | 1                  |
| N-CA-N-CA-C         | 111.00             | 97.17           | 1                  |
| CA-C-N              | 116.20             | 126.08          | 1                  |
| C-N-CA              | 121.70             | 112.81          | 1                  |
| N-CA-C              | 111.00             | 124.83          | 1                  |
| CA-C-N              | 116.20             | 106.32          | 1                  |
| N-CA-C-CA-N-CA-C    | 111.00             | 124.82          | 1                  |
| C-CA-C-N-C-N-CA     | 121.70             | 112.82          | 1                  |
| N-CA-C              | 113.30             | 127.61          | 1                  |
| C-CA-CB             | 110.10             | 119.48          | 1                  |
| N-CA-C              | 111.00             | 97.18           | 1                  |
| CA-C-C-CA-CA-CB-CG2 | 110.50             | 118.89          | 1                  |
| CA-C-C-N-CA         | 121.70             | 130.58          | 1                  |
| CA-CB-CG2           | 110.50             | 118.88          | 1                  |
| CA-C-O              | 120.80             | 129.18          | 1                  |
| CB-CG-CA-CB-CA-C-O  | 120.80             | 129.18          | 1                  |
| C-CA-CB             | 109.10             | 119.94          | 1                  |
| N-CA-C              | 111.00             | 124.80          | 1                  |
| C-CA-C-CA-CB        | 109.10             | 119.94          | 1                  |
| C-CA-C-CA-C-CA-CB   | 109.10             | 98.26           | 1                  |
| CA-C-N              | 116.20             | 106.34          | 1                  |
| C-CA-CA-C-N         | 116.20             | 106.34          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-CB-CG              | 112.60             | 107.67          | 1                  |
| C-CA-CB               | 110.10             | 119.46          | 3                  |
| N-CA-CB               | 110.50             | 118.88          | 1                  |
| C-N-C-N-C-CA-CA-CB-CG | 113.80             | 118.73          | 1                  |
| N-CA-CB               | 111.50             | 119.87          | 1                  |
| N-CA-C-CA-CA-C-CA-C-O | 120.80             | 129.17          | 1                  |
| CA-C-N-CA-CB          | 110.50             | 102.13          | 1                  |
| C-CA-CB               | 111.60             | 101.75          | 1                  |
| N-CA-CB               | 110.40             | 103.01          | 1                  |
| N-CA-C                | 111.00             | 97.21           | 1                  |
| C-N-C-CA-C-N-CA       | 121.70             | 130.56          | 1                  |
| N-CA-C                | 111.00             | 124.78          | 1                  |
| C-N-CA                | 121.70             | 112.84          | 1                  |
| C-CA-CB               | 110.10             | 119.45          | 1                  |
| N-CA-C                | 111.00             | 97.22           | 2                  |
| N-CA-CB               | 110.50             | 118.87          | 1                  |
| CA-CB-CG2             | 110.50             | 118.86          | 1                  |
| N-CA-C                | 113.30             | 127.57          | 1                  |
| C-N-C-CA-C-CA-CB      | 109.10             | 119.92          | 1                  |
| N-CA-C                | 111.00             | 124.77          | 1                  |
| CA-C-O                | 120.80             | 129.16          | 1                  |
| C-N-CA-C-O            | 120.80             | 112.44          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB-CG-CD     | 112.60             | 120.96          | 1                  |
| N-CA-CB           | 111.50             | 103.14          | 1                  |
| C-CA-C-N-CA-C-N   | 116.20             | 106.37          | 1                  |
| CA-C-N            | 116.20             | 126.03          | 1                  |
| C-N-CA-C-N        | 116.20             | 106.37          | 1                  |
| N-CA-CB           | 110.50             | 102.14          | 1                  |
| C-N-CA-C-N        | 116.20             | 126.03          | 1                  |
| C-CA-C-N-CA       | 121.70             | 112.85          | 1                  |
| C-CA-CB           | 110.10             | 100.76          | 1                  |
| C-N-C-CA-N-CA-CB  | 110.50             | 118.85          | 1                  |
| N-CA-C            | 111.00             | 97.24           | 1                  |
| C-CA-CA-C-O       | 120.80             | 112.45          | 1                  |
| CA-CB-CG2         | 110.50             | 118.85          | 1                  |
| CA-C-CA-C-C-CA-CB | 109.10             | 98.29           | 1                  |
| CA-C-N            | 116.20             | 106.38          | 1                  |
| C-CA-N-CA-C       | 111.00             | 97.25           | 1                  |
| C-N-CA            | 121.70             | 112.86          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 100.77          | 1                  |
| CA-N-CD           | 112.00             | 118.87          | 1                  |
| C-CA-CB           | 110.10             | 119.43          | 1                  |
| CA-C-N-CA-N-CA-CB | 103.00             | 108.40          | 1                  |
| N-CA-C            | 111.00             | 97.26           | 1                  |



| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                  | 110.10             | 119.42          | 2                  |
| C-N-CA                   | 121.70             | 112.87          | 2                  |
| N-CA-CA-C-N              | 116.20             | 106.39          | 1                  |
| C-N-CA-CB-CG             | 113.80             | 118.71          | 1                  |
| C-CA-N-CA-C              | 111.00             | 124.73          | 1                  |
| CA-CB-CG2                | 110.50             | 118.84          | 1                  |
| CA-C-O                   | 120.80             | 129.14          | 1                  |
| CA-C-N                   | 116.20             | 126.01          | 1                  |
| N-CA-C-CA-CB             | 110.10             | 100.78          | 1                  |
| CA-CB-CG2                | 110.50             | 118.83          | 1                  |
| C-CA-C-CA-CA-C-N         | 116.20             | 106.40          | 1                  |
| C-CA-CA-C-O              | 120.80             | 129.13          | 1                  |
| N-CA-N-CA-C              | 111.00             | 97.28           | 1                  |
| N-CA-CB                  | 110.50             | 102.17          | 1                  |
| N-CA-CB                  | 111.50             | 103.17          | 1                  |
| C-CA-CB                  | 110.50             | 117.85          | 1                  |
| CA-C-C-CA-CB             | 110.50             | 103.15          | 1                  |
| CA-C-CA-CB-CG            | 112.60             | 107.70          | 1                  |
| N-CA-N-CA-C              | 111.00             | 97.29           | 1                  |
| CA-N-CD                  | 112.00             | 118.86          | 1                  |
| C-N-CA-C-C-CA-C-N-CA-C-O | 120.80             | 129.12          | 1                  |
| N-CA-C-N-CA              | 121.70             | 130.51          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 119.40          | 1                  |
| CA-C-O            | 120.80             | 112.48          | 1                  |
| C-N-CA            | 121.70             | 112.89          | 1                  |
| N-CA-CB           | 110.50             | 102.18          | 1                  |
| CB-CG-CD          | 112.60             | 120.92          | 1                  |
| C-N-C-CA-CB       | 109.10             | 119.86          | 1                  |
| C-N-CA            | 121.70             | 130.50          | 1                  |
| C-CA-N-CA-C-N-CA  | 121.70             | 130.50          | 1                  |
| C-CA-CA-C-N       | 116.20             | 106.42          | 1                  |
| N-CA-CA-CB-CG2    | 110.50             | 118.81          | 1                  |
| C-CA-CB           | 110.10             | 100.81          | 1                  |
| N-CA-C            | 111.00             | 97.31           | 1                  |
| CA-C-N            | 116.20             | 106.42          | 1                  |
| C-CA-C-CA-CA-C-O  | 120.80             | 112.49          | 1                  |
| N-CA-CB           | 110.40             | 103.07          | 1                  |
| N-CA-C            | 111.00             | 124.68          | 1                  |
| C-N-C-CA-CB       | 110.10             | 119.38          | 1                  |
| C-CA-CB           | 110.10             | 119.38          | 1                  |
| CA-C-N-CA-C-CA-CB | 110.10             | 119.38          | 1                  |
| C-N-CA            | 121.70             | 130.49          | 1                  |
| N-CA-N-CA-C       | 111.00             | 124.67          | 1                  |
| C-CA-CB           | 110.10             | 100.82          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-C-CA-CB                | 110.10             | 119.37          | 1                  |
| N-CA-C                           | 111.00             | 124.67          | 1                  |
| N-CA-C                           | 111.00             | 124.66          | 2                  |
| N-CA-CB                          | 110.50             | 118.80          | 1                  |
| C-N-CA                           | 121.70             | 130.48          | 1                  |
| C-CA-CB                          | 110.10             | 119.37          | 2                  |
| N-CA-C-CA-N-CA-N-CA-C-CA-C-CA-CB | 110.10             | 100.83          | 1                  |
| N-CA-CB                          | 110.50             | 102.21          | 1                  |
| C-CA-CA-C-N                      | 116.20             | 125.95          | 1                  |
| C-N-C-CA-N-CA-C-CA-C-CA-CB       | 110.10             | 100.84          | 1                  |
| C-N-C-CA-C-N-CA                  | 121.70             | 130.47          | 1                  |
| C-CA-CB                          | 110.10             | 119.36          | 1                  |
| CA-C-O                           | 120.80             | 129.09          | 1                  |
| CA-C-O                           | 120.80             | 112.51          | 1                  |
| C-N-CD                           | 125.00             | 105.02          | 1                  |
| N-CA-C                           | 111.00             | 124.65          | 1                  |
| C-N-C-N-CA                       | 121.70             | 130.47          | 1                  |
| C-CA-N-CA-C-CA-CB                | 110.10             | 119.36          | 1                  |
| N-CA-C-N-CA                      | 121.70             | 130.47          | 1                  |
| C-N-CA-C-O                       | 120.80             | 129.08          | 1                  |
| C-CA-CB                          | 110.10             | 119.35          | 2                  |
| C-N-CA                           | 121.70             | 130.47          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA-C-C-CA-CB   | 111.60             | 101.86          | 1                  |
| C-N-CA                  | 121.70             | 112.94          | 3                  |
| N-CA-C                  | 111.00             | 124.63          | 1                  |
| C-CA-N-CA-N-CA-CA-CB-CG | 113.80             | 108.93          | 1                  |
| CA-CB-CG                | 113.80             | 108.93          | 1                  |
| C-CA-CB                 | 109.10             | 98.39           | 1                  |
| CA-CB-CG2               | 110.50             | 118.77          | 2                  |
| CA-CB-CG                | 113.80             | 118.67          | 1                  |
| N-CA-CB                 | 110.50             | 102.23          | 1                  |
| C-CA-CB                 | 109.10             | 119.80          | 1                  |
| C-CA-CB                 | 110.10             | 119.34          | 1                  |
| CA-C-O                  | 120.80             | 112.53          | 2                  |
| N-CA-CB                 | 111.50             | 103.23          | 1                  |
| C-N-CA                  | 121.70             | 112.95          | 2                  |
| N-CA-C-CA-N-CA-C-CA-CB  | 110.10             | 119.34          | 1                  |
| N-CA-C                  | 111.00             | 124.62          | 1                  |
| CA-CB-CG                | 113.80             | 118.66          | 1                  |
| C-CA-CB                 | 110.10             | 100.86          | 2                  |
| C-N-CD                  | 125.00             | 105.07          | 1                  |
| CA-C-O                  | 120.80             | 129.06          | 2                  |
| C-CA-CB                 | 110.10             | 119.33          | 1                  |
| N-CA-C                  | 111.00             | 124.60          | 2                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-CB-CG2             | 110.50             | 118.76          | 2                  |
| CA-C-N-CA-N-CA-C-N-CA | 121.70             | 112.96          | 1                  |
| C-N-CA                | 121.70             | 112.96          | 2                  |
| C-N-CA                | 121.70             | 130.44          | 1                  |
| C-CA-CB               | 109.10             | 98.42           | 1                  |
| C-CA-CB               | 110.10             | 119.32          | 2                  |
| C-CA-CB               | 110.10             | 100.88          | 2                  |
| CA-CB-CA-N-C-CA-CB    | 109.10             | 119.78          | 1                  |
| CA-CB-N-CA-CB         | 110.50             | 102.25          | 1                  |
| N-CA-C-N-CA           | 121.70             | 112.97          | 1                  |
| CA-C-O                | 120.80             | 129.05          | 1                  |
| CA-N-CD               | 112.00             | 118.79          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 119.32          | 1                  |
| CA-C-N                | 116.20             | 106.50          | 1                  |
| N-CA-CB               | 110.50             | 118.74          | 1                  |
| CA-C-N                | 116.20             | 125.90          | 1                  |
| CA-N-CA-C-C-CA-CB     | 110.50             | 117.77          | 1                  |
| CA-CB-CG2             | 110.50             | 118.74          | 1                  |
| CA-C-O                | 120.80             | 129.04          | 1                  |
| N-CA-C                | 111.00             | 124.57          | 1                  |
| N-CA-C-CA-C-CA-CB     | 110.10             | 119.30          | 1                  |
| C-CA-CB               | 110.10             | 119.30          | 3                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-C-N-CA       | 121.70             | 130.42          | 1                  |
| N-CA-CB                | 111.50             | 103.27          | 2                  |
| CA-CB-CA-C-O           | 120.80             | 112.57          | 1                  |
| CA-C-CA-CB-CA-C-C-N-CA | 121.70             | 112.98          | 1                  |
| N-CA-CA-C-O            | 120.80             | 112.57          | 1                  |
| CA-CB-CG               | 113.80             | 118.64          | 1                  |
| CA-N-CD                | 112.00             | 118.78          | 1                  |
| CA-C-O                 | 120.80             | 112.57          | 2                  |
| CA-C-O                 | 120.80             | 130.96          | 1                  |
| N-CA-CA-CB-CG          | 112.60             | 107.76          | 1                  |
| CA-C-O                 | 120.80             | 129.03          | 1                  |
| C-CA-C-CA-CB           | 109.10             | 119.74          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 100.91          | 2                  |
| CA-C-O                 | 120.80             | 112.58          | 2                  |
| CA-C-N                 | 116.20             | 125.87          | 1                  |
| C-CA-CA-C-N            | 116.20             | 125.87          | 1                  |
| N-CA-C                 | 111.00             | 124.54          | 1                  |
| N-CA-N-CA-C-CA-CB      | 110.10             | 100.91          | 1                  |
| N-CA-C                 | 111.00             | 124.53          | 1                  |
| CA-CB-CA-C-C-N-CA      | 121.70             | 130.40          | 1                  |
| CA-C-O                 | 120.80             | 112.59          | 3                  |
| C-N-C-CA-CB            | 109.10             | 119.73          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-O                 | 120.80             | 112.59          | 1                  |
| CA-CB-C-N-CA               | 121.70             | 113.01          | 1                  |
| C-N-CA                     | 121.70             | 130.39          | 3                  |
| C-CA-CB                    | 109.10             | 119.72          | 1                  |
| C-CA-CB                    | 110.10             | 100.93          | 1                  |
| CA-C-C-CA-CB               | 110.10             | 100.93          | 1                  |
| C-CA-CB                    | 110.10             | 119.27          | 1                  |
| CA-CB-CG                   | 112.60             | 107.78          | 1                  |
| CA-C-O                     | 120.80             | 112.60          | 1                  |
| C-N-CA                     | 121.70             | 113.02          | 1                  |
| CA-CB-C-N-C-CA-CB          | 110.10             | 119.26          | 1                  |
| N-CA-CB                    | 110.50             | 118.70          | 1                  |
| C-N-N-CA-CA-C-N            | 116.20             | 125.84          | 1                  |
| N-CA-C                     | 111.00             | 97.51           | 1                  |
| CA-C-C-CA-CB               | 110.10             | 100.94          | 1                  |
| N-CA-C-CA-CA-C-CA-N-CA-C-N | 116.20             | 125.84          | 1                  |
| C-CA-CB                    | 110.10             | 100.95          | 1                  |
| C-N-CA                     | 121.70             | 130.37          | 2                  |
| C-N-CA                     | 121.70             | 113.03          | 1                  |
| CA-C-N                     | 116.20             | 125.83          | 3                  |
| N-CD-CG                    | 103.20             | 95.98           | 1                  |
| C-CA-CB                    | 110.10             | 119.25          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-C-O                  | 120.80             | 112.62          | 3                  |
| CA-C-C-N-N-CD-CG        | 103.20             | 95.98           | 1                  |
| CG-CD-N-CA-CG-CD-CA-C-N | 116.20             | 125.82          | 1                  |
| C-N-CA                  | 121.70             | 130.36          | 4                  |
| C-CA-CB                 | 110.10             | 100.96          | 1                  |
| C-N-CA                  | 121.70             | 113.04          | 2                  |
| CA-CB-N-CA-C-CA-CB      | 110.10             | 119.24          | 1                  |
| CA-C-CA-C-C-CA-CB       | 110.10             | 100.96          | 1                  |
| CA-C-O                  | 120.80             | 128.98          | 2                  |
| C-CA-N-CA-C             | 111.00             | 97.54           | 1                  |
| C-N-C-CA-C-CA-CB        | 110.10             | 119.24          | 1                  |
| CA-C-N                  | 116.20             | 125.82          | 1                  |
| N-CA-CB                 | 110.50             | 118.67          | 1                  |
| CA-C-O                  | 120.80             | 130.89          | 1                  |
| N-CA-N-CD-CG            | 103.20             | 95.99           | 1                  |
| C-N-CA                  | 121.70             | 113.05          | 2                  |
| N-CD-CG                 | 103.20             | 95.99           | 1                  |
| C-CA-CA-CB-CG           | 112.60             | 107.80          | 1                  |
| C-CA-CB                 | 110.10             | 119.22          | 1                  |
| CA-C-C-N-CA             | 121.70             | 113.06          | 1                  |
| C-CA-CA-C-CA-C-O        | 120.80             | 128.96          | 1                  |
| C-CA-N-CA-CB            | 111.50             | 119.66          | 1                  |



| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-N-CA             | 121.70             | 130.34          | 1                  |
| CA-C-O             | 120.80             | 128.96          | 1                  |
| N-CA-CA-C-N-CA-CB  | 111.50             | 119.66          | 1                  |
| N-CA-CB            | 103.00             | 97.72           | 1                  |
| C-CA-CA-C-C-N-CA   | 121.70             | 130.34          | 1                  |
| C-CA-CA-C-N        | 116.20             | 106.60          | 1                  |
| CA-C-CA-CB-C-CA-CB | 110.10             | 100.98          | 1                  |
| N-CA-CB            | 111.50             | 103.34          | 1                  |
| CA-C-C-CA-CB       | 110.10             | 100.99          | 1                  |
| C-CA-CB            | 110.10             | 100.99          | 2                  |
| N-CA-N-CA-CB       | 111.50             | 119.65          | 1                  |
| CA-C-N             | 116.20             | 106.61          | 1                  |
| N-CA-CB            | 110.50             | 102.35          | 1                  |
| C-N-CA             | 121.70             | 130.33          | 1                  |
| C-N-CA-C-CA-CB-CG  | 112.60             | 107.81          | 1                  |
| CA-N-CA-C-O        | 120.80             | 112.65          | 1                  |
| CA-C-O             | 120.80             | 128.95          | 1                  |
| CA-C-N             | 116.20             | 125.78          | 1                  |
| C-N-CA             | 121.70             | 113.07          | 1                  |
| C-N-CA             | 121.70             | 130.32          | 1                  |
| C-CA-CB            | 110.10             | 119.20          | 1                  |
| C-CA-CB            | 110.10             | 101.00          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CA-CB-C-N-CA           | 121.70             | 130.32          | 1                  |
| CA-CB-CG               | 113.80             | 109.01          | 2                  |
| C-CA-CB                | 110.50             | 103.32          | 1                  |
| CA-C-N                 | 116.20             | 106.62          | 2                  |
| N-CA-CB                | 110.50             | 118.64          | 1                  |
| CA-C-CA-C-C-CA-CB      | 109.10             | 119.63          | 1                  |
| N-CA-C                 | 111.00             | 124.41          | 1                  |
| CA-C-O                 | 120.80             | 112.66          | 1                  |
| CA-C-C-N-CA            | 121.70             | 130.32          | 1                  |
| N-CA-CB                | 111.50             | 119.64          | 1                  |
| CA-C-CA-C-C-CA-CA-C-O  | 120.80             | 128.94          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 101.01          | 1                  |
| CA-C-N-CA-N-CA-C-CA-CB | 110.10             | 119.19          | 1                  |
| CA-CB-C-CA-CB          | 109.10             | 119.62          | 1                  |
| C-CA-C-CA-CB           | 110.10             | 119.19          | 1                  |
| CA-C-O                 | 120.80             | 112.67          | 1                  |
| CA-C-O                 | 120.80             | 128.93          | 1                  |
| CA-C-N                 | 116.20             | 106.64          | 2                  |
| C-CA-N-CA-CA-C-O       | 120.80             | 128.93          | 1                  |
| C-CA-CB                | 110.50             | 103.33          | 1                  |
| N-CA-CA-C-N            | 116.20             | 106.64          | 1                  |
| CA-CB-CG               | 112.60             | 107.82          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-C-CA-CA-C-N | 116.20             | 125.76          | 1                  |
| C-CA-CB               | 110.10             | 119.18          | 1                  |
| C-CA-N-CA-C           | 111.00             | 124.38          | 1                  |
| CA-C-O                | 120.80             | 112.68          | 2                  |
| C-CA-CB               | 110.10             | 119.17          | 2                  |
| CA-CB-CG              | 112.60             | 107.83          | 1                  |
| C-CA-CB               | 110.10             | 101.03          | 1                  |
| N-CA-CB               | 110.50             | 102.39          | 1                  |
| N-CA-C                | 111.00             | 124.36          | 1                  |
| C-N-C-N-C-CA-N-CA-CB  | 111.50             | 103.39          | 1                  |
| N-CA-CB               | 111.50             | 103.39          | 1                  |
| CA-C-C-CA-C-N-N-CA-C  | 111.00             | 124.36          | 1                  |
| C-CA-C-CA-C-CA-CB     | 110.10             | 119.16          | 1                  |
| C-CA-CA-C-N           | 116.20             | 125.74          | 1                  |
| C-CA-N-CA-CB          | 110.50             | 118.60          | 1                  |
| C-CA-CB               | 110.10             | 119.16          | 1                  |
| CA-N-CD               | 112.00             | 105.33          | 1                  |
| C-N-CA-C-CA-C-O       | 120.80             | 128.90          | 1                  |
| N-CA-C                | 111.00             | 124.34          | 1                  |
| C-N-C-N-N-CA-CB       | 111.50             | 103.40          | 1                  |
| CA-CB-CG              | 112.60             | 117.36          | 1                  |
| CA-CB-CG              | 112.60             | 107.84          | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB             | 110.10             | 119.15          | 1                  |
| CA-C-O                   | 120.80             | 112.70          | 1                  |
| C-CA-CA-C-CA-C-N         | 116.20             | 106.67          | 1                  |
| CA-C-N                   | 116.90             | 124.04          | 1                  |
| CA-CB-CG                 | 113.90             | 105.33          | 1                  |
| C-CA-C-CA-CA-CB-CA-CB-CG | 112.60             | 107.84          | 1                  |
| C-CA-C-CA-N-CA-CB        | 111.50             | 103.41          | 1                  |
| N-CA-C-CA-CB             | 110.10             | 119.14          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 119.14          | 1                  |
| N-CA-CB                  | 111.50             | 119.59          | 1                  |
| CA-C-N                   | 116.20             | 125.72          | 1                  |
| CA-CB-CG                 | 114.10             | 123.62          | 1                  |
| C-CA-CB                  | 110.10             | 101.06          | 1                  |
| C-CA-C-CA-C-CA-CB        | 110.10             | 101.06          | 1                  |
| C-CA-CB                  | 110.10             | 119.14          | 2                  |
| C-N-CA-C-N-CA-CB         | 111.50             | 103.41          | 1                  |
| C-N-CA                   | 121.70             | 113.14          | 2                  |
| CA-C-O                   | 120.80             | 128.89          | 1                  |
| C-CA-N-CA-CB             | 111.50             | 103.41          | 1                  |
| C-CA-CB                  | 111.60             | 102.09          | 1                  |
| C-N-CA-C-C-N-CA          | 121.70             | 130.26          | 1                  |
| CA-C-C-N-CA-CB-CG1       | 110.40             | 118.48          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                   | 113.90             | 105.34          | 1                  |
| N-CA-C                     | 111.00             | 97.69           | 1                  |
| N-CA-N-CA-C                | 111.00             | 97.69           | 1                  |
| CA-N-CD                    | 112.00             | 105.35          | 1                  |
| C-CA-CB                    | 110.10             | 119.13          | 1                  |
| C-N-CA                     | 121.70             | 113.15          | 6                  |
| C-CA-CB                    | 110.10             | 101.07          | 1                  |
| CA-C-N                     | 116.20             | 106.70          | 1                  |
| N-CA-C                     | 111.00             | 97.70           | 1                  |
| C-CA-CB                    | 110.10             | 119.12          | 1                  |
| C-N-CA                     | 121.70             | 130.25          | 2                  |
| CA-CB-CG                   | 112.60             | 107.85          | 1                  |
| N-CA-CA-CB-CG              | 113.80             | 118.55          | 1                  |
| CA-C-N-CA-N-CA-CB          | 103.00             | 97.78           | 1                  |
| C-CA-CB                    | 110.10             | 101.08          | 1                  |
| CA-C-N-CA-CB               | 110.50             | 118.57          | 1                  |
| C-N-CA                     | 121.70             | 130.24          | 2                  |
| C-CA-CB                    | 110.10             | 101.09          | 1                  |
| CA-C-O                     | 120.80             | 112.73          | 1                  |
| N-CA-CA-C-CA-CB-CG         | 113.80             | 118.54          | 1                  |
| N-CA-N-CA-C-N-C-CA-C-CA-CB | 110.10             | 119.11          | 1                  |
| N-CA-C                     | 111.00             | 97.72           | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| CA-C-C-N-CA              | 121.70             | 130.24          | 1                  |
| C-CA-CB                  | 110.10             | 119.11          | 4                  |
| CA-CB-N-CA-C             | 111.00             | 124.28          | 1                  |
| C-N-CA                   | 121.70             | 113.17          | 4                  |
| CA-N-CD                  | 112.00             | 105.36          | 1                  |
| C-N-CA                   | 121.70             | 130.23          | 2                  |
| C-CA-OE1-CD-CA-C-C-CA-CB | 110.10             | 101.10          | 1                  |
| C-N-C-CA-CB              | 110.10             | 101.10          | 1                  |
| CA-C-O                   | 120.80             | 112.75          | 1                  |
| C-CA-CB                  | 110.10             | 101.10          | 2                  |
| C-CA-C-CA-CB             | 110.50             | 103.39          | 1                  |
| CA-C-N                   | 116.20             | 106.73          | 1                  |
| C-CA-CA-C-N              | 116.20             | 106.73          | 1                  |
| N-CA-CA-CB-CG            | 112.60             | 107.86          | 1                  |
| C-CA-CB                  | 110.10             | 119.10          | 1                  |
| N-CA-CA-C-N-CA-CB        | 111.50             | 119.55          | 1                  |
| CA-C-C-CA-CB             | 110.10             | 101.10          | 1                  |
| C-CA-CA-C-O              | 120.80             | 128.85          | 1                  |
| N-CA-C                   | 111.00             | 97.74           | 1                  |
| C-N-C-N-N-CA-C           | 111.00             | 97.75           | 1                  |
| CA-C-O                   | 120.80             | 130.74          | 1                  |
| CA-C-O                   | 120.80             | 128.85          | 1                  |

