



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:10 AM UTC

PDB ID : 7CYD / pdb\_00007cyd  
EMDB ID : EMD-30497  
Title : Cryo-EM structures of Alphacoronavirus spike glycoprotein  
Authors : Song, X.; Shi, Y.; Ding, W.; Liu, Z.J.; Peng, G.  
Deposited on : 2020-09-03  
Resolution : 3.55 Å(reported)  
Based on initial model : 5SZS

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:

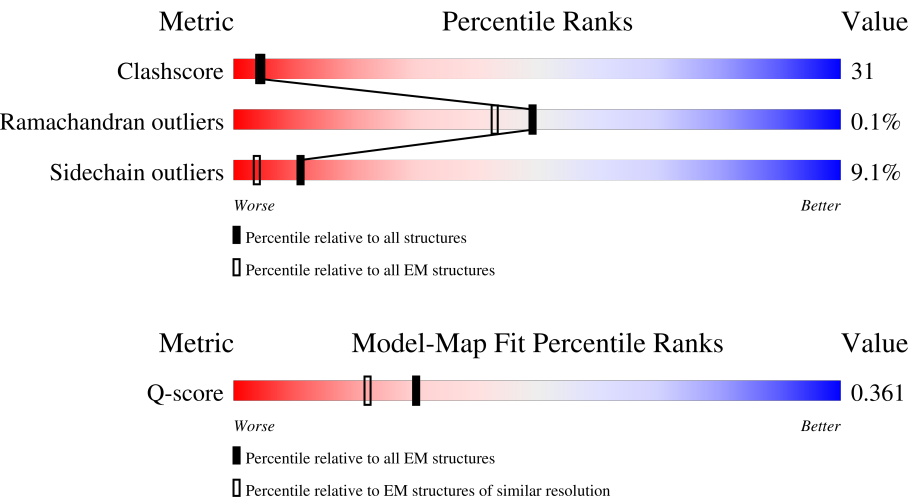
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.55 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 12819 ( 3.05 - 4.05 )                                    |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1116   |                  |
| 1   | B     | 1116   |                  |
| 1   | C     | 1116   |                  |
| 2   | D     | 7      |                  |

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| Mol | Chain | Length | Quality of chain                                                 |
|-----|-------|--------|------------------------------------------------------------------|
| 2   | F     | 7      | <div><div><div>43%</div><div>86%</div><div>14%</div></div></div> |
| 2   | H     | 7      | <div><div><div>29%</div><div>86%</div><div>14%</div></div></div> |
| 3   | E     | 3      | <div><div><div>33%</div><div>33%</div><div>33%</div></div></div> |
| 3   | G     | 3      | <div><div><div>33%</div><div>33%</div><div>33%</div></div></div> |
| 3   | I     | 3      | <div><div><div>33%</div><div>33%</div><div>33%</div></div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22320 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.

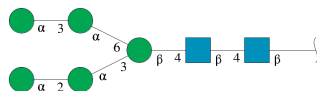
- Molecule 1 is a protein called Spike glycoprotein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 964      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7122  | 4504 | 1228 | 1353 | 37 |         |       |
| 1   | B     | 964      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7122  | 4504 | 1228 | 1353 | 37 |         |       |
| 1   | C     | 964      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7122  | 4504 | 1228 | 1353 | 37 |         |       |

There are 24 discrepancies between the modelled and reference sequences:

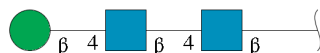
| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| A     | 642     | MET      | ARG    | variant | UNP P15423 |
| A     | 681     | ARG      | THR    | variant | UNP P15423 |
| A     | 765     | ALA      | VAL    | variant | UNP P15423 |
| A     | 775     | SER      | ALA    | variant | UNP P15423 |
| A     | 871     | ILE      | THR    | variant | UNP P15423 |
| A     | 937     | LEU      | ILE    | variant | UNP P15423 |
| A     | 971     | ARG      | THR    | variant | UNP P15423 |
| A     | 1005    | ILE      | MET    | variant | UNP P15423 |
| B     | 642     | MET      | ARG    | variant | UNP P15423 |
| B     | 681     | ARG      | THR    | variant | UNP P15423 |
| B     | 765     | ALA      | VAL    | variant | UNP P15423 |
| B     | 775     | SER      | ALA    | variant | UNP P15423 |
| B     | 871     | ILE      | THR    | variant | UNP P15423 |
| B     | 937     | LEU      | ILE    | variant | UNP P15423 |
| B     | 971     | ARG      | THR    | variant | UNP P15423 |
| B     | 1005    | ILE      | MET    | variant | UNP P15423 |
| C     | 642     | MET      | ARG    | variant | UNP P15423 |
| C     | 681     | ARG      | THR    | variant | UNP P15423 |
| C     | 765     | ALA      | VAL    | variant | UNP P15423 |
| C     | 775     | SER      | ALA    | variant | UNP P15423 |
| C     | 871     | ILE      | THR    | variant | UNP P15423 |
| C     | 937     | LEU      | ILE    | variant | UNP P15423 |
| C     | 971     | ARG      | THR    | variant | UNP P15423 |
| C     | 1005    | ILE      | MET    | variant | UNP P15423 |

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



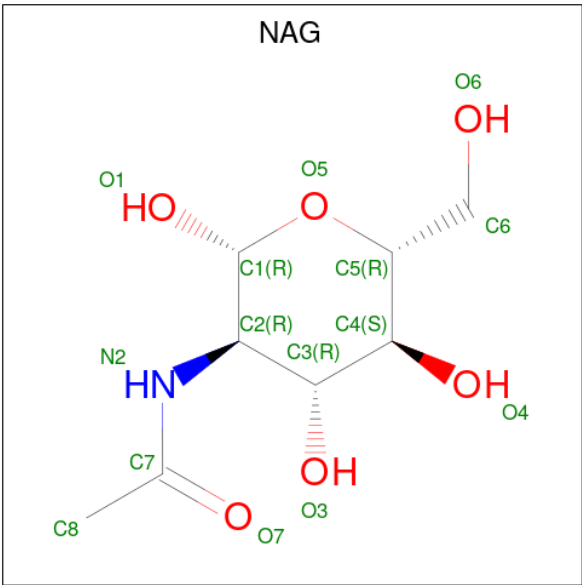
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 2   | D     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |
| 2   | F     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |
| 2   | H     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 3   | E     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 3   | G     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 3   | I     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |

- Molecule 4 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 |
|-----|-------|----------|-------|---|---|---|---------|
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

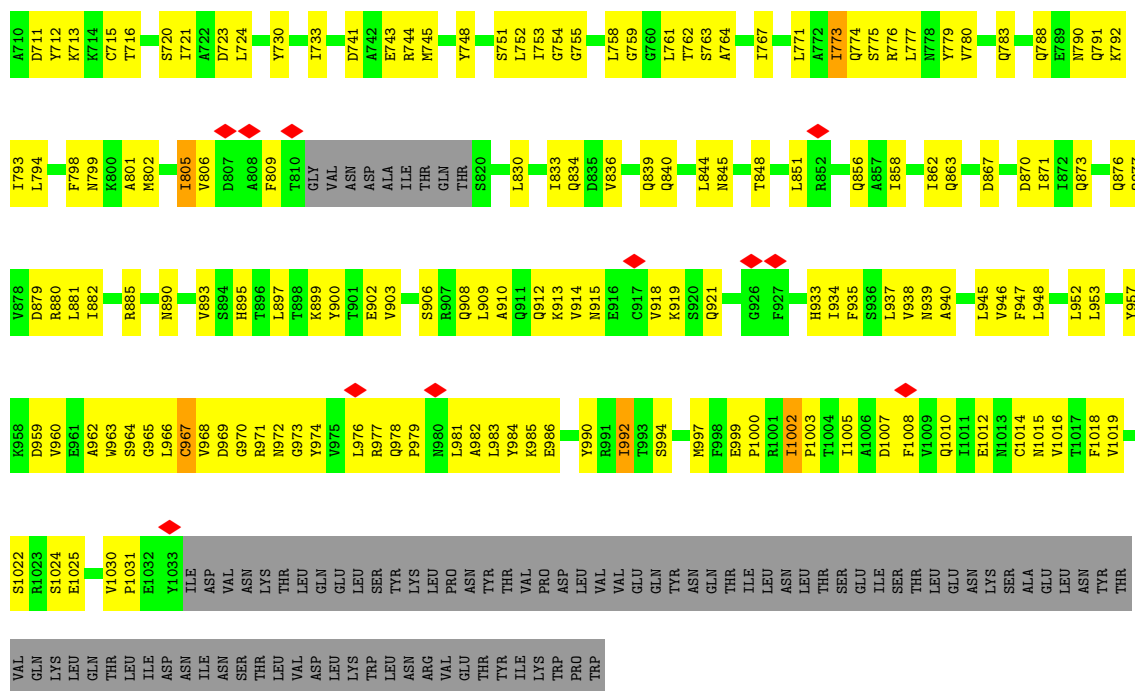
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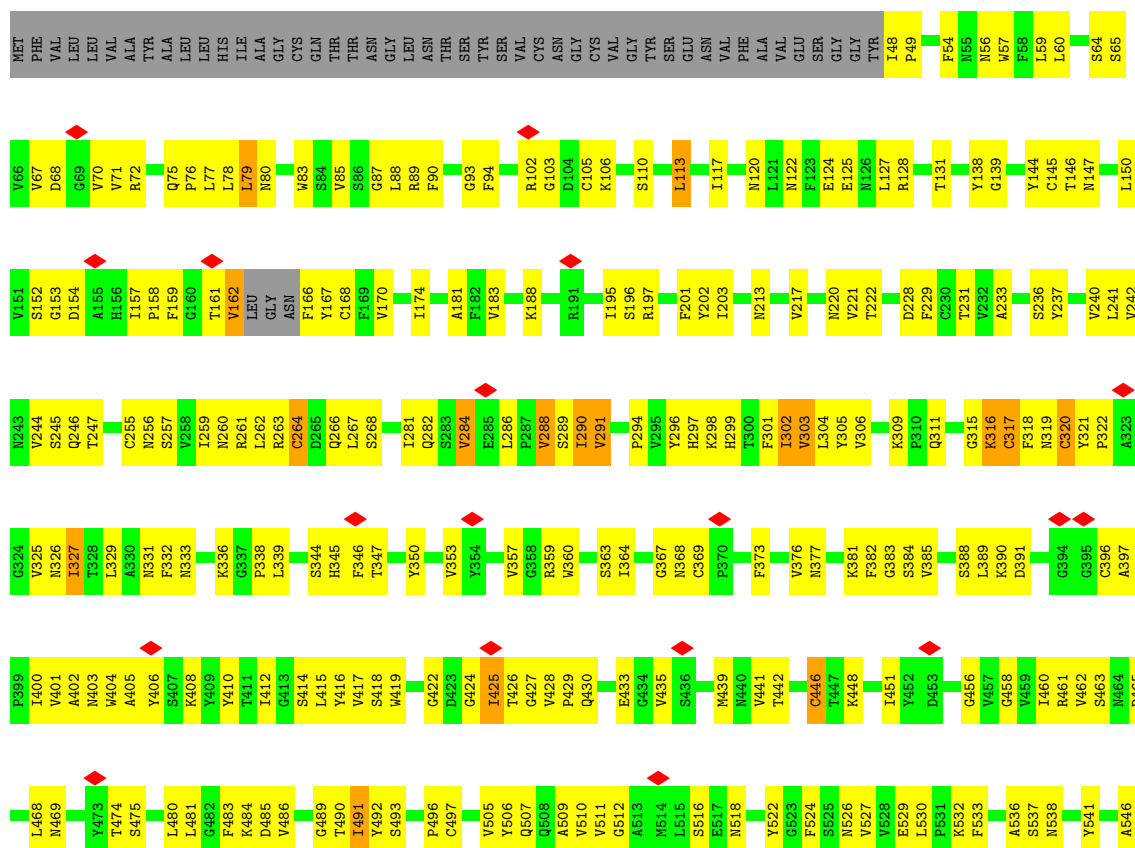
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

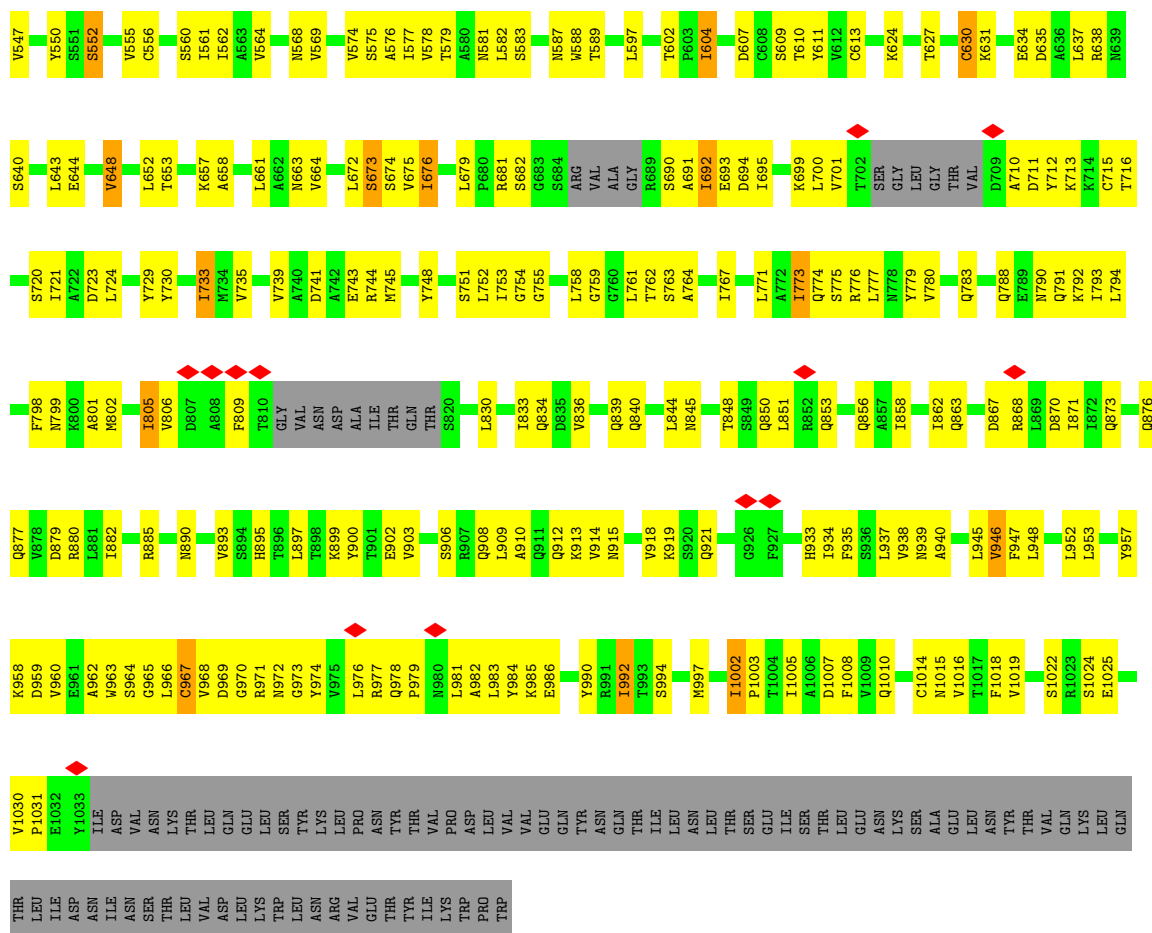






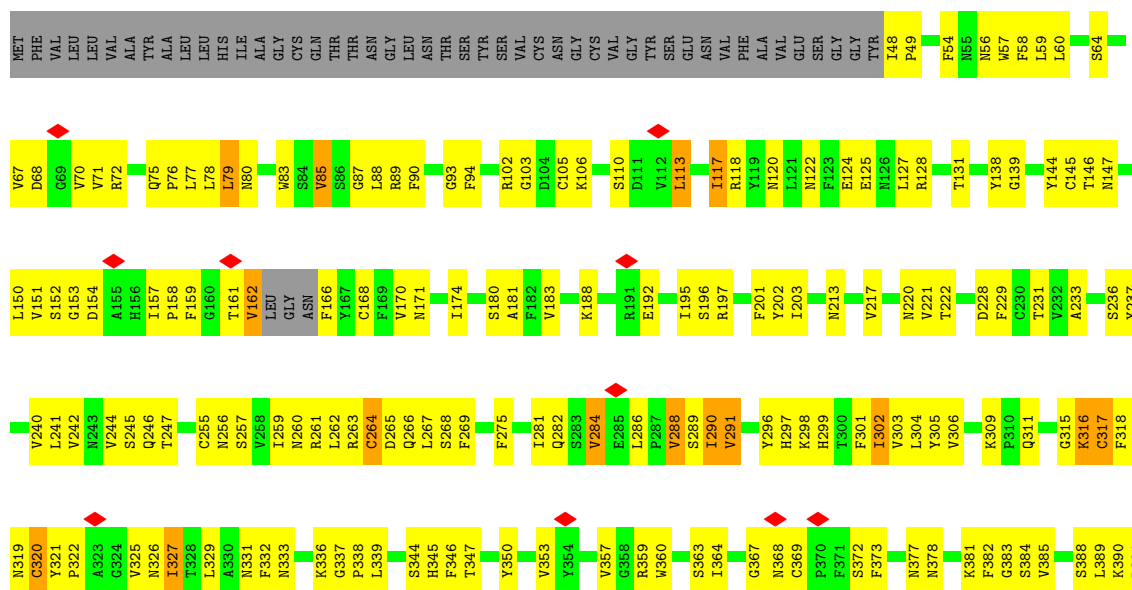
### • Molecule 1: Spike glycoprotein



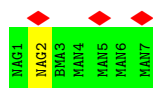


• Molecule 1: Spike glycoprotein

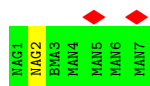
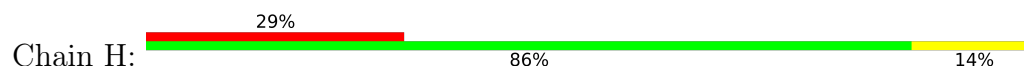
Chain C: 44% 40% 14%







- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 55513                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 2000                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 18000                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 23.498                                  | Depositor |
| Minimum map value                    | -10.870                                 | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 4                                       | Depositor |
| Map size (Å)                         | 280.0, 280.0, 280.0                     | wwPDB     |
| Map dimensions                       | 200, 200, 200                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.4, 1.4, 1.4                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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     | 0.51         | 1/7276 (0.0%)  | 0.77        | 2/9790 (0.0%)  |
| 1   | B     | 0.51         | 1/7276 (0.0%)  | 0.77        | 2/9790 (0.0%)  |
| 1   | C     | 0.51         | 1/7276 (0.0%)  | 0.77        | 2/9790 (0.0%)  |
| All | All   | 0.51         | 3/21828 (0.0%) | 0.77        | 6/29370 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 439 | MET  | C-N   | 10.31 | 1.47        | 1.33     |
| 1   | A     | 439 | MET  | C-N   | 10.31 | 1.47        | 1.33     |
| 1   | B     | 439 | MET  | C-N   | 10.27 | 1.47        | 1.33     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 93  | GLY  | CA-C-O  | -6.17 | 117.87      | 122.37   |
| 1   | A     | 93  | GLY  | CA-C-O  | -5.99 | 118.00      | 122.37   |
| 1   | B     | 93  | GLY  | CA-C-O  | -5.94 | 118.03      | 122.37   |
| 1   | A     | 318 | PHE  | CB-CA-C | -5.11 | 102.86      | 110.88   |
| 1   | B     | 318 | PHE  | CB-CA-C | -5.10 | 102.88      | 110.88   |
| 1   | C     | 318 | PHE  | CB-CA-C | -5.09 | 102.88      | 110.88   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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     | 7122  | 0        | 6276     | 442     | 0            |
| 1   | B     | 7122  | 0        | 6276     | 472     | 0            |
| 1   | C     | 7122  | 0        | 6275     | 459     | 0            |
| 2   | D     | 83    | 0        | 70       | 0       | 0            |
| 2   | F     | 83    | 0        | 70       | 0       | 0            |
| 2   | H     | 83    | 0        | 70       | 0       | 0            |
| 3   | E     | 39    | 0        | 34       | 8       | 0            |
| 3   | G     | 39    | 0        | 34       | 6       | 0            |
| 3   | I     | 39    | 0        | 34       | 7       | 0            |
| 4   | A     | 196   | 0        | 182      | 11      | 0            |
| 4   | B     | 196   | 0        | 182      | 20      | 0            |
| 4   | C     | 196   | 0        | 182      | 5       | 0            |
| All | All   | 22320 | 0        | 19685    | 1292    | 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 31.

