



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:42 AM UTC

PDB ID : 7CZP / pdb\_00007czp  
EMDB ID : EMD-30512  
Title : S protein of SARS-CoV-2 in complex bound with P2B-1A1  
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Zhou, Q.  
Deposited on : 2020-09-09  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

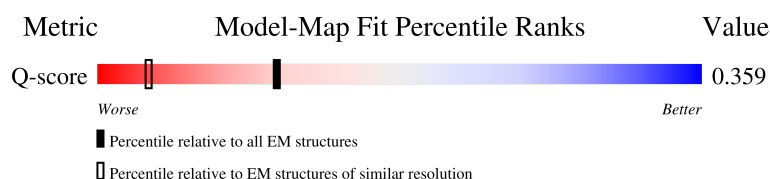
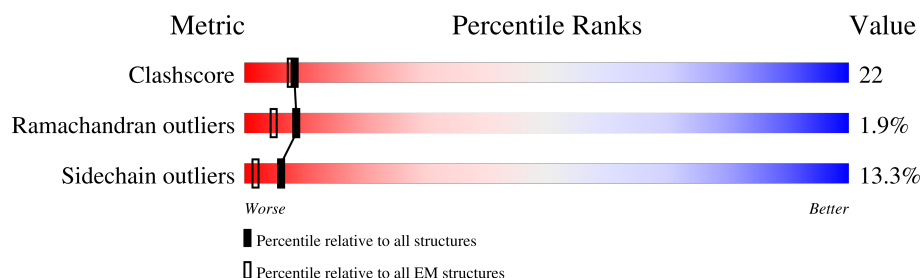
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.00 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                       | 14081 ( 2.50 - 3.50 )                                    |

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     | 1283   |  |
| 1   | B     | 1283   |  |
| 1   | C     | 1283   |  |
| 2   | H     | 450    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | J     | 450    |                  |
| 3   | L     | 216    |                  |
| 3   | N     | 216    |                  |
| 4   | D     | 2      |                  |
| 4   | E     | 2      |                  |
| 4   | F     | 2      |                  |
| 4   | G     | 2      |                  |
| 4   | I     | 2      |                  |
| 4   | K     | 2      |                  |
| 4   | M     | 2      |                  |
| 4   | O     | 2      |                  |
| 4   | P     | 2      |                  |
| 4   | Q     | 2      |                  |
| 4   | R     | 2      |                  |
| 4   | S     | 2      |                  |
| 4   | T     | 2      |                  |
| 4   | U     | 2      |                  |
| 4   | V     | 2      |                  |
| 4   | W     | 2      |                  |
| 4   | X     | 2      |                  |
| 4   | Y     | 2      |                  |
| 4   | Z     | 2      |                  |
| 4   | a     | 2      |                  |
| 4   | b     | 2      |                  |
| 4   | c     | 2      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | d     | 2      | 100%             |
|     |       |        | 100%             |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30946 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     | 1006     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7863  | 5019 | 1308 | 1500 | 36 |         |       |
| 1   | B     | 982      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7696  | 4920 | 1279 | 1462 | 35 |         |       |
| 1   | C     | 1004     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7853  | 5014 | 1307 | 1496 | 36 |         |       |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 986     | PRO      | LYS    | conflict       | UNP P0DTC2 |
| A     | 987     | PRO      | VAL    | conflict       | UNP P0DTC2 |
| A     | 1274    | LEU      | -      | expression tag | UNP P0DTC2 |
| A     | 1275    | GLU      | -      | expression tag | UNP P0DTC2 |
| A     | 1276    | ASP      | -      | expression tag | UNP P0DTC2 |
| A     | 1277    | TYR      | -      | expression tag | UNP P0DTC2 |
| A     | 1278    | LYS      | -      | expression tag | UNP P0DTC2 |
| A     | 1279    | ASP      | -      | expression tag | UNP P0DTC2 |
| A     | 1280    | ASP      | -      | expression tag | UNP P0DTC2 |
| A     | 1281    | ASP      | -      | expression tag | UNP P0DTC2 |
| A     | 1282    | ASP      | -      | expression tag | UNP P0DTC2 |
| A     | 1283    | LYS      | -      | expression tag | UNP P0DTC2 |
| B     | 986     | PRO      | LYS    | conflict       | UNP P0DTC2 |
| B     | 987     | PRO      | VAL    | conflict       | UNP P0DTC2 |
| B     | 1274    | LEU      | -      | expression tag | UNP P0DTC2 |
| B     | 1275    | GLU      | -      | expression tag | UNP P0DTC2 |
| B     | 1276    | ASP      | -      | expression tag | UNP P0DTC2 |
| B     | 1277    | TYR      | -      | expression tag | UNP P0DTC2 |
| B     | 1278    | LYS      | -      | expression tag | UNP P0DTC2 |
| B     | 1279    | ASP      | -      | expression tag | UNP P0DTC2 |
| B     | 1280    | ASP      | -      | expression tag | UNP P0DTC2 |
| B     | 1281    | ASP      | -      | expression tag | UNP P0DTC2 |
| B     | 1282    | ASP      | -      | expression tag | UNP P0DTC2 |
| B     | 1283    | LYS      | -      | expression tag | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 986     | PRO      | LYS    | conflict       | UNP P0DTC2 |
| C     | 987     | PRO      | VAL    | conflict       | UNP P0DTC2 |
| C     | 1274    | LEU      | -      | expression tag | UNP P0DTC2 |
| C     | 1275    | GLU      | -      | expression tag | UNP P0DTC2 |
| C     | 1276    | ASP      | -      | expression tag | UNP P0DTC2 |
| C     | 1277    | TYR      | -      | expression tag | UNP P0DTC2 |
| C     | 1278    | LYS      | -      | expression tag | UNP P0DTC2 |
| C     | 1279    | ASP      | -      | expression tag | UNP P0DTC2 |
| C     | 1280    | ASP      | -      | expression tag | UNP P0DTC2 |
| C     | 1281    | ASP      | -      | expression tag | UNP P0DTC2 |
| C     | 1282    | ASP      | -      | expression tag | UNP P0DTC2 |
| C     | 1283    | LYS      | -      | expression tag | UNP P0DTC2 |