| Angle type                              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| CA-N-CD                                 | 112.00             | 105.37          | 1                  |
| N-CA-CB                                 | 110.50             | 102.46          | 1                  |
| CA-C-N                                  | 116.20             | 125.66          | 1                  |
| C-CA-N-CA-CA-C-C-N-C-N-C-N-CA-CB-C-N-CA | 121.70             | 113.19          | 1                  |
| C-CA-C-N-CA                             | 121.70             | 130.21          | 1                  |
| C-N-CA                                  | 121.70             | 113.19          | 1                  |
| CB-CG-CD2                               | 131.20             | 125.05          | 1                  |
| N-CA-C-CA-CB                            | 110.10             | 101.12          | 1                  |
| CA-C-O                                  | 120.80             | 112.76          | 1                  |
| CA-CB-CG                                | 113.80             | 109.07          | 1                  |
| N-CA-CA-C-O                             | 120.80             | 128.84          | 1                  |
| CA-CB-CA-C-O                            | 120.80             | 128.83          | 1                  |
| CA-N-C-CA-N-CA-C                        | 111.00             | 124.23          | 1                  |
| CA-CB-CG1                               | 110.40             | 118.43          | 1                  |
| C-CA-CA-C-C-CA-C-CA-CB                  | 110.50             | 103.42          | 1                  |
| N-CA-CA-C-O                             | 120.80             | 128.83          | 1                  |
| N-CA-CB                                 | 110.50             | 102.47          | 1                  |
| CA-C-CA-CB-CG                           | 112.60             | 107.88          | 1                  |
| C-CA-CA-C-C-N-N-CA-CA-CB-CG             | 112.60             | 117.32          | 1                  |
| N-CA-CB                                 | 110.50             | 118.52          | 2                  |
| C-CA-CB                                 | 110.10             | 119.07          | 1                  |
| CA-C-O                                  | 120.80             | 128.82          | 2                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| CA-C-O               | 120.80             | 112.78          | 1                  |
| CA-CB-N-CA-CB        | 111.50             | 103.48          | 1                  |
| C-CA-CB              | 110.10             | 101.14          | 1                  |
| CA-CB-CG1            | 110.40             | 118.42          | 1                  |
| N-CA-C               | 111.00             | 124.21          | 1                  |
| C-CA-CB              | 110.10             | 119.06          | 5                  |
| C-CA-CB              | 111.40             | 120.36          | 1                  |
| C-CA-CB              | 111.60             | 102.17          | 2                  |
| CA-C-C-CA-C-N-CA     | 121.70             | 113.21          | 1                  |
| C-CA-N-CA-CB         | 111.50             | 119.52          | 1                  |
| N-CA-CB              | 103.00             | 97.81           | 1                  |
| N-CA-CB              | 111.50             | 119.52          | 1                  |
| CA-CB-CG             | 112.60             | 107.89          | 1                  |
| C-N-CA               | 121.70             | 113.21          | 1                  |
| C-N-CA               | 121.70             | 130.19          | 1                  |
| C-N-C-N-CA           | 121.70             | 113.22          | 1                  |
| C-CA-CB              | 109.10             | 119.47          | 1                  |
| C-N-N-CA-C-CA-CA-C-O | 120.80             | 128.81          | 1                  |
| C-N-CA               | 121.70             | 130.18          | 1                  |
| C-N-CA               | 121.70             | 113.22          | 1                  |
| C-CA-CB              | 110.10             | 101.15          | 1                  |
| CA-C-O               | 120.80             | 112.79          | 1                  |



| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| C-N-CA-N-CD             | 112.00             | 105.40          | 1                  |
| CA-C-C-N-CA             | 121.70             | 130.18          | 1                  |
| CA-CB-CG                | 113.80             | 118.51          | 1                  |
| C-CA-CB                 | 110.10             | 119.05          | 1                  |
| CA-C-N-CA-CB            | 110.50             | 118.51          | 1                  |
| N-CA-CA-CB-CB-CG-C-N-CA | 121.70             | 113.22          | 1                  |
| N-CA-CB                 | 110.50             | 102.50          | 2                  |
| C-CA-CA-C-N             | 116.20             | 125.61          | 1                  |
| N-CA-C                  | 111.00             | 124.18          | 1                  |
| C-N-CA                  | 121.70             | 113.23          | 1                  |
| C-N-CA-C-O              | 120.80             | 112.80          | 1                  |
| C-N-CA                  | 121.70             | 130.17          | 2                  |
| C-CA-CB                 | 110.10             | 101.16          | 1                  |
| CA-CB-CG                | 113.90             | 105.43          | 1                  |
| N-CA-CB                 | 103.00             | 97.83           | 1                  |
| C-CA-C-N-C-CA-CB        | 110.10             | 119.04          | 1                  |
| CA-C-N                  | 116.20             | 106.79          | 1                  |
| CA-CB-CG                | 112.60             | 107.90          | 2                  |
| C-N-CA-C-O              | 120.80             | 112.81          | 1                  |
| C-CA-CB                 | 111.40             | 102.47          | 1                  |
| C-CA-CB                 | 110.10             | 119.03          | 1                  |
| C-N-CA-C-N              | 116.20             | 106.80          | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                             | 110.50             | 118.49          | 1                  |
| C-N-N-CA-C                          | 111.00             | 97.84           | 1                  |
| C-CA-CA-C-N                         | 116.90             | 123.95          | 1                  |
| N-CA-CB                             | 111.50             | 119.49          | 2                  |
| C-N-CA-C-N                          | 116.20             | 125.60          | 1                  |
| C-CA-CB                             | 110.10             | 101.17          | 1                  |
| N-CA-C-N-CA                         | 121.70             | 130.16          | 1                  |
| CA-C-N-CA-CB                        | 110.50             | 118.49          | 1                  |
| N-CA-C-N-CA                         | 121.70             | 113.24          | 1                  |
| N-CA-C-N-CA-C-N                     | 116.20             | 125.60          | 1                  |
| N-CA-CB                             | 110.50             | 102.51          | 1                  |
| CA-C-O                              | 120.80             | 128.79          | 1                  |
| CA-C-N                              | 116.20             | 106.80          | 1                  |
| CA-C-N                              | 116.20             | 106.81          | 1                  |
| CA-CB-CG1                           | 110.40             | 118.39          | 2                  |
| C-CA-N-CA-CB                        | 110.50             | 102.52          | 1                  |
| C-CA-N-CA-CA-C-N-CA-OE1-CD-CA-CB-CG | 113.80             | 109.11          | 1                  |
| CA-CB-OG1                           | 109.60             | 102.56          | 1                  |
| CA-C-C-N-CA                         | 121.70             | 113.25          | 1                  |
| N-CA-CB                             | 111.50             | 103.52          | 1                  |
| C-CA-CB                             | 110.10             | 119.02          | 1                  |
| C-N-CA                              | 121.70             | 113.25          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-O                      | 120.80             | 112.82          | 1                  |
| C-CA-CA-C-C-CA-CB           | 110.10             | 101.18          | 1                  |
| N-CA-CB                     | 110.50             | 102.52          | 1                  |
| CB-CG-CD2                   | 131.20             | 125.10          | 1                  |
| C-N-CA                      | 121.70             | 113.26          | 1                  |
| CA-C-C-CA-CB-CG-CD          | 112.60             | 104.63          | 1                  |
| C-CA-CB                     | 111.40             | 102.49          | 2                  |
| C-N-CA-CB-CG                | 112.60             | 107.91          | 1                  |
| C-CA-N-CA-CB                | 103.00             | 97.84           | 1                  |
| N-CA-C                      | 111.00             | 124.13          | 2                  |
| C-N-CA                      | 121.70             | 130.14          | 1                  |
| C-N-CA-C-N-CA-CA-C-C-CA-CB  | 109.10             | 119.41          | 1                  |
| C-CA-CB                     | 109.10             | 119.41          | 1                  |
| C-CA-CB                     | 110.10             | 119.01          | 2                  |
| CA-C-N                      | 116.90             | 109.87          | 1                  |
| N-CA-CB                     | 110.50             | 102.53          | 1                  |
| CA-C-CA-CB-C-N-CA           | 121.70             | 113.26          | 1                  |
| N-CA-N-CA-C                 | 111.00             | 124.12          | 1                  |
| C-CA-CB                     | 110.10             | 119.00          | 2                  |
| CA-C-CA-C-O                 | 120.80             | 112.83          | 1                  |
| C-CA-CB                     | 110.50             | 117.53          | 1                  |
| C-CA-CA-C-C-N-CA-CB-N-CA-CB | 110.50             | 102.54          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-N-N-CA-C                  | 111.00             | 124.11          | 1                  |
| C-N-CA                      | 122.60             | 99.19           | 1                  |
| N-CA-N-CA-N-CA-C-CA-N-CA-CB | 111.50             | 119.46          | 1                  |
| C-N-CA                      | 121.70             | 130.12          | 2                  |
| C-N-CB-CG-CD                | 112.60             | 104.65          | 1                  |
| CB-CG-CD2                   | 131.20             | 125.12          | 1                  |
| CA-C-N                      | 116.90             | 109.88          | 1                  |
| C-CA-CB                     | 110.10             | 101.21          | 1                  |
| C-CA-CB                     | 109.10             | 119.39          | 2                  |
| CA-C-CA-CB-CG               | 112.60             | 107.92          | 1                  |
| N-CA-CA-C-N                 | 116.20             | 125.55          | 1                  |
| C-CA-CB                     | 110.10             | 118.99          | 1                  |
| C-CA-CA-C-N                 | 116.20             | 125.55          | 1                  |
| CA-C-O                      | 120.80             | 128.75          | 1                  |
| N-CA-C-CA-CB                | 111.40             | 120.28          | 1                  |
| CA-C-C-N-C-N-CA-CB-OG1      | 109.60             | 102.59          | 1                  |
| CA-C-N                      | 116.20             | 106.85          | 1                  |
| C-N-CA                      | 121.70             | 113.29          | 1                  |
| N-CA-CA-C-N                 | 116.20             | 106.86          | 1                  |
| C-N-C-CA-CB                 | 110.10             | 118.98          | 1                  |
| C-CA-CB                     | 110.10             | 101.22          | 1                  |
| CA-CB-CG                    | 112.60             | 107.93          | 2                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 110.50             | 118.44          | 1                  |
| CB-CG-N-CA-CB     | 110.50             | 118.44          | 1                  |
| CA-CB-OG1         | 109.60             | 102.60          | 1                  |
| CA-CB-CG1         | 110.40             | 118.34          | 1                  |
| OE1-CD-CA-C-O     | 120.80             | 128.74          | 1                  |
| C-CA-CA-CB-OG1    | 109.60             | 102.60          | 1                  |
| C-CA-CB           | 110.10             | 101.23          | 1                  |
| C-N-N-CA-C        | 111.00             | 124.07          | 1                  |
| CA-C-O            | 120.80             | 112.86          | 1                  |
| C-CA-CB           | 110.50             | 117.50          | 1                  |
| C-N-CA            | 122.60             | 99.27           | 1                  |
| CA-C-O            | 120.80             | 112.87          | 2                  |
| CA-C-CA-C-N       | 116.20             | 106.87          | 1                  |
| C-N-CA            | 121.70             | 130.10          | 1                  |
| C-CA-CB           | 110.10             | 118.96          | 4                  |
| CB-CG-CD2         | 131.20             | 125.14          | 2                  |
| CA-CB-N-CA-CA-C-N | 116.20             | 125.53          | 1                  |
| C-CA-CB           | 111.40             | 102.54          | 1                  |
| CA-C-O            | 120.80             | 128.73          | 1                  |
| C-CA-CB           | 110.10             | 101.24          | 2                  |
| C-CA-C-N-CA       | 121.70             | 130.09          | 1                  |
| N-CA-CB           | 111.50             | 119.43          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-C-CA-C-CA-CB | 111.60             | 102.27          | 1                  |
| CA-C-CA-C-O            | 120.80             | 128.73          | 1                  |
| CA-C-N                 | 116.20             | 106.88          | 2                  |
| CB-CG-N-CA-C-N-CA      | 121.70             | 113.31          | 1                  |
| CA-CB-C-CA-CA-CB-OG1   | 109.60             | 102.61          | 1                  |
| O-C-N                  | 123.00             | 115.54          | 1                  |
| N-CA-CB                | 110.50             | 102.58          | 2                  |
| N-CA-CB                | 110.50             | 118.42          | 1                  |
| N-CA-C                 | 111.00             | 124.05          | 1                  |
| CA-C-C-N-CA            | 121.70             | 113.31          | 1                  |
| C-CA-CB                | 110.10             | 101.25          | 3                  |
| N-CA-N-CA-CA-CB-OG1    | 109.60             | 102.61          | 1                  |
| CA-C-O                 | 120.80             | 128.72          | 1                  |
| N-CA-CA-CB-OG1         | 109.60             | 102.61          | 1                  |
| C-N-CA-N-CD            | 112.00             | 105.48          | 2                  |
| C-N-CA                 | 121.70             | 113.31          | 1                  |
| CA-CB-CG               | 112.60             | 117.26          | 1                  |
| CA-CB-CB-CG-CD2        | 131.20             | 125.14          | 1                  |
| C-N-CA                 | 121.70             | 113.32          | 2                  |
| C-CA-CB                | 109.10             | 98.85           | 1                  |
| CA-N-CD                | 112.00             | 105.48          | 1                  |
| C-N-C-CA-C-CA-C-CA-CB  | 110.10             | 101.25          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-N-C-N-CA            | 121.70             | 113.32          | 1                  |
| CA-CB-CG              | 112.60             | 107.94          | 1                  |
| CA-C-CA-C-O           | 120.80             | 112.88          | 1                  |
| C-N-C-N-N-CA-CB       | 110.50             | 102.59          | 1                  |
| C-N-CB-CG-C-CA-C-N-CA | 121.70             | 113.32          | 1                  |
| CA-C-N                | 116.20             | 125.51          | 1                  |
| CB-CG-CD2             | 131.20             | 125.15          | 2                  |
| CA-C-O                | 120.80             | 112.89          | 2                  |
| C-N-CA                | 121.70             | 130.08          | 2                  |
| CA-CB-CG              | 114.10             | 123.41          | 1                  |
| N-CA-CA-CB-CG         | 113.80             | 109.15          | 1                  |
| C-N-CA-C-N            | 116.20             | 125.51          | 1                  |
| N-CA-CB               | 111.50             | 119.41          | 2                  |
| N-CA-C-CA-C-CA-CB     | 109.10             | 119.34          | 1                  |
| C-CA-CB               | 110.10             | 101.26          | 1                  |
| C-CA-CB               | 111.40             | 120.24          | 1                  |
| N-CA-CB               | 110.50             | 102.59          | 4                  |
| N-CA-C                | 113.30             | 99.81           | 1                  |
| C-CA-C-N-CA           | 121.70             | 113.33          | 1                  |
| C-N-CA                | 121.70             | 113.33          | 2                  |
| C-N-C-N-CA            | 121.70             | 130.07          | 1                  |
| CA-C-O                | 120.80             | 128.70          | 3                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-N                      | 116.20             | 106.90          | 1                  |
| N-CA-N-CA-CB                | 110.50             | 102.60          | 1                  |
| CB-CG-CD2                   | 131.20             | 125.16          | 1                  |
| C-CA-CB                     | 110.10             | 118.93          | 1                  |
| OE1-CD-CA-CB-CG             | 112.60             | 107.95          | 1                  |
| N-CA-C                      | 111.00             | 124.01          | 1                  |
| C-CA-C-CA-C-CA-CB           | 110.10             | 101.27          | 1                  |
| N-CA-CA-C-CA-C-N-CA-C-CA-CB | 110.10             | 118.93          | 1                  |
| N-CA-N-CA-C-CA-CB           | 111.40             | 120.23          | 1                  |
| CA-CB-OG1                   | 109.60             | 102.63          | 2                  |
| CA-CB-CG                    | 113.80             | 109.16          | 1                  |
| N-CA-N-CA-CA-CB-C-CA-CB     | 110.10             | 101.28          | 1                  |
| C-N-C-CA-CB                 | 110.10             | 118.92          | 1                  |
| C-CA-C-CA-CB                | 110.10             | 101.28          | 1                  |
| C-N-CA                      | 122.60             | 99.39           | 1                  |
| C-N-CA                      | 121.70             | 130.06          | 1                  |
| CA-C-N                      | 116.20             | 106.92          | 1                  |
| C-CA-CB                     | 110.10             | 101.28          | 2                  |
| N-CA-C                      | 113.30             | 99.84           | 1                  |
| N-CA-C-CA-CB                | 110.10             | 101.28          | 1                  |
| CA-C-O                      | 120.80             | 128.69          | 2                  |
| N-CA-CB                     | 110.50             | 118.39          | 1                  |



| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-N-CA-CB             | 110.50             | 102.61          | 1                  |
| C-CA-CB                  | 110.10             | 118.92          | 1                  |
| C-N-CA                   | 122.60             | 99.40           | 1                  |
| C-CA-CB                  | 110.10             | 118.91          | 2                  |
| C-CA-C-N-N-CA-C-N-C-N-CA | 121.70             | 113.35          | 1                  |
| C-CA-CB                  | 110.10             | 101.29          | 2                  |
| N-CA-C                   | 111.00             | 123.98          | 2                  |
| CA-C-C-CA-CB             | 110.10             | 101.29          | 1                  |
| C-N-CA                   | 121.70             | 130.04          | 1                  |
| N-CA-CB                  | 110.50             | 118.38          | 1                  |
| C-CA-CB                  | 109.10             | 119.30          | 1                  |
| C-N-C-CA-CB              | 110.10             | 118.91          | 1                  |
| N-CA-CA-C-N              | 116.90             | 109.95          | 1                  |
| C-CA-C-CA-CB             | 109.10             | 119.29          | 1                  |
| CA-C-O                   | 120.80             | 112.92          | 1                  |
| CB-CG-CD2                | 131.20             | 125.18          | 1                  |
| C-CA-CB                  | 110.10             | 101.30          | 2                  |
| CA-CB-CG                 | 113.80             | 109.17          | 1                  |
| CB-CG-C-CA-CB            | 110.10             | 118.90          | 1                  |
| C-N-CA                   | 121.70             | 113.36          | 1                  |
| N-CA-N-CA-N-CA-C         | 111.00             | 123.97          | 1                  |
| N-CA-CA-CB-CG            | 113.80             | 109.17          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB          | 109.10             | 98.91           | 1                  |
| C-CA-CB               | 109.10             | 98.91           | 1                  |
| CA-CB-CG              | 112.60             | 107.97          | 1                  |
| N-CA-C-N-CA           | 121.70             | 130.03          | 1                  |
| N-CA-CB               | 111.50             | 119.37          | 2                  |
| C-N-CA-C-CB-CG-CA-C-O | 120.80             | 112.93          | 1                  |
| CA-C-C-CA-CB          | 110.50             | 117.44          | 1                  |
| N-CA-C                | 112.10             | 100.53          | 1                  |
| N-CA-N-CA-CB          | 110.50             | 102.63          | 2                  |
| C-CA-C-N-CA           | 121.70             | 113.37          | 1                  |
| N-CA-C                | 111.00             | 123.95          | 1                  |
| CA-C-CA-C-N           | 116.20             | 125.45          | 1                  |
| N-CA-CA-CB-CG         | 112.60             | 107.97          | 1                  |
| N-CA-CA-C-O           | 120.80             | 112.94          | 1                  |
| CB-CG-CD2             | 131.20             | 125.19          | 1                  |
| C-CA-N-CA-C           | 113.30             | 99.89           | 1                  |
| N-CA-CB               | 110.50             | 118.36          | 1                  |
| C-CA-CA-N-O-C-N       | 123.00             | 115.60          | 1                  |
| CA-C-O                | 120.80             | 112.94          | 2                  |
| C-N-CA                | 121.70             | 113.38          | 3                  |
| N-CA-C                | 111.00             | 98.05           | 1                  |
| N-CA-C                | 111.00             | 123.94          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-C-O                  | 120.80             | 128.66          | 1                  |
| C-CA-CB                 | 110.10             | 118.88          | 3                  |
| C-CA-CA-CB-N-CA-C-CA-CB | 110.10             | 101.32          | 1                  |
| CA-C-N-CA-CB            | 110.50             | 118.36          | 1                  |
| C-N-C-CA-CB             | 110.10             | 118.88          | 1                  |
| CA-C-C-N-CA             | 121.70             | 113.38          | 1                  |
| CA-C-O                  | 120.80             | 128.65          | 1                  |
| N-CA-C                  | 113.30             | 99.90           | 1                  |
| N-CA-CB                 | 110.50             | 118.35          | 1                  |
| CA-CB-CA-CB-CG          | 112.60             | 107.98          | 1                  |
| CA-C-N-CA-CA-C-O        | 120.80             | 112.95          | 1                  |
| N-CA-CB                 | 111.50             | 119.35          | 1                  |
| CA-CB-CG                | 112.60             | 107.98          | 1                  |
| CA-CB-OG1               | 109.60             | 102.67          | 1                  |
| C-N-N-CA-C              | 111.00             | 98.07           | 1                  |
| C-CA-CB                 | 110.10             | 118.87          | 1                  |
| N-CA-CB                 | 110.50             | 102.65          | 1                  |
| N-CA-CA-CB-CG           | 112.60             | 107.98          | 1                  |
| CA-C-O                  | 120.80             | 112.95          | 1                  |
| C-N-C-CA-CB             | 110.10             | 118.87          | 1                  |
| N-CA-C                  | 113.30             | 99.92           | 1                  |
| CA-C-N                  | 116.20             | 106.97          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| C-CA-CB          | 110.10             | 101.33          | 2                  |
| N-CA-CB          | 110.50             | 118.34          | 2                  |
| CA-C-O           | 120.80             | 112.96          | 1                  |
| N-CA-CB          | 111.50             | 119.34          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 101.34          | 1                  |
| C-CA-CB          | 110.10             | 101.34          | 1                  |
| N-CA-C-N-C-CA-CB | 109.10             | 98.95           | 1                  |
| N-CA-CB          | 110.50             | 102.66          | 1                  |
| C-N-CA           | 121.70             | 113.40          | 3                  |
| C-CA-CA-C-N      | 116.20             | 106.98          | 1                  |
| C-N-CA           | 121.70             | 130.00          | 1                  |
| CA-C-N           | 116.20             | 106.98          | 1                  |
| N-CA-C           | 111.00             | 98.09           | 1                  |
| N-CA-C           | 111.00             | 123.91          | 1                  |
| C-CA-CB          | 110.10             | 118.86          | 1                  |
| N-CA-C           | 113.30             | 99.94           | 1                  |
| C-N-CA           | 121.70             | 113.41          | 1                  |
| N-CA-CB          | 111.50             | 119.33          | 1                  |
| N-CA-CB          | 110.50             | 118.33          | 1                  |
| C-CA-CB          | 110.10             | 101.35          | 2                  |
| N-CA-CB          | 110.50             | 102.67          | 1                  |
| N-CA-N-CA-CB     | 110.50             | 118.33          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 118.85          | 1                  |
| CA-C-O                | 120.80             | 112.97          | 1                  |
| CA-CB-C-N-CA          | 121.70             | 113.41          | 1                  |
| N-CA-N-CA-C           | 111.00             | 123.89          | 1                  |
| CA-C-N                | 116.20             | 106.99          | 1                  |
| CA-C-O                | 120.80             | 128.63          | 1                  |
| N-CA-C                | 111.00             | 98.11           | 3                  |
| N-CA-N-CA-C           | 111.00             | 98.11           | 1                  |
| C-CA-CB               | 110.50             | 117.41          | 1                  |
| CA-CB-CG              | 112.60             | 108.00          | 3                  |
| N-CA-CB               | 103.00             | 97.94           | 2                  |
| N-CA-C                | 111.00             | 123.89          | 1                  |
| C-CA-CB               | 110.10             | 101.36          | 3                  |
| N-CA-CB               | 110.50             | 102.68          | 1                  |
| N-CA-CB               | 110.50             | 118.32          | 1                  |
| CA-C-O                | 120.80             | 128.62          | 2                  |
| N-CA-N-CA-C           | 112.10             | 100.60          | 1                  |
| C-N-CA                | 121.70             | 113.42          | 1                  |
| N-CA-C-CA-C-CA-C-N-CA | 121.70             | 113.42          | 1                  |
| N-CA-CB               | 111.50             | 119.32          | 1                  |
| C-CA-C-CA-CB          | 110.10             | 101.36          | 1                  |
| N-CA-C                | 111.00             | 98.12           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-CB-CG              | 112.60             | 117.20          | 1                  |
| CA-N-CD               | 112.00             | 118.44          | 1                  |
| CA-CB-C-N-CA          | 121.70             | 129.98          | 1                  |
| N-CA-CB               | 110.50             | 102.69          | 1                  |
| C-N-C-N-N-CA-CA-CB-CG | 112.60             | 117.20          | 1                  |
| CA-CB-CG              | 112.60             | 108.01          | 1                  |
| C-N-CA                | 121.70             | 113.43          | 1                  |
| C-N-C-CA-CB           | 110.10             | 101.37          | 1                  |
| C-CA-CA-CB-CA-C-O     | 120.80             | 128.61          | 1                  |
| N-CA-C                | 111.00             | 123.86          | 1                  |
| N-CA-CB               | 111.50             | 119.31          | 1                  |
| C-CA-CB               | 111.60             | 102.41          | 1                  |
| N-CA-CA-C-CA-C-O      | 120.80             | 112.99          | 1                  |
| CB-CG-CA-C-N          | 116.20             | 125.39          | 1                  |
| N-CA-CB               | 103.00             | 108.05          | 2                  |
| CB-CG-CD2             | 131.20             | 125.23          | 3                  |
| C-CA-CB               | 111.60             | 102.42          | 1                  |
| C-CA-C-N-C-N-CA       | 121.70             | 113.44          | 2                  |
| CA-C-N                | 116.20             | 107.02          | 1                  |
| CA-CB-N-CA-C          | 113.30             | 99.99           | 1                  |
| CA-C-O                | 120.80             | 128.60          | 1                  |
| N-CA-C                | 111.00             | 123.85          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-O           | 120.80             | 128.60          | 1                  |
| C-CA-C-CA-CB         | 111.60             | 102.42          | 1                  |
| CA-C-N               | 116.20             | 107.03          | 2                  |
| CA-C-C-N-C-CA-CA-C-O | 120.80             | 128.60          | 1                  |
| CA-N-CD              | 112.00             | 118.42          | 1                  |
| C-CA-CB              | 110.10             | 118.82          | 1                  |
| N-CA-C-N-CA          | 121.70             | 113.44          | 1                  |
| C-CA-N-CA-C          | 113.30             | 100.00          | 1                  |
| N-CA-C               | 111.00             | 123.84          | 1                  |
| N-CA-C               | 111.00             | 98.16           | 2                  |
| C-N-N-CA-C           | 111.00             | 123.84          | 1                  |
| CA-C-O               | 120.80             | 113.01          | 1                  |
| C-CA-C-CA-CB         | 110.10             | 118.81          | 1                  |
| CA-CB-C-CA-CB        | 111.60             | 102.43          | 1                  |
| C-N-C-N-C-N-CA       | 121.70             | 113.45          | 1                  |
| C-CA-CB              | 110.10             | 118.81          | 1                  |
| CA-CB-CG             | 112.60             | 108.02          | 2                  |
| C-N-CA               | 121.70             | 113.45          | 1                  |
| CA-C-O               | 120.80             | 128.59          | 2                  |
| N-CA-C-CA-C-N-CA     | 121.70             | 113.45          | 1                  |
| C-CA-CB              | 110.10             | 118.80          | 1                  |
| C-N-CA-CB-C-N-CA-C-N | 116.20             | 107.04          | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                   | 110.50             | 102.71          | 1                  |
| CA-C-N                    | 116.20             | 125.36          | 1                  |
| CB-CG-C-N-CA              | 121.70             | 129.94          | 1                  |
| N-CA-CB                   | 110.50             | 102.72          | 2                  |
| N-CA-C                    | 111.00             | 123.82          | 1                  |
| C-N-CA                    | 121.70             | 113.46          | 1                  |
| CA-C-O                    | 120.80             | 128.58          | 2                  |
| CA-C-N                    | 116.20             | 107.05          | 2                  |
| N-CA-CB                   | 111.50             | 119.28          | 1                  |
| C-CA-CB                   | 110.10             | 118.79          | 2                  |
| CB-CG-CD                  | 112.60             | 104.82          | 1                  |
| C-CA-CB                   | 111.60             | 102.45          | 1                  |
| N-CA-C                    | 111.00             | 98.19           | 1                  |
| N-CA-C-CA-CB              | 110.10             | 101.41          | 1                  |
| C-CA-CA-C-N               | 116.20             | 107.05          | 1                  |
| CB-CG-CD2                 | 131.20             | 125.25          | 1                  |
| C-N-CA-CB-CG              | 113.80             | 109.23          | 1                  |
| N-CA-C                    | 111.00             | 123.80          | 1                  |
| C-CA-C-CA-C-N-CA          | 121.70             | 113.47          | 1                  |
| C-N-N-CA-C-CA-C-CA-CA-C-N | 116.20             | 107.06          | 1                  |
| C-N-C-CA-CB               | 110.10             | 118.78          | 1                  |
| CA-C-N                    | 116.20             | 125.34          | 2                  |



| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 110.50             | 118.27          | 1                  |
| C-CA-CB           | 110.10             | 118.78          | 1                  |
| N-CA-C            | 111.00             | 123.79          | 3                  |
| CA-C-CG-CD-NE     | 112.00             | 101.95          | 1                  |
| CA-C-N            | 116.20             | 107.06          | 1                  |
| C-CA-C-CA-N-CA-CB | 110.50             | 102.73          | 1                  |
| CA-C-O            | 120.80             | 128.57          | 1                  |
| N-CA-CB           | 110.50             | 102.73          | 1                  |
| CB-CG-CD          | 112.60             | 104.84          | 1                  |
| N-CA-C-N-CA       | 121.70             | 113.48          | 1                  |
| CA-C-N            | 116.20             | 125.33          | 1                  |
| CA-C-O            | 120.80             | 128.56          | 5                  |
| C-N-CA            | 121.70             | 113.48          | 1                  |
| C-CA-CB           | 111.60             | 102.47          | 1                  |
| CA-CB-N-CA-C      | 111.00             | 123.78          | 1                  |
| N-CA-CB           | 111.50             | 103.74          | 1                  |
| CA-CB-CG          | 112.60             | 108.04          | 1                  |
| C-N-C-N-CA        | 121.70             | 113.48          | 1                  |
| C-CA-CB           | 110.10             | 118.77          | 1                  |
| CG-CD2-NE2        | 107.20             | 102.64          | 1                  |
| CA-C-N            | 116.20             | 107.07          | 1                  |
| N-CA-C            | 111.00             | 98.22           | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-C-O                | 120.80             | 113.04          | 1                  |
| C-CA-CA-CB-CG         | 112.60             | 108.04          | 1                  |
| C-N-CA                | 121.70             | 129.91          | 1                  |
| CA-C-O                | 120.80             | 113.05          | 1                  |
| CA-C-CA-CB-CA-C-O     | 120.80             | 128.55          | 1                  |
| N-CA-CB               | 110.50             | 102.75          | 1                  |
| N-CA-C-CA-CD2-NE2-CE1 | 109.00             | 104.44          | 1                  |
| C-CA-CD2-NE2-CE1      | 109.00             | 104.44          | 1                  |
| C-CA-CB               | 110.10             | 101.44          | 1                  |
| CA-C-O                | 120.80             | 128.55          | 1                  |
| C-N-CA                | 121.70             | 113.49          | 1                  |
| C-CA-C-N-CA           | 121.70             | 113.50          | 1                  |
| C-CA-N-CA-CB          | 110.40             | 117.23          | 1                  |
| N-CA-CB               | 111.50             | 103.75          | 1                  |
| N-CA-CA-C-C-CA-CB     | 110.10             | 101.44          | 1                  |
| C-CA-CB               | 111.40             | 102.74          | 1                  |
| N-CA-C                | 111.00             | 98.24           | 1                  |
| CA-C-O                | 120.80             | 128.54          | 1                  |
| CA-CB-CG              | 112.60             | 108.05          | 4                  |
| C-N-CD2-NE2-CE1       | 109.00             | 104.45          | 1                  |
| N-CA-CB               | 110.50             | 102.76          | 2                  |
| C-N-N-CA-CA-C-O       | 120.80             | 128.54          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-CB           | 110.50             | 118.24          | 1                  |
| C-N-CA            | 121.70             | 113.50          | 1                  |
| C-CA-CB           | 110.10             | 101.45          | 1                  |
| CA-C-N            | 116.90             | 110.07          | 1                  |
| CA-C-N            | 116.20             | 125.31          | 1                  |
| N-CA-CB           | 111.50             | 103.76          | 1                  |
| C-N-N-CA-CB       | 111.50             | 103.76          | 1                  |
| N-CA-C-N-CA       | 121.70             | 113.51          | 1                  |
| CA-C-O            | 120.80             | 113.06          | 1                  |
| N-CA-CB           | 103.00             | 97.99           | 1                  |
| CA-C-N            | 116.20             | 125.30          | 1                  |
| CA-CB-N-CA-C      | 111.00             | 123.74          | 1                  |
| C-CA-CB           | 110.10             | 101.46          | 1                  |
| CA-CB-CG          | 112.60             | 117.15          | 1                  |
| C-N-C-N-CA        | 121.70             | 113.51          | 1                  |
| CA-C-N            | 116.20             | 107.10          | 1                  |
| C-N-CA            | 121.70             | 113.51          | 1                  |
| C-CA-C-CA-CB      | 111.60             | 102.50          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 118.74          | 1                  |
| C-CA-C-CA-N-CA-CB | 103.00             | 98.00           | 1                  |
| C-N-CA            | 121.70             | 113.52          | 2                  |
| N-CA-C-CA-CB      | 110.10             | 118.74          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-C-N                     | 116.20             | 107.11          | 1                  |
| C-CA-CB                    | 110.10             | 118.74          | 1                  |
| CA-C-O                     | 120.80             | 128.53          | 1                  |
| C-CA-C-CA-C-N-N-CA-C-CA-CB | 110.10             | 101.47          | 1                  |
| CA-CB-CG                   | 113.80             | 109.26          | 1                  |
| C-CA-C-CA-N-CD-CG          | 103.20             | 96.39           | 1                  |
| CA-CB-CG                   | 112.60             | 108.06          | 1                  |
| N-CA-CB-CG-CD              | 112.60             | 120.32          | 1                  |
| CG-CD-NE                   | 112.00             | 102.01          | 1                  |
| OG1-CB-CG2                 | 109.30             | 118.38          | 1                  |
| C-N-CA                     | 121.70             | 129.88          | 1                  |
| C-CA-CB                    | 110.10             | 118.73          | 1                  |
| N-CD-CG                    | 103.20             | 96.39           | 1                  |
| CA-C-N-CA-CB               | 110.50             | 102.78          | 1                  |
| C-CA-CB                    | 110.10             | 101.47          | 1                  |
| CA-C-O                     | 120.80             | 128.52          | 2                  |
| N-CA-CB                    | 111.50             | 103.78          | 1                  |
| C-N-N-CA-CB                | 111.50             | 103.78          | 1                  |
| N-CA-C                     | 111.00             | 123.71          | 1                  |
| C-CA-C-N-CA                | 121.70             | 113.53          | 1                  |
| N-CA-CB                    | 110.50             | 102.78          | 1                  |
| CA-C-N                     | 116.20             | 107.12          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| CA-C-N                         | 116.20             | 125.28          | 1                  |
| C-N-CA                         | 121.70             | 113.53          | 3                  |
| N-CA-C-CA-CB                   | 111.60             | 102.52          | 1                  |
| C-CA-N-CA-CB                   | 111.50             | 119.21          | 1                  |
| N-CA-CB                        | 111.50             | 119.21          | 2                  |
| C-CA-CB                        | 110.10             | 118.72          | 1                  |
| C-CA-C-CA-CA-CB-CG-CD2-C-CA-CB | 110.10             | 118.72          | 1                  |
| CA-C-N                         | 116.20             | 107.13          | 1                  |
| CA-CB-C-N-CA                   | 121.70             | 113.54          | 1                  |
| N-CA-CB                        | 103.00             | 98.01           | 1                  |
| C-CA-C-CA-CB                   | 110.10             | 101.49          | 1                  |
| OG1-CB-CG2                     | 109.30             | 118.36          | 1                  |
| CA-CB-CG                       | 112.60             | 108.07          | 2                  |
| N-CA-CB                        | 103.00             | 107.98          | 1                  |
| N-CA-N-CA-C                    | 111.00             | 123.69          | 1                  |
| N-CA-C                         | 111.00             | 123.69          | 1                  |
| CA-C-N                         | 116.20             | 107.14          | 1                  |
| N-CA-C                         | 111.00             | 123.68          | 1                  |
| C-N-C-CA-CB                    | 110.10             | 118.71          | 1                  |
| CA-C-N                         | 116.20             | 125.26          | 1                  |
| C-N-CA                         | 121.70             | 113.55          | 1                  |
| C-CA-C-N-CA                    | 121.70             | 129.85          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CD2-NE2-N-CA-CB            | 110.50             | 102.80          | 1                  |
| CA-N-CA-CB-CG              | 112.60             | 108.07          | 1                  |
| N-CA-CA-C-O                | 120.80             | 128.50          | 1                  |
| N-CA-CB                    | 110.50             | 102.80          | 1                  |
| CA-C-C-CA-N-CA-C           | 111.00             | 98.33           | 1                  |
| N-CA-C-N-CA                | 121.70             | 113.55          | 1                  |
| C-CA-C-N-CA                | 121.70             | 113.55          | 1                  |
| CA-C-O                     | 120.80             | 128.49          | 1                  |
| C-N-CA-CB-CG               | 112.60             | 108.07          | 1                  |
| CG-CD2-C-CA-N-CA-CB        | 110.50             | 102.81          | 1                  |
| C-N-C-N-CA                 | 121.70             | 129.84          | 1                  |
| C-CA-CA-CB-CG              | 112.60             | 108.08          | 1                  |
| CA-CB-CG                   | 113.80             | 109.28          | 1                  |
| C-N-CA                     | 121.70             | 113.56          | 2                  |
| N-CA-C-N-CA                | 121.70             | 113.56          | 1                  |
| C-CA-CB                    | 110.10             | 118.69          | 1                  |
| N-CA-N-CA-CA-C-N-CA-C      | 111.00             | 123.66          | 1                  |
| CA-C-CA-C-CA-C-O           | 120.80             | 128.49          | 1                  |
| CA-C-CA-C-O                | 120.80             | 128.49          | 1                  |
| CA-C-N                     | 116.20             | 107.16          | 3                  |
| CA-C-C-CA-C-CA-C-CA-CA-C-N | 116.20             | 125.24          | 1                  |
| C-N-C-N-CA-C-O             | 120.80             | 128.48          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 111.00             | 123.65          | 1                  |
| C-N-N-CD-CG           | 103.20             | 96.42           | 1                  |
| N-CA-C                | 111.00             | 98.35           | 1                  |
| N-CA-CB               | 110.50             | 118.18          | 2                  |
| C-CA-CB               | 111.60             | 102.56          | 1                  |
| CA-N-CD               | 112.00             | 105.67          | 1                  |
| C-CA-C-CA-CA-C-CA-C-N | 116.20             | 125.24          | 1                  |
| N-CA-C-CA-CA-CB-CG    | 113.80             | 109.28          | 1                  |
| C-CA-CA-C-C-N-C-N-CA  | 121.70             | 129.83          | 1                  |
| C-N-C-N-CA            | 121.70             | 113.57          | 1                  |
| C-N-CA                | 121.70             | 129.83          | 1                  |
| C-CA-C-CA-C-CA-CB     | 110.10             | 118.68          | 1                  |
| CA-CB-CG              | 112.60             | 108.08          | 1                  |
| CA-C-O                | 120.80             | 128.48          | 1                  |
| C-CA-CB               | 110.10             | 101.52          | 2                  |
| C-CA-C-CA-CB          | 110.10             | 118.68          | 1                  |
| CD2-NE2-CE1           | 109.00             | 104.49          | 1                  |
| CA-C-N                | 116.20             | 125.23          | 1                  |
| C-N-CA                | 121.70             | 129.82          | 1                  |
| N-CA-C                | 111.00             | 123.63          | 1                  |
| CA-C-N                | 116.20             | 125.22          | 2                  |
| C-CA-CB               | 110.10             | 118.67          | 2                  |

| Angle type      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA     | 121.70             | 113.58          | 1                  |
| C-N-CA          | 121.70             | 113.58          | 2                  |
| N-CA-CB         | 110.50             | 118.17          | 1                  |
| C-CA-CB         | 110.10             | 101.53          | 1                  |
| CA-C-O          | 120.80             | 128.47          | 1                  |
| CA-CB-CG        | 113.90             | 105.78          | 1                  |
| C-N-CA-C-O      | 120.80             | 128.47          | 1                  |
| N-CA-CB         | 111.50             | 103.83          | 1                  |
| CA-CB-CG        | 104.50             | 95.93           | 1                  |
| CA-C-N          | 116.20             | 107.18          | 1                  |
| C-N-CD2-NE2-CE1 | 109.00             | 104.49          | 1                  |
| C-CA-CA-N-CD    | 112.00             | 105.69          | 1                  |
| N-CA-C          | 111.00             | 123.62          | 1                  |
| C-N-CA          | 121.70             | 113.59          | 1                  |
| C-CA-CB         | 110.10             | 101.54          | 3                  |
| C-N-C-N-C-CA-CB | 110.10             | 118.66          | 1                  |
| C-CA-CB         | 110.10             | 118.66          | 3                  |
| CB-CG-CD2       | 131.20             | 125.34          | 1                  |
| CA-C-N          | 116.20             | 125.21          | 1                  |
| N-CA-CB         | 110.50             | 102.84          | 1                  |
| CA-CB-CG        | 112.60             | 108.09          | 1                  |
| C-N-C-CA-CB     | 110.10             | 101.54          | 1                  |



| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                 | 112.60             | 108.10          | 1                  |
| C-CA-CA-C-N              | 116.20             | 125.21          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 118.66          | 1                  |
| CA-C-O                   | 120.80             | 113.14          | 1                  |
| CA-C-O                   | 120.80             | 128.45          | 2                  |
| CA-C-O                   | 120.80             | 111.34          | 1                  |
| CA-N-CD                  | 112.00             | 105.70          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 101.55          | 1                  |
| CA-C-N                   | 116.20             | 125.20          | 1                  |
| N-CA-C                   | 111.00             | 123.60          | 1                  |
| C-N-C-CA-CB              | 111.60             | 102.60          | 1                  |
| C-N-C-CA-CA-C-O          | 120.80             | 113.15          | 1                  |
| C-N-CA-C-C-CA-CB         | 110.10             | 118.65          | 1                  |
| N-CA-CB                  | 110.50             | 102.85          | 1                  |
| CD2-NE2-C-N-CA-C-C-CA-CB | 110.10             | 118.64          | 1                  |
| C-N-C-N-CA               | 121.70             | 113.61          | 1                  |
| C-CA-CB                  | 110.10             | 101.56          | 2                  |
| CA-CB-CA-CB-C-N-CA       | 121.70             | 129.79          | 1                  |
| N-CA-CB                  | 111.50             | 119.14          | 2                  |
| CA-C-C-CA-CB             | 110.10             | 101.56          | 1                  |
| C-N-CA-C-N               | 116.20             | 125.19          | 1                  |
| CA-C-N                   | 116.20             | 125.19          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| CA-C-O               | 120.80             | 128.44          | 1                  |
| C-CA-C-N-CA          | 121.70             | 129.79          | 1                  |
| C-CA-C-N-CA-C-C-N-CA | 121.70             | 113.61          | 1                  |
| NE-CZ-NH2            | 119.20             | 123.24          | 1                  |
| N-CA-N-CA-C          | 111.00             | 123.58          | 1                  |
| CA-CB-C-N-CA         | 121.70             | 129.78          | 1                  |
| N-CA-N-CA-CB         | 111.50             | 103.87          | 1                  |
| C-CA-CB              | 110.10             | 118.63          | 1                  |
| C-CA-CB              | 110.10             | 101.57          | 1                  |
| N-CA-C-CA-CB         | 110.10             | 101.57          | 1                  |
| CA-C-C-N-CA          | 121.70             | 113.62          | 1                  |
| C-N-CA               | 121.70             | 129.78          | 1                  |
| N-CA-C               | 111.00             | 98.43           | 1                  |
| N-CA-N-CA-CB         | 110.40             | 117.13          | 1                  |
| C-CA-CA-N-CD         | 112.00             | 105.72          | 1                  |
| CA-CB-CG             | 112.60             | 108.11          | 1                  |
| CD2-NE2-N-CA-C-CA-CB | 110.10             | 101.57          | 1                  |
| CA-C-O               | 120.80             | 113.17          | 1                  |
| C-N-CA-C-N           | 116.20             | 125.17          | 1                  |
| CA-C-N               | 116.20             | 125.17          | 1                  |
| N-CD-CG              | 103.20             | 96.47           | 1                  |
| CA-C-CA-CB-CG        | 113.80             | 109.31          | 1                  |

| Angle type  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| C-CA-C-CA-CB  | 109.10             | 118.97          | 1                  |
| CD2-NE2-CE1   | 109.00             | 104.51          | 1                  |
| CA-C-C-CA-C-N-C-CA-C-N-CA                           | 121.70             | 129.77          | 1                  |
| C-CA-CA-CB-CG                                       | 113.90             | 105.83          | 1                  |
| CD2-NE2-N-CA-CG-CD2-C-N-CA-C-CA-CB-N-CA-C-N-N-CA-CB | 111.50             | 119.12          | 1                  |
| CA-C-N  | 116.20             | 125.16          | 1                  |
| C-CA-C-CA-N-CA-C-CA-C-CA-C-CA-CB                    | 110.10             | 101.59          | 1                  |
| CA-CB-CG  | 113.80             | 109.32          | 1                  |
| CA-C-O  | 120.80             | 113.18          | 1                  |
| C-N-CA  | 121.70             | 129.76          | 1                  |
| N-CA-C-CA-N-CA-C-CA-CB                              | 110.10             | 118.61          | 1                  |
| N-CA-N-CA-CB  | 111.50             | 103.89          | 1                  |
| N-CA-N-CA-CB  | 110.50             | 102.89          | 1                  |
| N-CA-CB   | 110.40             | 103.68          | 2                  |
| CB-CG-CD  | 112.60             | 120.21          | 1                  |
| CA-CB-CD2-NE2-CE1                                   | 109.00             | 104.52          | 1                  |
| C-CA-CB   | 110.10             | 101.59          | 2                  |
| OE1-CD-OE2  | 122.90             | 112.16          | 1                  |
| C-CA-CB   | 110.10             | 101.60          | 2                  |
| CA-C-C-CA-CD2-NE2-CE1                               | 109.00             | 104.52          | 1                  |
| CA-C-O  | 120.80             | 128.41          | 2                  |
| C-CA-CB   | 110.10             | 118.60          | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| CD2-NE2-CE1              | 109.00             | 104.53          | 3                  |
| CA-N-CD                  | 112.00             | 105.74          | 1                  |
| C-CA-CD2-NE2-CE1         | 109.00             | 104.53          | 1                  |
| CA-CB-CG                 | 112.60             | 108.13          | 2                  |
| C-N-CA-CB-CG             | 112.60             | 108.13          | 1                  |
| C-CA-N-CA-C              | 111.00             | 98.48           | 1                  |
| CA-C-O                   | 120.80             | 111.41          | 1                  |
| C-N-CD2-NE2-CA-C-N       | 116.20             | 125.15          | 1                  |
| C-CA-CA-CB-CG            | 104.50             | 96.00           | 1                  |
| CA-C-N-CA-C              | 111.00             | 98.48           | 1                  |
| C-N-CA                   | 121.70             | 113.65          | 1                  |
| N-CA-C                   | 111.00             | 98.48           | 1                  |
| CA-C-N                   | 116.20             | 125.14          | 1                  |
| C-CA-C-N-CD2-NE2-CE1     | 109.00             | 104.53          | 1                  |
| C-CA-N-CA-CG-CD2-C-CA-CB | 111.40             | 102.91          | 1                  |
| C-N-CA-C-O               | 120.80             | 113.20          | 1                  |
| OG1-CB-CG2               | 109.30             | 118.24          | 1                  |
| C-CA-CB                  | 110.10             | 118.59          | 1                  |
| C-N-CA                   | 121.70             | 129.74          | 2                  |
| CD1-CG-CD2               | 110.80             | 100.97          | 1                  |
| CA-C-CA-C-CA-C-O         | 120.80             | 128.39          | 1                  |
| N-CA-CB                  | 110.50             | 102.91          | 2                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| CA-N-CD             | 112.00             | 105.75          | 1                  |
| OG1-CB-CG2          | 109.30             | 118.23          | 1                  |
| CA-C-N              | 116.20             | 125.13          | 1                  |
| N-CA-CA-C-N         | 116.20             | 125.13          | 1                  |
| N-CA-CA-C-N-CA-C    | 111.00             | 98.50           | 1                  |
| N-CA-C              | 111.00             | 98.50           | 2                  |
| CA-C-N              | 116.20             | 107.27          | 1                  |
| N-CA-CB             | 110.50             | 118.09          | 2                  |
| C-CA-CB             | 110.10             | 101.62          | 4                  |
| C-CA-CB             | 109.10             | 118.92          | 1                  |
| N-CA-C-CA-N-CA-C    | 111.00             | 123.50          | 1                  |
| C-N-CA              | 121.70             | 129.73          | 2                  |
| N-CA-CA-C-C-CA-CB   | 110.10             | 118.58          | 1                  |
| C-CA-CB             | 110.10             | 118.58          | 2                  |
| C-N-C-CA-C-N-CA     | 121.70             | 129.73          | 1                  |
| CA-CB-OG            | 111.10             | 102.18          | 2                  |
| N-CA-CD2-NE2-CA-C-O | 120.80             | 113.22          | 1                  |
| N-CA-C-CA-CB        | 110.10             | 118.57          | 1                  |
| CA-C-O              | 120.80             | 128.38          | 3                  |
| N-CA-C-CA-CB        | 111.40             | 102.93          | 1                  |
| CD2-NE2-CE1         | 109.00             | 104.54          | 2                  |
| C-N-N-CA-C-CA-CB    | 110.10             | 101.63          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| CD2-NE2-CA-C-CA-C-O    | 120.80             | 128.38          | 1                  |
| C-N-CA                 | 121.70             | 129.72          | 1                  |
| N-CA-C-CA-CB           | 110.10             | 101.63          | 1                  |
| CA-CB-CG               | 112.60             | 108.14          | 2                  |
| C-CA-CB                | 110.10             | 101.63          | 1                  |
| N-CA-CB                | 110.50             | 118.08          | 1                  |
| CA-N-C-CA-CB           | 110.10             | 118.57          | 1                  |
| CD1-CG-CD2             | 110.80             | 101.00          | 1                  |
| C-CA-CA-C-N-CA-C-CA-CB | 110.10             | 118.57          | 1                  |
| C-CA-N-CA-CB           | 110.50             | 118.07          | 1                  |
| C-CA-CA-CB-CG          | 113.80             | 109.35          | 1                  |
| C-N-CA                 | 121.70             | 113.68          | 1                  |
| CA-C-N                 | 116.20             | 125.11          | 1                  |
| CA-CB-CG               | 112.60             | 108.15          | 2                  |
| N-CA-CB                | 110.50             | 118.07          | 2                  |
| CA-C-O                 | 120.80             | 128.37          | 2                  |
| CA-C-O                 | 120.80             | 113.23          | 1                  |
| N-CA-C                 | 111.00             | 98.53           | 1                  |
| N-CA-N-CA-C            | 111.00             | 98.53           | 1                  |
| C-CA-C-N-CA            | 121.70             | 129.72          | 1                  |
| CA-CB-OG               | 111.10             | 102.19          | 1                  |
| CA-C-N-CA-CB           | 110.50             | 118.07          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.10             | 101.64          | 1                  |
| C-CA-N-CA-C       | 111.00             | 98.53           | 1                  |
| C-N-CA            | 121.70             | 113.69          | 2                  |
| CA-N-CD           | 112.00             | 105.77          | 1                  |
| N-CA-C            | 111.00             | 123.46          | 1                  |
| C-N-CA            | 121.70             | 129.71          | 2                  |
| C-CA-C-CA-C-N-CA  | 121.70             | 129.71          | 1                  |
| CA-C-O            | 120.80             | 128.36          | 1                  |
| N-CA-CB           | 110.50             | 102.94          | 2                  |
| C-CA-CB           | 110.10             | 101.65          | 4                  |
| CD2-NE2-CE1       | 109.00             | 104.55          | 1                  |
| CA-C-CD2-NE2-CE1  | 109.00             | 104.55          | 1                  |
| C-CA-CB           | 110.10             | 118.55          | 1                  |
| C-CA-CA-C-N-CA-CB | 110.50             | 102.94          | 1                  |
| C-N-CA            | 121.70             | 113.70          | 1                  |
| C-N-CA-C-C-CA-CB  | 110.10             | 101.65          | 1                  |
| C-N-N-CA-CB       | 110.50             | 118.06          | 1                  |
| C-CA-CA-CB-CG     | 112.60             | 108.15          | 1                  |
| N-CA-CB           | 110.40             | 103.73          | 1                  |
| CA-C-C-CA-CA-C-O  | 120.80             | 128.36          | 1                  |
| C-CA-C-CA-CB      | 110.10             | 101.65          | 1                  |
| C-N-CA-CB-OG      | 111.10             | 102.21          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-N-C-N-CA            | 121.70             | 129.70          | 1                  |
| C-CA-C-CA-CB          | 109.10             | 118.87          | 1                  |
| N-CA-C                | 111.00             | 98.56           | 1                  |
| N-CA-CA-C-CA-C-C-N-CA | 121.70             | 129.69          | 1                  |
| CA-CB-CG              | 112.60             | 108.16          | 1                  |
| C-CA-C-N-CA           | 121.70             | 113.71          | 1                  |
| N-CA-N-CA-C           | 111.00             | 98.57           | 1                  |
| N-CA-CB               | 110.50             | 102.95          | 1                  |
| C-N-C-N-CA            | 121.70             | 113.71          | 1                  |
| CA-C-O                | 120.80             | 113.25          | 1                  |
| N-CA-CA-CB-CG         | 113.80             | 109.36          | 1                  |
| C-CA-CA-CB-CG         | 113.80             | 109.36          | 1                  |
| C-N-CA                | 121.70             | 113.71          | 1                  |
| C-CA-CB               | 109.10             | 118.86          | 1                  |
| N-CA-CB               | 110.50             | 102.96          | 2                  |
| C-CA-CB               | 110.10             | 118.53          | 2                  |
| C-CA-CB               | 110.10             | 101.67          | 2                  |
| C-N-CA                | 121.70             | 129.69          | 1                  |
| CA-C-N-CA-C           | 111.00             | 123.42          | 1                  |
| C-CA-CA-C-N           | 116.20             | 107.33          | 1                  |
| CA-C-O                | 120.80             | 128.34          | 1                  |
| N-CA-CA-CB-CG         | 114.10             | 122.97          | 1                  |



