



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:27 AM UTC

PDB ID : 7VRV / pdb\_00007vrv  
EMDB ID : EMD-32107  
Title : VAS5 Spike (1 RBD up)  
Authors : Zhen, C.; Wang, X.  
Deposited on : 2021-10-25  
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

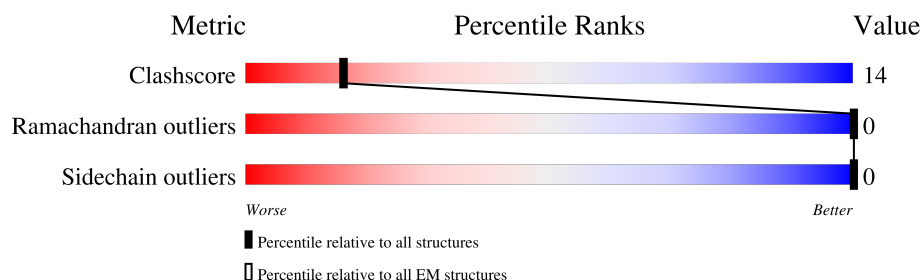
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1194   | 62% 29% 9%       |
| 1   | B     | 1194   | 63% 28% 9%       |
| 1   | C     | 1194   | 62% 29% 10%      |
| 2   | D     | 2      | 100%             |
| 2   | E     | 2      | 100%             |
| 2   | F     | 2      | 100%             |
| 2   | G     | 2      | 50% 50%          |
| 2   | H     | 2      | 100%             |
| 2   | I     | 2      | 100%             |

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| Mol | Chain | Length | Quality of chain                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------|
| 2   | J     | 2      |  100% |
| 2   | K     | 2      |  100% |
| 2   | L     | 2      |  100% |
| 2   | M     | 2      |  100% |
| 2   | N     | 2      |  100% |
| 2   | O     | 2      |  100% |
| 2   | P     | 2      |  100% |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1087     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8457  | 5395 | 1404 | 1620 | 38 |         |       |
| 1   | B     | 1091     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8485  | 5409 | 1416 | 1621 | 39 |         |       |
| 1   | C     | 1079     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8411  | 5363 | 1400 | 1611 | 37 |         |       |

There are 27 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | ?       | -        | ASN    | deletion            | UNP P0DTC2 |
| A     | ?       | -        | SER    | deletion            | UNP P0DTC2 |
| A     | ?       | -        | PRO    | deletion            | UNP P0DTC2 |
| A     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| A     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| A     | ?       | -        | ALA    | deletion            | UNP P0DTC2 |
| A     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| A     | 979     | PRO      | LYS    | engineered mutation | UNP P0DTC2 |
| A     | 980     | PRO      | VAL    | engineered mutation | UNP P0DTC2 |
| B     | ?       | -        | ASN    | deletion            | UNP P0DTC2 |
| B     | ?       | -        | SER    | deletion            | UNP P0DTC2 |
| B     | ?       | -        | PRO    | deletion            | UNP P0DTC2 |
| B     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| B     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| B     | ?       | -        | ALA    | deletion            | UNP P0DTC2 |
| B     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| B     | 979     | PRO      | LYS    | engineered mutation | UNP P0DTC2 |
| B     | 980     | PRO      | VAL    | engineered mutation | UNP P0DTC2 |
| C     | ?       | -        | ASN    | deletion            | UNP P0DTC2 |
| C     | ?       | -        | SER    | deletion            | UNP P0DTC2 |
| C     | ?       | -        | PRO    | deletion            | UNP P0DTC2 |
| C     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| C     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| C     | ?       | -        | ALA    | deletion            | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | ?       | -        | ARG    | deletion            | UNP P0DTC2 |
| C     | 979     | PRO      | LYS    | engineered mutation | UNP P0DTC2 |
| C     | 980     | PRO      | VAL    | engineered mutation | UNP P0DTC2 |

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 2   | D     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | E     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | F     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | G     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | H     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | I     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | J     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | K     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | L     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | M     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | N     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | O     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | P     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

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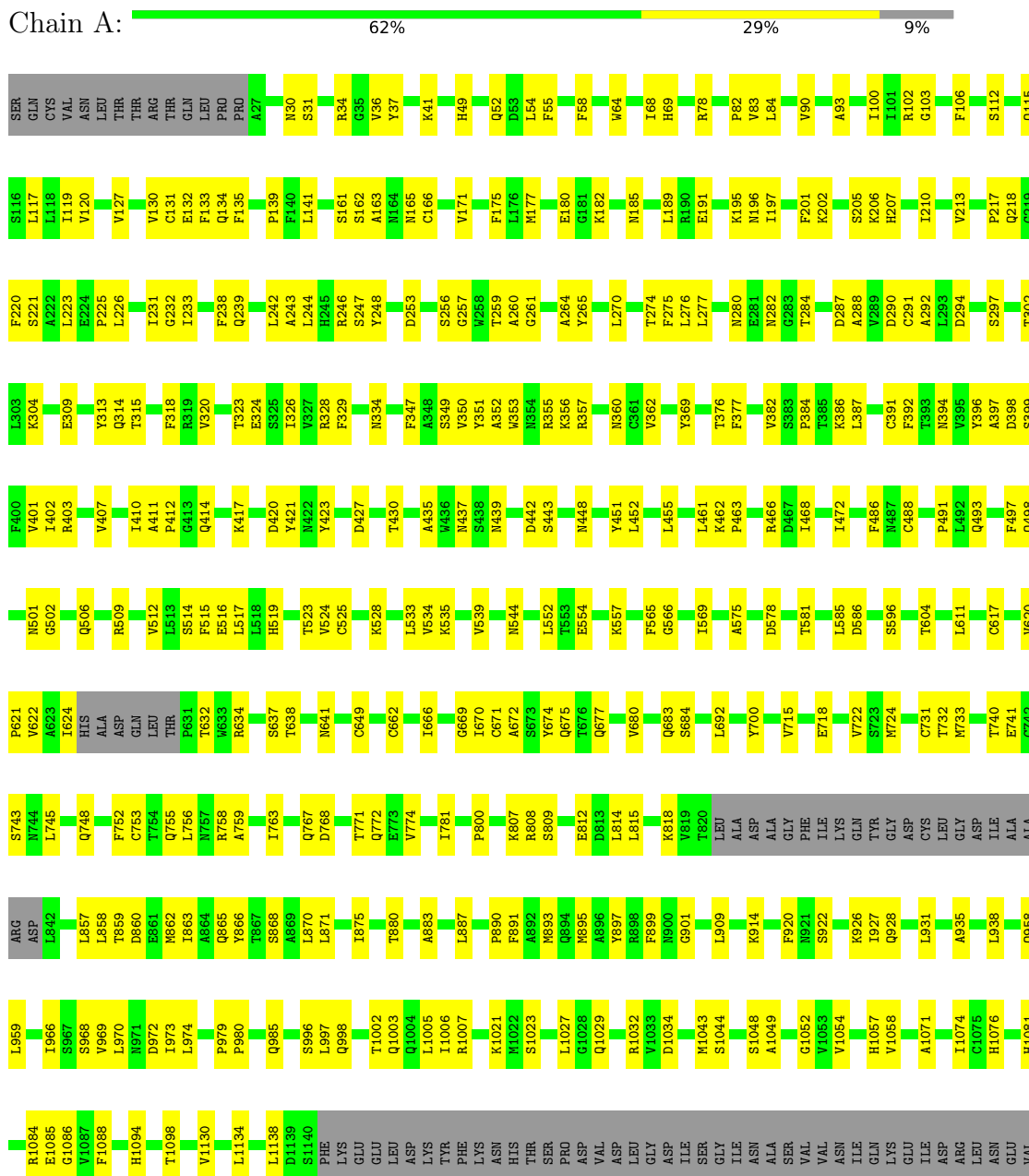
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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

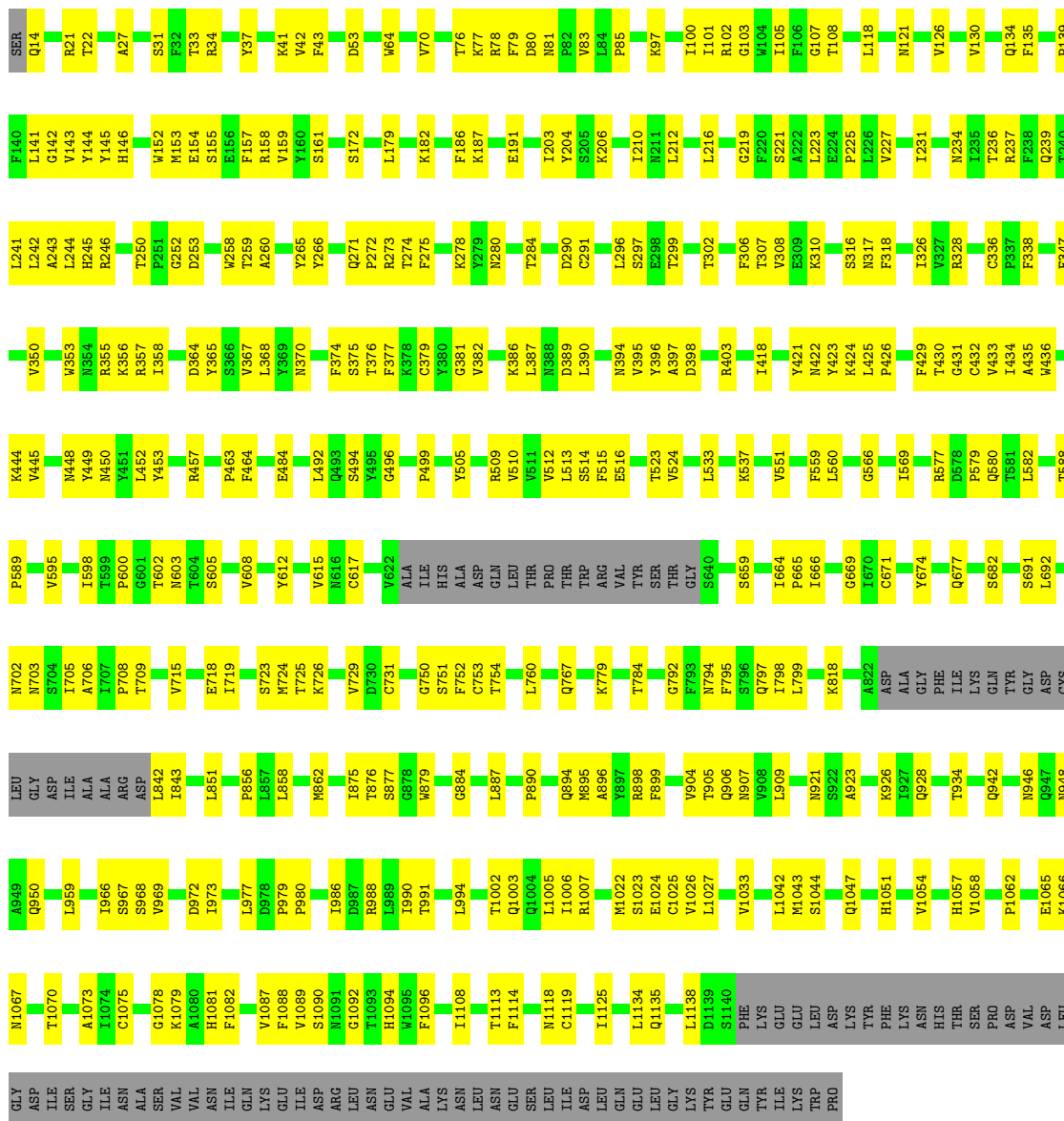
- Molecule 1: Spike glycoprotein



ALA  
LYS  
ASN  
LEU  
LEU  
ASN  
GLU  
SER  
LEU  
ILE  
ASP  
LEU  
LEU  
GLN  
GLU  
LEU  
GLY  
LYS  
TYR  
GLU  
GLN  
TYR  
ILE  
LYS  
TRP  
PRO

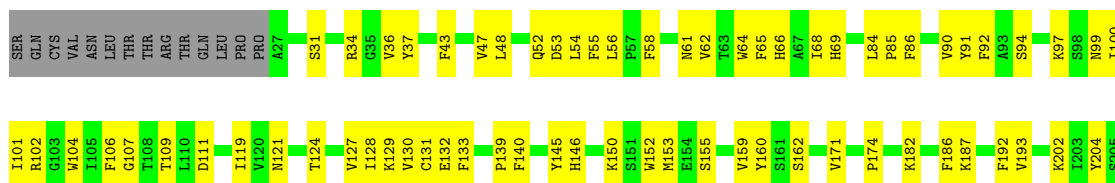
• Molecule 1: Spike glycoprotein

Chain B:  63% 28% 9%



• Molecule 1: Spike glycoprotein

Chain C:  62% 29% 10%





Chain F:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50%  50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