All (1292) 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:B:518:ASN:HD22 | 4:B:1206:NAG:C1  | 0.98                     | 1.56              |
| 1:A:518:ASN:HD22 | 4:A:1206:NAG:C1  | 0.91                     | 1.50              |
| 1:B:587:ASN:HD21 | 4:B:1212:NAG:C1  | 0.89                     | 1.50              |
| 1:C:245:SER:CB   | 3:I:2:NAG:O7     | 1.84                     | 1.26              |
| 1:A:245:SER:CB   | 3:E:2:NAG:O7     | 1.90                     | 1.18              |
| 1:B:775:SER:HB3  | 1:C:576:ALA:HB2  | 1.26                     | 1.17              |
| 1:C:774:GLN:HB3  | 1:C:783:GLN:HE22 | 1.17                     | 1.06              |
| 1:A:576:ALA:HB2  | 1:C:775:SER:HB3  | 1.37                     | 1.05              |
| 1:A:775:SER:HB3  | 1:B:576:ALA:HB2  | 1.35                     | 1.05              |
| 1:B:245:SER:CB   | 3:G:2:NAG:O7     | 2.03                     | 1.05              |
| 1:B:774:GLN:HB3  | 1:B:783:GLN:HE22 | 1.16                     | 1.04              |
| 1:A:774:GLN:HB3  | 1:A:783:GLN:HE22 | 1.16                     | 1.04              |
| 1:C:315:GLY:HA2  | 1:C:404:TRP:HZ2  | 1.21                     | 1.04              |
| 1:B:315:GLY:HA2  | 1:B:404:TRP:HZ2  | 1.22                     | 1.00              |
| 1:A:315:GLY:HA2  | 1:A:404:TRP:HZ2  | 1.22                     | 1.00              |
| 1:A:311:GLN:HG2  | 1:A:320:CYS:HA   | 1.48                     | 0.95              |
| 1:C:245:SER:HB2  | 3:I:2:NAG:O7     | 1.62                     | 0.95              |
| 1:B:311:GLN:HG2  | 1:B:320:CYS:HA   | 1.48                     | 0.94              |
| 1:A:908:GLN:O    | 1:A:912:GLN:HB2  | 1.69                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:311:GLN:HG2  | 1:C:320:CYS:HA   | 1.48                     | 0.93              |
| 1:C:908:GLN:O    | 1:C:912:GLN:HB2  | 1.69                     | 0.92              |
| 1:A:317:CYS:O    | 1:A:317:CYS:SG   | 2.28                     | 0.92              |
| 1:A:588:TRP:CD1  | 1:A:952:LEU:HA   | 2.05                     | 0.92              |
| 1:B:908:GLN:O    | 1:B:912:GLN:HB2  | 1.69                     | 0.91              |
| 1:A:533:PHE:HA   | 1:C:713:LYS:HD2  | 1.51                     | 0.91              |
| 1:C:317:CYS:O    | 1:C:317:CYS:SG   | 2.28                     | 0.91              |
| 1:B:317:CYS:SG   | 1:B:317:CYS:O    | 2.28                     | 0.90              |
| 1:C:588:TRP:CD1  | 1:C:952:LEU:HA   | 2.05                     | 0.90              |
| 1:A:245:SER:HB2  | 3:E:2:NAG:O7     | 1.70                     | 0.90              |
| 1:B:775:SER:HB3  | 1:C:576:ALA:CB   | 2.02                     | 0.90              |
| 1:B:588:TRP:CD1  | 1:B:952:LEU:HA   | 2.05                     | 0.90              |
| 1:A:266:GLN:OE1  | 1:C:631:LYS:NZ   | 2.06                     | 0.89              |
| 1:B:122:ASN:CG   | 4:B:1202:NAG:C1  | 2.45                     | 0.88              |
| 1:B:297:HIS:HA   | 1:B:345:HIS:CD2  | 2.11                     | 0.86              |
| 1:C:297:HIS:HA   | 1:C:345:HIS:CD2  | 2.11                     | 0.86              |
| 1:A:297:HIS:HA   | 1:A:345:HIS:CD2  | 2.11                     | 0.86              |
| 1:A:577:ILE:HD12 | 1:A:965:GLY:HA3  | 1.59                     | 0.85              |
| 1:C:577:ILE:HD12 | 1:C:965:GLY:HA3  | 1.59                     | 0.84              |
| 1:B:577:ILE:HD12 | 1:B:965:GLY:HA3  | 1.59                     | 0.84              |
| 1:A:316:LYS:HE2  | 1:A:316:LYS:HA   | 1.60                     | 0.84              |
| 1:C:316:LYS:HE2  | 1:C:316:LYS:HA   | 1.60                     | 0.83              |
| 1:C:245:SER:OG   | 3:I:2:NAG:O7     | 1.96                     | 0.83              |
| 1:B:316:LYS:HA   | 1:B:316:LYS:HE2  | 1.60                     | 0.83              |
| 1:B:245:SER:HB2  | 3:G:2:NAG:O7     | 1.79                     | 0.83              |
| 1:A:576:ALA:CB   | 1:C:775:SER:HB3  | 2.08                     | 0.82              |
| 1:B:75:GLN:HB2   | 1:B:77:LEU:HG    | 1.61                     | 0.82              |
| 1:C:75:GLN:HB2   | 1:C:77:LEU:HG    | 1.61                     | 0.82              |
| 1:B:315:GLY:HA2  | 1:B:404:TRP:CZ2  | 2.13                     | 0.82              |
| 1:A:1015:ASN:CG  | 4:A:1214:NAG:C1  | 2.53                     | 0.81              |
| 1:C:68:ASP:HA    | 1:C:245:SER:HA   | 1.62                     | 0.81              |
| 1:C:915:ASN:HA   | 1:C:919:LYS:HZ2  | 1.43                     | 0.81              |
| 1:A:75:GLN:HB2   | 1:A:77:LEU:HG    | 1.61                     | 0.81              |
| 1:A:775:SER:HB3  | 1:B:576:ALA:CB   | 2.09                     | 0.81              |
| 1:A:266:GLN:HA   | 1:C:631:LYS:HE2  | 1.63                     | 0.81              |
| 1:B:68:ASP:HA    | 1:B:245:SER:HA   | 1.62                     | 0.81              |
| 1:A:915:ASN:HA   | 1:A:919:LYS:HZ2  | 1.44                     | 0.80              |
| 1:C:522:TYR:HB2  | 1:C:538:ASN:HB2  | 1.63                     | 0.80              |
| 1:B:522:TYR:HB2  | 1:B:538:ASN:HB2  | 1.63                     | 0.80              |
| 1:C:879:ASP:HA   | 1:C:882:ILE:HG12 | 1.65                     | 0.79              |
| 1:A:68:ASP:HA    | 1:A:245:SER:HA   | 1.62                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:245:SER:OG   | 3:E:2:NAG:O7     | 1.99                     | 0.79              |
| 1:A:879:ASP:HA   | 1:A:882:ILE:HG12 | 1.64                     | 0.79              |
| 1:B:879:ASP:HA   | 1:B:882:ILE:HG12 | 1.64                     | 0.79              |
| 1:A:522:TYR:HB2  | 1:A:538:ASN:HB2  | 1.63                     | 0.79              |
| 1:B:144:TYR:HE2  | 4:B:1203:NAG:H2  | 1.48                     | 0.79              |
| 1:B:716:THR:O    | 1:C:461:ARG:NH1  | 2.16                     | 0.79              |
| 3:G:1:NAG:H2     | 3:G:1:NAG:H61    | 1.65                     | 0.78              |
| 3:I:1:NAG:H61    | 3:I:1:NAG:H2     | 1.65                     | 0.78              |
| 1:A:315:GLY:HA2  | 1:A:404:TRP:CZ2  | 2.13                     | 0.78              |
| 3:E:1:NAG:H2     | 3:E:1:NAG:H61    | 1.65                     | 0.78              |
| 1:A:1003:PRO:HB2 | 1:A:1031:PRO:HD2 | 1.66                     | 0.78              |
| 1:B:730:TYR:CD1  | 1:C:496:PRO:HG3  | 2.19                     | 0.77              |
| 1:B:541:TYR:O    | 1:B:541:TYR:CD1  | 2.38                     | 0.77              |
| 1:A:981:LEU:HD12 | 1:A:994:SER:HA   | 1.66                     | 0.77              |
| 1:C:1003:PRO:HB2 | 1:C:1031:PRO:HD2 | 1.66                     | 0.77              |
| 1:C:315:GLY:HA2  | 1:C:404:TRP:CZ2  | 2.13                     | 0.76              |
| 1:A:85:VAL:HG23  | 1:A:88:LEU:HG    | 1.67                     | 0.76              |
| 1:A:624:LYS:HG2  | 1:B:72:ARG:HE    | 1.50                     | 0.76              |
| 1:A:963:TRP:HE1  | 1:A:985:LYS:HB2  | 1.51                     | 0.76              |
| 1:B:700:LEU:HD23 | 1:B:700:LEU:O    | 1.85                     | 0.76              |
| 1:B:963:TRP:HE1  | 1:B:985:LYS:HB2  | 1.51                     | 0.76              |
| 1:C:541:TYR:O    | 1:C:541:TYR:CD1  | 2.38                     | 0.76              |
| 1:B:602:THR:CB   | 1:B:840:GLN:HE22 | 1.99                     | 0.76              |
| 1:B:1003:PRO:HB2 | 1:B:1031:PRO:HD2 | 1.66                     | 0.76              |
| 1:A:541:TYR:O    | 1:A:541:TYR:CD1  | 2.38                     | 0.76              |
| 1:C:602:THR:CB   | 1:C:840:GLN:HE22 | 1.99                     | 0.76              |
| 1:C:700:LEU:HD23 | 1:C:700:LEU:O    | 1.85                     | 0.76              |
| 1:C:848:THR:HA   | 1:C:851:LEU:HD12 | 1.68                     | 0.76              |
| 1:C:85:VAL:HG13  | 1:C:88:LEU:HG    | 1.67                     | 0.76              |
| 1:A:602:THR:CB   | 1:A:840:GLN:HE22 | 1.99                     | 0.75              |
| 1:C:981:LEU:HD12 | 1:C:994:SER:HA   | 1.66                     | 0.75              |
| 1:B:245:SER:OG   | 3:G:2:NAG:O7     | 2.04                     | 0.75              |
| 1:B:848:THR:HA   | 1:B:851:LEU:HD12 | 1.68                     | 0.75              |
| 1:B:85:VAL:HG23  | 1:B:88:LEU:HG    | 1.67                     | 0.75              |
| 1:B:383:GLY:HA3  | 1:B:422:GLY:HA3  | 1.67                     | 0.75              |
| 1:B:915:ASN:HA   | 1:B:919:LYS:HZ2  | 1.52                     | 0.75              |
| 1:B:981:LEU:HD12 | 1:B:994:SER:HA   | 1.66                     | 0.75              |
| 1:A:700:LEU:HD23 | 1:A:700:LEU:O    | 1.85                     | 0.74              |
| 1:A:848:THR:HA   | 1:A:851:LEU:HD12 | 1.68                     | 0.74              |
| 1:A:383:GLY:HA3  | 1:A:422:GLY:HA3  | 1.68                     | 0.74              |
| 1:C:963:TRP:HE1  | 1:C:985:LYS:HB2  | 1.51                     | 0.74              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:383:GLY:HA3   | 1:C:422:GLY:HA3  | 1.68                     | 0.74              |
| 1:A:113:LEU:H     | 1:A:113:LEU:HD22 | 1.52                     | 0.73              |
| 1:B:713:LYS:HD3   | 1:C:516:SER:HA   | 1.70                     | 0.73              |
| 1:C:76:PRO:HA     | 1:C:237:TYR:HA   | 1.70                     | 0.73              |
| 1:B:113:LEU:HD22  | 1:B:113:LEU:H    | 1.52                     | 0.73              |
| 1:C:806:VAL:HA    | 1:C:809:PHE:HD2  | 1.54                     | 0.73              |
| 1:C:113:LEU:H     | 1:C:113:LEU:HD22 | 1.52                     | 0.73              |
| 1:A:597:LEU:HD11  | 1:A:913:LYS:HZ1  | 1.54                     | 0.73              |
| 1:B:76:PRO:HA     | 1:B:237:TYR:HA   | 1.70                     | 0.73              |
| 1:B:713:LYS:HD2   | 1:C:533:PHE:HA   | 1.70                     | 0.72              |
| 1:B:1002:ILE:HD13 | 1:C:1010:GLN:HB3 | 1.71                     | 0.72              |
| 1:C:245:SER:HB3   | 3:I:2:NAG:O7     | 1.86                     | 0.72              |
| 1:C:597:LEU:HD11  | 1:C:913:LYS:HZ1  | 1.54                     | 0.72              |
| 1:B:631:LYS:HE2   | 1:C:266:GLN:HA   | 1.70                     | 0.72              |
| 1:B:518:ASN:HD22  | 4:B:1206:NAG:C2  | 1.96                     | 0.72              |
| 1:A:76:PRO:HA     | 1:A:237:TYR:HA   | 1.70                     | 0.72              |
| 1:B:1002:ILE:HD11 | 1:C:1010:GLN:H   | 1.54                     | 0.72              |
| 1:A:144:TYR:HE2   | 4:A:1203:NAG:H2  | 1.54                     | 0.72              |
| 1:B:597:LEU:HD11  | 1:B:913:LYS:HZ1  | 1.55                     | 0.72              |
| 1:B:806:VAL:HA    | 1:B:809:PHE:HD2  | 1.54                     | 0.71              |
| 1:A:157:ILE:HD12  | 1:A:158:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:992:ILE:HD11  | 1:A:1003:PRO:HA  | 1.72                     | 0.71              |
| 1:B:157:ILE:HD12  | 1:B:158:PRO:HD2  | 1.72                     | 0.71              |
| 1:C:862:ILE:HD12  | 1:C:862:ILE:H    | 1.56                     | 0.71              |
| 1:A:806:VAL:HA    | 1:A:809:PHE:HD2  | 1.54                     | 0.71              |
| 1:C:157:ILE:HD12  | 1:C:158:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:862:ILE:HD12  | 1:A:862:ILE:H    | 1.56                     | 0.70              |
| 1:A:974:TYR:HE1   | 1:A:1008:PHE:HA  | 1.57                     | 0.70              |
| 1:C:799:ASN:HA    | 1:C:802:MET:HG2  | 1.73                     | 0.70              |
| 1:C:627:THR:O     | 1:C:631:LYS:N    | 2.24                     | 0.70              |
| 1:A:799:ASN:HA    | 1:A:802:MET:HG2  | 1.73                     | 0.70              |
| 1:B:862:ILE:HD12  | 1:B:862:ILE:H    | 1.56                     | 0.70              |
| 1:B:316:LYS:HZ3   | 1:B:316:LYS:HB3  | 1.57                     | 0.70              |
| 1:B:974:TYR:HE1   | 1:B:1008:PHE:HA  | 1.57                     | 0.70              |
| 1:A:382:PHE:O     | 1:A:425:ILE:N    | 2.25                     | 0.70              |
| 1:A:245:SER:HB3   | 3:E:2:NAG:O7     | 1.91                     | 0.69              |
| 1:C:327:ILE:HD13  | 1:C:332:PHE:CE2  | 2.27                     | 0.69              |
| 1:A:627:THR:O     | 1:A:631:LYS:N    | 2.24                     | 0.69              |
| 1:B:799:ASN:HA    | 1:B:802:MET:HG2  | 1.73                     | 0.69              |
| 1:B:382:PHE:O     | 1:B:425:ILE:N    | 2.25                     | 0.69              |
| 1:B:992:ILE:HD11  | 1:B:1003:PRO:HA  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:644:GLU:O     | 1:A:648:VAL:HG12 | 1.93                     | 0.69              |
| 1:A:327:ILE:HD13  | 1:A:332:PHE:CE2  | 2.27                     | 0.69              |
| 1:B:644:GLU:O     | 1:B:648:VAL:HG12 | 1.93                     | 0.69              |
| 1:C:974:TYR:HE1   | 1:C:1008:PHE:HA  | 1.57                     | 0.69              |
| 1:B:188:LYS:HE2   | 1:C:489:GLY:N    | 2.07                     | 0.69              |
| 1:B:627:THR:O     | 1:B:631:LYS:N    | 2.24                     | 0.69              |
| 1:A:85:VAL:HG21   | 1:A:229:PHE:HB2  | 1.74                     | 0.69              |
| 1:B:327:ILE:HD13  | 1:B:332:PHE:CE2  | 2.27                     | 0.68              |
| 1:C:382:PHE:O     | 1:C:425:ILE:N    | 2.25                     | 0.68              |
| 1:A:188:LYS:HE2   | 1:B:489:GLY:N    | 2.08                     | 0.68              |
| 1:A:556:CYS:SG    | 1:A:562:ILE:HD11 | 2.34                     | 0.68              |
| 1:C:992:ILE:HD11  | 1:C:1003:PRO:HA  | 1.73                     | 0.68              |
| 1:C:302:ILE:HA    | 1:C:329:LEU:HG   | 1.75                     | 0.68              |
| 1:A:863:GLN:NE2   | 1:A:867:ASP:OD1  | 2.25                     | 0.68              |
| 1:B:131:THR:O     | 1:B:220:ASN:HB3  | 1.94                     | 0.68              |
| 1:B:556:CYS:SG    | 1:B:562:ILE:HD11 | 2.34                     | 0.68              |
| 1:B:863:GLN:NE2   | 1:B:867:ASP:OD1  | 2.25                     | 0.68              |
| 1:C:644:GLU:O     | 1:C:648:VAL:HG22 | 1.93                     | 0.68              |
| 1:B:85:VAL:HG21   | 1:B:229:PHE:HB2  | 1.75                     | 0.68              |
| 1:B:309:LYS:HE2   | 1:B:321:TYR:HB3  | 1.76                     | 0.68              |
| 1:C:85:VAL:HG11   | 1:C:229:PHE:HB2  | 1.74                     | 0.68              |
| 1:C:863:GLN:NE2   | 1:C:867:ASP:OD1  | 2.26                     | 0.68              |
| 1:A:131:THR:O     | 1:A:220:ASN:HB3  | 1.94                     | 0.68              |
| 1:A:338:PRO:HA    | 1:A:388:SER:HB2  | 1.76                     | 0.68              |
| 1:B:679:LEU:O     | 1:B:681:ARG:NH1  | 2.27                     | 0.68              |
| 1:C:113:LEU:HD22  | 1:C:113:LEU:N    | 2.09                     | 0.68              |
| 1:C:131:THR:O     | 1:C:220:ASN:HB3  | 1.94                     | 0.68              |
| 1:A:679:LEU:O     | 1:A:681:ARG:NH1  | 2.27                     | 0.68              |
| 1:A:302:ILE:HA    | 1:A:329:LEU:HG   | 1.75                     | 0.67              |
| 1:C:556:CYS:SG    | 1:C:562:ILE:HD11 | 2.33                     | 0.67              |
| 1:A:113:LEU:HD22  | 1:A:113:LEU:N    | 2.09                     | 0.67              |
| 1:A:1002:ILE:HD13 | 1:B:1010:GLN:HB3 | 1.77                     | 0.67              |
| 1:A:316:LYS:HB3   | 1:A:316:LYS:HZ3  | 1.59                     | 0.67              |
| 1:B:113:LEU:HD22  | 1:B:113:LEU:N    | 2.09                     | 0.67              |
| 1:C:338:PRO:HA    | 1:C:388:SER:HB2  | 1.76                     | 0.67              |
| 1:A:624:LYS:HG2   | 1:B:72:ARG:NE    | 2.09                     | 0.67              |
| 1:B:302:ILE:HA    | 1:B:329:LEU:HG   | 1.75                     | 0.67              |
| 1:A:588:TRP:CZ2   | 1:A:953:LEU:HB2  | 2.30                     | 0.67              |
| 1:A:774:GLN:HB3   | 1:A:783:GLN:NE2  | 2.01                     | 0.67              |
| 1:C:679:LEU:O     | 1:C:681:ARG:NH1  | 2.27                     | 0.66              |
| 1:A:694:ASP:OD1   | 1:A:695:ILE:HD13 | 1.96                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:311:GLN:HB2  | 1:B:321:TYR:HD2   | 1.61                     | 0.66              |
| 1:C:602:THR:CB   | 1:C:840:GLN:NE2   | 2.59                     | 0.66              |
| 1:C:694:ASP:OD1  | 1:C:695:ILE:HD13  | 1.96                     | 0.66              |
| 1:B:113:LEU:H    | 1:B:113:LEU:CD2   | 2.07                     | 0.66              |
| 1:C:113:LEU:H    | 1:C:113:LEU:CD2   | 2.07                     | 0.66              |
| 1:A:327:ILE:HD12 | 1:A:327:ILE:H     | 1.61                     | 0.66              |
| 1:B:338:PRO:HA   | 1:B:388:SER:HB2   | 1.76                     | 0.66              |
| 1:C:309:LYS:HE2  | 1:C:321:TYR:HB3   | 1.76                     | 0.66              |
| 1:A:602:THR:CB   | 1:A:840:GLN:NE2   | 2.59                     | 0.66              |
| 1:B:518:ASN:ND2  | 4:B:1206:NAG:C2   | 2.57                     | 0.66              |
| 1:C:311:GLN:HB2  | 1:C:321:TYR:HD2   | 1.61                     | 0.66              |
| 1:A:309:LYS:HE2  | 1:A:321:TYR:HB3   | 1.76                     | 0.66              |
| 1:A:113:LEU:H    | 1:A:113:LEU:CD2   | 2.08                     | 0.66              |
| 1:A:730:TYR:CD1  | 1:B:496:PRO:HG3   | 2.31                     | 0.66              |
| 1:A:150:LEU:HG   | 1:A:153:GLY:H     | 1.61                     | 0.65              |
| 1:C:588:TRP:CZ2  | 1:C:953:LEU:HB2   | 2.30                     | 0.65              |
| 1:A:532:LYS:HE3  | 1:C:711:ASP:H     | 1.61                     | 0.65              |
| 1:B:150:LEU:HG   | 1:B:153:GLY:H     | 1.61                     | 0.65              |
| 1:B:744:ARG:HH21 | 1:C:564:VAL:CB    | 2.09                     | 0.65              |
| 1:B:588:TRP:CZ2  | 1:B:953:LEU:HB2   | 2.30                     | 0.65              |
| 1:B:327:ILE:H    | 1:B:327:ILE:HD12  | 1.61                     | 0.65              |
| 1:C:144:TYR:HE2  | 4:C:1203:NAG:H2   | 1.62                     | 0.65              |
| 1:B:602:THR:CB   | 1:B:840:GLN:NE2   | 2.59                     | 0.65              |
| 1:C:316:LYS:HE2  | 1:C:316:LYS:CA    | 2.26                     | 0.65              |
| 1:C:327:ILE:HD12 | 1:C:327:ILE:H     | 1.61                     | 0.65              |
| 1:A:316:LYS:HE2  | 1:A:316:LYS:CA    | 2.26                     | 0.65              |
| 1:B:694:ASP:OD1  | 1:B:695:ILE:HD13  | 1.96                     | 0.65              |
| 1:B:971:ARG:NH2  | 1:B:1014:CYS:SG   | 2.70                     | 0.65              |
| 1:A:518:ASN:ND2  | 4:A:1206:NAG:C2   | 2.60                     | 0.65              |
| 1:A:1010:GLN:HB3 | 1:C:1002:ILE:HD13 | 1.77                     | 0.65              |
| 1:C:657:LYS:HA   | 1:C:764:ALA:HB1   | 1.79                     | 0.65              |
| 1:C:971:ARG:NH2  | 1:C:1014:CYS:SG   | 2.70                     | 0.65              |
| 1:A:311:GLN:HB2  | 1:A:321:TYR:HD2   | 1.61                     | 0.65              |
| 1:B:657:LYS:HA   | 1:B:764:ALA:HB1   | 1.79                     | 0.65              |
| 1:A:971:ARG:NH2  | 1:A:1014:CYS:SG   | 2.70                     | 0.64              |
| 1:B:579:THR:HA   | 1:B:962:ALA:O     | 1.98                     | 0.64              |
| 1:B:775:SER:CB   | 1:C:576:ALA:HB2   | 2.17                     | 0.64              |
| 1:A:588:TRP:NE1  | 1:A:952:LEU:HA    | 2.13                     | 0.64              |
| 1:B:144:TYR:CE2  | 4:B:1203:NAG:H2   | 2.30                     | 0.64              |
| 1:C:969:ASP:OD1  | 1:C:970:GLY:N     | 2.31                     | 0.64              |
| 1:A:631:LYS:HE2  | 1:B:266:GLN:HA    | 1.80                     | 0.64              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:579:THR:HA  | 1:C:962:ALA:O    | 1.98                     | 0.64              |
| 1:A:657:LYS:HA  | 1:A:764:ALA:HB1  | 1.79                     | 0.64              |
| 1:C:150:LEU:HG  | 1:C:153:GLY:H    | 1.61                     | 0.64              |
| 1:B:48:ILE:HD13 | 1:B:79:LEU:HD11  | 1.80                     | 0.64              |
| 1:B:588:TRP:NE1 | 1:B:952:LEU:HA   | 2.13                     | 0.64              |
| 1:B:774:GLN:HB3 | 1:B:783:GLN:NE2  | 2.01                     | 0.64              |
| 1:A:532:LYS:HG3 | 1:C:711:ASP:OD2  | 1.98                     | 0.64              |
| 1:C:346:PHE:HD1 | 1:C:427:GLY:O    | 1.81                     | 0.64              |
| 1:A:83:TRP:CD1  | 1:A:102:ARG:H    | 2.16                     | 0.63              |
| 1:C:588:TRP:NE1 | 1:C:952:LEU:HA   | 2.13                     | 0.63              |
| 1:A:485:ASP:OD1 | 1:A:490:THR:N    | 2.32                     | 0.63              |
| 1:A:346:PHE:HD1 | 1:A:427:GLY:O    | 1.81                     | 0.63              |
| 1:A:969:ASP:OD1 | 1:A:970:GLY:N    | 2.31                     | 0.63              |
| 1:B:475:SER:HB3 | 1:B:481:LEU:HD21 | 1.81                     | 0.63              |
| 1:C:85:VAL:H    | 1:C:231:THR:HA   | 1.63                     | 0.63              |
| 3:G:1:NAG:H2    | 3:G:1:NAG:C6     | 2.28                     | 0.63              |
| 1:B:85:VAL:H    | 1:B:231:THR:HA   | 1.63                     | 0.63              |
| 1:B:316:LYS:HE2 | 1:B:316:LYS:CA   | 2.26                     | 0.63              |
| 1:B:743:GLU:HG3 | 1:B:744:ARG:H    | 1.64                     | 0.63              |
| 1:A:475:SER:HB3 | 1:A:481:LEU:HD21 | 1.81                     | 0.63              |
| 1:A:579:THR:HA  | 1:A:962:ALA:O    | 1.98                     | 0.63              |
| 1:C:316:LYS:NZ  | 1:C:316:LYS:HB3  | 2.13                     | 0.63              |
| 1:C:743:GLU:HG3 | 1:C:744:ARG:H    | 1.64                     | 0.63              |
| 3:I:1:NAG:H2    | 3:I:1:NAG:C6     | 2.29                     | 0.63              |
| 1:B:346:PHE:HD1 | 1:B:427:GLY:O    | 1.82                     | 0.63              |
| 1:A:546:ALA:HB2 | 1:A:562:ILE:HD13 | 1.81                     | 0.62              |
| 1:A:921:GLN:HG2 | 1:A:933:HIS:HD2  | 1.63                     | 0.62              |
| 1:B:691:ALA:HA  | 1:B:694:ASP:OD2  | 1.99                     | 0.62              |
| 1:B:969:ASP:OD1 | 1:B:970:GLY:N    | 2.31                     | 0.62              |
| 1:C:546:ALA:HB2 | 1:C:562:ILE:HD13 | 1.81                     | 0.62              |
| 1:B:83:TRP:CD1  | 1:B:102:ARG:H    | 2.16                     | 0.62              |
| 1:B:485:ASP:OD1 | 1:B:490:THR:N    | 2.32                     | 0.62              |
| 1:B:546:ALA:HB2 | 1:B:562:ILE:HD13 | 1.81                     | 0.62              |
| 1:C:921:GLN:HG2 | 1:C:933:HIS:HD2  | 1.63                     | 0.62              |
| 1:A:48:ILE:HD13 | 1:A:79:LEU:HD11  | 1.80                     | 0.62              |
| 1:C:48:ILE:HD13 | 1:C:79:LEU:HD11  | 1.80                     | 0.62              |
| 1:C:83:TRP:CD1  | 1:C:102:ARG:H    | 2.16                     | 0.62              |
| 1:B:87:GLY:O    | 1:B:89:ARG:NH1   | 2.32                     | 0.62              |
| 1:B:316:LYS:HB3 | 1:B:316:LYS:NZ   | 2.13                     | 0.62              |
| 1:A:87:GLY:O    | 1:A:89:ARG:NH1   | 2.32                     | 0.62              |
| 1:A:316:LYS:HB3 | 1:A:316:LYS:NZ   | 2.13                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:485:ASP:OD1  | 1:A:489:GLY:N    | 2.33                     | 0.62              |
| 1:A:713:LYS:HD2  | 1:B:533:PHE:HA   | 1.82                     | 0.62              |
| 1:B:68:ASP:HA    | 1:B:244:VAL:O    | 1.99                     | 0.62              |
| 1:A:85:VAL:H     | 1:A:231:THR:HA   | 1.63                     | 0.62              |
| 1:A:691:ALA:HA   | 1:A:694:ASP:OD2  | 1.99                     | 0.62              |
| 1:A:68:ASP:HA    | 1:A:244:VAL:O    | 1.99                     | 0.62              |
| 1:C:475:SER:HB3  | 1:C:481:LEU:HD21 | 1.81                     | 0.62              |
| 3:E:1:NAG:H2     | 3:E:1:NAG:C6     | 2.29                     | 0.62              |
| 1:A:385:VAL:HA   | 1:A:419:TRP:HA   | 1.82                     | 0.62              |
| 1:B:921:GLN:HG2  | 1:B:933:HIS:HD2  | 1.63                     | 0.62              |
| 1:C:485:ASP:OD1  | 1:C:490:THR:N    | 2.32                     | 0.62              |
| 1:C:485:ASP:OD1  | 1:C:489:GLY:N    | 2.33                     | 0.62              |
| 1:C:974:TYR:CE1  | 1:C:1008:PHE:HA  | 2.35                     | 0.62              |
| 1:A:743:GLU:HG3  | 1:A:744:ARG:H    | 1.64                     | 0.61              |
| 1:A:871:ILE:HD12 | 1:A:871:ILE:H    | 1.65                     | 0.61              |
| 1:C:87:GLY:O     | 1:C:89:ARG:NH1   | 2.32                     | 0.61              |
| 1:C:385:VAL:HA   | 1:C:419:TRP:HA   | 1.82                     | 0.61              |
| 1:C:691:ALA:HA   | 1:C:694:ASP:OD2  | 1.99                     | 0.61              |
| 1:B:391:ASP:OD1  | 1:B:391:ASP:N    | 2.34                     | 0.61              |
| 1:A:159:PHE:HE2  | 1:A:221:VAL:HG13 | 1.65                     | 0.61              |
| 1:B:90:PHE:HZ    | 4:B:1204:NAG:H3  | 1.66                     | 0.61              |
| 1:B:871:ILE:HD12 | 1:B:871:ILE:H    | 1.65                     | 0.61              |
| 1:C:68:ASP:HA    | 1:C:244:VAL:O    | 1.99                     | 0.61              |
| 1:B:526:ASN:N    | 1:B:538:ASN:O    | 2.34                     | 0.61              |
| 1:A:124:GLU:OE1  | 1:A:124:GLU:N    | 2.27                     | 0.61              |
| 1:A:974:TYR:CE1  | 1:A:1008:PHE:HA  | 2.35                     | 0.61              |
| 1:B:297:HIS:HB2  | 1:B:433:GLU:HG3  | 1.83                     | 0.61              |
| 1:B:367:GLY:HA3  | 1:B:397:ALA:O    | 2.01                     | 0.61              |
| 1:B:485:ASP:OD1  | 1:B:489:GLY:N    | 2.33                     | 0.61              |
| 1:B:624:LYS:HG2  | 1:C:72:ARG:NE    | 2.15                     | 0.61              |
| 1:A:72:ARG:NE    | 1:C:624:LYS:HG2  | 2.16                     | 0.61              |
| 1:B:723:ASP:OD1  | 1:B:724:LEU:N    | 2.34                     | 0.61              |
| 1:A:297:HIS:HB2  | 1:A:433:GLU:HG3  | 1.82                     | 0.61              |
| 1:A:367:GLY:HA3  | 1:A:397:ALA:O    | 2.01                     | 0.61              |
| 1:B:587:ASN:CG   | 4:B:1212:NAG:C1  | 2.69                     | 0.61              |
| 1:C:774:GLN:HB3  | 1:C:783:GLN:NE2  | 2.01                     | 0.61              |
| 1:A:806:VAL:HA   | 1:A:809:PHE:CD2  | 2.36                     | 0.60              |
| 1:A:984:TYR:HE2  | 1:A:986:GLU:HB3  | 1.66                     | 0.60              |
| 1:B:159:PHE:HE2  | 1:B:221:VAL:HG13 | 1.65                     | 0.60              |
| 1:C:871:ILE:HD12 | 1:C:871:ILE:H    | 1.66                     | 0.60              |
| 1:A:391:ASP:N    | 1:A:391:ASP:OD1  | 2.34                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:583:SER:HB2  | 1:A:957:TYR:HB3  | 1.83                     | 0.60              |
| 1:B:125:GLU:OE1  | 1:B:161:THR:N    | 2.34                     | 0.60              |
| 1:C:159:PHE:HE2  | 1:C:221:VAL:HG13 | 1.65                     | 0.60              |
| 1:B:385:VAL:HA   | 1:B:419:TRP:HA   | 1.83                     | 0.60              |
| 1:A:526:ASN:N    | 1:A:538:ASN:O    | 2.34                     | 0.60              |
| 1:C:255:CYS:SG   | 1:C:261:ARG:HD2  | 2.41                     | 0.60              |
| 1:C:806:VAL:HA   | 1:C:809:PHE:CD2  | 2.36                     | 0.60              |
| 1:B:255:CYS:SG   | 1:B:261:ARG:HD2  | 2.41                     | 0.60              |
| 1:B:332:PHE:CD1  | 1:B:339:LEU:HD21 | 2.37                     | 0.60              |
| 1:B:711:ASP:H    | 1:C:532:LYS:HE3  | 1.66                     | 0.60              |
| 1:C:657:LYS:NZ   | 1:C:762:THR:O    | 2.35                     | 0.60              |
| 1:A:255:CYS:SG   | 1:A:261:ARG:HD2  | 2.41                     | 0.60              |
| 1:C:297:HIS:HB2  | 1:C:433:GLU:HG3  | 1.82                     | 0.60              |
| 1:A:332:PHE:CD1  | 1:A:339:LEU:HD21 | 2.37                     | 0.60              |
| 1:A:657:LYS:NZ   | 1:A:762:THR:O    | 2.35                     | 0.60              |
| 1:B:583:SER:HB2  | 1:B:957:TYR:HB3  | 1.83                     | 0.60              |
| 1:B:974:TYR:CE1  | 1:B:1008:PHE:HA  | 2.35                     | 0.60              |
| 1:C:332:PHE:CD1  | 1:C:339:LEU:HD21 | 2.37                     | 0.60              |
| 1:C:367:GLY:HA3  | 1:C:397:ALA:O    | 2.01                     | 0.60              |
| 1:C:526:ASN:N    | 1:C:538:ASN:O    | 2.34                     | 0.60              |
| 1:C:583:SER:HB2  | 1:C:957:TYR:HB3  | 1.83                     | 0.60              |
| 1:A:723:ASP:OD1  | 1:A:724:LEU:N    | 2.34                     | 0.59              |
| 1:B:70:VAL:HA    | 1:B:242:VAL:O    | 2.02                     | 0.59              |
| 1:C:984:TYR:HE2  | 1:C:986:GLU:HB3  | 1.66                     | 0.59              |
| 1:B:986:GLU:H    | 1:B:986:GLU:CD   | 2.09                     | 0.59              |
| 1:B:145:CYS:SG   | 1:B:146:THR:N    | 2.76                     | 0.59              |
| 1:C:1015:ASN:HB3 | 1:C:1018:PHE:CD2 | 2.37                     | 0.59              |
| 1:A:533:PHE:HB2  | 1:C:713:LYS:NZ   | 2.18                     | 0.59              |
| 1:A:986:GLU:CD   | 1:A:986:GLU:H    | 2.09                     | 0.59              |
| 1:B:877:GLN:HA   | 1:B:880:ARG:HG2  | 1.84                     | 0.59              |
| 1:B:1015:ASN:HB3 | 1:B:1018:PHE:CD2 | 2.37                     | 0.59              |
| 1:C:391:ASP:N    | 1:C:391:ASP:OD1  | 2.34                     | 0.59              |
| 1:C:316:LYS:N    | 1:C:316:LYS:HD2  | 2.18                     | 0.59              |
| 1:C:723:ASP:OD1  | 1:C:724:LEU:N    | 2.34                     | 0.59              |
| 1:C:986:GLU:H    | 1:C:986:GLU:CD   | 2.09                     | 0.59              |
| 1:A:144:TYR:CE2  | 4:A:1203:NAG:H2  | 2.38                     | 0.59              |
| 1:B:124:GLU:OE1  | 1:B:124:GLU:N    | 2.27                     | 0.59              |
| 1:B:984:TYR:HE2  | 1:B:986:GLU:HB3  | 1.66                     | 0.59              |
| 1:C:145:CYS:SG   | 1:C:146:THR:N    | 2.76                     | 0.59              |
| 1:C:877:GLN:HA   | 1:C:880:ARG:HG2  | 1.84                     | 0.59              |
| 1:A:70:VAL:HA    | 1:A:242:VAL:O    | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:546:ALA:HA    | 1:A:556:CYS:HA    | 1.85                     | 0.59              |
| 1:B:806:VAL:HA    | 1:B:809:PHE:CD2   | 2.36                     | 0.59              |
| 1:B:1007:ASP:OD1  | 1:C:977:ARG:NH2   | 2.36                     | 0.59              |
| 1:C:260:ASN:OD1   | 1:C:263:ARG:NH1   | 2.23                     | 0.59              |
| 1:A:83:TRP:H      | 1:A:103:GLY:HA3   | 1.68                     | 0.59              |
| 1:B:385:VAL:HG12  | 1:B:419:TRP:HB2   | 1.85                     | 0.59              |
| 1:A:72:ARG:HE     | 1:C:624:LYS:HG2   | 1.65                     | 0.59              |
| 1:A:332:PHE:HD1   | 1:A:339:LEU:HD21  | 1.68                     | 0.59              |
| 1:A:1015:ASN:HB3  | 1:A:1018:PHE:CD2  | 2.38                     | 0.59              |
| 1:C:332:PHE:HD1   | 1:C:339:LEU:HD21  | 1.68                     | 0.59              |
| 1:A:648:VAL:O     | 1:A:652:LEU:HG    | 2.03                     | 0.58              |
| 1:B:546:ALA:HA    | 1:B:556:CYS:HA    | 1.85                     | 0.58              |
| 1:C:359:ARG:CZ    | 1:C:405:ALA:H     | 2.16                     | 0.58              |
| 1:A:125:GLU:OE1   | 1:A:161:THR:N     | 2.34                     | 0.58              |
| 1:A:145:CYS:SG    | 1:A:146:THR:N     | 2.76                     | 0.58              |
| 1:B:359:ARG:CZ    | 1:B:405:ALA:H     | 2.16                     | 0.58              |
| 1:C:70:VAL:HA     | 1:C:242:VAL:O     | 2.03                     | 0.58              |
| 1:C:147:ASN:HA    | 1:C:166:PHE:CD1   | 2.39                     | 0.58              |
| 1:B:316:LYS:HD2   | 1:B:316:LYS:N     | 2.18                     | 0.58              |
| 1:B:327:ILE:HD11  | 1:B:389:LEU:HD13  | 1.85                     | 0.58              |
| 1:B:624:LYS:HG2   | 1:C:72:ARG:HE     | 1.68                     | 0.58              |
| 1:C:327:ILE:HD11  | 1:C:389:LEU:HD13  | 1.85                     | 0.58              |
| 1:A:713:LYS:HD3   | 1:B:516:SER:HA    | 1.86                     | 0.58              |
| 1:B:332:PHE:HD1   | 1:B:339:LEU:HD21  | 1.68                     | 0.58              |
| 1:B:657:LYS:NZ    | 1:B:762:THR:O     | 2.35                     | 0.58              |
| 1:C:320:CYS:SG    | 1:C:410:TYR:OH    | 2.57                     | 0.58              |
| 1:A:147:ASN:HA    | 1:A:166:PHE:CD1   | 2.38                     | 0.58              |
| 1:A:316:LYS:HD2   | 1:A:316:LYS:N     | 2.18                     | 0.58              |
| 1:A:877:GLN:HA    | 1:A:880:ARG:HG2   | 1.84                     | 0.58              |
| 1:B:147:ASN:HA    | 1:B:166:PHE:CD1   | 2.39                     | 0.58              |
| 1:B:568:ASN:ND2   | 4:B:1210:NAG:O5   | 2.35                     | 0.58              |
| 1:C:125:GLU:OE1   | 1:C:161:THR:N     | 2.34                     | 0.58              |
| 1:C:83:TRP:H      | 1:C:103:GLY:HA3   | 1.68                     | 0.58              |
| 1:A:327:ILE:HD11  | 1:A:389:LEU:HD13  | 1.85                     | 0.58              |
| 1:B:144:TYR:CD2   | 4:B:1203:NAG:H83  | 2.39                     | 0.58              |
| 1:A:440:ASN:CG    | 4:A:1207:NAG:C1   | 2.69                     | 0.58              |
| 1:A:1010:GLN:H    | 1:C:1002:ILE:HD11 | 1.68                     | 0.58              |
| 1:A:1002:ILE:HD11 | 1:B:1010:GLN:H    | 1.68                     | 0.57              |
| 1:B:146:THR:O     | 1:B:166:PHE:HA    | 2.04                     | 0.57              |
| 1:C:145:CYS:HA    | 1:C:168:CYS:HA    | 1.86                     | 0.57              |
| 1:A:146:THR:O     | 1:A:166:PHE:HA    | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:385:VAL:HG12 | 1:A:419:TRP:HB2  | 1.85                     | 0.57              |
| 1:A:533:PHE:CA   | 1:C:713:LYS:HD2  | 2.31                     | 0.57              |
| 1:B:648:VAL:O    | 1:B:652:LEU:HG   | 2.03                     | 0.57              |
| 1:A:145:CYS:HA   | 1:A:168:CYS:HA   | 1.86                     | 0.57              |
| 1:A:609:SER:O    | 1:A:613:CYS:HB2  | 2.05                     | 0.57              |
| 1:B:83:TRP:H     | 1:B:103:GLY:HA3  | 1.68                     | 0.57              |
| 1:B:195:ILE:HD13 | 1:B:201:PHE:HB2  | 1.87                     | 0.57              |
| 1:B:556:CYS:SG   | 1:B:560:SER:HB2  | 2.45                     | 0.57              |
| 1:C:939:ASN:OD1  | 1:C:940:ALA:N    | 2.36                     | 0.57              |
| 1:C:546:ALA:HA   | 1:C:556:CYS:HA   | 1.85                     | 0.57              |
| 1:A:359:ARG:CZ   | 1:A:405:ALA:H    | 2.16                     | 0.57              |
| 1:A:556:CYS:SG   | 1:A:560:SER:HB2  | 2.45                     | 0.57              |
| 1:C:385:VAL:HG22 | 1:C:419:TRP:HB2  | 1.85                     | 0.57              |
| 1:A:195:ILE:HD13 | 1:A:201:PHE:HB2  | 1.87                     | 0.57              |
| 1:C:195:ILE:HD13 | 1:C:201:PHE:HB2  | 1.87                     | 0.57              |
| 1:B:465:ASP:N    | 1:B:491:ILE:HD11 | 2.20                     | 0.57              |
| 1:C:146:THR:O    | 1:C:166:PHE:HA   | 2.04                     | 0.57              |
| 1:C:609:SER:O    | 1:C:613:CYS:HB2  | 2.05                     | 0.57              |
| 1:B:78:LEU:HB3   | 1:B:236:SER:OG   | 2.05                     | 0.56              |
| 1:A:465:ASP:N    | 1:A:491:ILE:HD11 | 2.20                     | 0.56              |
| 1:B:333:ASN:HD21 | 1:B:336:LYS:HZ3  | 1.53                     | 0.56              |
| 1:C:648:VAL:O    | 1:C:652:LEU:HG   | 2.03                     | 0.56              |
| 1:A:105:CYS:HB3  | 1:A:110:SER:HA   | 1.86                     | 0.56              |
| 1:A:247:THR:HA   | 1:B:469:ASN:OD1  | 2.05                     | 0.56              |
| 1:B:145:CYS:HA   | 1:B:168:CYS:HA   | 1.86                     | 0.56              |
| 1:B:609:SER:O    | 1:B:613:CYS:HB2  | 2.05                     | 0.56              |
| 1:B:939:ASN:OD1  | 1:B:940:ALA:N    | 2.36                     | 0.56              |
| 1:C:333:ASN:HD21 | 1:C:336:LYS:HZ3  | 1.52                     | 0.56              |
| 1:C:556:CYS:SG   | 1:C:560:SER:HB2  | 2.45                     | 0.56              |
| 1:A:346:PHE:HB3  | 1:A:428:VAL:CB   | 2.36                     | 0.56              |
| 1:C:105:CYS:HB3  | 1:C:110:SER:HA   | 1.86                     | 0.56              |
| 1:C:465:ASP:N    | 1:C:491:ILE:HD11 | 2.20                     | 0.56              |
| 1:B:282:GLN:HB2  | 1:B:284:VAL:HG12 | 1.87                     | 0.56              |
| 1:C:801:ALA:O    | 1:C:805:ILE:CB   | 2.54                     | 0.56              |
| 1:A:1005:ILE:HA  | 1:A:1008:PHE:CD2 | 2.41                     | 0.56              |
| 1:B:105:CYS:HB3  | 1:B:110:SER:HA   | 1.86                     | 0.56              |
| 1:C:85:VAL:HG13  | 1:C:88:LEU:H     | 1.71                     | 0.56              |
| 1:A:801:ALA:O    | 1:A:805:ILE:CB   | 2.54                     | 0.56              |
| 1:B:188:LYS:NZ   | 1:C:486:VAL:O    | 2.34                     | 0.56              |
| 1:B:360:TRP:NE1  | 1:B:402:ALA:HB1  | 2.21                     | 0.56              |
| 1:A:333:ASN:HD21 | 1:A:336:LYS:HZ3  | 1.53                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:346:PHE:HB3  | 1:C:428:VAL:CB   | 2.36                     | 0.56              |
| 1:A:78:LEU:HB3   | 1:A:236:SER:OG   | 2.05                     | 0.56              |
| 1:A:85:VAL:HG23  | 1:A:88:LEU:H     | 1.71                     | 0.56              |
| 1:B:346:PHE:HB3  | 1:B:428:VAL:CB   | 2.36                     | 0.56              |
| 1:C:78:LEU:HB3   | 1:C:236:SER:OG   | 2.05                     | 0.56              |
| 1:C:170:VAL:N    | 1:C:181:ALA:O    | 2.36                     | 0.56              |
| 1:C:316:LYS:HB3  | 1:C:316:LYS:HZ3  | 1.69                     | 0.56              |
| 1:A:385:VAL:H    | 1:A:425:ILE:HD12 | 1.72                     | 0.55              |
| 1:B:144:TYR:HE2  | 4:B:1203:NAG:C2  | 2.19                     | 0.55              |
| 1:B:801:ALA:O    | 1:B:805:ILE:CB   | 2.54                     | 0.55              |
| 1:B:968:VAL:H    | 1:B:973:GLY:HA2  | 1.72                     | 0.55              |
| 1:A:90:PHE:HZ    | 4:A:1204:NAG:H3  | 1.71                     | 0.55              |
| 1:A:1022:SER:OG  | 1:A:1024:SER:OG  | 2.24                     | 0.55              |
| 1:A:939:ASN:OD1  | 1:A:940:ALA:N    | 2.36                     | 0.55              |
| 1:A:968:VAL:H    | 1:A:973:GLY:HA2  | 1.72                     | 0.55              |
| 1:B:85:VAL:HG23  | 1:B:88:LEU:H     | 1.71                     | 0.55              |
| 1:C:776:ARG:HD3  | 1:C:935:PHE:HB3  | 1.88                     | 0.55              |
| 1:C:1005:ILE:HA  | 1:C:1008:PHE:CD2 | 2.41                     | 0.55              |
| 1:C:968:VAL:H    | 1:C:973:GLY:HA2  | 1.72                     | 0.55              |
| 1:A:289:SER:OG   | 1:A:442:THR:N    | 2.40                     | 0.55              |
| 1:B:1005:ILE:HA  | 1:B:1008:PHE:CD2 | 2.41                     | 0.55              |
| 1:A:576:ALA:HB2  | 1:C:775:SER:CB   | 2.24                     | 0.55              |
| 1:B:485:ASP:N    | 1:B:490:THR:O    | 2.27                     | 0.55              |
| 1:B:775:SER:HB3  | 1:C:576:ALA:CA   | 2.37                     | 0.55              |
| 1:C:360:TRP:NE1  | 1:C:402:ALA:HB1  | 2.21                     | 0.55              |
| 1:C:385:VAL:H    | 1:C:425:ILE:HD12 | 1.71                     | 0.55              |
| 1:A:458:GLY:HA2  | 1:A:497:CYS:HB3  | 1.89                     | 0.55              |
| 1:B:776:ARG:HD3  | 1:B:935:PHE:HB3  | 1.88                     | 0.55              |
| 1:A:776:ARG:HD3  | 1:A:935:PHE:HB3  | 1.88                     | 0.55              |
| 1:A:895:HIS:O    | 1:A:899:LYS:HD3  | 2.07                     | 0.55              |
| 1:A:346:PHE:HA   | 1:A:426:THR:C    | 2.32                     | 0.55              |
| 1:A:360:TRP:NE1  | 1:A:402:ALA:HB1  | 2.21                     | 0.55              |
| 1:C:895:HIS:O    | 1:C:899:LYS:HD3  | 2.07                     | 0.55              |
| 3:E:1:NAG:C6     | 3:E:1:NAG:C2     | 2.85                     | 0.55              |
| 1:C:282:GLN:HB2  | 1:C:284:VAL:HG12 | 1.87                     | 0.54              |
| 1:A:282:GLN:HB2  | 1:A:284:VAL:HG12 | 1.87                     | 0.54              |
| 1:A:297:HIS:CB   | 1:A:433:GLU:HG3  | 2.38                     | 0.54              |
| 1:B:297:HIS:CB   | 1:B:433:GLU:HG3  | 2.38                     | 0.54              |
| 1:B:527:VAL:HG23 | 1:B:537:SER:H    | 1.72                     | 0.54              |
| 1:C:527:VAL:HG13 | 1:C:537:SER:H    | 1.72                     | 0.54              |
| 1:B:289:SER:OG   | 1:B:442:THR:N    | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:791:GLN:O    | 1:B:794:LEU:HG   | 2.07                     | 0.54              |
| 1:B:895:HIS:O    | 1:B:899:LYS:HD3  | 2.07                     | 0.54              |
| 1:C:368:ASN:HD21 | 1:C:396:CYS:HA   | 1.73                     | 0.54              |
| 1:A:327:ILE:H    | 1:A:327:ILE:CD1  | 2.19                     | 0.54              |
| 1:A:527:VAL:HG23 | 1:A:537:SER:H    | 1.73                     | 0.54              |
| 1:A:791:GLN:O    | 1:A:794:LEU:HG   | 2.07                     | 0.54              |
| 1:C:289:SER:OG   | 1:C:442:THR:N    | 2.40                     | 0.54              |
| 1:C:458:GLY:HA2  | 1:C:497:CYS:HB3  | 1.89                     | 0.54              |
| 3:G:1:NAG:C6     | 3:G:1:NAG:C2     | 2.85                     | 0.54              |
| 1:A:311:GLN:HB2  | 1:A:321:TYR:CD2  | 2.43                     | 0.54              |
| 1:B:385:VAL:H    | 1:B:425:ILE:HD12 | 1.72                     | 0.54              |
| 1:C:346:PHE:HA   | 1:C:426:THR:C    | 2.32                     | 0.54              |
| 1:C:389:LEU:HA   | 1:C:415:LEU:HB2  | 1.90                     | 0.54              |
| 1:A:465:ASP:HB2  | 1:A:491:ILE:HD11 | 1.90                     | 0.54              |
| 1:A:597:LEU:HD11 | 1:A:913:LYS:NZ   | 2.23                     | 0.54              |
| 1:A:624:LYS:HE2  | 1:B:72:ARG:CD    | 2.38                     | 0.54              |
| 1:B:65:SER:HB3   | 1:C:470:GLY:HA3  | 1.90                     | 0.54              |
| 1:B:170:VAL:N    | 1:B:181:ALA:O    | 2.36                     | 0.54              |
| 1:B:316:LYS:CA   | 1:B:316:LYS:CE   | 2.85                     | 0.54              |
| 1:B:320:CYS:SG   | 1:B:410:TYR:OH   | 2.57                     | 0.54              |
| 1:C:506:TYR:N    | 1:C:509:ALA:O    | 2.34                     | 0.54              |
| 1:B:128:ARG:HH12 | 1:B:228:ASP:HB2  | 1.73                     | 0.54              |
| 1:B:260:ASN:OD1  | 1:B:263:ARG:NH1  | 2.23                     | 0.54              |
| 1:B:368:ASN:HD21 | 1:B:396:CYS:HA   | 1.73                     | 0.54              |
| 1:C:485:ASP:N    | 1:C:490:THR:O    | 2.27                     | 0.54              |
| 1:A:170:VAL:O    | 1:A:181:ALA:N    | 2.29                     | 0.54              |
| 1:B:346:PHE:HA   | 1:B:426:THR:C    | 2.32                     | 0.54              |
| 1:C:937:LEU:HB2  | 1:C:948:LEU:HB2  | 1.90                     | 0.54              |
| 1:A:937:LEU:HB2  | 1:A:948:LEU:HB2  | 1.90                     | 0.53              |
| 1:B:458:GLY:HA2  | 1:B:497:CYS:HB3  | 1.90                     | 0.53              |
| 1:B:694:ASP:OD1  | 1:B:695:ILE:N    | 2.42                     | 0.53              |
| 1:C:311:GLN:HB2  | 1:C:321:TYR:CD2  | 2.43                     | 0.53              |
| 1:A:403:ASN:HD21 | 1:A:406:TYR:HD1  | 1.56                     | 0.53              |
| 1:C:298:LYS:HG2  | 1:C:345:HIS:CE1  | 2.43                     | 0.53              |
| 1:C:791:GLN:O    | 1:C:794:LEU:HG   | 2.07                     | 0.53              |
| 1:A:893:VAL:O    | 1:A:897:LEU:HG   | 2.09                     | 0.53              |
| 1:B:465:ASP:HB2  | 1:B:491:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:893:VAL:O    | 1:B:897:LEU:HG   | 2.09                     | 0.53              |
| 1:B:937:LEU:HB2  | 1:B:948:LEU:HB2  | 1.90                     | 0.53              |
| 1:C:124:GLU:OE1  | 1:C:124:GLU:N    | 2.27                     | 0.53              |
| 3:I:1:NAG:C6     | 3:I:1:NAG:C2     | 2.85                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:ASN:OD1  | 1:A:263:ARG:NH1  | 2.23                     | 0.53              |
| 1:A:304:LEU:HD12 | 1:A:305:TYR:H    | 1.74                     | 0.53              |
| 1:B:298:LYS:HG2  | 1:B:345:HIS:CE1  | 2.43                     | 0.53              |
| 1:B:304:LEU:HD12 | 1:B:305:TYR:H    | 1.74                     | 0.53              |
| 1:B:311:GLN:HB2  | 1:B:321:TYR:CD2  | 2.43                     | 0.53              |
| 1:C:297:HIS:CB   | 1:C:433:GLU:HG3  | 2.38                     | 0.53              |
| 1:A:128:ARG:HH12 | 1:A:228:ASP:HB2  | 1.73                     | 0.53              |
| 1:A:368:ASN:HD21 | 1:A:396:CYS:HA   | 1.73                     | 0.53              |
| 1:A:298:LYS:HG2  | 1:A:345:HIS:CE1  | 2.43                     | 0.53              |
| 1:B:282:GLN:H    | 1:B:282:GLN:CD   | 2.17                     | 0.53              |
| 1:B:711:ASP:OD2  | 1:C:532:LYS:HG3  | 2.08                     | 0.53              |
| 1:C:893:VAL:O    | 1:C:897:LEU:HG   | 2.09                     | 0.53              |
| 1:C:541:TYR:HA   | 1:C:560:SER:OG   | 2.09                     | 0.53              |
| 1:A:170:VAL:N    | 1:A:181:ALA:O    | 2.36                     | 0.53              |
| 1:A:384:SER:H    | 1:A:425:ILE:HG13 | 1.74                     | 0.53              |
| 1:A:959:ASP:OD1  | 1:A:960:VAL:N    | 2.42                     | 0.53              |
| 1:B:306:VAL:HA   | 1:B:325:VAL:HA   | 1.90                     | 0.53              |
| 1:B:959:ASP:OD1  | 1:B:960:VAL:N    | 2.42                     | 0.53              |
| 1:C:128:ARG:HH12 | 1:C:228:ASP:HB2  | 1.73                     | 0.53              |
| 1:B:986:GLU:OE1  | 1:B:986:GLU:N    | 2.33                     | 0.53              |
| 1:C:983:LEU:HD11 | 1:C:990:TYR:HB3  | 1.91                     | 0.53              |
| 1:A:389:LEU:HA   | 1:A:415:LEU:HB2  | 1.90                     | 0.52              |
| 1:B:597:LEU:HD11 | 1:B:913:LYS:NZ   | 2.23                     | 0.52              |
| 1:B:607:ASP:OD1  | 1:B:609:SER:N    | 2.42                     | 0.52              |
| 1:C:306:VAL:HA   | 1:C:325:VAL:HA   | 1.90                     | 0.52              |
| 1:C:316:LYS:CA   | 1:C:316:LYS:CE   | 2.85                     | 0.52              |
| 1:C:959:ASP:OD1  | 1:C:960:VAL:N    | 2.42                     | 0.52              |
| 1:A:694:ASP:OD1  | 1:A:695:ILE:N    | 2.42                     | 0.52              |
| 1:A:788:GLN:O    | 1:A:792:LYS:NZ   | 2.43                     | 0.52              |
| 1:B:389:LEU:HA   | 1:B:415:LEU:HB2  | 1.90                     | 0.52              |
| 1:B:541:TYR:HA   | 1:B:560:SER:OG   | 2.09                     | 0.52              |
| 1:C:304:LEU:HD12 | 1:C:305:TYR:H    | 1.74                     | 0.52              |
| 1:C:465:ASP:HB2  | 1:C:491:ILE:HD11 | 1.90                     | 0.52              |
| 1:C:984:TYR:CE2  | 1:C:986:GLU:HB3  | 2.44                     | 0.52              |
| 3:E:1:NAG:H61    | 3:E:1:NAG:C2     | 2.38                     | 0.52              |
| 1:A:541:TYR:HA   | 1:A:560:SER:OG   | 2.09                     | 0.52              |
| 1:C:694:ASP:OD1  | 1:C:695:ILE:N    | 2.42                     | 0.52              |
| 1:A:282:GLN:H    | 1:A:282:GLN:CD   | 2.17                     | 0.52              |
| 1:A:588:TRP:CH2  | 1:A:953:LEU:HB2  | 2.45                     | 0.52              |
| 1:B:106:LYS:HG2  | 1:B:106:LYS:O    | 2.10                     | 0.52              |
| 1:B:403:ASN:HD21 | 1:B:406:TYR:HD1  | 1.56                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:690:SER:HB3  | 1:C:939:ASN:HD21 | 1.75                     | 0.52              |
| 1:B:682:SER:O    | 1:B:682:SER:OG   | 2.28                     | 0.52              |
| 1:B:788:GLN:O    | 1:B:792:LYS:NZ   | 2.43                     | 0.52              |
| 1:B:984:TYR:CE2  | 1:B:986:GLU:HB3  | 2.44                     | 0.52              |
| 1:C:597:LEU:HD11 | 1:C:913:LYS:NZ   | 2.23                     | 0.52              |
| 1:A:506:TYR:N    | 1:A:509:ALA:O    | 2.34                     | 0.52              |
| 1:C:282:GLN:H    | 1:C:282:GLN:CD   | 2.17                     | 0.52              |
| 1:C:588:TRP:CH2  | 1:C:953:LEU:HB2  | 2.45                     | 0.52              |
| 1:C:640:SER:HA   | 1:C:643:LEU:HD12 | 1.92                     | 0.52              |
| 1:A:306:VAL:HA   | 1:A:325:VAL:HA   | 1.90                     | 0.52              |
| 1:B:384:SER:H    | 1:B:425:ILE:HG13 | 1.74                     | 0.52              |
| 1:C:384:SER:H    | 1:C:425:ILE:HG13 | 1.74                     | 0.52              |
| 1:A:309:LYS:NZ   | 1:A:322:PRO:O    | 2.41                     | 0.52              |
| 1:B:611:TYR:CZ   | 1:B:851:LEU:HD21 | 2.45                     | 0.52              |
| 1:A:128:ARG:HB2  | 1:A:159:PHE:HD2  | 1.75                     | 0.52              |
| 1:A:971:ARG:HA   | 1:A:971:ARG:NE   | 2.25                     | 0.52              |
| 1:C:611:TYR:CZ   | 1:C:851:LEU:HD21 | 2.45                     | 0.52              |
| 1:A:228:ASP:OD1  | 1:A:229:PHE:N    | 2.43                     | 0.51              |
| 1:B:367:GLY:N    | 1:B:398:MET:SD   | 2.83                     | 0.51              |
| 1:B:1015:ASN:HB3 | 1:B:1018:PHE:CE2 | 2.46                     | 0.51              |
| 1:C:971:ARG:HA   | 1:C:971:ARG:NE   | 2.25                     | 0.51              |
| 1:A:1015:ASN:HB3 | 1:A:1018:PHE:CE2 | 2.46                     | 0.51              |
| 1:A:716:THR:O    | 1:B:461:ARG:NH1  | 2.39                     | 0.51              |
| 1:B:588:TRP:CH2  | 1:B:953:LEU:HB2  | 2.45                     | 0.51              |
| 1:B:870:ASP:HB2  | 1:B:873:GLN:HE22 | 1.76                     | 0.51              |
| 1:C:170:VAL:O    | 1:C:181:ALA:N    | 2.29                     | 0.51              |
| 1:C:921:GLN:OE1  | 1:C:934:ILE:HA   | 2.11                     | 0.51              |
| 1:C:986:GLU:OE1  | 1:C:986:GLU:N    | 2.33                     | 0.51              |
| 1:A:640:SER:HA   | 1:A:643:LEU:HD12 | 1.91                     | 0.51              |
| 1:A:690:SER:O    | 1:A:693:GLU:HG2  | 2.11                     | 0.51              |
| 1:A:983:LEU:HD11 | 1:A:990:TYR:HB3  | 1.91                     | 0.51              |
| 1:B:122:ASN:OD1  | 4:B:1202:NAG:C1  | 2.58                     | 0.51              |
| 1:B:890:ASN:HA   | 1:B:893:VAL:HG12 | 1.92                     | 0.51              |
| 1:B:983:LEU:HD11 | 1:B:990:TYR:HB3  | 1.91                     | 0.51              |
| 1:C:106:LYS:O    | 1:C:106:LYS:HG2  | 2.10                     | 0.51              |
| 1:C:474:THR:HA   | 1:C:480:LEU:HA   | 1.93                     | 0.51              |
| 1:A:106:LYS:O    | 1:A:106:LYS:HG2  | 2.09                     | 0.51              |
| 1:A:485:ASP:N    | 1:A:490:THR:O    | 2.27                     | 0.51              |
| 1:A:607:ASP:OD1  | 1:A:609:SER:N    | 2.42                     | 0.51              |
| 1:C:303:VAL:H    | 1:C:329:LEU:HA   | 1.76                     | 0.51              |
| 1:C:607:ASP:OD1  | 1:C:609:SER:N    | 2.42                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:690:SER:O    | 1:C:693:GLU:HG2   | 2.11                     | 0.51              |
| 1:A:611:TYR:CZ   | 1:A:851:LEU:HD21  | 2.45                     | 0.51              |
| 1:A:690:SER:HB3  | 1:A:939:ASN:HD21  | 1.75                     | 0.51              |
| 1:A:1008:PHE:CE2 | 1:A:1030:VAL:HG11 | 2.46                     | 0.51              |
| 1:B:144:TYR:OH   | 4:B:1203:NAG:O5   | 2.27                     | 0.51              |
| 1:B:921:GLN:OE1  | 1:B:934:ILE:HA    | 2.11                     | 0.51              |
| 1:B:971:ARG:HA   | 1:B:971:ARG:NE    | 2.25                     | 0.51              |
| 1:A:144:TYR:CD2  | 4:A:1203:NAG:H83  | 2.46                     | 0.51              |
| 1:B:389:LEU:HD23 | 1:B:389:LEU:H     | 1.76                     | 0.51              |
| 1:B:474:THR:HA   | 1:B:480:LEU:HA    | 1.93                     | 0.51              |
| 1:C:403:ASN:HD21 | 1:C:406:TYR:HD1   | 1.56                     | 0.51              |
| 1:C:788:GLN:O    | 1:C:792:LYS:NZ    | 2.43                     | 0.51              |
| 1:A:909:LEU:O    | 1:A:913:LYS:HG3   | 2.11                     | 0.51              |
| 1:A:984:TYR:CE2  | 1:A:986:GLU:HB3   | 2.44                     | 0.51              |
| 1:B:128:ARG:HB2  | 1:B:159:PHE:HD2   | 1.75                     | 0.51              |
| 1:B:506:TYR:N    | 1:B:509:ALA:O     | 2.34                     | 0.51              |
| 1:B:690:SER:O    | 1:B:693:GLU:HG2   | 2.10                     | 0.51              |
| 1:B:1022:SER:OG  | 1:B:1024:SER:OG   | 2.24                     | 0.51              |
| 1:C:228:ASP:OD1  | 1:C:229:PHE:N     | 2.43                     | 0.51              |
| 1:A:489:GLY:N    | 1:C:188:LYS:HE2   | 2.26                     | 0.51              |
| 1:B:228:ASP:OD1  | 1:B:229:PHE:N     | 2.43                     | 0.51              |
| 1:C:870:ASP:HB2  | 1:C:873:GLN:HE22  | 1.76                     | 0.51              |
| 1:C:890:ASN:HA   | 1:C:893:VAL:HG12  | 1.92                     | 0.51              |
| 1:C:909:LEU:O    | 1:C:913:LYS:HG3   | 2.11                     | 0.51              |
| 1:A:262:LEU:O    | 1:A:266:GLN:HG2   | 2.12                     | 0.50              |
| 1:A:367:GLY:N    | 1:A:398:MET:SD    | 2.83                     | 0.50              |
| 1:A:474:THR:HA   | 1:A:480:LEU:HA    | 1.93                     | 0.50              |
| 1:A:576:ALA:CA   | 1:C:775:SER:HB3   | 2.41                     | 0.50              |
| 1:B:640:SER:HA   | 1:B:643:LEU:HD12  | 1.91                     | 0.50              |
| 1:C:1015:ASN:HB3 | 1:C:1018:PHE:CE2  | 2.46                     | 0.50              |
| 1:A:154:ASP:OD1  | 1:A:154:ASP:N     | 2.44                     | 0.50              |
| 1:A:657:LYS:O    | 1:A:661:LEU:HD23  | 2.11                     | 0.50              |
| 1:C:316:LYS:N    | 1:C:316:LYS:CD    | 2.73                     | 0.50              |
| 1:A:550:TYR:HD2  | 1:A:552:SER:H     | 1.59                     | 0.50              |
| 1:A:890:ASN:HA   | 1:A:893:VAL:HG12  | 1.92                     | 0.50              |
| 1:C:389:LEU:H    | 1:C:389:LEU:HD23  | 1.76                     | 0.50              |
| 1:A:303:VAL:H    | 1:A:329:LEU:HA    | 1.76                     | 0.50              |
| 1:B:170:VAL:O    | 1:B:181:ALA:N     | 2.29                     | 0.50              |
| 1:B:262:LEU:O    | 1:B:266:GLN:HG2   | 2.12                     | 0.50              |
| 1:B:303:VAL:H    | 1:B:329:LEU:HA    | 1.76                     | 0.50              |
| 1:B:1008:PHE:CE2 | 1:B:1030:VAL:HG11 | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:367:GLY:N    | 1:C:398:MET:SD   | 2.83                     | 0.50              |
| 1:A:316:LYS:N    | 1:A:316:LYS:CD   | 2.73                     | 0.50              |
| 1:B:309:LYS:NZ   | 1:B:322:PRO:O    | 2.41                     | 0.50              |
| 1:C:327:ILE:HD12 | 1:C:327:ILE:N    | 2.26                     | 0.50              |
| 1:A:389:LEU:H    | 1:A:389:LEU:HD23 | 1.76                     | 0.50              |
| 1:A:402:ALA:HB3  | 1:A:410:TYR:HB2  | 1.93                     | 0.50              |
| 1:A:921:GLN:OE1  | 1:A:934:ILE:HA   | 2.11                     | 0.50              |
| 1:B:402:ALA:HB3  | 1:B:410:TYR:HB2  | 1.93                     | 0.50              |
| 1:B:550:TYR:HD2  | 1:B:552:SER:H    | 1.58                     | 0.50              |
| 1:B:711:ASP:H    | 1:C:532:LYS:CE   | 2.25                     | 0.50              |
| 1:C:168:CYS:HB2  | 1:C:183:VAL:CB   | 2.42                     | 0.50              |
| 1:A:316:LYS:NZ   | 1:A:316:LYS:CB   | 2.73                     | 0.50              |