| Angle type                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------|--------------------|-----------------|--------------------|
| N-CA-CD2-NE2-CE1              | 109.00             | 104.56          | 1                  |
| C-CA-CA-C-O                   | 120.80             | 113.26          | 1                  |
| N-CA-CB                       | 111.50             | 103.96          | 1                  |
| CA-C-N                        | 116.20             | 125.07          | 1                  |
| CA-C-CA-C-C-CA-CD2-NE2-CE1    | 109.00             | 104.57          | 1                  |
| N-CA-C                        | 111.00             | 123.41          | 1                  |
| CA-C-O                        | 120.80             | 113.26          | 1                  |
| CA-CB-C-CA-CA-C-O             | 120.80             | 113.26          | 1                  |
| N-CA-CB                       | 110.50             | 118.04          | 1                  |
| CD2-NE2-CE1                   | 109.00             | 104.57          | 3                  |
| C-N-CA                        | 121.70             | 113.72          | 1                  |
| C-CA-CB                       | 110.10             | 101.68          | 1                  |
| CA-C-N-CA-CB                  | 110.50             | 102.97          | 1                  |
| N-CA-CB                       | 110.50             | 102.97          | 1                  |
| CA-C-CA-C-C-CA-CB             | 110.10             | 101.68          | 1                  |
| CA-C-O                        | 120.80             | 128.33          | 2                  |
| CA-C-C-CA-N-CA-C-N-C-N-CA     | 121.70             | 113.73          | 1                  |
| C-CA-CB                       | 110.10             | 118.52          | 1                  |
| CA-C-N                        | 116.20             | 125.06          | 1                  |
| N-CA-CB                       | 110.50             | 118.03          | 1                  |
| C-CA-CB                       | 110.10             | 118.51          | 3                  |
| CA-C-C-CA-CA-C-C-N-C-N-CA-C-O | 120.80             | 111.50          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-CB            | 103.00             | 107.87          | 1                  |
| C-N-CA                  | 121.70             | 129.67          | 2                  |
| C-CA-C-CA-CB            | 110.10             | 101.69          | 1                  |
| C-CA-CB                 | 110.10             | 101.69          | 1                  |
| CA-C-N                  | 116.20             | 125.05          | 4                  |
| N-CA-CB                 | 110.50             | 118.02          | 1                  |
| N-CA-CB                 | 110.40             | 103.76          | 1                  |
| C-CA-CA-C-N             | 116.20             | 107.35          | 1                  |
| CA-CB-N-CA-N-CA-C       | 111.00             | 98.61           | 1                  |
| C-N-CA                  | 121.70             | 113.73          | 1                  |
| N-CA-CD2-NE2-CE1        | 109.00             | 104.58          | 1                  |
| C-CA-CB                 | 110.50             | 117.14          | 1                  |
| N-CA-NE-CZ-NH2          | 119.20             | 123.18          | 1                  |
| CA-C-O                  | 120.80             | 128.32          | 1                  |
| CA-CB-CG                | 112.60             | 108.18          | 1                  |
| N-CA-CB                 | 110.50             | 102.98          | 1                  |
| CA-CB-CG                | 113.80             | 109.38          | 1                  |
| CA-C-N                  | 116.20             | 107.36          | 1                  |
| N-CA-CB                 | 103.00             | 107.86          | 1                  |
| C-N-CA                  | 121.70             | 113.74          | 1                  |
| C-N-CA                  | 121.70             | 129.66          | 1                  |
| C-CA-CA-CB-CA-C-C-CA-CB | 110.10             | 101.70          | 1                  |

| Angle type               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                  | 111.40             | 119.80          | 1                  |
| N-CA-C                   | 111.00             | 123.37          | 1                  |
| N-CA-C-CA-C-CA-CB        | 110.10             | 101.70          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 101.70          | 1                  |
| N-CA-C                   | 113.30             | 100.49          | 1                  |
| C-N-CA-C-N               | 116.20             | 125.04          | 1                  |
| CA-CB-CG                 | 112.60             | 117.02          | 1                  |
| C-N-CA                   | 121.70             | 113.75          | 3                  |
| C-CA-CB                  | 110.10             | 118.49          | 3                  |
| C-CA-C-N-C-CA-CB         | 110.10             | 118.49          | 1                  |
| C-N-CA                   | 121.70             | 129.65          | 3                  |
| N-CA-C                   | 111.00             | 98.63           | 1                  |
| C-N-C-CA-CB              | 110.10             | 118.49          | 1                  |
| C-N-CA-C-O               | 120.80             | 128.31          | 1                  |
| C-N-C-CA-CB              | 110.10             | 101.71          | 1                  |
| C-CA-CB                  | 110.10             | 101.71          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 118.48          | 1                  |
| N-CA-C-N-C-N-C-N-C-CA-CB | 110.10             | 118.48          | 1                  |
| C-CA-CB                  | 110.10             | 118.48          | 1                  |
| C-CA-C-CA-CB             | 110.10             | 101.72          | 1                  |
| N-CA-C                   | 111.00             | 98.65           | 2                  |
| CA-C-O                   | 120.80             | 128.30          | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-C-N-N-CA-C-CA-CD2-NE2-CE1 | 109.00             | 104.59          | 1                  |
| C-CA-CD2-NE2-CE1                    | 109.00             | 104.59          | 1                  |
| C-N-N-CA-C-CA-CD2-NE2-CE1           | 109.00             | 104.59          | 1                  |
| C-N-CA                              | 121.70             | 113.77          | 1                  |
| N-CA-CA-C-N                         | 116.20             | 125.01          | 1                  |
| CD2-NE2-CE1                         | 109.00             | 104.59          | 1                  |
| CA-CB-CG                            | 112.60             | 108.19          | 1                  |
| N-CA-CB                             | 110.50             | 117.99          | 1                  |
| N-CA-CB                             | 103.00             | 98.15           | 1                  |
| C-CA-CB                             | 110.10             | 118.47          | 2                  |
| N-CA-C                              | 111.00             | 98.67           | 1                  |
| C-CA-C-N-CA                         | 121.70             | 113.77          | 1                  |
| CA-CB-CG                            | 114.10             | 122.91          | 1                  |
| CA-C-CA-C-N                         | 116.20             | 125.01          | 1                  |
| C-N-CA                              | 121.70             | 129.63          | 1                  |
| C-N-C-CA-C-CA-CB                    | 111.60             | 120.41          | 1                  |
| C-N-C-CA-C-N-N-CA-CB                | 110.50             | 103.02          | 1                  |
| N-CA-CB                             | 111.50             | 104.02          | 1                  |
| CA-C-C-N-CA                         | 121.70             | 129.62          | 1                  |
| CA-C-C-CA-CB                        | 110.10             | 101.74          | 1                  |
| NE-CZ-C-N-CA                        | 121.70             | 113.78          | 1                  |
| N-CA-C-CA-CB                        | 110.10             | 101.74          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| CA-C-N                           | 116.20             | 125.00          | 2                  |
| CA-CB-CA-C-N-CA-C-CA-CB          | 110.10             | 101.74          | 1                  |
| N-CA-CB                          | 110.50             | 117.98          | 2                  |
| C-N-CA                           | 121.70             | 113.78          | 1                  |
| C-CA-CB                          | 110.10             | 101.74          | 1                  |
| C-CA-CB                          | 110.10             | 118.46          | 1                  |
| CA-C-O                           | 120.80             | 128.28          | 1                  |
| CA-C-N-CA-N-CA-CB                | 103.00             | 107.84          | 1                  |
| N-CA-N-CA-CA-C-C-N-CA            | 121.70             | 129.61          | 1                  |
| CA-C-O                           | 120.80             | 113.33          | 1                  |
| C-CA-CB                          | 110.10             | 118.45          | 1                  |
| CA-C-CA-C-O                      | 120.80             | 128.27          | 1                  |
| N-CA-C                           | 111.00             | 123.31          | 1                  |
| N-CA-CB                          | 110.50             | 117.97          | 1                  |
| CA-CB-CG                         | 112.60             | 117.00          | 1                  |
| N-CA-C                           | 111.00             | 98.70           | 1                  |
| CA-CB-CG                         | 113.80             | 109.41          | 1                  |
| C-N-C-N-CA                       | 121.70             | 113.79          | 1                  |
| CA-C-C-CA-N-CA-N-CA-N-CA-C-CA-CB | 110.10             | 101.75          | 1                  |
| CA-C-CA-C-C-CA-CB                | 110.10             | 118.45          | 1                  |
| C-CA-CB                          | 110.10             | 101.75          | 1                  |
| N-CA-CA-CB-C-N-C-CA-CB           | 110.10             | 118.44          | 1                  |

| Angle type                   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------|--------------------|-----------------|--------------------|
| CD2-NE2-CE1                  | 109.00             | 104.61          | 2                  |
| C-N-N-CA-CB                  | 111.50             | 104.03          | 1                  |
| C-N-C-N-CA-C-C-N-N-CA-C-N-CA | 121.70             | 129.60          | 1                  |
| C-N-C-CA-C-CA-CB             | 110.10             | 118.44          | 1                  |
| CA-C-N-CA-C-CA-N-CA-CB       | 110.50             | 117.96          | 1                  |
| N-CA-CD1-CG-CD2              | 106.30             | 113.32          | 1                  |
| C-N-CA                       | 121.70             | 113.80          | 1                  |
| N-CA-CB                      | 103.00             | 98.17           | 1                  |
| C-CA-C-CA-CB                 | 110.10             | 101.77          | 1                  |
| C-CA-CB                      | 110.10             | 118.43          | 2                  |
| C-N-CD2-NE2-CE1              | 109.00             | 104.62          | 1                  |
| N-CA-CB                      | 110.50             | 117.95          | 1                  |
| N-CA-CA-CB-N-CA-C-CA-CB      | 110.10             | 118.43          | 1                  |
| N-CA-CA-C-O                  | 120.80             | 128.25          | 1                  |
| C-N-CA                       | 121.70             | 113.81          | 1                  |
| C-CA-CB                      | 110.10             | 101.77          | 1                  |
| N-CA-CB                      | 111.50             | 118.95          | 1                  |
| C-CA-CB                      | 111.40             | 103.07          | 1                  |
| C-CA-N-CA-C-CA-CB            | 110.10             | 101.78          | 1                  |
| N-CA-N-CA-C-N-CA             | 121.70             | 113.82          | 1                  |
| CD2-NE2-CE1                  | 109.00             | 104.62          | 1                  |
| C-CA-CB                      | 110.10             | 101.78          | 2                  |

| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| OD1-CG-ND2                           | 122.60             | 118.22          | 1                  |
| C-N-CA-C-CA-C-O                      | 120.80             | 128.25          | 1                  |
| C-CA-CB                              | 110.10             | 118.42          | 1                  |
| CA-C-C-N-CA                          | 121.70             | 129.58          | 1                  |
| N-CA-CB                              | 110.50             | 103.05          | 1                  |
| C-CA-CA-C-N                          | 116.20             | 107.44          | 1                  |
| C-N-CA                               | 121.70             | 113.82          | 1                  |
| C-CA-CD2-NE2-CE1                     | 109.00             | 104.62          | 1                  |
| C-N-CA                               | 121.70             | 129.58          | 1                  |
| C-CA-N-CA-CB                         | 110.50             | 103.06          | 1                  |
| C-N-C-CA-CB                          | 110.10             | 101.78          | 1                  |
| C-CA-C-N-CA                          | 121.70             | 129.58          | 1                  |
| C-CA-C-CA-N-CA-C                     | 111.00             | 98.75           | 1                  |
| C-CA-CB                              | 110.10             | 118.41          | 1                  |
| C-CA-C-CA-CB                         | 110.10             | 118.41          | 1                  |
| N-CA-C                               | 111.00             | 123.25          | 1                  |
| C-N-N-CA-C                           | 111.00             | 123.25          | 1                  |
| N-CA-CA-C-C-N-C-CA-CA-C-C-CA-N-CA-CB | 110.50             | 117.93          | 1                  |
| C-CA-CB                              | 111.40             | 119.71          | 1                  |
| C-N-CA                               | 121.70             | 113.83          | 2                  |
| C-N-C-N-CA                           | 121.70             | 113.83          | 1                  |
| C-CA-CD2-NE2-CE1                     | 109.00             | 104.63          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-N-CA-N-CA-C  | 111.00             | 123.23          | 1                  |
| C-N-CA            | 121.70             | 113.84          | 5                  |
| C-CA-CB           | 110.10             | 101.80          | 1                  |
| C-N-CA            | 121.70             | 129.56          | 3                  |
| OE1-CD-OE2        | 122.90             | 112.42          | 1                  |
| N-CA-CA-N-CD      | 112.00             | 105.88          | 1                  |
| C-CA-CA-C-O       | 120.80             | 113.37          | 1                  |
| N-CA-CB           | 111.50             | 104.07          | 1                  |
| N-CA-C-CA-CB      | 110.10             | 101.80          | 1                  |
| N-CA-CB           | 110.50             | 103.08          | 1                  |
| C-CA-CA-CB-N-CA-C | 111.00             | 98.77           | 1                  |
| CA-C-C-CA-CB      | 110.50             | 117.05          | 1                  |
| C-CA-CB           | 111.40             | 103.10          | 1                  |
| C-N-N-CA-CB       | 103.00             | 98.20           | 1                  |
| N-CA-CB           | 111.50             | 118.92          | 1                  |
| C-CA-CB           | 110.10             | 101.81          | 1                  |
| CA-C-C-CA-CB      | 110.10             | 118.39          | 1                  |
| C-CA-CB           | 111.60             | 120.33          | 1                  |
| C-CA-CB           | 110.50             | 117.05          | 1                  |
| N-CA-C            | 111.00             | 123.22          | 1                  |
| N-CA-CB           | 103.00             | 107.80          | 1                  |
| N-CA-N-CA-CB      | 111.50             | 104.08          | 1                  |



| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-C-CA-CA-C-N-CA-CD2-NE2-CE1 | 109.00             | 104.64          | 1                  |
| N-CA-CB                              | 110.50             | 117.92          | 1                  |
| N-CA-CA-C-N                          | 116.90             | 123.44          | 1                  |
| CA-C-CA-CB-CA-C-O                    | 120.80             | 128.22          | 1                  |
| N-CA-N-CA-C-N-CA                     | 121.70             | 113.85          | 1                  |
| CA-C-O                               | 120.80             | 128.22          | 1                  |
| CA-C-N                               | 116.20             | 124.92          | 1                  |
| CA-CB-CG                             | 112.60             | 108.24          | 1                  |
| N-CA-CB                              | 111.50             | 118.91          | 2                  |
| N-CA-C-N-N-CA-N-CA-N-CA-C            | 111.00             | 123.21          | 1                  |
| C-N-CA                               | 121.70             | 129.55          | 1                  |
| CA-C-O                               | 120.80             | 128.21          | 1                  |
| C-CA-CB                              | 109.10             | 99.51           | 1                  |
| C-CA-CB                              | 110.10             | 118.38          | 2                  |
| C-CA-CB                              | 110.10             | 101.82          | 2                  |
| CA-C-CA-CB-CG                        | 112.60             | 108.24          | 1                  |
| C-N-CA                               | 121.70             | 113.85          | 1                  |
| C-CA-CA-C-N                          | 116.20             | 107.48          | 1                  |
| N-CA-N-CA-CB                         | 103.00             | 107.79          | 1                  |
| N-CA-CB                              | 103.00             | 107.79          | 1                  |
| C-N-CA                               | 121.70             | 113.86          | 4                  |
| N-CA-C                               | 111.00             | 98.80           | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-O         | 120.80             | 128.21          | 1                  |
| OD1-CG-ND2         | 122.60             | 118.24          | 1                  |
| C-CA-CA-C-N-CA-CB  | 110.50             | 117.90          | 1                  |
| CA-C-N             | 116.20             | 107.49          | 1                  |
| C-CA-C-CA-CB       | 110.10             | 118.37          | 1                  |
| C-N-CA             | 121.70             | 129.54          | 1                  |
| CA-C-N             | 116.20             | 124.91          | 2                  |
| C-CA-C-N-CA        | 121.70             | 129.54          | 1                  |
| C-N-CA-C-N         | 116.20             | 124.91          | 1                  |
| C-CA-CD2-NE2-CE1   | 109.00             | 104.65          | 1                  |
| CA-C-O             | 120.80             | 113.40          | 2                  |
| OD1-CG-ND2         | 122.60             | 118.25          | 1                  |
| CA-C-CA-CB-CG      | 113.80             | 109.45          | 1                  |
| CA-N-CD            | 112.00             | 105.91          | 2                  |
| N-CA-CB            | 110.50             | 103.10          | 1                  |
| C-CA-CB            | 110.10             | 118.37          | 1                  |
| CA-C-CA-C-C-CA-CB  | 110.10             | 118.37          | 1                  |
| C-N-CA             | 121.70             | 113.87          | 2                  |
| CA-C-N-CA-CA-CB-CG | 112.60             | 108.25          | 1                  |
| N-CA-CB            | 110.50             | 117.89          | 1                  |
| CA-C-O             | 120.80             | 113.41          | 3                  |
| C-CA-CB            | 110.10             | 118.36          | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                   | 111.50             | 104.11          | 2                  |
| C-CA-CB                   | 109.10             | 99.53           | 1                  |
| CA-CB-CG                  | 113.80             | 109.45          | 1                  |
| N-CA-C                    | 111.00             | 123.17          | 1                  |
| N-CA-CB                   | 110.50             | 103.11          | 2                  |
| C-N-CA                    | 121.70             | 113.88          | 3                  |
| CA-C-O                    | 120.80             | 128.19          | 1                  |
| CA-CB-CG                  | 112.60             | 108.25          | 1                  |
| C-CA-CA-C-C-CA-N-CA-CB    | 110.50             | 117.89          | 1                  |
| C-CA-N-CA-C               | 111.00             | 123.17          | 1                  |
| C-CA-CA-C-O               | 120.80             | 113.41          | 1                  |
| CA-C-CD2-NE2-CE1          | 109.00             | 104.65          | 1                  |
| CA-N-CD                   | 112.00             | 105.92          | 1                  |
| C-CA-CB                   | 111.40             | 103.15          | 1                  |
| C-CA-CB                   | 110.10             | 118.35          | 1                  |
| C-CA-CB                   | 110.10             | 101.85          | 1                  |
| CA-C-C-CA-C-N-C-CA-C-N-CA | 121.70             | 129.52          | 1                  |
| N-CA-CB                   | 103.00             | 98.22           | 1                  |
| C-N-CA-C-O                | 120.80             | 128.18          | 1                  |
| CA-C-O                    | 120.80             | 113.42          | 1                  |
| CA-C-N                    | 116.20             | 124.88          | 1                  |
| CA-C-CA-C-C-CA-CB         | 110.10             | 101.85          | 1                  |

| Angle type                                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| C-CA-C-N-CA                                 | 121.70             | 113.89          | 1                  |
| N-CA-CA-CB-CG                               | 113.80             | 109.46          | 1                  |
| N-CA-C-CA-CB                                | 110.10             | 118.34          | 1                  |
| CA-N-CD                                     | 112.00             | 105.93          | 1                  |
| C-CA-CA-C-CA-C-N-CA-CA-C-CA-C-N-CA-CA-CB-CG | 113.60             | 121.84          | 1                  |
| OD1-CG-ND2                                  | 122.60             | 118.26          | 1                  |
| N-CA-CB                                     | 110.50             | 103.13          | 1                  |
| CA-C-CD2-NE2-N-CA-C-CA-N-CA-CB              | 110.50             | 103.13          | 1                  |
| N-CA-CB                                     | 110.40             | 103.90          | 1                  |
| C-CA-CB                                     | 110.10             | 118.34          | 2                  |
| CG-CD2-C-N-CA                               | 121.70             | 129.50          | 1                  |
| C-N-C-CA-CB                                 | 110.10             | 101.86          | 1                  |
| CA-C-O                                      | 120.80             | 113.43          | 1                  |
| CA-CB-CG                                    | 112.60             | 108.27          | 1                  |
| CA-C-N                                      | 116.20             | 107.53          | 1                  |
| C-CA-CB                                     | 110.10             | 101.87          | 2                  |
| C-N-N-CA-CB                                 | 110.50             | 103.14          | 1                  |
| CA-CB-CG                                    | 113.80             | 109.47          | 2                  |
| C-N-CA                                      | 121.70             | 129.50          | 1                  |
| C-N-C-CA-C-N-C-CA-N-CA-N-CA-CB              | 110.50             | 117.86          | 1                  |
| N-CA-C-N-CA                                 | 121.70             | 129.49          | 1                  |
| C-CA-CB                                     | 110.10             | 118.33          | 1                  |

| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB      | 110.10             | 118.32          | 1                  |
| C-CA-CB           | 110.10             | 101.88          | 3                  |
| C-CA-C-CA-CB      | 109.10             | 118.62          | 1                  |
| N-CA-CB           | 111.50             | 104.14          | 1                  |
| CA-C-O            | 120.80             | 128.16          | 2                  |
| C-CA-C-N-CA       | 121.70             | 129.49          | 1                  |
| CA-N-CD           | 112.00             | 105.94          | 1                  |
| C-CA-CA-C-O       | 120.80             | 128.16          | 1                  |
| C-N-C-N-CA        | 121.70             | 113.91          | 1                  |
| C-CA-CB           | 110.10             | 118.32          | 1                  |
| CA-C-C-CA-CB      | 110.10             | 101.88          | 1                  |
| CA-C-N-CA-CB      | 110.50             | 117.85          | 1                  |
| N-CA-CB           | 111.50             | 104.15          | 1                  |
| CA-C-O            | 120.80             | 128.15          | 1                  |
| N-CA-CA-C-CA-N-CD | 112.00             | 105.94          | 1                  |
| CA-C-N            | 116.90             | 110.41          | 1                  |
| CA-C-N            | 116.20             | 124.85          | 1                  |
| CA-CB-CG          | 112.60             | 108.28          | 1                  |
| CA-CB-CG2         | 110.40             | 117.75          | 1                  |
| N-CA-CB           | 110.40             | 103.91          | 1                  |
| C-N-CA            | 121.70             | 129.48          | 1                  |
| N-CA-CB           | 110.50             | 103.15          | 1                  |

| Angle type                   | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-N-CA                  | 121.70             | 113.92          | 2                  |
| C-CA-CB                      | 109.10             | 118.61          | 1                  |
| C-CA-C-N-CA-CB-CG            | 113.90             | 106.12          | 1                  |
| C-N-CA                       | 121.70             | 113.92          | 1                  |
| CA-CB-C-CA-CA-C-N-CA-CB      | 110.50             | 117.84          | 1                  |
| C-N-CA                       | 121.70             | 113.93          | 1                  |
| N-CA-CA-C-N                  | 116.90             | 123.38          | 1                  |
| N-CA-N-CA-CA-C-C-N-CA        | 121.70             | 113.93          | 1                  |
| C-N-CA                       | 121.70             | 129.47          | 2                  |
| C-N-CA-CB-CG                 | 112.60             | 108.28          | 1                  |
| C-CA-N-CA-CD-NE-CA-CB-C-N-CA | 121.70             | 113.93          | 1                  |
| C-CA-CB                      | 110.10             | 101.90          | 1                  |
| C-CA-C-N-C-CA-C-CA-CB        | 110.10             | 118.30          | 1                  |
| N-CA-CA-CB-CG                | 113.60             | 121.80          | 1                  |
| C-CA-CB                      | 110.50             | 116.97          | 1                  |
| N-CA-CB                      | 111.50             | 104.17          | 1                  |
| N-CA-CA-N-CD                 | 112.00             | 105.96          | 1                  |
| C-CA-N-CA-C-N-N-CA-CB        | 110.40             | 103.93          | 1                  |
| CA-C-N-CA-CB                 | 110.50             | 103.17          | 1                  |
| CA-CB-CG                     | 112.60             | 108.29          | 3                  |
| CA-C-CA-CB-CG2               | 110.40             | 117.73          | 1                  |
| N-CA-N-CA-CB                 | 110.50             | 117.83          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CD-NE-C-CA-CB              | 110.10             | 101.91          | 1                  |
| C-CA-C-CA-CB               | 110.10             | 101.91          | 1                  |
| CA-C-C-N-CA                | 121.70             | 129.46          | 1                  |
| N-CD-CG                    | 103.20             | 109.67          | 1                  |
| CA-C-O                     | 120.80             | 113.47          | 1                  |
| C-CA-CA-C-C-CA-N-CA-C      | 111.00             | 123.07          | 1                  |
| N-CA-CB                    | 110.50             | 117.83          | 1                  |
| CD2-NE2-CE1                | 109.00             | 104.69          | 1                  |
| C-CA-CB                    | 110.10             | 101.91          | 1                  |
| C-CA-CA-C-O                | 120.80             | 128.13          | 1                  |
| N-CA-CA-N-CD               | 112.00             | 105.97          | 1                  |
| C-N-CA-C-N-CA-CA-C-N       | 116.20             | 124.82          | 1                  |
| C-CA-CA-C-C-CA-N-CA-CB     | 110.40             | 103.94          | 1                  |
| N-CA-CA-CB-CG              | 112.60             | 108.29          | 1                  |
| N-CA-CB                    | 110.50             | 103.18          | 1                  |
| N-CA-CA-CB-CA-C-O          | 120.80             | 128.12          | 1                  |
| C-CA-CB                    | 110.10             | 118.28          | 2                  |
| CA-C-N                     | 116.90             | 110.44          | 1                  |
| CA-C-C-N-CA                | 121.70             | 113.95          | 1                  |
| CA-C-C-N-C-CA-N-CA-C-CA-CB | 110.10             | 118.28          | 1                  |
| C-CA-C-CA-CA-C-CA-C-N      | 116.20             | 107.59          | 1                  |
| C-CA-CA-C-C-CA-CB          | 110.10             | 101.92          | 1                  |

| Angle type                      | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------------|--------------------|-----------------|--------------------|
| C-CA-C-CA-C-CA-CB               | 110.10             | 101.92          | 1                  |
| C-CA-C-N-CA                     | 121.70             | 129.45          | 1                  |
| CA-CB-CG2                       | 110.40             | 117.72          | 1                  |
| C-N-CA                          | 121.70             | 129.45          | 1                  |
| C-CA-CB                         | 111.40             | 103.22          | 1                  |
| C-N-C-N-CA                      | 121.70             | 113.96          | 1                  |
| C-N-C-N-C-N-CA                  | 121.70             | 129.44          | 1                  |
| N-CA-C-CA-CB                    | 110.10             | 118.27          | 1                  |
| CA-C-N                          | 116.90             | 123.35          | 1                  |
| C-CA-C-CA-CB                    | 110.10             | 118.27          | 1                  |
| CA-N-CD                         | 112.00             | 105.98          | 1                  |
| C-CA-CB                         | 110.10             | 118.27          | 2                  |
| C-N-CA-CB-CG                    | 113.90             | 106.16          | 1                  |
| CA-CB-CG                        | 112.60             | 108.30          | 1                  |
| N-CA-N-CD-C-N-CA-C-CB-CG-CA-C-O | 120.80             | 113.49          | 1                  |
| CA-C-N                          | 116.20             | 124.80          | 1                  |
| CA-CB-CG                        | 114.10             | 122.70          | 1                  |
| CA-C-O                          | 120.80             | 113.49          | 2                  |
| N-CA-CB                         | 110.40             | 103.95          | 1                  |
| CG-CD2-CA-C-N-CA-CB             | 110.50             | 103.19          | 1                  |
| C-CA-CB                         | 110.10             | 101.94          | 4                  |
| N-CA-CB                         | 111.50             | 118.81          | 1                  |