## 4 Experimental information

| Property                             | Value                      | Source    |
|--------------------------------------|----------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE            | Depositor |
| Imposed symmetry                     | POINT, Not provided        |           |
| Number of particles used             | 57732                      | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF          | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY        | Depositor |
| Microscope                           | FEI TITAN                  | Depositor |
| Voltage (kV)                         | 300                        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                         | Depositor |
| Minimum defocus (nm)                 | 1200                       | Depositor |
| Maximum defocus (nm)                 | 1500                       | Depositor |
| Magnification                        | Not provided               |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k) | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | A     | 0.16         | 0/8657      | 0.37        | 0/11793        |
| 1   | B     | 0.16         | 0/8683      | 0.38        | 0/11828        |
| 1   | C     | 0.16         | 0/8610      | 0.39        | 1/11725 (0.0%) |
| All | All   | 0.16         | 0/25950     | 0.38        | 1/35346 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 130 | VAL  | N-CA-C | -5.87 | 106.77      | 112.29   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 8457  | 0        | 8202     | 273     | 0            |
| 1   | B     | 8485  | 0        | 8247     | 252     | 0            |
| 1   | C     | 8411  | 0        | 8157     | 256     | 0            |
| 2   | D     | 28    | 0        | 25       | 0       | 0            |
| 2   | E     | 28    | 0        | 25       | 1       | 0            |
| 2   | F     | 28    | 0        | 25       | 0       | 0            |
| 2   | G     | 28    | 0        | 25       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | H     | 28    | 0        | 25       | 0       | 0            |
| 2   | I     | 28    | 0        | 25       | 0       | 0            |
| 2   | J     | 28    | 0        | 25       | 0       | 0            |
| 2   | K     | 28    | 0        | 25       | 2       | 0            |
| 2   | L     | 28    | 0        | 25       | 0       | 0            |
| 2   | M     | 28    | 0        | 25       | 0       | 0            |
| 2   | N     | 28    | 0        | 25       | 0       | 0            |
| 2   | O     | 28    | 0        | 25       | 0       | 0            |
| 2   | P     | 28    | 0        | 25       | 0       | 0            |
| 3   | A     | 140   | 0        | 130      | 4       | 0            |
| 3   | B     | 140   | 0        | 130      | 2       | 0            |
| 3   | C     | 154   | 0        | 143      | 1       | 0            |
| All | All   | 26151 | 0        | 25334    | 736     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:391:CYS:HA   | 1:A:525:CYS:HB3   | 1.52                     | 0.90              |
| 1:C:107:GLY:O    | 1:C:237:ARG:HB2   | 1.75                     | 0.87              |
| 1:C:391:CYS:HA   | 1:C:525:CYS:HB3   | 1.55                     | 0.86              |
| 1:A:396:TYR:HB2  | 1:A:514:SER:HB3   | 1.58                     | 0.85              |
| 1:C:246:ARG:HG3  | 1:C:258:TRP:HA    | 1.61                     | 0.83              |
| 1:A:763:ILE:HD11 | 1:A:1005:LEU:HD23 | 1.62                     | 0.81              |
| 1:B:425:LEU:HD12 | 1:B:426:PRO:HD2   | 1.64                     | 0.80              |
| 1:A:1044:SER:HG  | 1:A:1057:HIS:HD1  | 1.32                     | 0.77              |
| 1:A:37:TYR:HB3   | 1:A:223:LEU:HB2   | 1.65                     | 0.77              |
| 1:A:604:THR:HG22 | 3:A:1306:NAG:H62  | 1.68                     | 0.76              |
| 1:A:617:CYS:N    | 1:A:649:CYS:SG    | 2.59                     | 0.75              |
| 1:A:106:PHE:HB2  | 1:A:117:LEU:HB2   | 1.68                     | 0.75              |
| 1:B:144:TYR:HB2  | 1:B:155:SER:HB3   | 1.68                     | 0.74              |
| 1:C:894:GLN:HE21 | 1:C:898:ARG:HH21  | 1.34                     | 0.73              |
| 1:A:733:MET:HE1  | 1:C:319:ARG:HD2   | 1.70                     | 0.72              |
| 1:B:1033:VAL:O   | 1:C:1023:SER:OG   | 2.07                     | 0.72              |
| 1:B:896:ALA:HB1  | 1:B:906:GLN:HB2   | 1.72                     | 0.71              |
| 1:B:898:ARG:NH1  | 1:B:1042:LEU:O    | 2.23                     | 0.71              |
| 1:A:355:ARG:NH2  | 1:A:357:ARG:HE    | 1.88                     | 0.71              |
| 1:A:781:ILE:HG21 | 1:A:865:GLN:HE21  | 1.56                     | 0.71              |
| 1:A:225:PRO:HG2  | 1:C:562:PHE:HZ    | 1.54                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:246:ARG:HH21 | 1:A:260:ALA:H     | 1.40                     | 0.70              |
| 1:C:724:MET:HE1  | 1:C:1007:ARG:HB3  | 1.73                     | 0.69              |
| 1:B:126:VAL:HB   | 1:B:172:SER:HB3   | 1.74                     | 0.69              |
| 1:C:795:PHE:HE1  | 1:C:920:PHE:HE2   | 1.41                     | 0.69              |
| 1:A:472:ILE:HA   | 1:A:491:PRO:HD3   | 1.74                     | 0.69              |
| 1:B:210:ILE:HG13 | 1:B:212:LEU:H     | 1.58                     | 0.69              |
| 1:B:431:GLY:HA3  | 1:B:513:LEU:O     | 1.93                     | 0.68              |
| 1:B:715:VAL:HG22 | 1:B:923:ALA:HB1   | 1.75                     | 0.68              |
| 1:B:139:PRO:HA   | 1:B:158:ARG:O     | 1.94                     | 0.68              |
| 1:B:70:VAL:HB    | 1:B:76:THR:HB     | 1.76                     | 0.68              |
| 1:A:722:VAL:HG21 | 1:A:774:VAL:HG11  | 1.75                     | 0.67              |
| 1:A:318:PHE:HE2  | 1:A:634:ARG:HH22  | 1.40                     | 0.67              |
| 1:A:1044:SER:OG  | 1:A:1057:HIS:ND1  | 2.23                     | 0.67              |
| 1:B:751:SER:OG   | 1:B:754:THR:OG1   | 2.13                     | 0.67              |
| 1:A:41:LYS:HB3   | 1:C:563:GLN:HB3   | 1.74                     | 0.67              |
| 1:B:669:GLY:HA3  | 1:C:862:MET:HE1   | 1.74                     | 0.67              |
| 1:B:449:TYR:HB3  | 1:B:494:SER:HB3   | 1.77                     | 0.67              |
| 1:A:134:GLN:HB2  | 1:A:162:SER:HB2   | 1.76                     | 0.66              |
| 1:A:666:ILE:HD11 | 1:A:672:ALA:HB2   | 1.76                     | 0.66              |
| 1:B:386:LYS:HB3  | 1:B:389:ASP:HB3   | 1.78                     | 0.66              |
| 1:B:1079:LYS:HA  | 1:B:1118:ASN:HA   | 1.76                     | 0.66              |
| 1:C:317:ASN:HA   | 1:C:594:GLY:HA2   | 1.77                     | 0.66              |
| 1:B:139:PRO:HB3  | 1:B:159:VAL:HA    | 1.78                     | 0.66              |
| 1:C:555:SER:HB3  | 1:C:586:ASP:HB2   | 1.78                     | 0.66              |
| 1:A:326:ILE:HD12 | 1:A:539:VAL:HG21  | 1.76                     | 0.65              |
| 1:A:430:THR:OG1  | 1:A:515:PHE:O     | 2.14                     | 0.65              |
| 1:C:389:ASP:OD1  | 1:C:528:LYS:NZ    | 2.29                     | 0.65              |
| 1:C:715:VAL:HG12 | 1:C:1058:VAL:HG22 | 1.77                     | 0.65              |
| 1:C:433:VAL:HG12 | 1:C:512:VAL:HG12  | 1.77                     | 0.65              |
| 1:C:784:THR:HG22 | 1:C:872:ALA:HB2   | 1.78                     | 0.65              |
| 1:B:290:ASP:O    | 1:B:297:SER:OG    | 2.16                     | 0.64              |
| 1:A:959:LEU:O    | 1:A:968:SER:OG    | 2.14                     | 0.64              |
| 1:A:1084:ARG:HG3 | 1:A:1085:GLU:HG2  | 1.78                     | 0.64              |
| 1:B:1081:HIS:HB3 | 1:B:1113:THR:HG21 | 1.80                     | 0.64              |
| 1:B:328:ARG:NH2  | 1:B:580:GLN:OE1   | 2.31                     | 0.64              |
| 1:C:58:PHE:HB2   | 1:C:293:LEU:HD11  | 1.80                     | 0.64              |
| 1:A:566:GLY:HA3  | 1:A:575:ALA:HB3   | 1.79                     | 0.64              |
| 1:B:296:LEU:HB2  | 1:B:608:VAL:HG11  | 1.79                     | 0.64              |
| 1:C:99:ASN:O     | 1:C:102:ARG:NH2   | 2.31                     | 0.64              |
| 1:C:452:LEU:HD22 | 1:C:492:LEU:HB3   | 1.79                     | 0.64              |
| 1:C:340:GLU:OE2  | 1:C:356:LYS:NZ    | 2.30                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:34:ARG:NH1   | 1:C:219:GLY:O     | 2.32                     | 0.63              |
| 1:C:401:VAL:HG22 | 1:C:509:ARG:HD3   | 1.79                     | 0.63              |
| 1:C:328:ARG:NH2  | 1:C:531:THR:O     | 2.32                     | 0.63              |
| 1:C:37:TYR:HB3   | 1:C:223:LEU:HB3   | 1.81                     | 0.63              |
| 1:C:551:VAL:HB   | 1:C:588:THR:O     | 1.98                     | 0.63              |
| 1:C:763:ILE:HD11 | 1:C:1005:LEU:HD23 | 1.81                     | 0.62              |
| 1:B:375:SER:HB2  | 1:B:436:TRP:HA    | 1.79                     | 0.62              |
| 1:B:615:VAL:HG23 | 1:B:617:CYS:H     | 1.63                     | 0.62              |
| 1:B:752:PHE:HD2  | 1:B:994:LEU:HD21  | 1.64                     | 0.62              |
| 1:C:329:PHE:O    | 1:C:580:GLN:NE2   | 2.30                     | 0.62              |
| 1:C:1003:GLN:HB3 | 1:C:1007:ARG:HH12 | 1.63                     | 0.62              |
| 1:A:30:ASN:O     | 1:A:218:GLN:NE2   | 2.32                     | 0.62              |
| 1:C:64:TRP:HE1   | 1:C:264:ALA:HB1   | 1.64                     | 0.62              |
| 3:B:1306:NAG:H3  | 3:B:1306:NAG:H83  | 1.82                     | 0.62              |
| 1:A:557:LYS:NZ   | 1:A:586:ASP:OD1   | 2.24                     | 0.62              |
| 1:B:715:VAL:HA   | 1:B:1057:HIS:O    | 2.00                     | 0.62              |
| 1:C:619:GLU:N    | 1:C:619:GLU:OE1   | 2.30                     | 0.62              |
| 1:A:34:ARG:NH1   | 1:A:221:SER:OG    | 2.33                     | 0.62              |
| 1:C:546:LEU:HD11 | 1:C:573:THR:HG21  | 1.82                     | 0.62              |
| 1:C:92:PHE:HZ    | 1:C:101:ILE:HD11  | 1.63                     | 0.61              |
| 1:C:351:TYR:HB3  | 1:C:453:TYR:HA    | 1.82                     | 0.61              |
| 1:B:350:VAL:HG21 | 1:B:418:ILE:HD12  | 1.82                     | 0.61              |
| 1:B:818:LYS:NZ   | 1:B:934:THR:O     | 2.30                     | 0.61              |
| 1:C:392:PHE:HB2  | 1:C:524:VAL:HG23  | 1.83                     | 0.61              |
| 1:B:81:ASN:O     | 1:B:239:GLN:NE2   | 2.33                     | 0.61              |
| 1:A:552:LEU:HD12 | 1:A:585:LEU:HB3   | 1.81                     | 0.61              |
| 1:A:920:PHE:HE1  | 1:A:1058:VAL:HG11 | 1.65                     | 0.61              |
| 1:A:127:VAL:HG22 | 1:A:171:VAL:HG13  | 1.83                     | 0.61              |
| 1:A:355:ARG:NH2  | 1:A:396:TYR:HD1   | 1.98                     | 0.61              |
| 1:A:748:GLN:OE1  | 1:C:962:ASN:ND2   | 2.29                     | 0.61              |
| 1:B:34:ARG:NH1   | 1:B:219:GLY:O     | 2.33                     | 0.60              |
| 1:B:724:MET:HG2  | 1:B:767:GLN:NE2   | 2.16                     | 0.60              |
| 1:C:818:LYS:HD2  | 1:C:935:ALA:HB2   | 1.83                     | 0.60              |
| 1:A:692:LEU:HD21 | 1:B:862:MET:HB2   | 1.83                     | 0.60              |
| 1:C:461:LEU:HD11 | 1:C:465:GLU:HB3   | 1.81                     | 0.60              |
| 1:B:875:ILE:HG13 | 1:B:876:THR:HG23  | 1.83                     | 0.60              |
| 1:A:384:PRO:HA   | 1:A:387:LEU:HD23  | 1.84                     | 0.60              |
| 1:B:969:VAL:HG12 | 1:B:972:ASP:H     | 1.66                     | 0.60              |
| 1:A:391:CYS:HA   | 1:A:525:CYS:CB    | 2.29                     | 0.60              |
| 1:B:1134:LEU:HG  | 1:B:1138:LEU:HD23 | 1.83                     | 0.60              |
| 1:C:454:ARG:NH1  | 1:C:455:LEU:O     | 2.35                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:97:LYS:HD2   | 1:B:182:LYS:HB2   | 1.84                     | 0.60              |
| 1:C:48:LEU:HB3   | 1:C:276:LEU:HD11  | 1.83                     | 0.60              |
| 1:C:86:PHE:HD1   | 1:C:90:VAL:HG13   | 1.67                     | 0.60              |
| 1:B:21:ARG:NE    | 1:B:79:PHE:O      | 2.33                     | 0.59              |
| 1:B:718:GLU:OE1  | 1:B:1057:HIS:NE2  | 2.35                     | 0.59              |
| 1:A:387:LEU:HD11 | 1:A:515:PHE:HE2   | 1.66                     | 0.59              |
| 1:A:883:ALA:HA   | 1:C:1039:GLY:HA2  | 1.85                     | 0.59              |
| 1:A:355:ARG:NH1  | 1:A:356:LYS:O     | 2.36                     | 0.59              |
| 1:B:308:VAL:H    | 1:B:602:THR:HB    | 1.67                     | 0.59              |
| 1:C:99:ASN:OD1   | 1:C:102:ARG:NH1   | 2.36                     | 0.59              |
| 1:C:328:ARG:HH11 | 1:C:580:GLN:HG3   | 1.68                     | 0.59              |
| 1:A:244:LEU:HB3  | 1:A:246:ARG:HH12  | 1.68                     | 0.59              |
| 1:A:369:TYR:OH   | 1:C:415:THR:O     | 2.20                     | 0.59              |
| 1:C:97:LYS:HE3   | 1:C:187:LYS:HB2   | 1.84                     | 0.59              |
| 1:C:967:SER:HB3  | 1:C:973:ILE:HG12  | 1.84                     | 0.59              |
| 1:A:352:ALA:HB2  | 1:A:468:ILE:HG21  | 1.84                     | 0.58              |
| 1:B:108:THR:OG1  | 1:B:234:ASN:O     | 2.21                     | 0.58              |
| 1:B:797:GLN:HG2  | 1:B:928:GLN:NE2   | 2.18                     | 0.58              |
| 1:C:245:HIS:CD2  | 1:C:254:SER:HB3   | 2.38                     | 0.58              |
| 1:B:445:VAL:HA   | 1:B:499:PRO:HG3   | 1.85                     | 0.58              |
| 1:A:675:GLN:O    | 1:A:684:SER:OG    | 2.20                     | 0.58              |
| 1:B:367:VAL:O    | 1:B:370:ASN:ND2   | 2.36                     | 0.58              |
| 1:A:120:VAL:HG11 | 3:A:1302:NAG:H82  | 1.84                     | 0.58              |
| 1:B:379:CYS:HA   | 1:B:432:CYS:HA    | 1.86                     | 0.58              |
| 1:A:355:ARG:HH11 | 1:A:356:LYS:H     | 1.51                     | 0.58              |
| 1:B:666:ILE:HG12 | 1:B:671:CYS:HA    | 1.85                     | 0.58              |
| 1:A:323:THR:HG23 | 1:A:324:GLU:OE1   | 2.04                     | 0.58              |
| 1:A:557:LYS:HD2  | 1:B:43:PHE:HE2    | 1.68                     | 0.58              |
| 1:A:768:ASP:OD2  | 1:A:772:GLN:NE2   | 2.36                     | 0.58              |
| 1:A:54:LEU:HD11  | 1:A:195:LYS:HD3   | 1.84                     | 0.58              |
| 1:A:1086:GLY:HA3 | 1:A:1098:THR:O    | 2.04                     | 0.58              |
| 1:B:899:PHE:HE1  | 1:B:1042:LEU:HD11 | 1.69                     | 0.58              |
| 1:C:731:CYS:SG   | 1:C:732:THR:N     | 2.76                     | 0.58              |
| 1:C:106:PHE:HD2  | 1:C:235:ILE:HG21  | 1.68                     | 0.58              |
| 1:A:31:SER:HA    | 1:A:218:GLN:HE22  | 1.68                     | 0.58              |
| 1:C:290:ASP:OD1  | 1:C:291:CYS:N     | 2.37                     | 0.57              |
| 1:C:204:TYR:HA   | 1:C:225:PRO:HA    | 1.86                     | 0.57              |
| 1:C:280:ASN:HD21 | 1:C:284:THR:HG1   | 1.48                     | 0.57              |
| 1:C:361:CYS:H    | 1:C:524:VAL:HG12  | 1.68                     | 0.57              |
| 1:B:80:ASP:O     | 1:B:265:TYR:OH    | 2.21                     | 0.57              |
| 1:B:310:LYS:HG3  | 1:B:664:ILE:HD11  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:815:LEU:HG    | 1:A:938:LEU:HD11  | 1.85                     | 0.57              |
| 1:A:895:MET:HB3   | 1:A:909:LEU:HD11  | 1.85                     | 0.57              |
| 1:A:731:CYS:SG    | 1:A:732:THR:N     | 2.78                     | 0.57              |
| 1:B:27:ALA:HB3    | 1:B:64:TRP:HB3    | 1.86                     | 0.57              |
| 1:B:731:CYS:HB2   | 1:B:753:CYS:HA    | 1.86                     | 0.57              |
| 1:A:420:ASP:O     | 1:A:461:LEU:N     | 2.37                     | 0.57              |
| 1:A:812:GLU:HA    | 1:A:815:LEU:HD13  | 1.86                     | 0.57              |
| 1:C:314:GLN:OE1   | 1:C:596:SER:OG    | 2.17                     | 0.57              |
| 1:C:280:ASN:ND2   | 1:C:284:THR:OG1   | 2.31                     | 0.57              |
| 1:C:1109:THR:HG22 | 1:C:1111:ASP:H    | 1.70                     | 0.57              |
| 1:B:299:THR:HA    | 1:B:302:THR:HG22  | 1.85                     | 0.57              |
| 1:B:316:SER:OG    | 1:B:317:ASN:N     | 2.37                     | 0.56              |
| 1:B:365:TYR:HB2   | 1:B:387:LEU:HD22  | 1.86                     | 0.56              |
| 1:B:14:GLN:NE2    | 1:B:253:ASP:OD1   | 2.38                     | 0.56              |
| 1:B:328:ARG:HB3   | 1:B:579:PRO:HG3   | 1.88                     | 0.56              |
| 1:C:53:ASP:OD1    | 1:C:54:LEU:N      | 2.36                     | 0.56              |
| 1:A:93:ALA:O      | 1:A:265:TYR:HB2   | 2.05                     | 0.56              |
| 1:C:31:SER:HB3    | 1:C:62:VAL:HG21   | 1.87                     | 0.56              |
| 1:C:404:GLY:HA2   | 1:C:508:TYR:CD2   | 2.41                     | 0.56              |
| 1:A:638:THR:OG1   | 1:A:641:ASN:ND2   | 2.35                     | 0.56              |
| 1:A:112:SER:OG    | 1:A:134:GLN:OE1   | 2.22                     | 0.56              |
| 1:A:276:LEU:HD11  | 1:A:304:LYS:HA    | 1.87                     | 0.56              |
| 1:B:246:ARG:NH2   | 1:B:252:GLY:O     | 2.39                     | 0.56              |
| 1:C:48:LEU:HD21   | 1:C:306:PHE:HB2   | 1.88                     | 0.56              |
| 1:C:127:VAL:HG12  | 1:C:127:VAL:O     | 2.06                     | 0.56              |
| 1:A:82:PRO:HG2    | 1:A:84:LEU:HD21   | 1.88                     | 0.56              |
| 1:A:1023:SER:HA   | 1:A:1027:LEU:HD12 | 1.87                     | 0.56              |
| 1:A:891:PHE:HZ    | 1:A:1043:MET:HE1  | 1.70                     | 0.55              |
| 1:B:858:LEU:HD22  | 1:B:862:MET:HE3   | 1.87                     | 0.55              |
| 1:C:899:PHE:HE1   | 1:C:1042:LEU:HD11 | 1.71                     | 0.55              |
| 1:B:34:ARG:HH22   | 1:B:219:GLY:H     | 1.52                     | 0.55              |
| 1:B:726:LYS:HD3   | 1:B:856:PRO:HA    | 1.87                     | 0.55              |
| 1:C:310:LYS:HA    | 1:C:599:THR:O     | 2.06                     | 0.55              |
| 1:B:702:ASN:OD1   | 1:B:703:ASN:N     | 2.39                     | 0.55              |
| 1:B:905:THR:OG1   | 1:B:907:ASN:OD1   | 2.21                     | 0.55              |
| 1:C:561:PRO:O     | 1:C:577:ARG:NH1   | 2.30                     | 0.55              |
| 1:A:733:MET:HE2   | 1:C:592:PHE:CD2   | 2.41                     | 0.55              |
| 1:C:681:ALA:HB1   | 1:C:684:SER:HB3   | 1.89                     | 0.55              |
| 1:C:426:PRO:HD2   | 1:C:429:PHE:HB2   | 1.88                     | 0.55              |
| 1:A:115:GLN:NE2   | 1:A:132:GLU:OE1   | 2.39                     | 0.55              |
| 1:A:292:ALA:HB1   | 1:A:632:THR:HB    | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:431:GLY:HA2  | 1:C:515:PHE:HD2   | 1.71                     | 0.55              |
| 1:A:185:ASN:HA   | 1:A:213:VAL:HG23  | 1.88                     | 0.55              |
| 1:A:866:TYR:HE1  | 1:C:692:LEU:HB3   | 1.71                     | 0.55              |
| 1:B:326:ILE:HD13 | 1:B:533:LEU:HA    | 1.89                     | 0.55              |
| 1:B:356:LYS:HB3  | 1:B:397:ALA:HB3   | 1.89                     | 0.54              |
| 1:C:52:GLN:HA    | 1:C:274:THR:HA    | 1.89                     | 0.54              |
| 1:A:674:TYR:OH   | 1:A:683:GLN:OE1   | 2.19                     | 0.54              |
| 1:B:355:ARG:NH1  | 1:B:398:ASP:OD2   | 2.39                     | 0.54              |
| 1:C:438:SER:OG   | 1:C:509:ARG:NH2   | 2.35                     | 0.54              |
| 1:A:127:VAL:HG13 | 1:A:171:VAL:HG22  | 1.89                     | 0.54              |
| 1:C:145:TYR:HA   | 1:C:152:TRP:HA    | 1.90                     | 0.54              |
| 1:C:859:THR:HG22 | 1:C:862:MET:HE3   | 1.88                     | 0.54              |
| 1:A:102:ARG:NH1  | 1:A:243:ALA:O     | 2.41                     | 0.54              |
| 1:A:131:CYS:HA   | 1:A:166:CYS:HB3   | 1.89                     | 0.54              |
| 1:C:437:ASN:HA   | 1:C:508:TYR:CD1   | 2.43                     | 0.54              |
| 1:A:133:PHE:HB2  | 1:A:135:PHE:HD1   | 1.73                     | 0.54              |
| 1:A:328:ARG:HH21 | 1:A:533:LEU:N     | 2.05                     | 0.54              |
| 1:C:567:ARG:NH1  | 1:C:571:ASP:OD1   | 2.41                     | 0.54              |
| 1:A:566:GLY:N    | 1:A:575:ALA:O     | 2.41                     | 0.54              |
| 1:B:143:VAL:HA   | 1:B:154:GLU:HA    | 1.90                     | 0.54              |
| 1:B:433:VAL:HG22 | 1:B:512:VAL:HG13  | 1.89                     | 0.53              |
| 1:C:917:ALA:O    | 1:C:921:ASN:ND2   | 2.41                     | 0.53              |
| 1:A:622:VAL:HG23 | 1:A:637:SER:HB3   | 1.90                     | 0.53              |
| 1:B:692:LEU:HD21 | 1:C:862:MET:HB2   | 1.90                     | 0.53              |
| 1:A:52:GLN:HB2   | 1:A:274:THR:HG22  | 1.90                     | 0.53              |
| 1:A:175:PHE:CE1  | 3:A:1302:NAG:H61  | 2.43                     | 0.53              |
| 1:A:290:ASP:OD1  | 1:A:292:ALA:N     | 2.40                     | 0.53              |
| 1:A:314:GLN:OE1  | 1:A:314:GLN:N     | 2.41                     | 0.53              |
| 1:B:21:ARG:HB2   | 1:B:79:PHE:H      | 1.73                     | 0.53              |
| 1:C:124:THR:OG1  | 1:C:174:PRO:O     | 2.26                     | 0.53              |
| 1:A:815:LEU:HD23 | 1:A:1049:ALA:HB2  | 1.90                     | 0.53              |
| 1:C:491:PRO:HG2  | 1:C:492:LEU:HD12  | 1.90                     | 0.53              |
| 1:A:569:ILE:HG21 | 1:B:842:LEU:HG    | 1.89                     | 0.53              |
| 1:A:752:PHE:O    | 1:A:756:LEU:HD12  | 2.08                     | 0.53              |
| 1:A:535:LYS:NZ   | 1:A:554:GLU:OE1   | 2.34                     | 0.53              |
| 1:B:97:LYS:HE3   | 1:B:186:PHE:HA    | 1.90                     | 0.53              |
| 1:C:1002:THR:O   | 1:C:1006:ILE:HD12 | 2.08                     | 0.53              |
| 1:A:486:PHE:CE1  | 1:B:377:PHE:HB3   | 2.44                     | 0.53              |
| 1:A:818:LYS:NZ   | 1:A:931:LEU:O     | 2.33                     | 0.53              |
| 1:A:417:LYS:HA   | 1:A:421:TYR:HD2   | 1.73                     | 0.53              |
| 1:B:595:VAL:HG23 | 1:B:612:TYR:HE1   | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:118:LEU:HD21  | 1:B:135:PHE:CZ    | 2.43                     | 0.52              |
| 1:B:966:ILE:HB    | 1:B:973:ILE:HD12  | 1.92                     | 0.52              |
| 1:C:1122:VAL:HG21 | 1:C:1125:ILE:HD12 | 1.91                     | 0.52              |
| 1:A:402:ILE:HD11  | 1:A:407:VAL:HA    | 1.90                     | 0.52              |
| 1:A:403:ARG:HA    | 1:A:497:PHE:HZ    | 1.75                     | 0.52              |
| 1:B:374:PHE:HA    | 1:B:434:ILE:HD11  | 1.90                     | 0.52              |
| 1:C:337:PRO:HB2   | 1:C:340:GLU:HG2   | 1.91                     | 0.52              |
| 1:B:967:SER:HB3   | 1:B:973:ILE:HD11  | 1.91                     | 0.52              |
| 1:C:749:TYR:OH    | 1:C:987:ASP:OD1   | 2.19                     | 0.52              |
| 1:A:246:ARG:NE    | 1:A:259:THR:H     | 2.08                     | 0.52              |
| 1:A:349:SER:HA    | 1:A:451:TYR:CE2   | 2.44                     | 0.52              |
| 1:A:401:VAL:HG22  | 1:A:509:ARG:HA    | 1.91                     | 0.52              |
| 1:A:800:PRO:HG2   | 1:A:868:SER:HB2   | 1.91                     | 0.52              |
| 1:C:119:ILE:HG12  | 1:C:128:ILE:HD13  | 1.90                     | 0.52              |
| 1:C:132:GLU:O     | 1:C:132:GLU:HG2   | 2.09                     | 0.52              |
| 1:A:205:SER:HB2   | 1:A:226:LEU:HG    | 1.92                     | 0.52              |
| 1:A:309:GLU:O     | 1:A:313:TYR:OH    | 2.20                     | 0.52              |
| 1:B:143:VAL:HG11  | 1:B:179:LEU:HD11  | 1.91                     | 0.52              |
| 1:B:452:LEU:HD23  | 1:B:492:LEU:HB3   | 1.92                     | 0.52              |
| 1:C:407:VAL:O     | 1:C:410:ILE:HG22  | 2.10                     | 0.52              |
| 1:A:818:LYS:HD3   | 1:A:935:ALA:HB2   | 1.91                     | 0.52              |
| 1:B:705:ILE:HD13  | 1:B:1087:VAL:HG11 | 1.92                     | 0.52              |
| 1:B:724:MET:HE2   | 1:B:948:ASN:HD22  | 1.74                     | 0.52              |
| 1:A:68:ILE:H      | 1:A:78:ARG:HB2    | 1.74                     | 0.52              |
| 1:C:472:ILE:HA    | 1:C:491:PRO:HD3   | 1.92                     | 0.52              |
| 1:B:715:VAL:HG12  | 1:B:1058:VAL:HG22 | 1.92                     | 0.51              |
| 1:A:320:VAL:HG13  | 1:A:624:ILE:HD11  | 1.93                     | 0.51              |
| 1:A:566:GLY:HA2   | 1:B:43:PHE:HB3    | 1.92                     | 0.51              |
| 1:A:755:GLN:HA    | 1:A:758:ARG:HE    | 1.75                     | 0.51              |
| 1:A:1094:HIS:CE1  | 2:G:2:NAG:H5      | 2.46                     | 0.51              |
| 1:B:942:GLN:NE2   | 1:B:946:ASN:OD1   | 2.37                     | 0.51              |
| 1:B:1025:CYS:HB3  | 1:B:1044:SER:OG   | 2.11                     | 0.51              |
| 1:C:344:ALA:HB3   | 1:C:347:PHE:CE1   | 2.44                     | 0.51              |
| 1:B:1003:GLN:HB3  | 1:B:1007:ARG:HH12 | 1.75                     | 0.51              |
| 1:C:642:VAL:HG22  | 1:C:651:ILE:HG22  | 1.92                     | 0.51              |
| 1:B:595:VAL:HG23  | 1:B:612:TYR:CE1   | 2.46                     | 0.51              |
| 1:B:1119:CYS:HB2  | 1:B:1125:ILE:HD13 | 1.92                     | 0.51              |
| 1:C:418:ILE:HA    | 1:C:422:ASN:HD21  | 1.75                     | 0.51              |
| 1:C:879:TRP:HB3   | 1:C:1028:GLY:HA2  | 1.93                     | 0.51              |
| 1:A:197:ILE:HG12  | 1:A:202:LYS:HZ2   | 1.75                     | 0.51              |
| 1:C:104:TRP:HB2   | 1:C:119:ILE:HD12  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:83:VAL:HG22   | 1:B:237:ARG:NH2   | 2.26                     | 0.51              |
| 1:A:90:VAL:HG21   | 1:A:238:PHE:CE1   | 2.45                     | 0.51              |
| 1:A:1034:ASP:HB3  | 1:B:1023:SER:HB2  | 1.92                     | 0.51              |
| 1:B:418:ILE:HA    | 1:B:422:ASN:HB2   | 1.93                     | 0.51              |
| 1:B:779:LYS:NZ    | 1:B:884:GLY:O     | 2.37                     | 0.51              |
| 1:A:246:ARG:HG3   | 1:A:259:THR:HG22  | 1.93                     | 0.51              |
| 1:A:347:PHE:CZ    | 1:A:399:SER:HB3   | 2.45                     | 0.51              |
| 1:B:1075:CYS:HA   | 1:B:1081:HIS:HD2  | 1.76                     | 0.51              |
| 1:A:244:LEU:HD13  | 1:A:246:ARG:HH22  | 1.76                     | 0.51              |
| 1:A:455:LEU:HB3   | 1:A:493:GLN:HE22  | 1.75                     | 0.51              |
| 1:C:271:GLN:OE1   | 1:C:273:ARG:NH2   | 2.44                     | 0.51              |
| 1:B:107:GLY:O     | 1:B:237:ARG:HB2   | 2.11                     | 0.50              |
| 1:B:589:PRO:HB3   | 1:C:848:PHE:CD1   | 2.47                     | 0.50              |
| 1:B:22:THR:N      | 1:B:77:LYS:O      | 2.32                     | 0.50              |
| 1:B:589:PRO:HB3   | 1:C:848:PHE:CG    | 2.45                     | 0.50              |
| 1:C:280:ASN:OD1   | 1:C:284:THR:N     | 2.44                     | 0.50              |
| 1:B:381:GLY:HA3   | 1:B:430:THR:HA    | 1.94                     | 0.50              |
| 1:B:959:LEU:O     | 1:B:968:SER:OG    | 2.29                     | 0.50              |
| 1:C:85:PRO:HA     | 1:C:237:ARG:HH21  | 1.77                     | 0.50              |
| 1:C:68:ILE:HD13   | 1:C:262:ALA:HA    | 1.93                     | 0.50              |
| 1:C:1097:VAL:HG11 | 1:C:1112:ASN:HD21 | 1.77                     | 0.50              |
| 1:A:196:ASN:HB3   | 1:A:201:PHE:HD1   | 1.76                     | 0.50              |
| 1:C:719:ILE:HG23  | 1:C:1054:VAL:HG12 | 1.94                     | 0.50              |
| 1:A:133:PHE:HB3   | 1:A:161:SER:H     | 1.76                     | 0.50              |
| 1:A:141:LEU:HB3   | 1:A:243:ALA:HB2   | 1.93                     | 0.50              |
| 1:B:290:ASP:OD1   | 1:B:291:CYS:N     | 2.45                     | 0.50              |
| 1:A:410:ILE:HG13  | 1:A:410:ILE:O     | 2.12                     | 0.50              |
| 1:A:1003:GLN:HB3  | 1:A:1007:ARG:HH12 | 1.77                     | 0.50              |
| 1:A:1134:LEU:O    | 1:A:1138:LEU:N    | 2.39                     | 0.50              |
| 1:B:105:ILE:HD11  | 1:B:241:LEU:HD21  | 1.94                     | 0.50              |
| 1:A:578:ASP:HB3   | 1:A:581:THR:O     | 2.12                     | 0.49              |
| 1:A:895:MET:HE2   | 1:A:895:MET:HA    | 1.93                     | 0.49              |
| 1:B:271:GLN:OE1   | 1:B:272:PRO:HD2   | 2.12                     | 0.49              |
| 1:B:347:PHE:HB2   | 1:B:509:ARG:NH2   | 2.27                     | 0.49              |
| 1:B:386:LYS:O     | 1:B:390:LEU:N     | 2.28                     | 0.49              |
| 1:B:706:ALA:HA    | 1:B:1067:ASN:HA   | 1.94                     | 0.49              |
| 1:B:923:ALA:HA    | 1:B:926:LYS:HG2   | 1.94                     | 0.49              |
| 1:C:795:PHE:CE1   | 1:C:920:PHE:HE2   | 2.25                     | 0.49              |
| 1:A:596:SER:HB2   | 1:A:611:LEU:HB3   | 1.94                     | 0.49              |
| 1:B:895:MET:HB3   | 1:B:909:LEU:HD11  | 1.93                     | 0.49              |
| 2:K:1:NAG:O3      | 2:K:2:NAG:N2      | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1032:ARG:HB2  | 1:B:1024:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:719:ILE:HG13  | 1:B:1054:VAL:HG23 | 1.95                     | 0.49              |
| 1:B:396:TYR:N     | 1:B:514:SER:O     | 2.31                     | 0.49              |
| 1:C:726:LYS:HE3   | 1:C:764:ALA:HB1   | 1.93                     | 0.49              |
| 1:A:502:GLY:O     | 1:A:506:GLN:HG3   | 2.12                     | 0.49              |
| 1:A:741:GLU:O     | 1:A:745:LEU:HD23  | 2.12                     | 0.49              |
| 1:A:1006:ILE:HG21 | 1:B:1005:LEU:HG   | 1.93                     | 0.49              |
| 1:A:392:PHE:CD1   | 1:A:517:LEU:HD21  | 2.47                     | 0.49              |
| 1:B:350:VAL:HG22  | 1:B:422:ASN:HB3   | 1.93                     | 0.49              |
| 1:B:879:TRP:HB2   | 1:B:1027:LEU:O    | 2.13                     | 0.49              |
| 1:C:541:PHE:CZ    | 1:C:587:ILE:HD13  | 2.48                     | 0.49              |
| 1:A:398:ASP:HB2   | 1:A:512:VAL:HG23  | 1.95                     | 0.49              |
| 1:A:486:PHE:HE1   | 1:B:377:PHE:HB3   | 1.76                     | 0.49              |
| 1:A:969:VAL:HG12  | 1:A:972:ASP:H     | 1.78                     | 0.49              |
| 1:B:103:GLY:HA3   | 1:B:241:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:1002:THR:O    | 1:A:1006:ILE:HG12 | 2.13                     | 0.49              |
| 1:A:376:THR:OG1   | 1:A:435:ALA:HB3   | 2.13                     | 0.48              |
| 1:A:501:ASN:OD1   | 1:A:502:GLY:N     | 2.38                     | 0.48              |
| 1:A:901:GLY:HA3   | 1:A:1029:GLN:HE22 | 1.77                     | 0.48              |
| 1:B:376:THR:OG1   | 1:B:435:ALA:O     | 2.23                     | 0.48              |
| 1:B:394:ASN:ND2   | 1:B:516:GLU:OE1   | 2.46                     | 0.48              |
| 1:B:448:ASN:OD1   | 1:B:450:ASN:ND2   | 2.37                     | 0.48              |
| 1:B:523:THR:HG23  | 1:B:524:VAL:HG23  | 1.95                     | 0.48              |
| 1:C:69:HIS:ND1    | 1:C:261:GLY:O     | 2.44                     | 0.48              |
| 1:C:403:ARG:O     | 1:C:407:VAL:HG23  | 2.13                     | 0.48              |
| 1:C:719:ILE:C     | 1:C:720:LEU:HD12  | 2.38                     | 0.48              |
| 1:A:462:LYS:HE2   | 1:A:463:PRO:HD2   | 1.95                     | 0.48              |
| 1:A:519:HIS:O     | 1:B:41:LYS:HD2    | 2.12                     | 0.48              |
| 1:B:204:TYR:HA    | 1:B:225:PRO:HA    | 1.95                     | 0.48              |
| 1:C:127:VAL:HA    | 1:C:171:VAL:HG22  | 1.94                     | 0.48              |
| 1:C:979:PRO:N     | 1:C:980:PRO:HD2   | 2.28                     | 0.48              |
| 1:A:857:LEU:HA    | 1:C:667:GLY:HA2   | 1.95                     | 0.48              |
| 1:A:1076:HIS:CD2  | 1:A:1130:VAL:HB   | 2.49                     | 0.48              |
| 1:C:809:SER:N     | 1:C:812:GLU:OE1   | 2.46                     | 0.48              |
| 1:B:203:ILE:HB    | 1:B:227:VAL:HG21  | 1.95                     | 0.48              |
| 1:C:309:GLU:HG2   | 1:C:310:LYS:H     | 1.78                     | 0.48              |
| 1:C:404:GLY:HA2   | 1:C:508:TYR:CE2   | 2.48                     | 0.48              |
| 1:C:1025:CYS:HB2  | 1:C:1041:HIS:CE1  | 2.48                     | 0.48              |
| 1:A:100:ILE:HG22  | 1:A:242:LEU:HD22  | 1.96                     | 0.48              |
| 1:C:379:CYS:HB3   | 1:C:382:VAL:O     | 2.14                     | 0.48              |
| 1:C:617:CYS:N     | 1:C:649:CYS:SG    | 2.87                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:328:ARG:HD3  | 1:A:578:ASP:OD1   | 2.14                     | 0.48              |
| 1:A:355:ARG:HH21 | 1:A:396:TYR:HD1   | 1.59                     | 0.48              |
| 1:C:812:GLU:HA   | 1:C:815:LEU:HB2   | 1.96                     | 0.48              |
| 3:A:1303:NAG:O5  | 1:C:558:LYS:NZ    | 2.46                     | 0.48              |
| 1:C:329:PHE:HE2  | 1:C:528:LYS:HB2   | 1.79                     | 0.48              |
| 1:C:347:PHE:CE2  | 1:C:399:SER:HB2   | 2.49                     | 0.48              |
| 1:C:53:ASP:HB3   | 1:C:55:PHE:CE1    | 2.49                     | 0.48              |
| 1:A:103:GLY:HA3  | 1:A:119:ILE:O     | 2.14                     | 0.47              |
| 1:B:1090:SER:OG  | 1:B:1092:GLY:O    | 2.32                     | 0.47              |
| 1:C:106:PHE:HB3  | 1:C:235:ILE:HD13  | 1.96                     | 0.47              |
| 1:C:543:PHE:CE2  | 1:C:576:VAL:HG11  | 2.49                     | 0.47              |
| 1:A:115:GLN:HB3  | 1:A:130:VAL:HG22  | 1.97                     | 0.47              |
| 1:A:922:SER:O    | 1:A:926:LYS:HG2   | 2.14                     | 0.47              |
| 1:A:468:ILE:HG13 | 1:A:468:ILE:O     | 2.14                     | 0.47              |
| 1:A:759:ALA:O    | 1:A:763:ILE:HG12  | 2.14                     | 0.47              |
| 1:C:290:ASP:OD2  | 1:C:293:LEU:HG    | 2.15                     | 0.47              |
| 1:A:290:ASP:OD1  | 1:A:291:CYS:N     | 2.47                     | 0.47              |
| 1:B:422:ASN:HD21 | 1:B:453:TYR:HB2   | 1.78                     | 0.47              |
| 1:B:566:GLY:HA2  | 1:C:43:PHE:H      | 1.77                     | 0.47              |
| 1:C:128:ILE:HG12 | 1:C:229:LEU:HD13  | 1.96                     | 0.47              |
| 1:C:308:VAL:O    | 1:C:602:THR:HG23  | 2.14                     | 0.47              |
| 1:A:662:CYS:HB2  | 1:A:671:CYS:HB3   | 1.61                     | 0.47              |
| 1:B:272:PRO:O    | 1:B:273:ARG:NH1   | 2.47                     | 0.47              |
| 1:C:358:ILE:HB   | 1:C:395:VAL:HB    | 1.96                     | 0.47              |
| 1:A:859:THR:HG22 | 1:A:862:MET:HE1   | 1.96                     | 0.47              |
| 1:B:559:PHE:O    | 1:B:577:ARG:NH2   | 2.48                     | 0.47              |
| 1:C:146:HIS:ND1  | 1:C:153:MET:HB2   | 2.29                     | 0.47              |
| 1:A:49:HIS:O     | 1:A:277:LEU:HD23  | 2.14                     | 0.47              |
| 1:B:338:PHE:HE2  | 1:B:364:ASP:H     | 1.63                     | 0.47              |
| 1:B:434:ILE:O    | 1:B:510:VAL:HA    | 2.15                     | 0.47              |
| 1:B:1073:ALA:O   | 1:B:1125:ILE:HG13 | 2.15                     | 0.47              |
| 1:C:56:LEU:HB2   | 1:C:270:LEU:HD23  | 1.97                     | 0.47              |
| 1:C:562:PHE:HA   | 1:C:577:ARG:HH22  | 1.80                     | 0.47              |
| 1:B:258:TRP:HZ3  | 1:B:260:ALA:HB2   | 1.79                     | 0.47              |
| 1:B:108:THR:HA   | 1:B:236:THR:HG22  | 1.97                     | 0.47              |
| 1:B:665:PRO:HB3  | 1:C:857:LEU:HD13  | 1.97                     | 0.47              |
| 1:B:899:PHE:HB3  | 1:B:904:VAL:HG13  | 1.96                     | 0.47              |