- Molecule 2 is a protein called Immunoglobulin heavy variable 4-59,Chain H of P2B-1A1,Anti-RhD monoclonal T125 gamma1 heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | H     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1669  | 1062 | 272 | 330 | 5 |         |       |
| 2   | J     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1669  | 1062 | 272 | 330 | 5 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| H     | 76      | LYS      | ASN    | conflict | UNP P01825 |
| H     | 108     | ASP      | HIS    | conflict | UNP Q5EFE5 |
| J     | 76      | LYS      | ASN    | conflict | UNP P01825 |
| J     | 108     | ASP      | HIS    | conflict | UNP Q5EFE5 |

- Molecule 3 is a protein called IG c181\_light\_IGLV2-14\_IGLJ3,IGL@ protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | L     | 213      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 986 | 263 | 326 | 5 |         |       |
| 3   | N     | 213      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 986 | 263 | 326 | 5 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| L     | 48      | PHE      | LEU    | conflict | UNP A0A5C2GM57 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| L     | 96      | ASN      | SER    | conflict | UNP A0A5C2GM57 |
| L     | 99      | PHE      | TRP    | conflict | UNP A0A5C2GM57 |
| L     | 100     | ALA      | VAL    | conflict | UNP A0A5C2GM57 |
| N     | 48      | PHE      | LEU    | conflict | UNP A0A5C2GM57 |
| N     | 96      | ASN      | SER    | conflict | UNP A0A5C2GM57 |
| N     | 99      | PHE      | TRP    | conflict | UNP A0A5C2GM57 |
| N     | 100     | ALA      | VAL    | conflict | UNP A0A5C2GM57 |

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



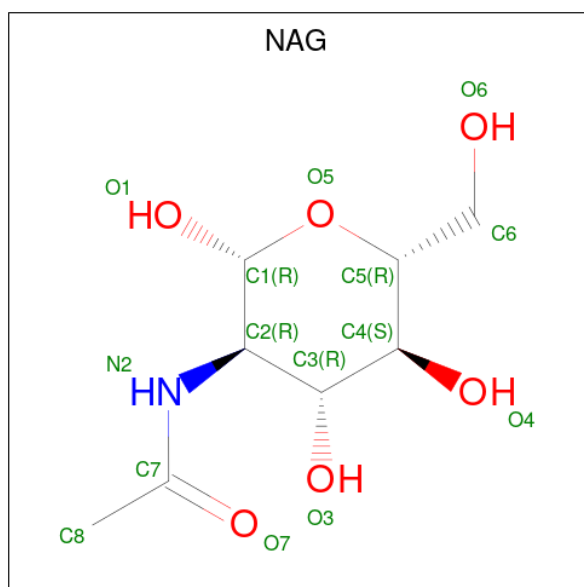
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 4   | D     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | E     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | F     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | G     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | I     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | K     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | M     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | O     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | P     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | Q     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | R     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | S     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | T     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 4   | U     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | V     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | W     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | X     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | Y     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | Z     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | a     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | b     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | c     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 4   | d     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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