| 1:A:524:PHE:HB2  | 1:A:538:ASN:HB3  | 1.93                     | 0.50              |
| 1:B:147:ASN:HB3  | 1:B:154:ASP:OD2  | 2.12                     | 0.50              |
| 1:B:296:TYR:O    | 1:B:345:HIS:NE2  | 2.45                     | 0.50              |
| 1:B:690:SER:HB3  | 1:B:939:ASN:HD21 | 1.75                     | 0.50              |
| 1:C:402:ALA:HB3  | 1:C:410:TYR:HB2  | 1.93                     | 0.50              |
| 1:A:113:LEU:N    | 1:A:113:LEU:CD2  | 2.73                     | 0.50              |
| 1:B:83:TRP:N     | 1:B:103:GLY:HA3  | 2.27                     | 0.50              |
| 1:B:168:CYS:HB2  | 1:B:183:VAL:CB   | 2.42                     | 0.50              |
| 1:B:288:VAL:CB   | 1:B:448:LYS:HB3  | 2.42                     | 0.50              |
| 1:B:299:HIS:ND1  | 1:B:301:PHE:HE1  | 2.10                     | 0.50              |
| 1:B:657:LYS:O    | 1:B:661:LEU:HD23 | 2.11                     | 0.50              |
| 1:C:299:HIS:ND1  | 1:C:301:PHE:HE1  | 2.10                     | 0.50              |
| 1:C:672:LEU:O    | 1:C:674:SER:N    | 2.45                     | 0.50              |
| 1:B:127:LEU:HD23 | 1:B:159:PHE:O    | 2.12                     | 0.50              |
| 1:C:288:VAL:CB   | 1:C:448:LYS:HB3  | 2.42                     | 0.50              |
| 1:C:296:TYR:O    | 1:C:345:HIS:NE2  | 2.45                     | 0.50              |
| 1:C:524:PHE:HB2  | 1:C:538:ASN:HB3  | 1.93                     | 0.50              |
| 1:C:657:LYS:O    | 1:C:661:LEU:HD23 | 2.11                     | 0.50              |
| 1:A:168:CYS:HB2  | 1:A:183:VAL:CB   | 2.42                     | 0.49              |
| 1:A:288:VAL:CB   | 1:A:448:LYS:HB3  | 2.42                     | 0.49              |
| 1:A:296:TYR:O    | 1:A:345:HIS:NE2  | 2.45                     | 0.49              |
| 1:A:298:LYS:H    | 1:A:345:HIS:CE1  | 2.30                     | 0.49              |
| 1:A:672:LEU:O    | 1:A:674:SER:N    | 2.45                     | 0.49              |
| 1:B:909:LEU:O    | 1:B:913:LYS:HG3  | 2.11                     | 0.49              |
| 1:C:360:TRP:CE2  | 1:C:402:ALA:HB1  | 2.47                     | 0.49              |
| 1:A:346:PHE:HD1  | 1:A:427:GLY:C    | 2.20                     | 0.49              |
| 1:B:113:LEU:N    | 1:B:113:LEU:CD2  | 2.73                     | 0.49              |
| 1:C:147:ASN:HB3  | 1:C:154:ASP:OD2  | 2.12                     | 0.49              |
| 1:A:299:HIS:ND1  | 1:A:301:PHE:HE1  | 2.10                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:315:GLY:CA   | 1:B:404:TRP:HZ2   | 2.10                     | 0.49              |
| 1:C:196:SER:OG   | 1:C:197:ARG:N     | 2.45                     | 0.49              |
| 1:C:910:ALA:O    | 1:C:914:VAL:HG13  | 2.12                     | 0.49              |
| 1:A:83:TRP:N     | 1:A:103:GLY:HA3   | 2.27                     | 0.49              |
| 1:A:127:LEU:HD23 | 1:A:159:PHE:O     | 2.12                     | 0.49              |
| 1:A:446:CYS:SG   | 1:A:497:CYS:HB2   | 2.53                     | 0.49              |
| 1:A:910:ALA:O    | 1:A:914:VAL:HG23  | 2.12                     | 0.49              |
| 1:B:908:GLN:O    | 1:B:912:GLN:CB    | 2.53                     | 0.49              |
| 1:C:83:TRP:N     | 1:C:103:GLY:HA3   | 2.27                     | 0.49              |
| 1:C:346:PHE:HD1  | 1:C:427:GLY:C     | 2.20                     | 0.49              |
| 1:C:1008:PHE:CE2 | 1:C:1030:VAL:HG21 | 2.46                     | 0.49              |
| 1:C:1024:SER:OG  | 1:C:1025:GLU:OE2  | 2.31                     | 0.49              |
| 1:A:870:ASP:HB2  | 1:A:873:GLN:HE22  | 1.76                     | 0.49              |
| 1:B:360:TRP:CE2  | 1:B:402:ALA:HB1   | 2.47                     | 0.49              |
| 1:C:256:ASN:OD1  | 1:C:257:SER:N     | 2.46                     | 0.49              |
| 1:C:262:LEU:O    | 1:C:266:GLN:HG2   | 2.12                     | 0.49              |
| 1:C:297:HIS:ND1  | 1:C:345:HIS:HB3   | 2.28                     | 0.49              |
| 1:A:188:LYS:NZ   | 1:B:486:VAL:O     | 2.45                     | 0.49              |
| 1:A:611:TYR:CE1  | 1:A:851:LEU:HD11  | 2.48                     | 0.49              |
| 1:C:127:LEU:HD23 | 1:C:159:PHE:O     | 2.12                     | 0.49              |
| 1:C:128:ARG:HB2  | 1:C:159:PHE:HD2   | 1.75                     | 0.49              |
| 1:C:291:VAL:CB   | 1:C:451:ILE:HG13  | 2.43                     | 0.49              |
| 1:C:400:ILE:HG13 | 1:C:414:SER:OG    | 2.13                     | 0.49              |
| 1:C:550:TYR:HD2  | 1:C:552:SER:H     | 1.59                     | 0.49              |
| 1:C:918:VAL:HG22 | 1:C:919:LYS:HD3   | 1.95                     | 0.49              |
| 1:A:578:VAL:HA   | 1:A:964:SER:OG    | 2.13                     | 0.49              |
| 1:B:346:PHE:HD1  | 1:B:427:GLY:C     | 2.20                     | 0.49              |
| 1:B:711:ASP:HB2  | 1:C:532:LYS:O     | 2.12                     | 0.49              |
| 1:C:298:LYS:H    | 1:C:345:HIS:CE1   | 2.30                     | 0.49              |
| 1:A:83:TRP:HB3   | 1:A:233:ALA:HA    | 1.94                     | 0.49              |
| 1:A:297:HIS:ND1  | 1:A:345:HIS:HB3   | 2.28                     | 0.49              |
| 1:B:512:GLY:HA2  | 1:B:536:ALA:O     | 2.13                     | 0.49              |
| 1:B:868:ARG:O    | 1:C:372:SER:OG    | 2.31                     | 0.49              |
| 1:C:311:GLN:CG   | 1:C:320:CYS:HA    | 2.34                     | 0.49              |
| 1:A:291:VAL:CB   | 1:A:451:ILE:HG13  | 2.43                     | 0.49              |
| 1:A:327:ILE:HD12 | 1:A:327:ILE:N     | 2.26                     | 0.49              |
| 1:A:524:PHE:HB2  | 1:A:538:ASN:C     | 2.38                     | 0.49              |
| 1:A:712:TYR:HA   | 1:A:715:CYS:SG    | 2.53                     | 0.49              |
| 1:A:290:ILE:HD12 | 1:A:290:ILE:N     | 2.28                     | 0.49              |
| 1:A:945:LEU:HB3  | 1:A:947:PHE:HE1   | 1.78                     | 0.49              |
| 1:A:986:GLU:OE1  | 1:A:986:GLU:N     | 2.33                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1024:SER:OG  | 1:A:1025:GLU:OE2 | 2.31                     | 0.49              |
| 1:B:154:ASP:OD1  | 1:B:154:ASP:N    | 2.44                     | 0.49              |
| 1:B:256:ASN:OD1  | 1:B:257:SER:N    | 2.46                     | 0.49              |
| 1:B:524:PHE:HB2  | 1:B:538:ASN:HB3  | 1.93                     | 0.49              |
| 1:B:578:VAL:HA   | 1:B:964:SER:OG   | 2.13                     | 0.49              |
| 1:C:446:CYS:SG   | 1:C:497:CYS:HB2  | 2.53                     | 0.49              |
| 1:A:404:TRP:HE3  | 1:A:408:LYS:HG3  | 1.78                     | 0.48              |
| 1:B:672:LEU:O    | 1:B:674:SER:N    | 2.45                     | 0.48              |
| 1:B:899:LYS:O    | 1:B:902:GLU:HG3  | 2.13                     | 0.48              |
| 1:C:512:GLY:HA2  | 1:C:536:ALA:O    | 2.13                     | 0.48              |
| 1:A:147:ASN:HB3  | 1:A:154:ASP:OD2  | 2.12                     | 0.48              |
| 1:A:400:ILE:HG13 | 1:A:414:SER:OG   | 2.13                     | 0.48              |
| 1:A:461:ARG:NH1  | 1:C:716:THR:O    | 2.45                     | 0.48              |
| 1:A:512:GLY:HA2  | 1:A:536:ALA:O    | 2.13                     | 0.48              |
| 1:B:147:ASN:O    | 1:B:166:PHE:N    | 2.46                     | 0.48              |
| 1:B:910:ALA:O    | 1:B:914:VAL:HG23 | 2.12                     | 0.48              |
| 1:B:1024:SER:OG  | 1:B:1025:GLU:OE2 | 2.31                     | 0.48              |
| 1:C:83:TRP:HB3   | 1:C:233:ALA:HA   | 1.94                     | 0.48              |
| 1:C:147:ASN:O    | 1:C:166:PHE:N    | 2.46                     | 0.48              |
| 1:C:611:TYR:CE1  | 1:C:851:LEU:HD11 | 2.48                     | 0.48              |
| 1:C:899:LYS:O    | 1:C:902:GLU:HG3  | 2.13                     | 0.48              |
| 1:C:1022:SER:OG  | 1:C:1024:SER:OG  | 2.24                     | 0.48              |
| 1:A:976:LEU:HG   | 1:A:978:GLN:O    | 2.14                     | 0.48              |
| 1:B:400:ILE:HG13 | 1:B:414:SER:OG   | 2.13                     | 0.48              |
| 1:B:712:TYR:HA   | 1:B:715:CYS:SG   | 2.53                     | 0.48              |
| 1:C:578:VAL:HA   | 1:C:964:SER:OG   | 2.13                     | 0.48              |
| 1:C:752:LEU:HD12 | 1:C:753:ILE:HG13 | 1.95                     | 0.48              |
| 1:C:946:VAL:C    | 1:C:947:PHE:HD1  | 2.21                     | 0.48              |
| 1:A:360:TRP:CE2  | 1:A:402:ALA:HB1  | 2.47                     | 0.48              |
| 1:B:446:CYS:SG   | 1:B:497:CYS:HB2  | 2.53                     | 0.48              |
| 1:B:691:ALA:O    | 1:B:695:ILE:HG12 | 2.14                     | 0.48              |
| 1:B:752:LEU:HD12 | 1:B:753:ILE:HG13 | 1.95                     | 0.48              |
| 1:B:856:GLN:HB3  | 1:B:880:ARG:HD3  | 1.95                     | 0.48              |
| 1:B:918:VAL:HG22 | 1:B:919:LYS:HD3  | 1.95                     | 0.48              |
| 1:A:83:TRP:HA    | 1:A:102:ARG:C    | 2.39                     | 0.48              |
| 1:A:196:SER:OG   | 1:A:197:ARG:N    | 2.45                     | 0.48              |
| 1:A:798:PHE:O    | 1:A:802:MET:HG2  | 2.14                     | 0.48              |
| 1:A:856:GLN:HB3  | 1:A:880:ARG:HD3  | 1.95                     | 0.48              |
| 1:B:196:SER:OG   | 1:B:197:ARG:N    | 2.45                     | 0.48              |
| 1:B:611:TYR:CE1  | 1:B:851:LEU:HD11 | 2.48                     | 0.48              |
| 1:B:790:ASN:HA   | 1:B:793:ILE:HG12 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:945:LEU:HB3  | 1:B:947:PHE:HE1  | 1.78                     | 0.48              |
| 1:C:309:LYS:NZ   | 1:C:322:PRO:O    | 2.41                     | 0.48              |
| 1:A:496:PRO:HG3  | 1:C:730:TYR:CD1  | 2.48                     | 0.48              |
| 1:A:577:ILE:HG13 | 1:A:577:ILE:O    | 2.13                     | 0.48              |
| 1:A:611:TYR:HE1  | 1:A:851:LEU:HD11 | 1.79                     | 0.48              |
| 1:A:790:ASN:HA   | 1:A:793:ILE:HG12 | 1.95                     | 0.48              |
| 1:A:833:ILE:HG13 | 1:A:834:GLN:N    | 2.28                     | 0.48              |
| 1:A:946:VAL:C    | 1:A:947:PHE:HD1  | 2.21                     | 0.48              |
| 1:B:291:VAL:CB   | 1:B:451:ILE:HG13 | 2.43                     | 0.48              |
| 1:B:833:ILE:HG13 | 1:B:834:GLN:N    | 2.28                     | 0.48              |
| 1:C:76:PRO:HG3   | 1:C:237:TYR:HE1  | 1.79                     | 0.48              |
| 1:C:290:ILE:HD12 | 1:C:290:ILE:N    | 2.28                     | 0.48              |
| 1:C:611:TYR:HE1  | 1:C:851:LEU:HD11 | 1.78                     | 0.48              |
| 1:C:691:ALA:O    | 1:C:695:ILE:HG12 | 2.14                     | 0.48              |
| 1:C:712:TYR:HA   | 1:C:715:CYS:SG   | 2.53                     | 0.48              |
| 1:A:316:LYS:CA   | 1:A:316:LYS:CE   | 2.85                     | 0.48              |
| 1:B:327:ILE:H    | 1:B:327:ILE:CD1  | 2.19                     | 0.48              |
| 1:B:404:TRP:HE3  | 1:B:408:LYS:HG3  | 1.78                     | 0.48              |
| 1:B:524:PHE:HB2  | 1:B:538:ASN:C    | 2.38                     | 0.48              |
| 1:B:798:PHE:O    | 1:B:802:MET:HG2  | 2.14                     | 0.48              |
| 1:C:404:TRP:HE3  | 1:C:408:LYS:HG3  | 1.78                     | 0.48              |
| 1:B:298:LYS:H    | 1:B:345:HIS:CE1  | 2.30                     | 0.48              |
| 1:C:261:ARG:HG3  | 1:C:261:ARG:HH11 | 1.79                     | 0.48              |
| 1:C:833:ILE:HG13 | 1:C:834:GLN:N    | 2.28                     | 0.48              |
| 1:A:899:LYS:O    | 1:A:902:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:908:GLN:O    | 1:A:912:GLN:CB   | 2.53                     | 0.48              |
| 1:B:297:HIS:ND1  | 1:B:345:HIS:HB3  | 2.28                     | 0.48              |
| 1:B:327:ILE:HD12 | 1:B:327:ILE:N    | 2.26                     | 0.48              |
| 1:B:505:VAL:HA   | 1:B:510:VAL:HA   | 1.96                     | 0.48              |
| 1:C:83:TRP:HA    | 1:C:102:ARG:C    | 2.39                     | 0.48              |
| 1:C:286:LEU:HD22 | 1:C:446:CYS:HB3  | 1.95                     | 0.48              |
| 1:C:577:ILE:HG13 | 1:C:577:ILE:O    | 2.13                     | 0.48              |
| 1:C:798:PHE:O    | 1:C:802:MET:HG2  | 2.14                     | 0.48              |
| 1:A:147:ASN:O    | 1:A:166:PHE:N    | 2.46                     | 0.48              |
| 1:B:85:VAL:CG2   | 1:B:229:PHE:HB2  | 2.44                     | 0.48              |
| 1:B:290:ILE:N    | 1:B:290:ILE:HD12 | 2.28                     | 0.48              |
| 1:B:713:LYS:NZ   | 1:C:533:PHE:HB2  | 2.28                     | 0.48              |
| 1:A:256:ASN:OD1  | 1:A:257:SER:N    | 2.46                     | 0.47              |
| 1:A:286:LEU:HD22 | 1:A:446:CYS:HB3  | 1.95                     | 0.47              |
| 1:A:505:VAL:HA   | 1:A:510:VAL:HA   | 1.96                     | 0.47              |
| 1:B:76:PRO:HG3   | 1:B:237:TYR:HE1  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:577:ILE:HG13 | 1:B:577:ILE:O    | 2.13                     | 0.47              |
| 1:B:611:TYR:HE1  | 1:B:851:LEU:HD11 | 1.78                     | 0.47              |
| 1:B:261:ARG:HH11 | 1:B:261:ARG:HG3  | 1.79                     | 0.47              |
| 1:C:524:PHE:HB2  | 1:C:538:ASN:C    | 2.38                     | 0.47              |
| 1:C:856:GLN:HB3  | 1:C:880:ARG:HD3  | 1.94                     | 0.47              |
| 1:C:976:LEU:HG   | 1:C:978:GLN:O    | 2.14                     | 0.47              |
| 1:A:564:VAL:CB   | 1:C:744:ARG:HH21 | 2.27                     | 0.47              |
| 1:B:83:TRP:HA    | 1:B:102:ARG:C    | 2.39                     | 0.47              |
| 1:B:83:TRP:HB3   | 1:B:233:ALA:HA   | 1.95                     | 0.47              |
| 1:A:94:PHE:HA    | 1:A:217:VAL:O    | 2.15                     | 0.47              |
| 1:B:78:LEU:O     | 1:B:80:ASN:ND2   | 2.47                     | 0.47              |
| 1:B:144:TYR:HD2  | 4:B:1203:NAG:H83 | 1.79                     | 0.47              |
| 1:B:946:VAL:C    | 1:B:947:PHE:HD1  | 2.22                     | 0.47              |
| 1:B:976:LEU:HG   | 1:B:978:GLN:O    | 2.14                     | 0.47              |
| 1:C:790:ASN:HA   | 1:C:793:ILE:HG12 | 1.95                     | 0.47              |
| 1:A:72:ARG:O     | 1:A:72:ARG:HG3   | 2.15                     | 0.47              |
| 1:A:78:LEU:O     | 1:A:80:ASN:ND2   | 2.47                     | 0.47              |
| 1:A:752:LEU:HD12 | 1:A:753:ILE:HG13 | 1.95                     | 0.47              |
| 1:C:94:PHE:HA    | 1:C:217:VAL:O    | 2.15                     | 0.47              |
| 1:A:918:VAL:HG12 | 1:A:919:LYS:HD3  | 1.95                     | 0.47              |
| 1:A:966:LEU:O    | 1:A:966:LEU:HD12 | 2.15                     | 0.47              |
| 1:B:390:LYS:O    | 1:B:416:TYR:HE1  | 1.98                     | 0.47              |
| 1:C:945:LEU:HB3  | 1:C:947:PHE:HE1  | 1.78                     | 0.47              |
| 1:A:360:TRP:CZ2  | 1:A:402:ALA:HB1  | 2.50                     | 0.47              |
| 1:A:624:LYS:HE2  | 1:B:72:ARG:HD3   | 1.97                     | 0.47              |
| 1:A:691:ALA:O    | 1:A:695:ILE:HG12 | 2.14                     | 0.47              |
| 1:A:775:SER:HB3  | 1:B:576:ALA:CA   | 2.44                     | 0.47              |
| 1:B:360:TRP:CZ2  | 1:B:402:ALA:HB1  | 2.50                     | 0.47              |
| 1:B:836:VAL:O    | 1:B:839:GLN:HG2  | 2.15                     | 0.47              |
| 1:B:976:LEU:HD12 | 1:B:976:LEU:HA   | 1.75                     | 0.47              |
| 1:C:78:LEU:O     | 1:C:80:ASN:ND2   | 2.47                     | 0.47              |
| 1:C:197:ARG:O    | 1:C:213:ASN:HA   | 2.15                     | 0.47              |
| 1:C:505:VAL:HA   | 1:C:510:VAL:HA   | 1.96                     | 0.47              |
| 1:C:966:LEU:HD12 | 1:C:966:LEU:O    | 2.15                     | 0.47              |
| 1:A:390:LYS:O    | 1:A:416:TYR:HE1  | 1.98                     | 0.47              |
| 1:A:59:LEU:HD23  | 1:A:60:LEU:N     | 2.30                     | 0.47              |
| 1:A:76:PRO:HG3   | 1:A:237:TYR:HE1  | 1.79                     | 0.47              |
| 1:B:94:PHE:HA    | 1:B:217:VAL:O    | 2.15                     | 0.47              |
| 1:B:286:LEU:HD22 | 1:B:446:CYS:HB3  | 1.95                     | 0.47              |
| 1:B:369:CYS:HB3  | 1:B:396:CYS:HB3  | 1.64                     | 0.47              |
| 1:C:836:VAL:O    | 1:C:839:GLN:HG2  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:261:ARG:HG3  | 1:A:261:ARG:HH11 | 1.79                     | 0.46              |
| 1:A:547:VAL:N    | 1:A:555:VAL:O    | 2.48                     | 0.46              |
| 1:B:921:GLN:HE21 | 1:B:921:GLN:HB2  | 1.56                     | 0.46              |
| 1:B:966:LEU:HD12 | 1:B:966:LEU:O    | 2.15                     | 0.46              |
| 1:C:144:TYR:CE2  | 4:C:1203:NAG:H2  | 2.46                     | 0.46              |
| 1:A:347:THR:N    | 1:A:427:GLY:HA2  | 2.31                     | 0.46              |
| 1:A:947:PHE:C    | 1:A:948:LEU:HD22 | 2.40                     | 0.46              |
| 1:B:159:PHE:CE2  | 1:B:221:VAL:HG13 | 2.49                     | 0.46              |
| 1:C:298:LYS:H    | 1:C:345:HIS:CG   | 2.34                     | 0.46              |
| 1:A:977:ARG:HG2  | 1:A:1007:ASP:HA  | 1.97                     | 0.46              |
| 1:C:347:THR:N    | 1:C:427:GLY:HA2  | 2.31                     | 0.46              |
| 1:C:360:TRP:CZ2  | 1:C:402:ALA:HB1  | 2.50                     | 0.46              |
| 1:C:390:LYS:O    | 1:C:416:TYR:HE1  | 1.98                     | 0.46              |
| 1:C:844:LEU:HD12 | 1:C:845:ASN:N    | 2.31                     | 0.46              |
| 1:C:976:LEU:HD12 | 1:C:976:LEU:HA   | 1.75                     | 0.46              |
| 1:A:146:THR:HA   | 1:A:154:ASP:O    | 2.16                     | 0.46              |
| 1:A:630:CYS:SG   | 1:A:631:LYS:N    | 2.89                     | 0.46              |
| 1:B:146:THR:HA   | 1:B:154:ASP:O    | 2.16                     | 0.46              |
| 1:C:630:CYS:SG   | 1:C:631:LYS:N    | 2.89                     | 0.46              |
| 1:A:128:ARG:HB3  | 1:A:222:THR:O    | 2.16                     | 0.46              |
| 1:A:197:ARG:O    | 1:A:213:ASN:HA   | 2.15                     | 0.46              |
| 1:A:320:CYS:SG   | 1:A:410:TYR:OH   | 2.57                     | 0.46              |
| 1:A:344:SER:OG   | 1:A:424:GLY:HA2  | 2.16                     | 0.46              |
| 1:A:635:ASP:HA   | 1:A:638:ARG:NH1  | 2.31                     | 0.46              |
| 1:B:128:ARG:HB3  | 1:B:222:THR:O    | 2.16                     | 0.46              |
| 1:B:966:LEU:HD13 | 1:B:1019:VAL:CG2 | 2.46                     | 0.46              |
| 1:C:154:ASP:OD1  | 1:C:154:ASP:N    | 2.44                     | 0.46              |
| 1:C:547:VAL:N    | 1:C:555:VAL:O    | 2.48                     | 0.46              |
| 1:A:682:SER:O    | 1:A:682:SER:OG   | 2.28                     | 0.46              |
| 1:A:966:LEU:HD13 | 1:A:1019:VAL:CG2 | 2.46                     | 0.46              |
| 1:B:197:ARG:O    | 1:B:213:ASN:HA   | 2.15                     | 0.46              |
| 1:B:966:LEU:HD13 | 1:B:1019:VAL:CB  | 2.46                     | 0.46              |
| 1:C:635:ASP:HA   | 1:C:638:ARG:NH1  | 2.31                     | 0.46              |
| 1:A:159:PHE:CE2  | 1:A:221:VAL:HG13 | 2.49                     | 0.46              |
| 1:A:658:ALA:HB1  | 1:A:751:SER:HA   | 1.98                     | 0.46              |
| 1:A:967:CYS:SG   | 1:A:1014:CYS:HA  | 2.56                     | 0.46              |
| 1:B:59:LEU:HD23  | 1:B:60:LEU:N     | 2.30                     | 0.46              |
| 1:B:72:ARG:O     | 1:B:72:ARG:HG3   | 2.15                     | 0.46              |
| 1:B:630:CYS:SG   | 1:B:631:LYS:N    | 2.88                     | 0.46              |
| 1:B:711:ASP:OD2  | 1:C:533:PHE:HB3  | 2.15                     | 0.46              |
| 1:C:72:ARG:HG3   | 1:C:72:ARG:O     | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:344:SER:OG   | 1:C:424:GLY:HA2  | 2.16                     | 0.46              |
| 1:C:966:LEU:HD13 | 1:C:1019:VAL:CG1 | 2.46                     | 0.46              |
| 1:B:90:PHE:CZ    | 4:B:1204:NAG:H3  | 2.48                     | 0.46              |
| 1:B:298:LYS:H    | 1:B:345:HIS:CG   | 2.34                     | 0.46              |
| 1:B:305:TYR:HB2  | 1:B:326:ASN:OD1  | 2.16                     | 0.46              |
| 1:B:316:LYS:N    | 1:B:316:LYS:CD   | 2.73                     | 0.46              |
| 1:C:966:LEU:HD13 | 1:C:1019:VAL:CB  | 2.46                     | 0.46              |
| 1:C:977:ARG:HG2  | 1:C:1007:ASP:HA  | 1.97                     | 0.46              |
| 1:A:298:LYS:H    | 1:A:345:HIS:CG   | 2.34                     | 0.46              |
| 1:B:547:VAL:N    | 1:B:555:VAL:O    | 2.48                     | 0.46              |
| 1:B:977:ARG:HG2  | 1:B:1007:ASP:HA  | 1.97                     | 0.46              |
| 1:C:128:ARG:HB3  | 1:C:222:THR:O    | 2.16                     | 0.46              |
| 1:C:359:ARG:HH22 | 1:C:403:ASN:CG   | 2.24                     | 0.46              |
| 1:C:529:GLU:HG2  | 1:C:530:LEU:H    | 1.81                     | 0.46              |
| 1:C:607:ASP:CG   | 1:C:610:THR:H    | 2.24                     | 0.46              |
| 1:C:947:PHE:C    | 1:C:948:LEU:HD22 | 2.40                     | 0.46              |
| 1:A:711:ASP:H    | 1:B:532:LYS:HE3  | 1.81                     | 0.46              |
| 1:A:775:SER:CB   | 1:B:576:ALA:HB2  | 2.25                     | 0.46              |
| 1:A:836:VAL:O    | 1:A:839:GLN:HG2  | 2.15                     | 0.46              |
| 1:A:966:LEU:HD13 | 1:A:1019:VAL:CB  | 2.46                     | 0.46              |
| 1:B:663:ASN:OD1  | 1:B:664:VAL:N    | 2.49                     | 0.46              |
| 1:C:315:GLY:CA   | 1:C:404:TRP:HZ2  | 2.10                     | 0.46              |
| 1:A:305:TYR:HB2  | 1:A:326:ASN:OD1  | 2.16                     | 0.45              |
| 1:A:657:LYS:HA   | 1:A:764:ALA:CB   | 2.46                     | 0.45              |
| 1:A:663:ASN:OD1  | 1:A:664:VAL:N    | 2.49                     | 0.45              |
| 1:B:344:SER:OG   | 1:B:424:GLY:HA2  | 2.16                     | 0.45              |
| 1:B:428:VAL:HG12 | 1:B:430:GLN:H    | 1.82                     | 0.45              |
| 1:B:947:PHE:C    | 1:B:948:LEU:HD22 | 2.40                     | 0.45              |
| 1:C:146:THR:HA   | 1:C:154:ASP:O    | 2.16                     | 0.45              |
| 1:A:428:VAL:HG12 | 1:A:430:GLN:H    | 1.81                     | 0.45              |
| 1:B:347:THR:N    | 1:B:427:GLY:HA2  | 2.31                     | 0.45              |
| 1:B:359:ARG:HH22 | 1:B:403:ASN:CG   | 2.24                     | 0.45              |
| 1:B:635:ASP:HA   | 1:B:638:ARG:NH1  | 2.31                     | 0.45              |
| 1:B:658:ALA:HB1  | 1:B:751:SER:HA   | 1.98                     | 0.45              |
| 1:C:59:LEU:HD23  | 1:C:60:LEU:N     | 2.30                     | 0.45              |
| 1:C:305:TYR:HB2  | 1:C:326:ASN:OD1  | 2.16                     | 0.45              |
| 1:C:663:ASN:OD1  | 1:C:664:VAL:N    | 2.49                     | 0.45              |
| 1:C:908:GLN:O    | 1:C:912:GLN:CB   | 2.53                     | 0.45              |
| 1:C:967:CYS:SG   | 1:C:1014:CYS:HA  | 2.56                     | 0.45              |
| 1:A:68:ASP:HB3   | 1:A:246:GLN:H    | 1.81                     | 0.45              |
| 1:B:529:GLU:HG2  | 1:B:530:LEU:H    | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:541:TYR:O    | 1:B:541:TYR:CG   | 2.70                     | 0.45              |
| 1:B:844:LEU:HD12 | 1:B:845:ASN:N    | 2.31                     | 0.45              |
| 1:C:128:ARG:NH1  | 1:C:228:ASP:HB2  | 2.31                     | 0.45              |
| 1:A:631:LYS:HZ1  | 1:B:266:GLN:CD   | 2.20                     | 0.45              |
| 1:B:867:ASP:CG   | 1:C:378:ASN:HD21 | 2.24                     | 0.45              |
| 1:C:85:VAL:CG1   | 1:C:229:PHE:HB2  | 2.44                     | 0.45              |
| 1:A:844:LEU:HD12 | 1:A:845:ASN:N    | 2.31                     | 0.45              |
| 1:B:56:ASN:ND2   | 1:B:122:ASN:HB2  | 2.32                     | 0.45              |
| 1:B:68:ASP:HB3   | 1:B:246:GLN:H    | 1.81                     | 0.45              |
| 1:C:138:TYR:CG   | 1:C:139:GLY:N    | 2.85                     | 0.45              |
| 1:C:527:VAL:HA   | 1:C:537:SER:O    | 2.17                     | 0.45              |
| 1:A:359:ARG:HH22 | 1:A:403:ASN:CG   | 2.24                     | 0.45              |
| 1:A:527:VAL:HA   | 1:A:537:SER:O    | 2.17                     | 0.45              |
| 1:B:76:PRO:HG3   | 1:B:237:TYR:CE1  | 2.52                     | 0.45              |
| 1:C:331:ASN:OD1  | 1:C:332:PHE:N    | 2.50                     | 0.45              |
| 1:A:76:PRO:HG3   | 1:A:237:TYR:CE1  | 2.52                     | 0.45              |
| 1:A:128:ARG:NH1  | 1:A:228:ASP:HB2  | 2.31                     | 0.45              |
| 1:A:331:ASN:OD1  | 1:A:332:PHE:N    | 2.50                     | 0.45              |
| 1:B:87:GLY:HA2   | 1:B:228:ASP:OD1  | 2.17                     | 0.45              |
| 1:B:588:TRP:CE2  | 1:B:589:THR:O    | 2.70                     | 0.45              |
| 1:B:657:LYS:HA   | 1:B:764:ALA:CB   | 2.46                     | 0.45              |
| 1:B:967:CYS:SG   | 1:B:1014:CYS:HA  | 2.56                     | 0.45              |
| 1:C:428:VAL:HG22 | 1:C:430:GLN:H    | 1.82                     | 0.45              |
| 1:C:802:MET:N    | 1:C:802:MET:SD   | 2.90                     | 0.45              |
| 1:A:85:VAL:CG2   | 1:A:229:PHE:HB2  | 2.44                     | 0.45              |
| 1:A:359:ARG:HH12 | 1:A:403:ASN:HB3  | 1.81                     | 0.45              |
| 1:B:448:LYS:HD2  | 1:B:456:GLY:O    | 2.17                     | 0.45              |
| 1:C:68:ASP:HB3   | 1:C:246:GLN:H    | 1.81                     | 0.45              |
| 1:C:162:VAL:N    | 1:C:188:LYS:O    | 2.50                     | 0.45              |
| 1:C:448:LYS:HD2  | 1:C:456:GLY:O    | 2.17                     | 0.45              |
| 1:A:588:TRP:CE2  | 1:A:589:THR:O    | 2.70                     | 0.45              |
| 1:B:128:ARG:NH1  | 1:B:228:ASP:HB2  | 2.31                     | 0.45              |
| 1:B:359:ARG:HH12 | 1:B:403:ASN:HB3  | 1.81                     | 0.45              |
| 1:B:404:TRP:HE3  | 1:B:408:LYS:CG   | 2.30                     | 0.45              |
| 1:B:518:ASN:CG   | 4:B:1206:NAG:C1  | 2.80                     | 0.45              |
| 1:C:56:ASN:ND2   | 1:C:122:ASN:HB2  | 2.32                     | 0.45              |
| 1:C:138:TYR:CD2  | 1:C:174:ILE:HG12 | 2.52                     | 0.45              |
| 1:C:144:TYR:CD2  | 4:C:1203:NAG:H83 | 2.52                     | 0.45              |
| 1:A:468:LEU:O    | 1:A:468:LEU:HD23 | 2.17                     | 0.44              |
| 1:A:607:ASP:CG   | 1:A:610:THR:H    | 2.24                     | 0.44              |
| 1:B:360:TRP:HE1  | 1:B:402:ALA:HB1  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:658:ALA:HB1  | 1:C:751:SER:HA   | 1.98                     | 0.44              |
| 1:A:138:TYR:CD2  | 1:A:174:ILE:HG12 | 2.52                     | 0.44              |
| 1:A:404:TRP:HE3  | 1:A:408:LYS:CG   | 2.30                     | 0.44              |
| 1:A:529:GLU:HG2  | 1:A:530:LEU:H    | 1.81                     | 0.44              |
| 1:B:162:VAL:N    | 1:B:188:LYS:O    | 2.50                     | 0.44              |
| 1:C:468:LEU:HD23 | 1:C:468:LEU:O    | 2.17                     | 0.44              |
| 1:C:541:TYR:O    | 1:C:541:TYR:CG   | 2.70                     | 0.44              |
| 1:A:56:ASN:ND2   | 1:A:122:ASN:HB2  | 2.32                     | 0.44              |
| 1:A:87:GLY:HA2   | 1:A:228:ASP:OD1  | 2.17                     | 0.44              |
| 1:A:275:PHE:O    | 1:C:638:ARG:HD2  | 2.17                     | 0.44              |
| 1:A:548:LEU:HA   | 1:A:548:LEU:HD23 | 1.71                     | 0.44              |
| 1:B:138:TYR:CG   | 1:B:139:GLY:N    | 2.85                     | 0.44              |
| 1:B:526:ASN:OD1  | 1:B:527:VAL:N    | 2.51                     | 0.44              |
| 1:B:867:ASP:CG   | 1:C:378:ASN:ND2  | 2.76                     | 0.44              |
| 1:C:359:ARG:HH12 | 1:C:403:ASN:HB3  | 1.81                     | 0.44              |
| 1:A:448:LYS:HD2  | 1:A:456:GLY:O    | 2.17                     | 0.44              |
| 1:A:607:ASP:OD1  | 1:A:607:ASP:C    | 2.60                     | 0.44              |
| 1:B:138:TYR:CD2  | 1:B:174:ILE:HG12 | 2.52                     | 0.44              |
| 1:B:607:ASP:OD1  | 1:B:607:ASP:C    | 2.60                     | 0.44              |
| 1:B:607:ASP:CG   | 1:B:610:THR:H    | 2.24                     | 0.44              |
| 1:B:802:MET:O    | 1:B:806:VAL:CB   | 2.66                     | 0.44              |
| 1:C:664:VAL:HG22 | 1:C:676:ILE:CD1  | 2.48                     | 0.44              |
| 1:C:972:ASN:HA   | 1:C:1010:GLN:HG3 | 1.99                     | 0.44              |
| 1:A:863:GLN:NE2  | 1:A:863:GLN:O    | 2.51                     | 0.44              |
| 1:B:1002:ILE:CD1 | 1:C:1010:GLN:H   | 2.27                     | 0.44              |
| 1:C:526:ASN:OD1  | 1:C:527:VAL:N    | 2.51                     | 0.44              |
| 1:C:588:TRP:CE2  | 1:C:589:THR:O    | 2.70                     | 0.44              |
| 1:C:657:LYS:HA   | 1:C:764:ALA:CB   | 2.46                     | 0.44              |
| 1:A:664:VAL:HG12 | 1:A:676:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:780:VAL:HG13 | 1:A:921:GLN:NE2  | 2.33                     | 0.44              |
| 1:B:331:ASN:OD1  | 1:B:332:PHE:N    | 2.50                     | 0.44              |
| 1:B:385:VAL:CA   | 1:B:419:TRP:HA   | 2.47                     | 0.44              |
| 1:C:802:MET:O    | 1:C:806:VAL:CB   | 2.66                     | 0.44              |
| 1:A:369:CYS:HB3  | 1:A:396:CYS:HB3  | 1.64                     | 0.44              |
| 1:A:463:SER:O    | 1:A:491:ILE:HG13 | 2.18                     | 0.44              |
| 1:B:527:VAL:HA   | 1:B:537:SER:O    | 2.17                     | 0.44              |
| 1:B:759:GLY:O    | 1:B:761:LEU:HG   | 2.18                     | 0.44              |
| 1:C:404:TRP:HE3  | 1:C:408:LYS:CG   | 2.30                     | 0.44              |
| 1:C:530:LEU:HD23 | 1:C:530:LEU:HA   | 1.87                     | 0.44              |
| 1:C:546:ALA:CB   | 1:C:562:ILE:HD13 | 2.47                     | 0.44              |
| 1:A:858:ILE:HG12 | 1:A:877:GLN:OE1  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:468:LEU:HD23 | 1:B:468:LEU:O    | 2.17                     | 0.44              |
| 1:B:518:ASN:ND2  | 4:B:1206:NAG:O7  | 2.51                     | 0.44              |
| 1:B:754:GLY:O    | 1:B:758:LEU:HB3  | 2.18                     | 0.44              |
| 1:C:76:PRO:HG3   | 1:C:237:TYR:CE1  | 2.52                     | 0.44              |
| 1:A:162:VAL:N    | 1:A:188:LYS:O    | 2.50                     | 0.44              |
| 1:A:673:SER:O    | 1:A:674:SER:C    | 2.61                     | 0.44              |
| 1:B:77:LEU:HD12  | 1:B:240:VAL:HG11 | 2.00                     | 0.44              |
| 1:B:463:SER:O    | 1:B:491:ILE:HG13 | 2.18                     | 0.44              |
| 1:B:710:ALA:HB1  | 1:C:532:LYS:HZ1  | 1.82                     | 0.44              |
| 1:C:316:LYS:NZ   | 1:C:316:LYS:CB   | 2.73                     | 0.44              |
| 1:C:607:ASP:OD1  | 1:C:607:ASP:C    | 2.60                     | 0.44              |
| 1:A:138:TYR:CG   | 1:A:139:GLY:N    | 2.85                     | 0.43              |
| 1:A:981:LEU:HG   | 1:A:982:ALA:H    | 1.83                     | 0.43              |
| 1:B:624:LYS:HG2  | 1:C:72:ARG:CZ    | 2.48                     | 0.43              |
| 1:B:802:MET:SD   | 1:B:802:MET:N    | 2.90                     | 0.43              |
| 1:C:87:GLY:HA2   | 1:C:228:ASP:OD1  | 2.17                     | 0.43              |
| 1:C:301:PHE:HB3  | 1:C:347:THR:CB   | 2.48                     | 0.43              |
| 1:C:790:ASN:OD1  | 1:C:791:GLN:N    | 2.51                     | 0.43              |
| 1:A:54:PHE:HB2   | 1:A:57:TRP:HB2   | 2.00                     | 0.43              |
| 1:A:350:TYR:HB2  | 1:A:373:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:802:MET:N    | 1:A:802:MET:SD   | 2.90                     | 0.43              |
| 1:B:780:VAL:HG13 | 1:B:921:GLN:NE2  | 2.32                     | 0.43              |
| 1:B:972:ASN:HA   | 1:B:1010:GLN:HG3 | 1.99                     | 0.43              |
| 1:C:359:ARG:NH2  | 1:C:403:ASN:OD1  | 2.52                     | 0.43              |
| 1:C:692:ILE:HD13 | 1:C:692:ILE:H    | 1.84                     | 0.43              |
| 1:C:830:LEU:HA   | 1:C:833:ILE:HG12 | 2.00                     | 0.43              |
| 1:C:863:GLN:NE2  | 1:C:863:GLN:O    | 2.51                     | 0.43              |
| 1:A:532:LYS:HG3  | 1:C:711:ASP:CG   | 2.42                     | 0.43              |
| 1:A:754:GLY:O    | 1:A:758:LEU:HB3  | 2.18                     | 0.43              |
| 1:A:759:GLY:O    | 1:A:761:LEU:HG   | 2.18                     | 0.43              |
| 1:B:301:PHE:HB3  | 1:B:347:THR:CB   | 2.48                     | 0.43              |
| 1:B:713:LYS:CD   | 1:C:516:SER:HA   | 2.46                     | 0.43              |
| 1:B:981:LEU:HG   | 1:B:982:ALA:H    | 1.83                     | 0.43              |
| 1:C:673:SER:O    | 1:C:674:SER:C    | 2.61                     | 0.43              |
| 1:A:264:CYS:O    | 1:A:267:LEU:HD22 | 2.19                     | 0.43              |
| 1:A:533:PHE:HB2  | 1:C:713:LYS:HZ3  | 1.82                     | 0.43              |
| 1:A:692:ILE:HD13 | 1:A:692:ILE:H    | 1.84                     | 0.43              |
| 1:A:972:ASN:HA   | 1:A:1010:GLN:HG3 | 1.99                     | 0.43              |
| 1:B:88:LEU:HD12  | 1:B:229:PHE:CD2  | 2.53                     | 0.43              |
| 1:B:90:PHE:CZ    | 4:B:1204:NAG:C1  | 3.01                     | 0.43              |
| 1:B:790:ASN:OD1  | 1:B:791:GLN:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:526:ASN:OD1  | 1:A:527:VAL:N    | 2.51                     | 0.43              |
| 1:B:188:LYS:HZ2  | 1:C:486:VAL:C    | 2.23                     | 0.43              |
| 1:B:391:ASP:HA   | 1:B:416:TYR:CE1  | 2.54                     | 0.43              |
| 1:B:664:VAL:HG12 | 1:B:676:ILE:CD1  | 2.48                     | 0.43              |
| 1:B:863:GLN:NE2  | 1:B:863:GLN:O    | 2.51                     | 0.43              |
| 1:C:90:PHE:HZ    | 4:C:1204:NAG:H3  | 1.84                     | 0.43              |
| 1:C:741:ASP:N    | 1:C:741:ASP:OD1  | 2.51                     | 0.43              |
| 1:A:385:VAL:CA   | 1:A:419:TRP:HA   | 2.47                     | 0.43              |
| 1:A:546:ALA:CB   | 1:A:562:ILE:HD13 | 2.47                     | 0.43              |
| 1:A:802:MET:O    | 1:A:806:VAL:CB   | 2.66                     | 0.43              |
| 1:A:900:TYR:HA   | 1:A:903:VAL:HG12 | 2.01                     | 0.43              |
| 1:B:54:PHE:HB2   | 1:B:57:TRP:HB2   | 2.01                     | 0.43              |
| 1:B:350:TYR:HB2  | 1:B:373:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:673:SER:O    | 1:B:674:SER:C    | 2.61                     | 0.43              |
| 1:B:692:ILE:H    | 1:B:692:ILE:HD13 | 1.84                     | 0.43              |
| 1:C:54:PHE:HB2   | 1:C:57:TRP:HB2   | 2.00                     | 0.43              |
| 1:C:159:PHE:CE2  | 1:C:221:VAL:HG13 | 2.49                     | 0.43              |
| 1:C:873:GLN:H    | 1:C:873:GLN:CD   | 2.25                     | 0.43              |
| 1:A:532:LYS:CE   | 1:C:711:ASP:H    | 2.30                     | 0.43              |
| 1:B:743:GLU:HG3  | 1:B:744:ARG:N    | 2.32                     | 0.43              |
| 1:C:369:CYS:HB3  | 1:C:396:CYS:HB3  | 1.64                     | 0.43              |
| 1:C:675:VAL:HA   | 1:C:690:SER:OG   | 2.18                     | 0.43              |
| 1:C:780:VAL:HG23 | 1:C:921:GLN:NE2  | 2.32                     | 0.43              |
| 1:C:805:ILE:HG12 | 1:C:809:PHE:HE2  | 1.84                     | 0.43              |
| 1:A:85:VAL:CB    | 1:A:229:PHE:HB2  | 2.49                     | 0.43              |
| 1:A:541:TYR:O    | 1:A:541:TYR:CG   | 2.70                     | 0.43              |
| 1:B:316:LYS:NZ   | 1:B:316:LYS:CB   | 2.73                     | 0.43              |
| 1:C:56:ASN:HD22  | 1:C:122:ASN:HB2  | 1.84                     | 0.43              |
| 1:C:463:SER:O    | 1:C:491:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:634:GLU:HA   | 1:C:637:LEU:HG   | 2.01                     | 0.43              |
| 1:A:391:ASP:HA   | 1:A:416:TYR:CE1  | 2.54                     | 0.43              |
| 1:B:359:ARG:NH2  | 1:B:403:ASN:OD1  | 2.51                     | 0.43              |
| 1:B:805:ILE:HG12 | 1:B:809:PHE:HE2  | 1.83                     | 0.43              |
| 1:B:858:ILE:HG12 | 1:B:877:GLN:OE1  | 2.18                     | 0.43              |
| 1:C:326:ASN:OD1  | 1:C:326:ASN:N    | 2.46                     | 0.43              |
| 1:C:360:TRP:HE1  | 1:C:402:ALA:HB1  | 1.82                     | 0.43              |
| 1:C:368:ASN:ND2  | 1:C:396:CYS:HA   | 2.34                     | 0.43              |
| 1:C:759:GLY:O    | 1:C:761:LEU:HG   | 2.18                     | 0.43              |
| 1:A:506:TYR:CE2  | 1:A:507:GLN:HG3  | 2.54                     | 0.43              |
| 1:B:49:PRO:HG3   | 1:B:106:LYS:NZ   | 2.34                     | 0.43              |
| 1:B:264:CYS:O    | 1:B:267:LEU:HD22 | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:298:LYS:HE3   | 1:B:298:LYS:HA   | 2.01                     | 0.43              |
| 1:B:546:ALA:CB    | 1:B:562:ILE:HD13 | 2.47                     | 0.43              |
| 1:B:900:TYR:HA    | 1:B:903:VAL:HG12 | 2.01                     | 0.43              |
| 1:C:88:LEU:HD12   | 1:C:229:PHE:CD2  | 2.53                     | 0.43              |
| 1:C:350:TYR:HB2   | 1:C:373:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:506:TYR:CE2   | 1:C:507:GLN:HG3  | 2.54                     | 0.43              |
| 1:C:876:GLN:O     | 1:C:879:ASP:OD1  | 2.37                     | 0.43              |
| 1:A:88:LEU:HD12   | 1:A:229:PHE:CD2  | 2.53                     | 0.42              |
| 1:A:390:LYS:O     | 1:A:416:TYR:CE1  | 2.72                     | 0.42              |
| 1:A:655:ASP:OD1   | 1:B:569:VAL:O    | 2.36                     | 0.42              |
| 1:B:56:ASN:HD22   | 1:B:122:ASN:HB2  | 1.84                     | 0.42              |
| 1:B:359:ARG:NH1   | 1:B:405:ALA:H    | 2.17                     | 0.42              |
| 1:B:638:ARG:HD2   | 1:C:275:PHE:O    | 2.19                     | 0.42              |
| 1:C:49:PRO:HG3    | 1:C:106:LYS:NZ   | 2.34                     | 0.42              |
| 1:A:301:PHE:HB3   | 1:A:347:THR:CB   | 2.48                     | 0.42              |
| 1:A:382:PHE:N     | 1:A:425:ILE:O    | 2.27                     | 0.42              |
| 1:A:773:ILE:H     | 1:A:773:ILE:HG12 | 1.67                     | 0.42              |
| 1:A:805:ILE:HG12  | 1:A:809:PHE:HE2  | 1.84                     | 0.42              |
| 1:C:57:TRP:CZ3    | 1:C:120:ASN:HB2  | 2.54                     | 0.42              |
| 1:C:75:GLN:HB2    | 1:C:77:LEU:CG    | 2.43                     | 0.42              |
| 1:C:384:SER:N     | 1:C:425:ILE:HG13 | 2.34                     | 0.42              |
| 1:C:462:VAL:HA    | 1:C:492:TYR:HD1  | 1.83                     | 0.42              |
| 1:C:981:LEU:HG    | 1:C:982:ALA:H    | 1.83                     | 0.42              |
| 1:C:1015:ASN:HD22 | 4:C:1214:NAG:H83 | 1.84                     | 0.42              |
| 1:A:77:LEU:HD12   | 1:A:240:VAL:HG11 | 2.00                     | 0.42              |
| 1:A:333:ASN:HD21  | 1:A:336:LYS:NZ   | 2.17                     | 0.42              |
| 1:A:385:VAL:O     | 1:A:419:TRP:HA   | 2.20                     | 0.42              |
| 1:A:634:GLU:HA    | 1:A:637:LEU:HG   | 2.01                     | 0.42              |
| 1:B:247:THR:HA    | 1:C:469:ASN:OD1  | 2.19                     | 0.42              |
| 1:B:752:LEU:O     | 1:B:755:GLY:N    | 2.52                     | 0.42              |
| 1:B:876:GLN:OE1   | 1:B:880:ARG:NH2  | 2.53                     | 0.42              |
| 1:C:682:SER:O     | 1:C:682:SER:OG   | 2.28                     | 0.42              |
| 1:C:754:GLY:O     | 1:C:758:LEU:HB3  | 2.18                     | 0.42              |
| 1:C:858:ILE:HG12  | 1:C:877:GLN:OE1  | 2.18                     | 0.42              |
| 1:A:462:VAL:HA    | 1:A:492:TYR:HD1  | 1.83                     | 0.42              |
| 1:A:790:ASN:OD1   | 1:A:791:GLN:N    | 2.51                     | 0.42              |
| 1:A:938:VAL:HG13  | 1:A:947:PHE:CD1  | 2.54                     | 0.42              |
| 1:B:299:HIS:HD1   | 1:B:301:PHE:HE1  | 1.67                     | 0.42              |
| 1:B:729:TYR:OH    | 1:C:499:PRO:HB2  | 2.19                     | 0.42              |
| 1:B:733:ILE:H     | 1:B:733:ILE:HG12 | 1.67                     | 0.42              |
| 1:B:876:GLN:O     | 1:B:879:ASP:OD1  | 2.37                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:938:VAL:HG13 | 1:B:947:PHE:CD1  | 2.54                     | 0.42              |
| 1:C:298:LYS:HE3  | 1:C:298:LYS:HA   | 2.01                     | 0.42              |
| 1:C:391:ASP:HA   | 1:C:416:TYR:CE1  | 2.54                     | 0.42              |
| 1:A:57:TRP:CZ3   | 1:A:120:ASN:HB2  | 2.54                     | 0.42              |
| 1:A:144:TYR:HE2  | 4:A:1203:NAG:C2  | 2.26                     | 0.42              |
| 1:A:360:TRP:HE1  | 1:A:402:ALA:HB1  | 1.82                     | 0.42              |
| 1:A:602:THR:O    | 1:A:604:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:805:ILE:HG12 | 1:A:809:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:806:VAL:O    | 1:A:809:PHE:HB2  | 2.20                     | 0.42              |
| 1:A:876:GLN:O    | 1:A:879:ASP:OD1  | 2.37                     | 0.42              |
| 1:B:72:ARG:HA    | 1:B:241:LEU:HA   | 2.01                     | 0.42              |
| 1:B:85:VAL:CB    | 1:B:229:PHE:HB2  | 2.49                     | 0.42              |
| 1:C:85:VAL:CB    | 1:C:229:PHE:HB2  | 2.49                     | 0.42              |
| 1:A:368:ASN:ND2  | 1:A:396:CYS:HA   | 2.34                     | 0.42              |
| 1:A:469:ASN:OD1  | 1:C:247:THR:HA   | 2.19                     | 0.42              |
| 1:A:830:LEU:HA   | 1:A:833:ILE:HG12 | 2.00                     | 0.42              |
| 1:B:462:VAL:HA   | 1:B:492:TYR:HD1  | 1.83                     | 0.42              |
| 1:B:805:ILE:HG12 | 1:B:809:PHE:CE2  | 2.55                     | 0.42              |
| 1:C:77:LEU:HD12  | 1:C:240:VAL:HG11 | 2.00                     | 0.42              |
| 1:C:527:VAL:HG13 | 1:C:536:ALA:HA   | 2.02                     | 0.42              |
| 1:A:49:PRO:HG3   | 1:A:106:LYS:NZ   | 2.34                     | 0.42              |
| 1:A:999:GLU:HA   | 1:A:1000:PRO:HD3 | 1.89                     | 0.42              |
| 1:B:56:ASN:HB3   | 1:B:120:ASN:OD1  | 2.20                     | 0.42              |
| 1:B:57:TRP:CZ3   | 1:B:120:ASN:HB2  | 2.54                     | 0.42              |
| 1:B:675:VAL:HA   | 1:B:690:SER:OG   | 2.18                     | 0.42              |
| 1:B:741:ASP:OD1  | 1:B:741:ASP:N    | 2.51                     | 0.42              |
| 1:B:873:GLN:H    | 1:B:873:GLN:CD   | 2.25                     | 0.42              |
| 1:C:752:LEU:O    | 1:C:755:GLY:N    | 2.53                     | 0.42              |
| 1:A:171:ASN:OD1  | 1:A:180:SER:OG   | 2.28                     | 0.42              |
| 1:A:516:SER:HA   | 1:C:713:LYS:HD3  | 2.01                     | 0.42              |
| 1:A:699:LYS:HG2  | 1:A:699:LYS:O    | 2.20                     | 0.42              |
| 1:A:741:ASP:OD1  | 1:A:741:ASP:N    | 2.51                     | 0.42              |
| 1:B:602:THR:O    | 1:B:604:ILE:HG12 | 2.20                     | 0.42              |
| 1:C:385:VAL:CA   | 1:C:419:TRP:HA   | 2.47                     | 0.42              |
| 1:C:506:TYR:CD2  | 1:C:507:GLN:HG3  | 2.55                     | 0.42              |
| 1:C:548:LEU:HD23 | 1:C:548:LEU:HA   | 1.71                     | 0.42              |
| 1:C:999:GLU:HA   | 1:C:1000:PRO:HD3 | 1.89                     | 0.42              |
| 1:A:675:VAL:HA   | 1:A:690:SER:OG   | 2.19                     | 0.42              |
| 1:B:390:LYS:O    | 1:B:416:TYR:CE1  | 2.72                     | 0.42              |
| 1:B:868:ARG:C    | 1:C:372:SER:OG   | 2.63                     | 0.42              |
| 1:C:72:ARG:HA    | 1:C:241:LEU:HA   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:900:TYR:HA   | 1:C:903:VAL:HG12 | 2.01                     | 0.42              |
| 1:C:921:GLN:HE21 | 1:C:921:GLN:HB2  | 1.56                     | 0.42              |
| 1:A:56:ASN:HB3   | 1:A:120:ASN:OD1  | 2.20                     | 0.42              |
| 1:A:298:LYS:HE3  | 1:A:298:LYS:HA   | 2.01                     | 0.42              |
| 1:A:359:ARG:NH2  | 1:A:403:ASN:OD1  | 2.52                     | 0.42              |
| 1:A:404:TRP:O    | 1:A:404:TRP:CG   | 2.73                     | 0.42              |
| 1:A:966:LEU:HB2  | 1:A:1019:VAL:H   | 1.85                     | 0.42              |
| 1:B:385:VAL:O    | 1:B:419:TRP:HA   | 2.20                     | 0.42              |
| 1:B:506:TYR:CE2  | 1:B:507:GLN:HG3  | 2.54                     | 0.42              |
| 1:B:518:ASN:HB2  | 4:B:1206:NAG:C1  | 2.50                     | 0.42              |
| 1:B:634:GLU:HA   | 1:B:637:LEU:HG   | 2.01                     | 0.42              |
| 1:C:264:CYS:O    | 1:C:267:LEU:HD22 | 2.19                     | 0.42              |
| 1:C:903:VAL:HA   | 1:C:906:SER:OG   | 2.20                     | 0.42              |
| 1:A:506:TYR:CD2  | 1:A:507:GLN:HG3  | 2.55                     | 0.41              |
| 1:B:346:PHE:CZ   | 1:B:381:LYS:HG2  | 2.55                     | 0.41              |
| 1:B:368:ASN:ND2  | 1:B:396:CYS:HA   | 2.34                     | 0.41              |
| 1:B:806:VAL:O    | 1:B:809:PHE:HB2  | 2.20                     | 0.41              |
| 1:B:830:LEU:HA   | 1:B:833:ILE:HG12 | 2.00                     | 0.41              |
| 1:C:385:VAL:O    | 1:C:419:TRP:HA   | 2.20                     | 0.41              |
| 1:A:185:ALA:HB2  | 1:B:294:PRO:HG2  | 2.02                     | 0.41              |
| 1:C:390:LYS:O    | 1:C:416:TYR:CE1  | 2.72                     | 0.41              |
| 1:C:805:ILE:HG12 | 1:C:809:PHE:CE2  | 2.55                     | 0.41              |
| 1:C:966:LEU:HB2  | 1:C:1019:VAL:H   | 1.85                     | 0.41              |
| 1:A:72:ARG:HA    | 1:A:241:LEU:HA   | 2.01                     | 0.41              |
| 1:A:752:LEU:O    | 1:A:755:GLY:N    | 2.52                     | 0.41              |
| 1:B:948:LEU:HD13 | 1:B:948:LEU:HA   | 1.94                     | 0.41              |
| 1:C:346:PHE:CZ   | 1:C:381:LYS:HG2  | 2.55                     | 0.41              |
| 1:C:938:VAL:HG13 | 1:C:947:PHE:CD1  | 2.54                     | 0.41              |
| 1:A:56:ASN:HD22  | 1:A:122:ASN:HB2  | 1.84                     | 0.41              |
| 1:A:346:PHE:CZ   | 1:A:381:LYS:HG2  | 2.55                     | 0.41              |
| 1:A:384:SER:N    | 1:A:425:ILE:HG13 | 2.34                     | 0.41              |
| 1:B:326:ASN:OD1  | 1:B:326:ASN:N    | 2.46                     | 0.41              |
| 1:B:631:LYS:HZ3  | 1:C:265:ASP:CG   | 2.29                     | 0.41              |
| 1:B:653:THR:O    | 1:B:748:TYR:HD1  | 2.04                     | 0.41              |
| 1:B:976:LEU:HD23 | 1:B:979:PRO:HA   | 2.02                     | 0.41              |
| 1:C:56:ASN:HB3   | 1:C:120:ASN:OD1  | 2.20                     | 0.41              |
| 1:C:60:LEU:HD23  | 1:C:60:LEU:HA    | 1.87                     | 0.41              |
| 1:C:876:GLN:OE1  | 1:C:880:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:721:ILE:HD13 | 1:C:493:SER:HB3  | 2.01                     | 0.41              |
| 1:B:966:LEU:HB2  | 1:B:1019:VAL:H   | 1.85                     | 0.41              |
| 1:A:510:VAL:HG23 | 1:A:510:VAL:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:771:LEU:HD12 | 1:A:771:LEU:HA   | 1.92                     | 0.41              |
| 1:A:903:VAL:HA   | 1:A:906:SER:OG   | 2.21                     | 0.41              |
| 1:B:311:GLN:CG   | 1:B:320:CYS:HA   | 2.34                     | 0.41              |
| 1:B:333:ASN:HD21 | 1:B:336:LYS:NZ   | 2.17                     | 0.41              |
| 1:C:359:ARG:NH1  | 1:C:405:ALA:H    | 2.17                     | 0.41              |
| 1:C:484:LYS:HA   | 1:C:491:ILE:HA   | 2.03                     | 0.41              |
| 1:C:602:THR:O    | 1:C:604:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:876:GLN:OE1  | 1:A:880:ARG:NH2  | 2.52                     | 0.41              |
| 1:B:384:SER:N    | 1:B:425:ILE:HG13 | 2.34                     | 0.41              |
| 1:B:699:LYS:O    | 1:B:699:LYS:HG2  | 2.20                     | 0.41              |
| 1:B:741:ASP:O    | 1:B:745:MET:HB3  | 2.21                     | 0.41              |
| 1:B:868:ARG:O    | 1:C:372:SER:N    | 2.52                     | 0.41              |
| 1:B:958:LYS:HD3  | 1:B:958:LYS:HA   | 1.97                     | 0.41              |
| 1:A:359:ARG:NH1  | 1:A:405:ALA:H    | 2.17                     | 0.41              |
| 1:A:721:ILE:HD13 | 1:B:493:SER:HB3  | 2.02                     | 0.41              |
| 1:A:976:LEU:HD23 | 1:A:979:PRO:HA   | 2.02                     | 0.41              |
| 1:B:483:PHE:CD1  | 1:B:483:PHE:C    | 2.99                     | 0.41              |
| 1:B:527:VAL:HG23 | 1:B:536:ALA:HA   | 2.02                     | 0.41              |
| 1:C:381:LYS:HE2  | 1:C:381:LYS:HB3  | 1.80                     | 0.41              |
| 1:C:806:VAL:O    | 1:C:809:PHE:HB2  | 2.20                     | 0.41              |
| 1:A:49:PRO:HG2   | 1:A:52:PHE:HD2   | 1.86                     | 0.41              |
| 1:A:166:PHE:O    | 1:A:167:TYR:HD1  | 2.04                     | 0.41              |
| 1:A:311:GLN:CG   | 1:A:320:CYS:HA   | 2.34                     | 0.41              |
| 1:A:527:VAL:HG23 | 1:A:536:ALA:HA   | 2.02                     | 0.41              |
| 1:A:532:LYS:NZ   | 1:C:711:ASP:O    | 2.52                     | 0.41              |
| 1:A:873:GLN:H    | 1:A:873:GLN:CD   | 2.25                     | 0.41              |
| 1:B:166:PHE:O    | 1:B:167:TYR:HD1  | 2.04                     | 0.41              |
| 1:B:377:ASN:O    | 1:B:429:PRO:HD3  | 2.21                     | 0.41              |
| 1:B:506:TYR:CD2  | 1:B:507:GLN:HG3  | 2.55                     | 0.41              |
| 1:B:530:LEU:HD11 | 1:B:561:ILE:HD12 | 2.03                     | 0.41              |
| 1:B:582:LEU:O    | 1:B:960:VAL:HG12 | 2.21                     | 0.41              |
| 1:B:830:LEU:HD23 | 1:B:833:ILE:HD11 | 2.03                     | 0.41              |
| 1:B:903:VAL:HA   | 1:B:906:SER:OG   | 2.21                     | 0.41              |
| 1:C:359:ARG:HG2  | 1:C:405:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:144:TYR:OH   | 4:A:1203:NAG:O5  | 2.34                     | 0.41              |
| 1:A:383:GLY:CA   | 1:A:422:GLY:HA3  | 2.46                     | 0.41              |
| 1:A:653:THR:O    | 1:A:748:TYR:HD1  | 2.04                     | 0.41              |
| 1:A:741:ASP:O    | 1:A:745:MET:HB3  | 2.21                     | 0.41              |
| 1:B:359:ARG:HG2  | 1:B:405:ALA:HB2  | 2.03                     | 0.41              |
| 1:B:484:LYS:HA   | 1:B:491:ILE:HA   | 2.03                     | 0.41              |
| 1:B:730:TYR:CG   | 1:C:496:PRO:HG3  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:850:GLN:HA   | 1:B:853:GLN:HG3  | 2.03                     | 0.41              |
| 1:C:699:LYS:O    | 1:C:699:LYS:HG2  | 2.20                     | 0.41              |
| 1:C:862:ILE:HD11 | 1:C:885:ARG:HH12 | 1.86                     | 0.41              |
| 1:A:408:LYS:HD3  | 1:A:410:TYR:CE1  | 2.56                     | 0.40              |
| 1:A:971:ARG:O    | 1:A:1012:GLU:HA  | 2.21                     | 0.40              |
| 1:B:261:ARG:HG3  | 1:B:261:ARG:NH1  | 2.36                     | 0.40              |
| 1:B:404:TRP:O    | 1:B:404:TRP:CG   | 2.73                     | 0.40              |
| 1:B:790:ASN:OD1  | 1:B:790:ASN:N    | 2.54                     | 0.40              |
| 1:C:56:ASN:HB2   | 1:C:120:ASN:HD21 | 1.86                     | 0.40              |
| 1:C:117:ILE:HG13 | 1:C:118:ARG:N    | 2.36                     | 0.40              |
| 1:C:767:ILE:O    | 1:C:768:PRO:C    | 2.64                     | 0.40              |
| 1:A:75:GLN:HB2   | 1:A:77:LEU:CG    | 2.43                     | 0.40              |
| 1:A:359:ARG:HG2  | 1:A:405:ALA:HB2  | 2.03                     | 0.40              |
| 1:C:377:ASN:O    | 1:C:429:PRO:HD3  | 2.21                     | 0.40              |
| 1:C:582:LEU:O    | 1:C:960:VAL:HG12 | 2.21                     | 0.40              |
| 1:C:653:THR:O    | 1:C:748:TYR:HD1  | 2.04                     | 0.40              |
| 1:A:90:PHE:CZ    | 4:A:1204:NAG:H3  | 2.54                     | 0.40              |
| 1:B:773:ILE:H    | 1:B:773:ILE:HG12 | 1.67                     | 0.40              |
| 1:B:776:ARG:HD3  | 1:B:935:PHE:CB   | 2.52                     | 0.40              |
| 1:C:263:ARG:HD2  | 1:C:269:PHE:HA   | 2.03                     | 0.40              |
| 1:C:741:ASP:O    | 1:C:745:MET:HB3  | 2.21                     | 0.40              |
| 1:C:743:GLU:HG3  | 1:C:744:ARG:N    | 2.32                     | 0.40              |
| 1:A:197:ARG:C    | 1:A:199:GLY:N    | 2.78                     | 0.40              |
| 1:A:581:ASN:O    | 1:A:582:LEU:HD23 | 2.22                     | 0.40              |
| 1:A:881:LEU:HD23 | 1:A:881:LEU:HA   | 1.92                     | 0.40              |
| 1:B:771:LEU:HD23 | 1:C:578:VAL:HG22 | 2.04                     | 0.40              |
| 1:B:862:ILE:HD11 | 1:B:885:ARG:HH12 | 1.86                     | 0.40              |
| 1:C:58:PHE:N     | 1:C:192:GLU:OE1  | 2.55                     | 0.40              |
| 1:C:171:ASN:OD1  | 1:C:180:SER:OG   | 2.28                     | 0.40              |
| 1:C:408:LYS:HD3  | 1:C:410:TYR:CE1  | 2.56                     | 0.40              |
| 1:C:824:GLN:OE1  | 1:C:824:GLN:N    | 2.55                     | 0.40              |
| 1:A:337:GLY:N    | 1:A:338:PRO:HD2  | 2.36                     | 0.40              |
| 1:A:836:VAL:HA   | 1:A:839:GLN:HG2  | 2.04                     | 0.40              |
| 1:A:862:ILE:HD11 | 1:A:885:ARG:HH12 | 1.86                     | 0.40              |
| 1:B:56:ASN:HB2   | 1:B:120:ASN:HD21 | 1.86                     | 0.40              |
| 1:B:188:LYS:NZ   | 1:C:486:VAL:C    | 2.80                     | 0.40              |
| 1:B:581:ASN:O    | 1:B:582:LEU:HD23 | 2.22                     | 0.40              |
| 1:B:870:ASP:HB2  | 1:B:873:GLN:NE2  | 2.36                     | 0.40              |
| 1:C:337:GLY:N    | 1:C:338:PRO:HD2  | 2.36                     | 0.40              |
| 1:C:377:ASN:HA   | 1:C:427:GLY:HA3  | 2.04                     | 0.40              |
| 1:C:836:VAL:HA   | 1:C:839:GLN:HG2  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:865:ILE:HA   | 1:C:865:ILE:HD13 | 1.87                     | 0.40              |
| 1:C:881:LEU:HD23 | 1:C:881:LEU:HA   | 1.92                     | 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     | 954/1116 (86%)  | 900 (94%)  | 53 (6%)  | 1 (0%)   | 48          | 79 |
| 1   | B     | 954/1116 (86%)  | 900 (94%)  | 53 (6%)  | 1 (0%)   | 48          | 79 |
| 1   | C     | 954/1116 (86%)  | 900 (94%)  | 53 (6%)  | 1 (0%)   | 48          | 79 |
| All | All   | 2862/3348 (86%) | 2700 (94%) | 159 (6%) | 3 (0%)   | 49          | 79 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 673 | SER  |
| 1   | B     | 673 | SER  |
| 1   | C     | 673 | SER  |