| 1:C:101:ILE:HA   | 1:C:242:LEU:HG    | 1.96                     | 0.47              |
| 1:C:109:THR:HG22 | 1:C:111:ASP:HB2   | 1.97                     | 0.47              |
| 1:C:133:PHE:HA   | 1:C:162:SER:HB3   | 1.95                     | 0.47              |
| 1:A:253:ASP:O    | 1:A:257:GLY:N     | 2.35                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:439:ASN:ND2  | 1:A:443:SER:OG   | 2.44                     | 0.47              |
| 1:A:752:PHE:O    | 1:A:755:GLN:HB2  | 2.15                     | 0.47              |
| 1:B:818:LYS:HE2  | 1:B:818:LYS:HB3  | 1.77                     | 0.47              |
| 1:C:146:HIS:HE1  | 1:C:155:SER:HB2  | 1.79                     | 0.47              |
| 1:C:611:LEU:HD22 | 1:C:666:ILE:HG23 | 1.95                     | 0.47              |
| 1:A:282:ASN:HB3  | 1:C:558:LYS:HD2  | 1.97                     | 0.46              |
| 1:A:891:PHE:CZ   | 1:A:1043:MET:HE1 | 2.48                     | 0.46              |
| 1:B:145:TYR:HB2  | 1:B:152:TRP:CH2  | 2.50                     | 0.46              |
| 1:C:1118:ASN:OD1 | 1:C:1120:ASP:N   | 2.48                     | 0.46              |
| 1:B:358:ILE:HB   | 1:B:395:VAL:HB   | 1.97                     | 0.46              |
| 1:B:659:SER:OG   | 1:B:691:SER:HB3  | 2.15                     | 0.46              |
| 1:A:247:SER:OG   | 1:A:248:TYR:N    | 2.48                     | 0.46              |
| 1:A:334:ASN:O    | 1:A:362:VAL:N    | 2.43                     | 0.46              |
| 1:A:360:ASN:H    | 1:A:523:THR:HB   | 1.79                     | 0.46              |
| 1:B:85:PRO:HA    | 1:B:237:ARG:HE   | 1.81                     | 0.46              |
| 1:B:702:ASN:HD22 | 3:B:1308:NAG:C7  | 2.27                     | 0.46              |
| 1:B:729:VAL:HG22 | 1:B:851:LEU:HB2  | 1.97                     | 0.46              |
| 1:B:1089:VAL:O   | 1:B:1096:PHE:N   | 2.41                     | 0.46              |
| 1:A:669:GLY:HA2  | 1:B:862:MET:HE1  | 1.96                     | 0.46              |
| 1:A:752:PHE:HE1  | 1:C:963:PHE:HE2  | 1.64                     | 0.46              |
| 1:B:280:ASN:OD1  | 1:B:284:THR:N    | 2.47                     | 0.46              |
| 1:B:709:THR:HG21 | 1:B:1066:LYS:HD3 | 1.97                     | 0.46              |
| 1:A:871:LEU:O    | 1:A:875:ILE:HG12 | 2.16                     | 0.46              |
| 1:A:958:GLN:HE22 | 1:B:750:GLY:HA3  | 1.80                     | 0.46              |
| 1:A:979:PRO:N    | 1:A:980:PRO:HD2  | 2.30                     | 0.46              |
| 1:B:424:LYS:HD3  | 1:B:463:PRO:HD3  | 1.98                     | 0.46              |
| 1:C:331:ASN:HB2  | 1:C:580:GLN:OE1  | 2.16                     | 0.46              |
| 1:C:806:SER:HB3  | 1:C:808:ARG:HG3  | 1.96                     | 0.46              |
| 1:A:115:GLN:NE2  | 1:A:165:ASN:O    | 2.45                     | 0.46              |
| 1:A:809:SER:N    | 1:A:812:GLU:OE2  | 2.48                     | 0.46              |
| 1:B:899:PHE:CE2  | 1:B:909:LEU:HD12 | 2.50                     | 0.46              |
| 1:B:979:PRO:N    | 1:B:980:PRO:HD2  | 2.31                     | 0.46              |
| 1:A:177:MET:HE2  | 1:A:177:MET:HB3  | 1.83                     | 0.46              |
| 1:A:392:PHE:HB2  | 1:A:524:VAL:HG13 | 1.98                     | 0.46              |
| 1:A:755:GLN:HG2  | 1:A:758:ARG:NH2  | 2.31                     | 0.46              |
| 1:B:357:ARG:NH1  | 1:B:358:ILE:O    | 2.49                     | 0.46              |
| 1:B:418:ILE:HD13 | 1:B:422:ASN:HD22 | 1.80                     | 0.46              |
| 1:C:192:PHE:HA   | 1:C:204:TYR:O    | 2.15                     | 0.46              |
| 1:A:64:TRP:HE1   | 1:A:264:ALA:HB1  | 1.81                     | 0.46              |
| 1:A:353:TRP:CE2  | 1:A:466:ARG:HB3  | 2.51                     | 0.46              |
| 1:A:401:VAL:HB   | 1:A:451:TYR:CZ   | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:79:PHE:HB2    | 1:B:258:TRP:CH2   | 2.51                     | 0.46              |
| 1:B:906:GLN:OE1   | 1:B:906:GLN:N     | 2.49                     | 0.46              |
| 1:C:328:ARG:NH1   | 1:C:530:SER:OG    | 2.48                     | 0.46              |
| 1:A:355:ARG:NH1   | 1:A:356:LYS:H     | 2.14                     | 0.46              |
| 1:A:677:GLN:HB3   | 1:A:680:VAL:O     | 2.16                     | 0.46              |
| 1:B:444:LYS:O     | 1:B:499:PRO:HD3   | 2.16                     | 0.46              |
| 1:B:274:THR:O     | 1:B:275:PHE:HD1   | 1.99                     | 0.45              |
| 1:B:792:GLY:O     | 1:B:921:ASN:ND2   | 2.50                     | 0.45              |
| 1:C:91:TYR:HA     | 1:C:193:VAL:HG22  | 1.97                     | 0.45              |
| 1:C:139:PRO:HD2   | 1:C:140:PHE:CD1   | 2.51                     | 0.45              |
| 1:C:206:LYS:HB2   | 1:C:223:LEU:HD12  | 1.96                     | 0.45              |
| 1:C:554:GLU:N     | 1:C:554:GLU:OE1   | 2.49                     | 0.45              |
| 1:A:68:ILE:HA     | 1:A:261:GLY:O     | 2.16                     | 0.45              |
| 1:B:307:THR:HA    | 1:B:602:THR:HG21  | 1.98                     | 0.45              |
| 1:B:426:PRO:HG3   | 1:B:464:PHE:CZ    | 2.51                     | 0.45              |
| 1:C:92:PHE:HE2    | 1:C:94:SER:HB3    | 1.80                     | 0.45              |
| 1:B:484:GLU:OE1   | 1:B:484:GLU:N     | 2.50                     | 0.45              |
| 1:B:705:ILE:HG13  | 1:C:889:ILE:HD13  | 1.97                     | 0.45              |
| 1:B:1026:VAL:HG22 | 1:B:1044:SER:O    | 2.16                     | 0.45              |
| 1:C:365:TYR:CD2   | 1:C:368:LEU:HD12  | 2.51                     | 0.45              |
| 1:C:569:ILE:H     | 1:C:569:ILE:HD12  | 1.82                     | 0.45              |
| 1:C:763:ILE:O     | 1:C:767:GLN:HG2   | 2.17                     | 0.45              |
| 1:A:133:PHE:HA    | 1:A:162:SER:HB3   | 1.97                     | 0.45              |
| 1:A:141:LEU:HD23  | 1:A:243:ALA:HB2   | 1.98                     | 0.45              |
| 1:A:326:ILE:HD11  | 1:A:534:VAL:HG12  | 1.97                     | 0.45              |
| 1:A:1076:HIS:CE1  | 1:A:1130:VAL:H    | 2.34                     | 0.45              |
| 1:B:78:ARG:NE     | 1:B:80:ASP:OD2    | 2.46                     | 0.45              |
| 1:B:1094:HIS:CE1  | 2:K:2:NAG:H3      | 2.52                     | 0.45              |
| 1:C:139:PRO:C     | 1:C:159:VAL:HG12  | 2.41                     | 0.45              |
| 1:B:382:VAL:HG11  | 1:B:515:PHE:HZ    | 1.80                     | 0.45              |
| 1:C:1022:MET:SD   | 1:C:1026:VAL:HG11 | 2.57                     | 0.45              |
| 1:A:722:VAL:HG12  | 1:A:1052:GLY:HA2  | 1.99                     | 0.45              |
| 1:A:866:TYR:CE1   | 1:C:692:LEU:HB3   | 2.52                     | 0.45              |
| 1:A:206:LYS:HG3   | 1:A:207:HIS:N     | 2.31                     | 0.45              |
| 1:B:206:LYS:HE2   | 1:B:221:SER:HB2   | 1.99                     | 0.45              |
| 1:B:395:VAL:HA    | 1:B:515:PHE:HB3   | 1.98                     | 0.45              |
| 1:B:723:SER:O     | 1:B:1051:HIS:HB3  | 2.17                     | 0.45              |
| 1:C:490:PHE:CG    | 1:C:491:PRO:HD2   | 2.51                     | 0.45              |
| 1:A:246:ARG:HH21  | 1:A:260:ALA:N     | 2.11                     | 0.45              |
| 1:A:355:ARG:NH1   | 1:A:397:ALA:H     | 2.14                     | 0.45              |
| 1:B:100:ILE:HG13  | 1:B:243:ALA:H     | 1.82                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:101:ILE:O     | 1:B:101:ILE:HG13 | 2.17                     | 0.45              |
| 1:C:426:PRO:HG3   | 1:C:463:PRO:HB3  | 1.98                     | 0.45              |
| 1:C:594:GLY:O     | 1:C:613:GLN:HG2  | 2.17                     | 0.45              |
| 1:C:723:SER:O     | 1:C:1051:HIS:HB3 | 2.17                     | 0.45              |
| 1:A:355:ARG:NH2   | 1:A:396:TYR:HA   | 2.31                     | 0.45              |
| 1:B:595:VAL:HG13  | 1:B:595:VAL:O    | 2.16                     | 0.45              |
| 1:B:950:GLN:HE22  | 1:C:758:ARG:NE   | 2.15                     | 0.45              |
| 1:C:417:LYS:H     | 1:C:417:LYS:HD2  | 1.81                     | 0.45              |
| 1:C:924:ILE:HA    | 1:C:927:ILE:HG22 | 1.99                     | 0.45              |
| 1:C:1020:THR:HG22 | 1:C:1024:GLU:OE1 | 2.17                     | 0.45              |
| 1:B:130:VAL:HG21  | 1:B:231:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:58:PHE:CZ     | 1:A:275:PHE:HE1  | 2.35                     | 0.44              |
| 1:A:130:VAL:HG13  | 1:A:166:CYS:HB2  | 1.99                     | 0.44              |
| 1:A:814:LEU:HD11  | 1:A:928:GLN:NE2  | 2.32                     | 0.44              |
| 1:C:107:GLY:H     | 1:C:235:ILE:HG23 | 1.82                     | 0.44              |
| 1:A:519:HIS:CD2   | 1:B:42:VAL:HG23  | 2.53                     | 0.44              |
| 1:C:202:LYS:HE3   | 1:C:202:LYS:HB3  | 1.84                     | 0.44              |
| 1:C:1089:VAL:O    | 1:C:1095:TRP:HA  | 2.16                     | 0.44              |
| 1:B:569:ILE:HG12  | 1:C:47:VAL:HG11  | 1.99                     | 0.44              |
| 1:B:1078:GLY:O    | 1:B:1119:CYS:N   | 2.48                     | 0.44              |
| 1:C:396:TYR:HB2   | 1:C:514:SER:HB2  | 1.98                     | 0.44              |
| 1:C:662:CYS:SG    | 1:C:690:MET:HG3  | 2.57                     | 0.44              |
| 1:A:724:MET:CG    | 1:A:767:GLN:HE22 | 2.30                     | 0.44              |
| 1:A:958:GLN:OE1   | 1:B:750:GLY:HA3  | 2.18                     | 0.44              |
| 1:B:31:SER:HA     | 1:B:216:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:334:ASN:O     | 1:C:362:VAL:N    | 2.50                     | 0.44              |
| 1:A:55:PHE:HA     | 1:A:270:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:862:MET:SD    | 1:A:862:MET:N    | 2.91                     | 0.44              |
| 1:B:449:TYR:CZ    | 1:B:496:GLY:HA2  | 2.53                     | 0.44              |
| 1:B:1108:ILE:HD12 | 1:B:1108:ILE:H   | 1.83                     | 0.44              |
| 1:C:294:ASP:HB3   | 1:C:295:PRO:HD2  | 2.00                     | 0.44              |
| 1:C:972:ASP:O     | 1:C:975:SER:OG   | 2.30                     | 0.44              |
| 1:C:1135:GLN:N    | 1:C:1136:PRO:HD2 | 2.33                     | 0.44              |
| 1:A:970:LEU:O     | 1:A:974:LEU:HG   | 2.18                     | 0.44              |
| 1:B:102:ARG:HB3   | 1:B:121:ASN:O    | 2.17                     | 0.44              |
| 1:C:65:PHE:HE2    | 1:C:84:LEU:HD21  | 1.81                     | 0.44              |
| 1:C:146:HIS:CE1   | 1:C:155:SER:HB2  | 2.53                     | 0.44              |
| 1:C:202:LYS:HG2   | 1:C:228:ASP:HB3  | 1.99                     | 0.44              |
| 1:C:560:LEU:N     | 1:C:563:GLN:HE21 | 2.15                     | 0.44              |
| 1:C:675:GLN:OE1   | 1:C:676:THR:N    | 2.51                     | 0.44              |
| 1:A:350:VAL:HG21  | 1:A:402:ILE:HG22 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:733:MET:HE2  | 1:C:592:PHE:CG    | 2.52                     | 0.44              |
| 1:B:37:TYR:OH    | 1:B:53:ASP:OD2    | 2.16                     | 0.44              |
| 1:C:439:ASN:HA   | 1:C:507:PRO:HG2   | 2.00                     | 0.44              |
| 1:B:875:ILE:HG13 | 1:B:876:THR:N     | 2.32                     | 0.44              |
| 1:C:395:VAL:HG23 | 1:C:524:VAL:HG21  | 1.99                     | 0.44              |
| 1:A:394:ASN:HB2  | 1:A:516:GLU:OE1   | 2.18                     | 0.43              |
| 1:A:753:CYS:HA   | 1:A:756:LEU:HD13  | 1.99                     | 0.43              |
| 1:B:336:CYS:O    | 1:B:338:PHE:N     | 2.51                     | 0.43              |
| 1:A:180:GLU:HB3  | 1:A:182:LYS:HE3   | 2.00                     | 0.43              |
| 1:A:304:LYS:HE2  | 1:A:304:LYS:HB3   | 1.71                     | 0.43              |
| 1:A:392:PHE:HD1  | 1:A:517:LEU:HD21  | 1.82                     | 0.43              |
| 1:B:146:HIS:NE2  | 1:B:153:MET:HB3   | 2.33                     | 0.43              |
| 1:B:560:LEU:HD23 | 1:B:560:LEU:HA    | 1.83                     | 0.43              |
| 1:C:36:VAL:HG21  | 1:C:220:PHE:CE1   | 2.54                     | 0.43              |
| 1:C:344:ALA:HB3  | 1:C:347:PHE:HE1   | 1.83                     | 0.43              |
| 1:C:705:ILE:HG23 | 1:C:1068:PHE:HB2  | 1.99                     | 0.43              |
| 1:C:846:GLN:HG2  | 1:C:952:LEU:HD22  | 2.00                     | 0.43              |
| 1:B:403:ARG:HD3  | 1:B:505:TYR:HA    | 2.00                     | 0.43              |
| 1:B:858:LEU:HA   | 1:B:862:MET:HE2   | 1.99                     | 0.43              |
| 1:B:1082:PHE:HB2 | 1:B:1114:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:294:ASP:OD1  | 1:A:297:SER:OG    | 2.29                     | 0.43              |
| 1:B:118:LEU:HD21 | 1:B:135:PHE:HZ    | 1.83                     | 0.43              |
| 1:B:615:VAL:C    | 1:B:617:CYS:H     | 2.25                     | 0.43              |
| 1:C:329:PHE:HE1  | 1:C:544:ASN:H     | 1.66                     | 0.43              |
| 1:C:409:GLN:NE2  | 1:C:415:THR:O     | 2.52                     | 0.43              |
| 1:A:351:TYR:CD1  | 1:A:452:LEU:HB2   | 2.54                     | 0.43              |
| 1:A:442:ASP:C    | 1:A:448:ASN:HD22  | 2.26                     | 0.43              |
| 1:A:958:GLN:HG2  | 1:A:996:SER:OG    | 2.19                     | 0.43              |
| 1:B:551:VAL:CG1  | 1:B:588:THR:HB    | 2.49                     | 0.43              |
| 1:A:287:ASP:OD1  | 1:A:288:ALA:N     | 2.51                     | 0.43              |
| 1:A:355:ARG:CZ   | 1:A:396:TYR:HA    | 2.47                     | 0.43              |
| 1:A:382:VAL:HA   | 1:B:977:LEU:HD23  | 2.01                     | 0.43              |
| 1:A:958:GLN:O    | 1:A:958:GLN:NE2   | 2.52                     | 0.43              |
| 1:A:966:ILE:HB   | 1:A:973:ILE:HD13  | 2.00                     | 0.43              |
| 1:B:250:THR:O    | 1:B:250:THR:OG1   | 2.31                     | 0.43              |
| 1:B:425:LEU:HD11 | 1:B:429:PHE:CE1   | 2.54                     | 0.43              |
| 1:B:1082:PHE:C   | 1:B:1113:THR:HG23 | 2.44                     | 0.43              |
| 1:C:66:HIS:NE2   | 1:C:68:ILE:HG13   | 2.33                     | 0.43              |
| 1:C:448:ASN:ND2  | 1:C:497:PHE:O     | 2.47                     | 0.43              |
| 1:A:666:ILE:HD12 | 1:A:670:ILE:HG22  | 2.00                     | 0.43              |
| 1:B:21:ARG:HE    | 1:B:79:PHE:HB3    | 1.84                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:117:LEU:HD11 | 1:A:233:ILE:HG21  | 2.00                     | 0.43              |
| 1:A:859:THR:H    | 1:A:862:MET:HE1   | 1.84                     | 0.43              |
| 1:A:1086:GLY:CA  | 1:A:1098:THR:O    | 2.66                     | 0.43              |
| 1:B:894:GLN:HE22 | 1:B:898:ARG:NH2   | 2.15                     | 0.43              |
| 1:C:129:LYS:HD3  | 1:C:131:CYS:HB2   | 2.00                     | 0.43              |
| 1:C:388:ASN:HB2  | 1:C:527:PRO:HD2   | 2.00                     | 0.43              |
| 1:A:69:HIS:HB3   | 1:A:261:GLY:H     | 1.84                     | 0.43              |
| 1:A:196:ASN:HB3  | 1:A:201:PHE:CD1   | 2.54                     | 0.43              |
| 1:A:355:ARG:NH1  | 1:A:356:LYS:C     | 2.77                     | 0.43              |
| 1:A:865:GLN:NE2  | 1:C:692:LEU:HD12  | 2.34                     | 0.43              |
| 1:C:133:PHE:CD2  | 1:C:160:TYR:HB2   | 2.53                     | 0.43              |
| 1:C:202:LYS:NZ   | 1:C:228:ASP:HB3   | 2.34                     | 0.43              |
| 1:C:206:LYS:HD3  | 1:C:224:GLU:OE1   | 2.19                     | 0.43              |
| 1:C:546:LEU:HD13 | 1:C:565:PHE:CE2   | 2.53                     | 0.43              |
| 1:A:83:VAL:HG23  | 1:A:239:GLN:HE21  | 1.83                     | 0.42              |
| 1:A:197:ILE:HG12 | 1:A:202:LYS:NZ    | 2.33                     | 0.42              |
| 1:A:565:PHE:HB2  | 1:B:42:VAL:HG22   | 2.01                     | 0.42              |
| 1:B:79:PHE:CZ    | 1:B:242:LEU:HB2   | 2.54                     | 0.42              |
| 1:B:843:ILE:HD12 | 1:B:843:ILE:H     | 1.84                     | 0.42              |
| 1:C:452:LEU:HD23 | 1:C:493:GLN:C     | 2.44                     | 0.42              |
| 1:A:78:ARG:NE    | 1:A:78:ARG:HA     | 2.34                     | 0.42              |
| 1:A:386:LYS:HD2  | 1:A:386:LYS:HA    | 1.84                     | 0.42              |
| 1:A:756:LEU:HD22 | 1:A:997:LEU:HG    | 2.01                     | 0.42              |
| 1:B:317:ASN:OD1  | 1:B:318:PHE:N     | 2.52                     | 0.42              |
| 1:B:784:THR:HG21 | 1:B:799:LEU:HD22  | 2.00                     | 0.42              |
| 1:C:97:LYS:CG    | 1:C:182:LYS:HB2   | 2.49                     | 0.42              |
| 1:C:912:ASN:O    | 1:C:916:ILE:HG12  | 2.19                     | 0.42              |
| 1:A:437:ASN:ND2  | 1:A:439:ASN:OD1   | 2.40                     | 0.42              |
| 1:A:897:TYR:CZ   | 1:C:1100:ARG:HG2  | 2.54                     | 0.42              |
| 1:B:204:TYR:HB3  | 1:B:223:LEU:HB3   | 2.01                     | 0.42              |
| 1:B:353:TRP:CD1  | 1:B:353:TRP:H     | 2.37                     | 0.42              |
| 1:B:986:ILE:O    | 1:B:990:ILE:HG12  | 2.19                     | 0.42              |
| 1:B:1002:THR:O   | 1:B:1006:ILE:HG12 | 2.20                     | 0.42              |
| 1:C:85:PRO:HD2   | 1:C:269:TYR:OH    | 2.20                     | 0.42              |
| 1:C:310:LYS:HB2  | 1:C:664:ILE:HD11  | 2.01                     | 0.42              |
| 1:A:280:ASN:OD1  | 1:A:284:THR:N     | 2.48                     | 0.42              |
| 1:A:329:PHE:CE2  | 1:A:528:LYS:HB2   | 2.54                     | 0.42              |
| 1:A:377:PHE:HE1  | 1:A:384:PRO:HB3   | 1.84                     | 0.42              |
| 1:B:418:ILE:O    | 1:B:423:TYR:N     | 2.44                     | 0.42              |
| 1:B:600:PRO:HB3  | 1:B:674:TYR:HB3   | 2.02                     | 0.42              |
| 1:B:894:GLN:HE22 | 1:B:898:ARG:NE    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:438:SER:OG    | 1:C:438:SER:O     | 2.32                     | 0.42              |
| 1:C:659:SER:OG    | 1:C:691:SER:HB3   | 2.19                     | 0.42              |
| 1:C:899:PHE:HB3   | 1:C:904:VAL:HG13  | 2.01                     | 0.42              |
| 1:C:641:ASN:ND2   | 1:C:654:GLU:OE2   | 2.53                     | 0.42              |
| 1:C:1022:MET:HE1  | 1:C:1046:PRO:HB3  | 2.01                     | 0.42              |
| 1:A:34:ARG:HD3    | 1:A:34:ARG:HA     | 1.92                     | 0.42              |
| 1:A:412:PRO:HB3   | 1:A:427:ASP:HA    | 2.01                     | 0.42              |
| 1:A:700:TYR:HE1   | 1:B:890:PRO:HA    | 1.84                     | 0.42              |
| 1:A:870:LEU:HD23  | 1:A:870:LEU:HA    | 1.86                     | 0.42              |
| 1:A:880:THR:HG21  | 1:A:887:LEU:HD12  | 2.00                     | 0.42              |
| 1:B:1070:THR:OG1  | 1:B:1088:PHE:O    | 2.38                     | 0.42              |
| 1:A:210:ILE:HG21  | 1:A:217:PRO:HG3   | 2.02                     | 0.42              |
| 1:B:396:TYR:HB2   | 1:B:514:SER:OG    | 2.19                     | 0.42              |
| 1:B:760:LEU:HD23  | 1:B:760:LEU:HA    | 1.83                     | 0.42              |
| 1:B:877:SER:HA    | 1:B:887:LEU:O     | 2.19                     | 0.42              |
| 1:C:598:ILE:HB    | 1:C:609:ALA:HB3   | 2.01                     | 0.42              |
| 1:B:191:GLU:HG2   | 1:B:223:LEU:HD11  | 2.02                     | 0.42              |
| 1:C:453:TYR:CZ    | 1:C:493:GLN:HB3   | 2.55                     | 0.42              |
| 1:A:1003:GLN:HB3  | 1:A:1007:ARG:NH1  | 2.34                     | 0.42              |
| 1:B:33:THR:OG1    | 1:B:219:GLY:O     | 2.24                     | 0.42              |
| 1:B:102:ARG:HH21  | 1:B:141:LEU:HB3   | 1.85                     | 0.42              |
| 1:B:425:LEU:HD11  | 1:B:429:PHE:CD1   | 2.55                     | 0.42              |
| 1:C:159:VAL:HG23  | 1:C:160:TYR:CD2   | 2.55                     | 0.42              |
| 1:C:538:CYS:HB3   | 1:C:551:VAL:HG23  | 2.01                     | 0.42              |
| 1:A:756:LEU:HD11  | 1:A:998:GLN:OE1   | 2.20                     | 0.42              |
| 1:B:245:HIS:HB2   | 1:B:259:THR:HG23  | 2.02                     | 0.42              |
| 1:B:421:TYR:HD1   | 1:B:457:ARG:HD3   | 1.85                     | 0.42              |
| 1:B:1043:MET:HE3  | 1:B:1058:VAL:HG21 | 2.02                     | 0.42              |
| 1:C:102:ARG:HD2   | 1:C:121:ASN:O     | 2.19                     | 0.42              |
| 1:C:339:GLY:O     | 1:C:343:ASN:HB2   | 2.20                     | 0.42              |
| 1:C:388:ASN:OD1   | 1:C:388:ASN:N     | 2.52                     | 0.42              |
| 1:C:759:ALA:O     | 1:C:763:ILE:HG12  | 2.20                     | 0.42              |
| 1:C:1098:THR:HG23 | 1:C:1104:GLU:H    | 1.85                     | 0.42              |
| 1:A:162:SER:OG    | 1:A:163:ALA:N     | 2.53                     | 0.41              |
| 1:A:763:ILE:O     | 1:A:767:GLN:HG3   | 2.20                     | 0.41              |
| 1:A:914:LYS:HD2   | 1:A:914:LYS:HA    | 1.77                     | 0.41              |
| 1:B:1047:GLN:HB2  | 1:B:1054:VAL:CG1  | 2.49                     | 0.41              |
| 1:C:662:CYS:HB2   | 1:C:671:CYS:HB3   | 1.66                     | 0.41              |
| 1:C:1003:GLN:HB3  | 1:C:1007:ARG:NH1  | 2.31                     | 0.41              |
| 2:G:1:NAG:O3      | 2:G:2:NAG:N2      | 2.52                     | 0.41              |
| 1:A:349:SER:HA    | 1:A:451:TYR:HE2   | 1.84                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:411:ALA:HB3  | 1:A:414:GLN:HG3   | 2.02                     | 0.41              |
| 1:A:807:LYS:HA   | 1:A:807:LYS:HD2   | 1.91                     | 0.41              |
| 1:A:808:ARG:NH2  | 1:A:860:ASP:OD2   | 2.53                     | 0.41              |
| 1:A:890:PRO:HD3  | 1:C:704:SER:O     | 2.19                     | 0.41              |
| 1:B:278:LYS:HB2  | 1:B:306:PHE:CZ    | 2.55                     | 0.41              |
| 1:B:598:ILE:HG21 | 1:B:666:ILE:HD12  | 2.01                     | 0.41              |
| 1:C:86:PHE:HB2   | 1:C:238:PHE:HB2   | 2.03                     | 0.41              |
| 1:C:150:LYS:HD3  | 1:C:150:LYS:HA    | 1.80                     | 0.41              |
| 1:C:277:LEU:HB3  | 1:C:285:ILE:HD12  | 2.02                     | 0.41              |
| 1:C:457:ARG:HE   | 1:C:457:ARG:HB2   | 1.67                     | 0.41              |
| 1:C:498:GLN:O    | 1:C:501:ASN:HB2   | 2.20                     | 0.41              |
| 1:C:899:PHE:CE1  | 1:C:1042:LEU:HD11 | 2.54                     | 0.41              |
| 1:C:1086:GLY:HA3 | 1:C:1098:THR:O    | 2.21                     | 0.41              |
| 1:A:302:THR:HG21 | 1:A:315:THR:HA    | 2.02                     | 0.41              |
| 1:A:862:MET:HB3  | 1:C:692:LEU:HD21  | 2.03                     | 0.41              |
| 1:B:794:ASN:H    | 1:B:921:ASN:HD21  | 1.68                     | 0.41              |
| 1:B:1135:GLN:HA  | 1:B:1138:LEU:HG   | 2.02                     | 0.41              |
| 1:A:634:ARG:HA   | 1:A:634:ARG:HD3   | 1.80                     | 0.41              |
| 1:A:863:ILE:HG22 | 1:A:1048:SER:HB2  | 2.02                     | 0.41              |
| 1:B:134:GLN:O    | 1:B:161:SER:OG    | 2.32                     | 0.41              |
| 1:B:157:PHE:H    | 1:B:158:ARG:HH11  | 1.69                     | 0.41              |
| 1:B:1022:MET:O   | 1:B:1026:VAL:HB   | 2.20                     | 0.41              |
| 1:B:1082:PHE:O   | 1:B:1113:THR:HG23 | 2.21                     | 0.41              |
| 1:C:377:PHE:CD1  | 1:C:434:ILE:HG12  | 2.55                     | 0.41              |
| 2:E:1:NAG:H61    | 2:E:2:NAG:H82     | 2.03                     | 0.41              |
| 1:A:135:PHE:HD2  | 1:A:139:PRO:HB3   | 1.86                     | 0.41              |
| 1:B:157:PHE:C    | 1:B:158:ARG:HD2   | 2.45                     | 0.41              |
| 1:B:677:GLN:N    | 1:B:682:SER:O     | 2.51                     | 0.41              |
| 1:B:708:PRO:HA   | 1:B:1065:GLU:HA   | 2.03                     | 0.41              |
| 1:C:159:VAL:HG23 | 1:C:160:TYR:HD2   | 1.86                     | 0.41              |
| 1:C:295:PRO:HD3  | 1:C:633:TRP:HZ3   | 1.85                     | 0.41              |
| 1:C:425:LEU:HD23 | 1:C:425:LEU:HA    | 1.86                     | 0.41              |
| 1:A:718:GLU:CD   | 1:A:1021:LYS:HE2  | 2.46                     | 0.41              |
| 1:B:187:LYS:HA   | 1:B:187:LYS:HD3   | 1.83                     | 0.41              |
| 1:B:967:SER:OG   | 1:B:968:SER:N     | 2.53                     | 0.41              |
| 1:C:186:PHE:H    | 1:C:213:VAL:HG22  | 1.86                     | 0.41              |
| 1:C:404:GLY:HA2  | 1:C:508:TYR:HD2   | 1.84                     | 0.41              |
| 1:C:581:THR:O    | 1:C:583:GLU:N     | 2.52                     | 0.41              |
| 1:A:893:MET:SD   | 1:C:1072:PRO:HB3  | 2.60                     | 0.41              |
| 1:B:795:PHE:CG   | 1:B:798:ILE:HD11  | 2.55                     | 0.41              |
| 1:B:988:ARG:O    | 1:B:991:THR:HG22  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:41:LYS:HD2   | 1:C:562:PHE:CE1   | 2.56                     | 0.41              |
| 1:A:430:THR:OG1  | 1:A:430:THR:O     | 2.36                     | 0.41              |
| 1:A:472:ILE:HD11 | 1:A:488:CYS:C     | 2.46                     | 0.41              |
| 1:A:715:VAL:HG11 | 1:A:927:ILE:HG21  | 2.01                     | 0.41              |
| 1:A:966:ILE:HG12 | 1:A:985:GLN:NE2   | 2.36                     | 0.41              |
| 1:B:310:LYS:HB2  | 1:B:600:PRO:O     | 2.21                     | 0.41              |
| 1:C:437:ASN:HA   | 1:C:508:TYR:HD1   | 1.86                     | 0.41              |
| 1:C:502:GLY:O    | 1:C:506:GLN:N     | 2.53                     | 0.41              |
| 1:C:1054:VAL:C   | 1:C:1055:PHE:HD1  | 2.28                     | 0.41              |
| 1:A:36:VAL:HG11  | 1:A:220:PHE:CZ    | 2.56                     | 0.41              |
| 1:A:83:VAL:HA    | 1:A:239:GLN:HG3   | 2.03                     | 0.41              |
| 1:A:112:SER:HA   | 1:A:132:GLU:HG3   | 2.02                     | 0.41              |
| 1:A:231:ILE:HG13 | 1:A:232:GLY:N     | 2.36                     | 0.41              |
| 1:A:752:PHE:HE1  | 1:C:963:PHE:CE2   | 2.39                     | 0.41              |
| 1:A:865:GLN:CD   | 1:C:692:LEU:HD12  | 2.46                     | 0.41              |
| 1:B:191:GLU:OE2  | 1:B:206:LYS:HB3   | 2.21                     | 0.41              |
| 1:B:603:ASN:O    | 1:B:605:SER:N     | 2.53                     | 0.41              |
| 1:B:615:VAL:HG23 | 1:B:617:CYS:N     | 2.34                     | 0.41              |
| 1:C:61:ASN:OD1   | 3:C:1301:NAG:H83  | 2.20                     | 0.41              |
| 1:C:133:PHE:CE2  | 1:C:160:TYR:HB2   | 2.56                     | 0.41              |
| 1:C:385:THR:HG23 | 1:C:386:LYS:HG2   | 2.01                     | 0.41              |
| 1:A:197:ILE:HG23 | 1:A:202:LYS:HZ1   | 1.86                     | 0.41              |
| 1:A:423:TYR:HE2  | 1:A:512:VAL:HG21  | 1.86                     | 0.41              |
| 1:A:498:GLN:O    | 1:A:501:ASN:HB2   | 2.21                     | 0.41              |
| 1:B:537:LYS:N    | 1:B:551:VAL:HG23  | 2.36                     | 0.41              |
| 1:C:309:GLU:HG2  | 1:C:310:LYS:N     | 2.36                     | 0.41              |
| 1:C:899:PHE:CD1  | 1:C:1042:LEU:HD21 | 2.56                     | 0.41              |
| 1:A:771:THR:HG22 | 1:A:858:LEU:HD12  | 2.03                     | 0.40              |
| 1:B:577:ARG:NH1  | 1:B:582:LEU:HD22  | 2.36                     | 0.40              |
| 1:B:894:GLN:HE22 | 1:B:898:ARG:HH21  | 1.68                     | 0.40              |
| 1:A:253:ASP:N    | 1:A:256:SER:HB3   | 2.36                     | 0.40              |
| 1:B:64:TRP:CD1   | 1:B:266:TYR:HE2   | 2.39                     | 0.40              |
| 1:B:142:GLY:HA3  | 1:B:244:LEU:HB2   | 2.03                     | 0.40              |
| 1:B:236:THR:O    | 1:B:237:ARG:HD2   | 2.21                     | 0.40              |
| 1:B:708:PRO:HB3  | 1:B:1062:PRO:HB3  | 2.03                     | 0.40              |
| 1:B:797:GLN:HG2  | 1:B:928:GLN:HE21  | 1.83                     | 0.40              |
| 1:B:797:GLN:HE21 | 1:B:928:GLN:HE22  | 1.69                     | 0.40              |
| 1:C:100:ILE:O    | 1:C:102:ARG:HG2   | 2.21                     | 0.40              |
| 1:C:613:GLN:O    | 1:C:615:VAL:N     | 2.54                     | 0.40              |
| 1:C:988:ARG:O    | 1:C:991:THR:HG22  | 2.20                     | 0.40              |
| 1:A:328:ARG:HH21 | 1:A:533:LEU:H     | 1.66                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:620:VAL:N    | 1:A:621:PRO:HD2   | 2.36                     | 0.40              |
| 1:A:740:THR:O    | 1:A:743:SER:OG    | 2.28                     | 0.40              |
| 1:A:815:LEU:HD21 | 1:A:1054:VAL:HG21 | 2.04                     | 0.40              |
| 1:B:725:THR:OG1  | 1:B:948:ASN:OD1   | 2.39                     | 0.40              |
| 1:A:189:LEU:HG   | 1:A:191:GLU:OE1   | 2.22                     | 0.40              |
| 1:A:1074:ILE:O   | 1:A:1081:HIS:N    | 2.55                     | 0.40              |
| 1:B:894:GLN:HE22 | 1:B:898:ARG:HE    | 1.68                     | 0.40              |
| 1:C:355:ARG:NH1  | 1:C:398:ASP:OD2   | 2.54                     | 0.40              |
| 1:C:538:CYS:HB3  | 1:C:551:VAL:CG2   | 2.51                     | 0.40              |
| 1:C:795:PHE:HE1  | 1:C:920:PHE:CE2   | 2.30                     | 0.40              |
| 1:A:37:TYR:OH    | 1:A:54:LEU:O      | 2.39                     | 0.40              |
| 1:A:329:PHE:HA   | 1:A:544:ASN:HD21  | 1.87                     | 0.40              |
| 1:A:486:PHE:HZ   | 1:B:368:LEU:HD12  | 1.86                     | 0.40              |
| 1:A:899:PHE:CE2  | 1:A:909:LEU:HD12  | 2.57                     | 0.40              |
| 1:A:1071:ALA:O   | 1:A:1088:PHE:HB2  | 2.22                     | 0.40              |
| 1:C:381:GLY:HA3  | 1:C:430:THR:HB    | 2.04                     | 0.40              |
| 1:C:418:ILE:HA   | 1:C:422:ASN:ND2   | 2.35                     | 0.40              |
| 1:C:1022:MET:O   | 1:C:1026:VAL:HB   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 1081/1194 (90%) | 1009 (93%) | 72 (7%)  | 0        | 100         | 100 |
| 1   | B     | 1085/1194 (91%) | 1021 (94%) | 64 (6%)  | 0        | 100         | 100 |
| 1   | C     | 1073/1194 (90%) | 993 (92%)  | 80 (8%)  | 0        | 100         | 100 |
| All | All   | 3239/3582 (90%) | 3023 (93%) | 216 (7%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 942/1041 (90%)  | 942 (100%)  | 0        | 100         | 100 |
| 1   | B     | 946/1041 (91%)  | 946 (100%)  | 0        | 100         | 100 |
| 1   | C     | 937/1041 (90%)  | 937 (100%)  | 0        | 100         | 100 |
| All | All   | 2825/3123 (90%) | 2825 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 99   | ASN  |
| 1   | A     | 165  | ASN  |
| 1   | A     | 239  | GLN  |
| 1   | A     | 498  | GLN  |
| 1   | A     | 580  | GLN  |
| 1   | A     | 849  | ASN  |
| 1   | A     | 865  | GLN  |
| 1   | A     | 919  | GLN  |
| 1   | A     | 985  | GLN  |
| 1   | A     | 1029 | GLN  |
| 1   | A     | 1076 | HIS  |
| 1   | B     | 164  | ASN  |
| 1   | B     | 414  | GLN  |
| 1   | B     | 422  | ASN  |
| 1   | B     | 437  | ASN  |
| 1   | B     | 460  | ASN  |
| 1   | B     | 542  | ASN  |
| 1   | B     | 675  | GLN  |
| 1   | B     | 755  | GLN  |
| 1   | B     | 865  | GLN  |
| 1   | B     | 921  | ASN  |
| 1   | B     | 928  | GLN  |
| 1   | B     | 1041 | HIS  |
| 1   | B     | 1047 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1081 | HIS  |
| 1   | B     | 1094 | HIS  |
| 1   | C     | 122  | ASN  |
| 1   | C     | 894  | GLN  |
| 1   | C     | 928  | GLN  |
| 1   | C     | 958  | GLN  |
| 1   | C     | 998  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | NAG  | D     | 1   | 1,2  | 14,14,15     | 0.19 | 0           | 17,19,21    | 0.63 | 0           |
| 2   | NAG  | D     | 2   | 2    | 14,14,15     | 0.24 | 0           | 17,19,21    | 0.47 | 0           |
| 2   | NAG  | E     | 1   | 1,2  | 14,14,15     | 0.19 | 0           | 17,19,21    | 0.45 | 0           |
| 2   | NAG  | E     | 2   | 2    | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.44 | 0           |
| 2   | NAG  | F     | 1   | 1,2  | 14,14,15     | 0.36 | 0           | 17,19,21    | 0.67 | 0           |
| 2   | NAG  | F     | 2   | 2    | 14,14,15     | 0.28 | 0           | 17,19,21    | 0.54 | 0           |
| 2   | NAG  | G     | 1   | 1,2  | 14,14,15     | 0.38 | 0           | 17,19,21    | 0.70 | 1 (5%)      |
| 2   | NAG  | G     | 2   | 2    | 14,14,15     | 0.26 | 0           | 17,19,21    | 0.54 | 0           |
| 2   | NAG  | H     | 1   | 1,2  | 14,14,15     | 0.30 | 0           | 17,19,21    | 0.47 | 0           |
| 2   | NAG  | H     | 2   | 2    | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.53 | 0           |
| 2   | NAG  | I     | 1   | 1,2  | 14,14,15     | 0.26 | 0           | 17,19,21    | 0.41 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAG  | I     | 2   | 2    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.44 | 0        |
| 2   | NAG  | J     | 1   | 1,2  | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.38 | 0        |
| 2   | NAG  | J     | 2   | 2    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.39 | 0        |
| 2   | NAG  | K     | 1   | 1,2  | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.65 | 0        |
| 2   | NAG  | K     | 2   | 2    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.48 | 0        |
| 2   | NAG  | L     | 1   | 1,2  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.40 | 0        |
| 2   | NAG  | L     | 2   | 2    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.45 | 0        |
| 2   | NAG  | M     | 1   | 1,2  | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.55 | 0        |
| 2   | NAG  | M     | 2   | 2    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.54 | 0        |
| 2   | NAG  | N     | 1   | 1,2  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.39 | 0        |
| 2   | NAG  | N     | 2   | 2    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.42 | 0        |
| 2   | NAG  | O     | 1   | 1,2  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.52 | 0        |
| 2   | NAG  | O     | 2   | 2    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.47 | 0        |
| 2   | NAG  | P     | 1   | 1,2  | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.49 | 0        |
| 2   | NAG  | P     | 2   | 2    | 14,14,15     | 0.52 | 0        | 17,19,21    | 0.51 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | NAG  | D     | 1   | 1,2  | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 2   | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | E     | 1   | 1,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | E     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | F     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | F     | 2   | 2    | -       | 3/6/23/26 | 0/1/1/1 |
| 2   | NAG  | G     | 1   | 1,2  | -       | 3/6/23/26 | 0/1/1/1 |
| 2   | NAG  | G     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | H     | 1   | 1,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | H     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | I     | 1   | 1,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | I     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | J     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | J     | 2   | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | K     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | K     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | L     | 1   | 1,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | L     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | NAG  | M     | 1   | 1,2  | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | M     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | N     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | N     | 2   | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | O     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | O     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | P     | 1   | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | P     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | G     | 1   | NAG  | C1-O5-C5 | 2.00 | 114.87      | 112.19   |