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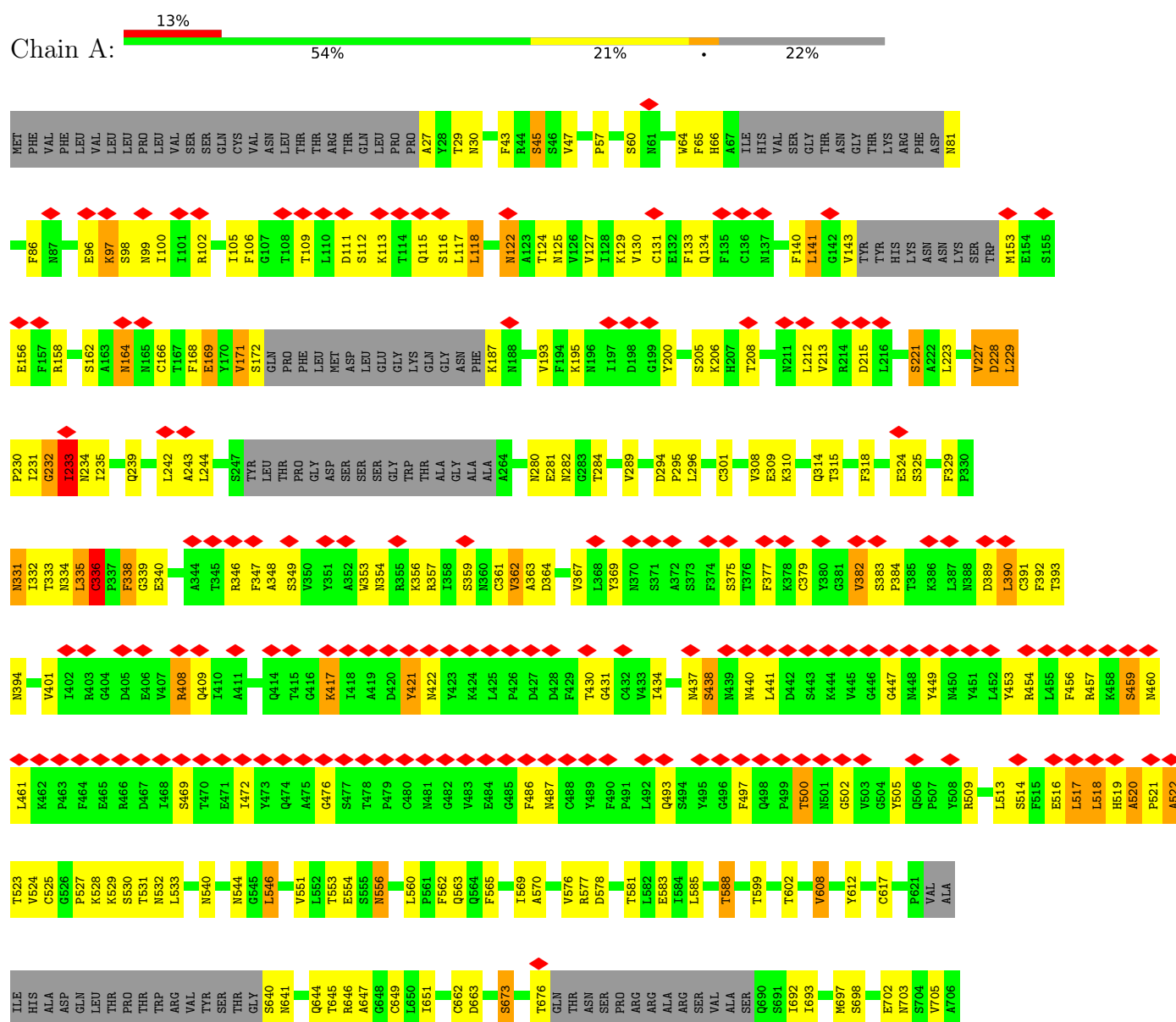
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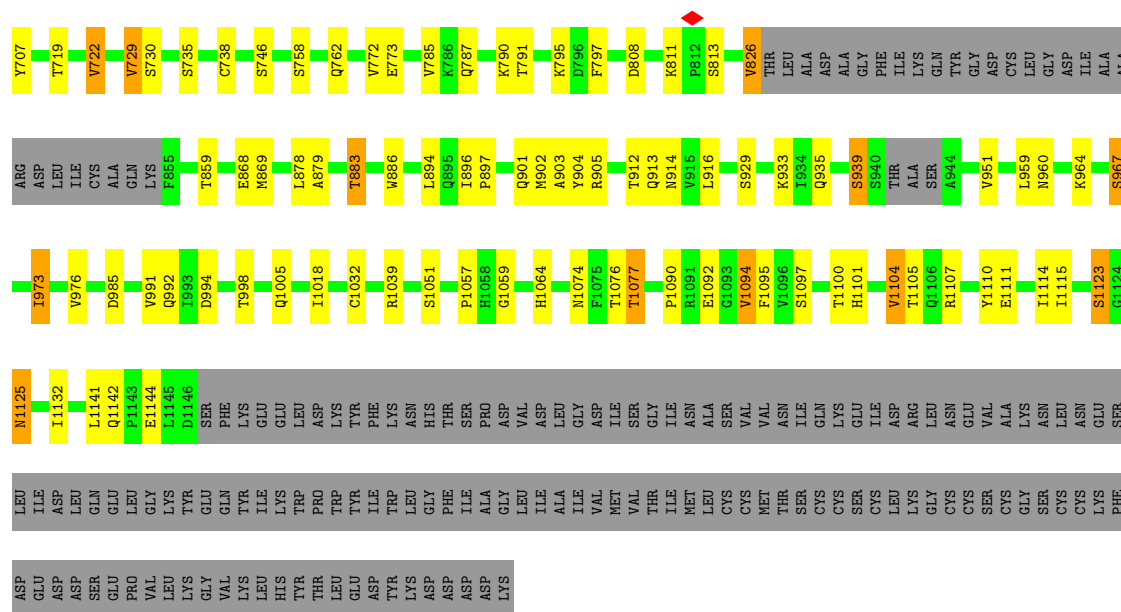
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 5   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 5   | C     | 1        | Total | C | N | O | 0       |
|     |       |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