### 5.3.2 Protein sidechains [i](#)

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     | 727/969 (75%)   | 662 (91%)  | 65 (9%)  | 9           | 33 |
| 1   | B     | 732/969 (76%)   | 665 (91%)  | 67 (9%)  | 8           | 32 |
| 1   | C     | 731/969 (75%)   | 664 (91%)  | 67 (9%)  | 8           | 32 |
| All | All   | 2190/2907 (75%) | 1991 (91%) | 199 (9%) | 11          | 33 |

All (199) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 64  | SER  |
| 1   | A     | 67  | VAL  |
| 1   | A     | 71  | VAL  |
| 1   | A     | 79  | LEU  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 117 | ILE  |
| 1   | A     | 141 | VAL  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 152 | SER  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 202 | TYR  |
| 1   | A     | 203 | ILE  |
| 1   | A     | 259 | ILE  |
| 1   | A     | 264 | CYS  |
| 1   | A     | 268 | SER  |
| 1   | A     | 281 | ILE  |
| 1   | A     | 284 | VAL  |
| 1   | A     | 288 | VAL  |
| 1   | A     | 290 | ILE  |
| 1   | A     | 302 | ILE  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 316 | LYS  |
| 1   | A     | 317 | CYS  |
| 1   | A     | 319 | ASN  |
| 1   | A     | 320 | CYS  |
| 1   | A     | 327 | ILE  |
| 1   | A     | 341 | VAL  |
| 1   | A     | 357 | VAL  |
| 1   | A     | 363 | SER  |
| 1   | A     | 364 | ILE  |
| 1   | A     | 376 | VAL  |
| 1   | A     | 412 | ILE  |
| 1   | A     | 418 | SER  |
| 1   | A     | 425 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 432  | VAL  |
| 1   | A     | 435  | VAL  |
| 1   | A     | 441  | VAL  |
| 1   | A     | 446  | CYS  |
| 1   | A     | 460  | ILE  |
| 1   | A     | 491  | ILE  |
| 1   | A     | 552  | SER  |
| 1   | A     | 564  | VAL  |
| 1   | A     | 569  | VAL  |
| 1   | A     | 574  | VAL  |
| 1   | A     | 575  | SER  |
| 1   | A     | 604  | ILE  |
| 1   | A     | 606  | VAL  |
| 1   | A     | 630  | CYS  |
| 1   | A     | 648  | VAL  |
| 1   | A     | 676  | ILE  |
| 1   | A     | 692  | ILE  |
| 1   | A     | 701  | VAL  |
| 1   | A     | 720  | SER  |
| 1   | A     | 733  | ILE  |
| 1   | A     | 763  | SER  |
| 1   | A     | 767  | ILE  |
| 1   | A     | 773  | ILE  |
| 1   | A     | 777  | LEU  |
| 1   | A     | 779  | TYR  |
| 1   | A     | 805  | ILE  |
| 1   | A     | 967  | CYS  |
| 1   | A     | 992  | ILE  |
| 1   | A     | 997  | MET  |
| 1   | A     | 1002 | ILE  |
| 1   | A     | 1016 | VAL  |
| 1   | B     | 64   | SER  |
| 1   | B     | 67   | VAL  |
| 1   | B     | 71   | VAL  |
| 1   | B     | 79   | LEU  |
| 1   | B     | 113  | LEU  |
| 1   | B     | 117  | ILE  |
| 1   | B     | 152  | SER  |
| 1   | B     | 162  | VAL  |
| 1   | B     | 202  | TYR  |
| 1   | B     | 203  | ILE  |
| 1   | B     | 259  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 264 | CYS  |
| 1   | B     | 268 | SER  |
| 1   | B     | 281 | ILE  |
| 1   | B     | 284 | VAL  |
| 1   | B     | 288 | VAL  |
| 1   | B     | 290 | ILE  |
| 1   | B     | 291 | VAL  |
| 1   | B     | 302 | ILE  |
| 1   | B     | 303 | VAL  |
| 1   | B     | 316 | LYS  |
| 1   | B     | 317 | CYS  |
| 1   | B     | 319 | ASN  |
| 1   | B     | 320 | CYS  |
| 1   | B     | 327 | ILE  |
| 1   | B     | 353 | VAL  |
| 1   | B     | 357 | VAL  |
| 1   | B     | 363 | SER  |
| 1   | B     | 364 | ILE  |
| 1   | B     | 376 | VAL  |
| 1   | B     | 401 | VAL  |
| 1   | B     | 412 | ILE  |
| 1   | B     | 417 | VAL  |
| 1   | B     | 418 | SER  |
| 1   | B     | 425 | ILE  |
| 1   | B     | 435 | VAL  |
| 1   | B     | 441 | VAL  |
| 1   | B     | 446 | CYS  |
| 1   | B     | 460 | ILE  |
| 1   | B     | 491 | ILE  |
| 1   | B     | 511 | VAL  |
| 1   | B     | 552 | SER  |
| 1   | B     | 564 | VAL  |
| 1   | B     | 574 | VAL  |
| 1   | B     | 575 | SER  |
| 1   | B     | 604 | ILE  |
| 1   | B     | 630 | CYS  |
| 1   | B     | 648 | VAL  |
| 1   | B     | 676 | ILE  |
| 1   | B     | 692 | ILE  |
| 1   | B     | 701 | VAL  |
| 1   | B     | 720 | SER  |
| 1   | B     | 733 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 735  | VAL  |
| 1   | B     | 739  | VAL  |
| 1   | B     | 763  | SER  |
| 1   | B     | 767  | ILE  |
| 1   | B     | 773  | ILE  |
| 1   | B     | 777  | LEU  |
| 1   | B     | 779  | TYR  |
| 1   | B     | 805  | ILE  |
| 1   | B     | 946  | VAL  |
| 1   | B     | 967  | CYS  |
| 1   | B     | 992  | ILE  |
| 1   | B     | 997  | MET  |
| 1   | B     | 1002 | ILE  |
| 1   | B     | 1016 | VAL  |
| 1   | C     | 64   | SER  |
| 1   | C     | 67   | VAL  |
| 1   | C     | 71   | VAL  |
| 1   | C     | 79   | LEU  |
| 1   | C     | 85   | VAL  |
| 1   | C     | 113  | LEU  |
| 1   | C     | 117  | ILE  |
| 1   | C     | 151  | VAL  |
| 1   | C     | 152  | SER  |
| 1   | C     | 162  | VAL  |
| 1   | C     | 202  | TYR  |
| 1   | C     | 203  | ILE  |
| 1   | C     | 259  | ILE  |
| 1   | C     | 264  | CYS  |
| 1   | C     | 268  | SER  |
| 1   | C     | 281  | ILE  |
| 1   | C     | 284  | VAL  |
| 1   | C     | 288  | VAL  |
| 1   | C     | 290  | ILE  |
| 1   | C     | 291  | VAL  |
| 1   | C     | 302  | ILE  |
| 1   | C     | 316  | LYS  |
| 1   | C     | 317  | CYS  |
| 1   | C     | 319  | ASN  |
| 1   | C     | 320  | CYS  |
| 1   | C     | 327  | ILE  |
| 1   | C     | 353  | VAL  |
| 1   | C     | 357  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 363  | SER  |
| 1   | C     | 364  | ILE  |
| 1   | C     | 412  | ILE  |
| 1   | C     | 417  | VAL  |
| 1   | C     | 418  | SER  |
| 1   | C     | 425  | ILE  |
| 1   | C     | 435  | VAL  |
| 1   | C     | 441  | VAL  |
| 1   | C     | 446  | CYS  |
| 1   | C     | 460  | ILE  |
| 1   | C     | 491  | ILE  |
| 1   | C     | 511  | VAL  |
| 1   | C     | 552  | SER  |
| 1   | C     | 564  | VAL  |
| 1   | C     | 569  | VAL  |
| 1   | C     | 574  | VAL  |
| 1   | C     | 575  | SER  |
| 1   | C     | 604  | ILE  |
| 1   | C     | 606  | VAL  |
| 1   | C     | 630  | CYS  |
| 1   | C     | 676  | ILE  |
| 1   | C     | 692  | ILE  |
| 1   | C     | 701  | VAL  |
| 1   | C     | 720  | SER  |
| 1   | C     | 733  | ILE  |
| 1   | C     | 739  | VAL  |
| 1   | C     | 763  | SER  |
| 1   | C     | 767  | ILE  |
| 1   | C     | 773  | ILE  |
| 1   | C     | 777  | LEU  |
| 1   | C     | 779  | TYR  |
| 1   | C     | 805  | ILE  |
| 1   | C     | 914  | VAL  |
| 1   | C     | 951  | VAL  |
| 1   | C     | 967  | CYS  |
| 1   | C     | 992  | ILE  |
| 1   | C     | 997  | MET  |
| 1   | C     | 1002 | ILE  |
| 1   | C     | 1016 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | ASN  |
| 1   | A     | 333 | ASN  |
| 1   | A     | 502 | GLN  |
| 1   | A     | 508 | GLN  |
| 1   | A     | 518 | ASN  |
| 1   | A     | 783 | GLN  |
| 1   | A     | 840 | GLN  |
| 1   | A     | 856 | GLN  |
| 1   | A     | 863 | GLN  |
| 1   | A     | 912 | GLN  |
| 1   | A     | 933 | HIS  |
| 1   | B     | 80  | ASN  |
| 1   | B     | 200 | HIS  |
| 1   | B     | 502 | GLN  |
| 1   | B     | 508 | GLN  |
| 1   | B     | 518 | ASN  |
| 1   | B     | 587 | ASN  |
| 1   | B     | 731 | ASN  |
| 1   | B     | 783 | GLN  |
| 1   | B     | 840 | GLN  |
| 1   | B     | 856 | GLN  |
| 1   | B     | 863 | GLN  |
| 1   | B     | 933 | HIS  |
| 1   | C     | 80  | ASN  |
| 1   | C     | 200 | HIS  |
| 1   | C     | 333 | ASN  |
| 1   | C     | 378 | ASN  |
| 1   | C     | 502 | GLN  |
| 1   | C     | 508 | GLN  |
| 1   | C     | 783 | GLN  |
| 1   | C     | 840 | GLN  |
| 1   | C     | 856 | GLN  |
| 1   | C     | 863 | GLN  |
| 1   | C     | 933 | HIS  |

### 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 ⓘ

30 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     | 0.42 | 0           | 17,19,21    | 0.80 | 0           |
| 2   | NAG  | D     | 2   | 2    | 14,14,15     | 0.38 | 0           | 17,19,21    | 1.13 | 1 (5%)      |
| 2   | BMA  | D     | 3   | 2    | 11,11,12     | 0.31 | 0           | 15,15,17    | 0.90 | 0           |
| 2   | MAN  | D     | 4   | 2    | 11,11,12     | 0.26 | 0           | 15,15,17    | 0.85 | 0           |
| 2   | MAN  | D     | 5   | 2    | 11,11,12     | 0.22 | 0           | 15,15,17    | 0.61 | 0           |
| 2   | MAN  | D     | 6   | 2    | 11,11,12     | 0.36 | 0           | 15,15,17    | 0.87 | 0           |
| 2   | MAN  | D     | 7   | 2    | 11,11,12     | 0.22 | 0           | 15,15,17    | 0.48 | 0           |
| 3   | NAG  | E     | 1   | 1,3  | 14,14,15     | 0.28 | 0           | 17,19,21    | 0.86 | 1 (5%)      |
| 3   | NAG  | E     | 2   | 3    | 14,14,15     | 0.29 | 0           | 17,19,21    | 0.54 | 0           |
| 3   | BMA  | E     | 3   | 3    | 11,11,12     | 0.27 | 0           | 15,15,17    | 0.52 | 0           |
| 2   | NAG  | F     | 1   | 1,2  | 14,14,15     | 0.42 | 0           | 17,19,21    | 0.79 | 0           |
| 2   | NAG  | F     | 2   | 2    | 14,14,15     | 0.36 | 0           | 17,19,21    | 1.13 | 1 (5%)      |
| 2   | BMA  | F     | 3   | 2    | 11,11,12     | 0.31 | 0           | 15,15,17    | 0.89 | 0           |
| 2   | MAN  | F     | 4   | 2    | 11,11,12     | 0.26 | 0           | 15,15,17    | 0.85 | 0           |
| 2   | MAN  | F     | 5   | 2    | 11,11,12     | 0.22 | 0           | 15,15,17    | 0.61 | 0           |
| 2   | MAN  | F     | 6   | 2    | 11,11,12     | 0.38 | 0           | 15,15,17    | 0.87 | 0           |
| 2   | MAN  | F     | 7   | 2    | 11,11,12     | 0.22 | 0           | 15,15,17    | 0.49 | 0           |
| 3   | NAG  | G     | 1   | 1,3  | 14,14,15     | 0.28 | 0           | 17,19,21    | 0.86 | 1 (5%)      |
| 3   | NAG  | G     | 2   | 3    | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.53 | 0           |
| 3   | BMA  | G     | 3   | 3    | 11,11,12     | 0.24 | 0           | 15,15,17    | 0.51 | 0           |
| 2   | NAG  | H     | 1   | 1,2  | 14,14,15     | 0.42 | 0           | 17,19,21    | 0.80 | 0           |
| 2   | NAG  | H     | 2   | 2    | 14,14,15     | 0.38 | 0           | 17,19,21    | 1.12 | 1 (5%)      |
| 2   | BMA  | H     | 3   | 2    | 11,11,12     | 0.31 | 0           | 15,15,17    | 0.89 | 0           |
| 2   | MAN  | H     | 4   | 2    | 11,11,12     | 0.25 | 0           | 15,15,17    | 0.86 | 0           |
| 2   | MAN  | H     | 5   | 2    | 11,11,12     | 0.22 | 0           | 15,15,17    | 0.61 | 0           |
| 2   | MAN  | H     | 6   | 2    | 11,11,12     | 0.38 | 0           | 15,15,17    | 0.88 | 0           |
| 2   | MAN  | H     | 7   | 2    | 11,11,12     | 0.22 | 0           | 15,15,17    | 0.48 | 0           |
| 3   | NAG  | I     | 1   | 1,3  | 14,14,15     | 0.29 | 0           | 17,19,21    | 0.85 | 1 (5%)      |
| 3   | NAG  | I     | 2   | 3    | 14,14,15     | 0.29 | 0           | 17,19,21    | 0.54 | 0           |
| 3   | BMA  | I     | 3   | 3    | 11,11,12     | 0.27 | 0           | 15,15,17    | 0.52 | 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  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | BMA  | D     | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | MAN  | D     | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | MAN  | D     | 5   | 2    | -       | 1/2/19/22 | 1/1/1/1 |
| 2   | MAN  | D     | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | MAN  | D     | 7   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | E     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | E     | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | NAG  | F     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | F     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | BMA  | F     | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | MAN  | F     | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | MAN  | F     | 5   | 2    | -       | 1/2/19/22 | 1/1/1/1 |
| 2   | MAN  | F     | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | MAN  | F     | 7   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | G     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | G     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | G     | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | NAG  | H     | 1   | 1,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | H     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | BMA  | H     | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | MAN  | H     | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | MAN  | H     | 5   | 2    | -       | 1/2/19/22 | 1/1/1/1 |
| 2   | MAN  | H     | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | MAN  | H     | 7   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | I     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | I     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | I     | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |

There are no bond length outliers.

All (6) bond angle outliers are listed below:



| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | H     | 2   | NAG  | C2-N2-C7 | -2.79 | 119.16      | 122.90   |
| 2   | F     | 2   | NAG  | C2-N2-C7 | -2.78 | 119.18      | 122.90   |
| 2   | D     | 2   | NAG  | C2-N2-C7 | -2.74 | 119.23      | 122.90   |
| 3   | E     | 1   | NAG  | C1-O5-C5 | 2.67  | 115.77      | 112.19   |
| 3   | G     | 1   | NAG  | C1-O5-C5 | 2.64  | 115.72      | 112.19   |
| 3   | I     | 1   | NAG  | C1-O5-C5 | 2.60  | 115.67      | 112.19   |

There are no chirality outliers.

All (51) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | E     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | E     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | G     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | G     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | I     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | E     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | E     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | G     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | G     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | I     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | D     | 3   | BMA  | C4-C5-C6-O6 |
| 2   | F     | 3   | BMA  | C4-C5-C6-O6 |
| 2   | H     | 3   | BMA  | C4-C5-C6-O6 |
| 2   | D     | 1   | NAG  | C8-C7-N2-C2 |
| 2   | D     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | F     | 1   | NAG  | C8-C7-N2-C2 |
| 2   | F     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | H     | 1   | NAG  | C8-C7-N2-C2 |
| 2   | H     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | E     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | G     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | D     | 1   | NAG  | O7-C7-N2-C2 |
| 2   | D     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | F     | 1   | NAG  | O7-C7-N2-C2 |
| 2   | F     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | H     | 1   | NAG  | O7-C7-N2-C2 |
| 2   | H     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | E     | 1   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | G     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | D     | 5   | MAN  | O5-C5-C6-O6 |
| 2   | F     | 5   | MAN  | O5-C5-C6-O6 |
| 2   | H     | 5   | MAN  | O5-C5-C6-O6 |
| 2   | D     | 3   | BMA  | O5-C5-C6-O6 |
| 2   | F     | 3   | BMA  | O5-C5-C6-O6 |
| 2   | H     | 3   | BMA  | O5-C5-C6-O6 |
| 2   | D     | 7   | MAN  | O5-C5-C6-O6 |
| 2   | F     | 7   | MAN  | O5-C5-C6-O6 |
| 2   | H     | 7   | MAN  | O5-C5-C6-O6 |
| 3   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | G     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | I     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | E     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | G     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | E     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | G     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | I     | 3   | BMA  | C4-C5-C6-O6 |

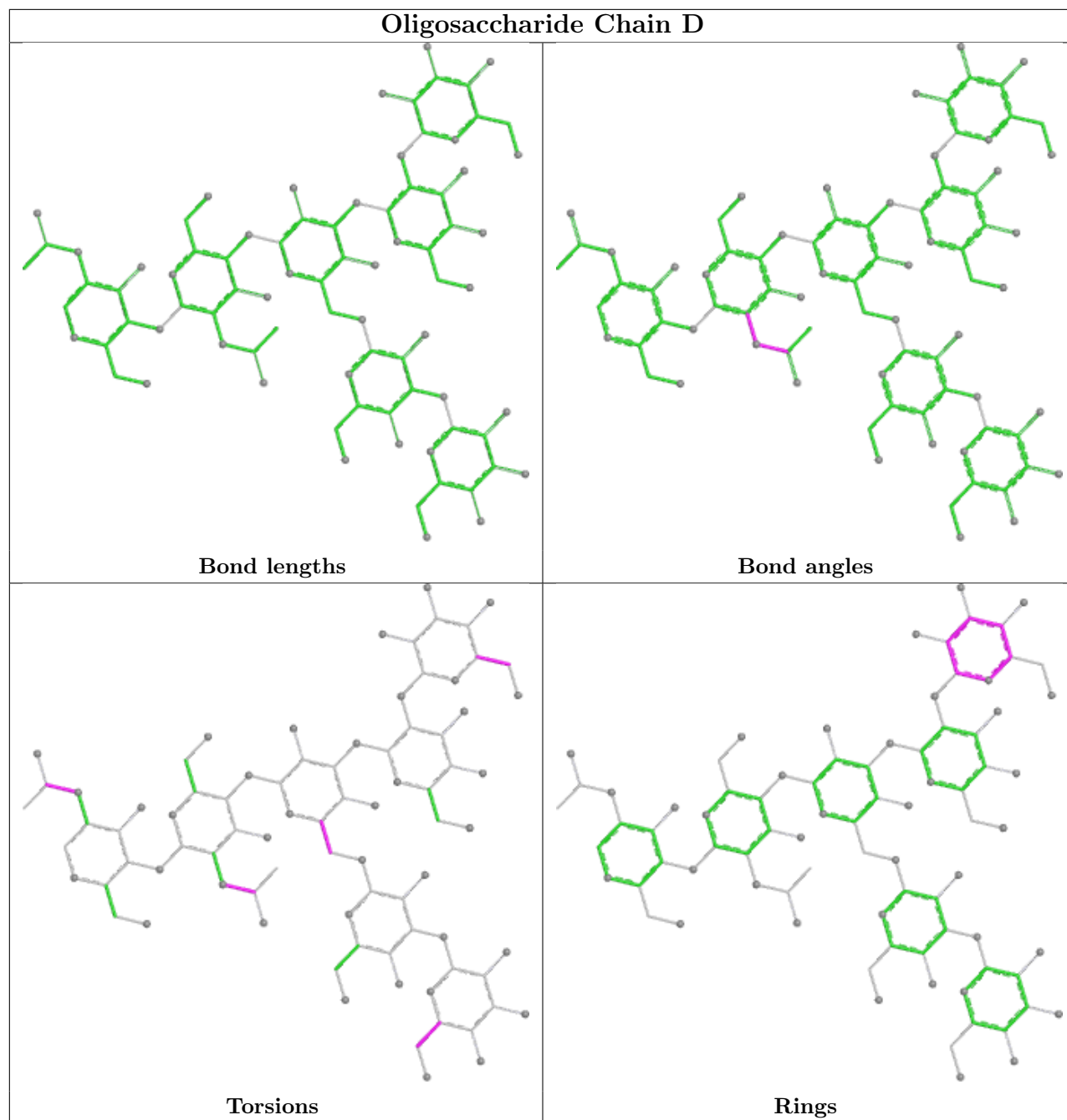
All (3) ring outliers are listed below:

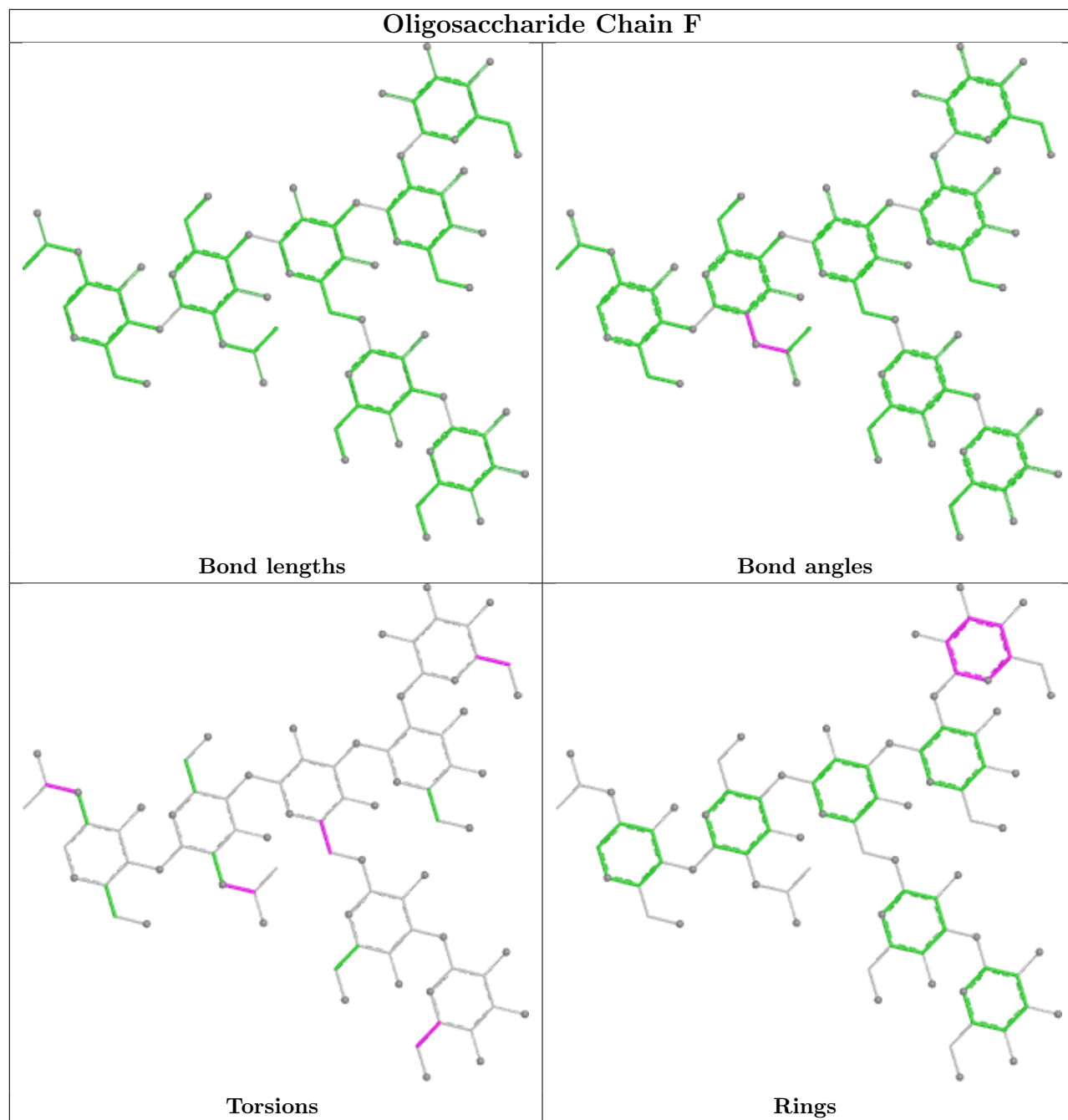
| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 2   | H     | 5   | MAN  | C1-C2-C3-C4-C5-O5 |
| 2   | F     | 5   | MAN  | C1-C2-C3-C4-C5-O5 |
| 2   | D     | 5   | MAN  | C1-C2-C3-C4-C5-O5 |

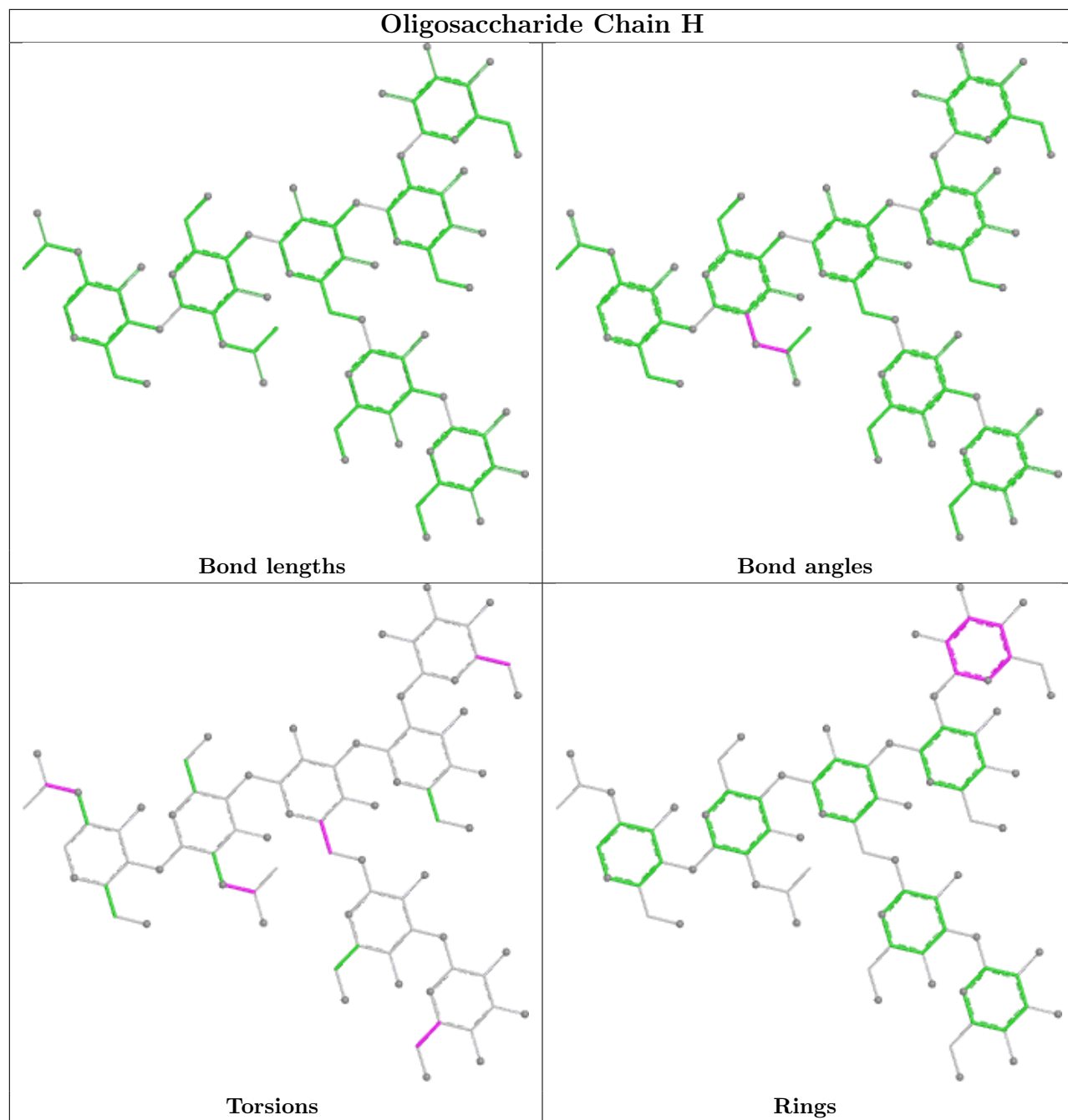
6 monomers are involved in 21 short contacts:

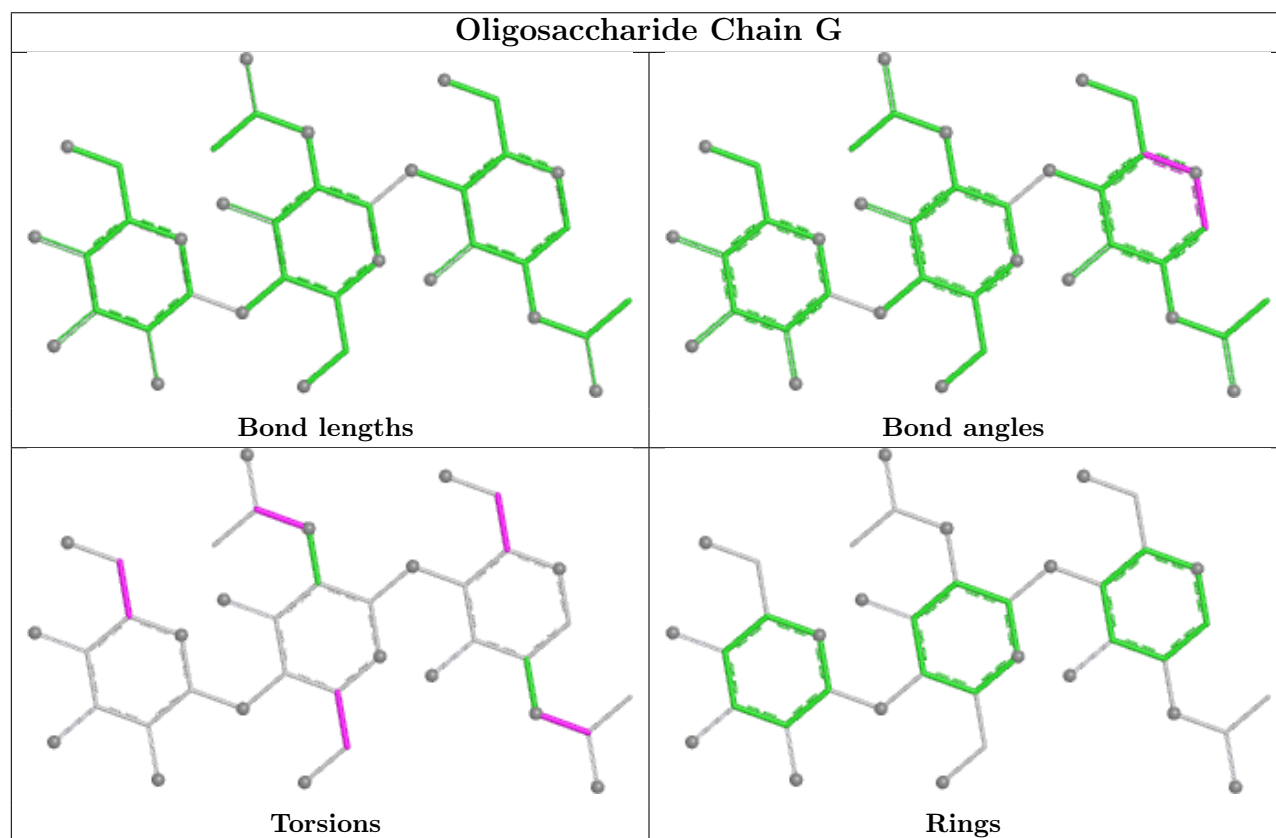
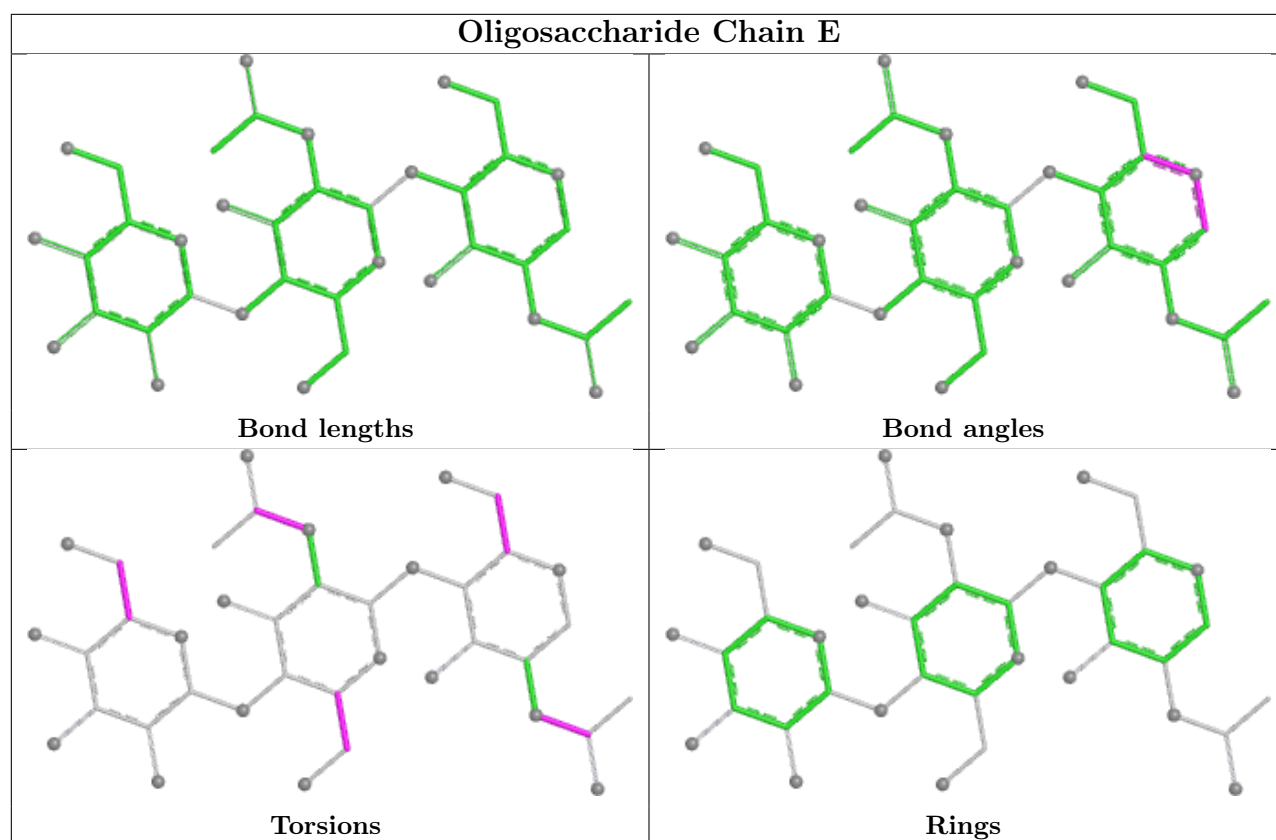
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | G     | 1   | NAG  | 3       | 0            |
| 3   | I     | 2   | NAG  | 4       | 0            |
| 3   | I     | 1   | NAG  | 3       | 0            |
| 3   | G     | 2   | NAG  | 3       | 0            |
| 3   | E     | 1   | NAG  | 4       | 0            |
| 3   | E     | 2   | NAG  | 4       | 0            |

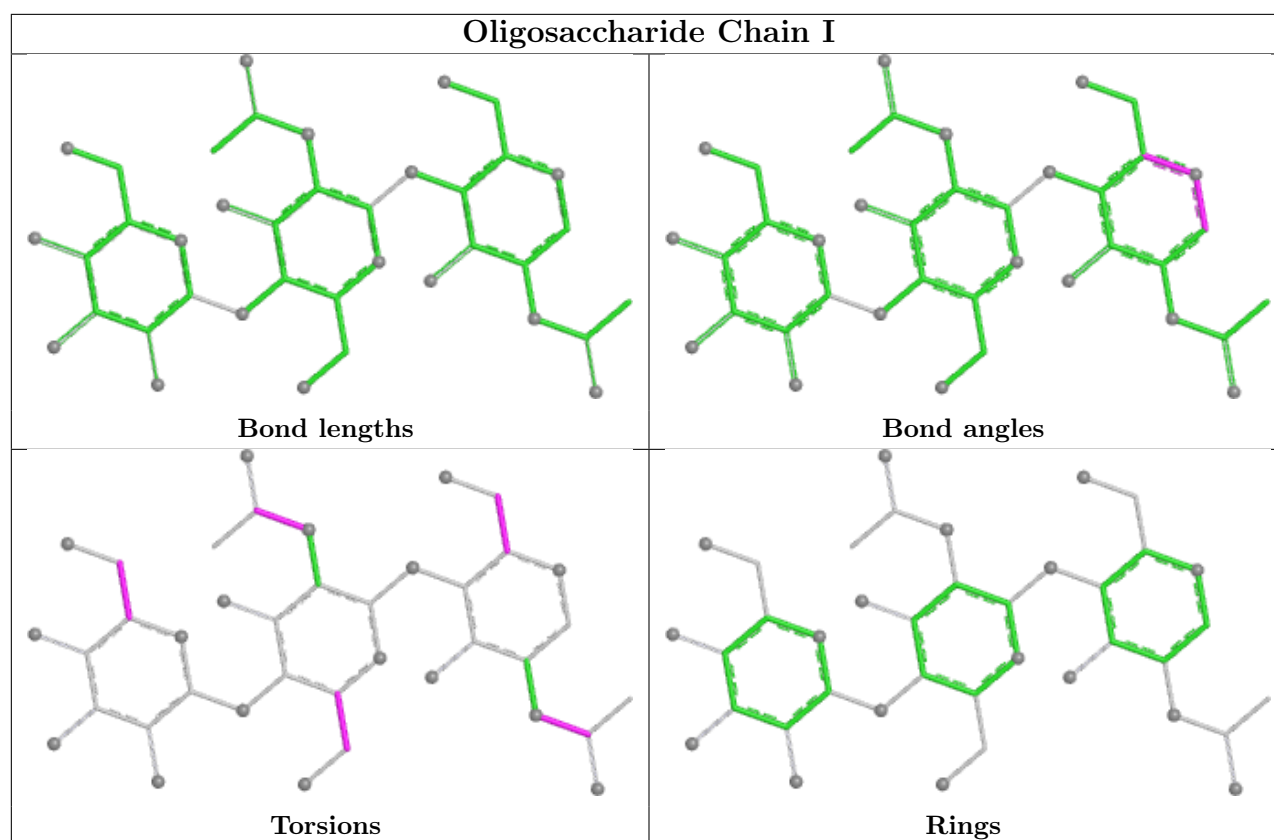
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

42 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 | $\# Z  > 2$ |
| 4   | NAG  | B     | 1209 | 1    | 14,14,15     | 0.44 | 0           | 17,19,21    | 0.47 | 0           |
| 4   | NAG  | C     | 1201 | 1    | 14,14,15     | 0.68 | 1 (7%)      | 17,19,21    | 0.38 | 0           |
| 4   | NAG  | A     | 1207 | 1    | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.90 | 1 (5%)      |
| 4   | NAG  | A     | 1202 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.38 | 0           |
| 4   | NAG  | A     | 1209 | 1    | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.47 | 0           |
| 4   | NAG  | B     | 1206 | 1    | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.44 | 0           |
| 4   | NAG  | B     | 1211 | 1    | 14,14,15     | 0.31 | 0           | 17,19,21    | 0.40 | 0           |
| 4   | NAG  | C     | 1213 | 1    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.67 | 1 (5%)      |
| 4   | NAG  | A     | 1208 | 1    | 14,14,15     | 0.69 | 1 (7%)      | 17,19,21    | 0.43 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | A     | 1206 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.44 | 0        |
| 4   | NAG  | B     | 1204 | 1    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.40 | 0        |
| 4   | NAG  | C     | 1210 | 1    | 14,14,15     | 1.26 | 1 (7%)   | 17,19,21    | 2.00 | 2 (11%)  |
| 4   | NAG  | B     | 1205 | 1    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 4   | NAG  | C     | 1214 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.40 | 0        |
| 4   | NAG  | A     | 1214 | 1    | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.38 | 0        |
| 4   | NAG  | A     | 1205 | 1    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 4   | NAG  | C     | 1211 | 1    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.41 | 0        |
| 4   | NAG  | B     | 1201 | 1    | 14,14,15     | 0.70 | 1 (7%)   | 17,19,21    | 0.37 | 0        |
| 4   | NAG  | C     | 1212 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 4   | NAG  | B     | 1214 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.38 | 0        |
| 4   | NAG  | B     | 1213 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.66 | 1 (5%)   |
| 4   | NAG  | B     | 1210 | 1    | 14,14,15     | 1.26 | 1 (7%)   | 17,19,21    | 2.01 | 2 (11%)  |
| 4   | NAG  | A     | 1211 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.40 | 0        |
| 4   | NAG  | A     | 1212 | 1    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 4   | NAG  | C     | 1202 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.37 | 0        |
| 4   | NAG  | C     | 1203 | 1    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | B     | 1208 | 1    | 14,14,15     | 0.69 | 1 (7%)   | 17,19,21    | 0.44 | 0        |
| 4   | NAG  | A     | 1213 | 1    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.66 | 1 (5%)   |
| 4   | NAG  | C     | 1209 | 1    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.48 | 0        |
| 4   | NAG  | A     | 1210 | 1    | 14,14,15     | 1.26 | 1 (7%)   | 17,19,21    | 2.00 | 2 (11%)  |
| 4   | NAG  | C     | 1207 | 1    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.90 | 1 (5%)   |
| 4   | NAG  | A     | 1204 | 1    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.40 | 0        |
| 4   | NAG  | A     | 1203 | 1    | 14,14,15     | 0.46 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | B     | 1202 | 1    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.37 | 0        |
| 4   | NAG  | C     | 1208 | 1    | 14,14,15     | 0.68 | 1 (7%)   | 17,19,21    | 0.44 | 0        |
| 4   | NAG  | A     | 1201 | 1    | 14,14,15     | 0.70 | 1 (7%)   | 17,19,21    | 0.38 | 0        |
| 4   | NAG  | B     | 1212 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.70 | 1 (5%)   |
| 4   | NAG  | C     | 1204 | 1    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.39 | 0        |
| 4   | NAG  | C     | 1205 | 1    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 4   | NAG  | C     | 1206 | 1    | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.45 | 0        |
| 4   | NAG  | B     | 1203 | 1    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | B     | 1207 | 1    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.89 | 1 (5%)   |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | NAG  | B     | 1209 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1201 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1207 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1202 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1209 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1206 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1211 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1213 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1208 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1206 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1204 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1210 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1205 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1214 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1214 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1205 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1211 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1201 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1212 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1214 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1213 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1210 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1211 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1212 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1202 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1203 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1208 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1213 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1209 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1210 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1207 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1204 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1203 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1202 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1208 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | NAG  | A     | 1201 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1212 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1204 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1205 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1206 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1203 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1207 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4   | C     | 1210 | NAG  | C1-C2 | 4.29  | 1.58        | 1.52     |
| 4   | A     | 1210 | NAG  | C1-C2 | 4.28  | 1.58        | 1.52     |
| 4   | B     | 1210 | NAG  | C1-C2 | 4.28  | 1.58        | 1.52     |
| 4   | A     | 1208 | NAG  | O5-C1 | -2.30 | 1.39        | 1.43     |
| 4   | B     | 1208 | NAG  | O5-C1 | -2.28 | 1.39        | 1.43     |
| 4   | A     | 1201 | NAG  | O5-C1 | -2.23 | 1.40        | 1.43     |
| 4   | C     | 1208 | NAG  | O5-C1 | -2.23 | 1.40        | 1.43     |
| 4   | B     | 1201 | NAG  | O5-C1 | -2.20 | 1.40        | 1.43     |
| 4   | C     | 1201 | NAG  | O5-C1 | -2.16 | 1.40        | 1.43     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 4   | B     | 1210 | NAG  | C1-O5-C5 | 6.94 | 121.49      | 112.19   |
| 4   | A     | 1210 | NAG  | C1-O5-C5 | 6.94 | 121.48      | 112.19   |
| 4   | C     | 1210 | NAG  | C1-O5-C5 | 6.92 | 121.46      | 112.19   |
| 4   | B     | 1210 | NAG  | C4-C3-C2 | 4.03 | 116.93      | 111.02   |
| 4   | C     | 1210 | NAG  | C4-C3-C2 | 4.02 | 116.91      | 111.02   |
| 4   | A     | 1210 | NAG  | C4-C3-C2 | 4.02 | 116.90      | 111.02   |
| 4   | C     | 1207 | NAG  | C1-O5-C5 | 3.24 | 116.53      | 112.19   |
| 4   | A     | 1207 | NAG  | C1-O5-C5 | 3.22 | 116.51      | 112.19   |
| 4   | B     | 1207 | NAG  | C1-O5-C5 | 3.20 | 116.48      | 112.19   |
| 4   | A     | 1212 | NAG  | C1-O5-C5 | 2.38 | 115.37      | 112.19   |
| 4   | C     | 1212 | NAG  | C1-O5-C5 | 2.38 | 115.37      | 112.19   |
| 4   | B     | 1212 | NAG  | C1-O5-C5 | 2.33 | 115.31      | 112.19   |
| 4   | C     | 1205 | NAG  | C1-O5-C5 | 2.25 | 115.20      | 112.19   |
| 4   | A     | 1205 | NAG  | C1-O5-C5 | 2.25 | 115.19      | 112.19   |
| 4   | B     | 1205 | NAG  | C1-O5-C5 | 2.23 | 115.17      | 112.19   |
| 4   | C     | 1213 | NAG  | C1-O5-C5 | 2.17 | 115.10      | 112.19   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 4   | B     | 1213 | NAG  | C1-O5-C5 | 2.16 | 115.08      | 112.19   |
| 4   | A     | 1213 | NAG  | C1-O5-C5 | 2.15 | 115.06      | 112.19   |

There are no chirality outliers.

All (105) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | A     | 1210 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1210 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1210 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1208 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1208 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1208 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1205 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1205 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1205 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1206 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1206 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1206 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1210 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1210 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1210 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1203 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1203 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1203 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1208 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1208 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1208 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1204 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1204 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1204 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1203 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1203 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1205 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1203 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1205 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1205 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1206 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1213 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1206 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1213 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1206 | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | C     | 1213 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1202 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1202 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1202 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1213 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1213 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1213 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1204 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1204 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1204 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1202 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1207 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1202 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1207 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1202 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1207 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1207 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1207 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1207 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1202 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1202 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1203 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1203 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1214 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1214 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1202 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1202 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1203 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1203 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1214 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1214 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 1202 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 1202 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 1203 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 1203 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 1214 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 1214 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1214 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1214 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1214 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1214 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1214 | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | C     | 1214 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1212 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1211 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1211 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1212 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1211 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1212 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1201 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1201 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1201 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1212 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1212 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1212 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1205 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 1210 | NAG  | C3-C2-N2-C7 |
| 4   | B     | 1205 | NAG  | C3-C2-N2-C7 |
| 4   | B     | 1210 | NAG  | C3-C2-N2-C7 |
| 4   | C     | 1205 | NAG  | C3-C2-N2-C7 |
| 4   | C     | 1210 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 1201 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1201 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1201 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1211 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1211 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1211 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1205 | NAG  | C1-C2-N2-C7 |
| 4   | B     | 1205 | NAG  | C1-C2-N2-C7 |
| 4   | C     | 1205 | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

14 monomers are involved in 36 short contacts:

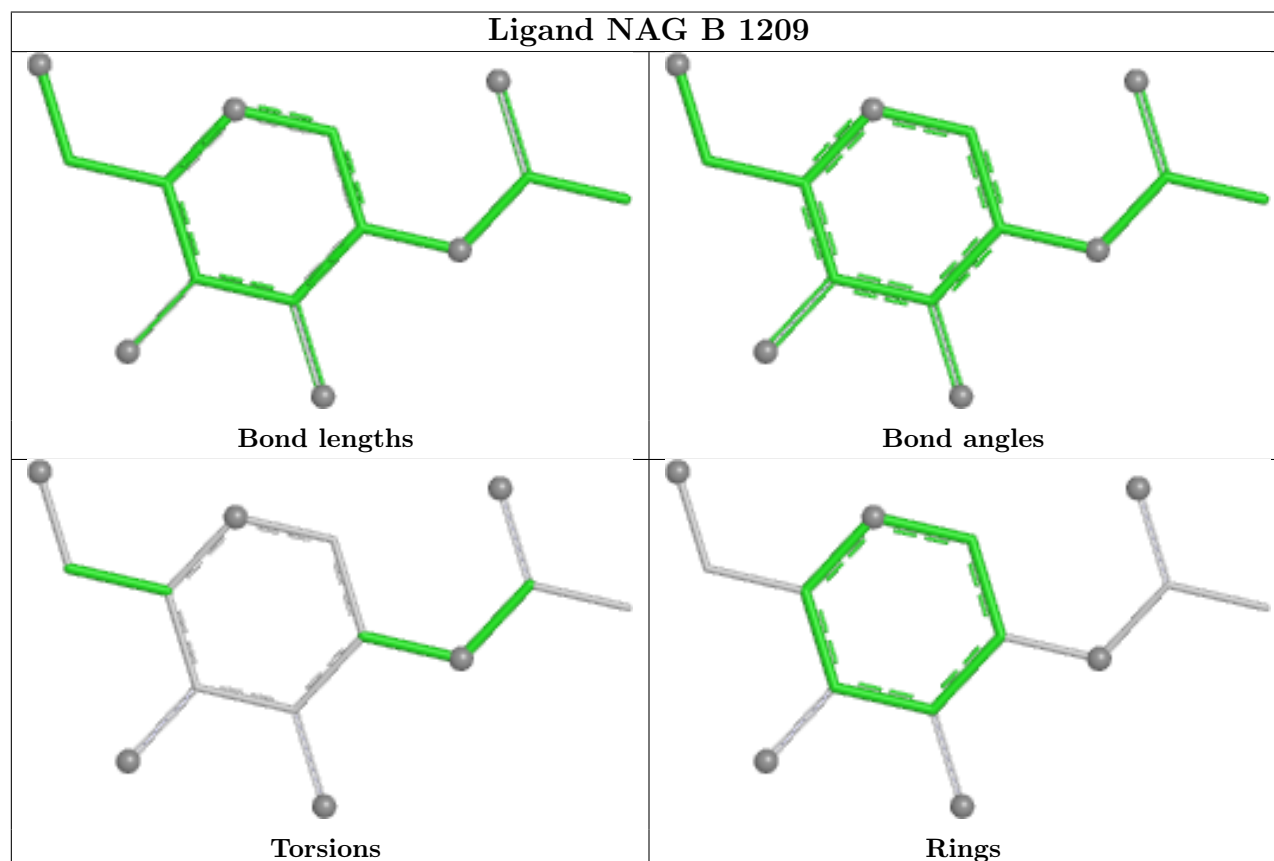
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1207 | NAG  | 1       | 0            |
| 4   | B     | 1206 | NAG  | 6       | 0            |
| 4   | A     | 1206 | NAG  | 2       | 0            |
| 4   | B     | 1204 | NAG  | 3       | 0            |
| 4   | C     | 1214 | NAG  | 1       | 0            |
| 4   | A     | 1214 | NAG  | 1       | 0            |
| 4   | B     | 1210 | NAG  | 1       | 0            |
| 4   | C     | 1203 | NAG  | 3       | 0            |
| 4   | A     | 1204 | NAG  | 2       | 0            |

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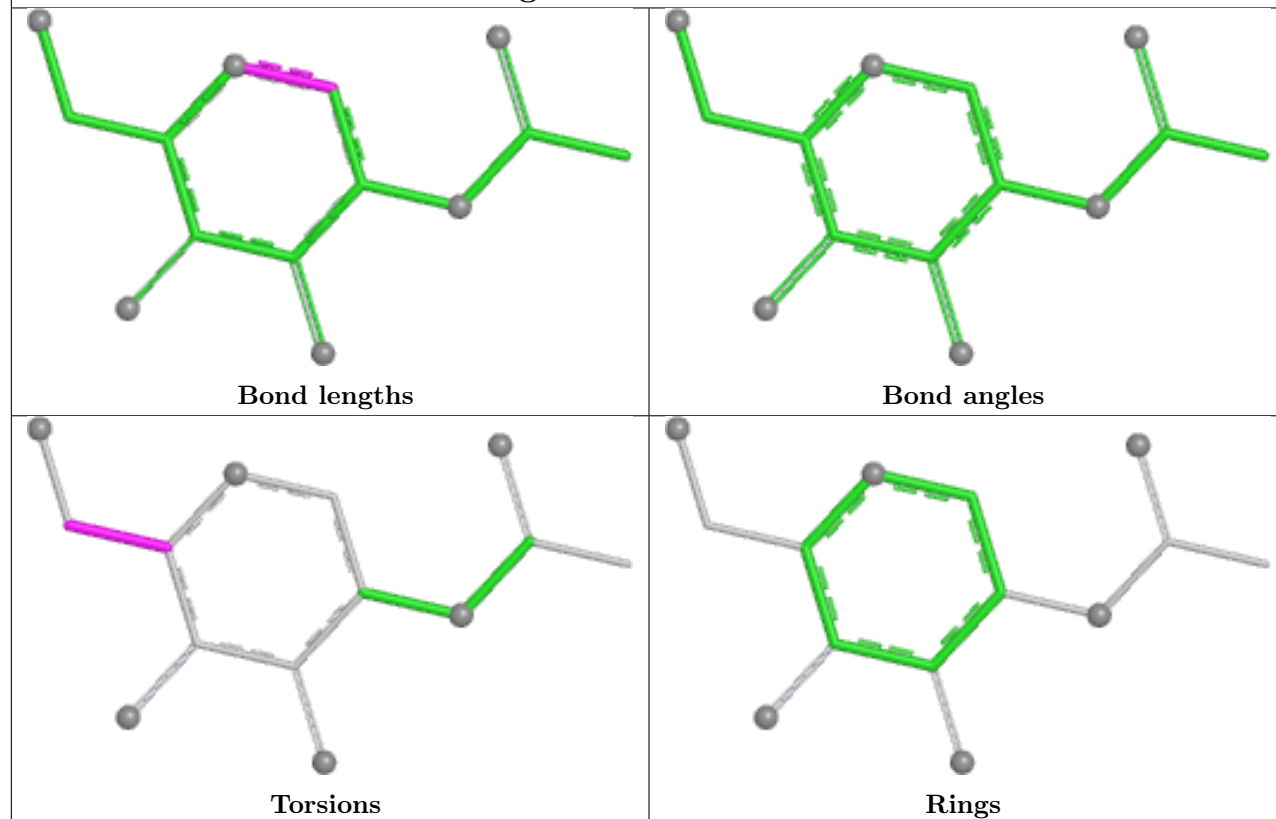
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1203 | NAG  | 5       | 0            |
| 4   | B     | 1202 | NAG  | 2       | 0            |
| 4   | B     | 1212 | NAG  | 2       | 0            |
| 4   | C     | 1204 | NAG  | 1       | 0            |
| 4   | B     | 1203 | NAG  | 6       | 0            |

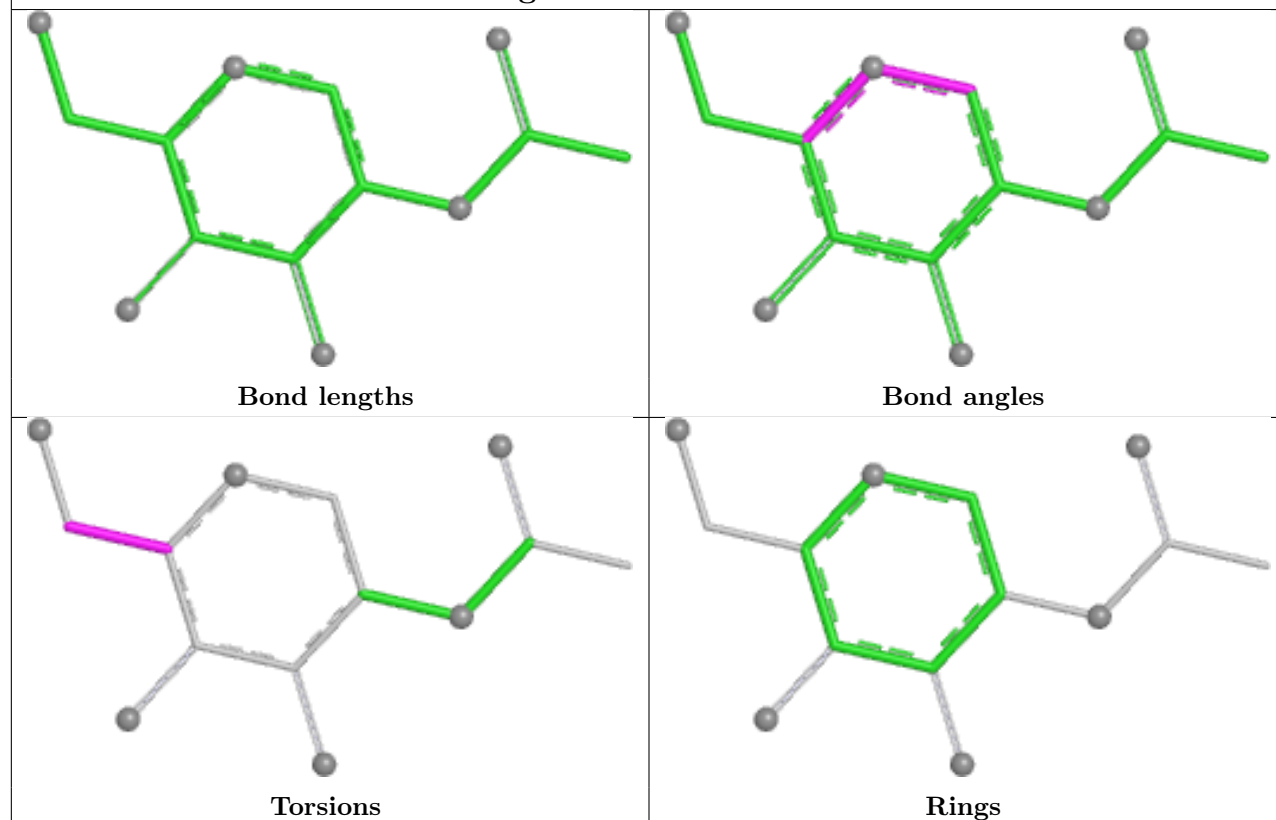
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



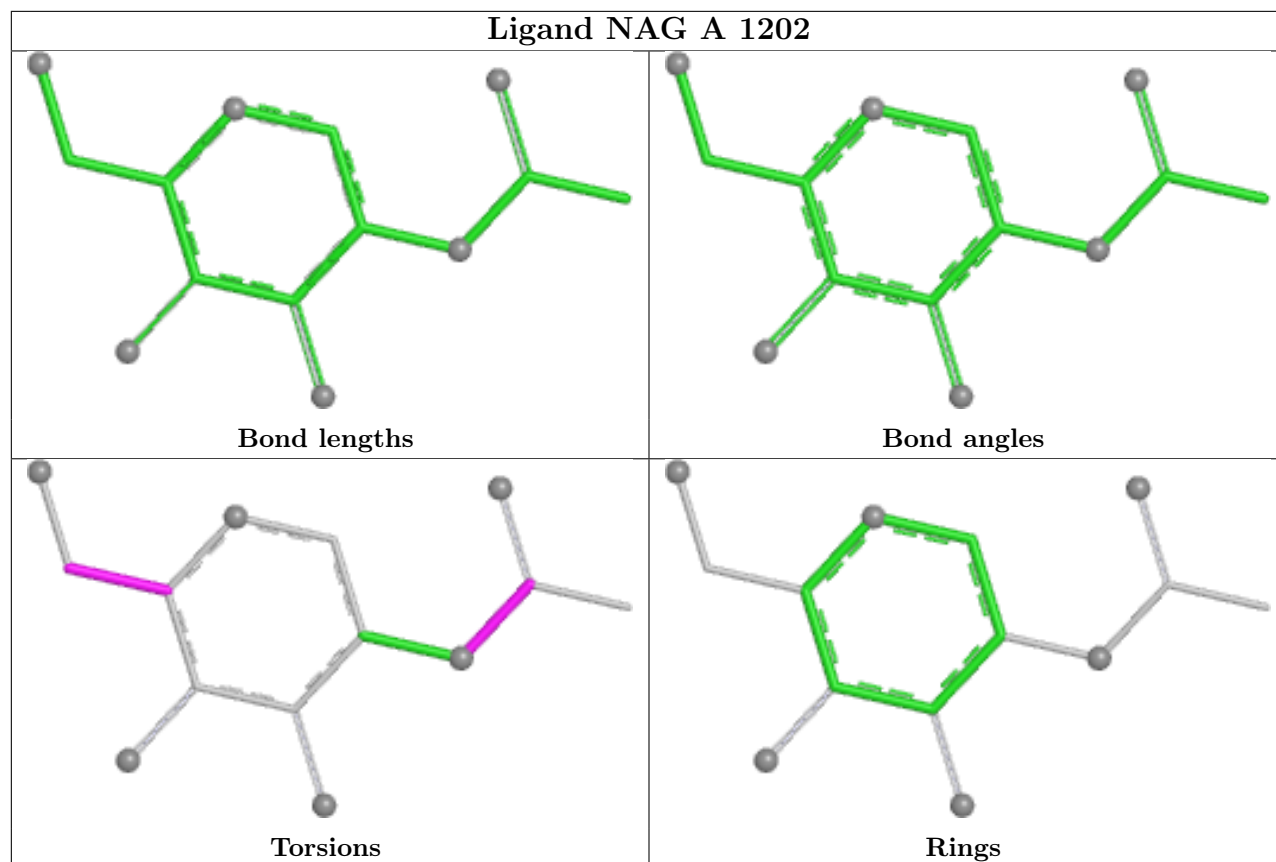
## Ligand NAG C 1201



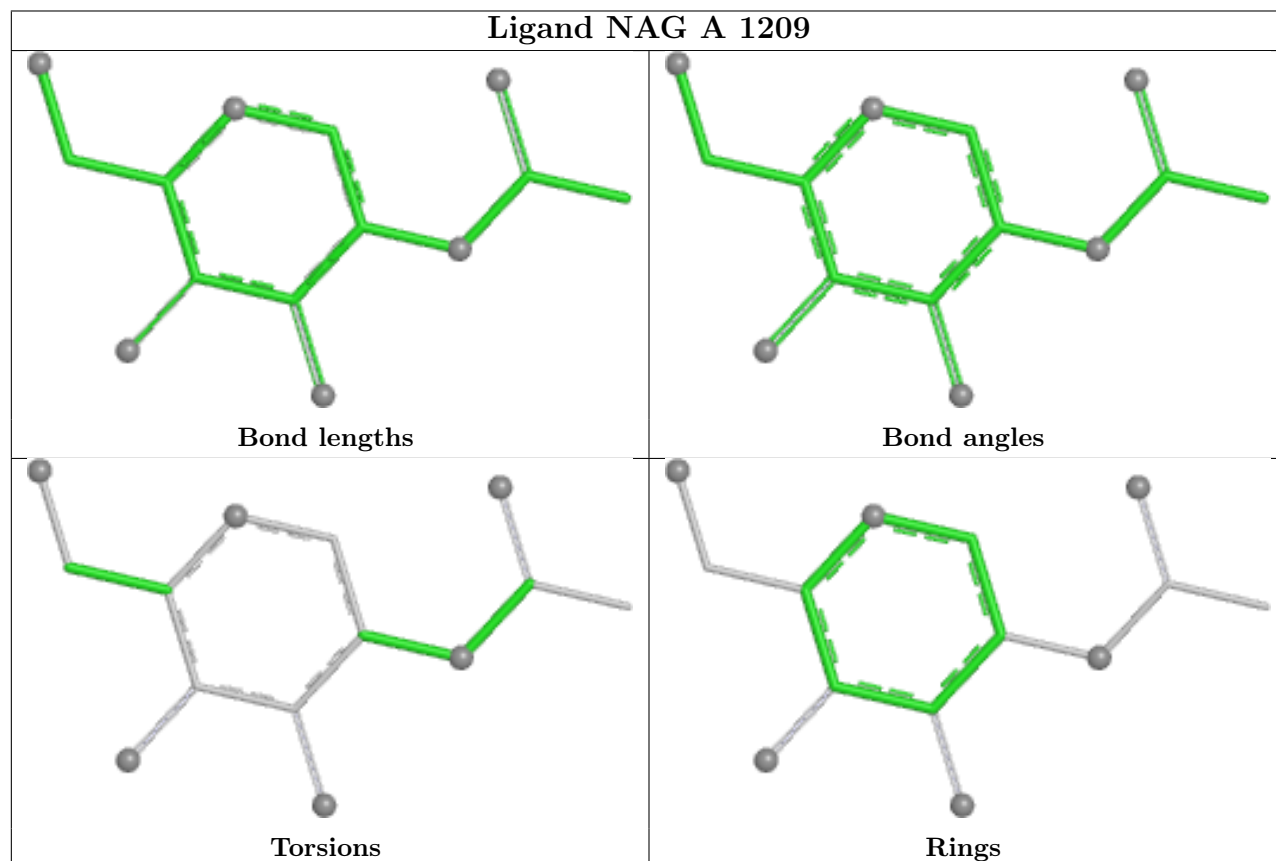
## Ligand NAG A 1207



## Ligand NAG A 1202

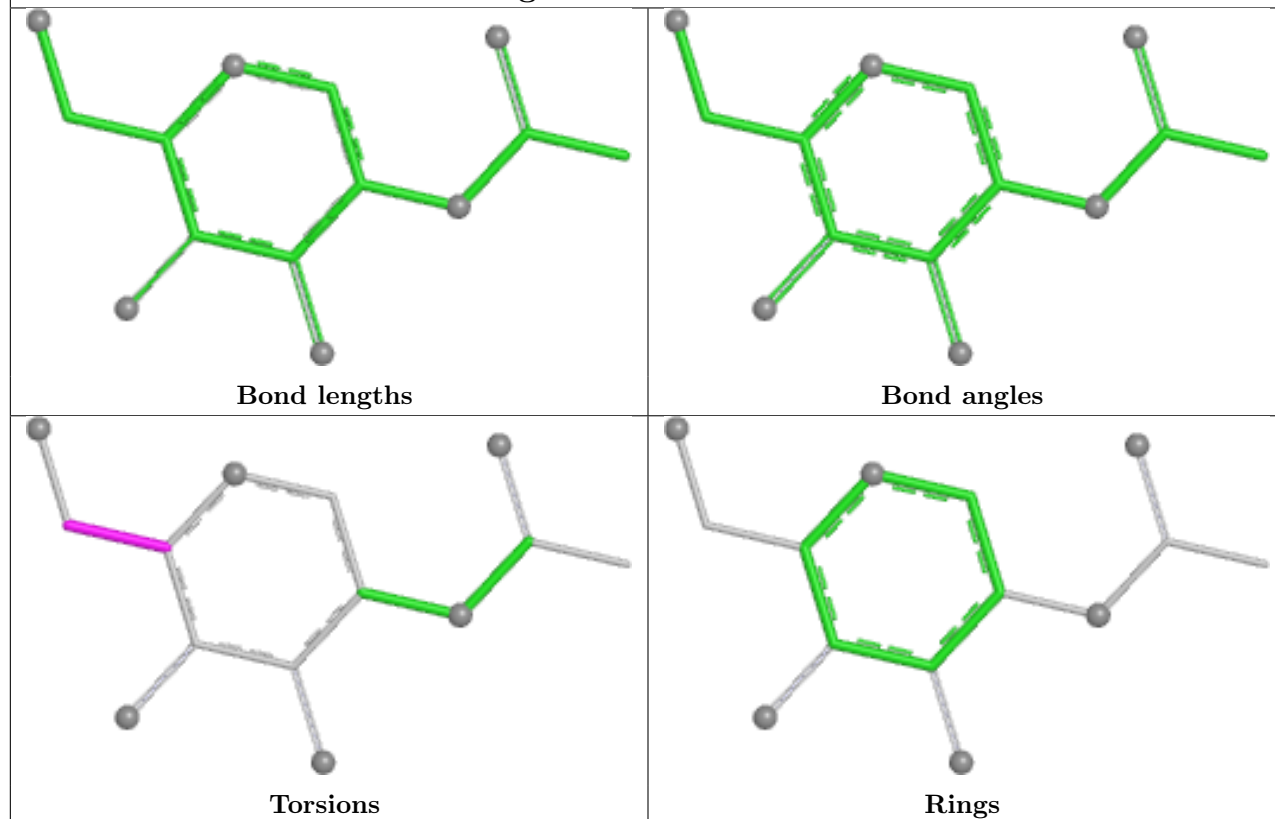


## Ligand NAG A 1209

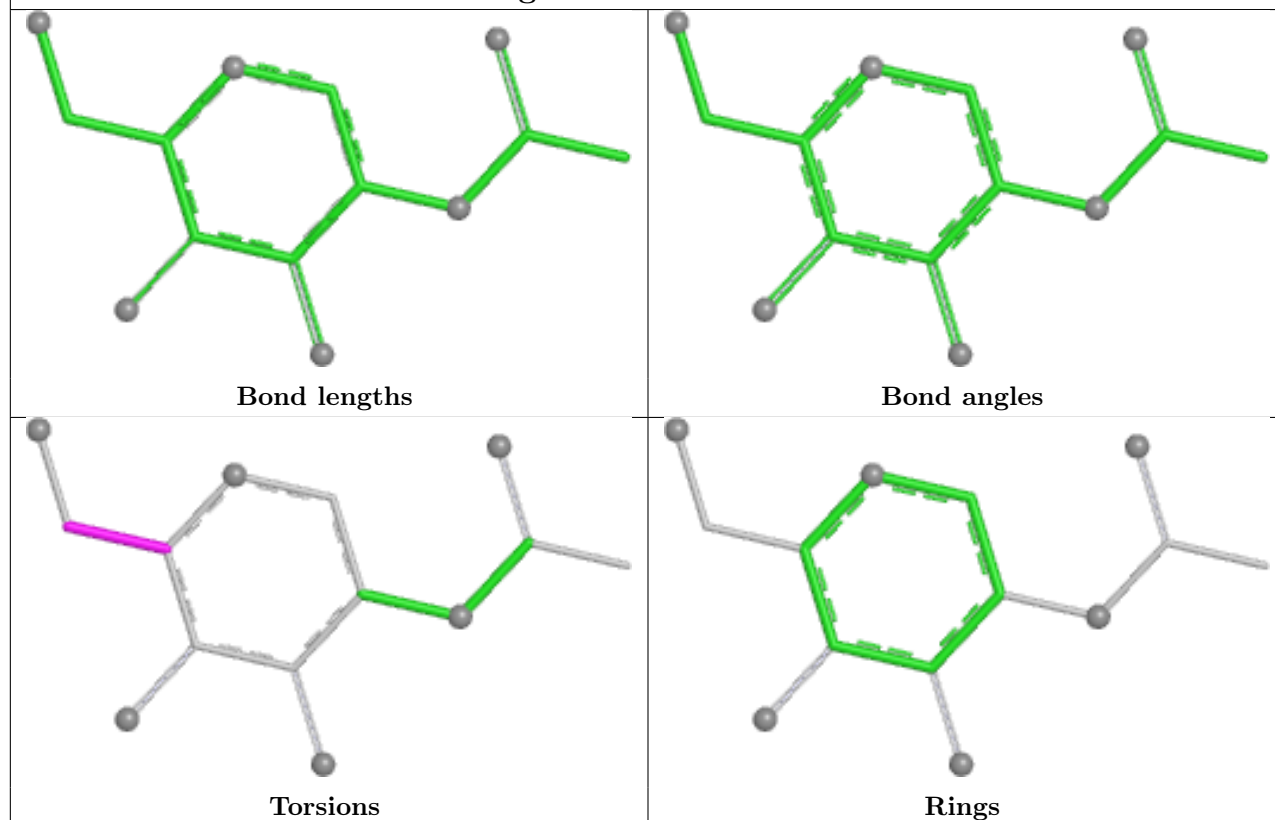


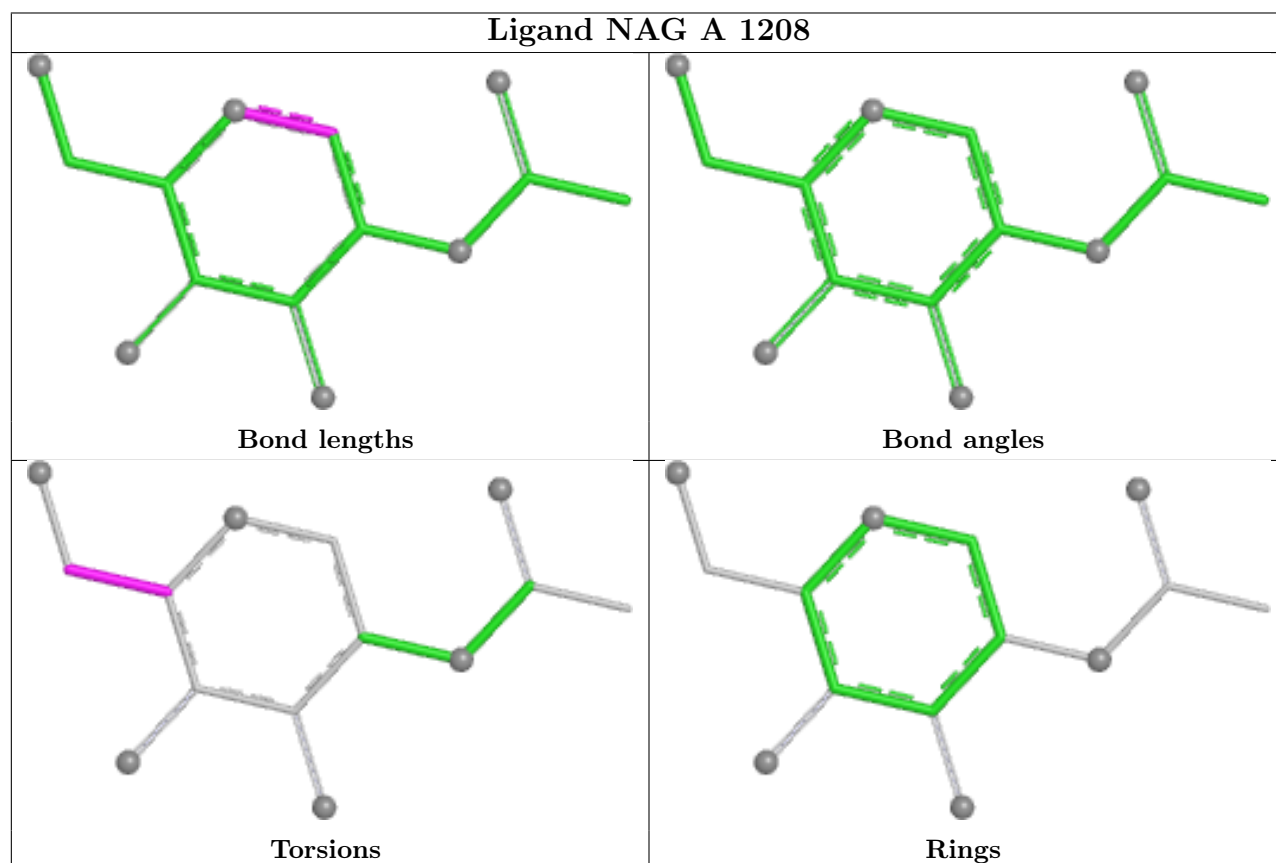
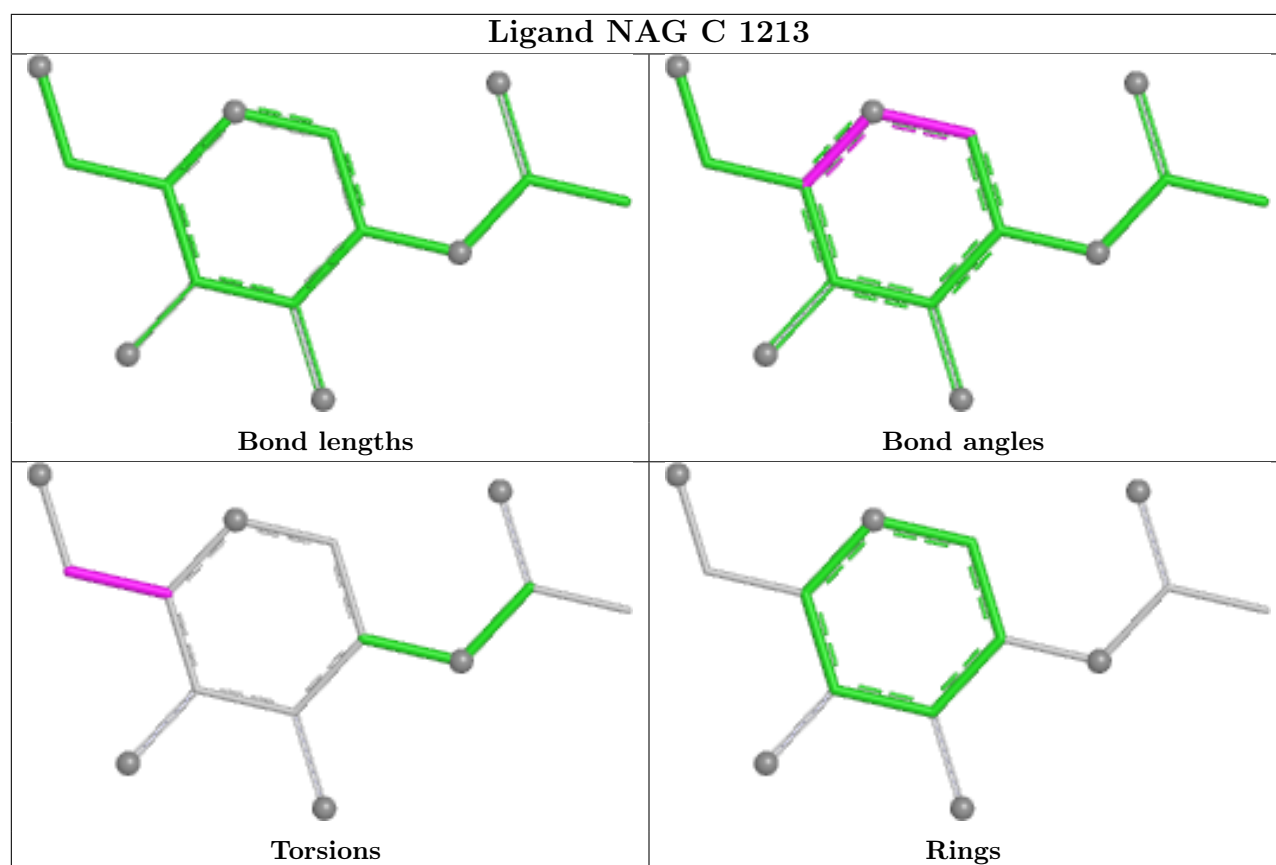