There are no chirality outliers.

All (53) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | E     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | M     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | O     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | K     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | K     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | M     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | K     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | H     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | G     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | M     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | M     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | G     | 1   | NAG  | C8-C7-N2-C2 |
| 2   | G     | 1   | NAG  | O7-C7-N2-C2 |
| 2   | K     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | K     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | G     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | D     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | O     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | G     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | H     | 1   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | I     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | D     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | I     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | L     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | D     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | N     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | F     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | H     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | J     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | N     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | I     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | O     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | M     | 1   | NAG  | C1-C2-N2-C7 |
| 2   | O     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | K     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | N     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | J     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | D     | 1   | NAG  | C3-C2-N2-C7 |
| 2   | F     | 1   | NAG  | C3-C2-N2-C7 |
| 2   | F     | 2   | NAG  | C3-C2-N2-C7 |
| 2   | H     | 2   | NAG  | C3-C2-N2-C7 |
| 2   | M     | 1   | NAG  | C3-C2-N2-C7 |
| 2   | M     | 2   | NAG  | C3-C2-N2-C7 |
| 2   | E     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | P     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | P     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | D     | 1   | NAG  | C1-C2-N2-C7 |
| 2   | F     | 1   | NAG  | C1-C2-N2-C7 |
| 2   | F     | 2   | NAG  | C1-C2-N2-C7 |
| 2   | H     | 2   | NAG  | C1-C2-N2-C7 |
| 2   | J     | 1   | NAG  | C1-C2-N2-C7 |
| 2   | M     | 2   | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

6 monomers are involved in 5 short contacts:

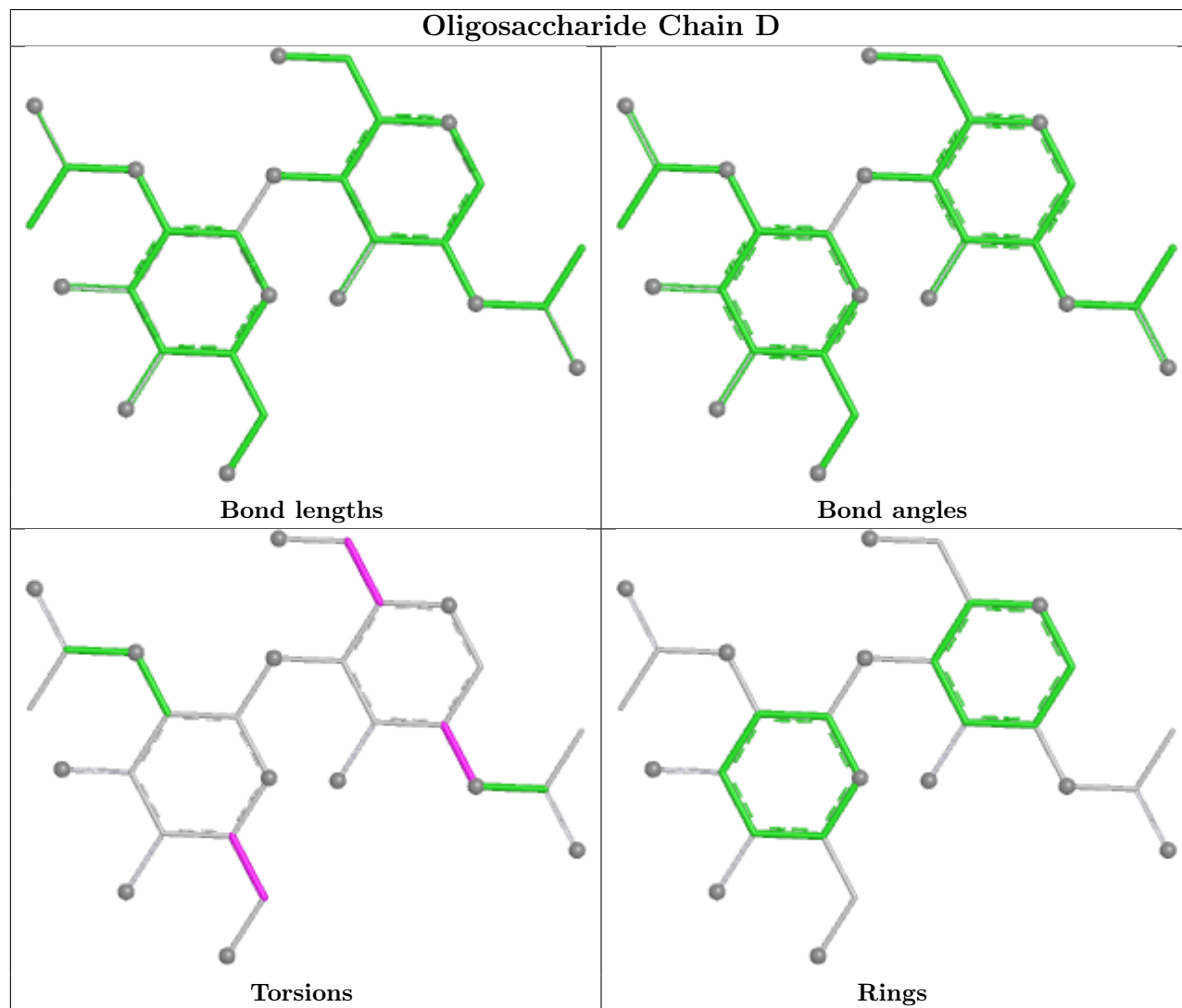
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | E     | 1   | NAG  | 1       | 0            |
| 2   | E     | 2   | NAG  | 1       | 0            |
| 2   | G     | 2   | NAG  | 2       | 0            |
| 2   | G     | 1   | NAG  | 1       | 0            |
| 2   | K     | 1   | NAG  | 1       | 0            |

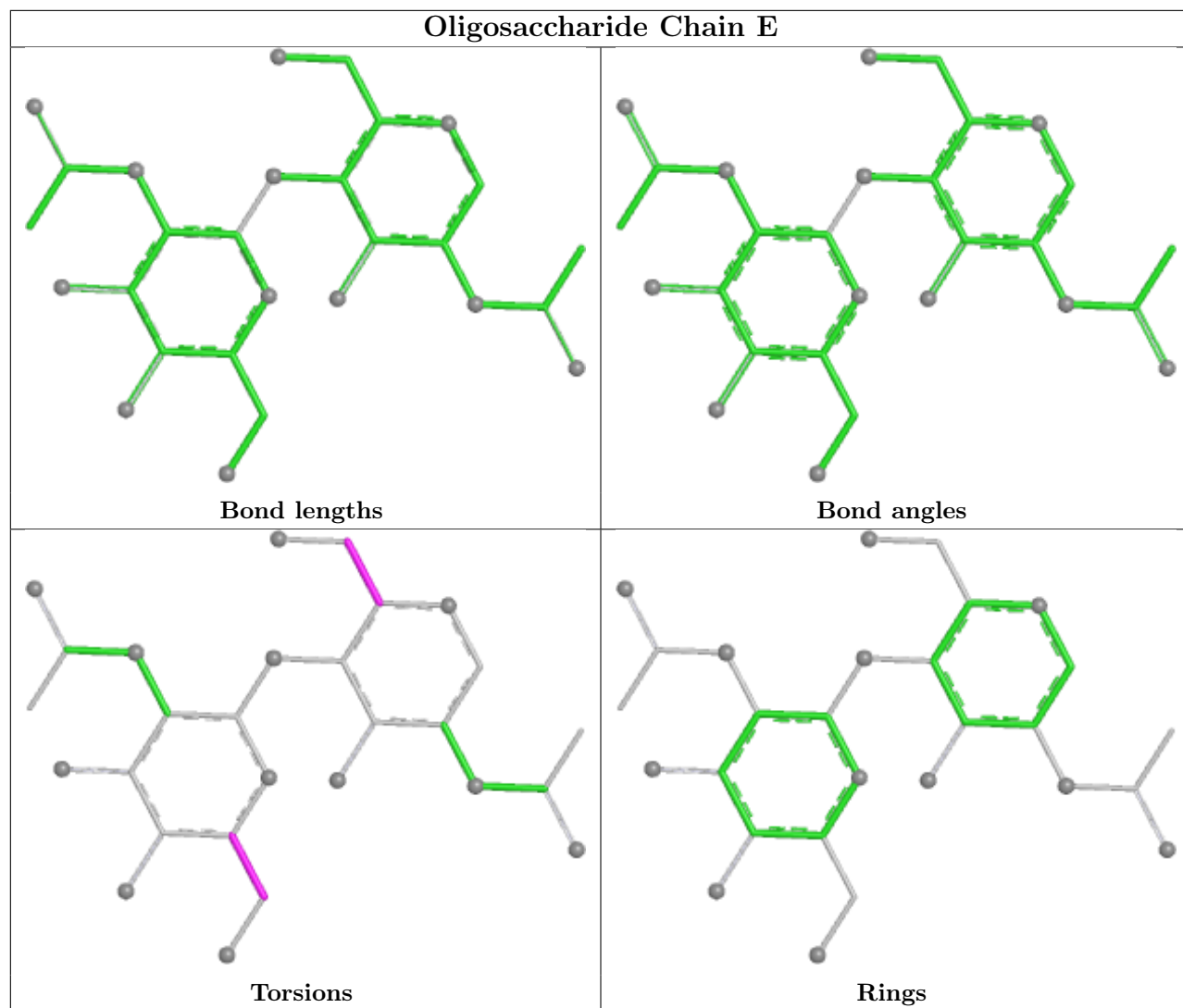
*Continued on next page...*

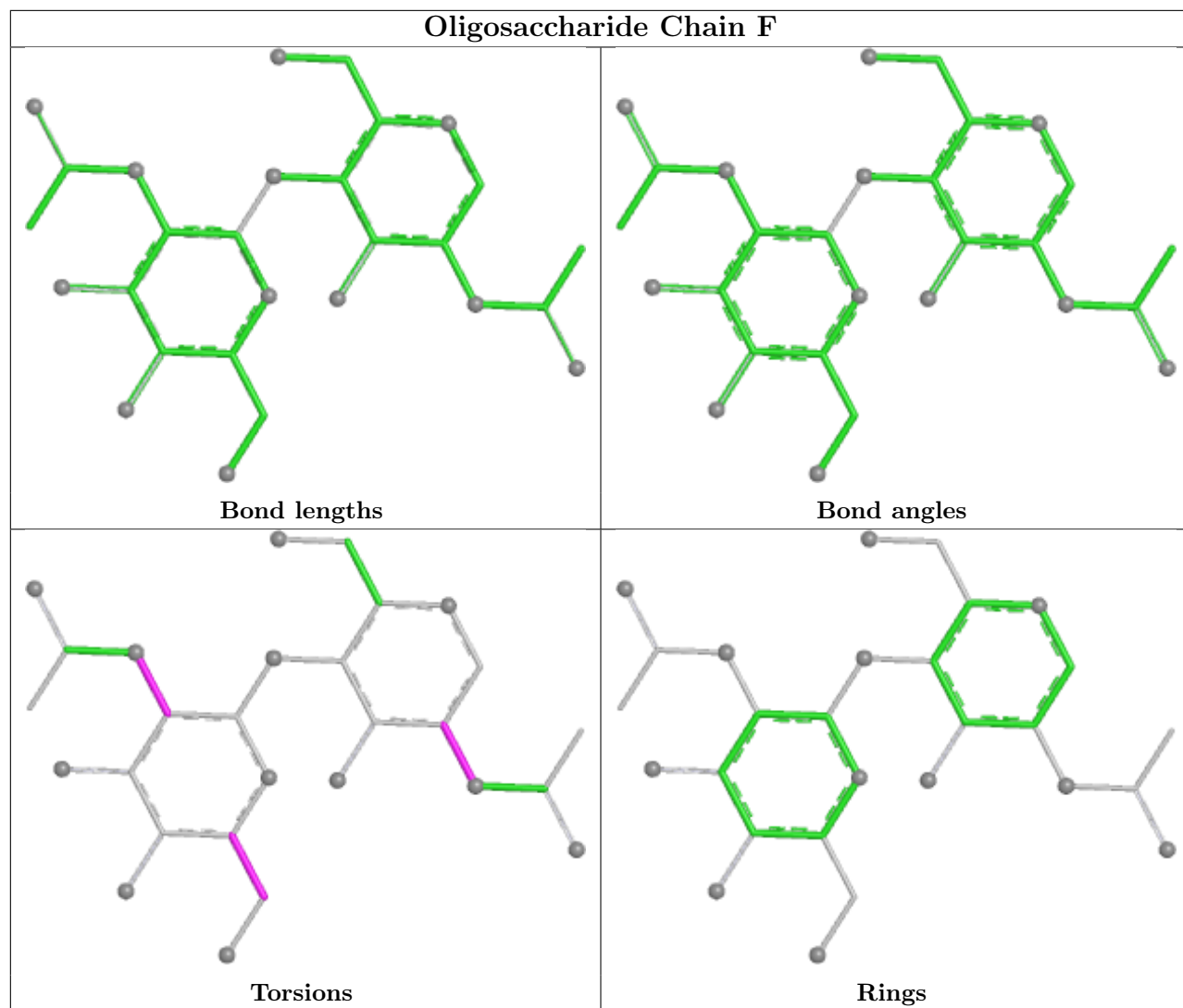
Continued from previous page...

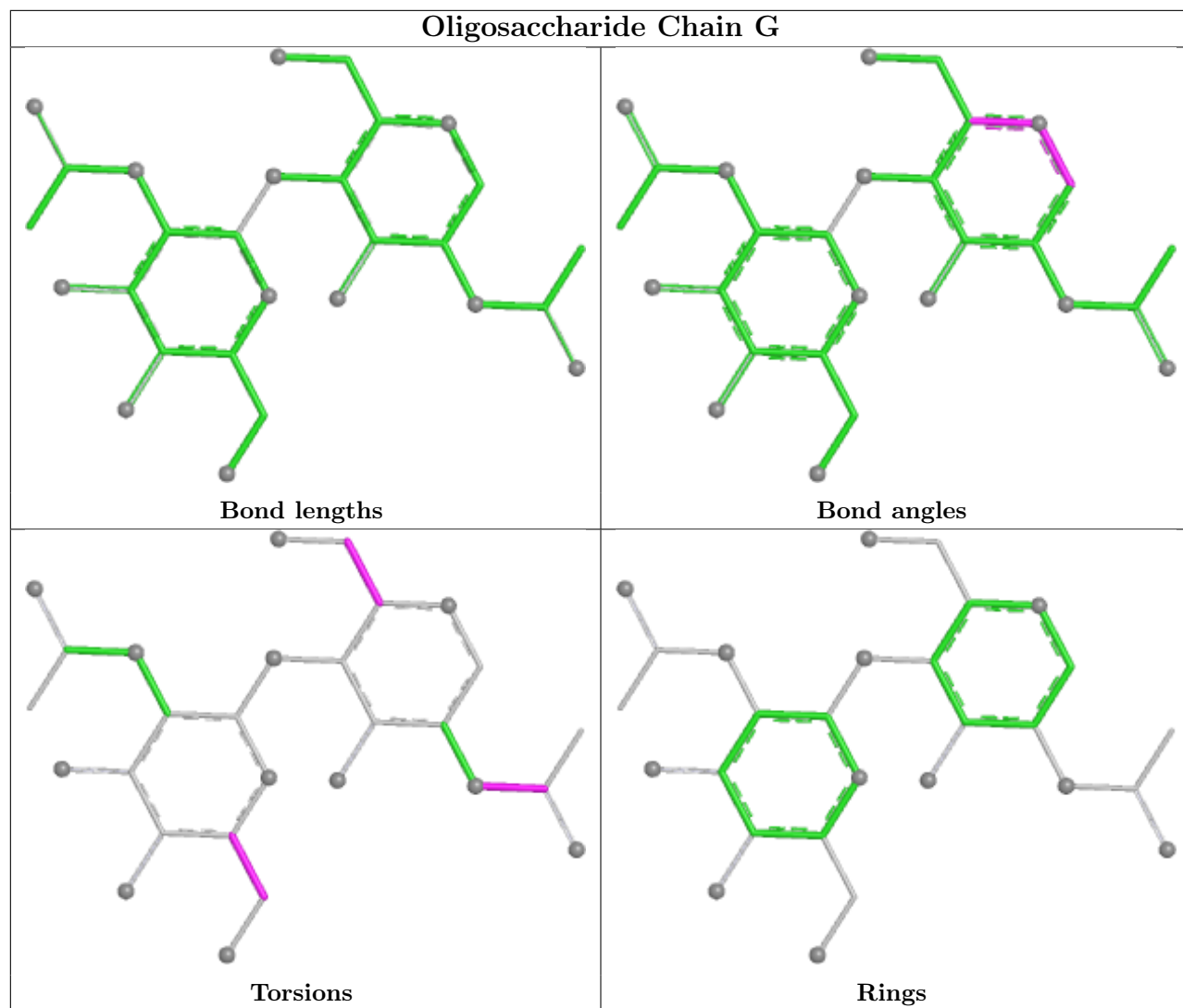
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | K     | 2   | NAG  | 2       | 0            |

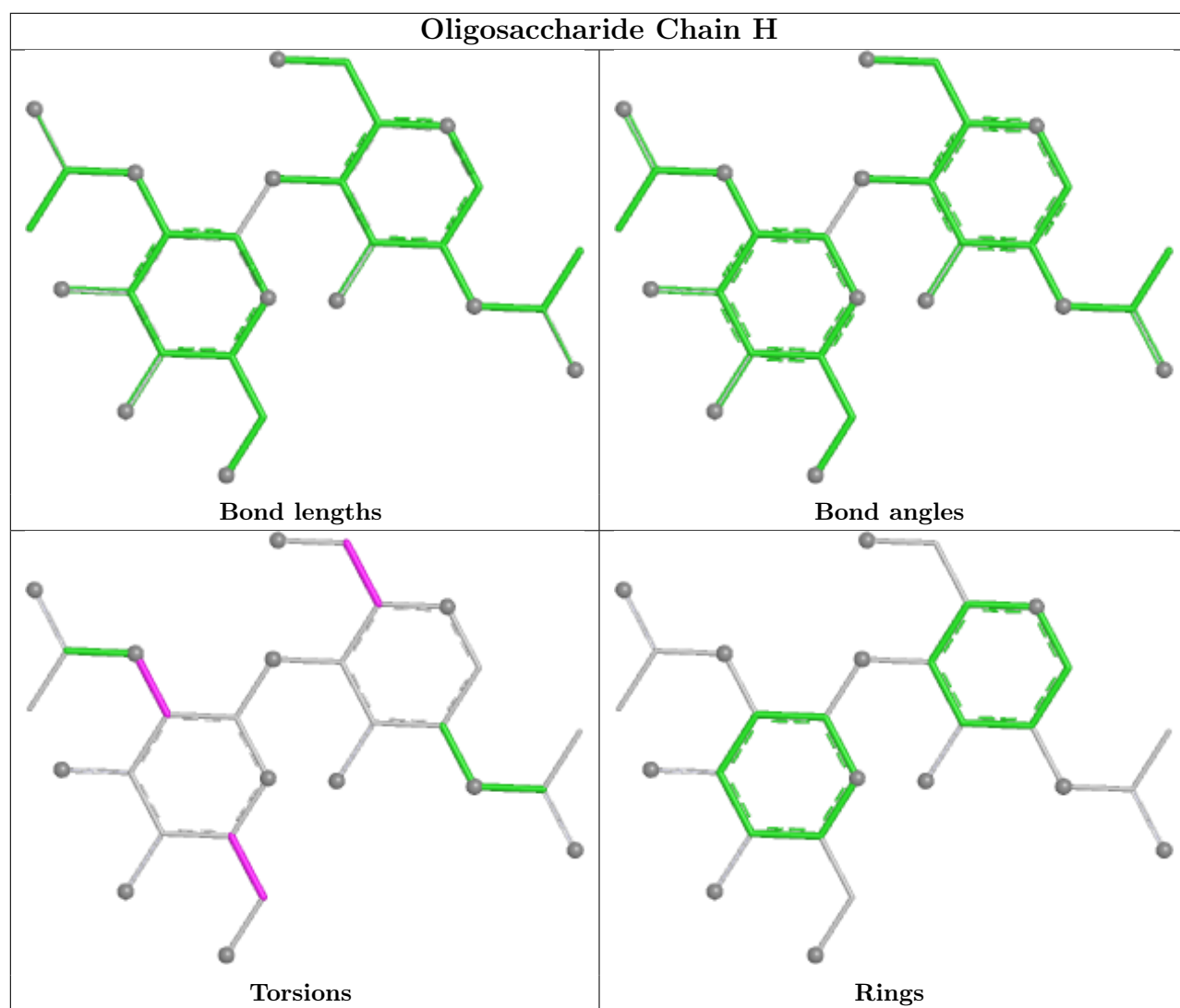
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