### 3 Residue-property plots

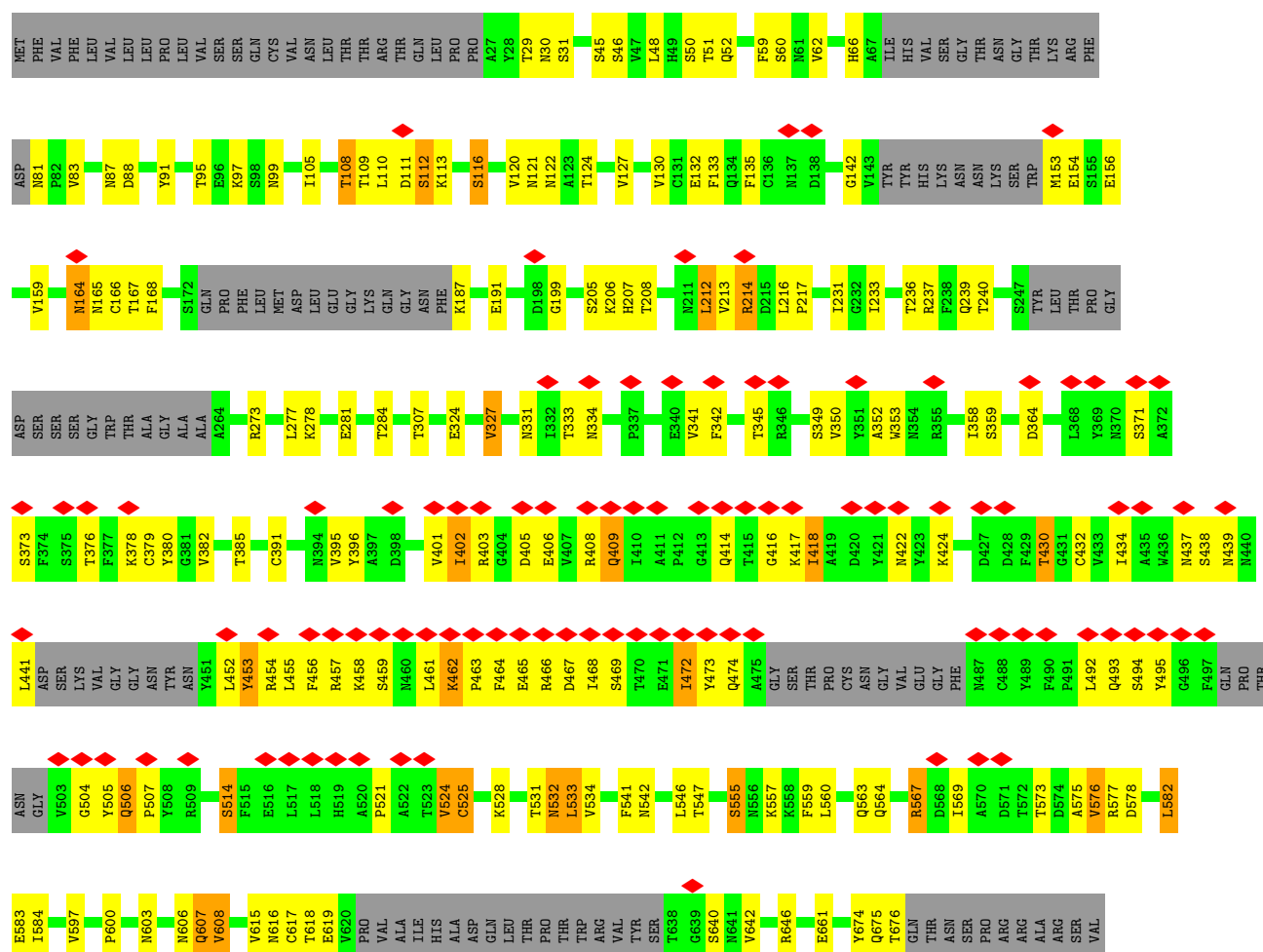
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Spike glycoprotein