## Ligand NAG B 1206

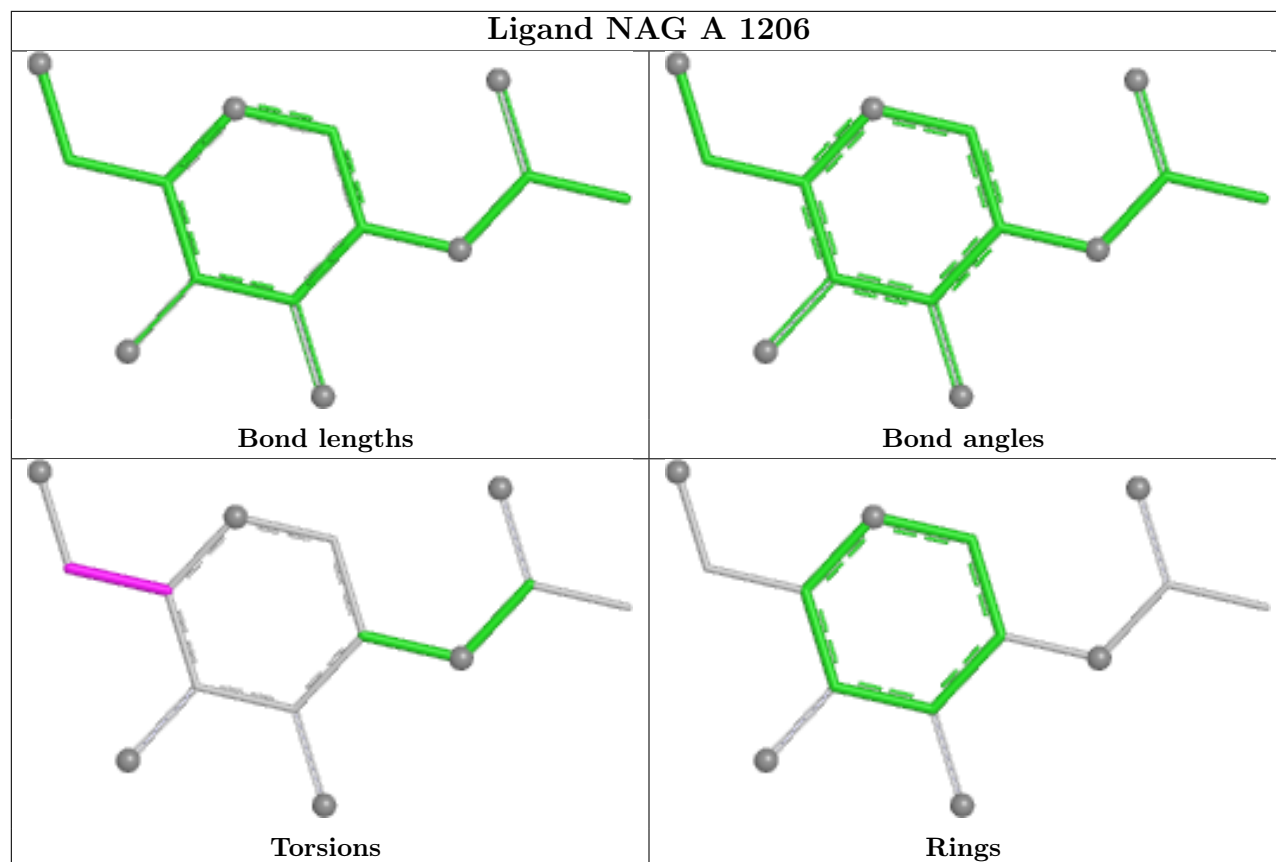


## Ligand NAG B 1211

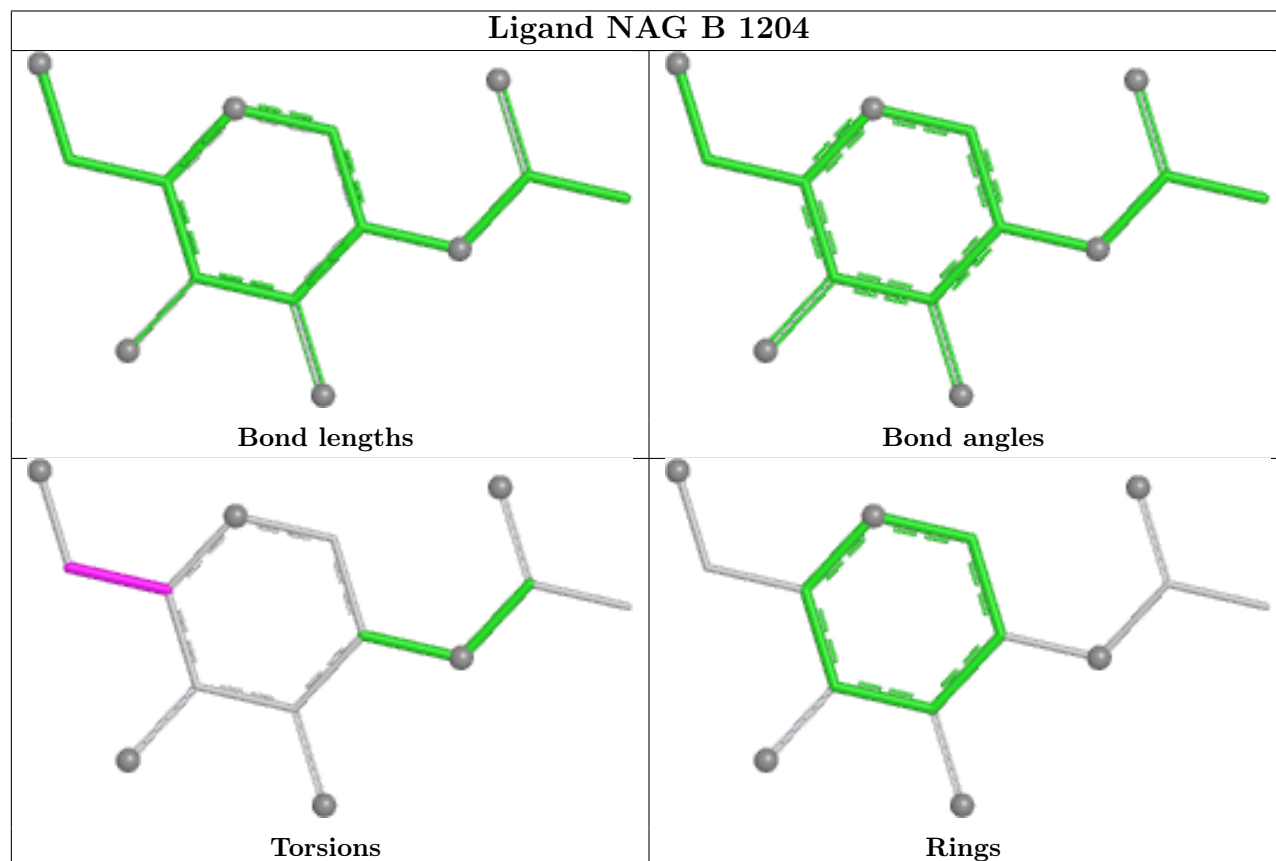




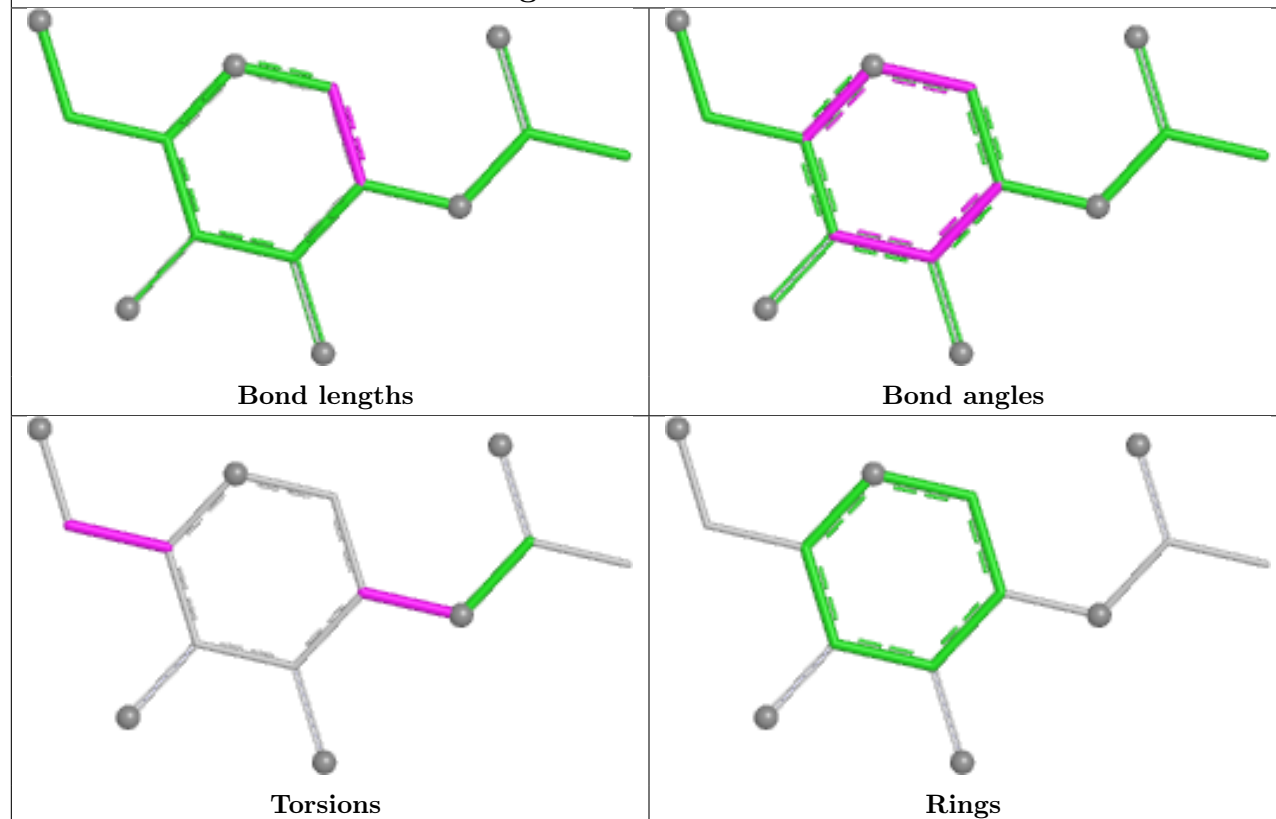
## Ligand NAG A 1206



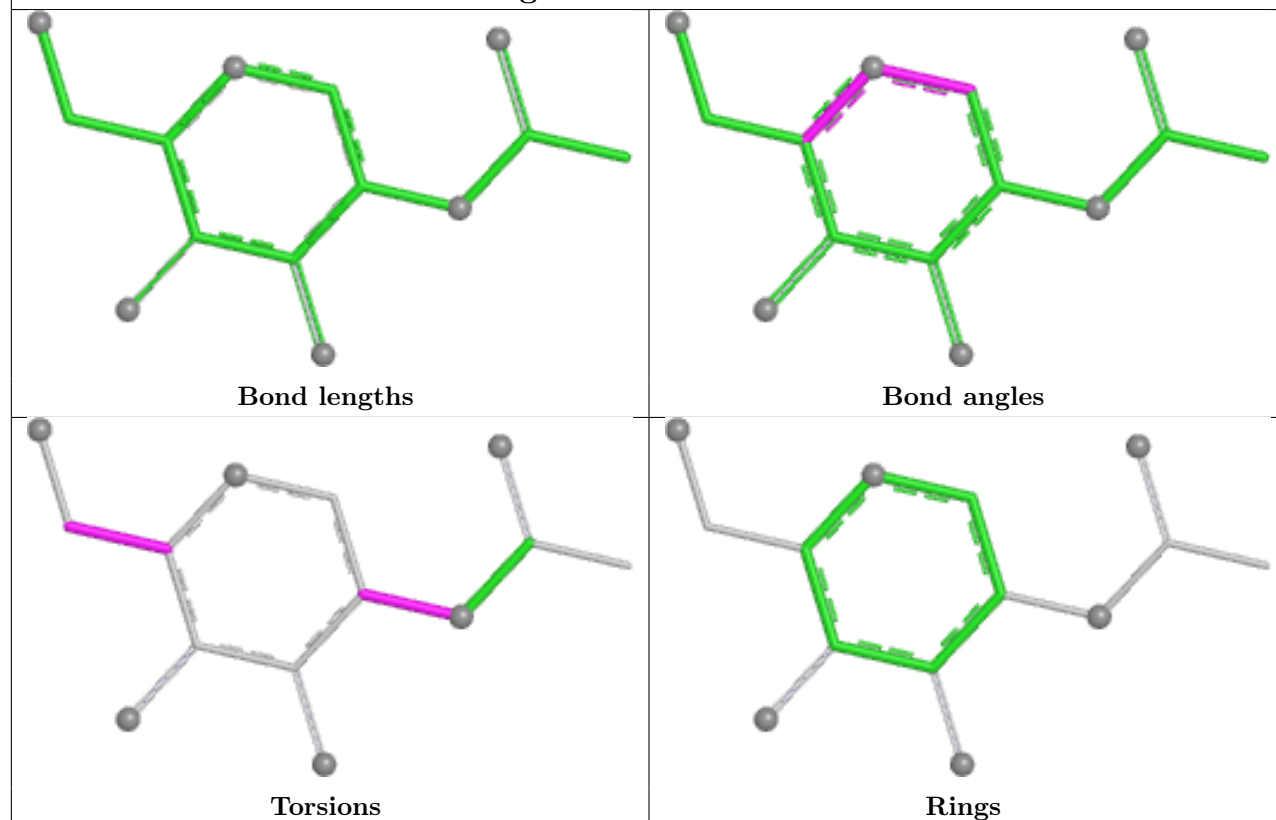
## Ligand NAG B 1204



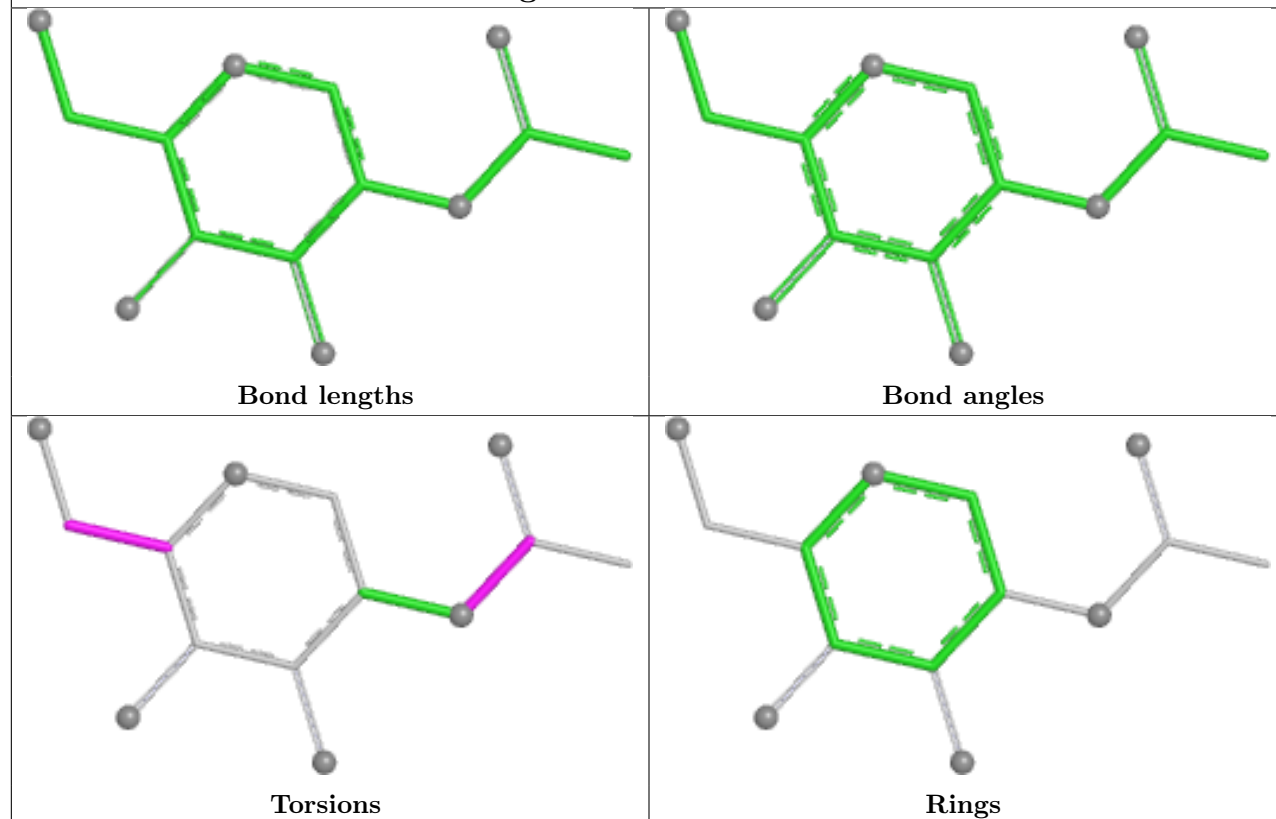
## Ligand NAG C 1210



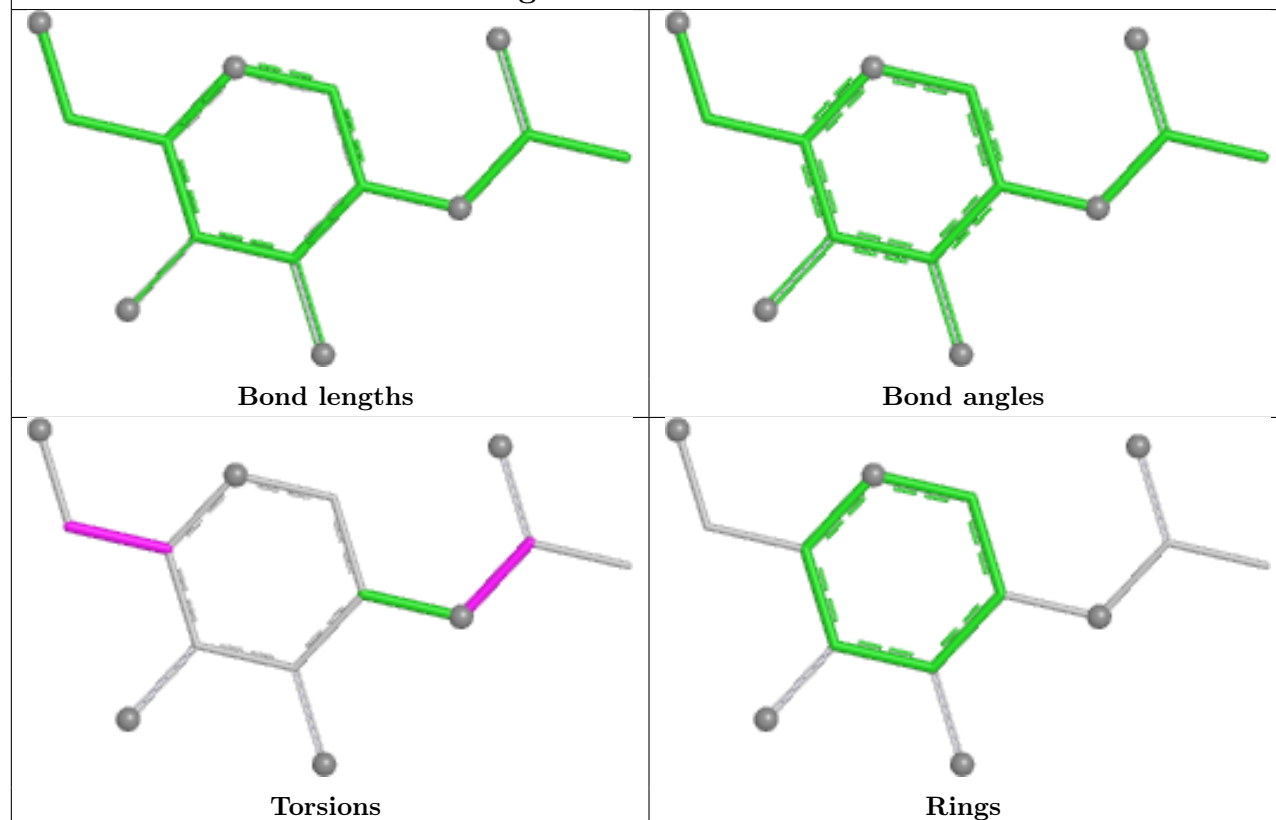
## Ligand NAG B 1205



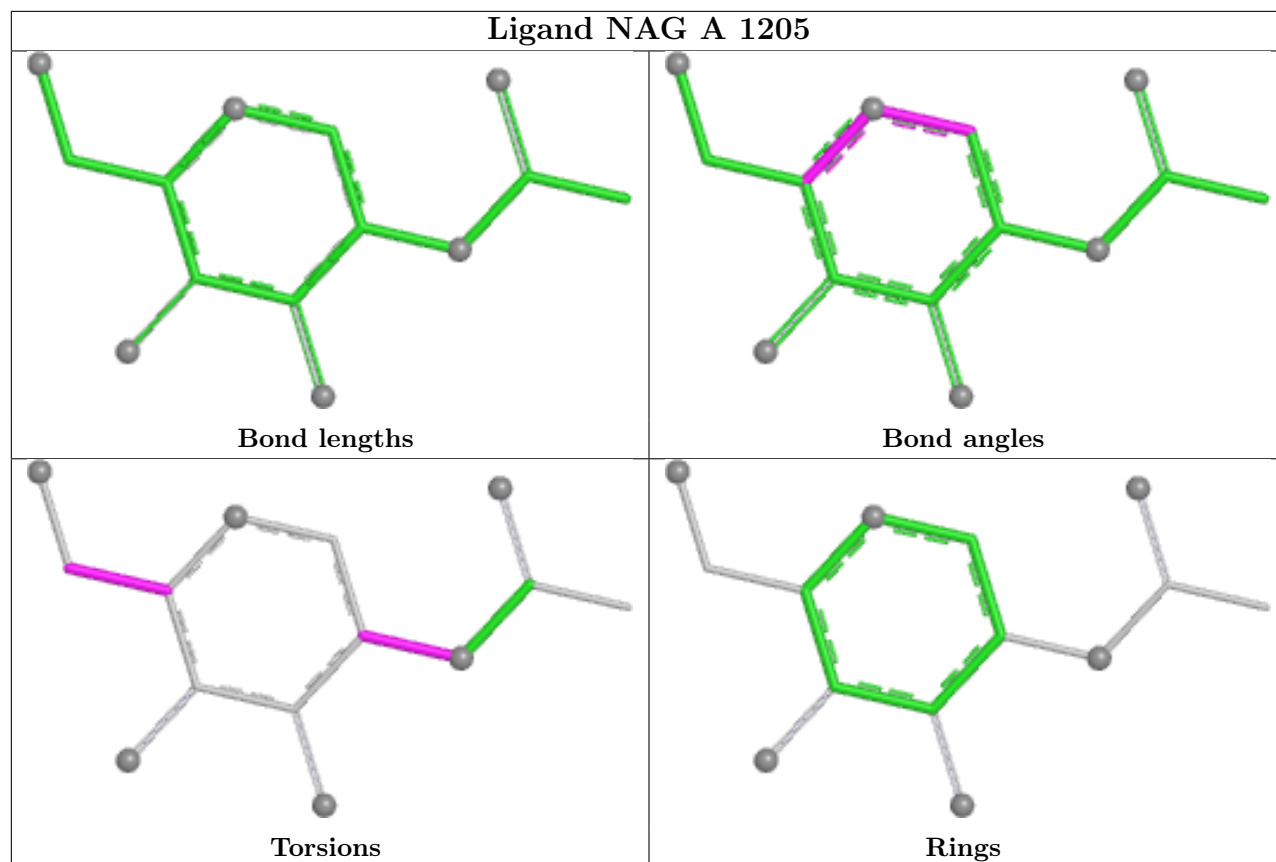
## Ligand NAG C 1214



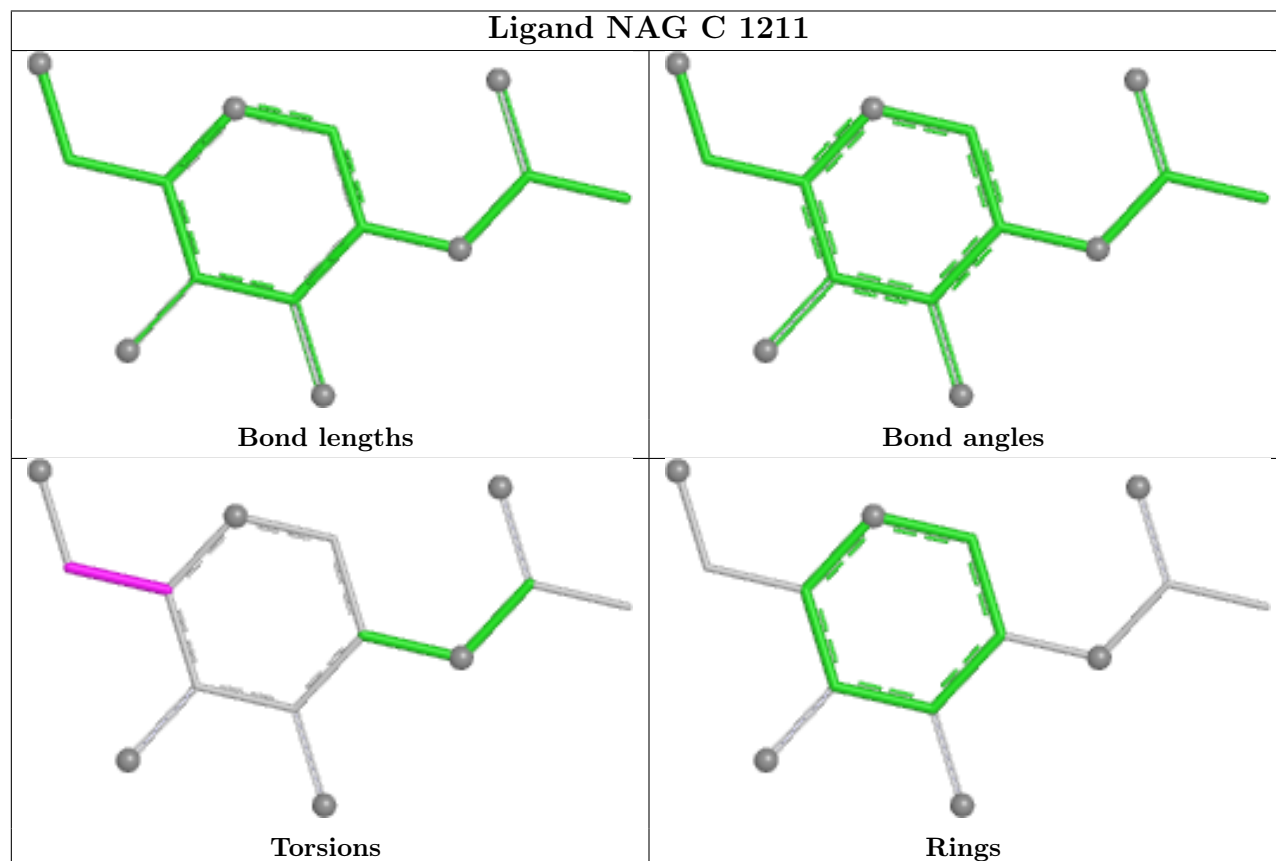
## Ligand NAG A 1214



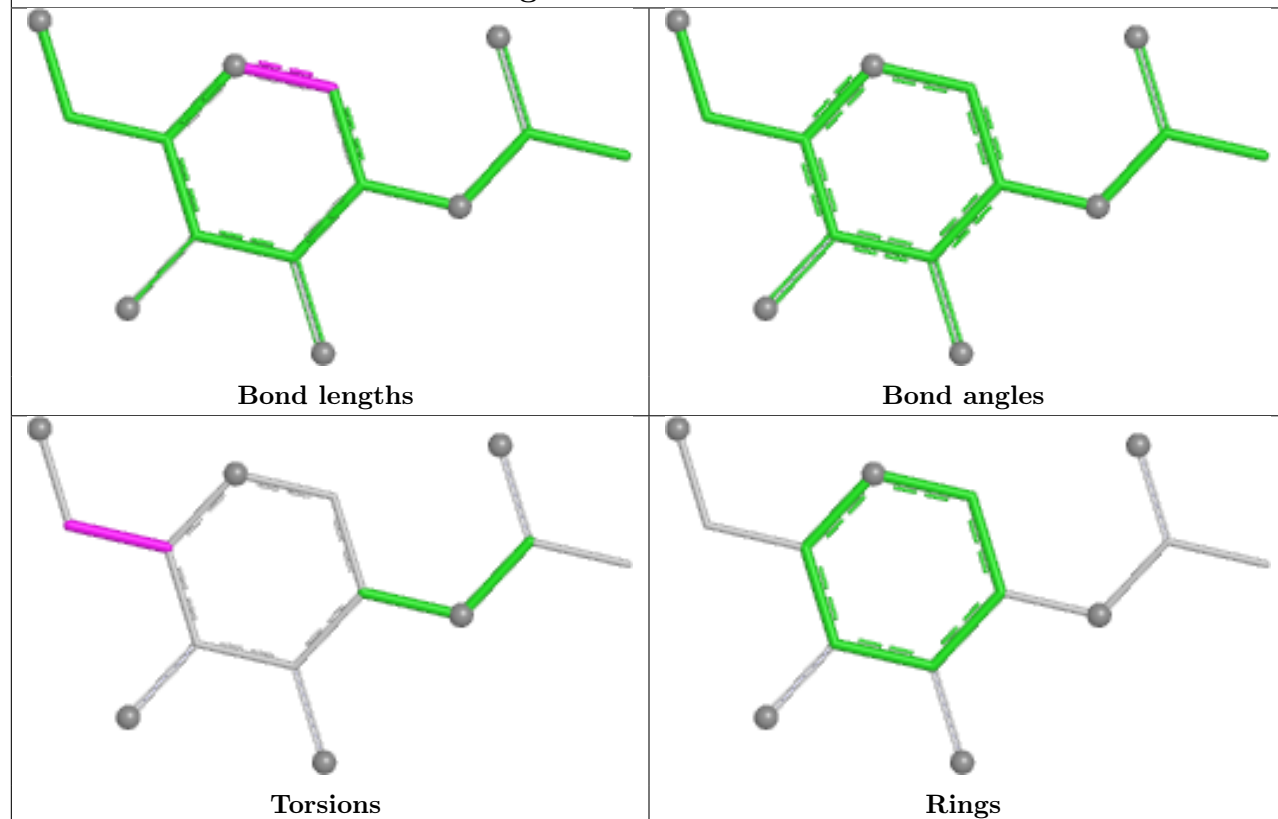
## Ligand NAG A 1205



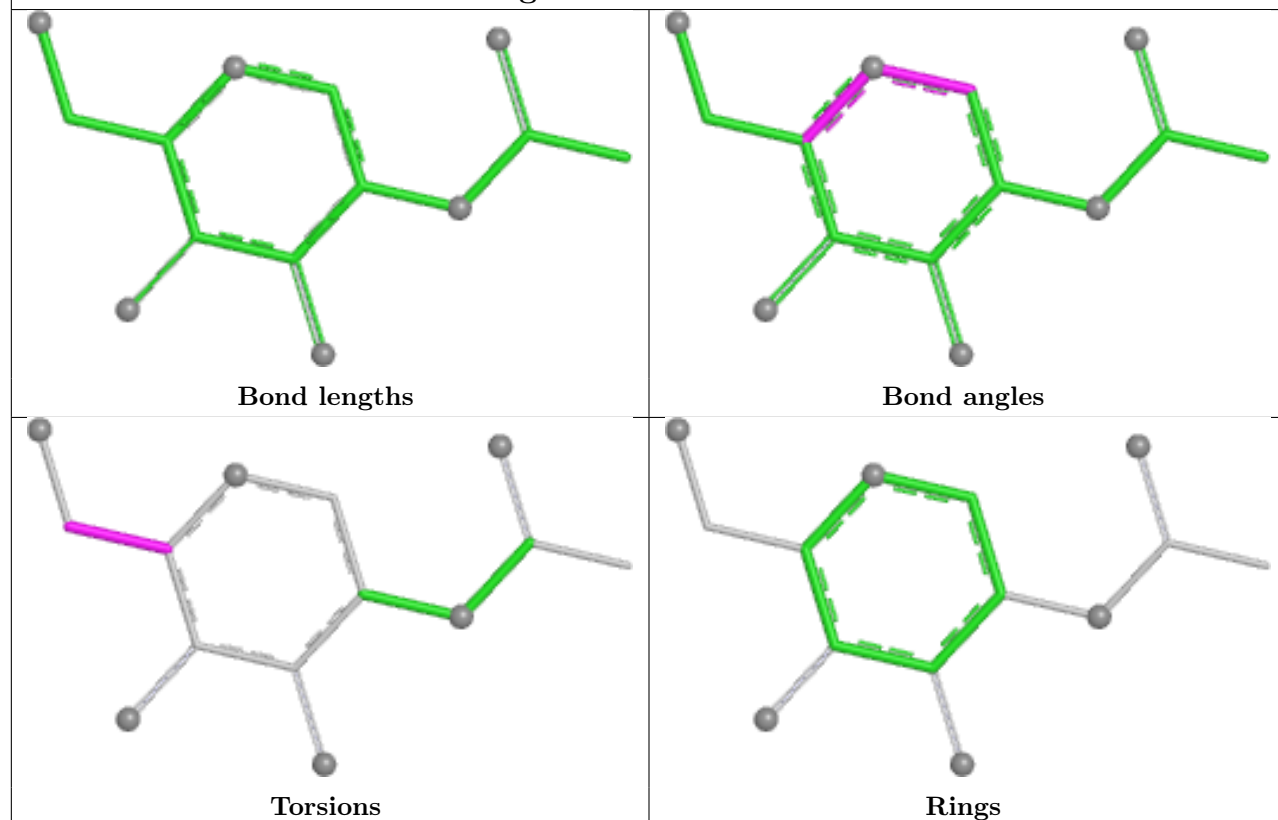
## Ligand NAG C 1211

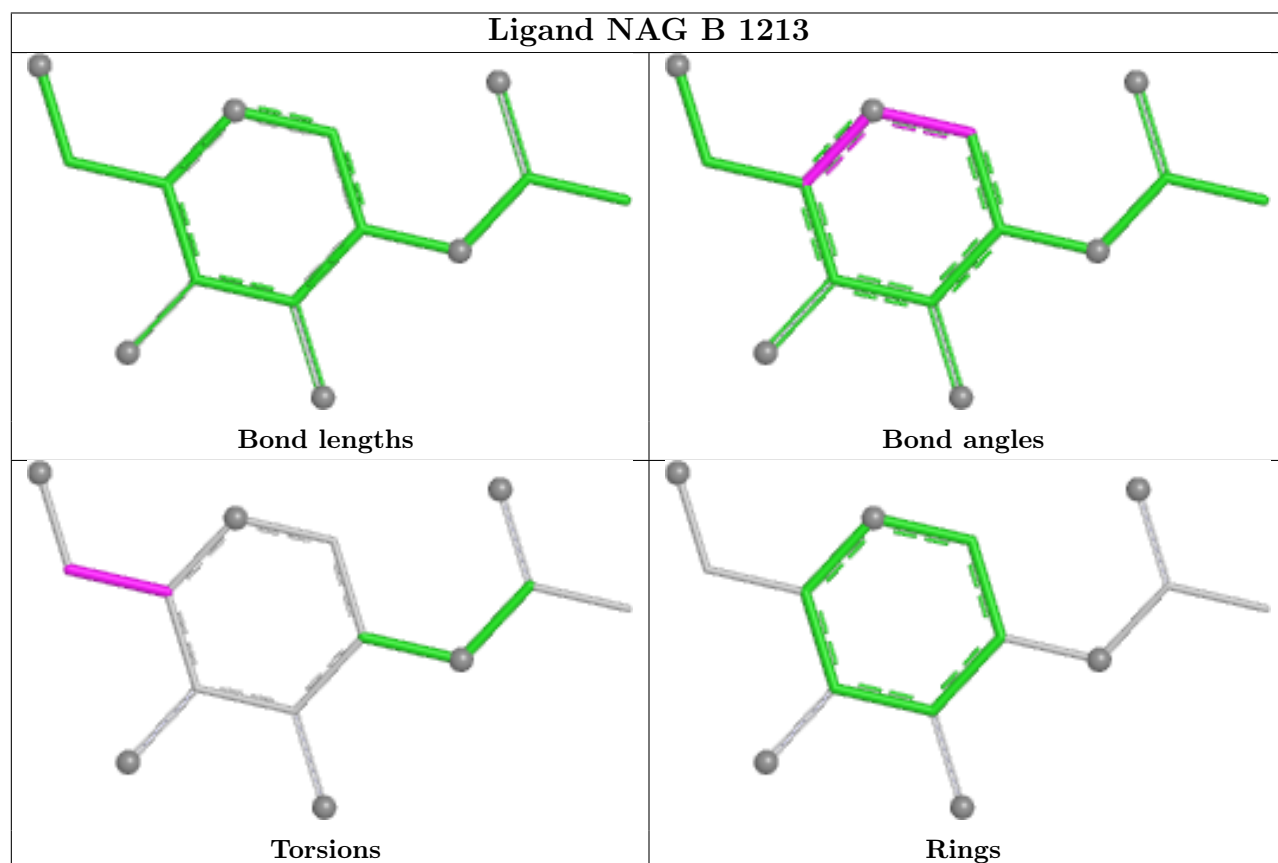
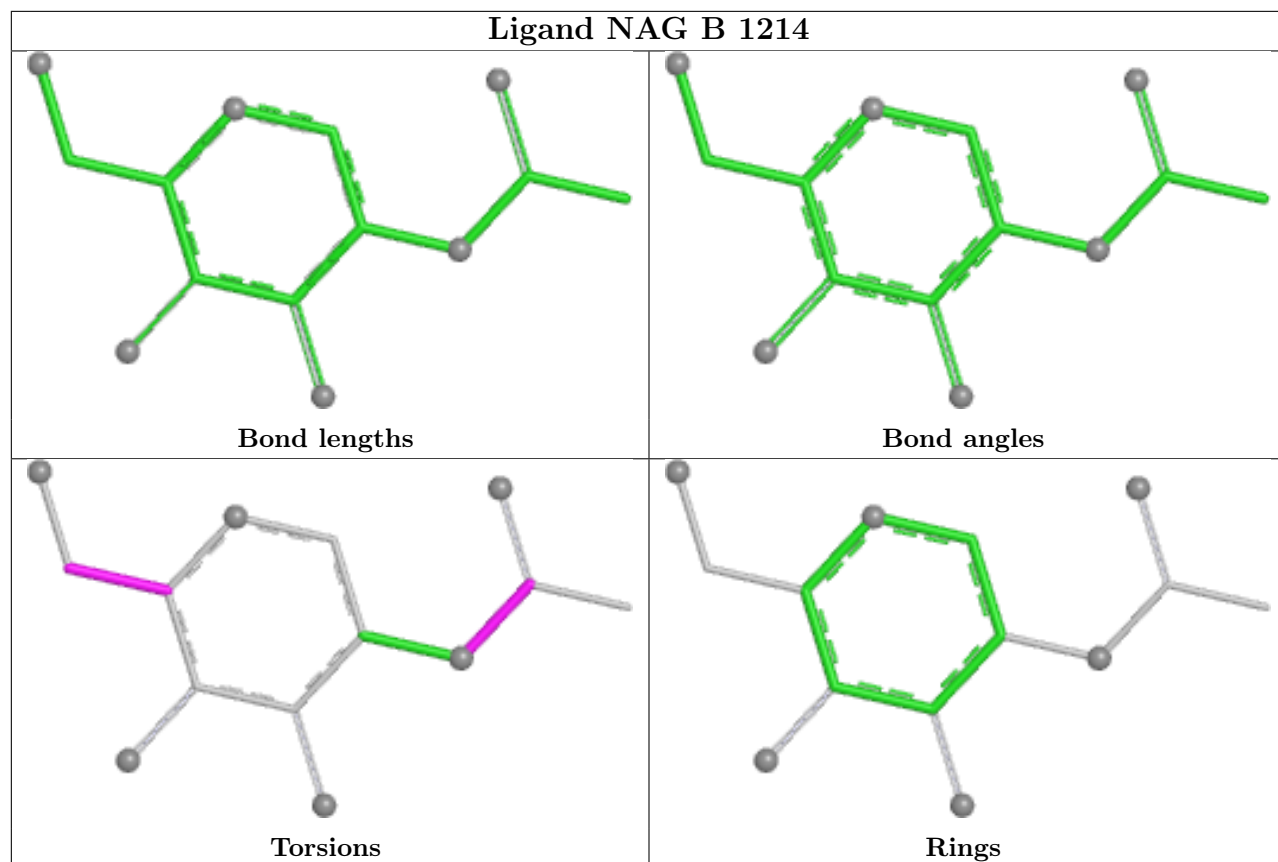