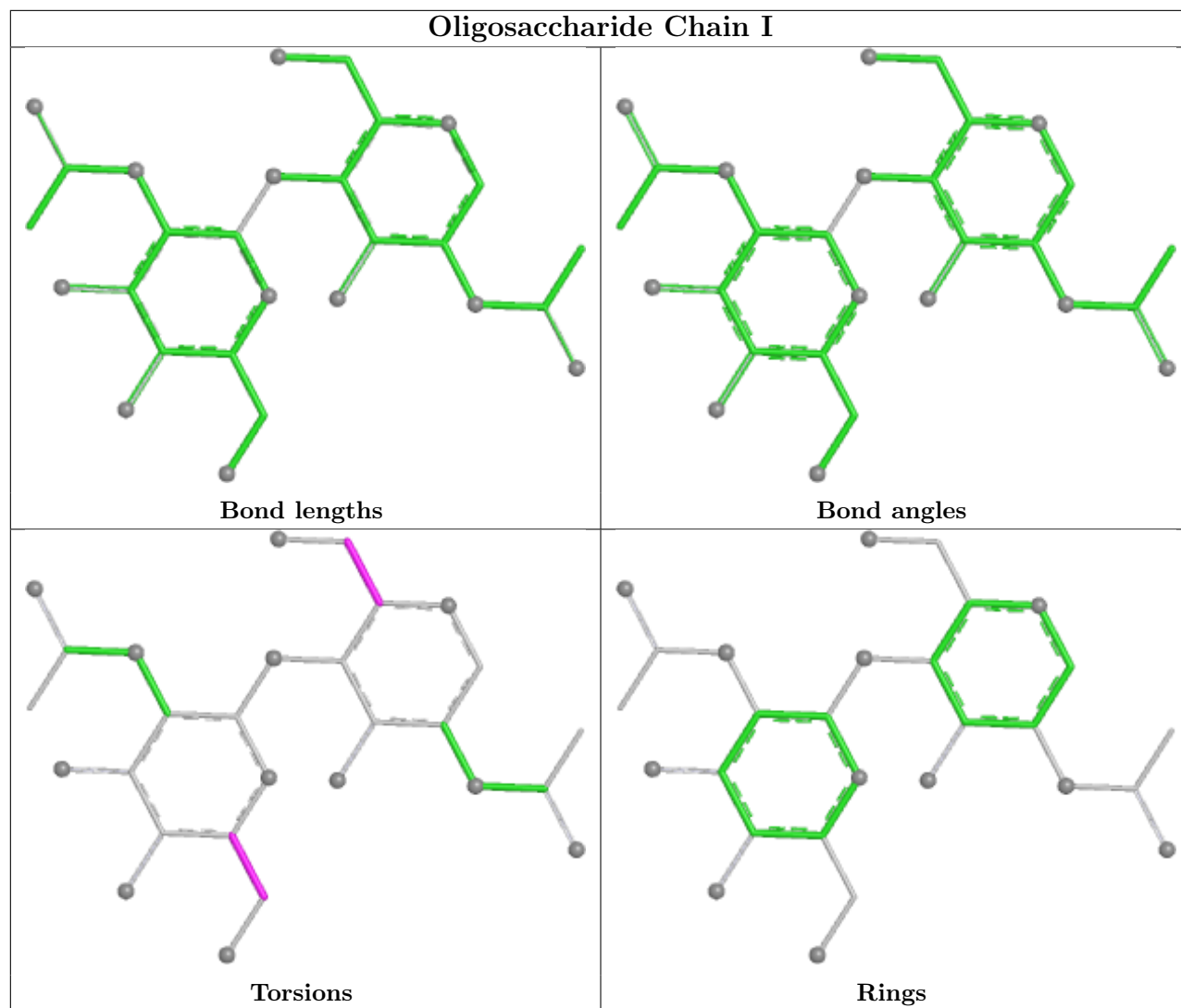


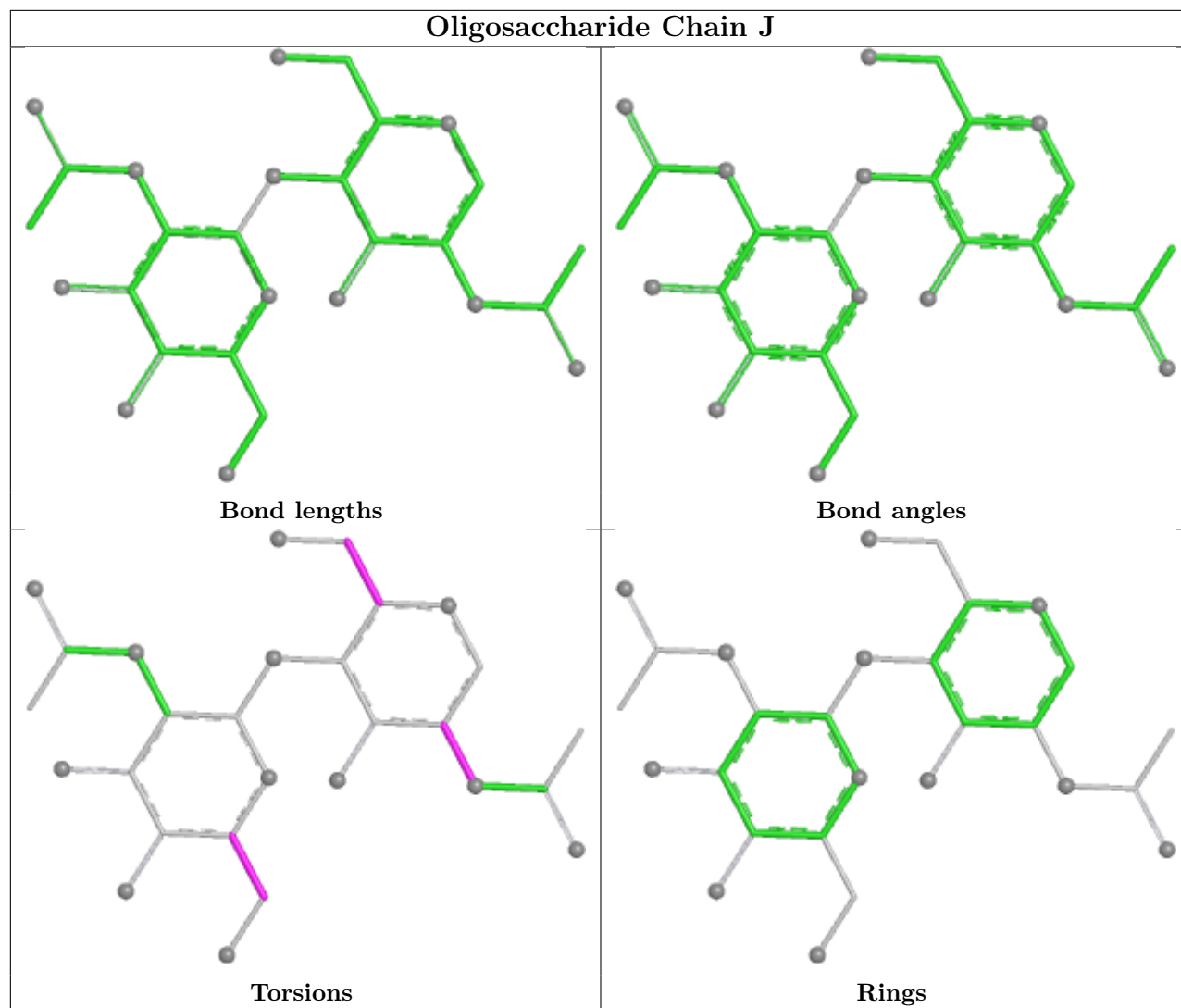


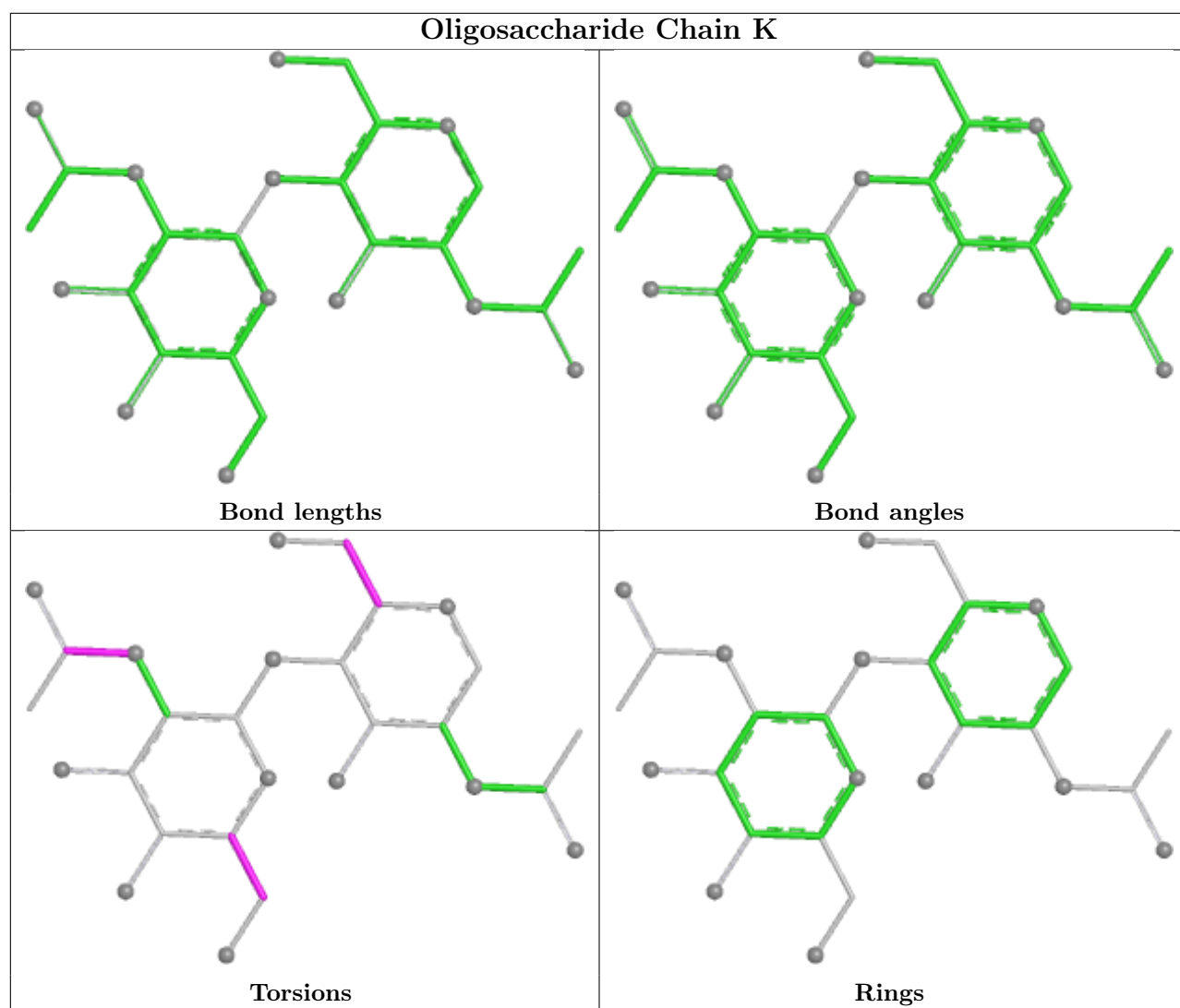


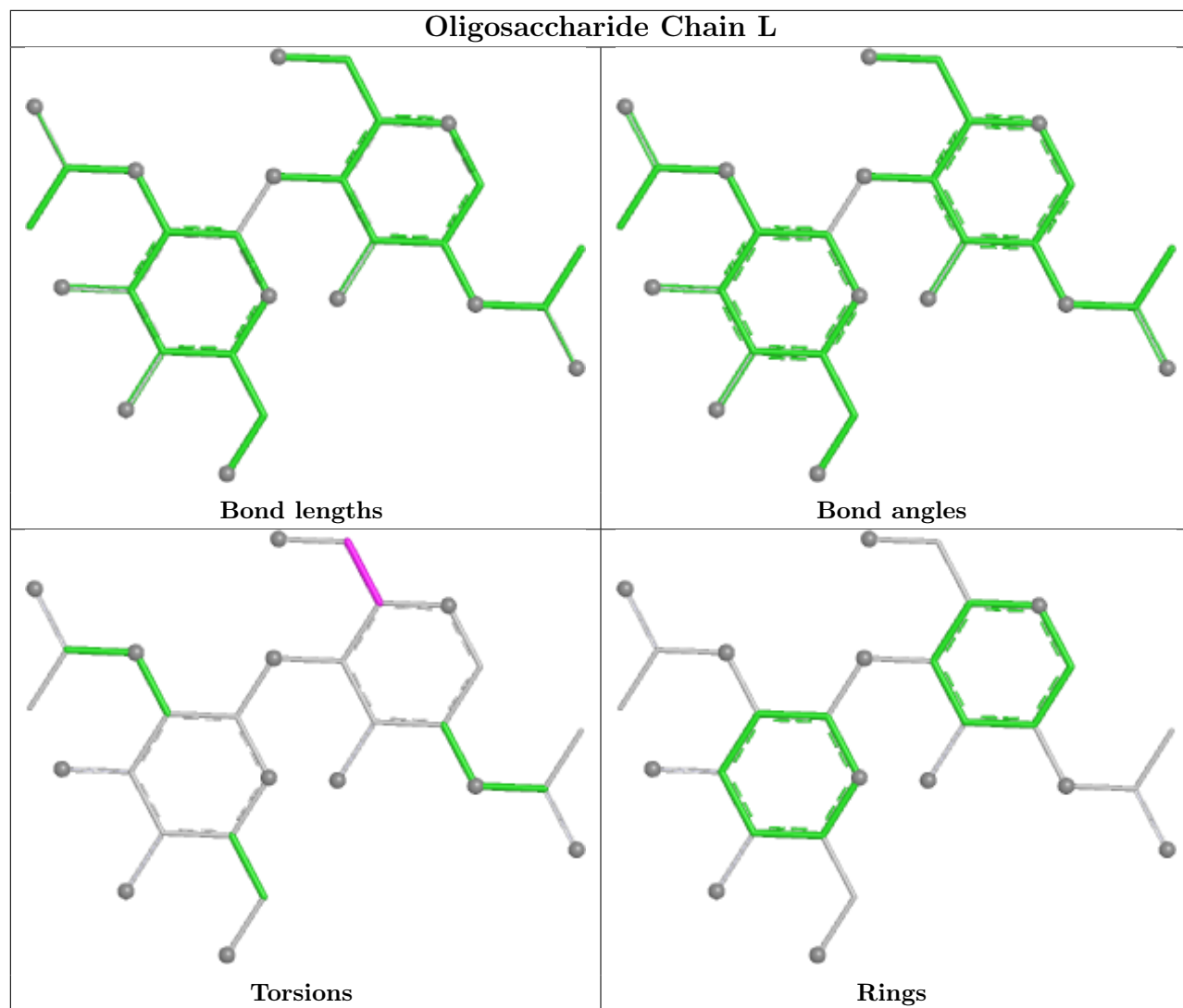


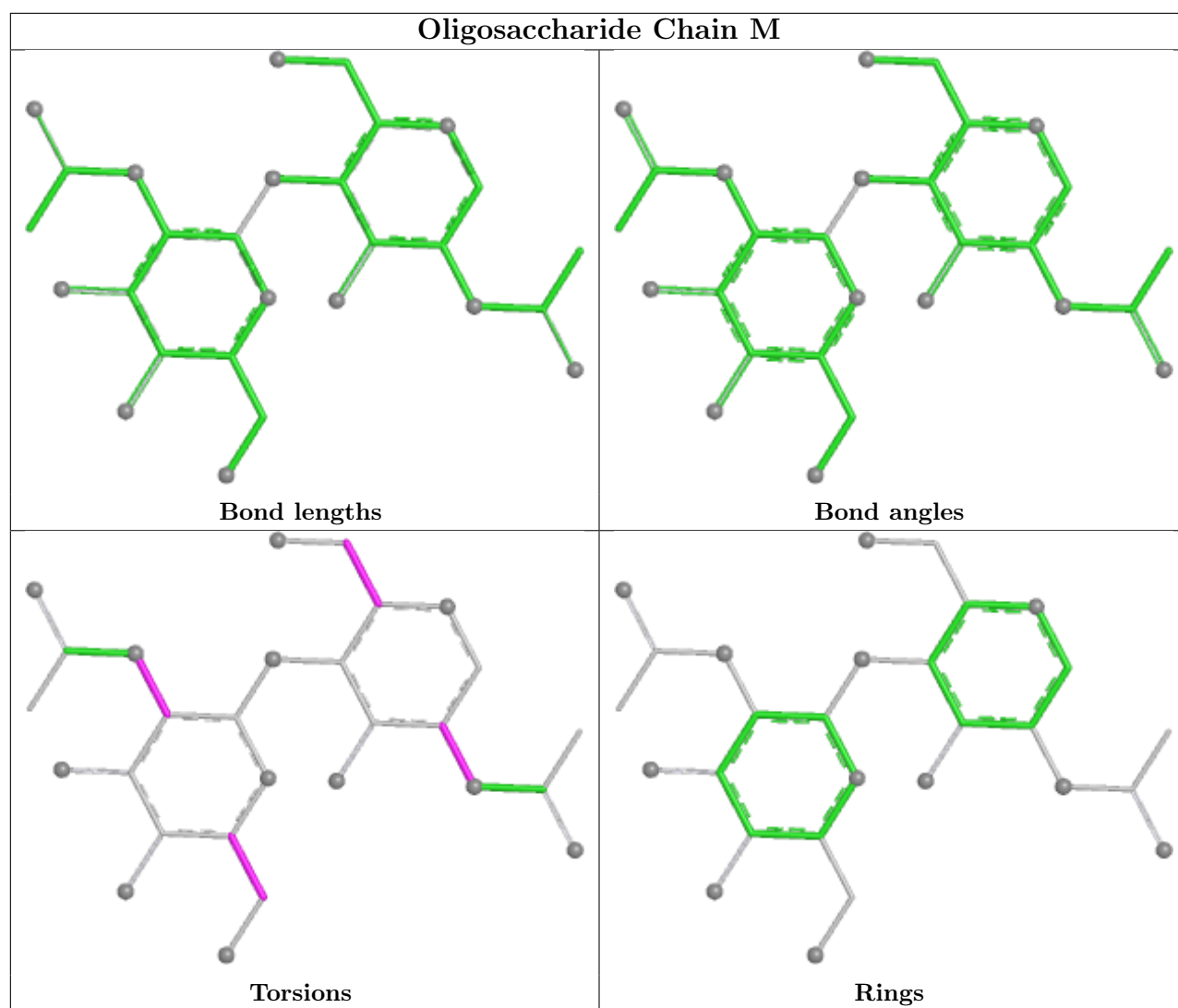


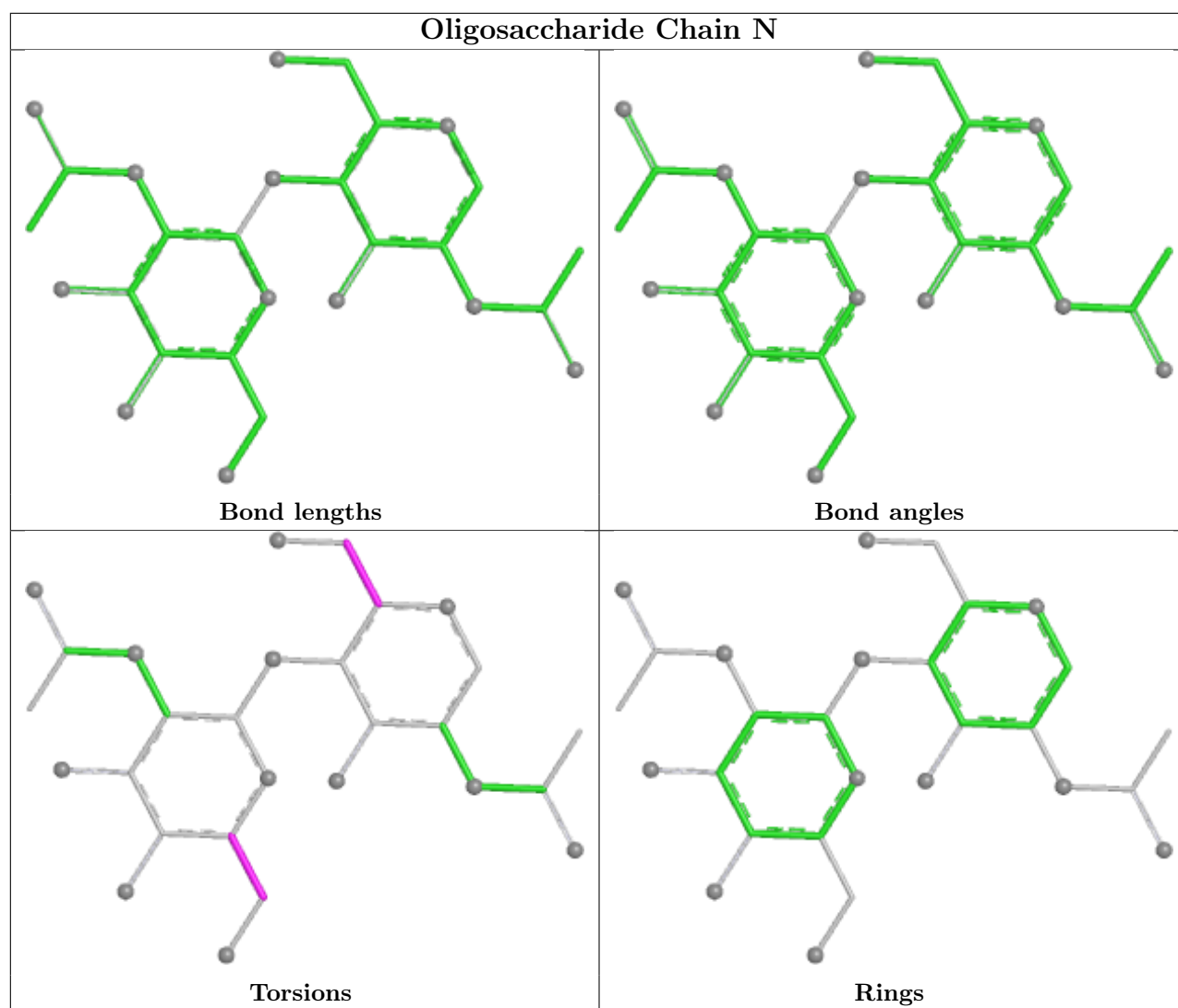


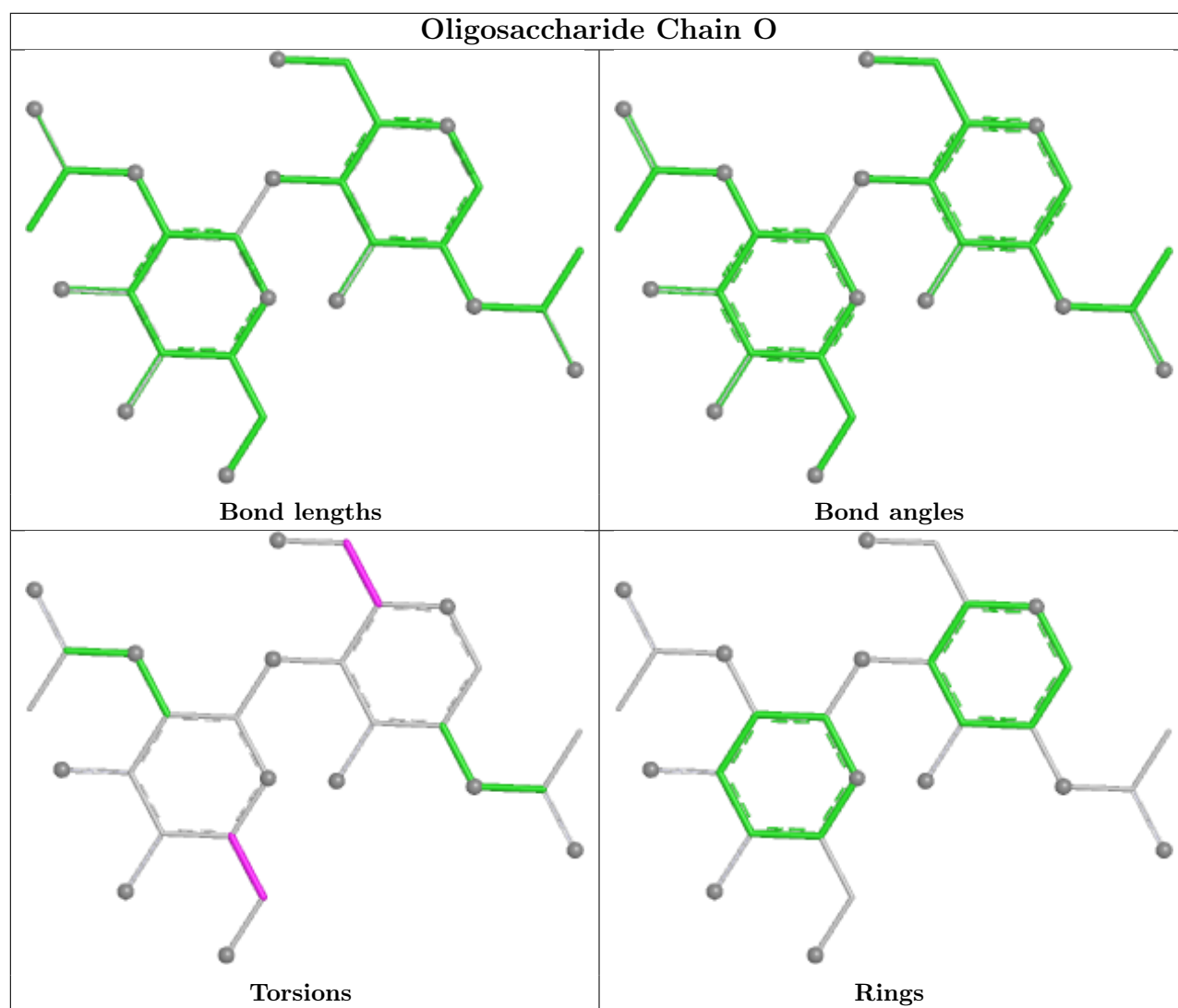


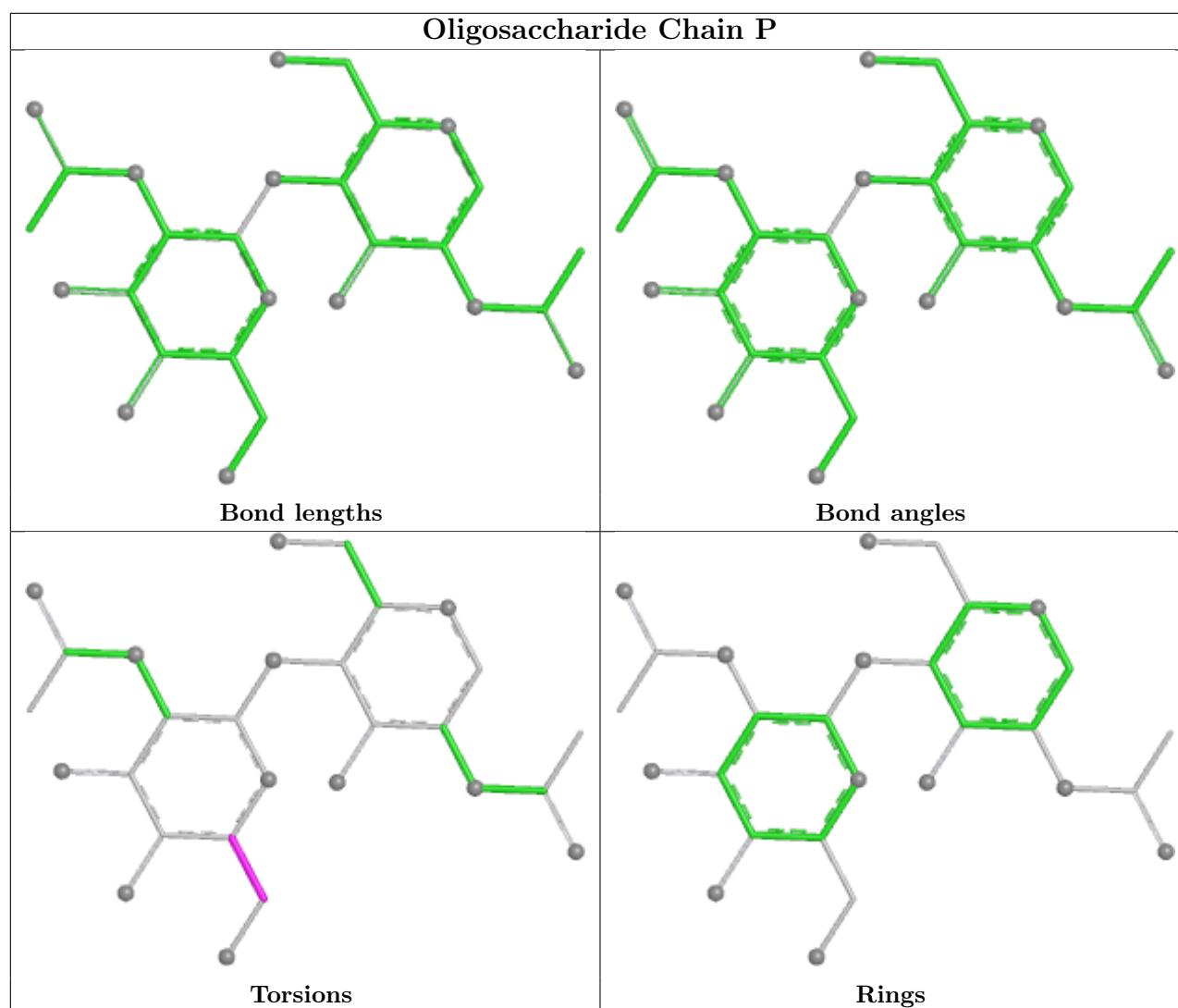












## 5.6 Ligand geometry [i](#)

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | NAG  | B     | 1301 | 1    | 14,14,15     | 0.30 | 0           | 17,19,21    | 0.43 | 0           |
| 3   | NAG  | B     | 1304 | 1    | 14,14,15     | 0.27 | 0           | 17,19,21    | 0.41 | 0           |
| 3   | NAG  | C     | 1308 | 1    | 14,14,15     | 0.24 | 0           | 17,19,21    | 0.42 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | B     | 1307 | 1    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | B     | 1302 | 1    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | A     | 1303 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | C     | 1311 | 1    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.52 | 0        |
| 3   | NAG  | C     | 1310 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | A     | 1305 | 1    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.40 | 0        |
| 3   | NAG  | C     | 1309 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.59 | 0        |
| 3   | NAG  | C     | 1307 | 1    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.51 | 0        |
| 3   | NAG  | A     | 1302 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.32 | 0        |
| 3   | NAG  | B     | 1303 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.39 | 0        |
| 3   | NAG  | A     | 1304 | 1    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.37 | 0        |
| 3   | NAG  | B     | 1309 | 1    | 14,14,15     | 0.17 | 0        | 17,19,21    | 0.47 | 0        |
| 3   | NAG  | B     | 1305 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.57 | 0        |
| 3   | NAG  | C     | 1306 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.61 | 0        |
| 3   | NAG  | A     | 1309 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.39 | 0        |
| 3   | NAG  | B     | 1310 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.53 | 0        |
| 3   | NAG  | C     | 1302 | 1    | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.42 | 0        |
| 3   | NAG  | A     | 1308 | 1    | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.40 | 0        |
| 3   | NAG  | A     | 1306 | 1    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.31 | 0        |
| 3   | NAG  | C     | 1303 | 1    | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.53 | 0        |
| 3   | NAG  | A     | 1307 | 1    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.49 | 0        |
| 3   | NAG  | C     | 1305 | 1    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.44 | 0        |
| 3   | NAG  | B     | 1306 | 1    | 14,14,15     | 0.69 | 1 (7%)   | 17,19,21    | 1.37 | 2 (11%)  |
| 3   | NAG  | A     | 1310 | 1    | 14,14,15     | 0.17 | 0        | 17,19,21    | 0.41 | 0        |
| 3   | NAG  | B     | 1308 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.67 | 1 (5%)   |
| 3   | NAG  | A     | 1301 | 1    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.43 | 0        |
| 3   | NAG  | C     | 1301 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.38 | 0        |
| 3   | NAG  | C     | 1304 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.43 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | NAG  | B     | 1301 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1304 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1308 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1307 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1302 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1303 | 1    | -       | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | NAG  | C     | 1311 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1310 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1305 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1309 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1307 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1302 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1303 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1304 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1309 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1305 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1306 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1309 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1310 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1302 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1308 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1306 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1303 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1307 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1305 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1306 | 1    | -       | 6/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1310 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 1308 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1301 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1301 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 1304 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | B     | 1306 | NAG  | C1-C2 | 2.38 | 1.55        | 1.52     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 3   | B     | 1306 | NAG  | C2-N2-C7 | 4.46 | 128.88      | 122.90   |
| 3   | B     | 1308 | NAG  | C1-O5-C5 | 2.28 | 115.25      | 112.19   |
| 3   | B     | 1306 | NAG  | C1-C2-N2 | 2.11 | 113.76      | 110.43   |

There are no chirality outliers.

All (72) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | B     | 1309 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1302 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1305 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1303 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1302 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1301 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1310 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1302 | NAG  | O5-C5-C6-O6 |
| 3   | B     | 1307 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1309 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1304 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1310 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1302 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1309 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1301 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1305 | NAG  | O5-C5-C6-O6 |
| 3   | B     | 1303 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1310 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1304 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1301 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1309 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1308 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1307 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1301 | NAG  | O5-C5-C6-O6 |
| 3   | B     | 1307 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1307 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1308 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1303 | NAG  | C8-C7-N2-C2 |
| 3   | A     | 1303 | NAG  | O7-C7-N2-C2 |
| 3   | B     | 1301 | NAG  | C8-C7-N2-C2 |
| 3   | B     | 1301 | NAG  | O7-C7-N2-C2 |
| 3   | B     | 1304 | NAG  | C8-C7-N2-C2 |
| 3   | B     | 1304 | NAG  | O7-C7-N2-C2 |
| 3   | B     | 1305 | NAG  | C8-C7-N2-C2 |
| 3   | B     | 1305 | NAG  | O7-C7-N2-C2 |
| 3   | B     | 1306 | NAG  | C8-C7-N2-C2 |
| 3   | B     | 1306 | NAG  | O7-C7-N2-C2 |
| 3   | C     | 1301 | NAG  | C8-C7-N2-C2 |
| 3   | C     | 1301 | NAG  | O7-C7-N2-C2 |
| 3   | C     | 1308 | NAG  | C8-C7-N2-C2 |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | C     | 1308 | NAG  | O7-C7-N2-C2 |
| 3   | C     | 1311 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1306 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1310 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1302 | NAG  | O5-C5-C6-O6 |
| 3   | B     | 1306 | NAG  | O5-C5-C6-O6 |
| 3   | B     | 1304 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1304 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1303 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1307 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1303 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1307 | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1303 | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1307 | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1311 | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1307 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 1311 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1307 | NAG  | C3-C2-N2-C7 |
| 3   | B     | 1306 | NAG  | C3-C2-N2-C7 |
| 3   | C     | 1303 | NAG  | C3-C2-N2-C7 |
| 3   | C     | 1306 | NAG  | C3-C2-N2-C7 |
| 3   | C     | 1307 | NAG  | C3-C2-N2-C7 |
| 3   | C     | 1309 | NAG  | C3-C2-N2-C7 |
| 3   | B     | 1305 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1305 | NAG  | O5-C5-C6-O6 |
| 3   | A     | 1304 | NAG  | C4-C5-C6-O6 |
| 3   | B     | 1306 | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1306 | NAG  | C1-C2-N2-C7 |
| 3   | C     | 1309 | NAG  | C1-C2-N2-C7 |
| 3   | B     | 1306 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1311 | NAG  | C3-C2-N2-C7 |
| 3   | A     | 1304 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

6 monomers are involved in 7 short contacts:

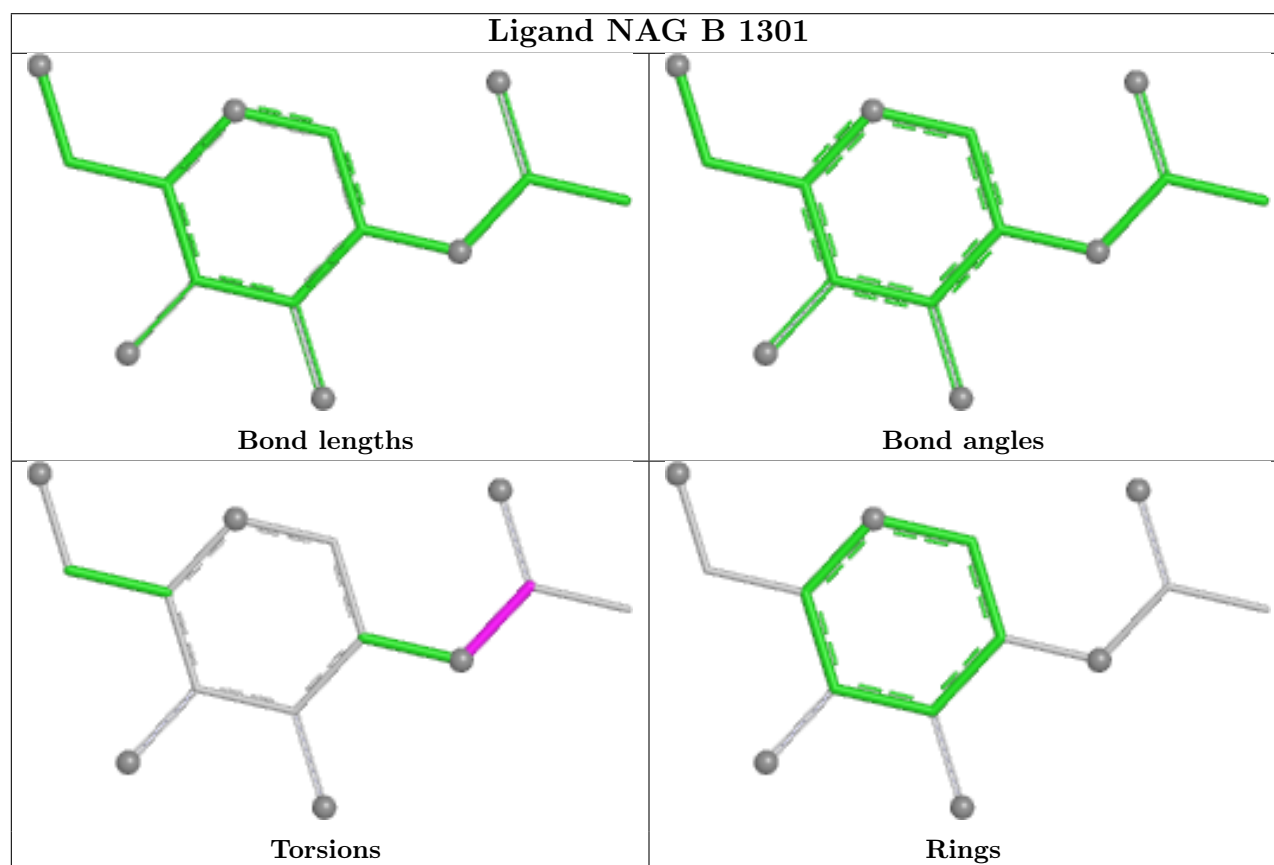
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 1303 | NAG  | 1       | 0            |
| 3   | A     | 1302 | NAG  | 2       | 0            |
| 3   | A     | 1306 | NAG  | 1       | 0            |
| 3   | B     | 1306 | NAG  | 1       | 0            |
| 3   | B     | 1308 | NAG  | 1       | 0            |

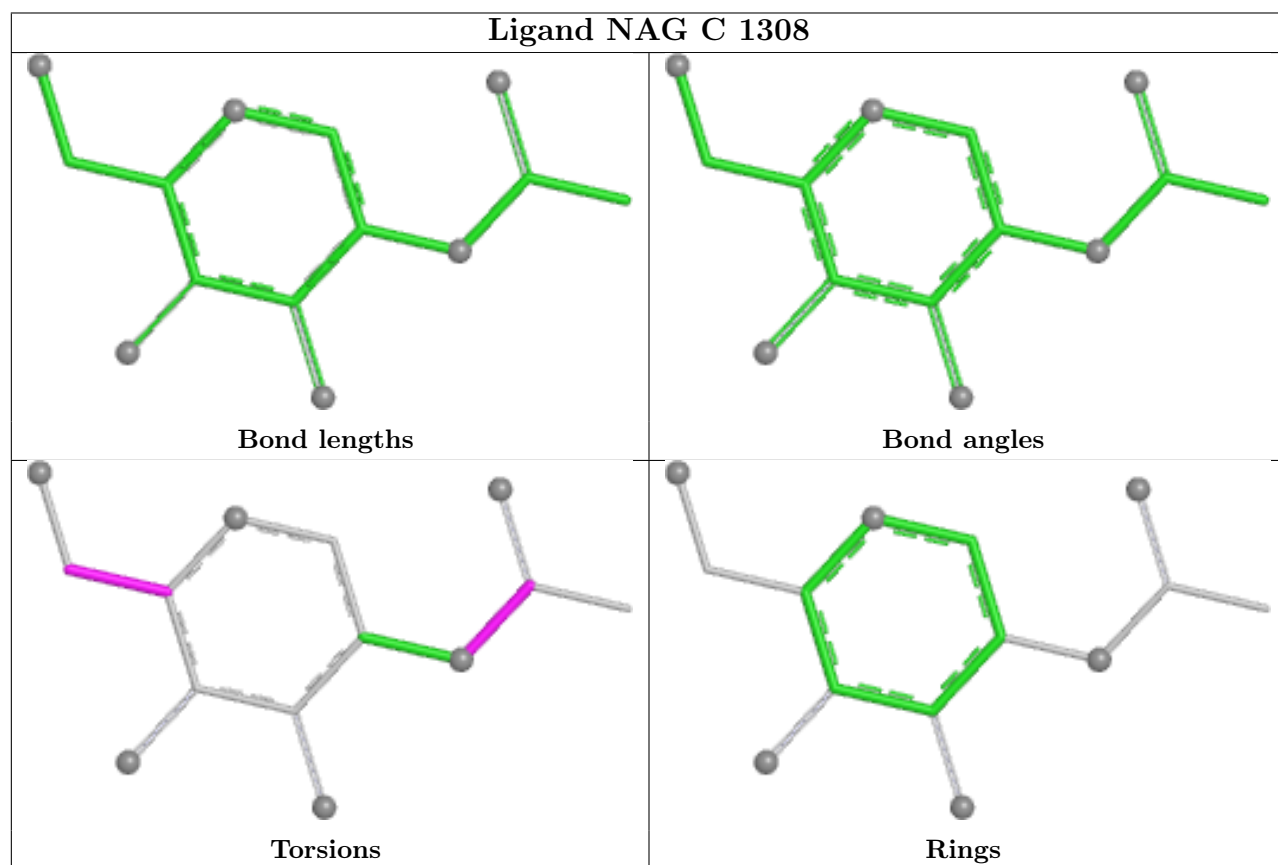
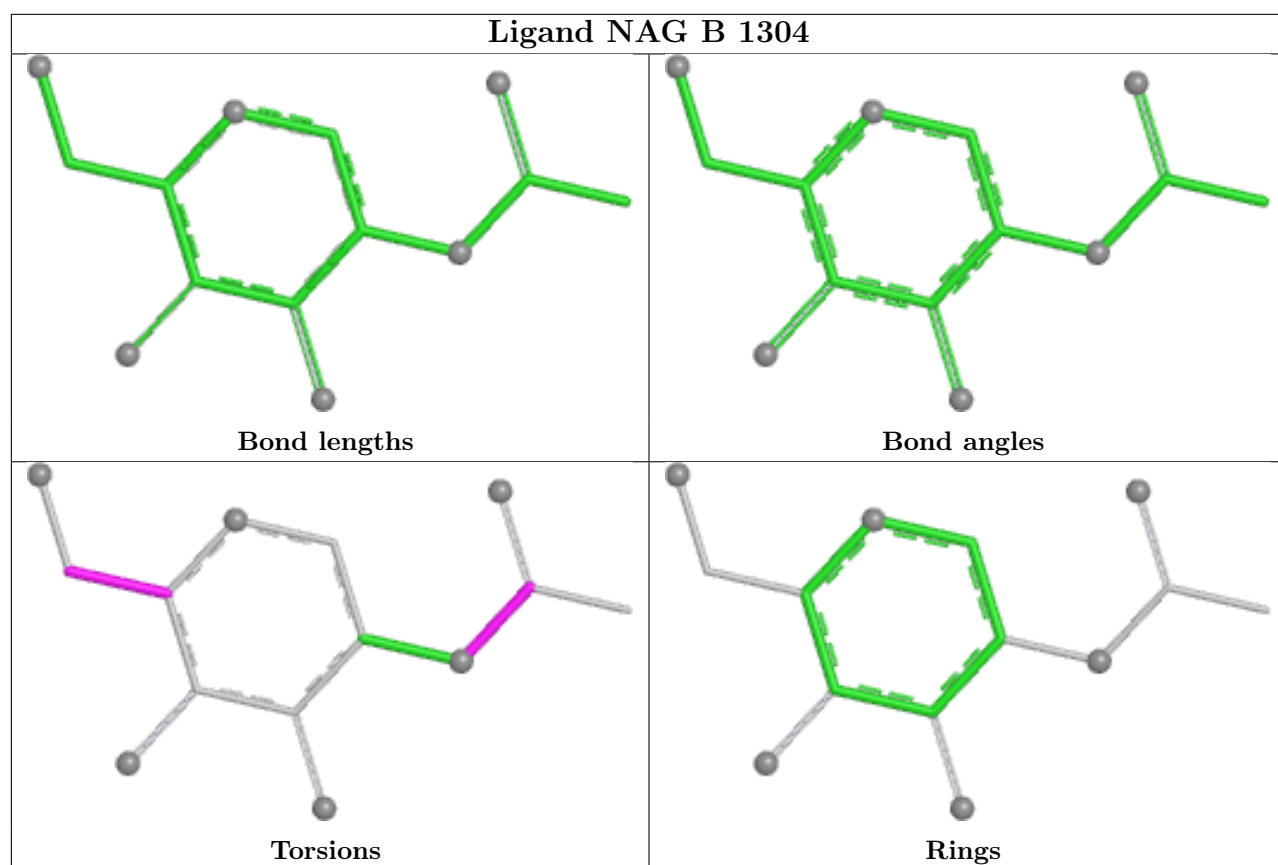
*Continued on next page...*