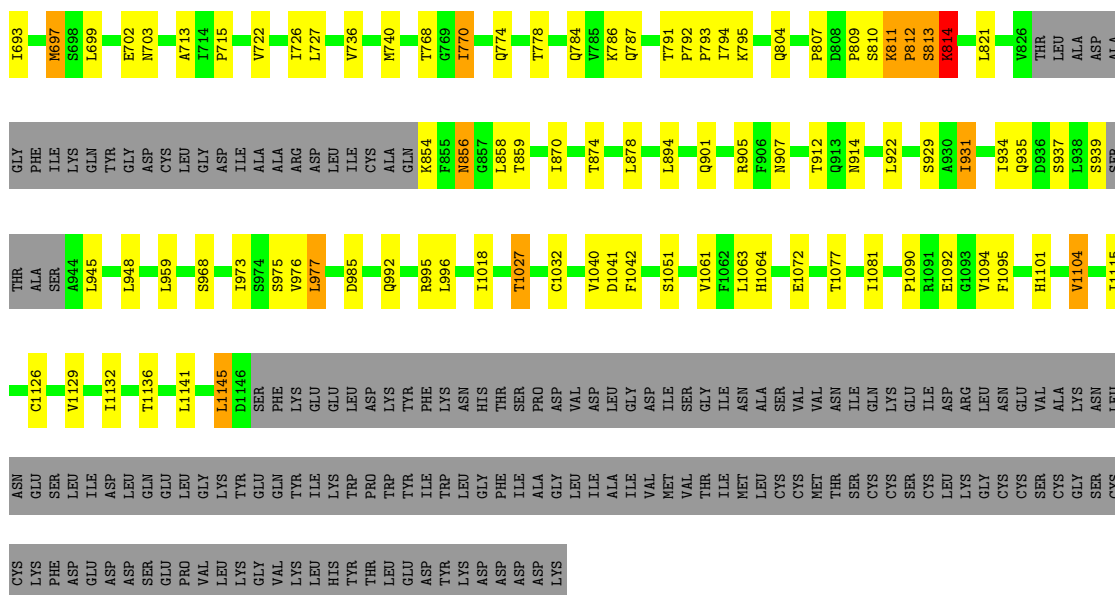




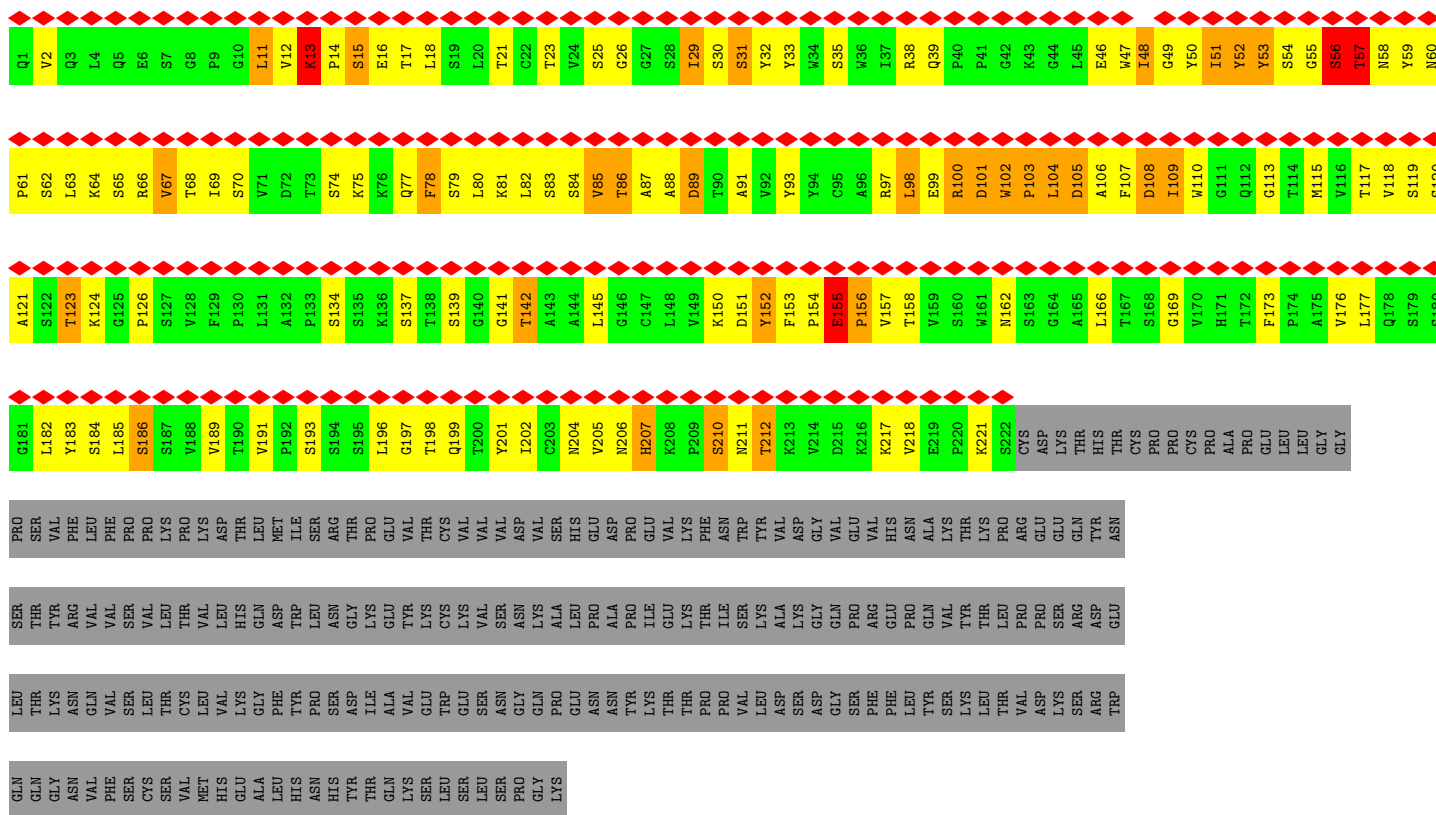
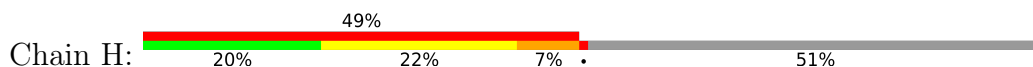
• Molecule 1: Spike glycoprotein