## Ligand NAG B 1201



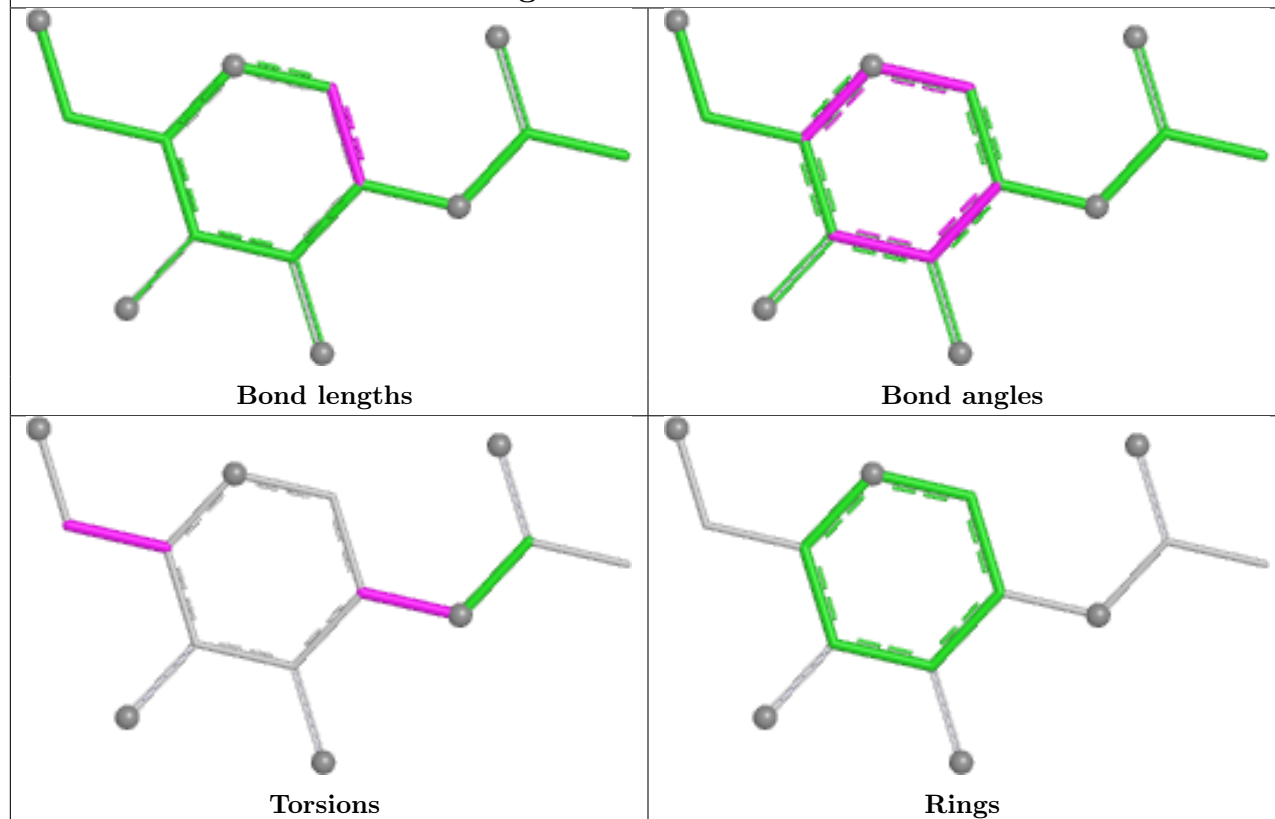
## Ligand NAG C 1212



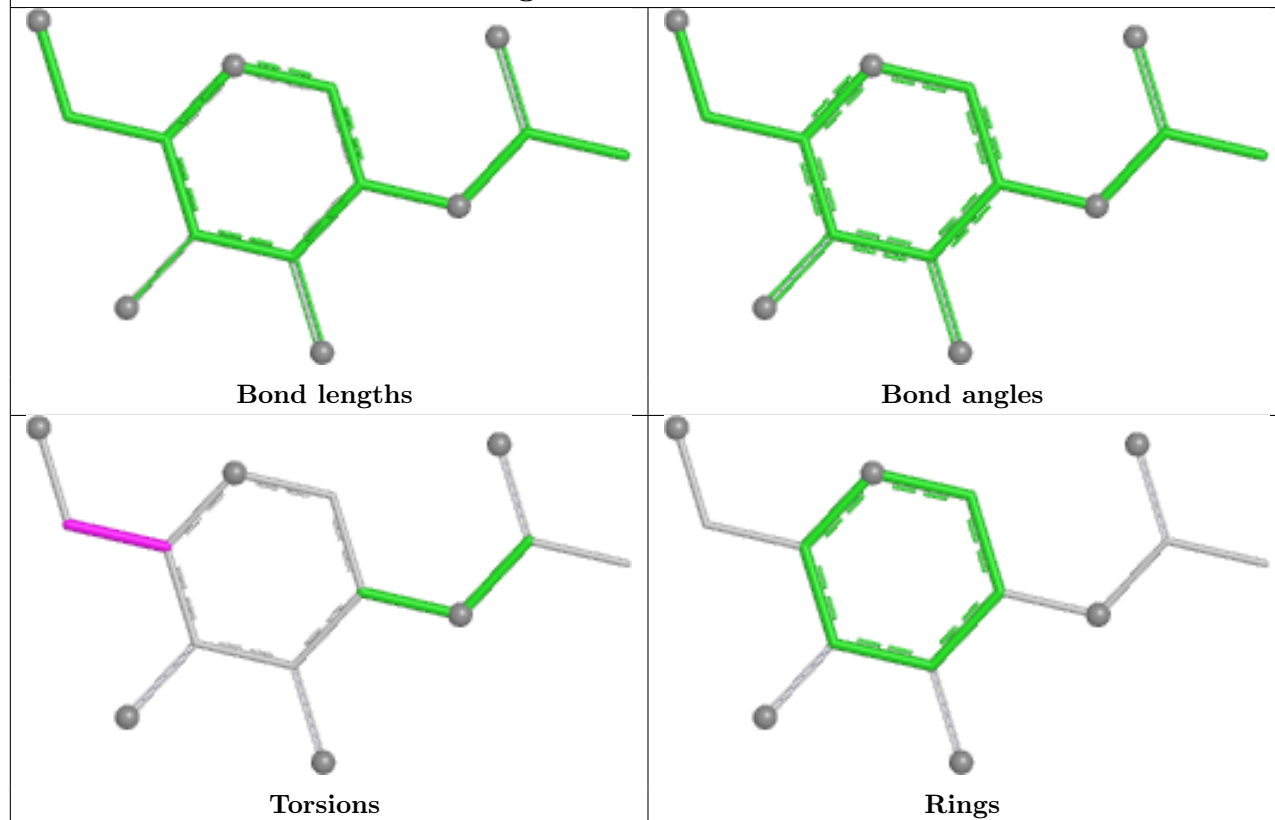


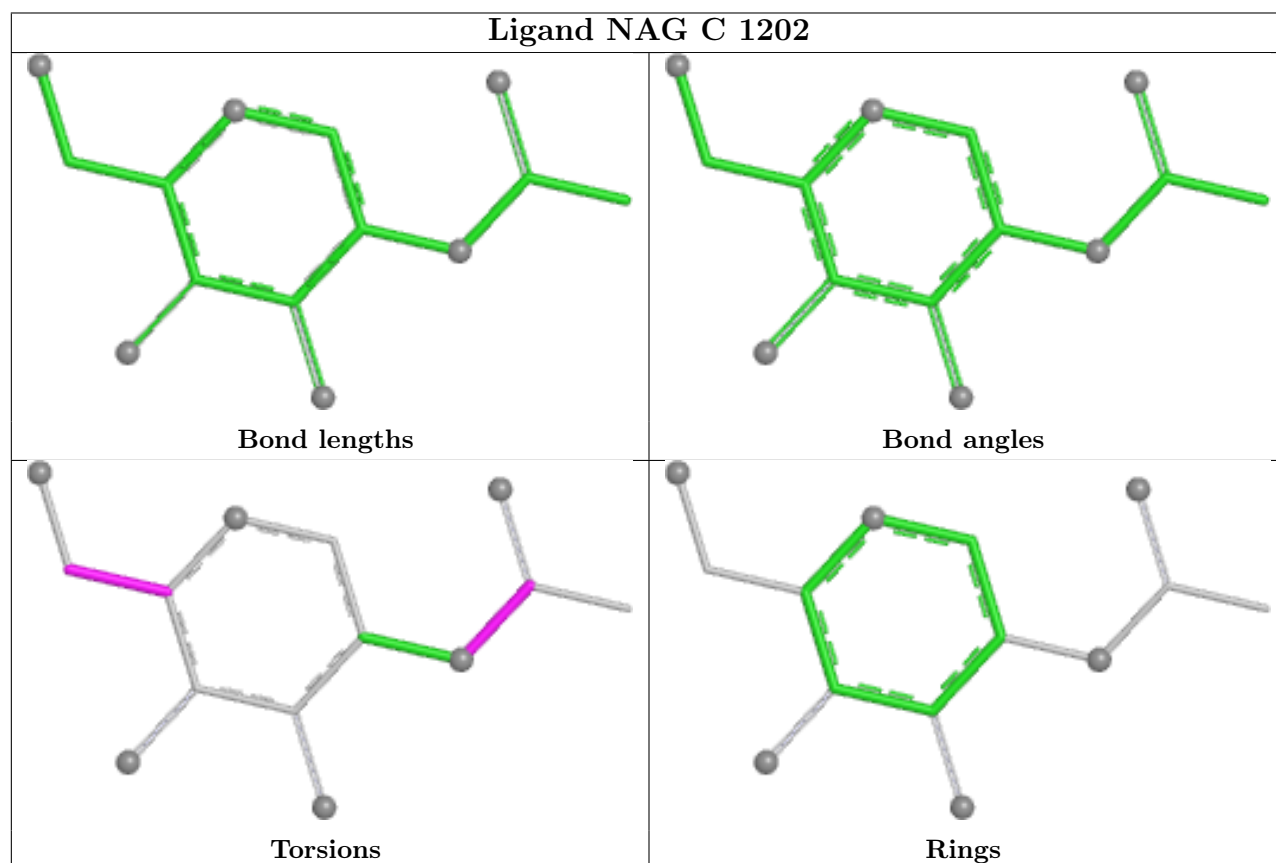
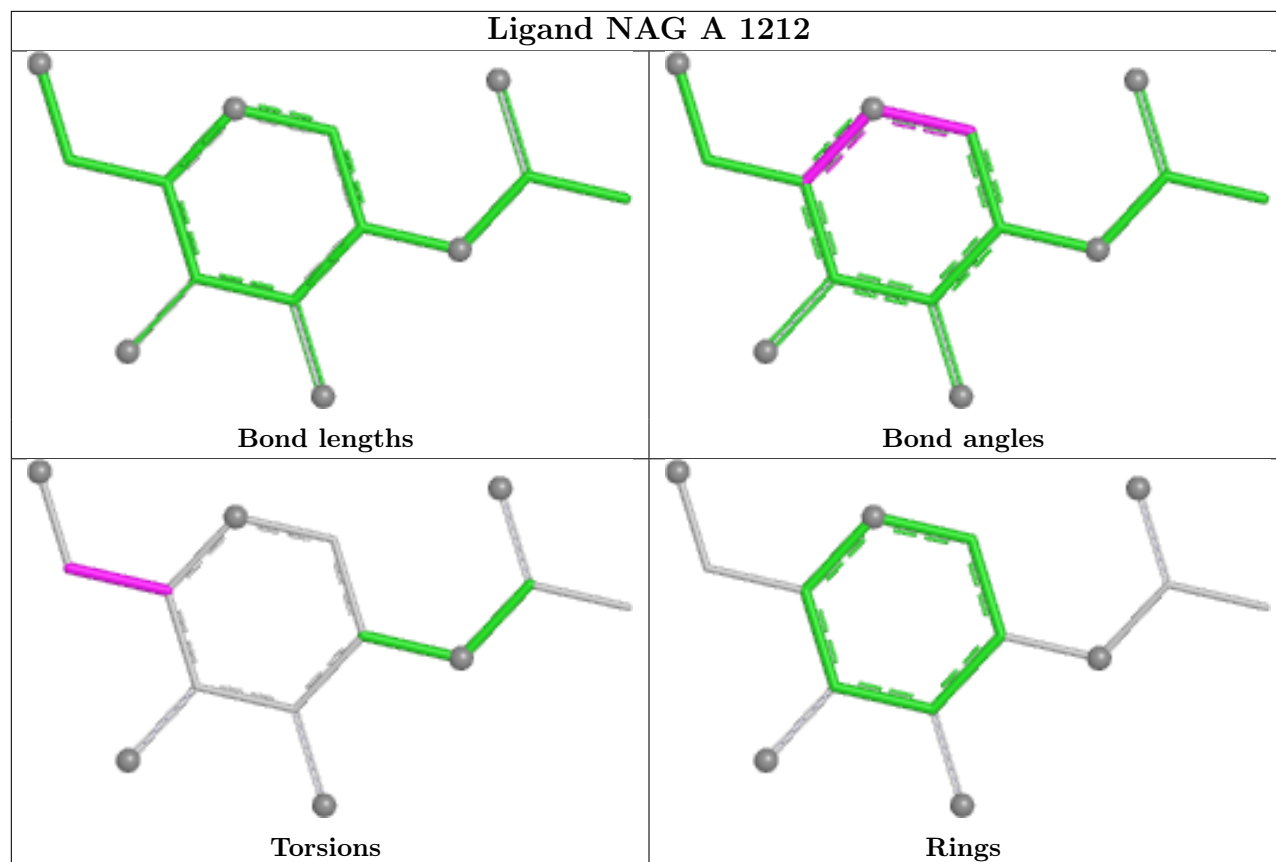


## Ligand NAG B 1210

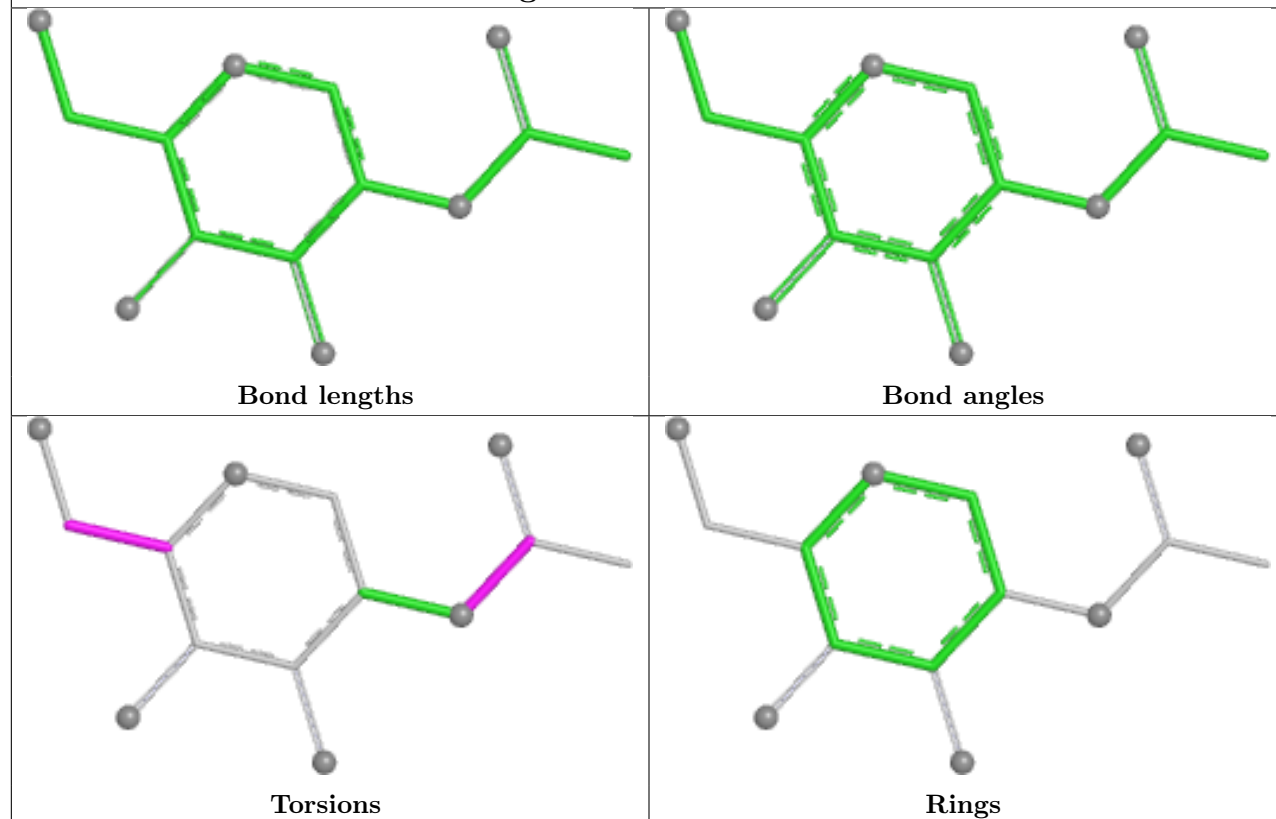


## Ligand NAG A 1211

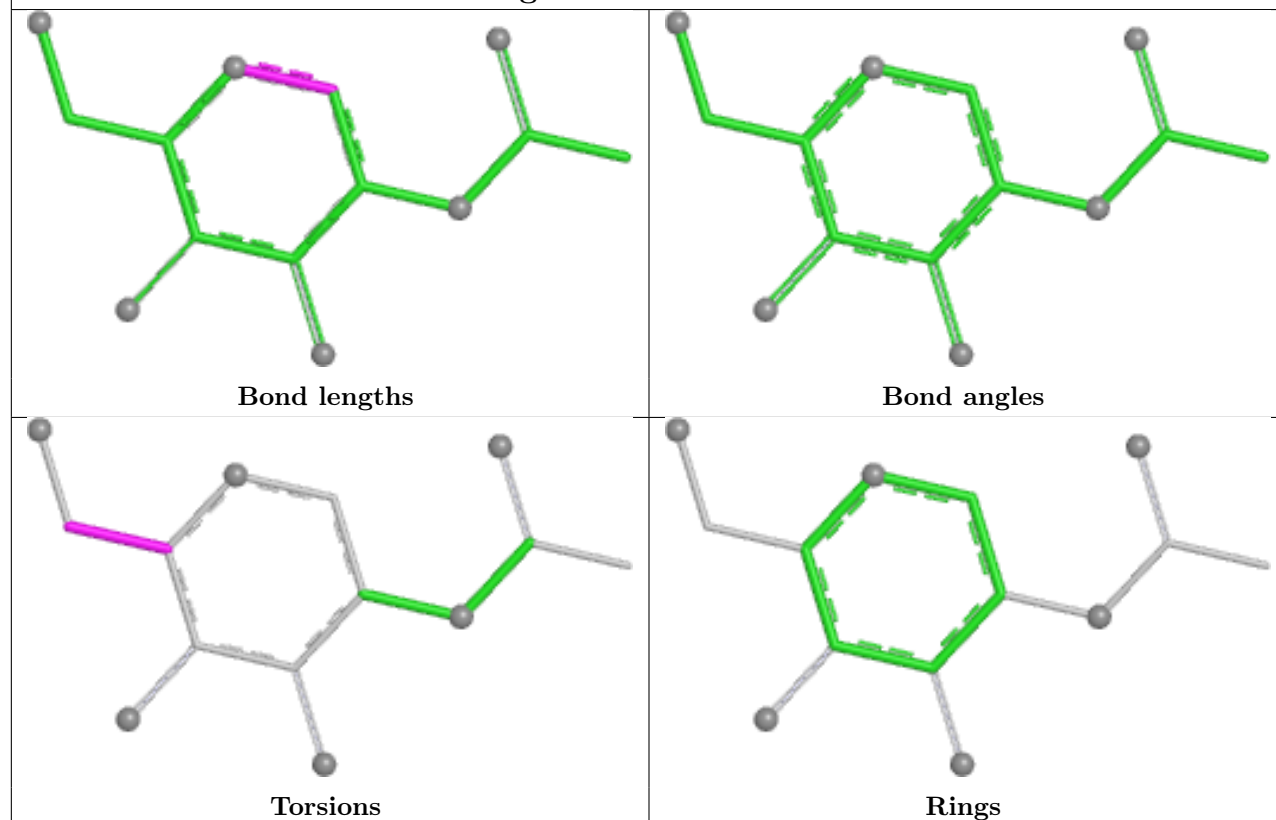




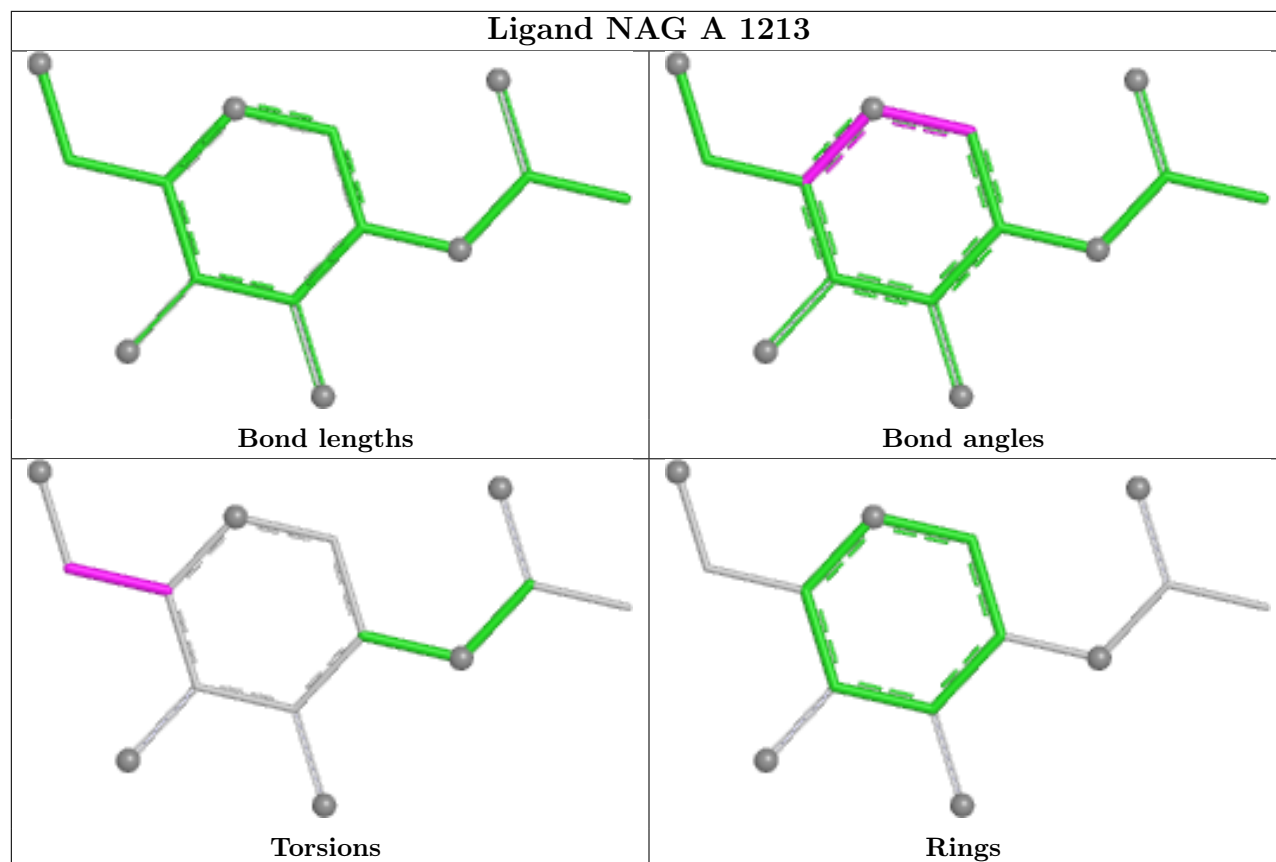
## Ligand NAG C 1203



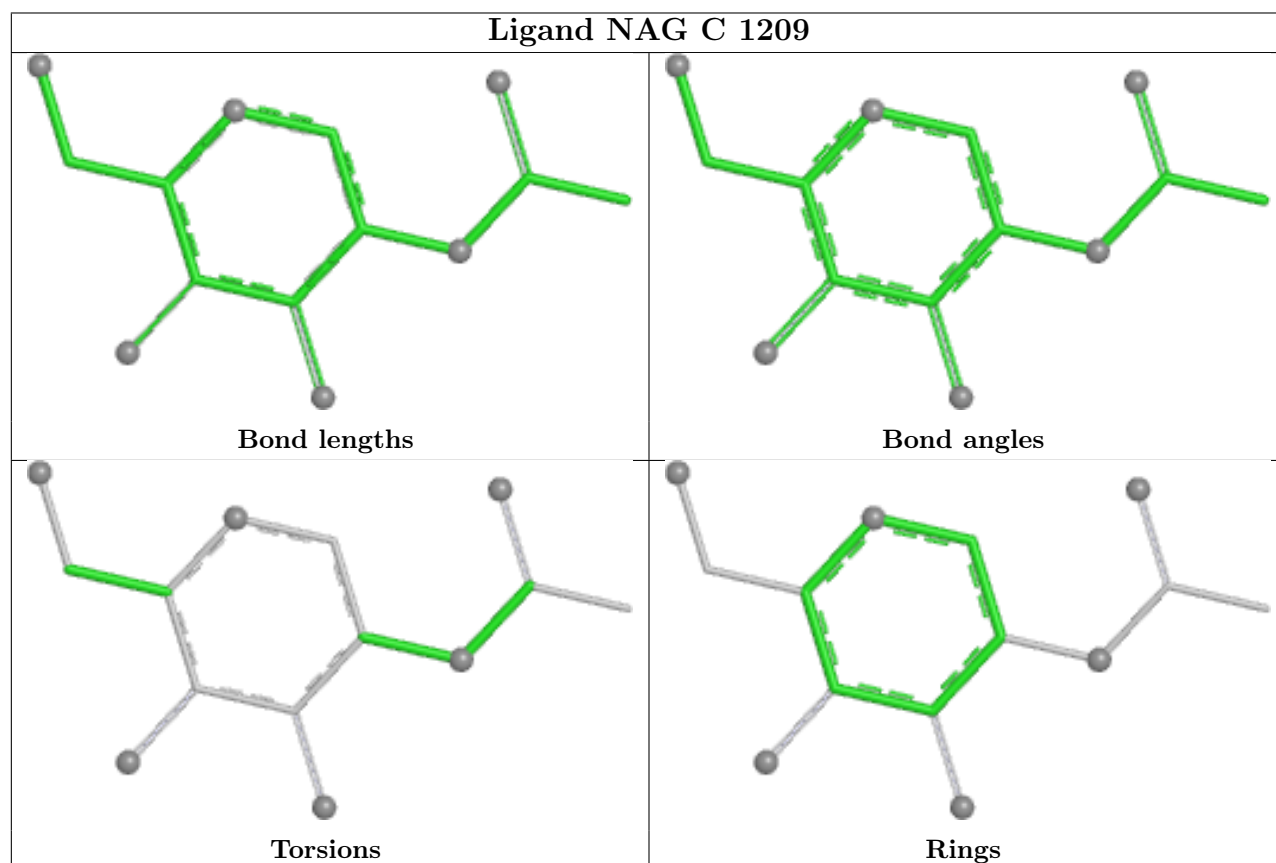
## Ligand NAG B 1208



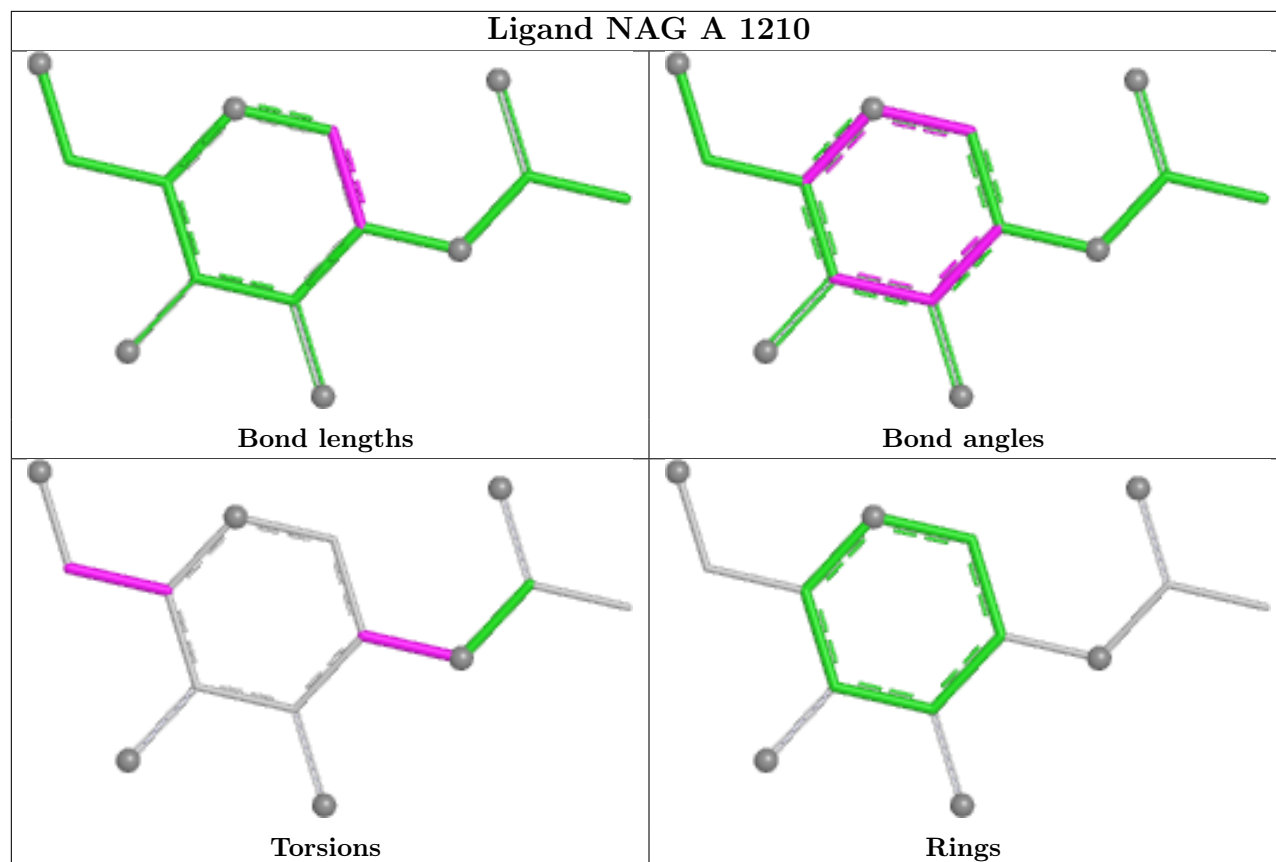
## Ligand NAG A 1213



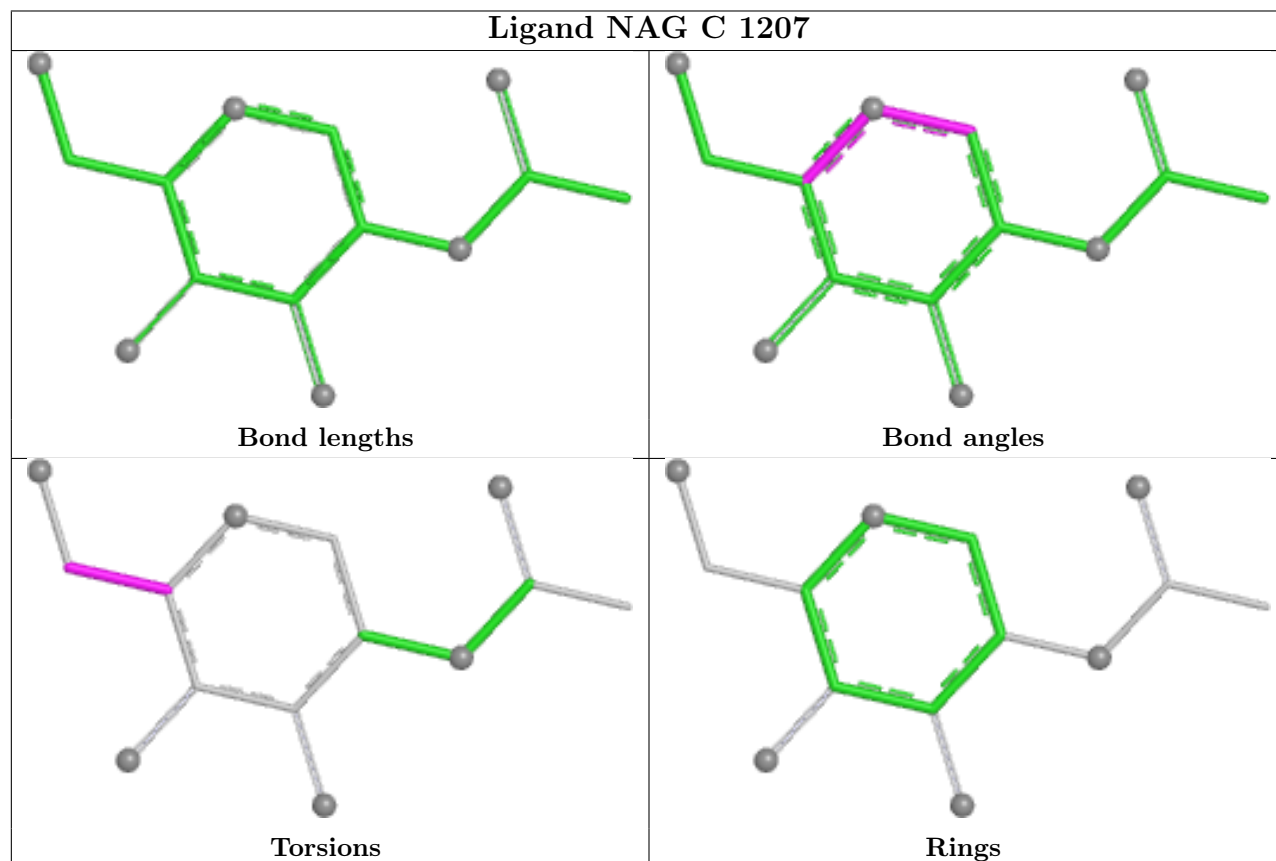
## Ligand NAG C 1209

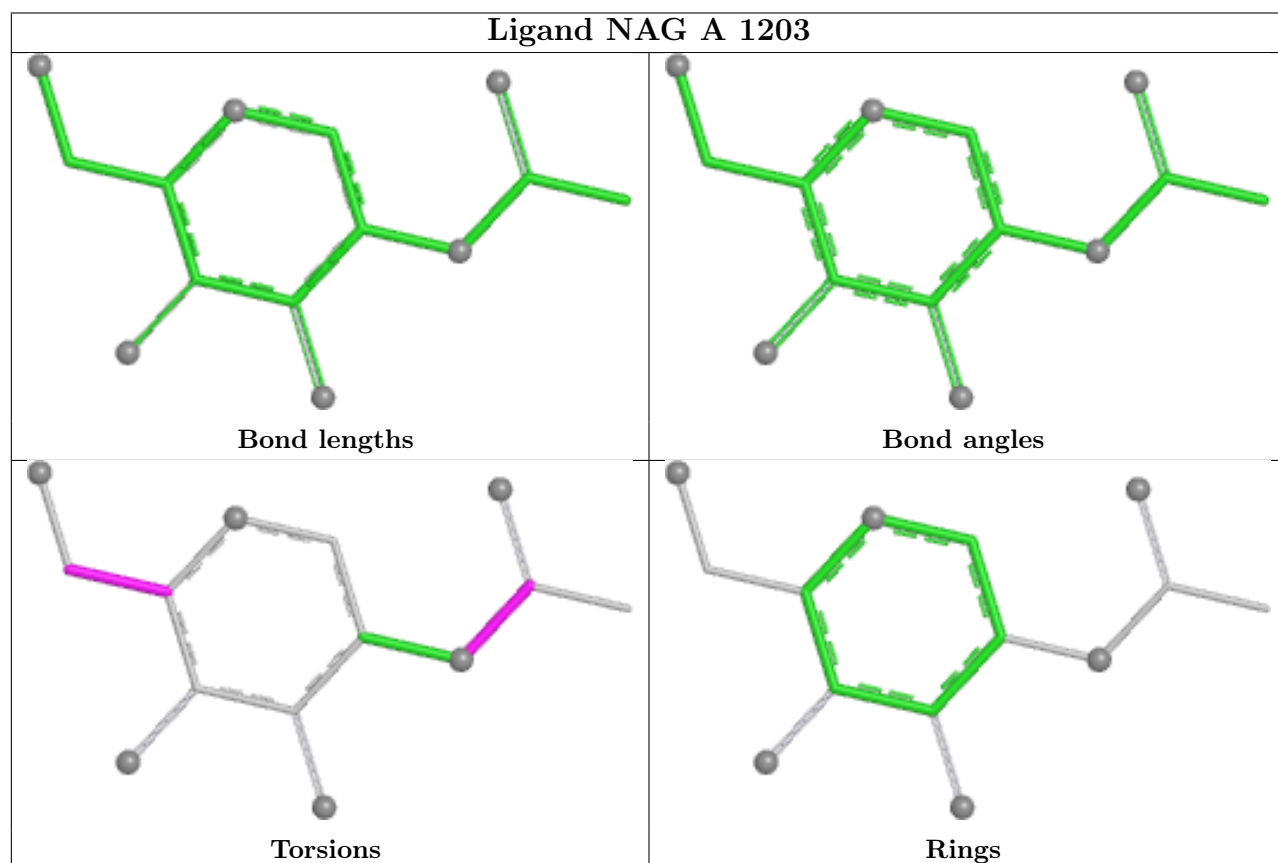
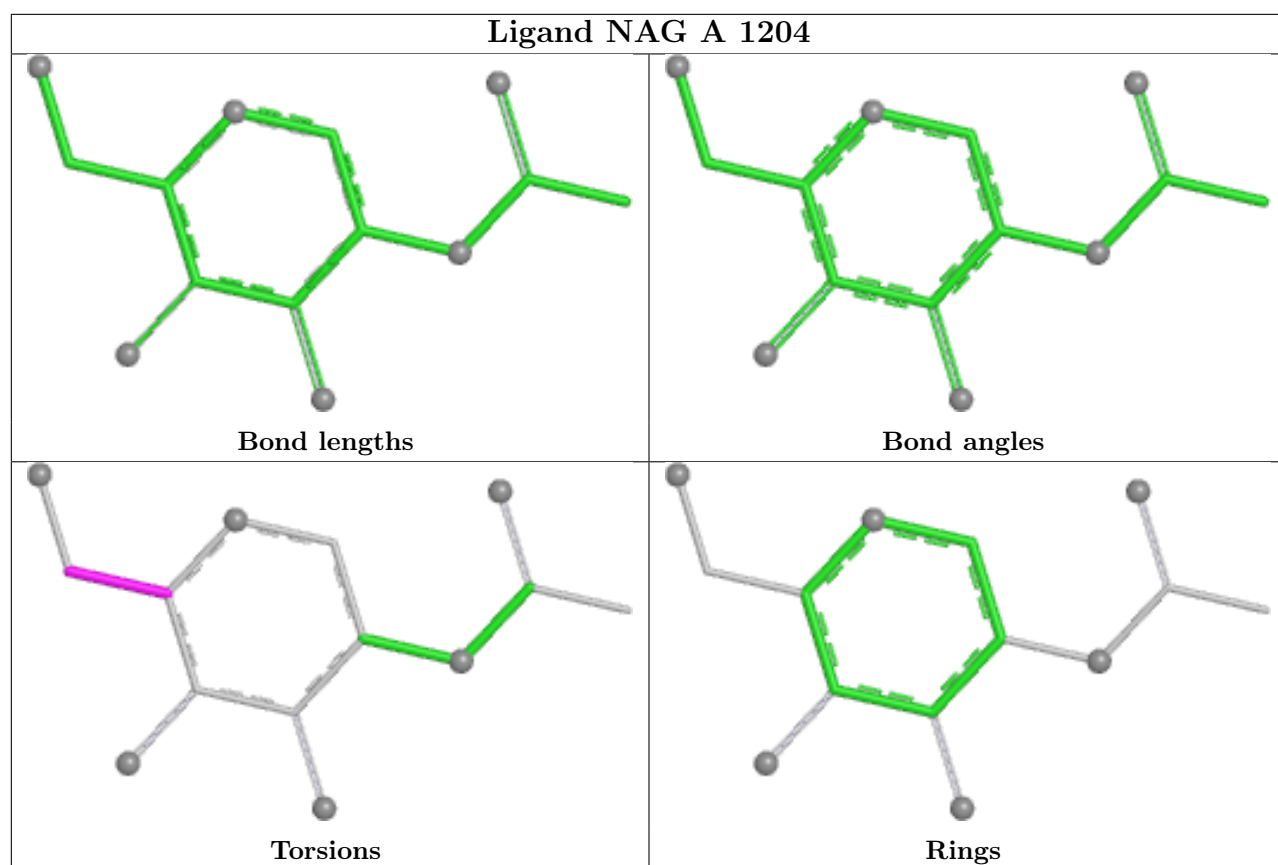