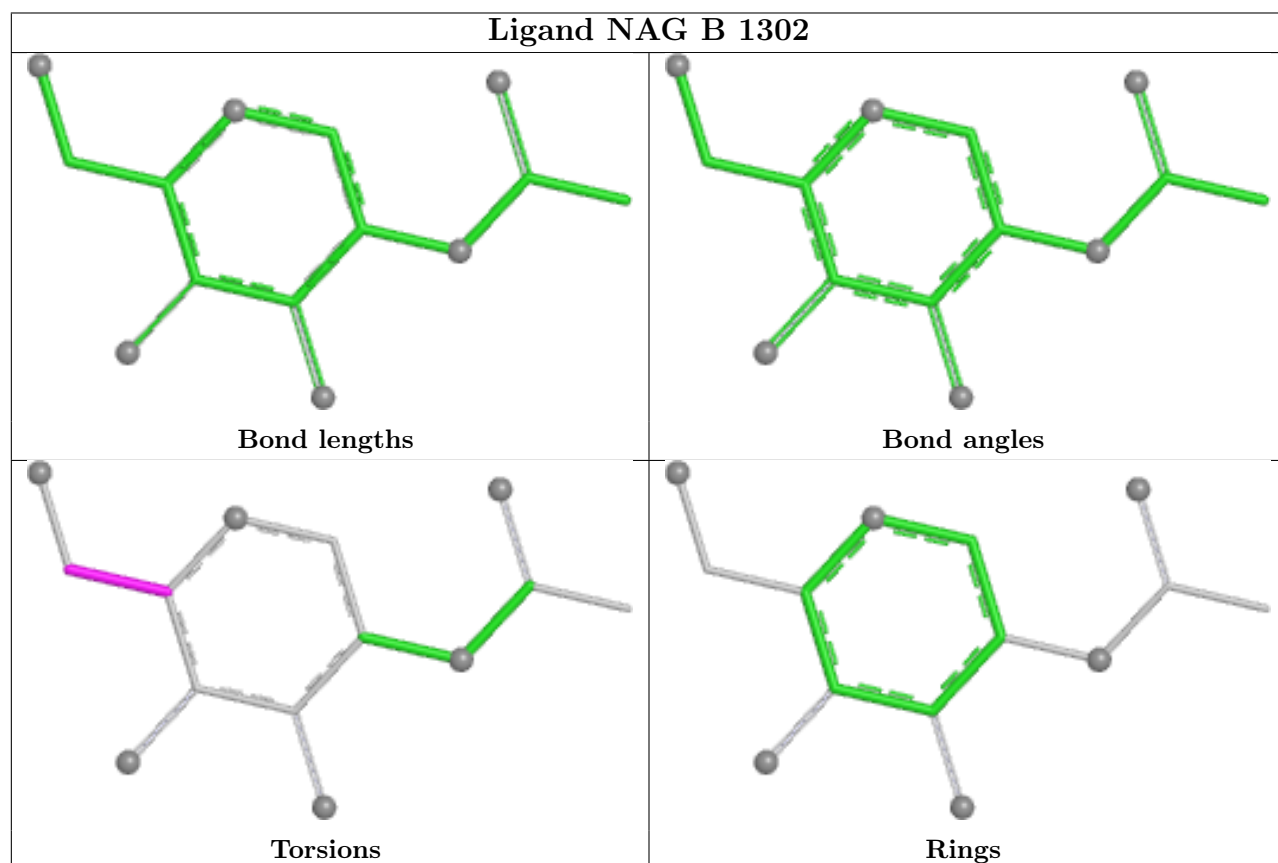
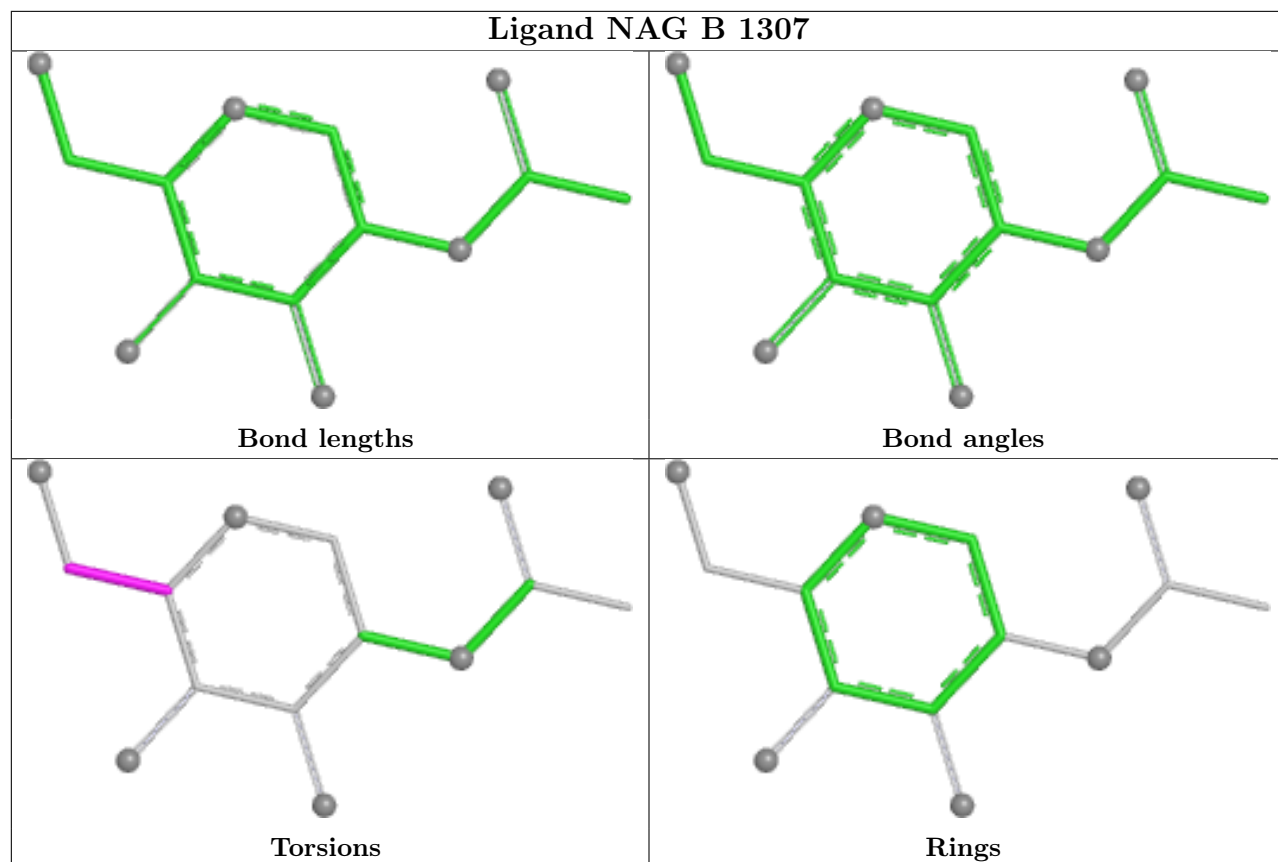
Continued from previous page...

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | C     | 1301 | NAG  | 1       | 0            |

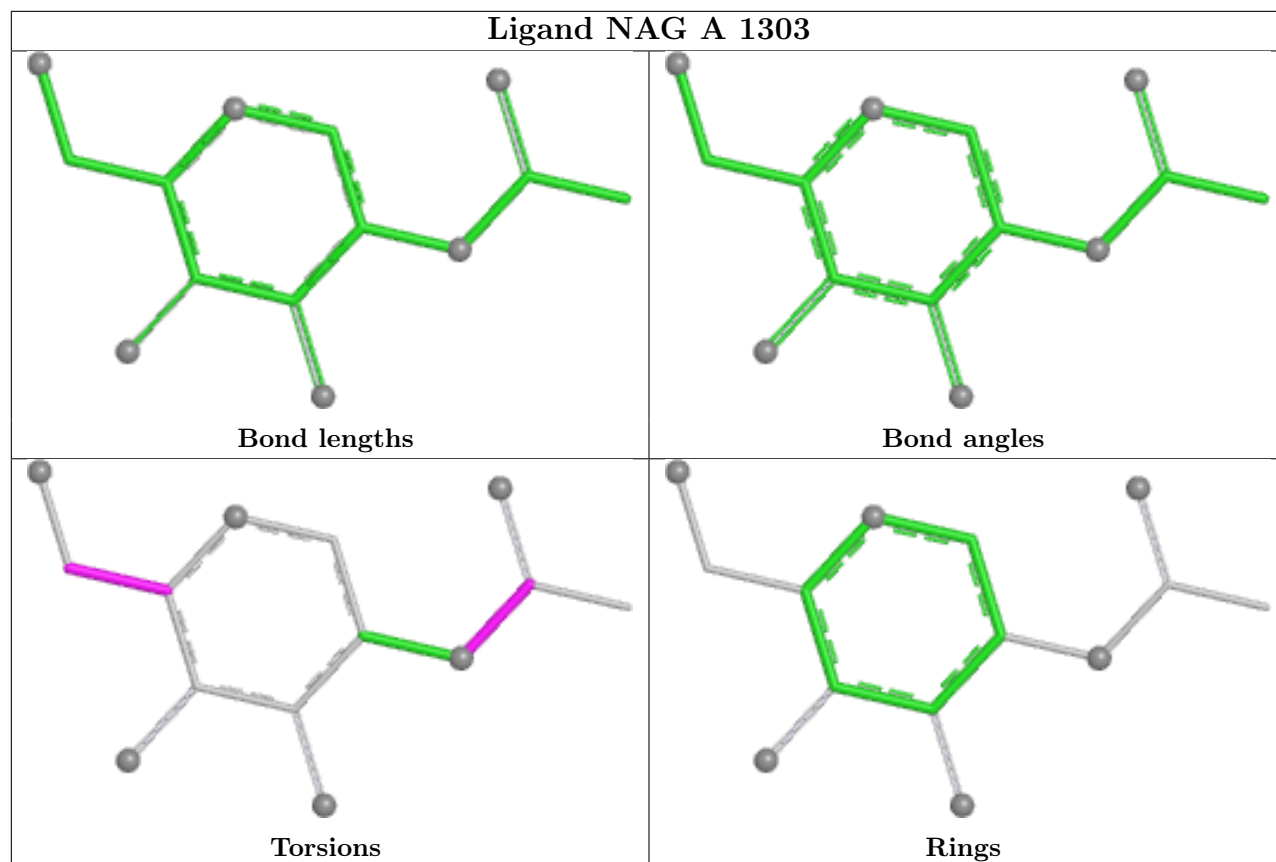
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



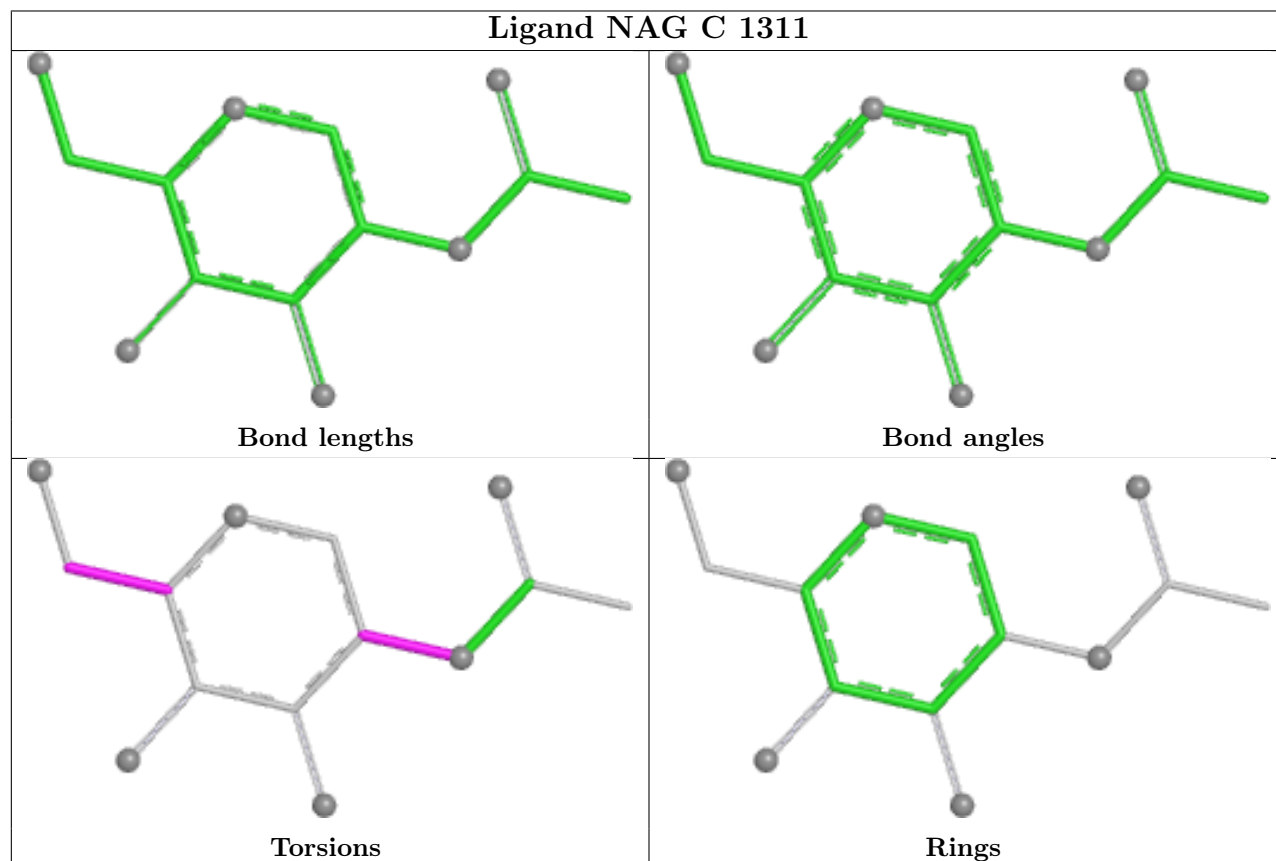


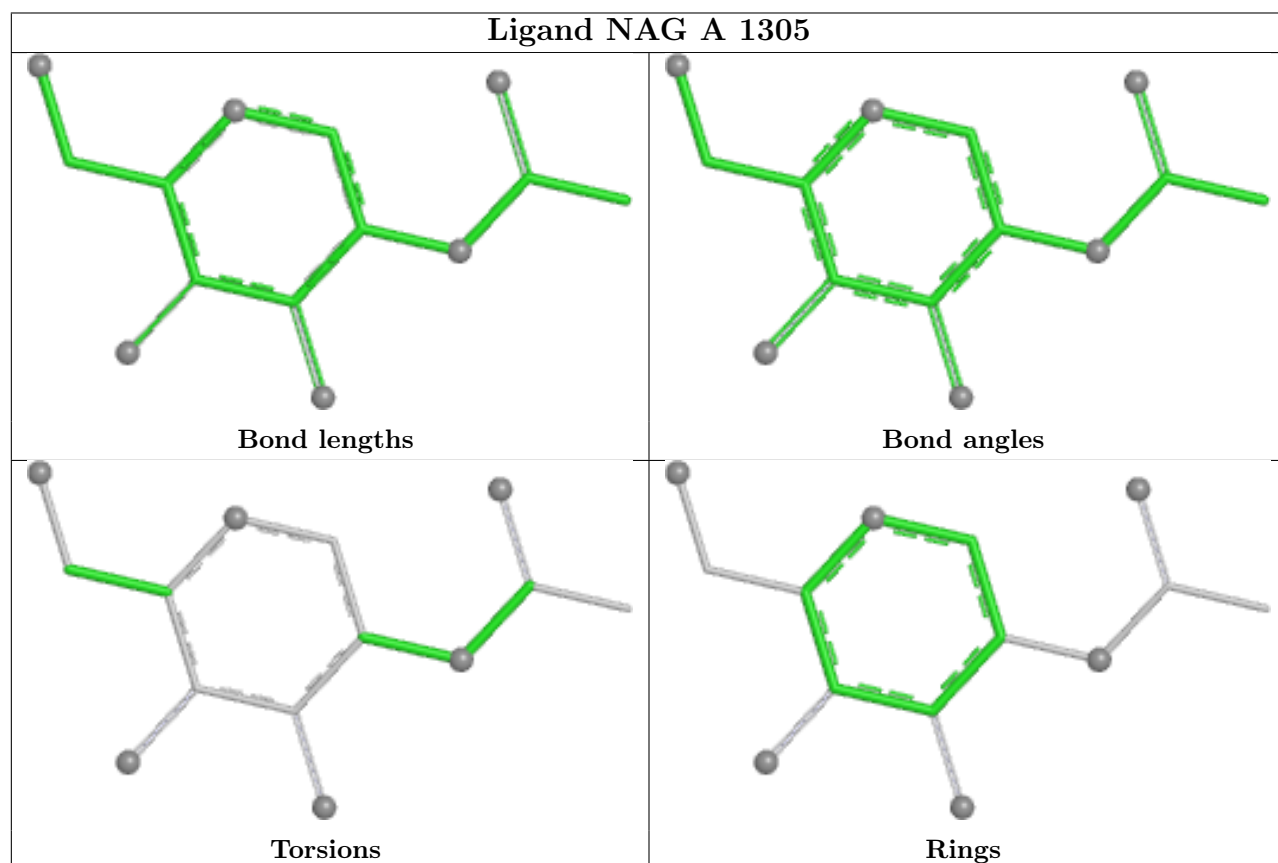
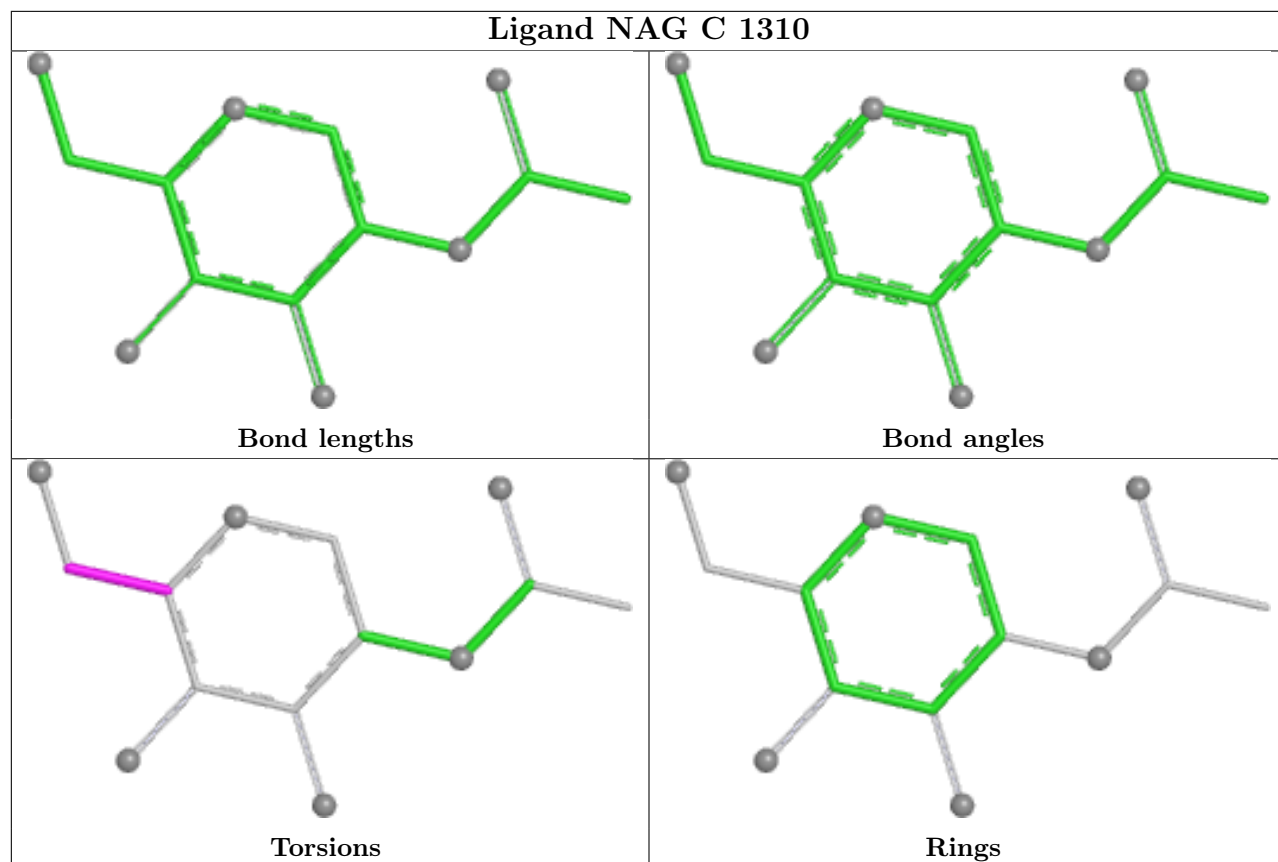


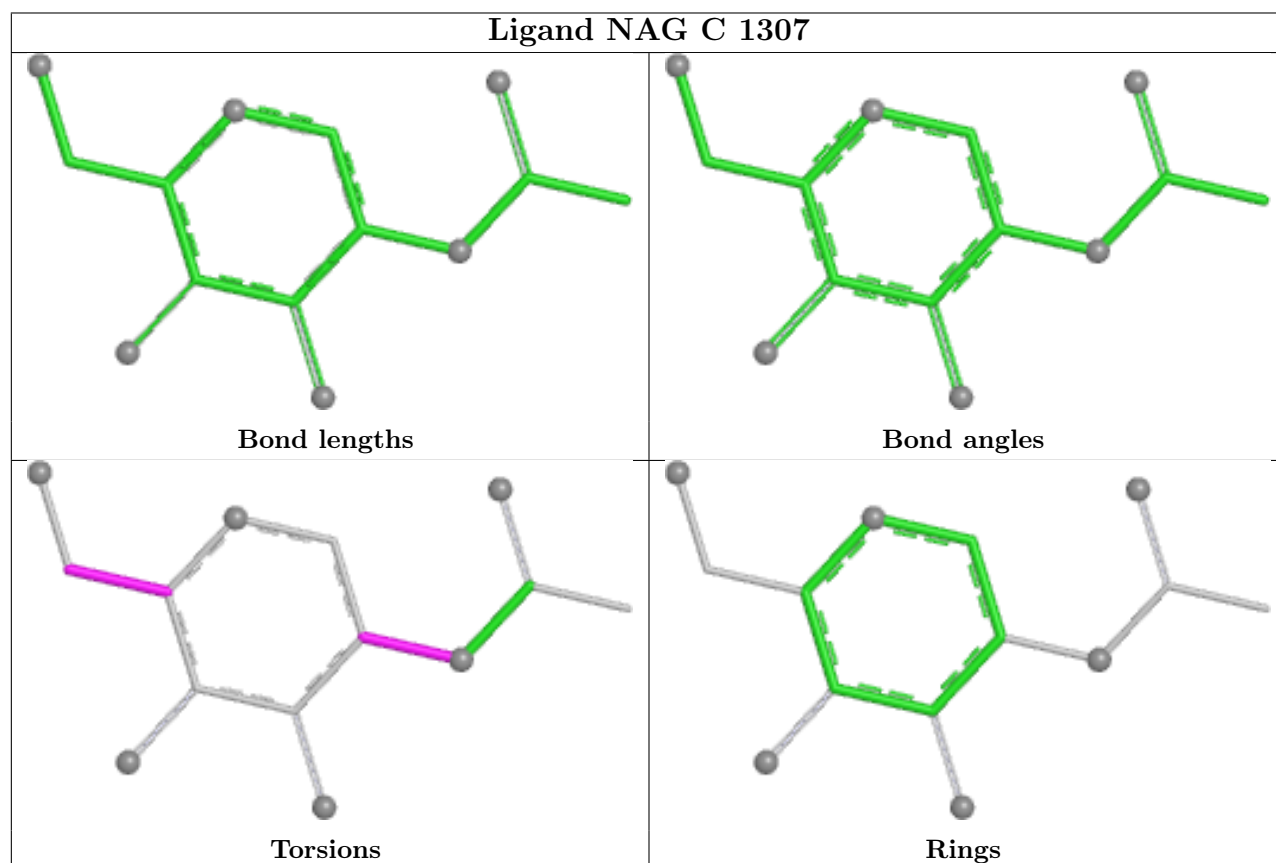
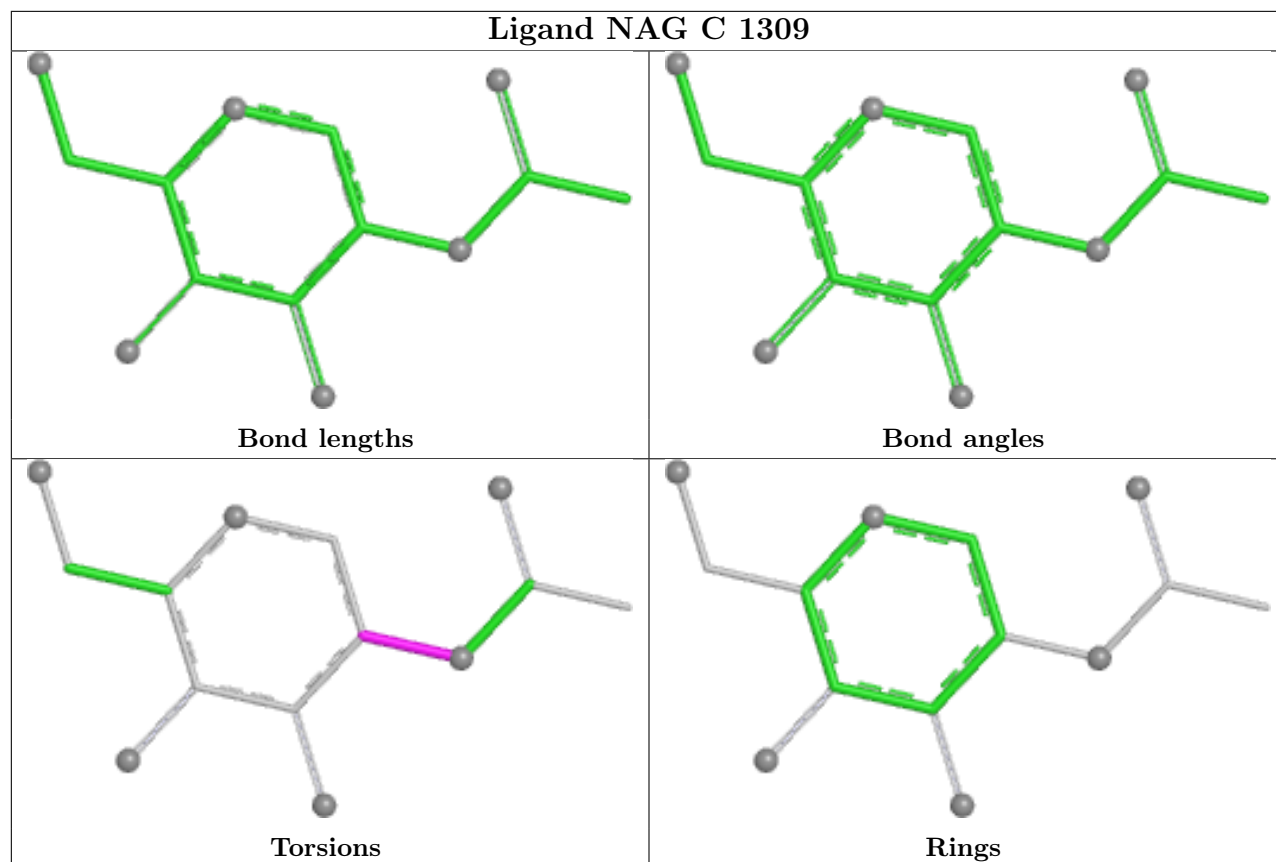
## Ligand NAG A 1303