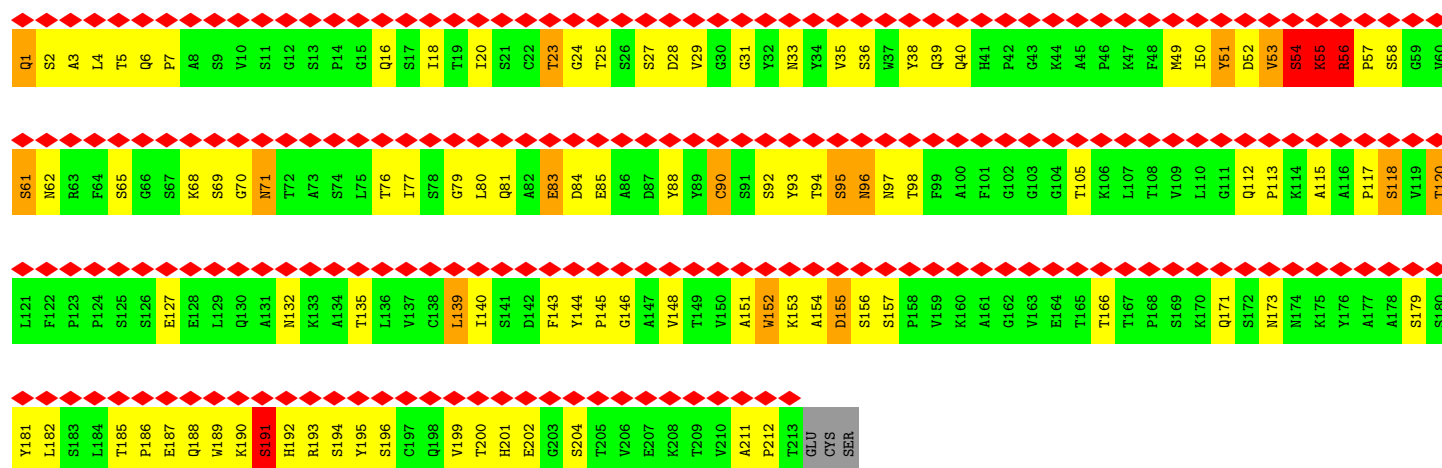


- Molecule 2: Immunoglobulin heavy variable 4-59, Chain H of P2B-1A1, Anti-RhD monoclonal T125 gamma1 heavy chain