| Angle type                                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|--------------------|-----------------|--------------------|
| CA-C-O                                      | 120.80             | 113.50          | 2                  |
| N-CA-C                                      | 111.00             | 98.97           | 1                  |
| C-CA-CB                                     | 110.10             | 118.26          | 1                  |
| C-N-C-CA-N-CA-C                             | 111.00             | 98.97           | 1                  |
| C-N-C-N-CA                                  | 121.70             | 113.97          | 1                  |
| CA-CB-CG                                    | 112.60             | 108.31          | 1                  |
| N-CA-CB                                     | 110.50             | 103.20          | 1                  |
| CA-N-CD                                     | 112.00             | 105.99          | 1                  |
| N-CA-C                                      | 111.00             | 123.02          | 1                  |
| CA-C-C-N-CA                                 | 121.70             | 129.43          | 1                  |
| N-CA-CB                                     | 103.00             | 107.72          | 1                  |
| CA-C-CA-CB-CG                               | 112.60             | 108.31          | 1                  |
| N-CA-CD2-NE2-C-N-CA-C-C-N-C-CA-CA-C-N-CA-CB | 111.50             | 118.80          | 1                  |
| N-CA-CA-CB-CG                               | 112.60             | 108.31          | 1                  |
| N-CA-C                                      | 111.00             | 98.98           | 1                  |
| C-CA-CB                                     | 111.40             | 103.25          | 1                  |
| N-CD-CG                                     | 103.20             | 96.76           | 1                  |
| C-CA-CB                                     | 110.50             | 116.94          | 1                  |
| NE-CZ-C-N-C-N-C-N-N-CA-CB                   | 110.50             | 103.21          | 1                  |
| C-CA-CB                                     | 110.10             | 101.95          | 1                  |
| N-CA-C                                      | 111.00             | 98.99           | 1                  |
| N-CA-C-N-C-N-C-CA-CB                        | 110.10             | 101.95          | 1                  |

| Angle type                     | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------|--------------------|-----------------|--------------------|
| N-CA-C-N-CA                    | 121.70             | 129.42          | 1                  |
| CA-C-N                         | 116.20             | 124.78          | 1                  |
| C-CA-N-CA-C-N-N-CD-CG          | 103.20             | 109.63          | 1                  |
| CA-C-O                         | 120.80             | 113.51          | 1                  |
| C-N-CA-C-N                     | 116.20             | 107.62          | 1                  |
| CA-N-CD                        | 112.00             | 106.00          | 1                  |
| C-N-CA                         | 121.70             | 129.42          | 1                  |
| CA-C-N                         | 116.20             | 124.77          | 1                  |
| C-CA-CB                        | 110.10             | 118.24          | 3                  |
| C-N-C-CA-CB                    | 111.40             | 103.26          | 1                  |
| C-CA-CB                        | 110.10             | 101.96          | 1                  |
| CA-C-O                         | 120.80             | 128.08          | 2                  |
| CA-C-CA-C-O                    | 120.80             | 113.52          | 1                  |
| C-N-CA-C-N                     | 116.20             | 124.77          | 1                  |
| CA-C-O                         | 120.80             | 113.52          | 2                  |
| CG-CD2-C-N-C-N-C-N-CA-C-CA-C-N | 116.20             | 107.63          | 1                  |
| CA-C-C-N-CA                    | 121.70             | 113.99          | 1                  |
| CD2-NE2-CE1                    | 109.00             | 104.72          | 1                  |
| N-CA-CA-C-N                    | 116.20             | 124.76          | 1                  |
| CA-C-N                         | 116.20             | 124.76          | 1                  |
| CA-C-N                         | 116.20             | 107.64          | 2                  |
| CA-C-N-CA-CA-C-N               | 116.20             | 124.76          | 1                  |

| Angle type                               | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| CA-C-N                                   | 116.90             | 123.32          | 1                  |
| N-CA-C                                   | 111.00             | 99.01           | 1                  |
| C-CA-CB                                  | 110.10             | 101.97          | 2                  |
| C-N-C-CA-C-N-N-CA-CA-C-O                 | 120.80             | 113.53          | 1                  |
| C-N-CA                                   | 121.70             | 129.40          | 2                  |
| N-CA-C-CA-CB                             | 110.10             | 101.97          | 1                  |
| N-CA-C                                   | 111.00             | 122.98          | 1                  |
| CA-CB-CA-CB-CG2                          | 110.40             | 117.67          | 1                  |
| C-CA-CB                                  | 111.40             | 103.27          | 1                  |
| CA-C-O                                   | 120.80             | 113.53          | 3                  |
| C-CA-C-N-C-N-CA-C-C-CA-CA-CB-C-N-N-CA-CB | 110.50             | 103.23          | 1                  |
| CA-C-C-CA-CB                             | 110.10             | 118.22          | 1                  |
| C-CA-C-CA-CB                             | 110.10             | 118.22          | 1                  |
| CA-CB-CG                                 | 113.80             | 109.53          | 1                  |
| C-CA-CB                                  | 110.10             | 101.98          | 1                  |
| C-N-C-N-N-CA-CB                          | 111.50             | 118.77          | 1                  |
| C-N-C-CA-CB                              | 110.10             | 118.22          | 1                  |
| N-CA-CB                                  | 110.50             | 103.24          | 4                  |
| N-CA-CB                                  | 110.50             | 117.76          | 2                  |
| C-N-C-N-N-CA-C                           | 111.00             | 122.96          | 1                  |
| CA-C-N-CA-CB                             | 110.50             | 117.76          | 1                  |
| CA-C-C-CA-N-CA-C                         | 111.00             | 122.96          | 1                  |

| Angle type                                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--|--------------------|-----------------|--------------------|
| C-N-CA   | 121.70             | 114.01          | 1                  |
| CA-C-O   | 120.80             | 128.06          | 1                  |
| C-CA-C-N-CA                                      | 121.70             | 129.39          | 1                  |
| C-N-CA   | 121.70             | 129.38          | 1                  |
| CA-C-N   | 116.20             | 107.66          | 1                  |
| CA-CB-N-CA-CA-C-C-N-N-CD-C-N-N-CA-C              | 111.00             | 122.95          | 1                  |
| C-N-N-CA-C                                       | 113.30             | 125.67          | 1                  |
| C-N-C-CA-CA-C-O                                  | 120.80             | 113.55          | 1                  |
| N-CA-C-N-CA                                      | 121.70             | 129.38          | 1                  |
| N-CA-CA-C-O                                      | 120.80             | 128.05          | 1                  |
| CA-C-N   | 116.20             | 107.67          | 1                  |
| N-CA-C   | 111.00             | 122.94          | 1                  |
| CA-C-CA-C-O                                      | 120.80             | 113.55          | 1                  |
| CA-CB-C-N-CA-C-N                                 | 116.20             | 107.67          | 1                  |
| CA-C-CA-N-CD                                     | 112.00             | 106.03          | 1                  |
| C-CA-C-CA-CB                                     | 110.10             | 118.20          | 1                  |
| CA-C-O   | 120.80             | 113.55          | 1                  |
| N-CA-CB  | 110.50             | 103.25          | 1                  |
| N-CA-N-CA-NE-CZ-C-N-CA-CB-CA-C-CA-C-C-CA-C-CA-CB | 110.10             | 102.00          | 1                  |
| CA-CB-CG   | 113.80             | 109.54          | 1                  |
| C-CA-CB  | 110.10             | 102.00          | 1                  |
| C-CA-CG-CD2-C-N-CA                               | 121.70             | 129.37          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                | 113.90             | 106.23          | 1                  |
| C-CA-CA-CB-CG           | 112.60             | 108.34          | 1                  |
| N-CA-C                  | 111.00             | 122.93          | 1                  |
| C-N-N-CA-CB             | 111.50             | 104.26          | 1                  |
| CA-C-C-CA-C-CA-CB       | 110.10             | 118.19          | 1                  |
| C-N-CA-C-N              | 116.20             | 107.68          | 1                  |
| C-CA-CB                 | 110.10             | 118.19          | 1                  |
| N-CA-C                  | 111.00             | 122.92          | 1                  |
| N-CA-C                  | 113.30             | 125.65          | 1                  |
| C-N-CA-C-N              | 116.20             | 107.69          | 1                  |
| CA-CB-C-N-CA            | 121.70             | 114.04          | 1                  |
| CA-C-C-CA-CB            | 110.10             | 118.19          | 1                  |
| CA-CB-CB-CG-CD2-NE2-CE1 | 109.00             | 104.74          | 1                  |
| N-CA-C                  | 111.00             | 99.09           | 3                  |
| C-CA-CB                 | 110.10             | 118.18          | 2                  |
| C-CA-C-CA-CB            | 110.10             | 102.02          | 1                  |
| CA-C-C-CA-C-N-CA-C-O    | 120.80             | 113.57          | 1                  |
| CA-CB-CG                | 113.90             | 106.24          | 1                  |
| N-CA-CB                 | 110.50             | 117.73          | 1                  |
| CA-C-N                  | 116.20             | 107.69          | 1                  |
| C-N-N-CA-CB             | 110.50             | 103.27          | 1                  |
| C-N-C-N-CA              | 121.70             | 114.05          | 2                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB         | 110.10             | 118.18          | 1                  |
| N-CA-CB              | 111.50             | 104.27          | 1                  |
| CA-C-O               | 120.80             | 128.03          | 2                  |
| C-N-CA               | 121.70             | 129.35          | 1                  |
| CA-C-N               | 116.20             | 107.70          | 4                  |
| C-CA-CB              | 111.40             | 103.33          | 1                  |
| CA-CB-N-CA-C         | 113.30             | 125.62          | 1                  |
| N-CA-CB              | 110.50             | 117.72          | 1                  |
| CA-CB-CG             | 112.60             | 108.35          | 1                  |
| C-N-C-CA-CB          | 109.10             | 99.75           | 1                  |
| CA-C-O               | 120.80             | 113.58          | 3                  |
| CA-C-C-CA-CB         | 110.10             | 118.17          | 1                  |
| C-N-N-CA-CB          | 110.50             | 117.72          | 1                  |
| CA-C-CA-C-O          | 120.80             | 113.58          | 1                  |
| C-CA-CA-C-N          | 116.20             | 124.70          | 1                  |
| C-CA-C-CA-CB         | 111.40             | 103.33          | 1                  |
| C-N-N-CA-CB          | 110.40             | 104.03          | 1                  |
| N-CA-C-CA-C-N-CA-C-N | 116.20             | 124.69          | 1                  |
| CB-CG-C-CA-CB        | 111.60             | 120.09          | 1                  |
| C-N-CA               | 121.70             | 129.34          | 1                  |
| CA-C-CB-CG-CA-C-N    | 116.20             | 107.71          | 1                  |
| C-N-CA               | 121.70             | 114.06          | 1                  |

| Angle type                       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                          | 110.10             | 118.16          | 2                  |
| CA-C-N                           | 116.20             | 107.71          | 1                  |
| NE-CZ-CA-C-C-N-C-CA-CB           | 111.40             | 103.34          | 1                  |
| CA-C-O                           | 120.80             | 113.59          | 1                  |
| N-CA-CB                          | 111.50             | 104.29          | 2                  |
| N-CA-CB                          | 110.50             | 103.29          | 1                  |
| CA-CB-CA-CB-C-N-C-CA-C-N-C-CA-CB | 109.10             | 99.77           | 1                  |
| CA-C-N                           | 116.20             | 107.72          | 2                  |
| CA-C-N                           | 116.20             | 124.68          | 1                  |
| C-CA-N-CA-CB                     | 111.50             | 104.29          | 1                  |
| C-N-C-CA-CB                      | 110.10             | 118.16          | 1                  |
| C-CA-CB                          | 110.10             | 102.04          | 2                  |
| CA-CB-OG                         | 111.10             | 102.62          | 1                  |
| CA-CB-CG                         | 112.60             | 108.36          | 1                  |
| C-N-CA                           | 121.70             | 129.33          | 1                  |
| C-CA-CB                          | 110.10             | 102.05          | 1                  |
| C-N-CA                           | 121.70             | 114.07          | 1                  |
| C-CA-CB                          | 111.60             | 120.08          | 1                  |
| CA-C-CA-C-N                      | 116.20             | 107.72          | 1                  |
| N-CA-C                           | 111.00             | 99.13           | 1                  |
| C-N-C-CA-CB                      | 110.10             | 118.15          | 1                  |
| N-CA-CB                          | 110.50             | 103.30          | 2                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-CB                | 111.50             | 118.70          | 1                  |
| N-CA-C                 | 111.00             | 99.14           | 1                  |
| CA-C-O                 | 120.80             | 128.00          | 1                  |
| C-CA-C-N-CA-C-N        | 116.20             | 107.73          | 1                  |
| C-N-CA                 | 121.70             | 114.08          | 2                  |
| N-CA-CA-C-O            | 120.80             | 128.00          | 1                  |
| C-N-CA                 | 121.70             | 129.32          | 3                  |
| C-CA-CB                | 110.10             | 118.15          | 1                  |
| C-N-CA-C-N             | 116.20             | 107.73          | 1                  |
| N-CA-C                 | 113.30             | 125.58          | 1                  |
| CA-C-N-CA-CB           | 110.50             | 117.70          | 1                  |
| N-CA-C                 | 111.00             | 122.86          | 1                  |
| CA-C-CA-CB-C-CA-CA-C-N | 116.20             | 107.73          | 1                  |
| N-CA-C                 | 111.00             | 122.85          | 1                  |
| CA-C-N                 | 116.20             | 124.66          | 1                  |
| CG-CD2-NE2             | 107.20             | 102.97          | 1                  |
| N-CA-CB                | 111.50             | 104.31          | 1                  |
| CA-N-CD                | 112.00             | 106.08          | 1                  |
| C-CA-C-N-CA            | 121.70             | 114.08          | 1                  |
| CA-C-O                 | 120.80             | 127.99          | 1                  |
| C-CA-CB                | 110.10             | 118.14          | 1                  |
| CA-C-N                 | 116.20             | 107.74          | 2                  |



| Angle type                           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                              | 109.10             | 99.79           | 1                  |
| CA-C-N-CA-CB                         | 110.40             | 104.05          | 1                  |
| C-CA-C-CA-CA-C-CA-C-N                | 116.20             | 107.74          | 1                  |
| C-CA-C-N-C-CA-CB                     | 109.10             | 99.80           | 1                  |
| C-CA-CA-C-N-CA-C                     | 111.00             | 122.84          | 1                  |
| CA-C-CA-C-C-CA-C-N-CA-CB-N-CA-C-N-CA | 121.70             | 129.31          | 1                  |
| CD-NE-CZ                             | 124.40             | 118.48          | 1                  |
| C-CA-N-CA-C                          | 111.00             | 99.17           | 1                  |
| CA-C-CA-C-O                          | 120.80             | 127.98          | 1                  |
| C-N-CA-C-C-CA-CB                     | 110.10             | 102.07          | 1                  |
| C-N-N-CA-C                           | 111.00             | 122.83          | 1                  |
| C-CA-CB                              | 110.10             | 102.08          | 1                  |
| N-CA-C                               | 111.00             | 99.17           | 1                  |
| CA-C-O                               | 120.80             | 113.62          | 1                  |
| C-N-CA-CB-CG                         | 112.60             | 108.38          | 1                  |
| CB-CG-CD                             | 112.60             | 105.42          | 1                  |
| N-CA-CA-N-CD                         | 112.00             | 106.09          | 1                  |
| CA-C-O                               | 120.80             | 127.98          | 1                  |
| CA-C-CA-CB-C-CA-CB                   | 110.50             | 116.83          | 1                  |
| C-N-N-CA-CA-C-C-CA-CB                | 110.10             | 102.08          | 1                  |
| CA-CB-CG                             | 112.60             | 108.38          | 1                  |
| CA-N-C-N-N-CA-CA-CB-CG               | 113.90             | 106.31          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-N-CA                     | 121.70             | 114.11          | 1                  |
| CA-C-N                     | 116.20             | 107.76          | 1                  |
| CA-CB-C-CA-CB              | 110.10             | 118.11          | 1                  |
| CA-C-C-CA-CB               | 110.10             | 102.09          | 1                  |
| C-CA-CB                    | 110.10             | 102.09          | 2                  |
| N-CD-CG                    | 103.20             | 96.87           | 1                  |
| C-CA-C-N-CA                | 121.70             | 114.11          | 1                  |
| N-CA-C-N-C-CA-CB           | 110.50             | 116.83          | 1                  |
| N-CA-CB                    | 110.50             | 103.33          | 1                  |
| CA-C-N                     | 116.20             | 107.77          | 3                  |
| CA-C-CA-C-N                | 116.20             | 107.77          | 1                  |
| C-CA-CB                    | 110.10             | 118.11          | 1                  |
| CA-C-C-N-CA                | 121.70             | 114.11          | 1                  |
| N-CA-C                     | 111.00             | 99.20           | 1                  |
| CA-C-C-N-C-N-C-CA-CB       | 110.10             | 102.09          | 1                  |
| N-CA-C-CA-CA-C-C-N-C-CA-CB | 110.10             | 102.09          | 1                  |
| C-N-CA                     | 121.70             | 114.12          | 2                  |
| CA-CB-OG                   | 111.10             | 102.67          | 1                  |
| C-CA-CB                    | 110.10             | 102.10          | 3                  |
| C-N-CA-C-CB-CG-CD          | 112.60             | 105.44          | 1                  |
| C-CA-CB                    | 110.10             | 118.10          | 1                  |
| C-N-CA                     | 121.70             | 129.28          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| CA-CB-CG                   | 113.80             | 109.59          | 1                  |
| CA-C-O                     | 120.80             | 127.96          | 3                  |
| CA-C-O                     | 120.80             | 113.64          | 1                  |
| C-CA-CB                    | 111.60             | 120.02          | 1                  |
| CA-C-N                     | 116.20             | 107.78          | 1                  |
| C-CA-C-N-CA                | 121.70             | 114.12          | 1                  |
| N-CA-C-CA-C-CA-C-CA-C-N-CA | 121.70             | 129.28          | 1                  |
| C-CA-CB                    | 111.40             | 119.40          | 1                  |
| C-CA-C-CA-CB               | 110.10             | 118.10          | 1                  |
| C-N-C-CA-CB                | 110.10             | 102.10          | 1                  |
| N-CA-N-CA-C-CA-CB          | 110.10             | 102.10          | 1                  |
| C-CA-C-CA-C-CA-CB          | 110.10             | 102.10          | 1                  |
| N-CA-CB                    | 110.50             | 117.65          | 1                  |
| CA-CB-CG                   | 114.10             | 105.69          | 1                  |
| C-CA-CB                    | 110.10             | 118.09          | 1                  |
| N-CA-CB                    | 111.50             | 104.35          | 1                  |
| N-CA-C                     | 111.00             | 99.22           | 1                  |
| C-CA-CB                    | 110.50             | 116.81          | 1                  |
| N-CA-C-N-CA                | 121.70             | 114.13          | 1                  |
| C-CA-CB                    | 110.10             | 102.11          | 3                  |
| C-N-CA-CB-OG1              | 109.60             | 103.29          | 1                  |
| C-N-CA                     | 121.70             | 129.27          | 1                  |

| Angle type           | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------|--------------------|-----------------|--------------------|
| C-N-C-N-CA           | 121.70             | 114.13          | 1                  |
| C-CA-C-CA-CB         | 110.10             | 118.09          | 1                  |
| CA-C-C-N-CA-CB-CG    | 114.10             | 105.69          | 1                  |
| C-CA-C-N-C-N-CA      | 121.70             | 114.13          | 1                  |
| CA-C-O               | 120.80             | 127.95          | 1                  |
| CA-C-CA-C-O          | 120.80             | 113.65          | 1                  |
| CA-C-O               | 120.80             | 113.65          | 1                  |
| C-N-CA-C-N           | 116.20             | 124.61          | 1                  |
| CA-C-O               | 120.80             | 113.66          | 2                  |
| C-CA-CB              | 110.10             | 118.08          | 2                  |
| N-CA-N-CA-C-N-C-N-CA | 121.70             | 114.14          | 1                  |
| C-CA-CA-C-N          | 116.20             | 107.80          | 1                  |
| C-CA-CB              | 110.10             | 102.12          | 3                  |
| N-CA-C-CA-C-N-C-N-CA | 121.70             | 114.14          | 1                  |
| CA-C-CA-C-N          | 116.20             | 107.80          | 1                  |
| C-CA-CA-N-CD         | 112.00             | 106.12          | 1                  |
| C-CA-C-N-CA          | 121.70             | 114.14          | 1                  |
| C-N-CA               | 121.70             | 114.14          | 1                  |
| CA-CB-CG             | 113.90             | 106.34          | 1                  |
| C-CA-C-CA-CB         | 110.10             | 118.08          | 1                  |
| C-N-CA               | 121.70             | 129.26          | 1                  |
| C-CA-CB              | 110.50             | 104.20          | 1                  |

| Angle type                    | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-C-CA-CB             | 110.50             | 104.20          | 1                  |
| CA-C-CA-C-CA-CB-CA-C-CA-CB-CG | 112.60             | 108.40          | 1                  |
| CD-NE-CZ                      | 124.40             | 118.53          | 1                  |
| C-N-CA                        | 121.70             | 129.25          | 1                  |
| CA-CB-CG                      | 112.60             | 108.41          | 2                  |
| N-CA-N-CA-N-CA-C              | 111.00             | 99.26           | 1                  |
| CA-C-C-CA-CB                  | 110.10             | 102.13          | 1                  |
| C-CA-CB                       | 110.10             | 118.07          | 1                  |
| N-CA-C                        | 111.00             | 99.26           | 3                  |
| N-CA-CB                       | 111.50             | 118.63          | 1                  |
| CA-C-O                        | 120.80             | 113.67          | 1                  |
| C-CA-CB                       | 111.40             | 119.37          | 1                  |
| CA-C-C-N-C-CA-CB              | 110.10             | 102.13          | 1                  |
| C-N-C-CA-CB                   | 110.10             | 102.13          | 1                  |
| C-N-CA                        | 121.70             | 114.15          | 1                  |
| C-CA-C-CA-CB                  | 110.10             | 102.14          | 1                  |
| C-N-CA                        | 121.70             | 114.16          | 2                  |
| CA-N-N-CA-N-CA-C-CA-CB        | 110.10             | 102.14          | 1                  |
| CA-N-CD                       | 112.00             | 106.13          | 1                  |
| C-CA-C-N-CA-C-O               | 120.80             | 113.68          | 1                  |
| N-CA-CB                       | 110.50             | 117.62          | 2                  |
| CA-C-N                        | 116.20             | 124.58          | 1                  |

| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| CA-C-N-CA-CB              | 111.50             | 118.62          | 1                  |
| CA-C-N                    | 116.20             | 107.82          | 1                  |
| CA-N-CD                   | 112.00             | 106.14          | 1                  |
| C-N-CA                    | 121.70             | 129.24          | 1                  |
| C-N-C-CA-CB               | 110.10             | 118.06          | 1                  |
| C-N-N-CA-CB               | 111.50             | 118.62          | 1                  |
| N-CA-CA-C-N               | 116.20             | 107.82          | 1                  |
| N-CA-C                    | 111.00             | 99.27           | 1                  |
| C-CA-N-CA-C               | 111.00             | 99.27           | 1                  |
| C-N-C-CA-CB               | 110.10             | 102.14          | 1                  |
| C-CA-C-N-C-CA-CA-C-N-CA-C | 111.00             | 99.28           | 1                  |
| C-CA-CA-C-O               | 120.80             | 113.68          | 1                  |
| N-CA-CA-C-CA-C-C-CA-CB    | 110.10             | 102.15          | 1                  |
| N-CA-CA-C-O               | 120.80             | 113.68          | 1                  |
| N-CA-C-CA-C-CA-CB         | 110.10             | 102.15          | 1                  |
| CA-C-O                    | 120.80             | 113.69          | 1                  |
| C-CA-CB                   | 110.10             | 102.15          | 2                  |
| CA-C-O                    | 120.80             | 127.91          | 2                  |
| N-CA-CB                   | 110.50             | 103.39          | 1                  |
| N-CA-C                    | 111.00             | 99.28           | 1                  |
| C-CA-C-CA-CB              | 110.10             | 102.15          | 1                  |
| C-N-CA                    | 121.70             | 129.23          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-C-CA-CB     | 110.10             | 102.15          | 1                  |
| N-CA-CB          | 111.50             | 118.61          | 1                  |
| N-CA-C           | 111.00             | 99.29           | 1                  |
| C-CA-N-CA-C      | 111.00             | 99.29           | 1                  |
| N-CA-CB          | 110.50             | 117.61          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 118.04          | 1                  |
| N-CA-C           | 111.00             | 122.71          | 1                  |
| C-N-CA-C-O       | 120.80             | 113.69          | 1                  |
| C-CA-CB          | 110.10             | 118.04          | 3                  |
| C-N-CA           | 121.70             | 114.18          | 1                  |
| CA-C-N-CA-CB     | 110.50             | 103.39          | 1                  |
| CA-CB-C-CA-CB    | 110.10             | 118.04          | 1                  |
| C-N-CA-C-O       | 120.80             | 127.90          | 1                  |
| C-N-CA-CB-N-CA-C | 112.10             | 122.55          | 1                  |
| N-CA-CB          | 110.50             | 117.60          | 2                  |
| CB-CG-CD         | 112.60             | 105.50          | 1                  |
| CA-C-C-N-CA-C-N  | 116.20             | 107.85          | 1                  |
| C-CA-CB          | 110.10             | 102.16          | 1                  |
| CA-C-O           | 120.80             | 127.90          | 1                  |
| C-CA-CA-CB-CG    | 112.60             | 108.42          | 1                  |
| C-CA-CB          | 110.10             | 118.03          | 4                  |
| N-CA-CB          | 110.40             | 104.14          | 1                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| N-CA-C              | 111.00             | 122.69          | 2                  |
| C-CA-CB             | 110.10             | 102.17          | 2                  |
| C-N-C-N-CA-C-C-N-CA | 121.70             | 129.21          | 1                  |
| N-CA-C-N-C-CA-CB    | 110.10             | 102.17          | 1                  |
| N-CA-CB             | 110.50             | 117.59          | 1                  |
| N-CA-C              | 112.10             | 122.53          | 1                  |
| C-CA-C-CA-CB        | 110.10             | 102.17          | 1                  |
| C-N-CA              | 121.70             | 129.21          | 1                  |
| C-N-CA-C-CA-C-N     | 116.20             | 107.86          | 1                  |
| C-CA-C-CA-CB        | 111.60             | 119.94          | 1                  |
| C-CA-CB             | 110.10             | 102.18          | 3                  |
| CA-C-O              | 120.80             | 127.89          | 1                  |
| C-CA-CB             | 110.10             | 118.02          | 1                  |
| CA-C-N              | 116.20             | 107.86          | 1                  |
| CA-C-O              | 120.80             | 113.71          | 1                  |
| N-CA-CB             | 111.50             | 118.59          | 1                  |
| C-N-CA              | 121.70             | 114.20          | 2                  |
| CA-C-CA-C-O         | 120.80             | 127.89          | 1                  |
| CA-C-N              | 116.20             | 124.54          | 1                  |
| C-CA-C-CA-CB        | 111.40             | 103.48          | 1                  |
| C-N-N-CA-C          | 111.00             | 99.33           | 1                  |
| N-CA-C              | 111.00             | 99.33           | 2                  |



| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| N-CA-C                 | 112.10             | 101.68          | 1                  |
| CA-CB-C-CA-CB          | 110.10             | 102.18          | 1                  |
| N-CA-CB                | 110.50             | 103.42          | 2                  |
| N-CA-CB                | 110.50             | 117.58          | 2                  |
| CA-C-O                 | 120.80             | 127.88          | 3                  |
| CA-CB-CG               | 114.10             | 105.77          | 1                  |
| CA-C-O                 | 120.80             | 113.72          | 3                  |
| C-N-C-CA-CB            | 110.10             | 118.01          | 1                  |
| C-CA-C-CA-C-CA-C-CA-CB | 110.10             | 118.01          | 1                  |
| N-CA-C-CA-N-CA-C       | 113.30             | 101.23          | 1                  |
| CA-C-C-CA-CB           | 111.40             | 103.49          | 1                  |
| N-CA-C                 | 111.00             | 99.34           | 1                  |
| OE1-CD-NE2             | 122.60             | 118.44          | 2                  |
| C-N-C-CA-CB            | 109.10             | 118.26          | 1                  |
| C-CA-CB                | 110.10             | 102.19          | 2                  |
| C-N-CA-C-N             | 116.20             | 107.88          | 2                  |
| N-CA-C                 | 111.00             | 99.35           | 1                  |
| CA-N-CD                | 112.00             | 106.18          | 1                  |
| N-CA-CB                | 110.50             | 117.57          | 1                  |
| CA-N-C-N-N-CA-C        | 111.00             | 122.65          | 1                  |
| N-CA-CB                | 110.50             | 103.43          | 2                  |
| CA-C-CA-CB-OG1         | 109.60             | 103.36          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| N-CA-C                | 112.10             | 101.70          | 1                  |
| N-CA-CA-C-N           | 116.20             | 124.52          | 1                  |
| C-CA-CB               | 110.10             | 102.20          | 2                  |
| CA-CB-CG              | 114.10             | 105.78          | 1                  |
| N-CA-C                | 111.00             | 99.36           | 4                  |
| C-CA-CB               | 110.10             | 118.00          | 2                  |
| N-CA-C-N-CA           | 121.70             | 114.22          | 2                  |
| C-CA-CB               | 111.40             | 119.30          | 1                  |
| N-CA-C                | 111.00             | 122.64          | 1                  |
| CA-C-N                | 116.20             | 107.89          | 2                  |
| N-CA-C-CA-CA-C-C-N-CA | 121.70             | 129.18          | 1                  |
| CA-CB-CG              | 112.60             | 108.44          | 1                  |
| C-CA-CB               | 109.10             | 118.24          | 1                  |
| N-CA-CB               | 110.50             | 103.44          | 1                  |
| C-N-CA                | 121.70             | 114.22          | 1                  |
| OD1-CG-ND2            | 122.60             | 118.44          | 1                  |
| C-CA-CB               | 111.40             | 103.51          | 1                  |
| C-N-N-CA-C            | 111.00             | 99.37           | 1                  |
| CA-C-O                | 120.80             | 113.74          | 2                  |
| N-CA-C                | 111.00             | 122.63          | 3                  |
| CA-C-N                | 116.20             | 124.51          | 1                  |
| CA-C-C-CA-CB          | 110.10             | 117.99          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| C-N-CA           | 121.70             | 129.18          | 1                  |
| C-CA-CB          | 110.10             | 117.99          | 2                  |
| CA-C-N           | 116.20             | 124.50          | 1                  |
| N-CA-C           | 112.10             | 122.48          | 1                  |
| C-CA-CA-C-CA-C-O | 120.80             | 127.86          | 1                  |
| CA-CB-CG         | 113.90             | 106.43          | 1                  |
| N-CA-C           | 111.00             | 99.38           | 2                  |
| CA-C-O           | 120.80             | 127.86          | 1                  |
| C-N-CA           | 121.70             | 129.17          | 1                  |
| CA-N-C-N-N-CA-C  | 112.10             | 101.72          | 1                  |
| CA-C-N           | 116.90             | 123.13          | 1                  |
| C-N-CA           | 121.70             | 114.23          | 1                  |
| C-CA-CB          | 110.10             | 102.22          | 4                  |
| CA-C-O           | 120.80             | 127.85          | 4                  |
| N-CA-C           | 113.30             | 101.27          | 1                  |
| C-CA-CB          | 110.10             | 117.98          | 1                  |
| CA-C-N-CA-C      | 111.00             | 99.39           | 1                  |
| CA-C-N           | 116.20             | 107.90          | 1                  |
| CA-CB-CG         | 112.60             | 108.45          | 1                  |
| C-N-CA           | 121.70             | 129.16          | 2                  |
| N-CA-C           | 111.00             | 99.39           | 3                  |
| CA-C-O           | 120.80             | 113.75          | 1                  |

| Angle type             | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                | 111.40             | 119.28          | 1                  |
| CA-CB-CG               | 112.60             | 116.75          | 1                  |
| CA-CB-CG               | 114.10             | 105.81          | 3                  |
| N-CA-CB                | 110.50             | 103.46          | 1                  |
| C-N-CA                 | 122.60             | 143.32          | 1                  |
| C-CA-CB                | 111.40             | 119.27          | 1                  |
| C-N-N-CA-C             | 111.00             | 99.40           | 1                  |
| N-CA-C-CA-CB           | 110.50             | 116.71          | 1                  |
| C-CA-CB                | 110.10             | 117.97          | 1                  |
| CA-CB-OG1              | 109.60             | 103.39          | 2                  |
| N-CA-C-N-CA            | 121.70             | 129.15          | 1                  |
| CB-CG-CD               | 112.60             | 105.56          | 2                  |
| CA-C-C-CA-CB           | 111.40             | 103.53          | 1                  |
| C-N-CA-CB-CG           | 112.60             | 108.46          | 1                  |
| C-CA-CB                | 109.10             | 118.21          | 1                  |
| C-CA-CB                | 110.50             | 116.71          | 1                  |
| CA-CB-CA-C-CA-C-C-N-CA | 121.70             | 129.15          | 1                  |
| C-CA-CB                | 110.10             | 102.24          | 4                  |
| CA-C-N                 | 116.20             | 124.47          | 1                  |
| C-CA-CB                | 111.40             | 119.26          | 2                  |
| C-CA-CB                | 110.10             | 117.96          | 1                  |
| C-N-CA                 | 122.60             | 143.27          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-C-CA-CB                | 110.10             | 117.96          | 1                  |
| C-CA-CB                     | 110.50             | 104.30          | 2                  |
| N-CA-N-CA-CB                | 110.50             | 117.53          | 1                  |
| C-CA-CB                     | 110.10             | 117.95          | 2                  |
| CA-C-N                      | 116.20             | 107.93          | 1                  |
| C-N-CA                      | 121.70             | 114.26          | 1                  |
| N-CA-C                      | 111.00             | 99.43           | 2                  |
| CA-C-N-CA-CA-C-C-CA-CB      | 111.40             | 103.55          | 1                  |
| N-CA-CB                     | 110.50             | 103.48          | 2                  |
| CA-C-O                      | 120.80             | 113.78          | 1                  |
| C-CA-CB                     | 110.10             | 102.25          | 2                  |
| C-N-CA                      | 121.70             | 129.14          | 1                  |
| CB-CG-CD                    | 112.60             | 105.58          | 1                  |
| CA-C-N-CA-C                 | 111.00             | 99.43           | 1                  |
| C-CA-CA-C-N                 | 116.20             | 107.94          | 1                  |
| CA-CB-CG                    | 113.80             | 117.93          | 1                  |
| N-CA-CA-N-C-CA-C-CA-C-CA-CB | 109.10             | 118.18          | 1                  |
| CA-C-N                      | 116.20             | 124.46          | 1                  |
| C-CA-C-CA-CA-CB-OG1         | 109.60             | 103.41          | 1                  |
| N-CA-C                      | 111.00             | 99.44           | 1                  |
| CA-CB-CG                    | 114.10             | 105.85          | 2                  |
| CA-C-N-CA-C                 | 112.10             | 101.78          | 1                  |

| Angle type              | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------|--------------------|-----------------|--------------------|
| CA-C-N                  | 116.20             | 124.45          | 1                  |
| CA-CB-C-CA-CB           | 111.60             | 103.35          | 1                  |
| CA-C-N                  | 116.20             | 107.95          | 1                  |
| CB-CG-CD                | 112.60             | 105.59          | 1                  |
| CA-C-O                  | 120.80             | 127.81          | 1                  |
| C-N-CA                  | 121.70             | 129.12          | 2                  |
| N-CA-C                  | 111.00             | 122.55          | 1                  |
| N-CA-CB                 | 110.50             | 117.51          | 2                  |
| C-N-N-CA-C              | 111.00             | 122.55          | 1                  |
| CA-C-O                  | 120.80             | 113.79          | 2                  |
| CA-C-N                  | 116.90             | 123.08          | 1                  |
| CA-C-N-CA-C             | 111.00             | 122.54          | 1                  |
| CA-CB-CG                | 112.60             | 116.72          | 1                  |
| N-CA-C                  | 111.00             | 99.46           | 1                  |
| CA-CB-CG                | 112.60             | 108.48          | 1                  |
| CA-CB-CG                | 113.80             | 117.92          | 1                  |
| C-N-CA                  | 121.70             | 114.28          | 2                  |
| C-CA-CB                 | 110.10             | 102.27          | 4                  |
| N-CA-CB                 | 110.50             | 103.49          | 1                  |
| N-CA-N-CA-C-CA-CB       | 110.10             | 117.93          | 1                  |
| CA-C-CA-CB-C-CA-C-CA-CB | 111.40             | 103.57          | 1                  |
| N-CA-CB                 | 110.50             | 103.50          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| N-CA-C                     | 113.30             | 101.35          | 1                  |
| N-CA-CB                    | 110.50             | 117.50          | 2                  |
| C-CA-CA-C-CA-C-C-N-C-CA-CB | 110.10             | 102.27          | 1                  |
| N-CA-C                     | 111.00             | 99.47           | 1                  |
| C-CA-CB                    | 110.10             | 102.28          | 3                  |
| C-CA-CB                    | 111.40             | 103.58          | 1                  |
| CA-C-N                     | 116.20             | 124.43          | 2                  |
| N-CA-CB                    | 111.50             | 104.50          | 1                  |
| C-N-CA                     | 121.70             | 114.29          | 1                  |
| N-CA-C                     | 112.10             | 122.39          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 102.28          | 1                  |
| C-CA-CB                    | 110.10             | 117.92          | 1                  |
| C-N-C-N-C-N-N-CA-CB        | 110.50             | 117.49          | 1                  |
| CA-CB-CG                   | 114.10             | 105.87          | 2                  |
| CA-CB-CG                   | 112.60             | 116.71          | 1                  |
| C-CA-CA-CB-CG              | 112.60             | 108.49          | 1                  |
| C-N-CA                     | 121.70             | 114.30          | 1                  |
| CA-C-O                     | 120.80             | 113.81          | 1                  |
| CA-C-C-N-C-N-CA            | 121.70             | 129.10          | 1                  |
| N-CD-CG                    | 103.20             | 109.37          | 1                  |
| OD1-CG-ND2                 | 122.60             | 118.49          | 1                  |
| C-CA-CB                    | 110.10             | 117.91          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| N-CA-CA-C-N                | 116.20             | 107.98          | 1                  |
| N-CA-C-CA-C-CA-CB          | 110.10             | 117.91          | 1                  |
| CA-CB-CG                   | 112.60             | 108.49          | 1                  |
| CA-C-N                     | 116.20             | 124.42          | 1                  |
| N-CA-N-CA-C                | 111.00             | 99.50           | 1                  |
| C-N-CA                     | 121.70             | 114.31          | 3                  |
| N-CA-CB                    | 111.50             | 118.48          | 1                  |
| CA-C-O                     | 120.80             | 127.78          | 2                  |
| C-CA-CB                    | 110.10             | 102.30          | 2                  |
| CA-C-CA-CB-CG              | 113.80             | 117.91          | 1                  |
| N-CA-CB                    | 110.50             | 117.48          | 1                  |
| C-N-C-N-CA                 | 121.70             | 129.09          | 1                  |
| C-N-N-CA-CB                | 111.50             | 104.52          | 1                  |
| C-N-N-CA-C                 | 111.00             | 99.50           | 1                  |
| N-CA-C                     | 111.00             | 99.50           | 1                  |
| C-CA-CB                    | 110.10             | 117.90          | 2                  |
| N-CA-CA-CB-CG              | 112.60             | 108.49          | 1                  |
| CA-C-CA-C-C-CA-CB          | 110.10             | 102.30          | 1                  |
| C-N-CA-C-C-CA-CA-C-O       | 120.80             | 127.78          | 1                  |
| N-CA-C                     | 111.00             | 122.49          | 1                  |
| CB-CG-C-N-N-CA-N-CA-N-CA-C | 111.00             | 99.51           | 1                  |
| N-CA-CA-CB-CG              | 114.10             | 105.90          | 1                  |



| Angle type        | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------|--------------------|-----------------|--------------------|
| C-CA-CB           | 110.50             | 116.65          | 1                  |
| CA-C-O            | 120.80             | 113.83          | 3                  |
| C-N-C-N-CA        | 121.70             | 114.32          | 1                  |
| N-CA-CB           | 110.50             | 117.47          | 2                  |
| N-CA-CB           | 111.50             | 118.47          | 1                  |
| CA-C-N            | 116.20             | 108.00          | 2                  |
| C-CA-CB           | 110.10             | 117.89          | 1                  |
| OE1-CD-NE2        | 122.60             | 118.50          | 1                  |
| CA-C-CA-C-N       | 116.20             | 108.00          | 1                  |
| CA-CB-CG          | 112.60             | 108.50          | 1                  |
| N-CA-CB           | 103.00             | 107.51          | 1                  |
| C-N-CA            | 121.70             | 114.32          | 1                  |
| C-N-CA            | 121.70             | 129.08          | 1                  |
| C-CA-CA-C-N       | 116.20             | 124.40          | 1                  |
| C-CA-CB           | 110.10             | 102.31          | 1                  |
| N-CA-C            | 111.00             | 99.53           | 2                  |
| C-CA-N-CA-CB      | 110.50             | 103.53          | 1                  |
| C-CA-CB           | 110.10             | 117.88          | 3                  |
| N-CA-C-CA-C-CA-CB | 111.40             | 103.62          | 1                  |
| CA-C-N            | 116.20             | 124.39          | 1                  |
| C-CA-CB           | 110.10             | 102.32          | 4                  |
| CA-N-N-CD-CG      | 103.20             | 109.34          | 1                  |

| Angle type       | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------|--------------------|-----------------|--------------------|
| N-CA-CB          | 110.50             | 117.46          | 1                  |
| N-CA-CA-C-N      | 116.20             | 108.01          | 1                  |
| CA-C-O           | 120.80             | 113.84          | 1                  |
| N-CA-CB          | 110.50             | 103.54          | 2                  |
| CA-CB-OG1        | 109.60             | 103.46          | 1                  |
| C-N-C-CA-CA-C-O  | 120.80             | 127.76          | 1                  |
| C-N-CA           | 121.70             | 114.33          | 2                  |
| CA-C-O           | 120.80             | 127.76          | 1                  |
| CA-C-CB-CG-CD    | 112.60             | 119.56          | 1                  |
| N-CA-C           | 111.00             | 122.45          | 2                  |
| N-CA-C-N-C-CA-CB | 110.10             | 102.33          | 1                  |
| C-CA-CB          | 111.40             | 103.63          | 1                  |
| C-CA-CB          | 110.10             | 117.87          | 3                  |
| C-N-CA           | 121.70             | 129.06          | 1                  |
| C-CA-N-CA-C      | 111.00             | 122.45          | 1                  |
| CA-C-N           | 116.20             | 108.02          | 1                  |
| CA-C-N-CA-CA-C-O | 120.80             | 113.85          | 1                  |
| C-N-CA           | 121.70             | 114.34          | 2                  |
| N-CA-CB          | 110.50             | 103.55          | 1                  |
| CA-C-O           | 120.80             | 127.75          | 1                  |
| C-N-C-N-CA       | 121.70             | 129.06          | 1                  |
| N-CA-C-CA-CB     | 110.10             | 102.33          | 1                  |

| Angle type          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------|--------------------|-----------------|--------------------|
| N-CA-C              | 111.00             | 99.56           | 2                  |
| CA-C-C-CA-CB        | 110.10             | 117.86          | 1                  |
| CA-CB-N-CA-C        | 111.00             | 99.56           | 1                  |
| N-CA-CB             | 111.50             | 118.44          | 1                  |
| C-CA-CB             | 111.60             | 103.43          | 1                  |
| C-CA-CB             | 110.10             | 102.34          | 2                  |
| CA-C-C-N-CA         | 121.70             | 114.35          | 1                  |
| CA-C-C-CA-C-N-CA    | 121.70             | 129.05          | 1                  |
| N-CA-C              | 111.00             | 99.57           | 1                  |
| CA-CB-CG            | 112.60             | 108.52          | 1                  |
| CA-CB-CA-C-O        | 120.80             | 113.86          | 1                  |
| CA-C-N              | 116.20             | 124.36          | 1                  |
| C-CA-CB-CG-CD       | 112.60             | 105.66          | 1                  |
| N-CA-C              | 111.00             | 122.43          | 2                  |
| C-CA-CB             | 111.40             | 119.15          | 1                  |
| C-N-C-CA-CB         | 110.10             | 102.35          | 1                  |
| CA-C-N-CA-C         | 111.00             | 99.58           | 1                  |
| C-CA-C-CA-CB        | 110.10             | 117.85          | 1                  |
| N-CA-C-CA-CB        | 110.10             | 117.85          | 1                  |
| N-CA-C-N-C-N-CA-C-O | 120.80             | 127.73          | 1                  |
| CA-C-N              | 116.20             | 108.05          | 2                  |
| C-N-C-CA-CB         | 111.60             | 103.45          | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| C-N-C-N-CA         | 121.70             | 114.36          | 1                  |
| N-CA-CB            | 110.50             | 117.43          | 1                  |
| CA-C-C-CA-CB       | 110.10             | 102.36          | 1                  |
| C-CA-CB            | 110.10             | 117.84          | 3                  |
| CA-C-C-CA-CB       | 110.10             | 117.84          | 1                  |
| C-CA-CB            | 111.40             | 103.66          | 1                  |
| N-CA-C             | 111.00             | 122.41          | 1                  |
| CA-C-C-N-CA        | 121.70             | 114.37          | 1                  |
| N-CA-CA-C-C-N-CA   | 121.70             | 114.37          | 1                  |
| C-CA-CB            | 110.10             | 102.36          | 1                  |
| C-CA-C-CA-CB       | 110.10             | 117.84          | 1                  |
| CA-C-O             | 120.80             | 113.88          | 1                  |
| C-CA-CB            | 111.60             | 103.46          | 1                  |
| C-CA-N-CA-CB       | 111.50             | 118.42          | 1                  |
| C-N-N-CA-C         | 111.00             | 122.40          | 1                  |
| C-N-C-N-CA         | 121.70             | 129.03          | 1                  |
| N-CA-CA-CB-C-CA-CB | 110.10             | 102.37          | 1                  |
| N-CA-C             | 111.00             | 122.39          | 1                  |
| C-N-CA             | 121.70             | 114.38          | 1                  |
| CA-C-C-CA-CB       | 110.10             | 117.83          | 1                  |
| N-CA-CB            | 110.50             | 103.58          | 1                  |
| C-N-CA-C-O         | 120.80             | 113.88          | 1                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| C-CA-CB               | 110.10             | 117.83          | 2                  |
| N-CA-C                | 111.00             | 99.61           | 2                  |
| N-CA-N-CA-C           | 113.30             | 101.50          | 1                  |
| C-N-CA                | 121.70             | 129.02          | 1                  |
| N-CA-CB               | 110.50             | 103.59          | 2                  |
| C-N-N-CA-CA-C-N       | 116.20             | 124.33          | 1                  |
| C-CA-C-CA-C-CA-CB     | 110.10             | 117.82          | 1                  |
| C-N-C-CA-C-CA-CB      | 110.10             | 117.82          | 1                  |
| N-CA-C-CA-CB          | 110.10             | 117.82          | 1                  |
| CA-N-CD               | 112.00             | 106.31          | 1                  |
| C-CA-CB               | 109.10             | 100.16          | 1                  |
| CA-CB-CG              | 113.80             | 117.86          | 1                  |
| C-CA-C-N-CA           | 121.70             | 129.02          | 1                  |
| N-CA-C                | 111.00             | 99.62           | 1                  |
| CA-CB-C-N-CA          | 121.70             | 129.01          | 1                  |
| CA-CB-CG              | 114.10             | 122.23          | 1                  |
| C-N-CA                | 121.70             | 114.39          | 3                  |
| CA-C-CA-C-C-N-CA      | 121.70             | 114.39          | 1                  |
| C-CA-C-N-N-CA-C-CA-CB | 110.10             | 117.82          | 1                  |
| CB-CG-CD              | 112.60             | 119.51          | 1                  |
| C-N-C-CA-CB           | 109.10             | 118.04          | 1                  |
| N-CA-C                | 111.00             | 99.63           | 1                  |

| Angle type                          | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-------------------------------------|--------------------|-----------------|--------------------|
| C-N-CA-C-N                          | 116.20             | 108.08          | 1                  |
| C-CA-CB                             | 110.10             | 117.82          | 1                  |
| C-CA-CB-CG-CD                       | 112.60             | 119.50          | 1                  |
| N-CA-CA-C-CA-C-CA-C-C-N-CA          | 121.70             | 114.39          | 1                  |
| C-CA-CB                             | 110.10             | 102.39          | 2                  |
| N-CA-CB                             | 111.50             | 104.60          | 2                  |
| CA-C-O                              | 120.80             | 127.70          | 1                  |
| C-CA-C-CA-CB                        | 110.10             | 117.81          | 1                  |
| N-CA-C-CA-C-CA-CB                   | 110.10             | 102.39          | 1                  |
| C-CA-CA-C-O                         | 120.80             | 127.70          | 1                  |
| C-CA-N-CA-CA-C-C-N-C-CA-C-CA-N-CA-C | 111.00             | 99.64           | 1                  |
| C-N-C-CA-CB                         | 111.40             | 103.69          | 1                  |
| C-CA-N-CA-C-N-C-N-CA-C-C-CA-CB      | 109.10             | 100.18          | 1                  |
| C-N-CA                              | 121.70             | 114.40          | 2                  |
| C-CA-CA-CB-CG                       | 112.60             | 116.65          | 1                  |
| CA-CB-CG                            | 113.80             | 117.85          | 1                  |
| CA-C-C-CA-CB                        | 110.10             | 117.80          | 1                  |
| CA-C-C-CA-CB                        | 110.10             | 102.40          | 2                  |
| C-N-CA                              | 121.70             | 129.00          | 2                  |
| N-CA-C                              | 111.00             | 122.35          | 2                  |
| C-N-CA-C-C-CA-CB                    | 110.10             | 102.40          | 1                  |
| C-CA-CB                             | 110.50             | 116.58          | 1                  |

| Angle type                 | Observed angle (°) | Ideal angle (°) | Number of outliers |
|----------------------------|--------------------|-----------------|--------------------|
| C-N-CA                     | 121.70             | 114.41          | 2                  |
| C-CA-CB                    | 110.10             | 117.80          | 1                  |
| N-CA-CB                    | 110.50             | 117.39          | 1                  |
| C-N-N-CA-CA-CB-CG          | 112.60             | 108.55          | 1                  |
| ND1-CE1-C-CA-C-N-CA        | 121.70             | 114.41          | 1                  |
| C-N-N-CA-CB                | 111.50             | 118.39          | 1                  |
| N-CA-C-CA-CB               | 111.40             | 103.71          | 1                  |
| N-CA-C-CA-CB               | 110.10             | 102.41          | 1                  |
| C-CA-CB                    | 110.10             | 117.79          | 1                  |
| CA-C-O                     | 120.80             | 113.92          | 1                  |
| N-CA-C                     | 111.00             | 99.66           | 1                  |
| CA-C-N                     | 116.20             | 124.30          | 1                  |
| C-CA-CB                    | 110.10             | 102.41          | 1                  |
| CB-CG-CD                   | 112.60             | 119.48          | 1                  |
| CA-CB-C-N-C-CA-C-N-N-CA-CB | 110.50             | 117.38          | 1                  |
| N-CA-N-CA-CB               | 110.50             | 103.62          | 1                  |
| CA-CB-CG                   | 112.60             | 108.55          | 1                  |
| CA-C-OD1-CG-C-CA-CB        | 111.40             | 103.71          | 1                  |
| N-CA-CA-C-N                | 116.20             | 108.11          | 1                  |
| CA-C-CA-C-N                | 116.20             | 124.29          | 1                  |
| C-N-CA                     | 121.70             | 114.42          | 1                  |
| N-CA-CA-CB-N-CA-CA-CB-CG   | 113.90             | 106.62          | 1                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| CA-C-N                      | 116.20             | 124.29          | 1                  |
| C-CA-CB                     | 110.10             | 102.42          | 1                  |
| CA-C-CA-C-C-CA-CA-CB-CG     | 113.80             | 117.84          | 1                  |
| CA-CB-CG                    | 112.60             | 108.56          | 1                  |
| C-N-N-CA-CA-C-N             | 116.20             | 124.28          | 1                  |
| C-CA-C-N-CA                 | 121.70             | 114.42          | 1                  |
| N-CA-CA-C-O                 | 120.80             | 127.67          | 1                  |
| C-N-CA-C-CA-C-N             | 116.20             | 108.12          | 1                  |
| CA-C-O                      | 120.80             | 127.67          | 1                  |
| CA-C-N                      | 116.90             | 122.96          | 1                  |
| C-N-CA                      | 121.70             | 128.97          | 2                  |
| CB-CG-C-CA-CB               | 110.10             | 102.42          | 1                  |
| CA-CB-CG                    | 114.10             | 122.18          | 1                  |
| C-N-CA-C-O                  | 120.80             | 127.67          | 2                  |
| CA-CB-C-N-CA-C-CA-C-C-CA-CB | 110.10             | 117.78          | 1                  |
| N-CA-CB                     | 110.50             | 117.37          | 1                  |
| CA-C-N                      | 116.20             | 108.12          | 1                  |
| C-CA-CB                     | 110.50             | 116.56          | 1                  |
| C-N-C-CA-CB                 | 110.10             | 102.43          | 1                  |
| CB-CG-CA-C-O                | 120.80             | 127.67          | 1                  |
| C-N-CA-C-O                  | 120.80             | 113.93          | 1                  |
| C-CA-OD1-CG-N-CA-CB         | 110.50             | 103.64          | 1                  |



| Angle type                | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---------------------------|--------------------|-----------------|--------------------|
| OD1-CG-ND2                | 122.60             | 118.56          | 1                  |
| N-CA-C-N-CA               | 121.70             | 114.43          | 1                  |
| N-CA-C                    | 111.00             | 99.70           | 2                  |
| CA-CB-C-N-C-CA-CB         | 111.40             | 119.07          | 1                  |
| N-CA-OE1-CD-C-CA-CB       | 110.10             | 102.43          | 1                  |
| C-CA-N-CA-CB              | 110.40             | 104.35          | 1                  |
| C-N-CA                    | 121.70             | 114.44          | 4                  |
| N-CA-C                    | 111.00             | 122.30          | 1                  |
| CA-C-CA-CB-N-CA-CB        | 103.00             | 107.44          | 1                  |
| CA-C-O                    | 120.80             | 113.94          | 1                  |
| CA-CB-N-CA-C              | 111.00             | 122.30          | 1                  |
| OE1-CD-NE2                | 122.60             | 118.57          | 1                  |
| N-CA-CB                   | 110.50             | 117.36          | 1                  |
| N-CA-N-CA-C               | 111.00             | 122.29          | 1                  |
| CA-C-N-CA-C               | 111.00             | 122.29          | 1                  |
| N-CA-C                    | 111.00             | 122.29          | 1                  |
| CB-CG-OE1-CD-C-N-CA-CB-CG | 112.60             | 108.57          | 1                  |
| N-CA-C-N-N-CA-C-N-C-CA-CB | 110.50             | 116.55          | 1                  |
| CA-C-C-N-CG-CD2-NE2       | 107.20             | 103.17          | 1                  |
| CA-CB-CG                  | 112.60             | 108.57          | 2                  |
| CA-C-O                    | 120.80             | 113.95          | 1                  |
| N-CA-C                    | 111.00             | 122.28          | 1                  |