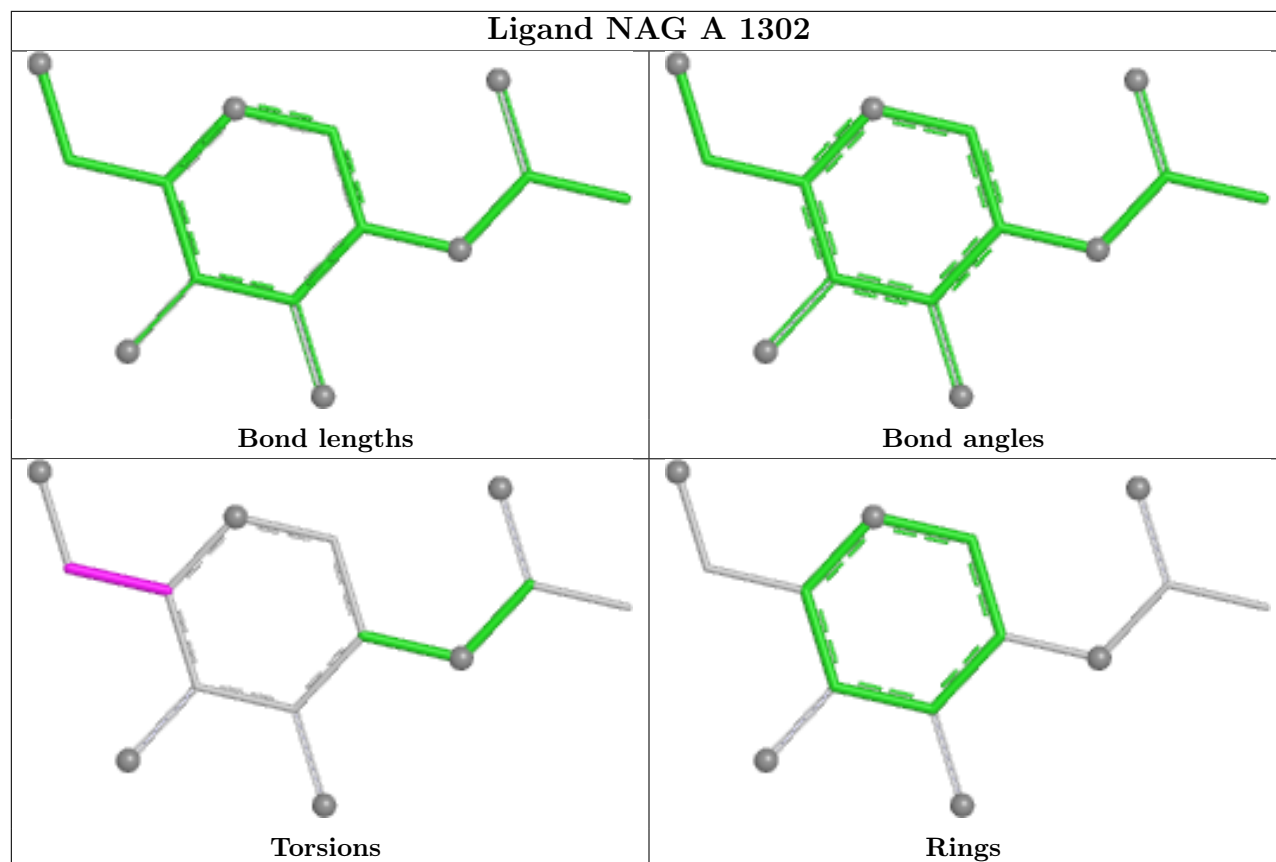
## Ligand NAG C 1311



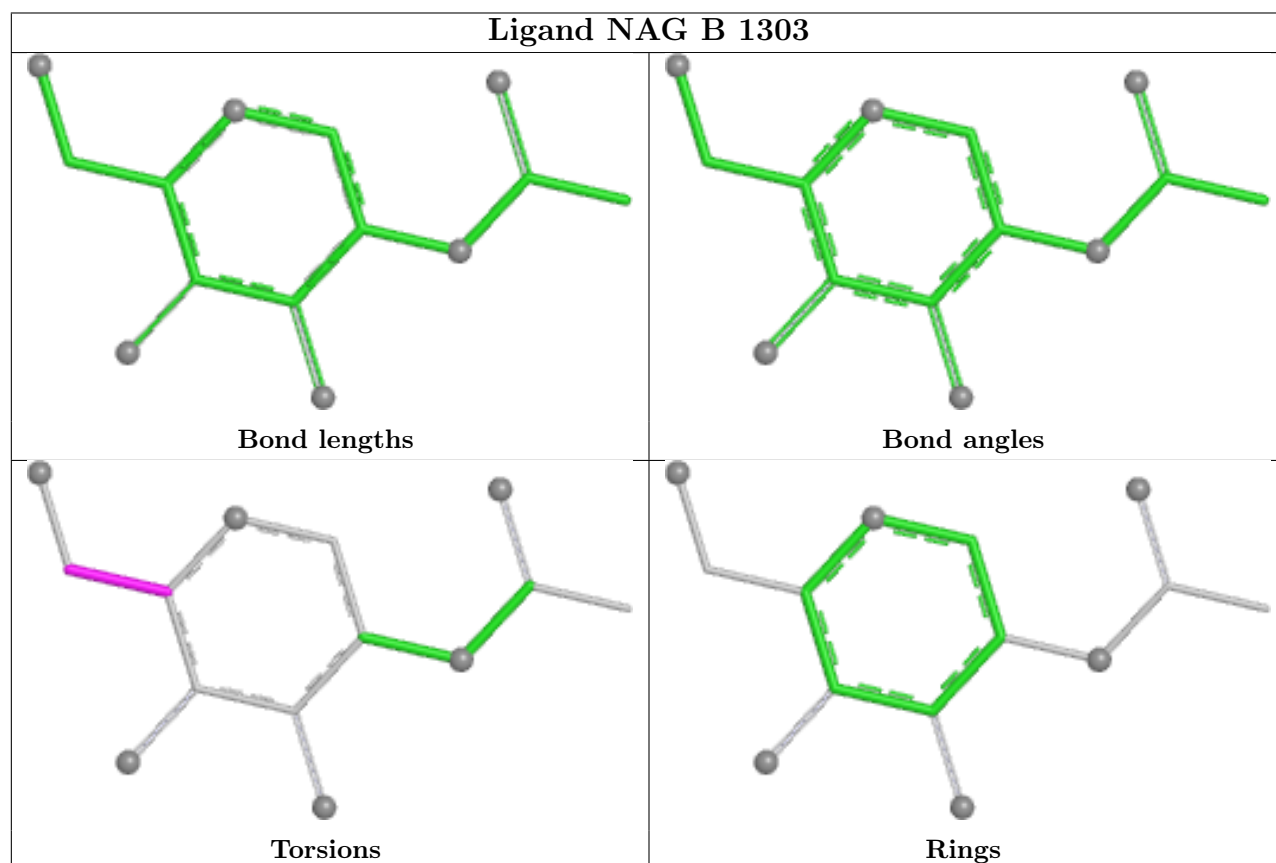


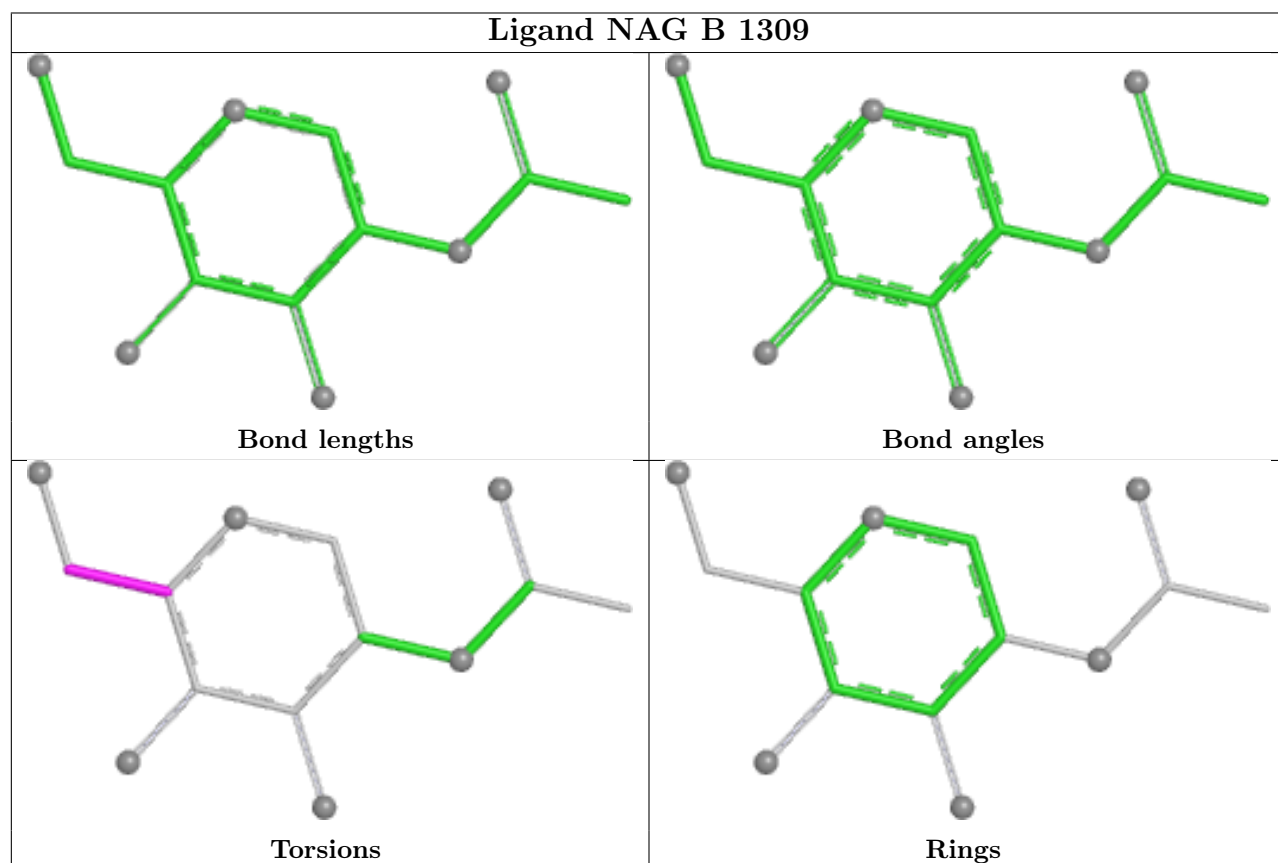
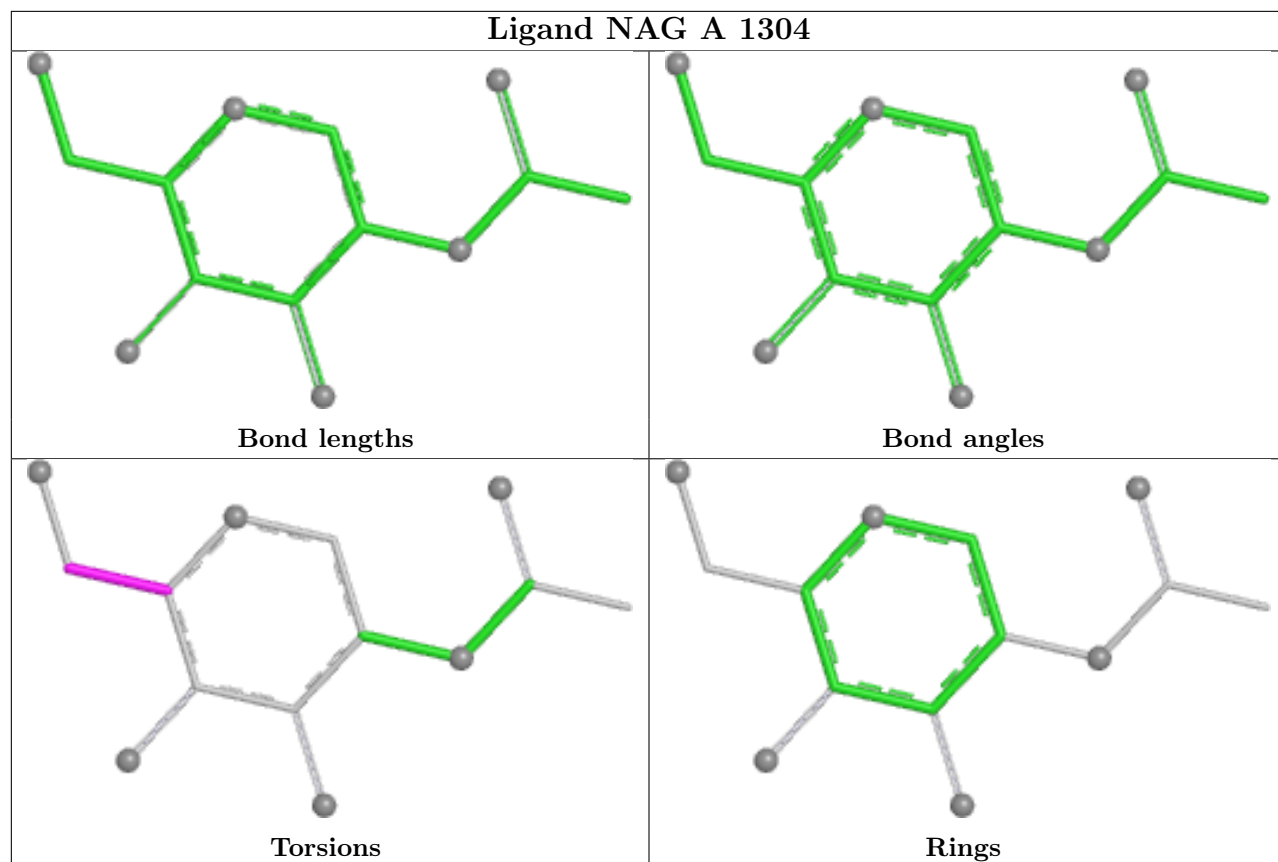