- Molecule 2: Immunoglobulin heavy variable 4-59, Chain H of P2B-1A1, Anti-RhD monoclonal T125 gamma1 heavy chain





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



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



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



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



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

Chain I:  50% 50%



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

Chain K:  50% 50%



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

Chain M:  50% 50%



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

Chain O:  50% 50% 50%



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

Chain P:  50% 100%



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

Chain Q:  50% 50%



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

Chain R:  50% 50%



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

Chain S: 100%



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

Chain T: 50% 100%



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

Chain U: 50% 50%



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

Chain V: 100% 100%



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

Chain W: 50% 50% 50%



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

Chain X: 50% 50%



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

Chain Y:  100%



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

Chain Z:  50% 50%



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

Chain a:  100%



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

Chain b:  50% 100%



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

Chain c:  100% 100%



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

Chain d:  100% 100%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 146875                                  | 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 ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.215                                   | Depositor |
| Minimum map value                    | -0.115                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size (Å)                         | 313.056, 313.056, 313.056               | wwPDB     |
| Map dimensions                       | 288, 288, 288                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.087, 1.087, 1.087                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.52         | 0/8039      | 0.61        | 2/10936 (0.0%)  |
| 1   | B     | 0.43         | 0/7864      | 0.59        | 2/10691 (0.0%)  |
| 1   | C     | 0.52         | 0/8028      | 0.60        | 2/10919 (0.0%)  |
| 2   | H     | 0.52         | 0/1713      | 0.69        | 0/2340          |
| 2   | J     | 0.52         | 0/1713      | 0.69        | 0/2340          |
| 3   | L     | 0.50         | 0/1619      | 0.62        | 4/2207 (0.2%)   |
| 3   | N     | 0.50         | 0/1619      | 0.62        | 4/2207 (0.2%)   |
| All | All   | 0.50         | 0/30595     | 0.61        | 14/41640 (0.0%) |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 538 | CYS  | N-CA-C | -6.20 | 100.86      | 110.10   |
| 3   | L     | 191 | SER  | N-CA-C | 6.18  | 117.81      | 111.14   |
| 3   | N     | 191 | SER  | N-CA-C | 6.15  | 117.79      | 111.14   |
| 3   | N     | 118 | SER  | N-CA-C | -6.01 | 99.40       | 108.96   |
| 3   | L     | 118 | SER  | N-CA-C | -6.01 | 99.40       | 108.96   |
| 1   | A     | 86  | PHE  | CA-C-N | 5.91  | 132.82      | 121.54   |
| 1   | A     | 86  | PHE  | C-N-CA | 5.91  | 132.82      | 121.54   |
| 1   | C     | 156 | GLU  | N-CA-C | 5.86  | 115.83      | 108.45   |
| 3   | N     | 56  | ARG  | CA-C-N | -5.70 | 114.06      | 119.76   |
| 3   | N     | 56  | ARG  | C-N-CA | -5.70 | 114.06      | 119.76   |
| 3   | L     | 56  | ARG  | CA-C-N | -5.70 | 114.06      | 119.76   |
| 3   | L     | 56  | ARG  | C-N-CA | -5.70 | 114.06      | 119.76   |
| 1   | B     | 212 | LEU  | CA-C-N | -5.37 | 117.66      | 123.08   |
| 1   | B     | 212 | LEU  | C-N-CA | -5.37 | 117.66      | 123.08   |