## Ligand NAG A 1210

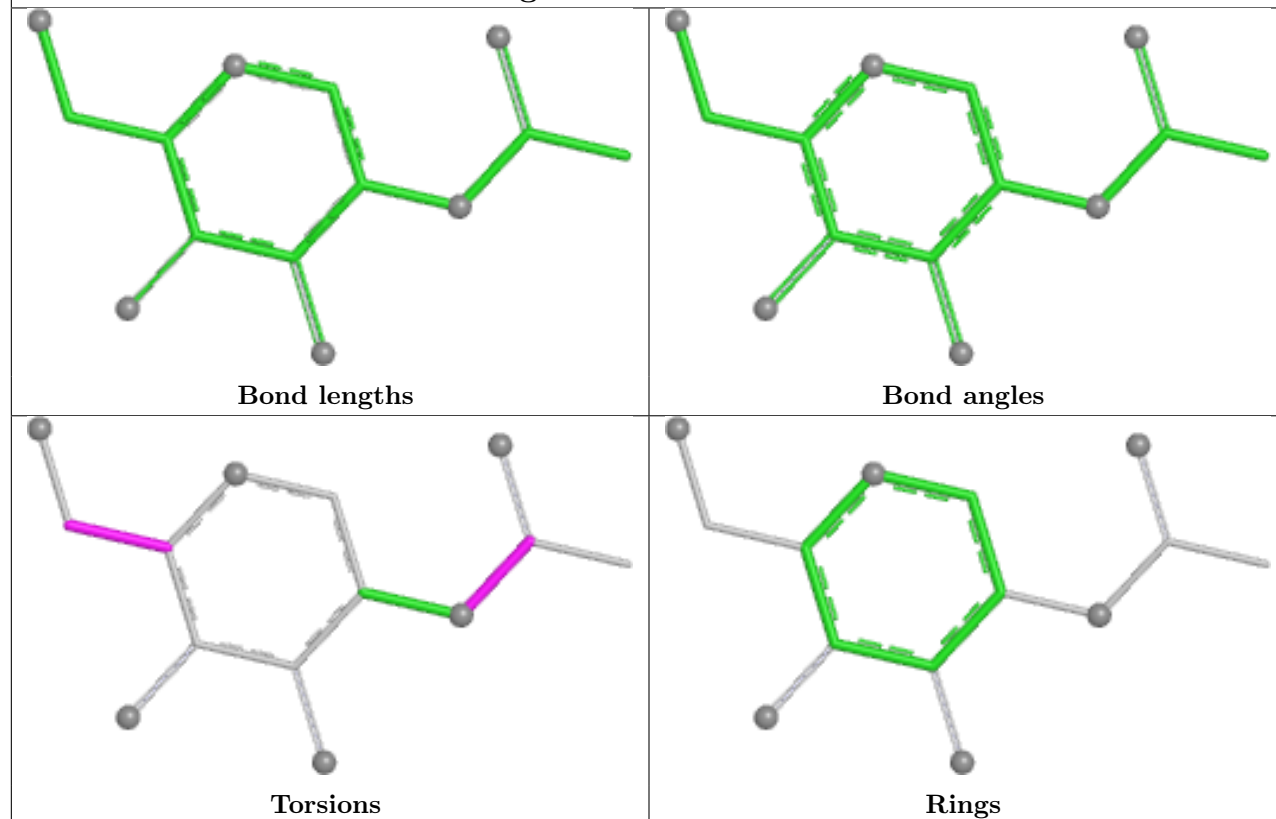


## Ligand NAG C 1207

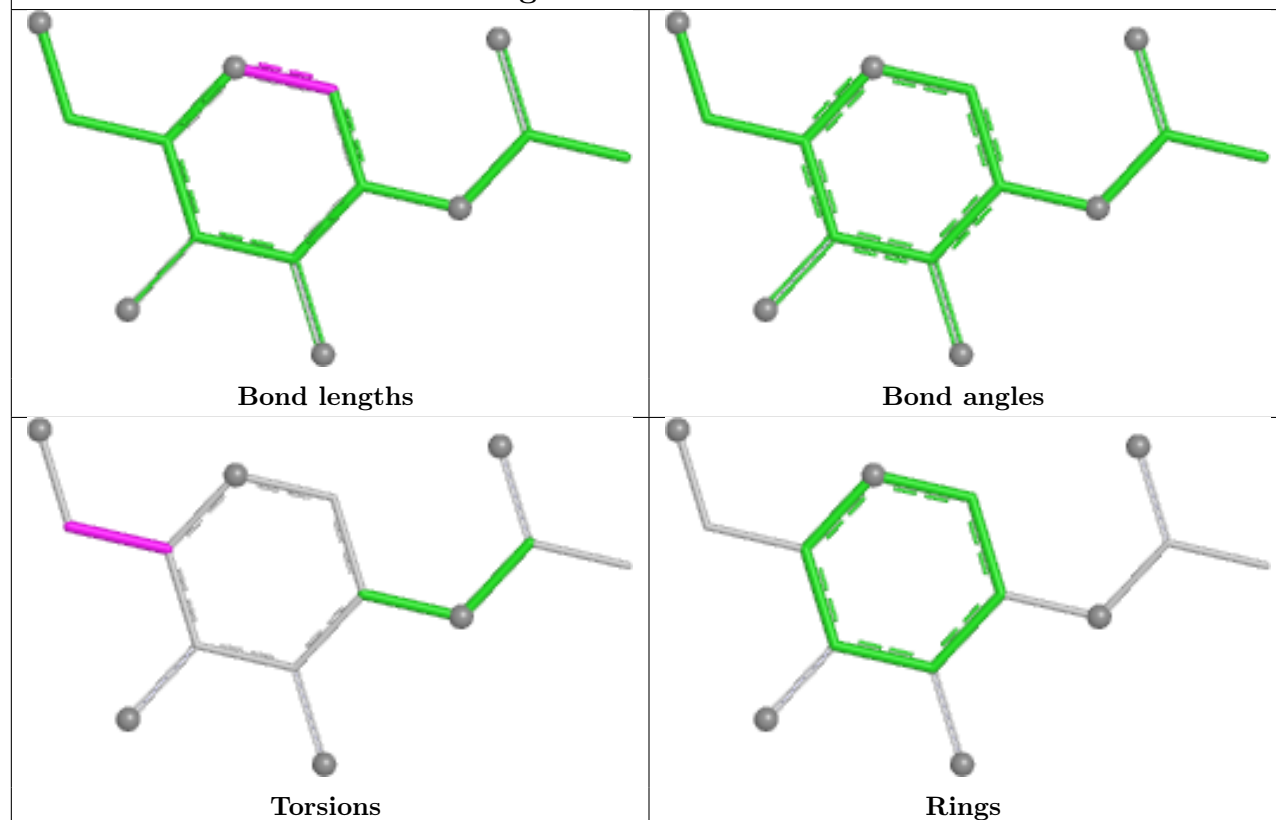




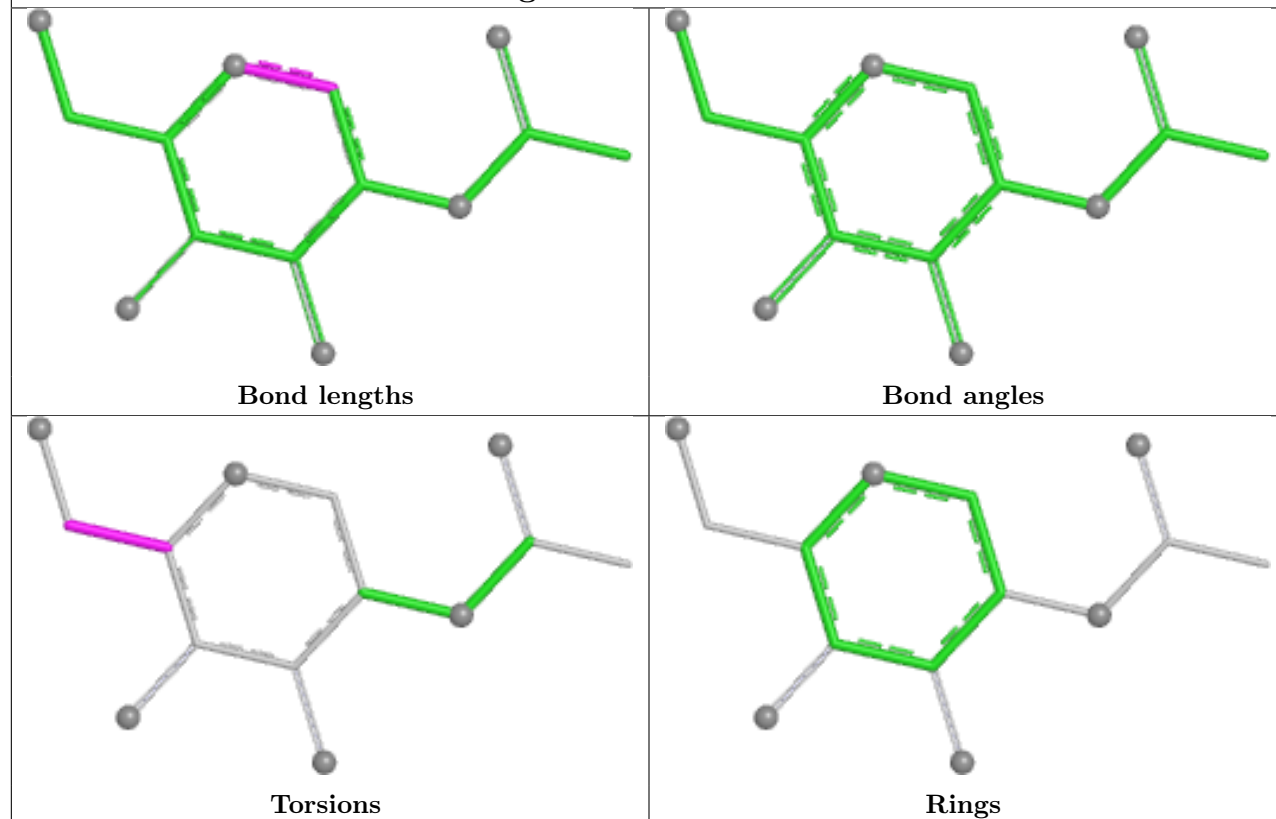
## Ligand NAG B 1202



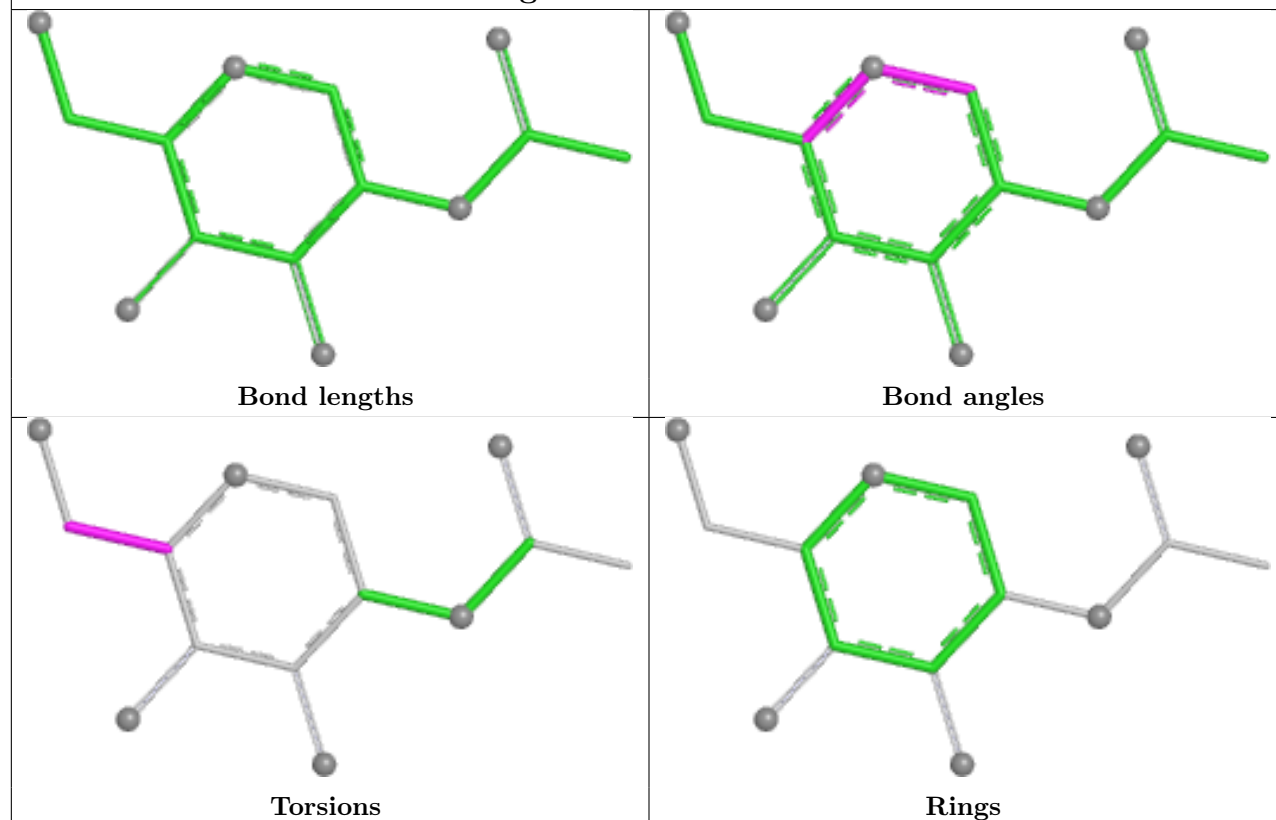
## Ligand NAG C 1208



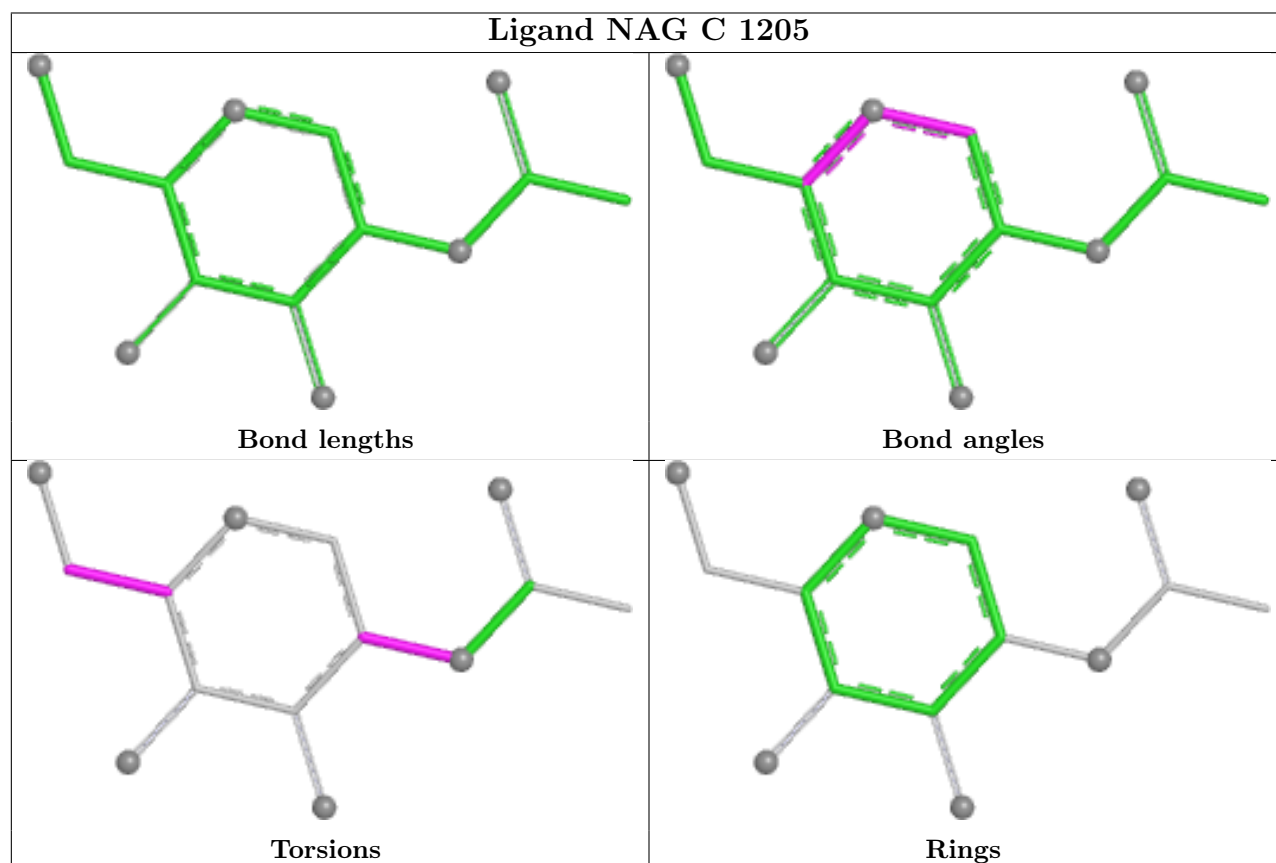
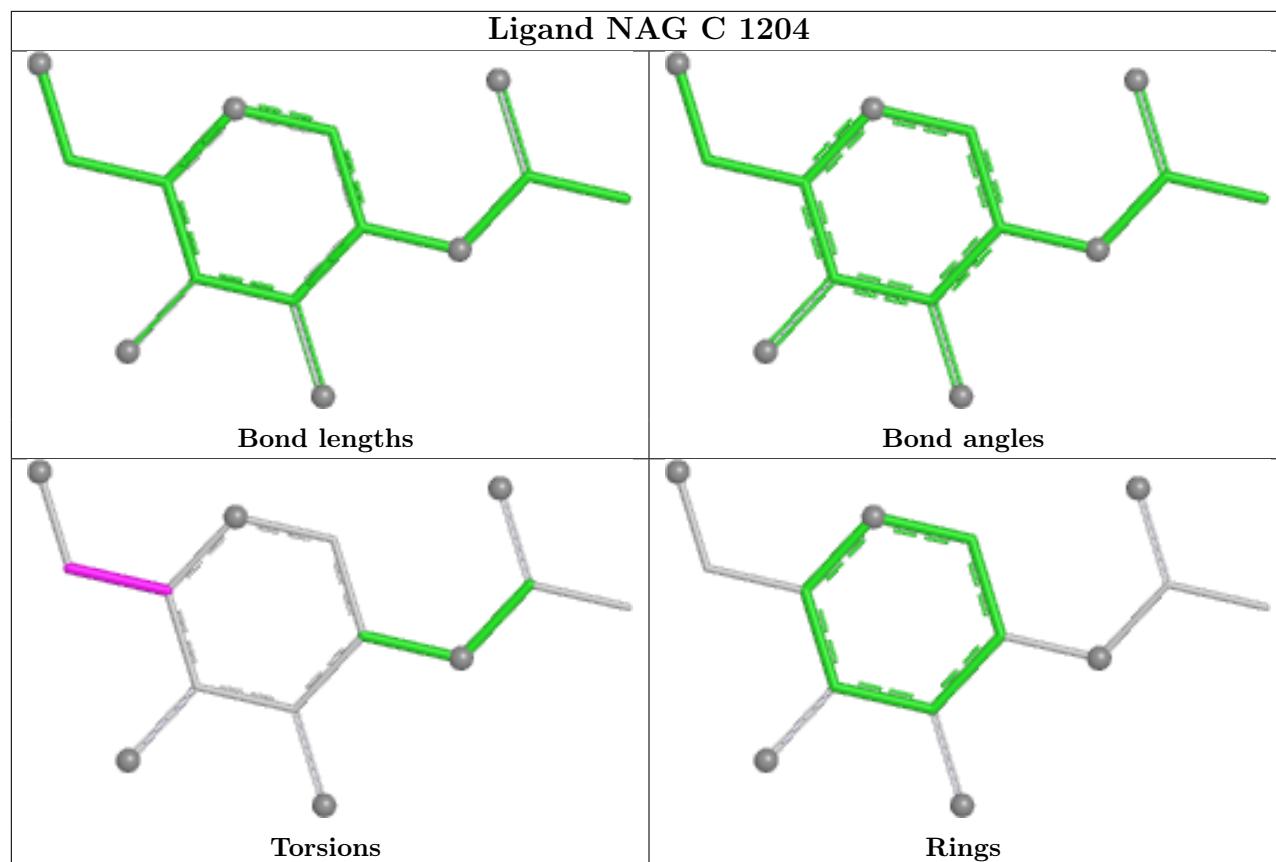
## Ligand NAG A 1201

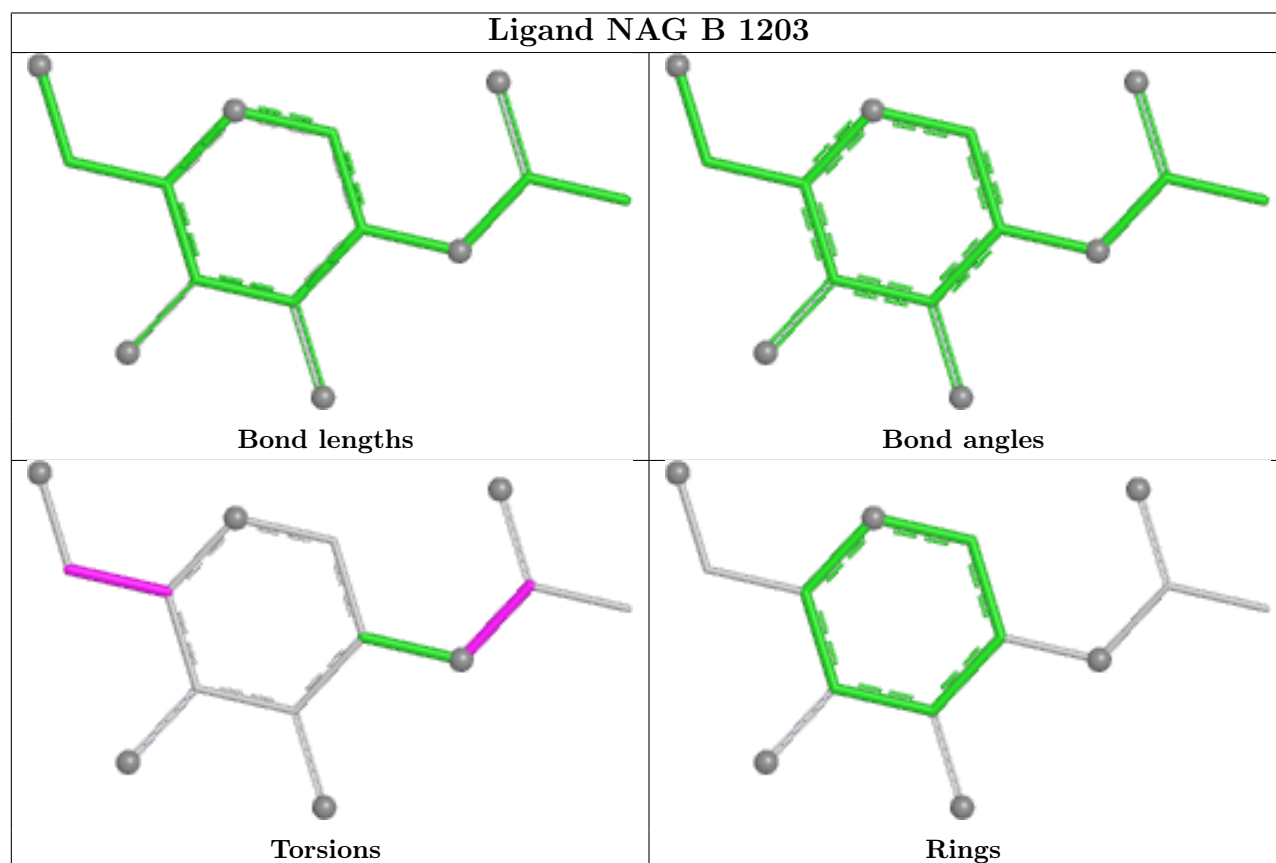
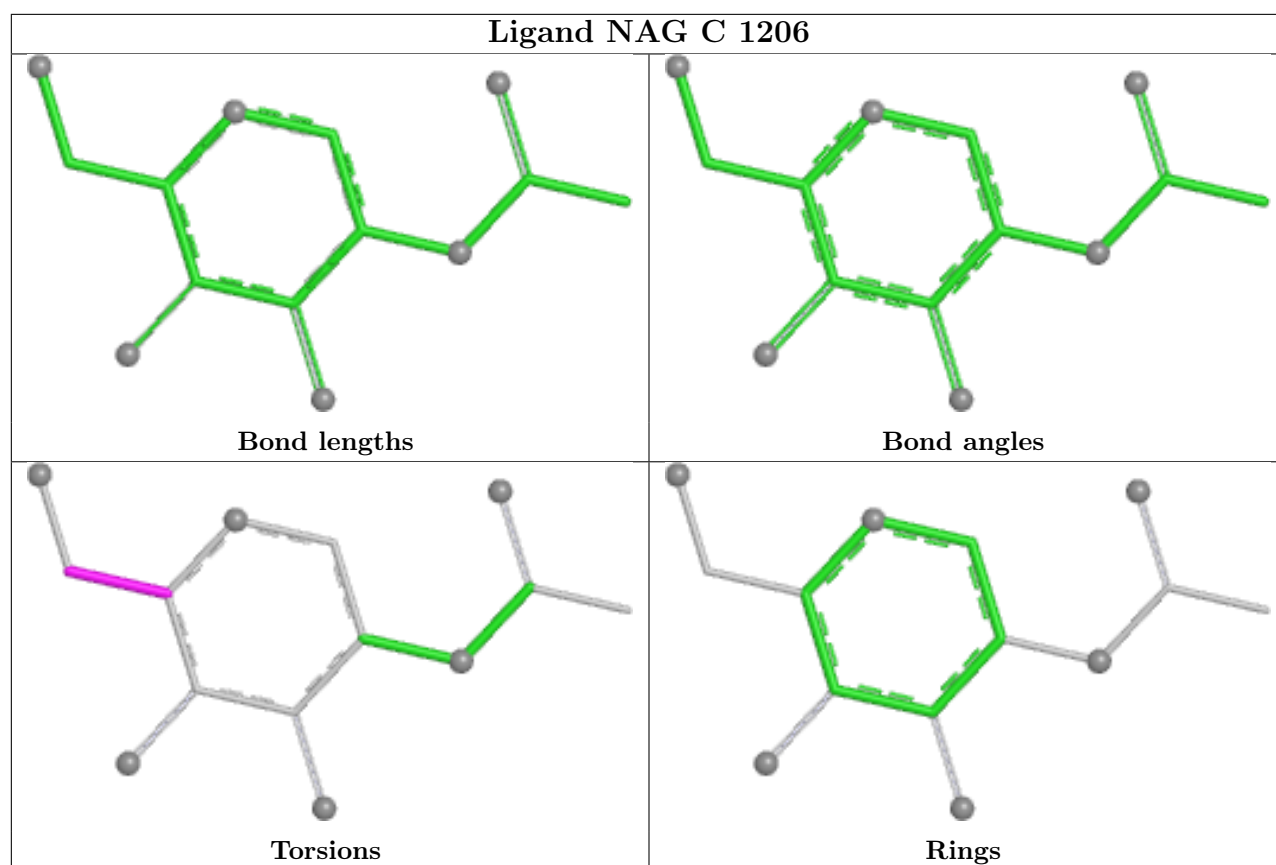


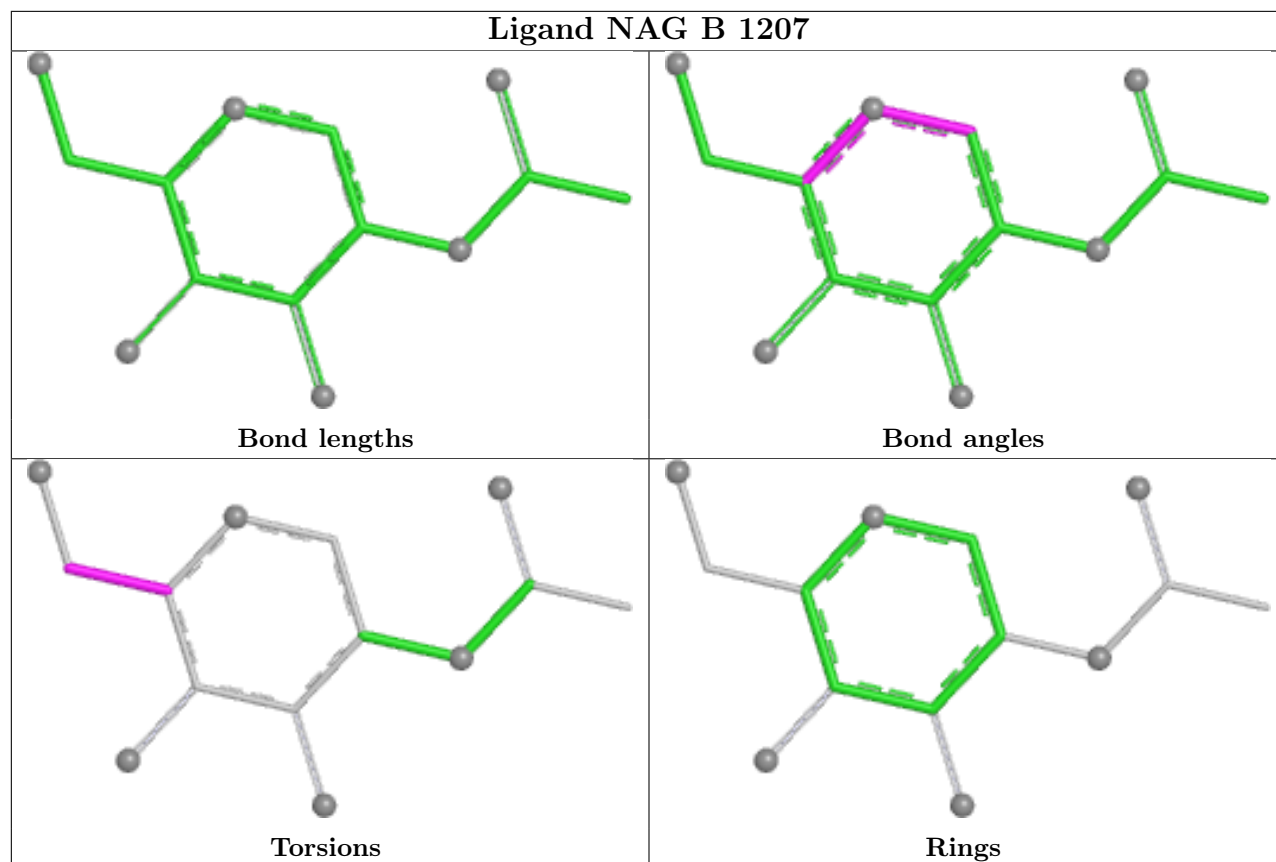
## Ligand NAG B 1212











## 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.

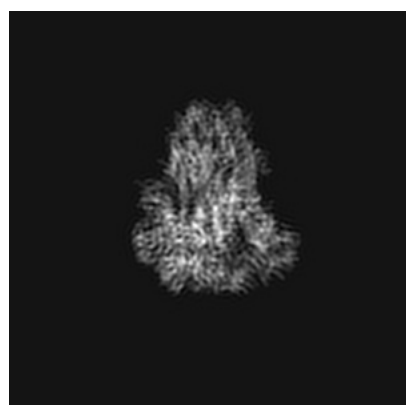
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30497. These allow visual inspection of the internal detail of the map and identification of artifacts.

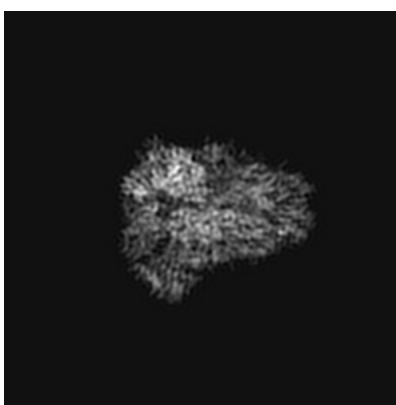
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

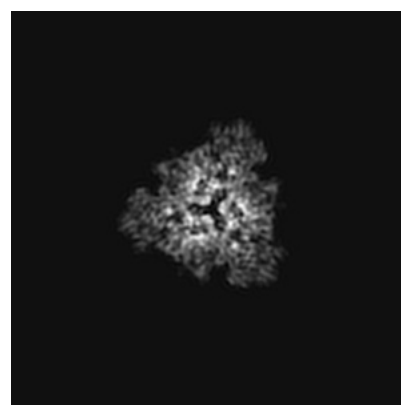
#### 6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 110



Y Index: 96

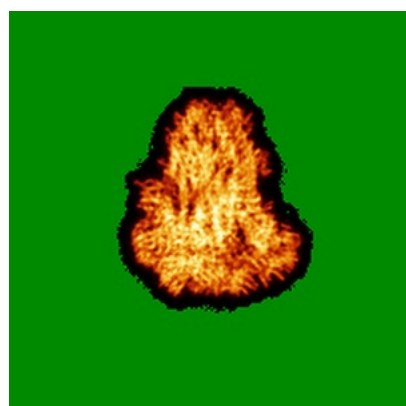


Z Index: 85

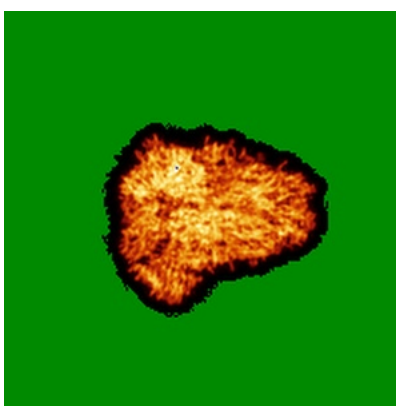
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

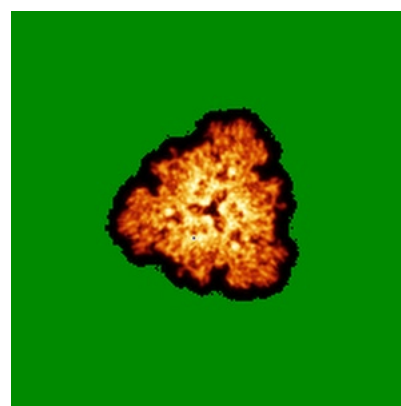
### 6.4.1 Primary map



X



Y

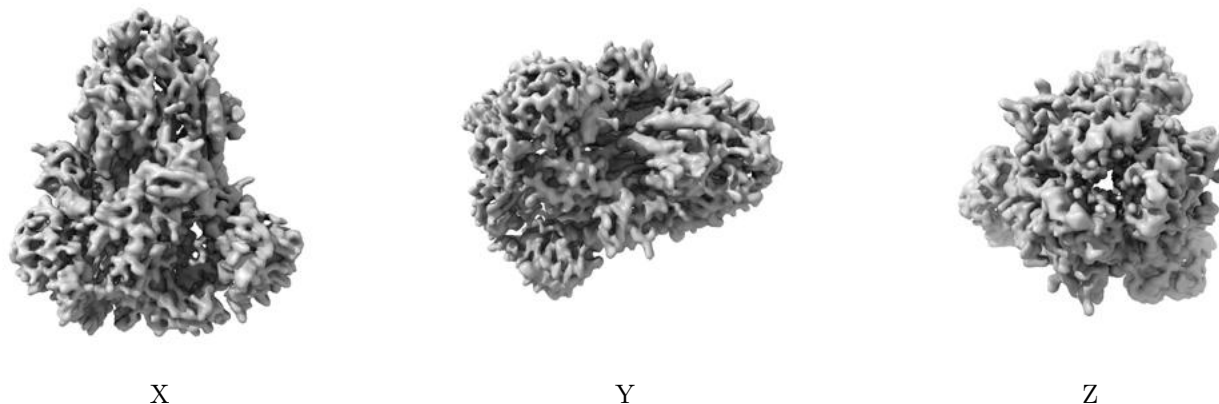


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

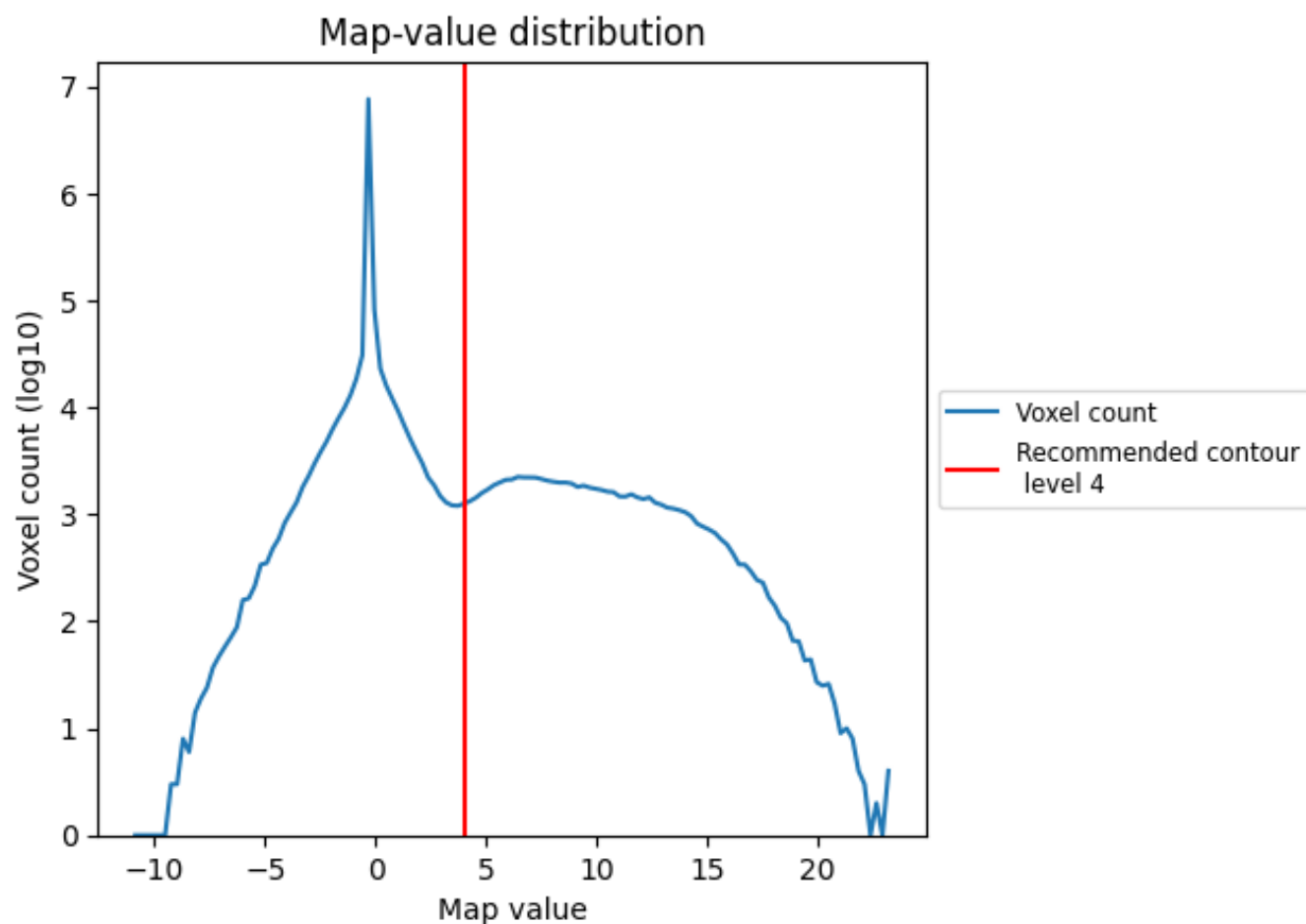
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

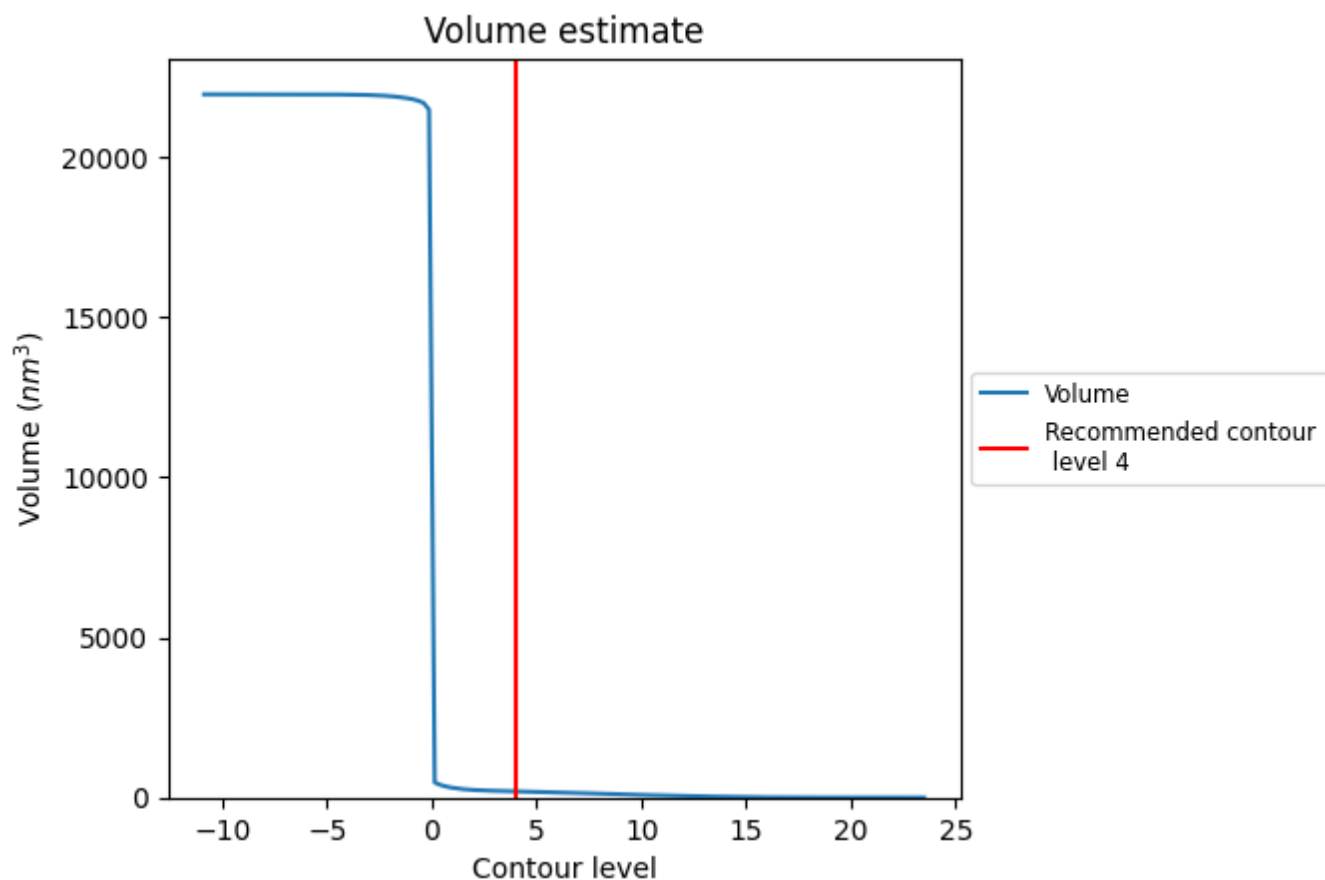
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

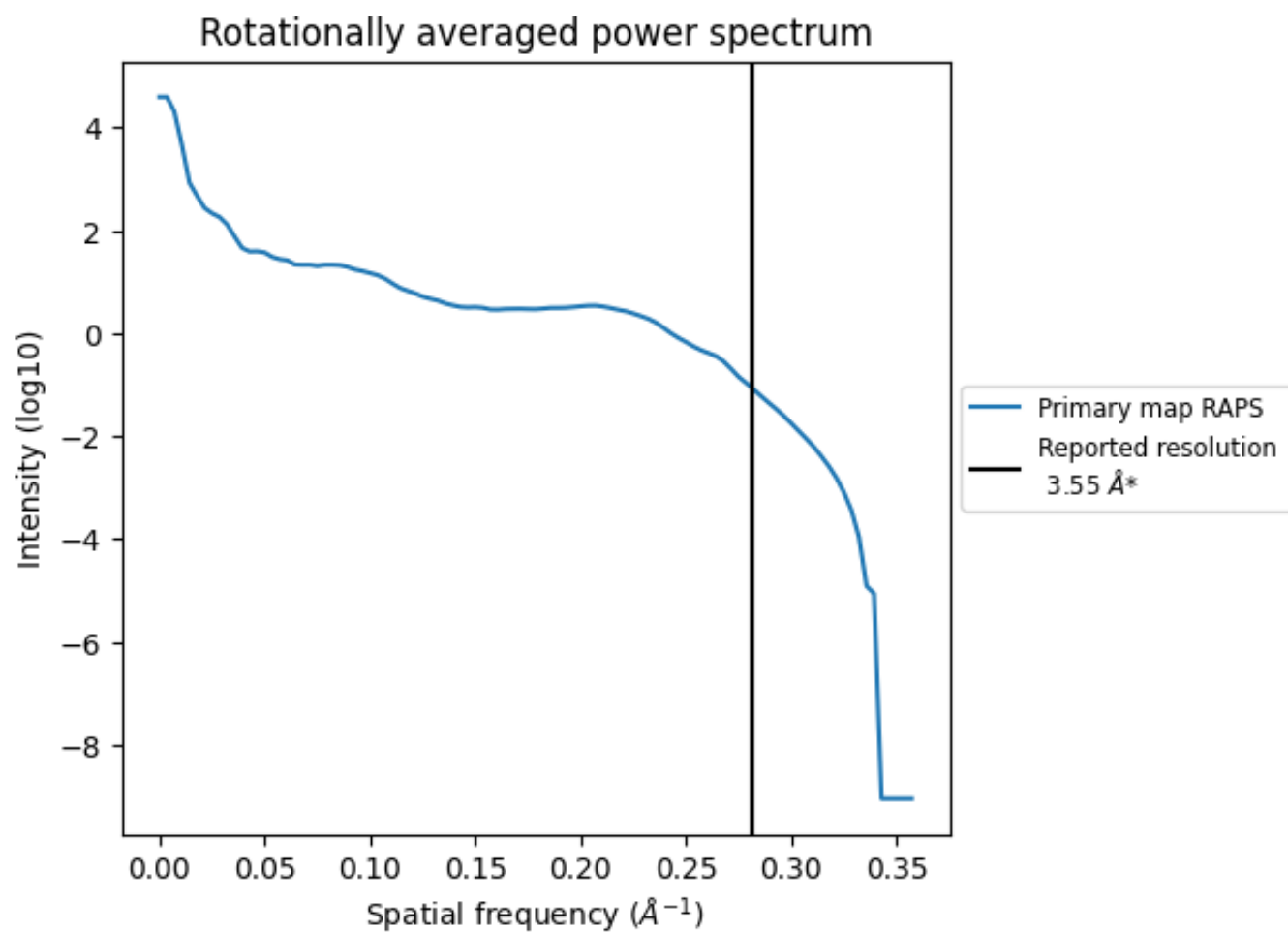


The volume at the recommended contour level is 198 nm<sup>3</sup>; this corresponds to an approximate mass of 179 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.282 Å<sup>-1</sup>

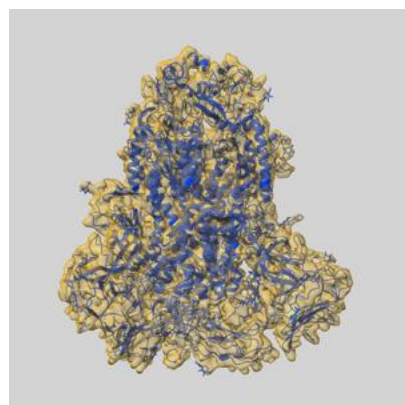
## 8 Fourier-Shell correlation

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

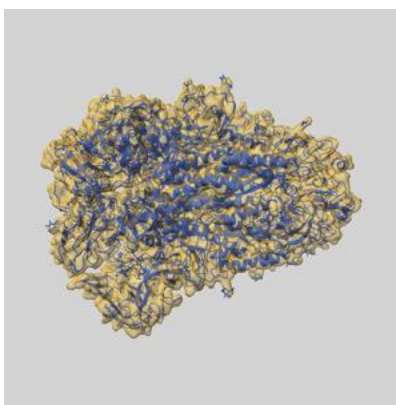
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30497 and PDB model 7CYD. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

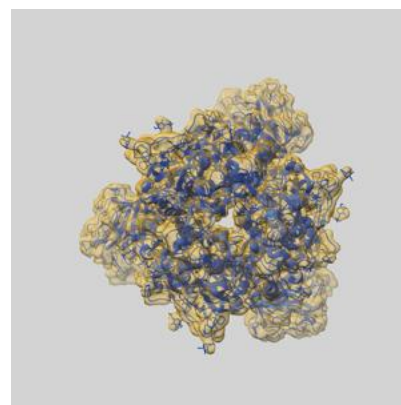
### 9.1 Map-model overlay [i](#)



X



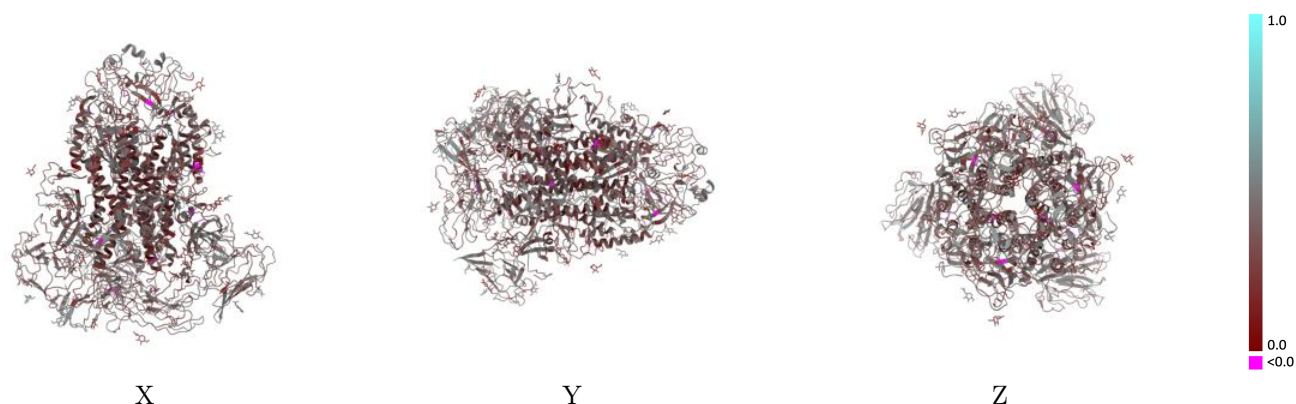
Y



Z

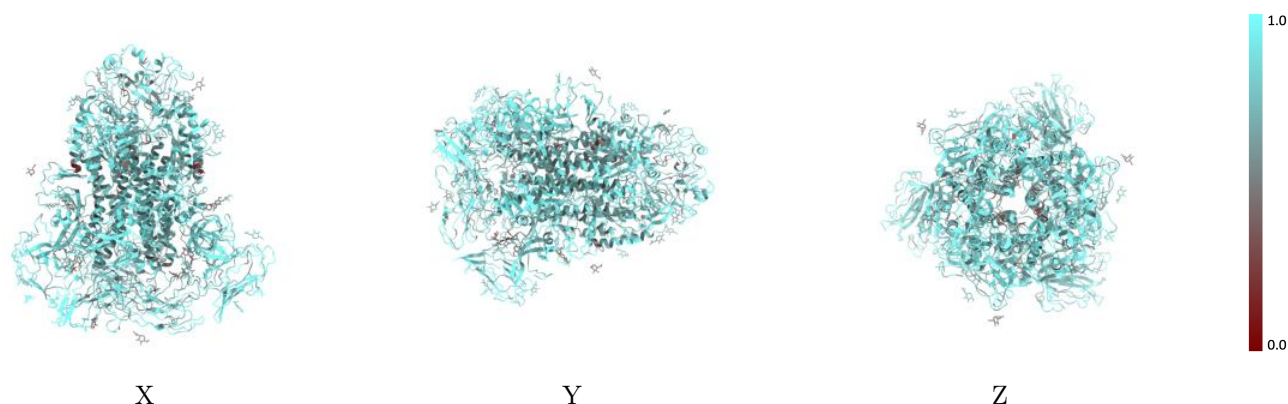
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



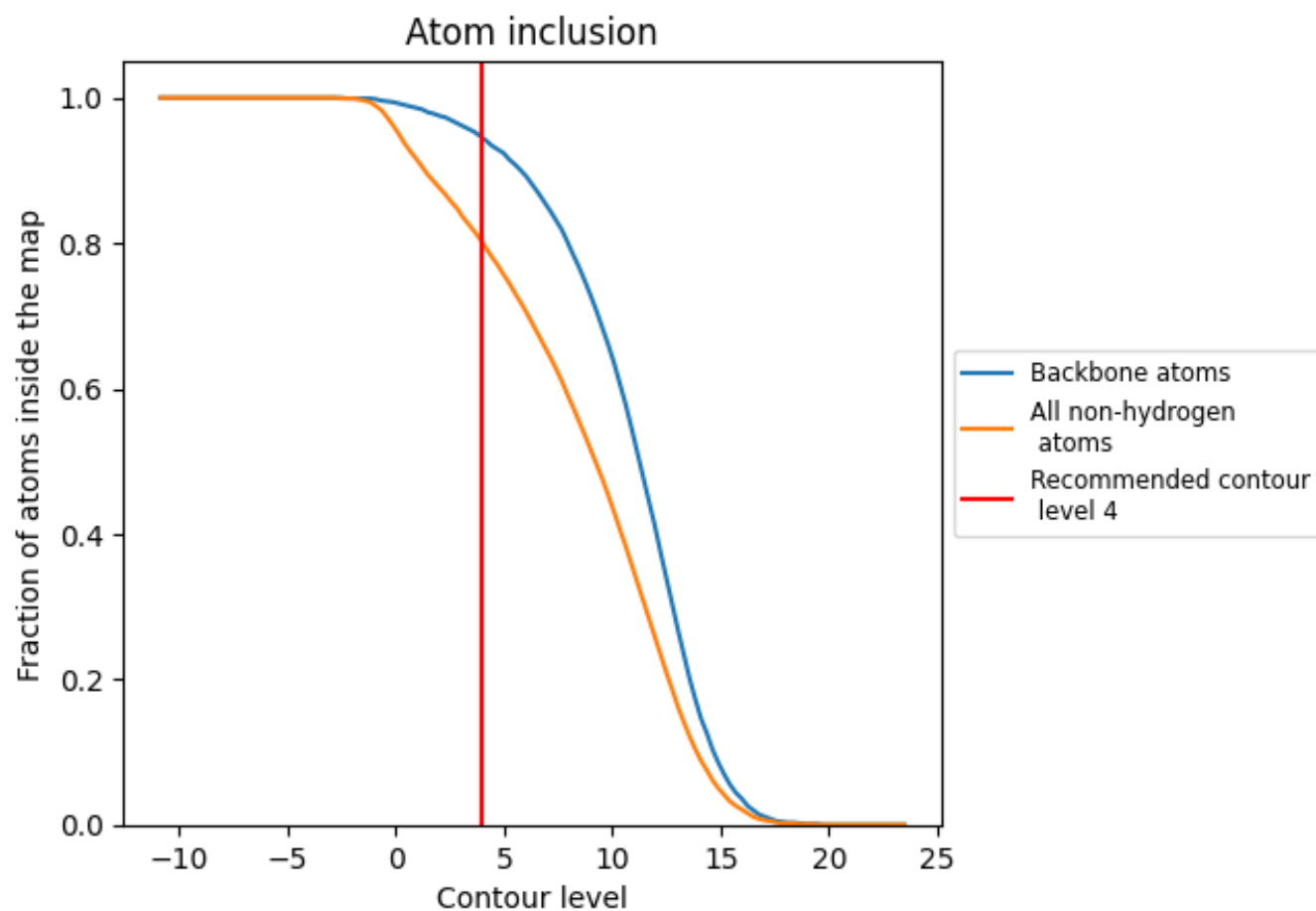
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8010 | <div></div> 0.3610 |
| A     | <div></div> 0.8050 | <div></div> 0.3650 |
| B     | <div></div> 0.8060 | <div></div> 0.3610 |
| C     | <div></div> 0.8070 | <div></div> 0.3610 |
| D     | <div></div> 0.5300 | <div></div> 0.2830 |
| E     | <div></div> 0.4870 | <div></div> 0.2430 |
| F     | <div></div> 0.4700 | <div></div> 0.2670 |
| G     | <div></div> 0.4870 | <div></div> 0.2380 |
| H     | <div></div> 0.5180 | <div></div> 0.2860 |
| I     | <div></div> 0.5130 | <div></div> 0.2510 |