## Ligand NAG A 1302

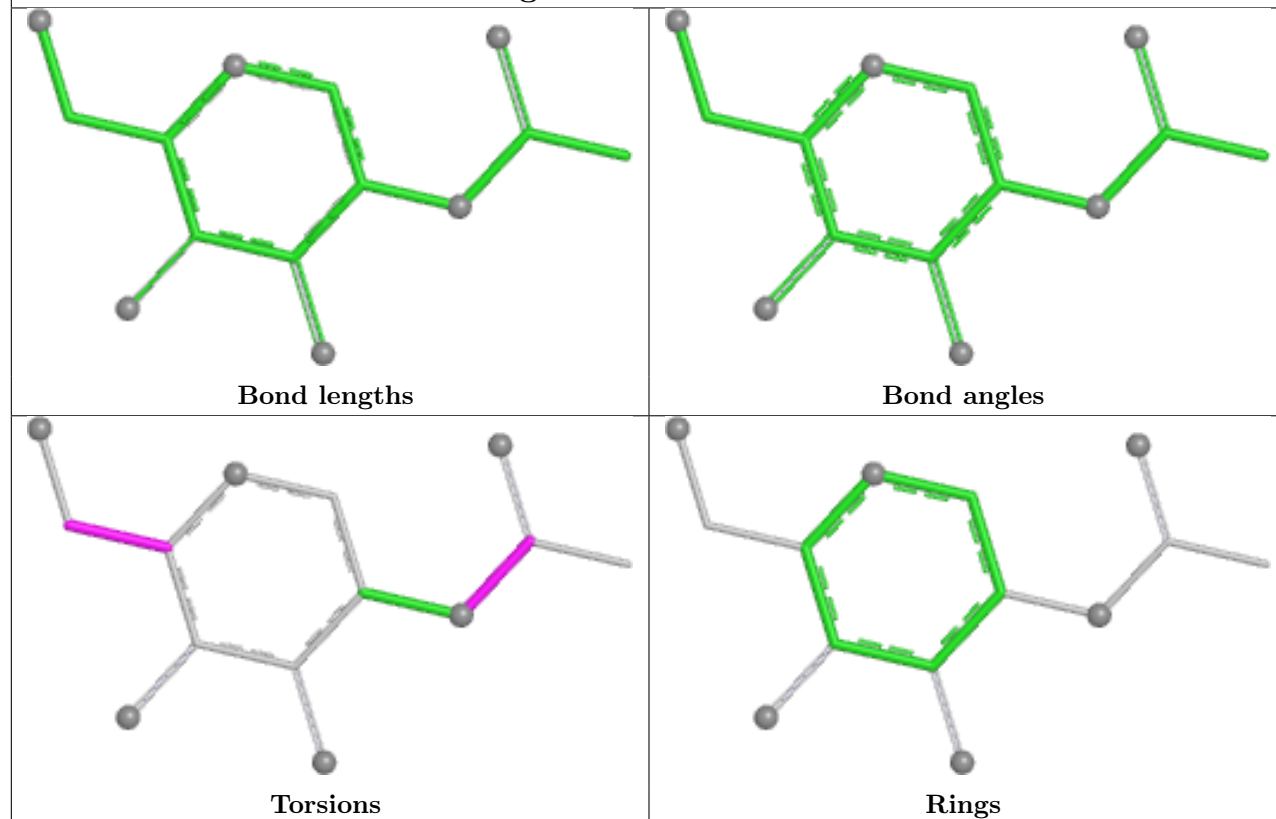


## Ligand NAG B 1303

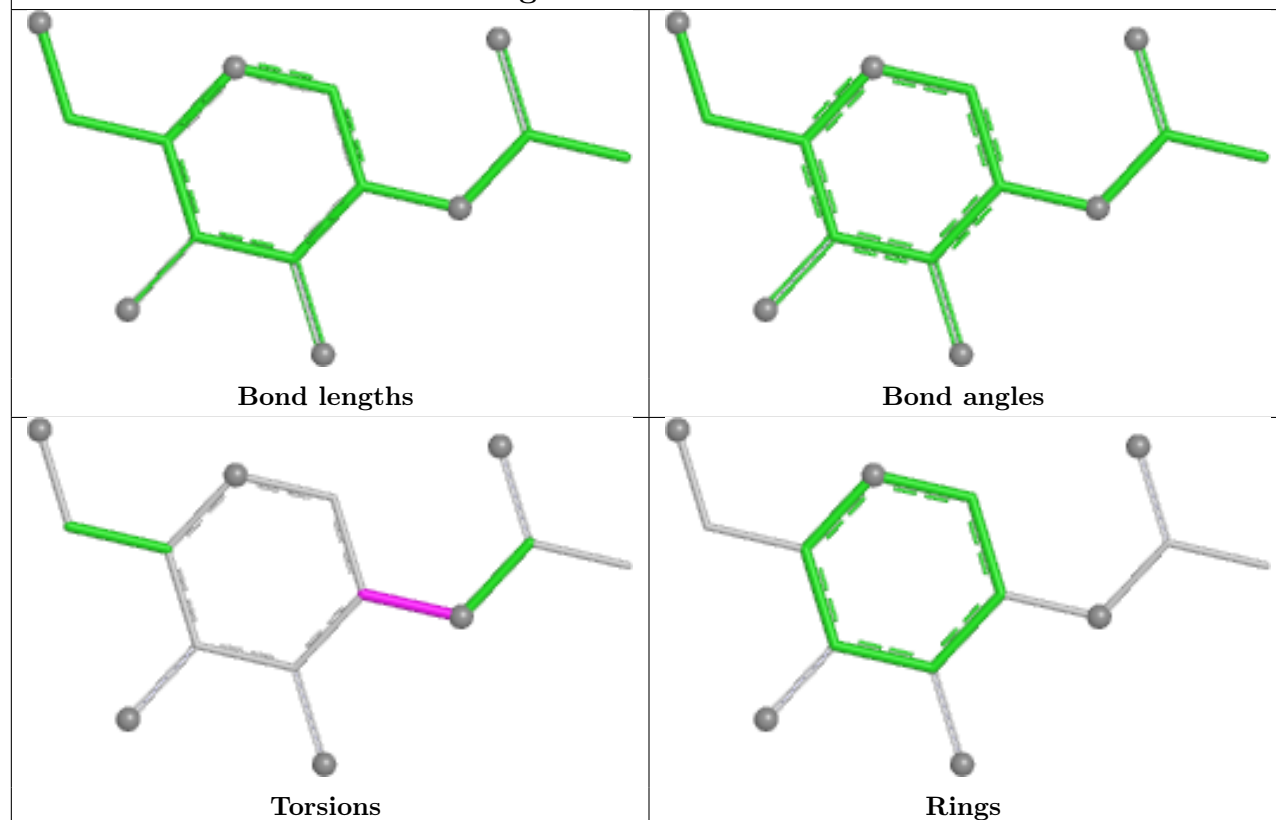




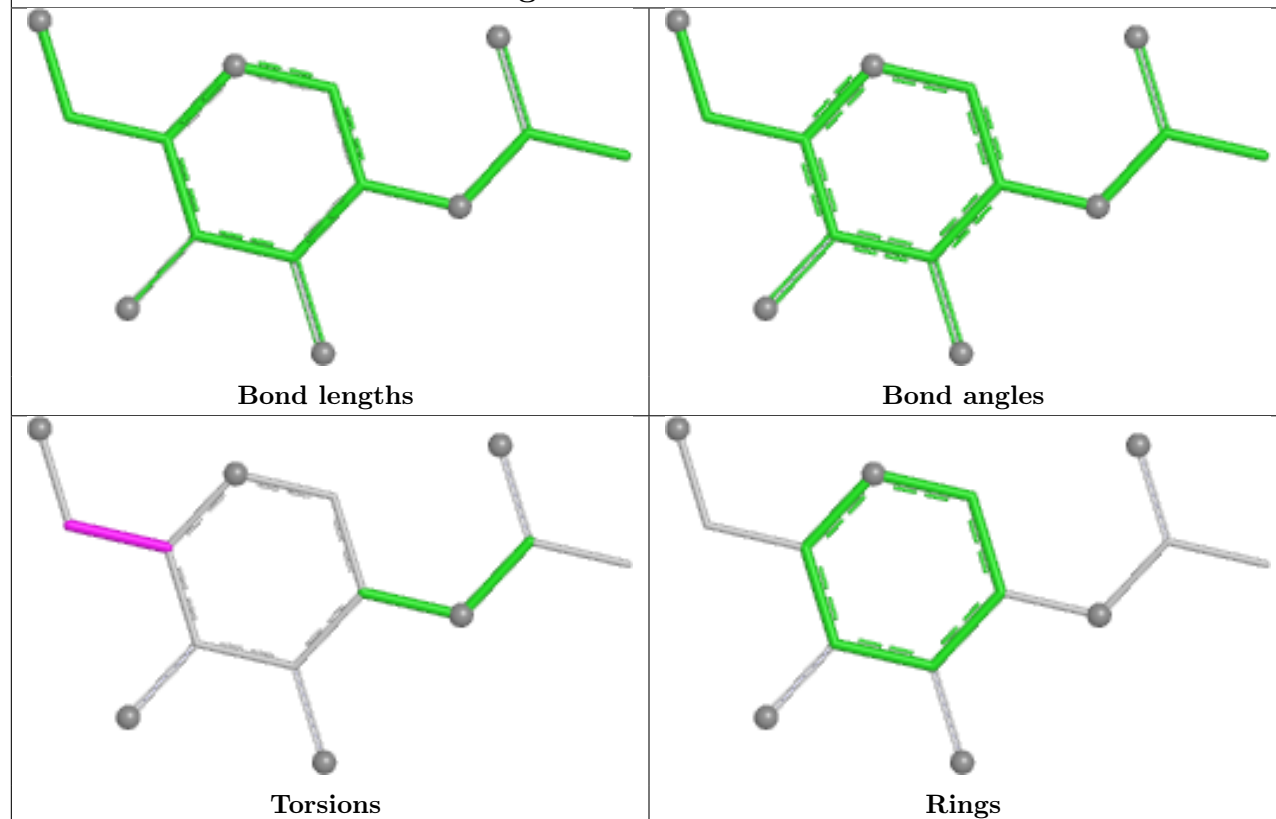
## Ligand NAG B 1305



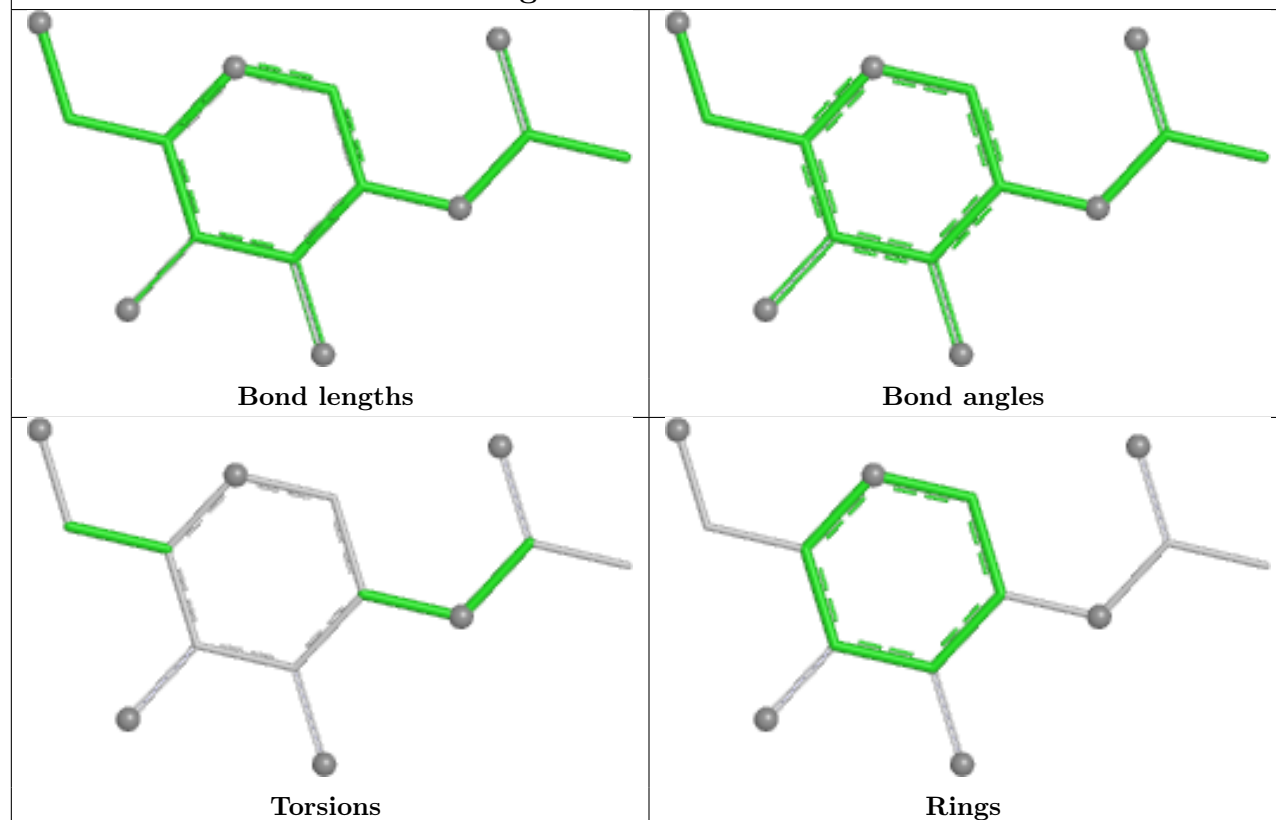
## Ligand NAG C 1306



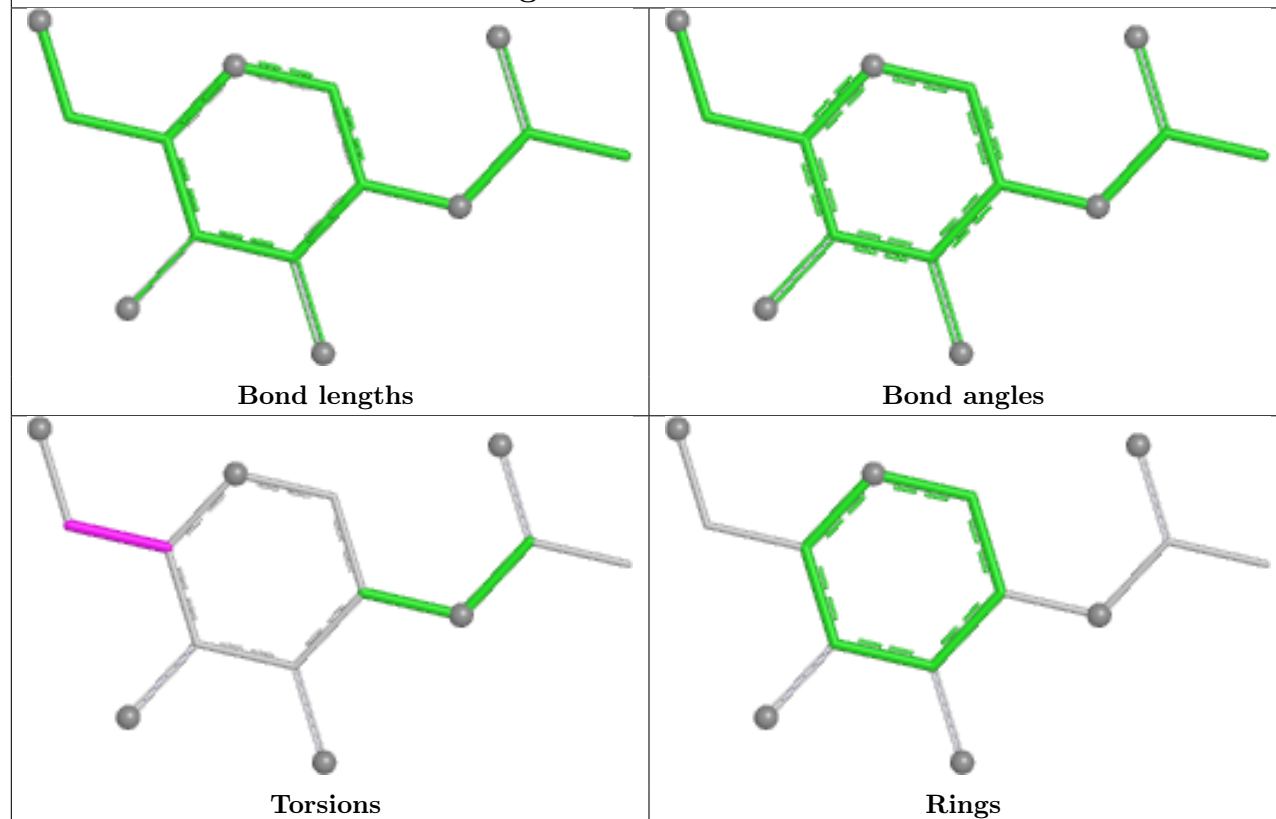
## Ligand NAG A 1309



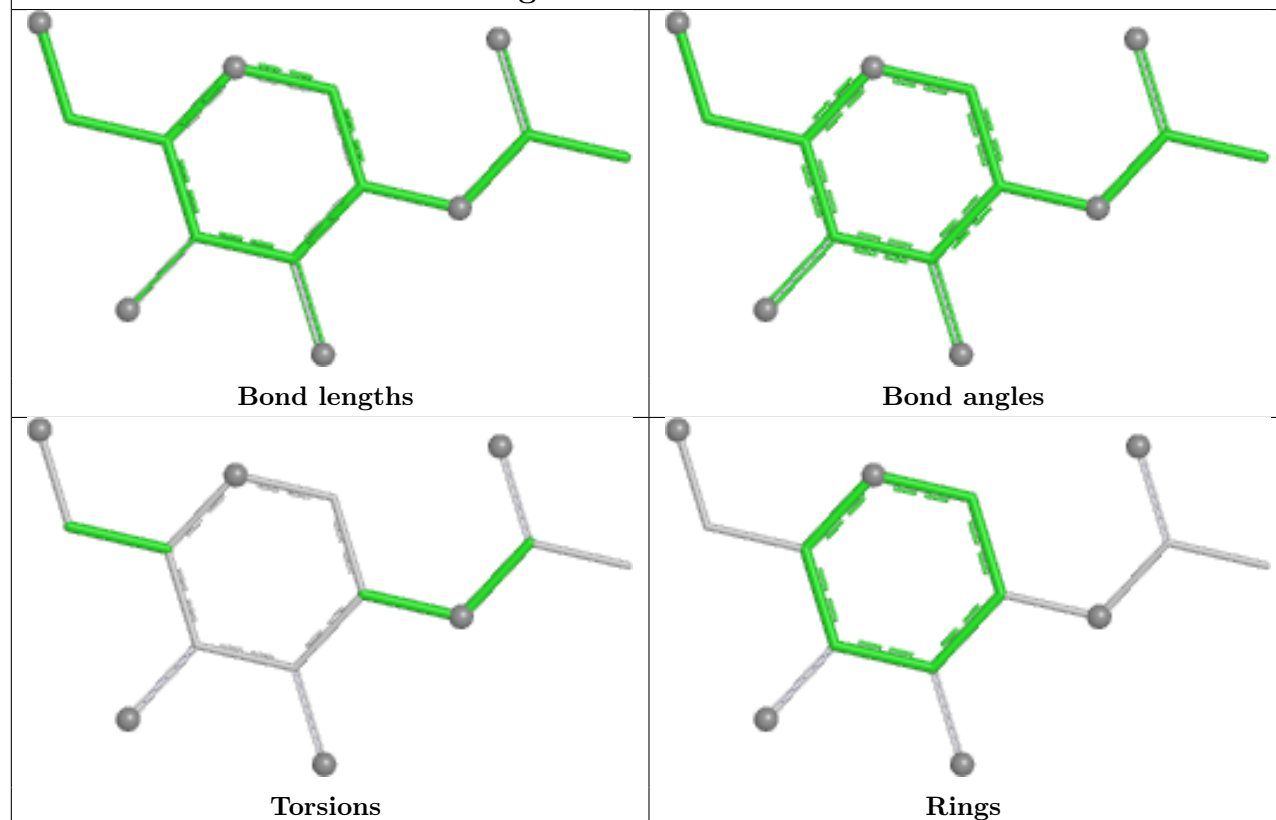
## Ligand NAG B 1310



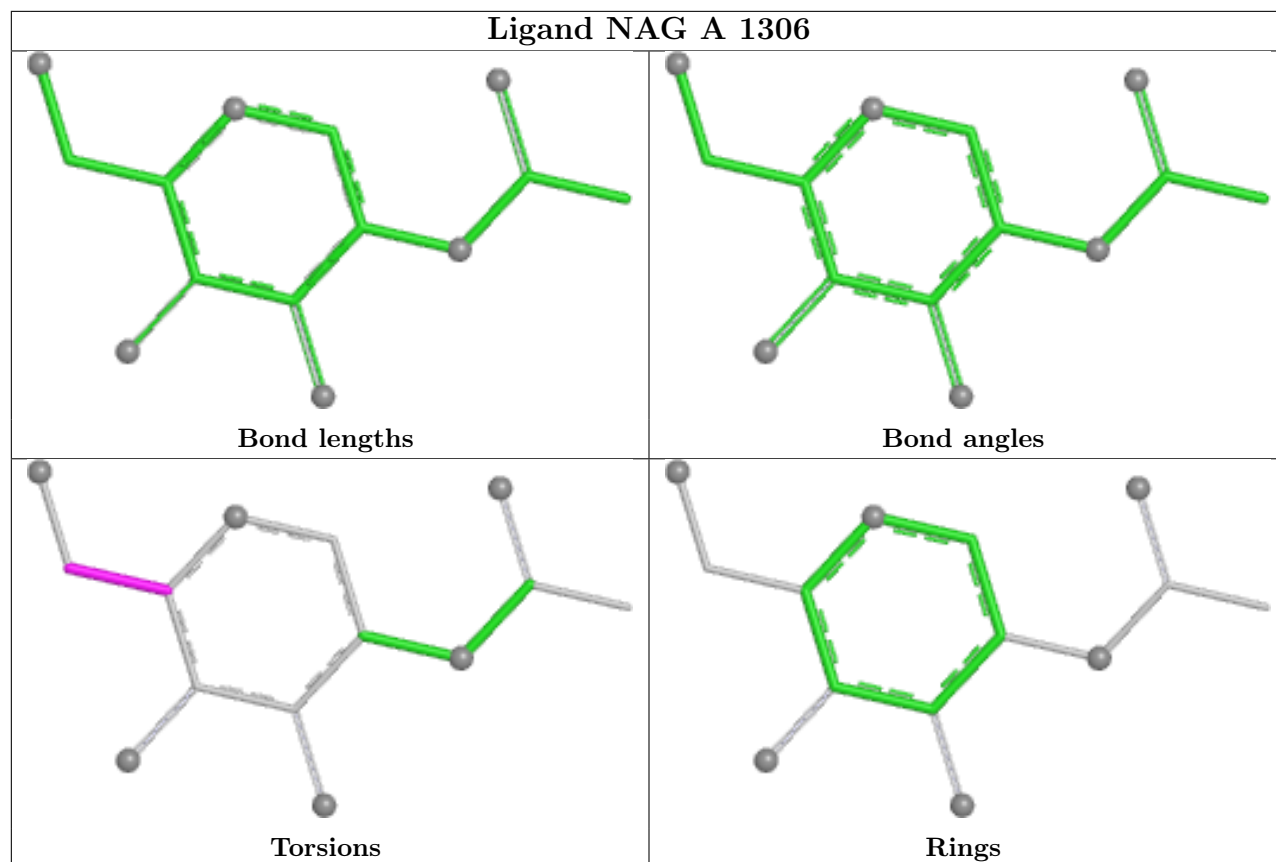
## Ligand NAG C 1302



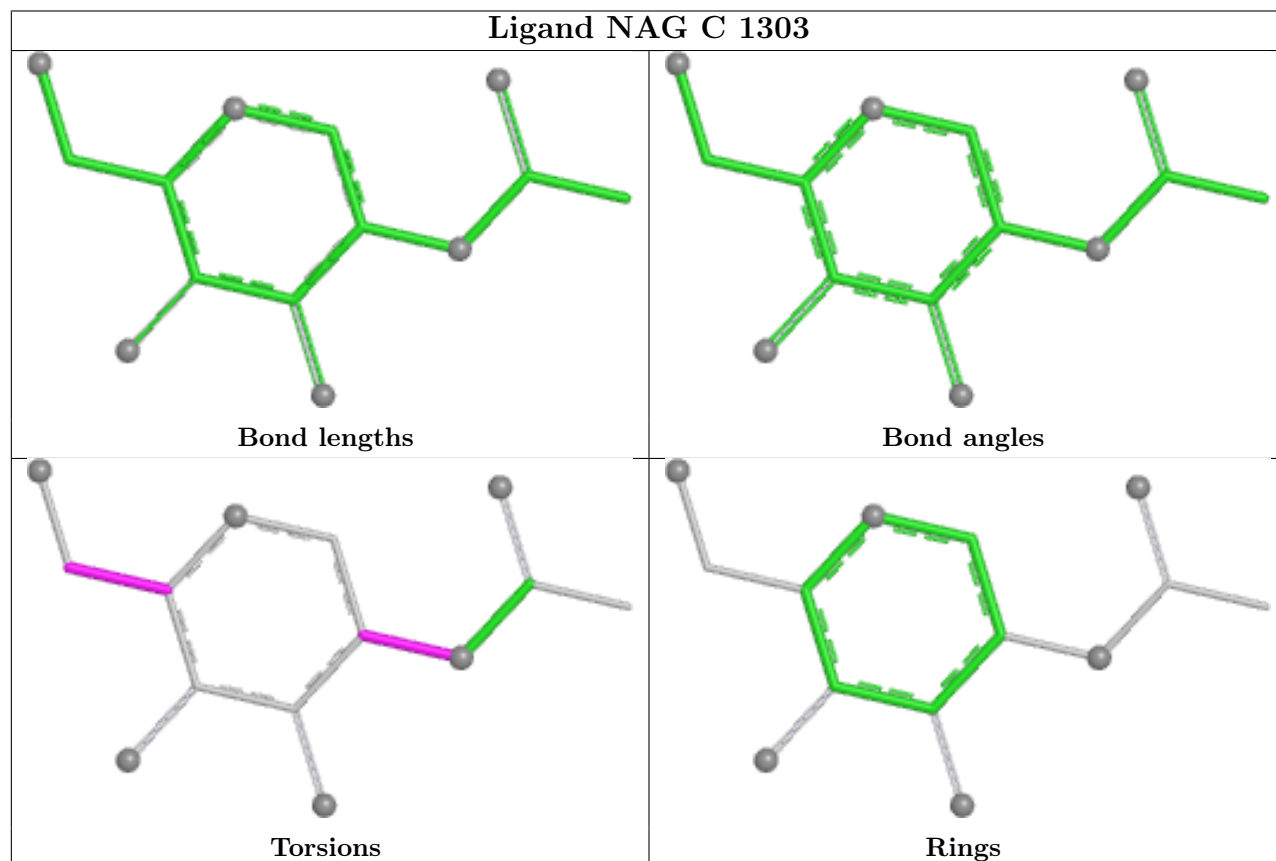
## Ligand NAG A 1308



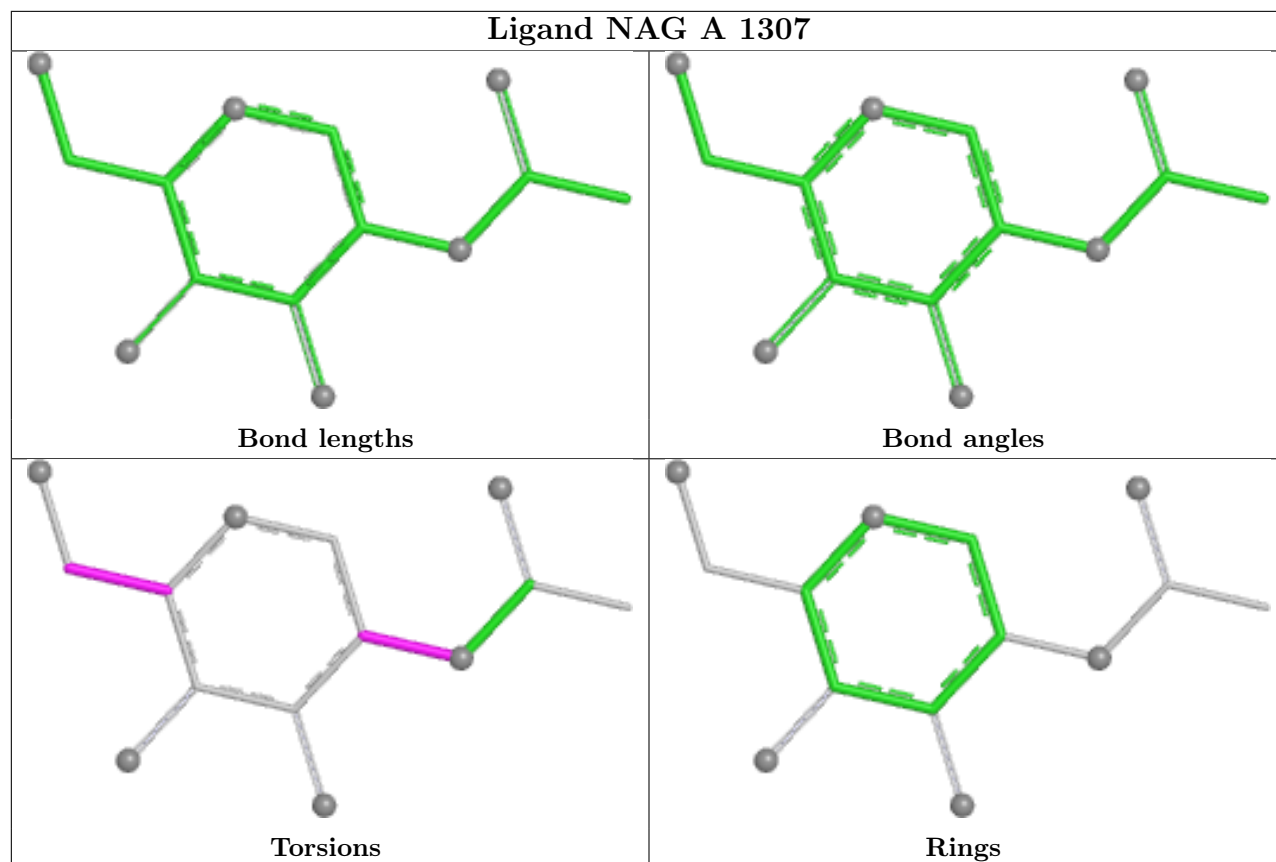
## Ligand NAG A 1306



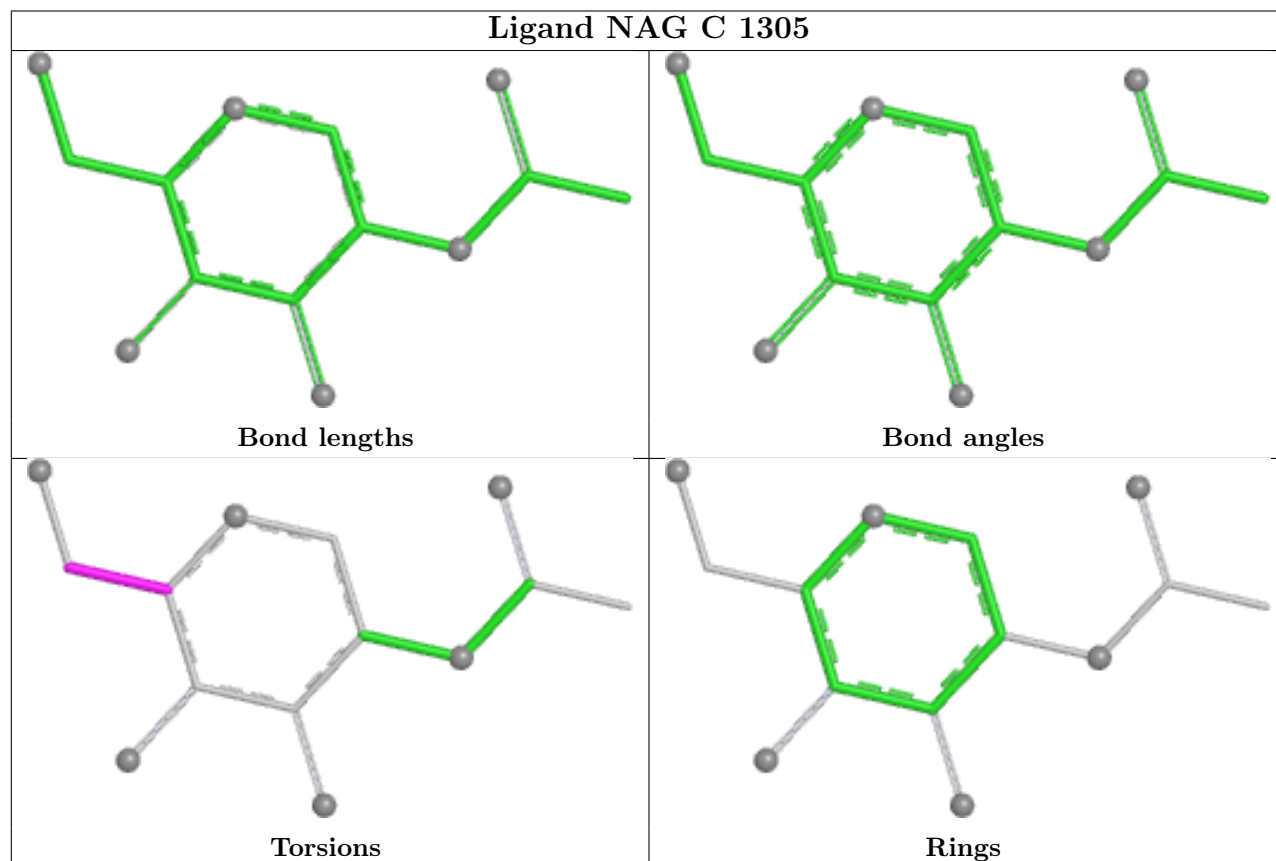
## Ligand NAG C 1303



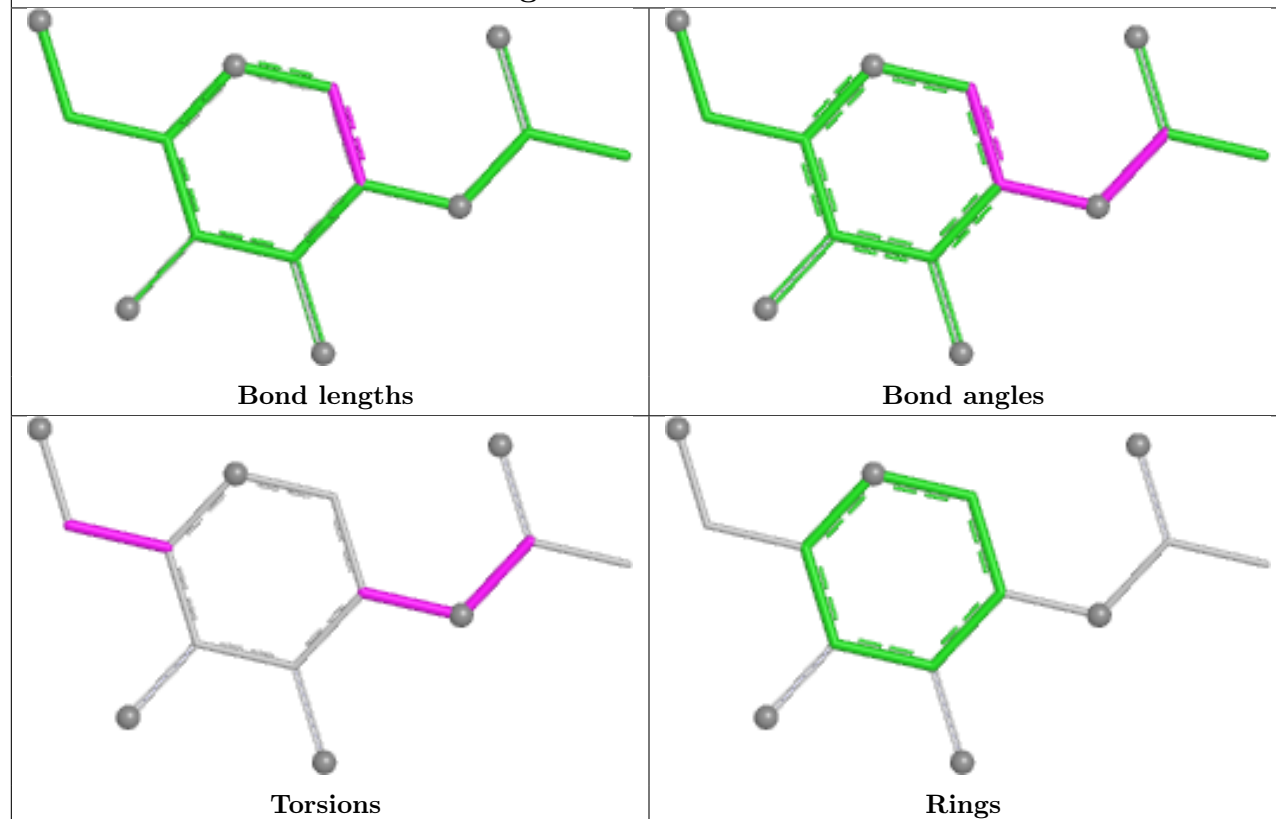
## Ligand NAG A 1307



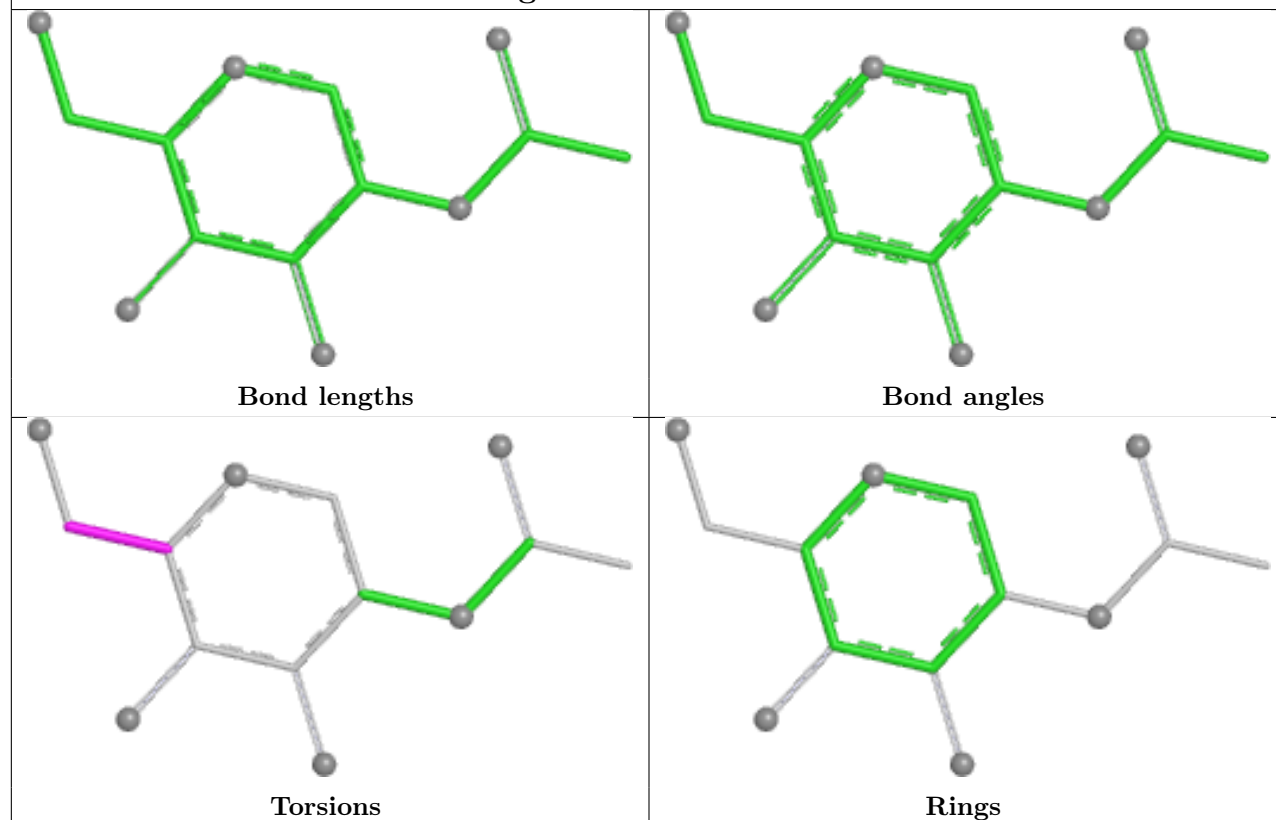
## Ligand NAG C 1305

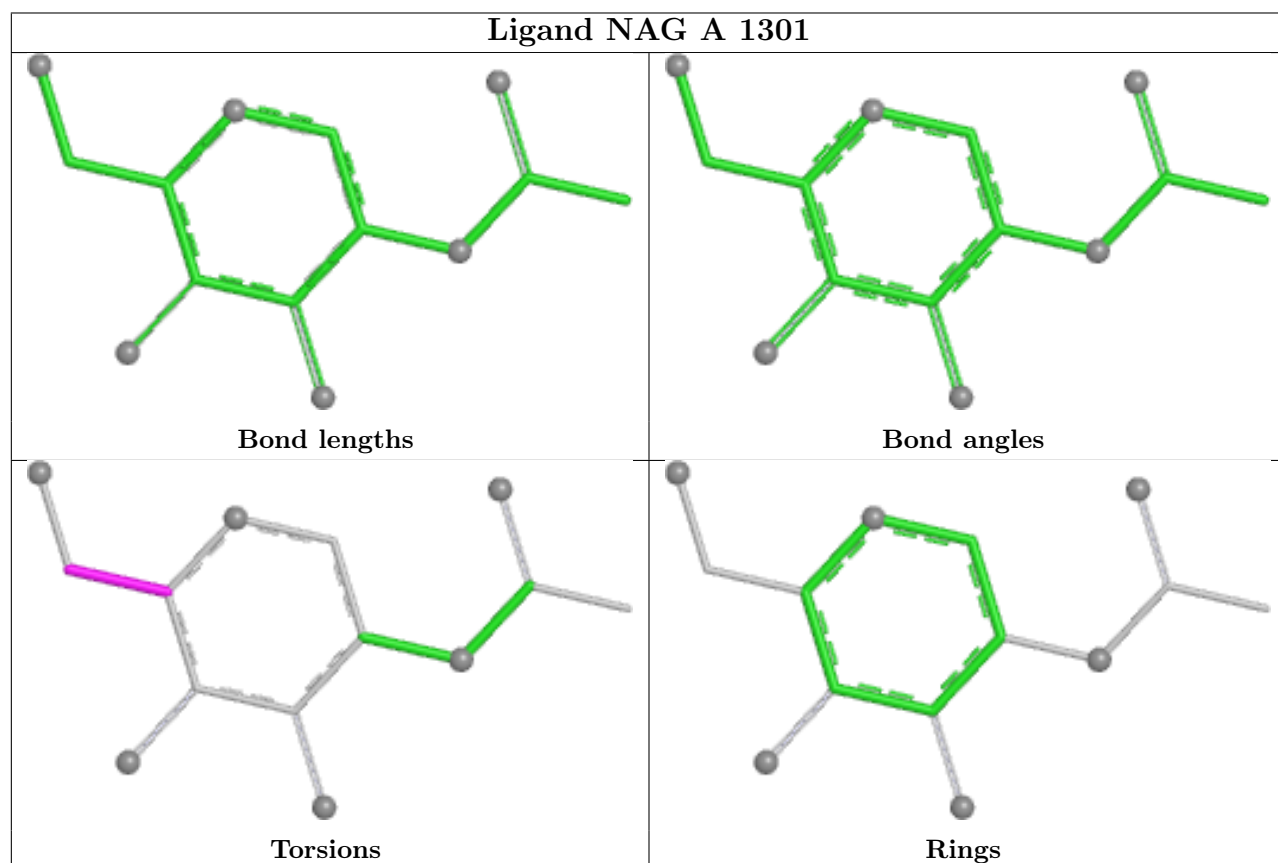
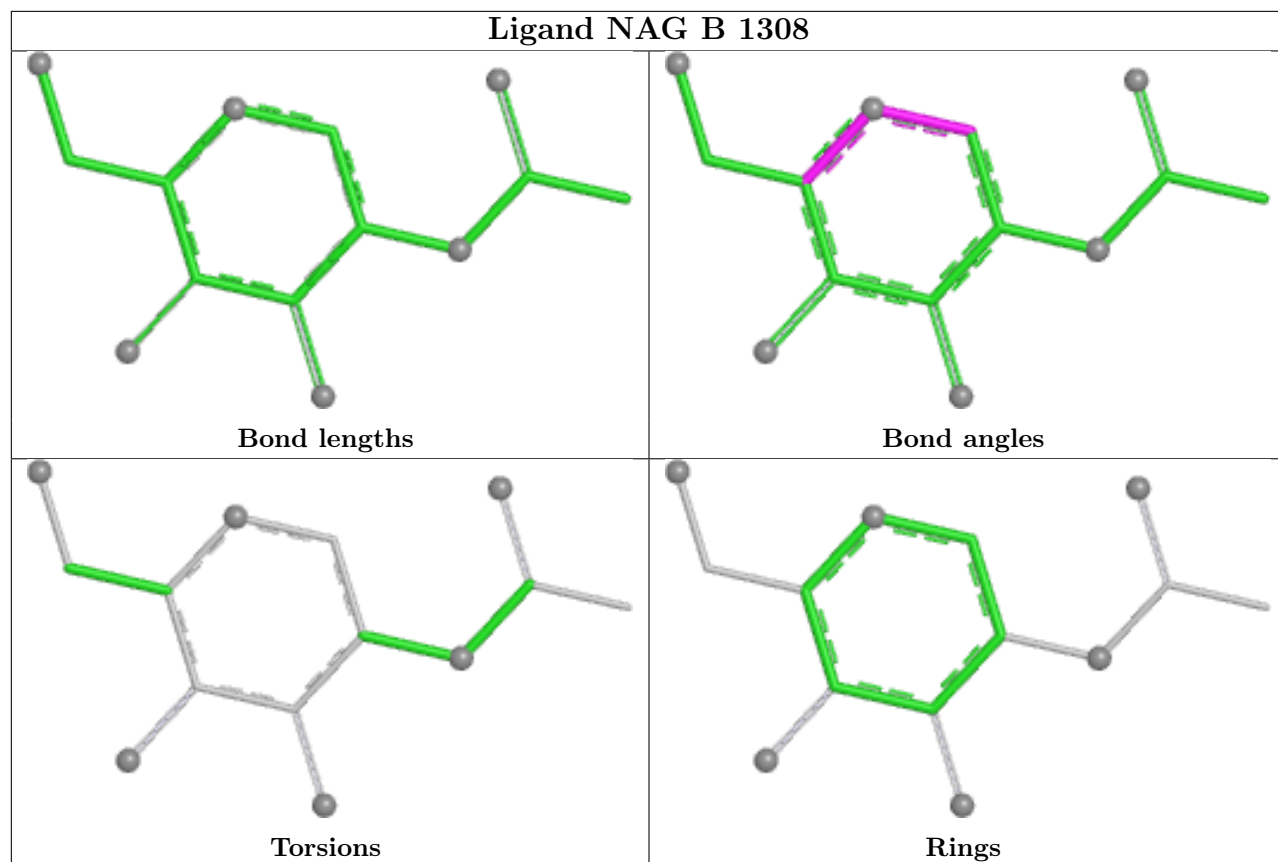


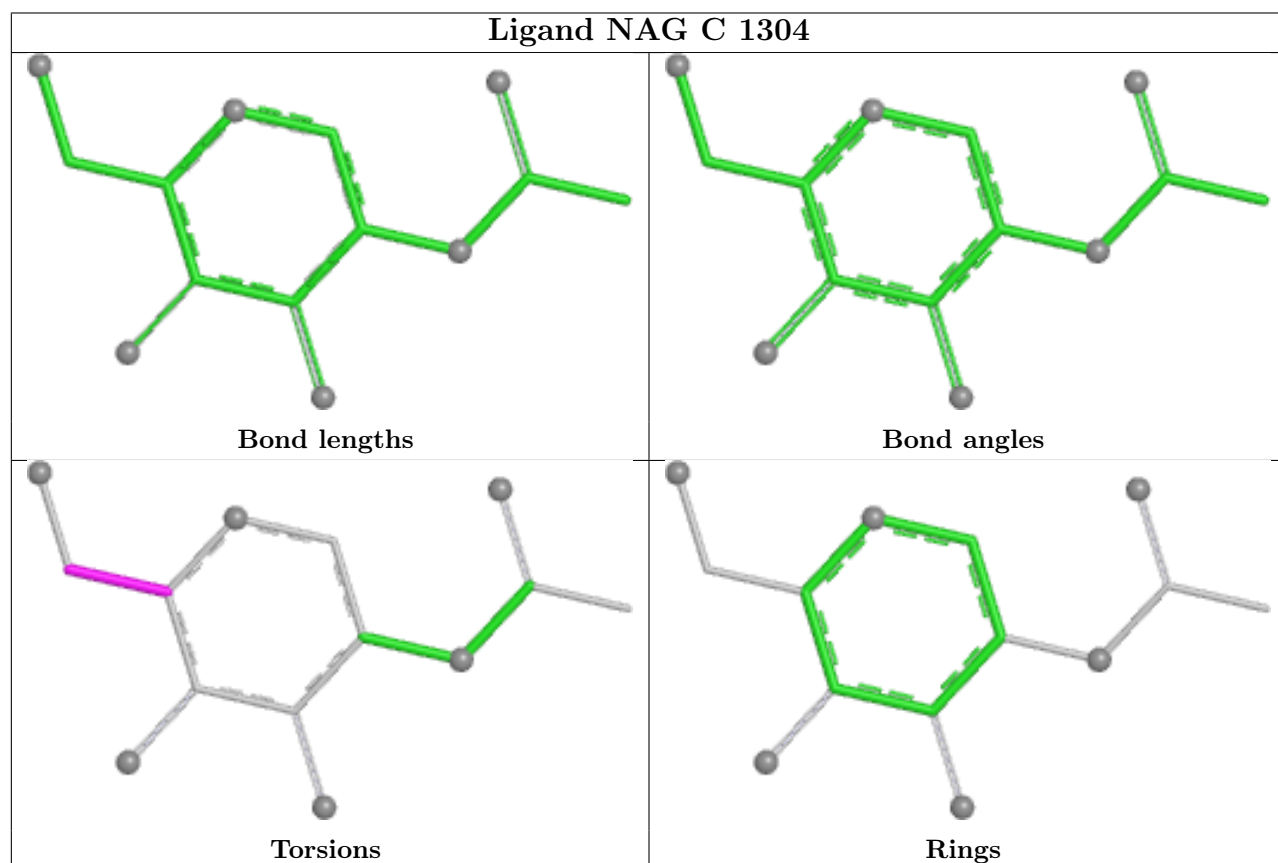
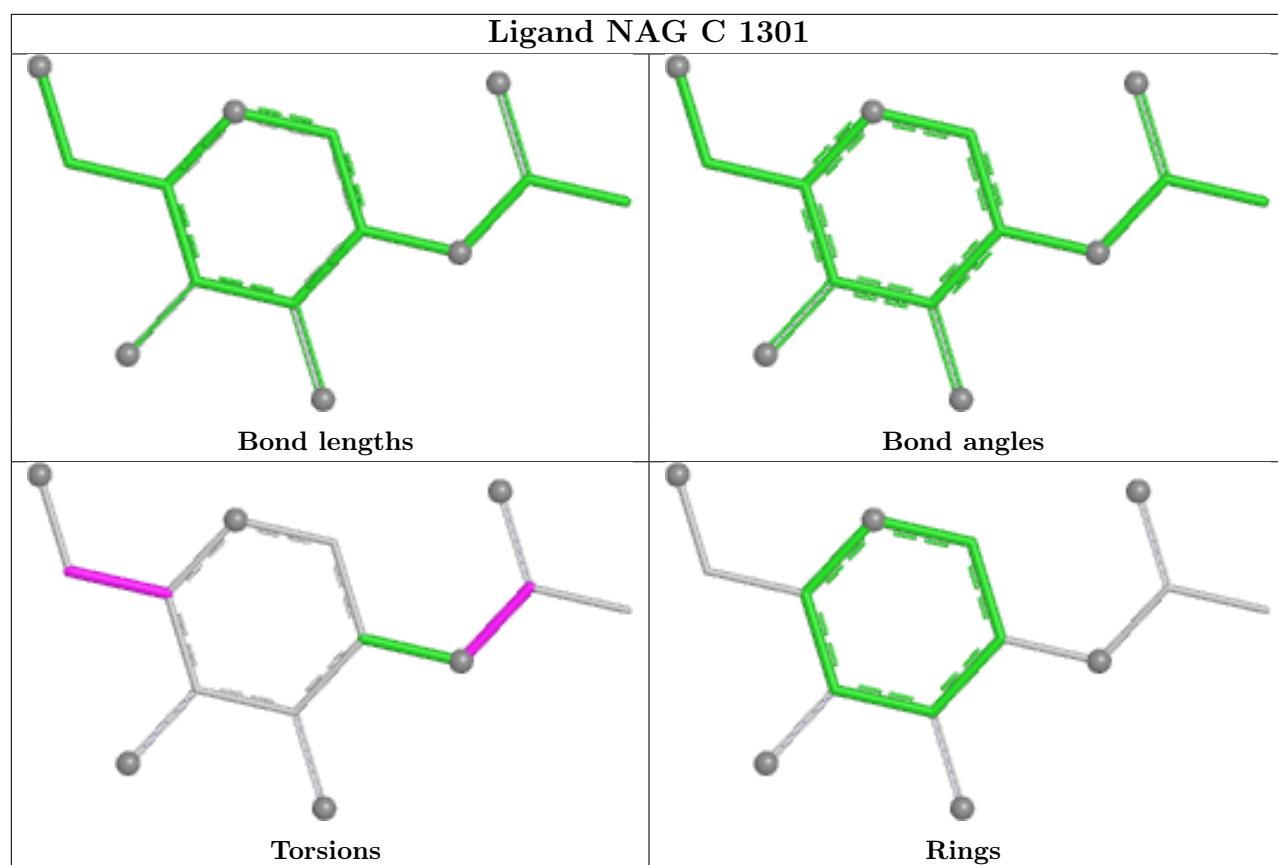
## Ligand NAG B 1306



## Ligand NAG A 1310







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32107. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.