| Angle type                         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|------------------------------------|--------------------|-----------------|--------------------|
| C-CA-CA-C-O                        | 120.80             | 113.95          | 2                  |
| C-N-CA                             | 121.70             | 114.45          | 3                  |
| CA-CB-C-CA-CB                      | 110.10             | 102.44          | 1                  |
| C-N-CA-C-O                         | 120.80             | 113.95          | 1                  |
| C-CA-CA-C-C-CA-C-CA-CG-CD1-NE1     | 110.20             | 104.96          | 1                  |
| CA-C-O                             | 120.80             | 127.65          | 1                  |
| C-N-CA                             | 121.70             | 128.95          | 1                  |
| N-CA-C                             | 111.00             | 99.73           | 1                  |
| C-CA-CB                            | 110.10             | 117.75          | 1                  |
| ND1-CE1-NE2                        | 108.40             | 112.43          | 1                  |
| CA-C-O                             | 120.80             | 127.64          | 1                  |
| N-CA-CB                            | 111.50             | 104.66          | 1                  |
| CA-C-O                             | 120.80             | 113.96          | 1                  |
| CA-CB-CG                           | 113.90             | 106.65          | 1                  |
| N-CA-C                             | 111.00             | 122.27          | 1                  |
| CA-C-CA-C-CA-C-C-N-OD1-CG-CB-CG-CD | 112.60             | 105.76          | 1                  |
| N-CA-C                             | 111.00             | 99.74           | 1                  |
| CA-C-N                             | 116.90             | 122.93          | 2                  |
| CA-CB-CA-C-C-N-ND1-CE1-NE2         | 108.40             | 112.42          | 1                  |
| N-CA-N-CA-CB                       | 111.50             | 118.34          | 1                  |
| N-CA-C                             | 111.00             | 122.26          | 1                  |
| C-N-CA                             | 121.70             | 114.46          | 2                  |

| Angle type                  | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------------|--------------------|-----------------|--------------------|
| C-CA-CB                     | 110.50             | 116.53          | 1                  |
| CA-C-O                      | 120.80             | 113.97          | 1                  |
| C-N-C-N-N-CA-CB             | 110.50             | 117.33          | 1                  |
| CA-CB-C-N-CA-C-N-CA-N-CA-CB | 110.50             | 103.67          | 1                  |
| C-CA-CB                     | 109.10             | 117.94          | 1                  |
| C-N-CA                      | 121.70             | 128.93          | 1                  |
| C-CA-CB                     | 110.10             | 102.46          | 1                  |
| C-CA-CB                     | 110.10             | 102.47          | 3                  |
| N-CA-CA-C-C-N-CA            | 121.70             | 128.93          | 1                  |
| N-CA-C                      | 111.00             | 122.25          | 1                  |
| OE1-CD-NE2                  | 122.60             | 126.62          | 1                  |
| CA-CB-CA-C-O                | 120.80             | 113.97          | 1                  |
| CA-C-O                      | 120.80             | 127.63          | 1                  |
| CA-CB-CG                    | 113.80             | 117.82          | 1                  |
| C-N-C-N-CA                  | 121.70             | 114.47          | 1                  |
| C-CA-CB                     | 110.50             | 104.48          | 1                  |
| C-N-C-CA-CB                 | 110.10             | 102.47          | 1                  |
| CA-C-CA-C-N                 | 116.20             | 124.23          | 1                  |
| OD1-CG-ND2                  | 122.60             | 118.59          | 1                  |
| N-CA-C                      | 111.00             | 122.24          | 1                  |
| CA-C-CA-C-C-CA-CB           | 110.10             | 117.72          | 1                  |
| C-CA-CB                     | 110.10             | 117.72          | 1                  |

| Angle type         | Observed angle (°) | Ideal angle (°) | Number of outliers |
|--------------------|--------------------|-----------------|--------------------|
| CA-C-O             | 120.80             | 127.62          | 1                  |
| N-CA-C             | 111.00             | 122.23          | 1                  |
| C-N-CA             | 121.70             | 128.92          | 1                  |
| C-CA-C-CA-CB       | 111.40             | 119.02          | 1                  |
| N-CA-CB            | 110.40             | 104.38          | 1                  |
| N-CA-C-CA-CB       | 110.10             | 102.48          | 1                  |
| C-CA-CB            | 110.10             | 102.48          | 1                  |
| C-N-CA             | 121.70             | 114.48          | 1                  |
| N-CA-N-CA-CB       | 110.50             | 117.32          | 1                  |
| N-CA-OE1-CD-N-CA-C | 111.00             | 122.23          | 1                  |
| CA-C-C-N-CA        | 121.70             | 128.92          | 1                  |
| C-N-C-N-CA         | 121.70             | 128.92          | 1                  |
| C-N-C-CA-CA-C-O    | 120.80             | 127.61          | 1                  |
| C-N-CA             | 121.70             | 114.49          | 3                  |
| C-CA-CB            | 111.40             | 119.01          | 2                  |
| CA-C-O             | 120.80             | 127.61          | 1                  |
| CA-C-CA-C-O        | 120.80             | 113.99          | 1                  |
| CA-C-C-CA-CB       | 110.50             | 104.49          | 1                  |
| C-N-C-N-CA         | 121.70             | 128.91          | 1                  |
| C-N-CA             | 121.70             | 128.91          | 2                  |
| C-N-C-CA-CB        | 111.60             | 103.59          | 1                  |
| C-CA-CB            | 109.10             | 117.91          | 2                  |

| Angle type            | Observed angle (°) | Ideal angle (°) | Number of outliers |
|-----------------------|--------------------|-----------------|--------------------|
| CA-C-N                | 116.20             | 108.19          | 1                  |
| CA-C-CA-C-N-CA-CA-C-N | 116.20             | 124.21          | 1                  |
| C-N-C-CA-CB           | 110.10             | 117.71          | 1                  |
| C-CA-CB               | 110.10             | 102.49          | 3                  |
| N-CA-C                | 112.10             | 102.09          | 1                  |
| N-CA-C-CA-C-CA-CA-C-N | 116.20             | 108.19          | 1                  |
| CA-C-N                | 116.20             | 124.21          | 1                  |
| N-CA-C-N-N-CA-CB      | 110.50             | 117.30          | 1                  |
| N-CA-N-CA-C           | 111.00             | 99.79           | 1                  |
| C-N-CA                | 121.70             | 128.90          | 1                  |
| N-CA-C                | 111.00             | 122.20          | 1                  |
| N-CA-C                | 111.00             | 99.80           | 1                  |
| N-CA-CA-C-C-CA-CB     | 110.10             | 117.70          | 1                  |
| OD1-CG-C-CA-CB        | 110.10             | 117.70          | 1                  |
| CB-CG-CD              | 112.60             | 105.80          | 1                  |

### Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

| Model ID | Clash score | Number of clashes |
|----------|-------------|-------------------|
| 1        | 721.14      | 144774            |

All 144774 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        | 24713    | 21896   | 1749    | 1068     |

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        | 22485    | 19361   | 1715    | 1409     |

Detailed list of outliers are tabulated below.

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 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       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | K1    | 589        | 0.0LYS       |
| 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       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | L1    | 105        | 0.0GLN       |
| 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    | 473        | 0.0ILE       |
| 1        | L1    | 510        | 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       |



| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | M1    | 196        | 0.0LEU       |
| 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       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | M1    | 376        | 0.0ILE       |
| 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       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | O1    | 313        | 0.0ASN       |
| 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       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | R1    | 235        | 0.0MET       |
| 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       |
| 1        | 91    | 11         | 0.0THR       |
| 1        | 91    | 38         | 0.0THR       |
| 1        | 91    | 46         | 0.0LYS       |
| 1        | 91    | 70         | 0.0PHE       |
| 1        | W1    | 10         | 0.0SER       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | W1    | 12         | 0.0ARG       |
| 1        | W1    | 79         | 0.0MET       |
| 1        | W1    | 89         | 0.0GLU       |
| 1        | W1    | 147        | 0.0GLU       |
| 1        | W1    | 161        | 0.0LEU       |
| 1        | W1    | 251        | 0.0SER       |
| 1        | W1    | 264        | 0.0LEU       |
| 1        | W1    | 270        | 0.0PRO       |
| 1        | W1    | 274        | 0.0ASN       |
| 1        | W1    | 275        | 0.0PRO       |
| 1        | W1    | 334        | 0.0LEU       |
| 1        | W1    | 337        | 0.0ILE       |
| 1        | W1    | 343        | 0.0GLN       |
| 1        | W1    | 366        | 0.0ILE       |
| 1        | W1    | 428        | 0.0ASN       |
| 1        | W1    | 435        | 0.0ASN       |
| 1        | W1    | 439        | 0.0GLU       |
| 1        | W1    | 524        | 0.0LYS       |
| 1        | W1    | 528        | 0.0GLN       |
| 1        | W1    | 547        | 0.0ASN       |
| 1        | W1    | 548        | 0.0SER       |
| 1        | W1    | 552        | 0.0SER       |
| 1        | W1    | 566        | 0.0GLU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | W1    | 574        | 0.0THR       |
| 1        | W1    | 576        | 0.0GLU       |
| 1        | V1    | 1117       | 0.0TYR       |
| 1        | V1    | 1126       | 0.0LEU       |
| 1        | V1    | 1212       | 0.0ARG       |
| 1        | V1    | 1215       | 0.0GLU       |
| 1        | V1    | 1295       | 0.0VAL       |
| 1        | V1    | 1308       | 0.0GLU       |
| 1        | V1    | 1321       | 0.0MET       |
| 1        | V1    | 1332       | 0.0LYS       |
| 1        | V1    | 1333       | 0.0ASP       |
| 1        | V1    | 1388       | 0.0GLU       |
| 1        | V1    | 1429       | 0.0LYS       |
| 1        | V1    | 1437       | 0.0VAL       |
| 1        | V1    | 1455       | 0.0ASN       |
| 1        | J1    | 637        | 0.0LEU       |
| 1        | J1    | 638        | 0.0ASP       |
| 1        | J1    | 727        | 0.0SER       |
| 1        | J1    | 788        | 0.0ASP       |
| 1        | J1    | 797        | 0.0LEU       |
| 1        | J1    | 798        | 0.0ASN       |
| 1        | 92    | 11         | 0.0THR       |
| 1        | 92    | 46         | 0.0LYS       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | 92    | 49         | 0.0ASN       |
| 1        | 92    | 70         | 0.0PHE       |
| 1        | W2    | 10         | 0.0SER       |
| 1        | W2    | 11         | 0.0PRO       |
| 1        | W2    | 79         | 0.0MET       |
| 1        | W2    | 89         | 0.0GLU       |
| 1        | W2    | 108        | 0.0GLU       |
| 1        | W2    | 109        | 0.0PRO       |
| 1        | W2    | 110        | 0.0LYS       |
| 1        | W2    | 147        | 0.0GLU       |
| 1        | W2    | 161        | 0.0LEU       |
| 1        | W2    | 251        | 0.0SER       |
| 1        | W2    | 264        | 0.0LEU       |
| 1        | W2    | 270        | 0.0PRO       |
| 1        | W2    | 274        | 0.0ASN       |
| 1        | W2    | 275        | 0.0PRO       |
| 1        | W2    | 334        | 0.0LEU       |
| 1        | W2    | 337        | 0.0ILE       |
| 1        | W2    | 343        | 0.0GLN       |
| 1        | W2    | 366        | 0.0ILE       |
| 1        | W2    | 428        | 0.0ASN       |
| 1        | W2    | 435        | 0.0ASN       |
| 1        | W2    | 437        | 0.0SER       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | W2    | 438        | 0.0SER       |
| 1        | W2    | 524        | 0.0LYS       |
| 1        | W2    | 530        | 0.0HIS       |
| 1        | W2    | 547        | 0.0ASN       |
| 1        | W2    | 548        | 0.0SER       |
| 1        | W2    | 552        | 0.0SER       |
| 1        | W2    | 566        | 0.0GLU       |
| 1        | W2    | 575        | 0.0ASN       |
| 1        | W2    | 577        | 0.0TRP       |
| 1        | V2    | 1126       | 0.0LEU       |
| 1        | V2    | 1239       | 0.0PHE       |
| 1        | V2    | 1295       | 0.0VAL       |
| 1        | V2    | 1308       | 0.0GLU       |
| 1        | V2    | 1382       | 0.0VAL       |
| 1        | V2    | 1387       | 0.0LYS       |
| 1        | V2    | 1388       | 0.0GLU       |
| 1        | V2    | 1437       | 0.0VAL       |
| 1        | J2    | 638        | 0.0ASP       |
| 1        | J2    | 742        | 0.0GLN       |
| 1        | J2    | 788        | 0.0ASP       |
| 1        | J2    | 789        | 0.0GLU       |
| 1        | A1    | 28         | 0.0ASN       |
| 1        | A1    | 37         | 0.0LEU       |



| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | A1    | 38         | 0.0ASN       |
| 1        | A1    | 39         | 0.0ASN       |
| 1        | A1    | 227        | 0.0THR       |
| 1        | A1    | 237        | 0.0HIS       |
| 1        | A1    | 242        | 0.0LYS       |
| 1        | A1    | 288        | 0.0GLU       |
| 1        | A1    | 303        | 0.0LEU       |
| 1        | A1    | 313        | 0.0THR       |
| 1        | A1    | 625        | 0.0GLU       |
| 1        | A1    | 439        | 0.0SER       |
| 1        | A1    | 443        | 0.0GLN       |
| 1        | A1    | 683        | 0.0THR       |
| 1        | A1    | 468        | 0.0PHE       |
| 1        | A1    | 746        | 0.0PRO       |
| 1        | A1    | 747        | 0.0PHE       |
| 1        | A1    | 754        | 0.0ARG       |
| 1        | A1    | 765        | 0.0ASP       |
| 1        | A1    | 561        | 0.0GLN       |
| 1        | A1    | 600        | 0.0ASN       |
| 1        | A1    | 601        | 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        | H1    | 304        | 0.0THR       |
| 1        | H1    | 319        | 0.0THR       |
| 1        | H1    | 324        | 0.0TYR       |
| 1        | H1    | 327        | 0.0PRO       |
| 1        | H1    | 330        | 0.0VAL       |
| 1        | H1    | 347        | 0.0THR       |
| 1        | H1    | 422        | 0.0LEU       |
| 1        | H1    | 423        | 0.0LYS       |
| 1        | H1    | 505        | 0.0ARG       |
| 1        | I1    | 270        | 0.0PRO       |
| 1        | I1    | 271        | 0.0PRO       |
| 1        | I1    | 276        | 0.0GLU       |
| 1        | I1    | 317        | 0.0LYS       |
| 1        | I1    | 349        | 0.0THR       |
| 1        | I1    | 353        | 0.0LEU       |
| 1        | I1    | 359        | 0.0THR       |
| 1        | I1    | 369        | 0.0LEU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | I1    | 370        | 0.0ASP       |
| 1        | I1    | 375        | 0.0LYS       |
| 1        | I1    | 433        | 0.0LYS       |
| 1        | I1    | 436        | 0.0LEU       |
| 1        | I1    | 445        | 0.0GLU       |
| 1        | I1    | 446        | 0.0GLU       |
| 1        | J3    | 637        | 0.0LEU       |
| 1        | J3    | 743        | 0.0GLN       |
| 1        | J3    | 788        | 0.0ASP       |
| 1        | J3    | 789        | 0.0GLU       |
| 1        | A2    | 28         | 0.0ASN       |
| 1        | A2    | 37         | 0.0LEU       |
| 1        | A2    | 227        | 0.0THR       |
| 1        | A2    | 237        | 0.0HIS       |
| 1        | A2    | 288        | 0.0GLU       |
| 1        | A2    | 303        | 0.0LEU       |
| 1        | A2    | 313        | 0.0THR       |
| 1        | A2    | 625        | 0.0GLU       |
| 1        | A2    | 439        | 0.0SER       |
| 1        | A2    | 443        | 0.0GLN       |
| 1        | A2    | 683        | 0.0THR       |
| 1        | A2    | 468        | 0.0PHE       |
| 1        | A2    | 746        | 0.0PRO       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | A2    | 747        | 0.0PHE       |
| 1        | A2    | 754        | 0.0ARG       |
| 1        | A2    | 765        | 0.0ASP       |
| 1        | A2    | 561        | 0.0GLN       |
| 1        | C1    | 2          | 0.0LYS       |
| 1        | C1    | 41         | 0.0LYS       |
| 1        | C1    | 60         | 0.0ASP       |
| 1        | C1    | 66         | 0.0VAL       |
| 1        | C1    | 82         | 0.0ASN       |
| 1        | C1    | 97         | 0.0THR       |
| 1        | C1    | 110        | 0.0ARG       |
| 1        | C1    | 117        | 0.0VAL       |
| 1        | C1    | 128        | 0.0THR       |
| 1        | C1    | 131        | 0.0TYR       |
| 1        | C1    | 132        | 0.0GLN       |
| 1        | C1    | 136        | 0.0LYS       |
| 1        | C1    | 153        | 0.0THR       |
| 1        | C1    | 183        | 0.0ARG       |
| 1        | C1    | 208        | 0.0LYS       |
| 1        | C1    | 209        | 0.0ASN       |
| 1        | C1    | 256        | 0.0HIS       |
| 1        | C1    | 260        | 0.0MET       |
| 1        | C1    | 293        | 0.0PRO       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C1    | 306        | 0.0VAL       |
| 1        | C1    | 307        | 0.0ASP       |
| 1        | C1    | 330        | 0.0SER       |
| 1        | C1    | 333        | 0.0GLU       |
| 1        | C1    | 334        | 0.0GLN       |
| 1        | C1    | 360        | 0.0LEU       |
| 1        | C1    | 362        | 0.0ASP       |
| 1        | C1    | 420        | 0.0LEU       |
| 1        | C1    | 441        | 0.0TYR       |
| 1        | C1    | 442        | 0.0SER       |
| 1        | C1    | 464        | 0.0ASN       |
| 1        | C1    | 495        | 0.0GLU       |
| 1        | C1    | 522        | 0.0GLU       |
| 1        | C1    | 562        | 0.0THR       |
| 1        | C1    | 633        | 0.0HIS       |
| 1        | C1    | 658        | 0.0ARG       |
| 1        | C1    | 664        | 0.0ARG       |
| 1        | C1    | 666        | 0.0VAL       |
| 1        | C1    | 670        | 0.0PRO       |
| 1        | C1    | 704        | 0.0TYR       |
| 1        | C1    | 718        | 0.0ASN       |
| 1        | C1    | 725        | 0.0GLU       |
| 1        | C1    | 745        | 0.0PHE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C1    | 748        | 0.0VAL       |
| 1        | C1    | 752        | 0.0VAL       |
| 1        | C1    | 753        | 0.0ASP       |
| 1        | C1    | 770        | 0.0ASN       |
| 1        | C1    | 778        | 0.0THR       |
| 1        | C1    | 783        | 0.0LEU       |
| 1        | C1    | 818        | 0.0PRO       |
| 1        | C1    | 827        | 0.0VAL       |
| 1        | C1    | 842        | 0.0LEU       |
| 1        | C1    | 864        | 0.0GLU       |
| 1        | C1    | 881        | 0.0THR       |
| 1        | C1    | 892        | 0.0LEU       |
| 1        | C1    | 917        | 0.0GLN       |
| 1        | C1    | 920        | 0.0ASN       |
| 1        | C1    | 924        | 0.0LEU       |
| 1        | C1    | 947        | 0.0GLU       |
| 1        | C1    | 962        | 0.0PRO       |
| 1        | C1    | 971        | 0.0GLU       |
| 1        | C1    | 974        | 0.0LEU       |
| 1        | C1    | 982        | 0.0THR       |
| 1        | C1    | 1011       | 0.0THR       |
| 1        | C1    | 1016       | 0.0PRO       |
| 1        | C1    | 1017       | 0.0ASN       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C1    | 1063       | 0.0TYR       |
| 1        | C1    | 1070       | 0.0TYR       |
| 1        | C1    | 1072       | 0.0VAL       |
| 1        | C1    | 1074       | 0.0LEU       |
| 1        | C1    | 1078       | 0.0LEU       |
| 1        | C1    | 1087       | 0.0CYS       |
| 1        | C1    | 1091       | 0.0GLU       |
| 1        | C1    | 1093       | 0.0LEU       |
| 1        | C1    | 1100       | 0.0PRO       |
| 1        | C1    | 1102       | 0.0ASN       |
| 1        | C1    | 1106       | 0.0VAL       |
| 1        | C1    | 1110       | 0.0TYR       |
| 1        | C1    | 1126       | 0.0ARG       |
| 1        | C1    | 1183       | 0.0THR       |
| 1        | C1    | 1226       | 0.0ARG       |
| 1        | C1    | 1254       | 0.0SER       |
| 1        | C1    | 1274       | 0.0SER       |
| 1        | C1    | 1290       | 0.0LYS       |
| 1        | C1    | 1325       | 0.0LYS       |
| 1        | C1    | 1356       | 0.0THR       |
| 1        | C1    | 1377       | 0.0THR       |
| 1        | C1    | 1396       | 0.0LEU       |
| 1        | C1    | 1404       | 0.0ASP       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C1    | 1405       | 0.0LEU       |
| 1        | C1    | 1414       | 0.0PHE       |
| 1        | C1    | 1415       | 0.0GLU       |
| 1        | C1    | 1433       | 0.0SER       |
| 1        | C1    | 1436       | 0.0VAL       |
| 1        | C1    | 1459       | 0.0LYS       |
| 1        | C1    | 1461       | 0.0ASN       |
| 1        | H2    | 304        | 0.0THR       |
| 1        | H2    | 319        | 0.0THR       |
| 1        | H2    | 324        | 0.0TYR       |
| 1        | H2    | 327        | 0.0PRO       |
| 1        | H2    | 330        | 0.0VAL       |
| 1        | H2    | 347        | 0.0THR       |
| 1        | H2    | 422        | 0.0LEU       |
| 1        | H2    | 423        | 0.0LYS       |
| 1        | H2    | 505        | 0.0ARG       |
| 1        | I2    | 270        | 0.0PRO       |
| 1        | I2    | 276        | 0.0GLU       |
| 1        | I2    | 317        | 0.0LYS       |
| 1        | I2    | 349        | 0.0THR       |
| 1        | I2    | 353        | 0.0LEU       |
| 1        | I2    | 359        | 0.0THR       |
| 1        | I2    | 369        | 0.0LEU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | I2    | 370        | 0.0ASP       |
| 1        | I2    | 375        | 0.0LYS       |
| 1        | I2    | 433        | 0.0LYS       |
| 1        | I2    | 436        | 0.0LEU       |
| 1        | I2    | 445        | 0.0GLU       |
| 1        | I2    | 446        | 0.0GLU       |
| 1        | J4    | 637        | 0.0LEU       |
| 1        | J4    | 743        | 0.0GLN       |
| 1        | J4    | 788        | 0.0ASP       |
| 1        | J4    | 789        | 0.0GLU       |
| 1        | d1    | 121        | 0.0ARG       |
| 1        | d1    | 140        | 0.0THR       |
| 1        | d1    | 146        | 0.0PHE       |
| 1        | d1    | 177        | 0.0VAL       |
| 1        | d1    | 190        | 0.0GLN       |
| 1        | d1    | 194        | 0.0LEU       |
| 1        | d1    | 196        | 0.0ILE       |
| 1        | d1    | 204        | 0.0VAL       |
| 1        | d1    | 207        | 0.0THR       |
| 1        | d1    | 211        | 0.0LEU       |
| 1        | d1    | 222        | 0.0GLN       |
| 1        | d1    | 245        | 0.0SER       |
| 1        | d1    | 246        | 0.0LEU       |



| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | d1    | 277        | 0.0LEU       |
| 1        | d1    | 278        | 0.0LYS       |
| 1        | d1    | 354        | 0.0PRO       |
| 1        | d1    | 362        | 0.0ILE       |
| 1        | d1    | 364        | 0.0HIS       |
| 1        | d1    | 404        | 0.0LEU       |
| 1        | d1    | 424        | 0.0SER       |
| 1        | d1    | 508        | 0.0ILE       |
| 1        | d1    | 534        | 0.0MET       |
| 1        | d1    | 535        | 0.0LYS       |
| 1        | d1    | 536        | 0.0VAL       |
| 1        | d1    | 596        | 0.0LEU       |
| 1        | d1    | 612        | 0.0VAL       |
| 1        | d1    | 614        | 0.0LEU       |
| 1        | d1    | 623        | 0.0LEU       |
| 1        | d1    | 649        | 0.0ARG       |
| 1        | d1    | 664        | 0.0LEU       |
| 1        | d1    | 699        | 0.0ILE       |
| 1        | d1    | 704        | 0.0GLU       |
| 1        | d1    | 716        | 0.0PRO       |
| 1        | d1    | 771        | 0.0ASP       |
| 1        | d1    | 773        | 0.0ARG       |
| 1        | d1    | 1186       | 0.0LEU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | d1    | 1195       | 0.0LYS       |
| 1        | d1    | 848        | 0.0LEU       |
| 1        | d1    | 857        | 0.0LEU       |
| 1        | d1    | 860        | 0.0ARG       |
| 1        | d1    | 1243       | 0.0CYS       |
| 1        | d1    | 1258       | 0.0LEU       |
| 1        | d1    | 928        | 0.0VAL       |
| 1        | d1    | 1078       | 0.0ARG       |
| 1        | d1    | 1092       | 0.0TYR       |
| 1        | d1    | 1108       | 0.0ASN       |
| 1        | d1    | 1109       | 0.0ASN       |
| 1        | A3    | 28         | 0.0ASN       |
| 1        | A3    | 37         | 0.0LEU       |
| 1        | A3    | 227        | 0.0THR       |
| 1        | A3    | 237        | 0.0HIS       |
| 1        | A3    | 288        | 0.0GLU       |
| 1        | A3    | 303        | 0.0LEU       |
| 1        | A3    | 313        | 0.0THR       |
| 1        | A3    | 625        | 0.0GLU       |
| 1        | A3    | 439        | 0.0SER       |
| 1        | A3    | 443        | 0.0GLN       |
| 1        | A3    | 683        | 0.0THR       |
| 1        | A3    | 468        | 0.0PHE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | A3    | 746        | 0.0PRO       |
| 1        | A3    | 747        | 0.0PHE       |
| 1        | A3    | 754        | 0.0ARG       |
| 1        | A3    | 765        | 0.0ASP       |
| 1        | A3    | 561        | 0.0GLN       |
| 1        | C2    | 2          | 0.0LYS       |
| 1        | C2    | 41         | 0.0LYS       |
| 1        | C2    | 60         | 0.0ASP       |
| 1        | C2    | 66         | 0.0VAL       |
| 1        | C2    | 82         | 0.0ASN       |
| 1        | C2    | 97         | 0.0THR       |
| 1        | C2    | 110        | 0.0ARG       |
| 1        | C2    | 117        | 0.0VAL       |
| 1        | C2    | 128        | 0.0THR       |
| 1        | C2    | 131        | 0.0TYR       |
| 1        | C2    | 132        | 0.0GLN       |
| 1        | C2    | 136        | 0.0LYS       |
| 1        | C2    | 153        | 0.0THR       |
| 1        | C2    | 183        | 0.0ARG       |
| 1        | C2    | 208        | 0.0LYS       |
| 1        | C2    | 209        | 0.0ASN       |
| 1        | C2    | 256        | 0.0HIS       |
| 1        | C2    | 260        | 0.0MET       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C2    | 293        | 0.0PRO       |
| 1        | C2    | 306        | 0.0VAL       |
| 1        | C2    | 307        | 0.0ASP       |
| 1        | C2    | 330        | 0.0SER       |
| 1        | C2    | 333        | 0.0GLU       |
| 1        | C2    | 334        | 0.0GLN       |
| 1        | C2    | 360        | 0.0LEU       |
| 1        | C2    | 362        | 0.0ASP       |
| 1        | C2    | 420        | 0.0LEU       |
| 1        | C2    | 441        | 0.0TYR       |
| 1        | C2    | 442        | 0.0SER       |
| 1        | C2    | 464        | 0.0ASN       |
| 1        | C2    | 495        | 0.0GLU       |
| 1        | C2    | 522        | 0.0GLU       |
| 1        | C2    | 562        | 0.0THR       |
| 1        | C2    | 633        | 0.0HIS       |
| 1        | C2    | 658        | 0.0ARG       |
| 1        | C2    | 664        | 0.0ARG       |
| 1        | C2    | 666        | 0.0VAL       |
| 1        | C2    | 670        | 0.0PRO       |
| 1        | C2    | 704        | 0.0TYR       |
| 1        | C2    | 718        | 0.0ASN       |
| 1        | C2    | 725        | 0.0GLU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C2    | 745        | 0.0PHE       |
| 1        | C2    | 748        | 0.0VAL       |
| 1        | C2    | 752        | 0.0VAL       |
| 1        | C2    | 753        | 0.0ASP       |
| 1        | C2    | 770        | 0.0ASN       |
| 1        | C2    | 778        | 0.0THR       |
| 1        | C2    | 783        | 0.0LEU       |
| 1        | C2    | 818        | 0.0PRO       |
| 1        | C2    | 827        | 0.0VAL       |
| 1        | C2    | 842        | 0.0LEU       |
| 1        | C2    | 864        | 0.0GLU       |
| 1        | C2    | 881        | 0.0THR       |
| 1        | C2    | 892        | 0.0LEU       |
| 1        | C2    | 917        | 0.0GLN       |
| 1        | C2    | 920        | 0.0ASN       |
| 1        | C2    | 924        | 0.0LEU       |
| 1        | C2    | 947        | 0.0GLU       |
| 1        | C2    | 962        | 0.0PRO       |
| 1        | C2    | 971        | 0.0GLU       |
| 1        | C2    | 974        | 0.0LEU       |
| 1        | C2    | 982        | 0.0THR       |
| 1        | C2    | 1011       | 0.0THR       |
| 1        | C2    | 1016       | 0.0PRO       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C2    | 1017       | 0.0ASN       |
| 1        | C2    | 1063       | 0.0TYR       |
| 1        | C2    | 1070       | 0.0TYR       |
| 1        | C2    | 1072       | 0.0VAL       |
| 1        | C2    | 1074       | 0.0LEU       |
| 1        | C2    | 1078       | 0.0LEU       |
| 1        | C2    | 1087       | 0.0CYS       |
| 1        | C2    | 1091       | 0.0GLU       |
| 1        | C2    | 1093       | 0.0LEU       |
| 1        | C2    | 1100       | 0.0PRO       |
| 1        | C2    | 1102       | 0.0ASN       |
| 1        | C2    | 1106       | 0.0VAL       |
| 1        | C2    | 1110       | 0.0TYR       |
| 1        | C2    | 1126       | 0.0ARG       |
| 1        | C2    | 1180       | 0.0GLU       |
| 1        | C2    | 1183       | 0.0THR       |
| 1        | C2    | 1226       | 0.0ARG       |
| 1        | C2    | 1254       | 0.0SER       |
| 1        | C2    | 1274       | 0.0SER       |
| 1        | C2    | 1290       | 0.0LYS       |
| 1        | C2    | 1325       | 0.0LYS       |
| 1        | C2    | 1356       | 0.0THR       |
| 1        | C2    | 1377       | 0.0THR       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | C2    | 1396       | 0.0LEU       |
| 1        | C2    | 1404       | 0.0ASP       |
| 1        | C2    | 1405       | 0.0LEU       |
| 1        | C2    | 1414       | 0.0PHE       |
| 1        | C2    | 1415       | 0.0GLU       |
| 1        | C2    | 1433       | 0.0SER       |
| 1        | C2    | 1436       | 0.0VAL       |
| 1        | C2    | 1459       | 0.0LYS       |
| 1        | C2    | 1461       | 0.0ASN       |
| 1        | H3    | 304        | 0.0THR       |
| 1        | H3    | 319        | 0.0THR       |
| 1        | H3    | 324        | 0.0TYR       |
| 1        | H3    | 327        | 0.0PRO       |
| 1        | H3    | 330        | 0.0VAL       |
| 1        | H3    | 347        | 0.0THR       |
| 1        | H3    | 422        | 0.0LEU       |
| 1        | H3    | 423        | 0.0LYS       |
| 1        | H3    | 505        | 0.0ARG       |
| 1        | I3    | 270        | 0.0PRO       |
| 1        | I3    | 276        | 0.0GLU       |
| 1        | I3    | 317        | 0.0LYS       |
| 1        | I3    | 349        | 0.0THR       |
| 1        | I3    | 353        | 0.0LEU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | I3    | 359        | 0.0THR       |
| 1        | I3    | 369        | 0.0LEU       |
| 1        | I3    | 370        | 0.0ASP       |
| 1        | I3    | 375        | 0.0LYS       |
| 1        | I3    | 433        | 0.0LYS       |
| 1        | I3    | 436        | 0.0LEU       |
| 1        | I3    | 445        | 0.0GLU       |
| 1        | I3    | 446        | 0.0GLU       |
| 1        | J5    | 637        | 0.0LEU       |
| 1        | J5    | 743        | 0.0GLN       |
| 1        | J5    | 788        | 0.0ASP       |
| 1        | J5    | 789        | 0.0GLU       |
| 1        | d2    | 121        | 0.0ARG       |
| 1        | d2    | 140        | 0.0THR       |
| 1        | d2    | 146        | 0.0PHE       |
| 1        | d2    | 177        | 0.0VAL       |
| 1        | d2    | 190        | 0.0GLN       |
| 1        | d2    | 194        | 0.0LEU       |
| 1        | d2    | 196        | 0.0ILE       |
| 1        | d2    | 204        | 0.0VAL       |
| 1        | d2    | 207        | 0.0THR       |
| 1        | d2    | 211        | 0.0LEU       |
| 1        | d2    | 222        | 0.0GLN       |



| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | d2    | 245        | 0.0SER       |
| 1        | d2    | 246        | 0.0LEU       |
| 1        | d2    | 277        | 0.0LEU       |
| 1        | d2    | 278        | 0.0LYS       |
| 1        | d2    | 354        | 0.0PRO       |
| 1        | d2    | 362        | 0.0ILE       |
| 1        | d2    | 364        | 0.0HIS       |
| 1        | d2    | 404        | 0.0LEU       |
| 1        | d2    | 424        | 0.0SER       |
| 1        | d2    | 508        | 0.0ILE       |
| 1        | d2    | 534        | 0.0MET       |
| 1        | d2    | 535        | 0.0LYS       |
| 1        | d2    | 536        | 0.0VAL       |
| 1        | d2    | 596        | 0.0LEU       |
| 1        | d2    | 612        | 0.0VAL       |
| 1        | d2    | 614        | 0.0LEU       |
| 1        | d2    | 623        | 0.0LEU       |
| 1        | d2    | 649        | 0.0ARG       |
| 1        | d2    | 664        | 0.0LEU       |
| 1        | d2    | 699        | 0.0ILE       |
| 1        | d2    | 704        | 0.0GLU       |
| 1        | d2    | 716        | 0.0PRO       |
| 1        | d2    | 771        | 0.0ASP       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | d2    | 773        | 0.0ARG       |
| 1        | d2    | 1186       | 0.0LEU       |
| 1        | d2    | 1195       | 0.0LYS       |
| 1        | d2    | 848        | 0.0LEU       |
| 1        | d2    | 857        | 0.0LEU       |
| 1        | d2    | 860        | 0.0ARG       |
| 1        | d2    | 1243       | 0.0CYS       |
| 1        | d2    | 1258       | 0.0LEU       |
| 1        | d2    | 928        | 0.0VAL       |
| 1        | d2    | 1078       | 0.0ARG       |
| 1        | d2    | 1092       | 0.0TYR       |
| 1        | d2    | 1108       | 0.0ASN       |
| 1        | d2    | 1109       | 0.0ASN       |
| 1        | A4    | 28         | 0.0ASN       |
| 1        | A4    | 37         | 0.0LEU       |
| 1        | A4    | 38         | 0.0ASN       |
| 1        | A4    | 39         | 0.0ASN       |
| 1        | A4    | 227        | 0.0THR       |
| 1        | A4    | 237        | 0.0HIS       |
| 1        | A4    | 242        | 0.0LYS       |
| 1        | A4    | 288        | 0.0GLU       |
| 1        | A4    | 303        | 0.0LEU       |
| 1        | A4    | 313        | 0.0THR       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | A4    | 625        | 0.0GLU       |
| 1        | A4    | 439        | 0.0SER       |
| 1        | A4    | 443        | 0.0GLN       |
| 1        | A4    | 683        | 0.0THR       |
| 1        | A4    | 468        | 0.0PHE       |
| 1        | A4    | 746        | 0.0PRO       |
| 1        | A4    | 747        | 0.0PHE       |
| 1        | A4    | 754        | 0.0ARG       |
| 1        | A4    | 765        | 0.0ASP       |
| 1        | A4    | 561        | 0.0GLN       |
| 1        | A4    | 600        | 0.0ASN       |
| 1        | A4    | 601        | 0.0ILE       |
| 1        | B2    | 25         | 0.0ARG       |
| 1        | B2    | 58         | 0.0THR       |
| 1        | B2    | 71         | 0.0PRO       |
| 1        | B2    | 75         | 0.0GLN       |
| 1        | B2    | 77         | 0.0PHE       |
| 1        | B2    | 103        | 0.0PHE       |
| 1        | B2    | 110        | 0.0ILE       |
| 1        | B2    | 136        | 0.0SER       |
| 1        | B2    | 156        | 0.0LEU       |
| 1        | B2    | 165        | 0.0VAL       |
| 1        | B2    | 182        | 0.0VAL       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | B2    | 186        | 0.0THR       |
| 1        | B2    | 211        | 0.0GLN       |
| 1        | B2    | 267        | 0.0SER       |
| 1        | B2    | 269        | 0.0ASP       |
| 1        | B2    | 270        | 0.0VAL       |
| 1        | B2    | 290        | 0.0VAL       |
| 1        | B2    | 292        | 0.0THR       |
| 1        | B2    | 303        | 0.0PRO       |
| 1        | B2    | 320        | 0.0PRO       |
| 1        | B2    | 336        | 0.0LYS       |
| 1        | B2    | 337        | 0.0LEU       |
| 1        | B2    | 344        | 0.0LEU       |
| 1        | B2    | 345        | 0.0PRO       |
| 1        | B2    | 348        | 0.0ILE       |
| 1        | B2    | 357        | 0.0ASP       |
| 1        | B2    | 358        | 0.0THR       |
| 1        | B2    | 359        | 0.0GLU       |
| 1        | B2    | 374        | 0.0THR       |
| 1        | B2    | 377        | 0.0SER       |
| 1        | B2    | 378        | 0.0LEU       |
| 1        | B2    | 380        | 0.0ASP       |
| 1        | B2    | 389        | 0.0PRO       |
| 1        | B2    | 396        | 0.0SER       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | B2    | 402        | 0.0PRO       |
| 1        | B2    | 403        | 0.0PRO       |
| 1        | B2    | 404        | 0.0ASN       |
| 1        | B2    | 405        | 0.0CYS       |
| 1        | B2    | 418        | 0.0LEU       |
| 1        | B2    | 441        | 0.0LEU       |
| 1        | B2    | 442        | 0.0LEU       |
| 1        | B2    | 447        | 0.0ASP       |
| 1        | B2    | 469        | 0.0ILE       |
| 1        | B2    | 497        | 0.0ARG       |
| 1        | B2    | 515        | 0.0PRO       |
| 1        | B2    | 516        | 0.0ASN       |
| 1        | B2    | 527        | 0.0LYS       |
| 1        | B2    | 574        | 0.0LEU       |
| 1        | B2    | 576        | 0.0ASN       |
| 1        | B2    | 590        | 0.0LYS       |
| 1        | B2    | 650        | 0.0THR       |
| 1        | B2    | 653        | 0.0ASP       |
| 1        | B2    | 654        | 0.0SER       |
| 1        | B2    | 656        | 0.0ASP       |
| 1        | B2    | 661        | 0.0THR       |
| 1        | B2    | 675        | 0.0LYS       |
| 1        | B2    | 676        | 0.0ILE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | B2    | 680        | 0.0LYS       |
| 1        | B2    | 691        | 0.0ASN       |
| 1        | B2    | 707        | 0.0ASN       |
| 1        | B2    | 715        | 0.0LEU       |
| 1        | B2    | 730        | 0.0TYR       |
| 1        | B2    | 731        | 0.0THR       |
| 1        | B2    | 772        | 0.0LEU       |
| 1        | B2    | 776        | 0.0LEU       |
| 1        | B2    | 782        | 0.0PRO       |
| 1        | B2    | 802        | 0.0SER       |
| 1        | B2    | 815        | 0.0GLN       |
| 1        | B2    | 829        | 0.0ASP       |
| 1        | B2    | 847        | 0.0SER       |
| 1        | B2    | 849        | 0.0PRO       |
| 1        | B2    | 858        | 0.0GLU       |
| 1        | B2    | 875        | 0.0LYS       |
| 1        | B2    | 889        | 0.0ASP       |
| 1        | B2    | 896        | 0.0LYS       |
| 1        | B2    | 898        | 0.0GLU       |
| 1        | B2    | 903        | 0.0ASP       |
| 1        | B2    | 913        | 0.0LYS       |
| 1        | B2    | 919        | 0.0VAL       |
| 1        | B2    | 929        | 0.0SER       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | B2    | 934        | 0.0SER       |
| 1        | B2    | 940        | 0.0LEU       |
| 1        | B2    | 941        | 0.0ASN       |
| 1        | B2    | 943        | 0.0THR       |
| 1        | B2    | 948        | 0.0LEU       |
| 1        | B2    | 949        | 0.0ASN       |
| 1        | B2    | 957        | 0.0TYR       |
| 1        | B2    | 960        | 0.0PRO       |
| 1        | B2    | 971        | 0.0SER       |
| 1        | B2    | 1018       | 0.0THR       |
| 1        | B2    | 1023       | 0.0ASP       |
| 1        | B2    | 1029       | 0.0VAL       |
| 1        | B2    | 1061       | 0.0ILE       |
| 1        | B2    | 1066       | 0.0ASN       |
| 1        | B2    | 1077       | 0.0LEU       |
| 1        | B2    | 1081       | 0.0PHE       |
| 1        | B2    | 1096       | 0.0VAL       |
| 1        | B2    | 1097       | 0.0ILE       |
| 1        | B2    | 1119       | 0.0GLU       |
| 1        | B2    | 1400       | 0.0PRO       |
| 1        | B2    | 1170       | 0.0ILE       |
| 1        | B2    | 1172       | 0.0ASP       |
| 1        | B2    | 1173       | 0.0GLU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | B2    | 1182       | 0.0THR       |
| 1        | B2    | 1192       | 0.0PRO       |
| 1        | B2    | 1224       | 0.0PHE       |
| 1        | B2    | 1226       | 0.0PRO       |
| 1        | B2    | 1507       | 0.0LEU       |
| 1        | B2    | 1508       | 0.0SER       |
| 1        | B2    | 1264       | 0.0LYS       |
| 1        | B2    | 1530       | 0.0LYS       |
| 1        | B2    | 1278       | 0.0LEU       |
| 1        | B2    | 1303       | 0.0TYR       |
| 1        | B2    | 1305       | 0.0HIS       |
| 1        | B2    | 1306       | 0.0ASP       |
| 1        | B2    | 1342       | 0.0LEU       |
| 1        | B2    | 1652       | 0.0PHE       |
| 1        | D2    | 101        | 0.0SER       |
| 1        | D2    | 142        | 0.0ASP       |
| 1        | D2    | 175        | 0.0ASN       |
| 1        | D2    | 177        | 0.0ILE       |
| 1        | D2    | 194        | 0.0VAL       |
| 1        | D2    | 203        | 0.0LYS       |
| 1        | D2    | 210        | 0.0ASN       |
| 1        | D2    | 222        | 0.0GLN       |
| 1        | D2    | 246        | 0.0LEU       |



| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | D2    | 269        | 0.0SER       |
| 1        | D2    | 278        | 0.0LYS       |
| 1        | D2    | 343        | 0.0ILE       |
| 1        | D2    | 349        | 0.0SER       |
| 1        | D2    | 354        | 0.0PRO       |
| 1        | D2    | 367        | 0.0HIS       |
| 1        | D2    | 413        | 0.0THR       |
| 1        | D2    | 431        | 0.0LYS       |
| 1        | D2    | 504        | 0.0VAL       |
| 1        | D2    | 511        | 0.0VAL       |
| 1        | D2    | 539        | 0.0ILE       |
| 1        | D2    | 541        | 0.0ILE       |
| 1        | D2    | 550        | 0.0LEU       |
| 1        | D2    | 569        | 0.0SER       |
| 1        | D2    | 570        | 0.0THR       |
| 1        | D2    | 602        | 0.0ASP       |
| 1        | D2    | 614        | 0.0MET       |
| 1        | D2    | 615        | 0.0TYR       |
| 1        | D2    | 626        | 0.0LEU       |
| 1        | D2    | 668        | 0.0LYS       |
| 1        | D2    | 673        | 0.0ILE       |
| 1        | D2    | 719        | 0.0PRO       |
| 1        | D2    | 774        | 0.0ASP       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | D2    | 813        | 0.0SER       |
| 1        | D2    | 820        | 0.0LEU       |
| 1        | D2    | 829        | 0.0GLU       |
| 1        | D2    | 830        | 0.0ILE       |
| 1        | D2    | 845        | 0.0LEU       |
| 1        | D2    | 854        | 0.0LEU       |
| 1        | D2    | 863        | 0.0LEU       |
| 1        | D2    | 866        | 0.0ARG       |
| 1        | D2    | 991        | 0.0THR       |
| 1        | D2    | 998        | 0.0THR       |
| 1        | D2    | 1005       | 0.0VAL       |
| 1        | D2    | 1299       | 0.0LYS       |
| 1        | D2    | 1300       | 0.0SER       |
| 1        | D2    | 1301       | 0.0SER       |
| 1        | D2    | 1041       | 0.0HIS       |
| 1        | D2    | 1081       | 0.0ARG       |
| 1        | D2    | 1083       | 0.0SER       |
| 1        | D2    | 1099       | 0.0THR       |
| 1        | D2    | 1113       | 0.0LEU       |
| 1        | D2    | 1114       | 0.0LYS       |
| 1        | H4    | 304        | 0.0THR       |
| 1        | H4    | 319        | 0.0THR       |
| 1        | H4    | 324        | 0.0TYR       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | H4    | 327        | 0.0PRO       |
| 1        | H4    | 330        | 0.0VAL       |
| 1        | H4    | 347        | 0.0THR       |
| 1        | H4    | 422        | 0.0LEU       |
| 1        | H4    | 423        | 0.0LYS       |
| 1        | H4    | 505        | 0.0ARG       |
| 1        | I4    | 270        | 0.0PRO       |
| 1        | I4    | 271        | 0.0PRO       |
| 1        | I4    | 276        | 0.0GLU       |
| 1        | I4    | 317        | 0.0LYS       |
| 1        | I4    | 349        | 0.0THR       |
| 1        | I4    | 353        | 0.0LEU       |
| 1        | I4    | 359        | 0.0THR       |
| 1        | I4    | 369        | 0.0LEU       |
| 1        | I4    | 370        | 0.0ASP       |
| 1        | I4    | 375        | 0.0LYS       |
| 1        | I4    | 433        | 0.0LYS       |
| 1        | I4    | 436        | 0.0LEU       |
| 1        | I4    | 445        | 0.0GLU       |
| 1        | I4    | 446        | 0.0GLU       |
| 1        | J6    | 637        | 0.0LEU       |
| 1        | J6    | 743        | 0.0GLN       |
| 1        | J6    | 788        | 0.0ASP       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | J6    | 789        | 0.0GLU       |
| 1        | K2    | 58         | 0.0ILE       |
| 1        | K2    | 106        | 0.0ILE       |
| 1        | K2    | 165        | 0.0ASN       |
| 1        | K2    | 182        | 0.0LYS       |
| 1        | K2    | 225        | 0.0LYS       |
| 1        | K2    | 239        | 0.0LEU       |
| 1        | K2    | 281        | 0.0GLU       |
| 1        | K2    | 363        | 0.0LYS       |
| 1        | K2    | 411        | 0.0ILE       |
| 1        | K2    | 416        | 0.0LYS       |
| 1        | K2    | 430        | 0.0ILE       |
| 1        | K2    | 472        | 0.0ILE       |
| 1        | K2    | 529        | 0.0ILE       |
| 1        | K2    | 531        | 0.0LYS       |
| 1        | K2    | 565        | 0.0ILE       |
| 1        | K2    | 581        | 0.0ASP       |
| 1        | K2    | 589        | 0.0LYS       |
| 1        | K2    | 632        | 0.0ILE       |
| 1        | K2    | 633        | 0.0LEU       |
| 1        | K2    | 678        | 0.0ILE       |
| 1        | K2    | 682        | 0.0GLU       |
| 1        | K2    | 687        | 0.0LEU       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | K2    | 714        | 0.0GLU       |
| 1        | K2    | 793        | 0.0LEU       |
| 1        | K2    | 802        | 0.0VAL       |
| 1        | K2    | 814        | 0.0ASN       |
| 1        | K2    | 849        | 0.0LYS       |
| 1        | K2    | 856        | 0.0ILE       |
| 1        | K2    | 858        | 0.0GLU       |
| 1        | K2    | 865        | 0.0GLU       |
| 1        | K2    | 939        | 0.0LYS       |
| 1        | L2    | 7          | 0.0THR       |
| 1        | L2    | 11         | 0.0ASP       |
| 1        | L2    | 20         | 0.0GLN       |
| 1        | L2    | 45         | 0.0ASP       |
| 1        | L2    | 58         | 0.0GLU       |
| 1        | L2    | 64         | 0.0LEU       |
| 1        | L2    | 73         | 0.0ASN       |
| 1        | L2    | 75         | 0.0ASP       |
| 1        | L2    | 105        | 0.0GLN       |
| 1        | L2    | 115        | 0.0GLU       |
| 1        | L2    | 128        | 0.0THR       |
| 1        | L2    | 153        | 0.0THR       |
| 1        | L2    | 212        | 0.0THR       |
| 1        | L2    | 224        | 0.0ILE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | L2    | 255        | 0.0SER       |
| 1        | L2    | 261        | 0.0GLN       |
| 1        | L2    | 271        | 0.0SER       |
| 1        | L2    | 285        | 0.0ILE       |
| 1        | L2    | 330        | 0.0ILE       |
| 1        | L2    | 344        | 0.0SER       |
| 1        | L2    | 352        | 0.0MET       |
| 1        | L2    | 380        | 0.0SER       |
| 1        | L2    | 399        | 0.0LEU       |
| 1        | L2    | 408        | 0.0ILE       |
| 1        | L2    | 426        | 0.0ILE       |
| 1        | L2    | 527        | 0.0ILE       |
| 1        | M2    | 94         | 0.0LEU       |
| 1        | M2    | 152        | 0.0ILE       |
| 1        | M2    | 168        | 0.0SER       |
| 1        | M2    | 179        | 0.0LEU       |
| 1        | M2    | 188        | 0.0SER       |
| 1        | M2    | 196        | 0.0LEU       |
| 1        | M2    | 201        | 0.0LEU       |
| 1        | M2    | 206        | 0.0THR       |
| 1        | M2    | 209        | 0.0CYS       |
| 1        | M2    | 211        | 0.0ILE       |
| 1        | M2    | 215        | 0.0ILE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | M2    | 228        | 0.0GLU       |
| 1        | M2    | 230        | 0.0LEU       |
| 1        | M2    | 231        | 0.0PHE       |
| 1        | M2    | 260        | 0.0LEU       |
| 1        | M2    | 262        | 0.0SER       |
| 1        | M2    | 266        | 0.0SER       |
| 1        | M2    | 268        | 0.0LEU       |
| 1        | M2    | 272        | 0.0SER       |
| 1        | M2    | 279        | 0.0ILE       |
| 1        | M2    | 300        | 0.0ARG       |
| 1        | M2    | 303        | 0.0THR       |
| 1        | M2    | 316        | 0.0GLN       |
| 1        | M2    | 324        | 0.0ARG       |
| 1        | M2    | 325        | 0.0VAL       |
| 1        | M2    | 327        | 0.0SER       |
| 1        | M2    | 329        | 0.0GLU       |
| 1        | M2    | 368        | 0.0ILE       |
| 1        | M2    | 376        | 0.0ILE       |
| 1        | M2    | 382        | 0.0SER       |
| 1        | M2    | 384        | 0.0ASN       |
| 1        | M2    | 390        | 0.0ARG       |
| 1        | M2    | 391        | 0.0LEU       |
| 1        | M2    | 399        | 0.0PHE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | M2    | 407        | 0.0ARG       |
| 1        | N2    | 15         | 0.0LYS       |
| 1        | N2    | 36         | 0.0HIS       |
| 1        | N2    | 39         | 0.0ILE       |
| 1        | N2    | 40         | 0.0ASP       |
| 1        | N2    | 132        | 0.0ILE       |
| 1        | N2    | 206        | 0.0VAL       |
| 1        | N2    | 208        | 0.0GLN       |
| 1        | N2    | 210        | 0.0ARG       |
| 1        | N2    | 256        | 0.0ASP       |
| 1        | O2    | 61         | 0.0ILE       |
| 1        | O2    | 80         | 0.0THR       |
| 1        | O2    | 125        | 0.0LEU       |
| 1        | O2    | 154        | 0.0MET       |
| 1        | O2    | 168        | 0.0ASP       |
| 1        | O2    | 183        | 0.0LEU       |
| 1        | O2    | 226        | 0.0ARG       |
| 1        | O2    | 313        | 0.0ASN       |
| 1        | O2    | 314        | 0.0LEU       |
| 1        | O2    | 295        | 0.0THR       |
| 1        | P2    | 90         | 0.0ASN       |
| 1        | P2    | 92         | 0.0THR       |
| 1        | P2    | 184        | 0.0VAL       |



| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | P2    | 214        | 0.0ASP       |
| 1        | P2    | 225        | 0.0VAL       |
| 1        | P2    | 269        | 0.0ILE       |
| 1        | P2    | 329        | 0.0VAL       |
| 1        | P2    | 332        | 0.0THR       |
| 1        | P2    | 384        | 0.0ASP       |
| 1        | P2    | 419        | 0.0LEU       |
| 1        | P2    | 427        | 0.0THR       |
| 1        | P2    | 456        | 0.0ILE       |
| 1        | P2    | 470        | 0.0TYR       |
| 1        | R2    | 103        | 0.0SER       |
| 1        | R2    | 138        | 0.0VAL       |
| 1        | R2    | 148        | 0.0GLN       |
| 1        | R2    | 151        | 0.0VAL       |
| 1        | R2    | 159        | 0.0LEU       |
| 1        | R2    | 164        | 0.0LYS       |
| 1        | R2    | 185        | 0.0THR       |
| 1        | R2    | 235        | 0.0MET       |
| 1        | R2    | 246        | 0.0PHE       |
| 1        | R2    | 256        | 0.0LEU       |
| 1        | R2    | 281        | 0.0VAL       |
| 1        | R2    | 285        | 0.0THR       |
| 1        | R2    | 299        | 0.0ILE       |

| Model ID | Chain | Residue ID | Residue type |
|----------|-------|------------|--------------|
| 1        | R2    | 312        | 0.0GLU       |
| 1        | R2    | 341        | 0.0ASP       |
| 1        | R2    | 375        | 0.0VAL       |
| 1        | R2    | 379        | 0.0PHE       |
| 1        | R2    | 399        | 0.0SER       |
| 1        | R2    | 561        | 0.0GLN       |
| 1        | R2    | 576        | 0.0ILE       |
| 1        | R2    | 609        | 0.0VAL       |
| 1        | R2    | 615        | 0.0THR       |
| 1        | R2    | 634        | 0.0LEU       |
| 1        | R2    | 661        | 0.0VAL       |
| 1        | R2    | 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.

#### *Acknowledgements*

*Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation*

*metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*