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     | 7863  | 0        | 7657     | 284     | 0            |
| 1   | B     | 7696  | 0        | 7514     | 144     | 0            |
| 1   | C     | 7853  | 0        | 7652     | 293     | 0            |
| 2   | H     | 1669  | 0        | 1651     | 210     | 0            |
| 2   | J     | 1669  | 0        | 1651     | 212     | 0            |
| 3   | L     | 1580  | 0        | 1517     | 142     | 0            |
| 3   | N     | 1580  | 0        | 1517     | 147     | 0            |
| 4   | D     | 28    | 0        | 25       | 0       | 0            |
| 4   | E     | 28    | 0        | 25       | 2       | 0            |
| 4   | F     | 28    | 0        | 25       | 0       | 0            |
| 4   | G     | 28    | 0        | 25       | 1       | 0            |
| 4   | I     | 28    | 0        | 25       | 1       | 0            |
| 4   | K     | 28    | 0        | 25       | 0       | 0            |
| 4   | M     | 28    | 0        | 25       | 0       | 0            |
| 4   | O     | 28    | 0        | 25       | 1       | 0            |
| 4   | P     | 28    | 0        | 25       | 0       | 0            |
| 4   | Q     | 28    | 0        | 25       | 0       | 0            |
| 4   | R     | 28    | 0        | 25       | 0       | 0            |
| 4   | S     | 28    | 0        | 25       | 1       | 0            |
| 4   | T     | 28    | 0        | 25       | 0       | 0            |
| 4   | U     | 28    | 0        | 25       | 0       | 0            |
| 4   | V     | 28    | 0        | 25       | 2       | 0            |
| 4   | W     | 28    | 0        | 25       | 1       | 0            |
| 4   | X     | 28    | 0        | 25       | 0       | 0            |
| 4   | Y     | 28    | 0        | 25       | 0       | 0            |
| 4   | Z     | 28    | 0        | 25       | 1       | 0            |
| 4   | a     | 28    | 0        | 25       | 2       | 0            |
| 4   | b     | 28    | 0        | 25       | 0       | 0            |
| 4   | c     | 28    | 0        | 25       | 3       | 0            |
| 4   | d     | 28    | 0        | 25       | 3       | 0            |
| 5   | A     | 126   | 0        | 117      | 4       | 0            |
| 5   | B     | 154   | 0        | 142      | 10      | 0            |
| 5   | C     | 112   | 0        | 104      | 2       | 0            |
| All | All   | 30946 | 0        | 30097    | 1324    | 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 22.

All (1324) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:13:LYS:HD2   | 2:J:14:PRO:CD    | 1.31                     | 1.57              |
| 2:H:13:LYS:HD2   | 2:H:14:PRO:CD    | 1.31                     | 1.53              |
| 2:J:154:PRO:HG3  | 2:J:207:HIS:CE1  | 1.42                     | 1.50              |
| 2:H:154:PRO:HG3  | 2:H:207:HIS:CE1  | 1.42                     | 1.48              |
| 5:B:1410:NAG:O4  | 5:B:1411:NAG:C1  | 1.63                     | 1.46              |
| 2:H:13:LYS:CD    | 2:H:14:PRO:HD2   | 1.42                     | 1.45              |
| 1:A:230:PRO:CB   | 1:C:521:PRO:HG2  | 1.46                     | 1.45              |
| 2:J:13:LYS:CD    | 2:J:14:PRO:HD2   | 1.42                     | 1.45              |
| 1:C:456:PHE:CE1  | 3:N:55:LYS:HD2   | 1.64                     | 1.31              |
| 1:A:456:PHE:CE1  | 3:L:55:LYS:HD2   | 1.65                     | 1.30              |
| 2:J:121:ALA:HB1  | 2:J:153:PHE:CE2  | 1.68                     | 1.26              |
| 2:H:121:ALA:HB1  | 2:H:153:PHE:CE2  | 1.68                     | 1.25              |
| 2:H:51:ILE:HD11  | 2:H:69:ILE:CG2   | 1.66                     | 1.25              |
| 2:J:51:ILE:HD11  | 2:J:69:ILE:CG2   | 1.66                     | 1.24              |
| 3:L:56:ARG:HH21  | 3:L:62:ASN:CB    | 1.51                     | 1.22              |
| 3:N:56:ARG:HH21  | 3:N:62:ASN:CB    | 1.51                     | 1.20              |
| 2:H:51:ILE:HD11  | 2:H:69:ILE:CB    | 1.72                     | 1.19              |
| 2:H:52:TYR:HE1   | 2:H:53:TYR:CE2   | 1.61                     | 1.18              |
| 1:A:200:TYR:CE1  | 1:C:521:PRO:HB2  | 1.78                     | 1.17              |
| 2:J:51:ILE:HD11  | 2:J:69:ILE:CB    | 1.72                     | 1.17              |
| 2:J:52:TYR:HE1   | 2:J:53:TYR:CE2   | 1.61                     | 1.17              |
| 2:H:62:SER:HB3   | 3:L:1:GLN:HB2    | 1.25                     | 1.17              |
| 1:A:230:PRO:CB   | 1:C:521:PRO:CG   | 2.23                     | 1.16              |
| 2:H:121:ALA:CB   | 2:H:153:PHE:CE2  | 2.29                     | 1.15              |
| 1:A:340:GLU:OE2  | 1:A:356:LYS:HE2  | 1.47                     | 1.15              |
| 2:J:121:ALA:CB   | 2:J:153:PHE:CE2  | 2.28                     | 1.15              |
| 1:A:227:VAL:HG11 | 1:A:229:LEU:HD23 | 1.19                     | 1.14              |
| 2:J:62:SER:HB3   | 3:N:1:GLN:HB2    | 1.25                     | 1.14              |
| 1:C:340:GLU:OE2  | 1:C:356:LYS:HE2  | 1.47                     | 1.14              |
| 1:C:523:THR:HG22 | 1:C:524:VAL:H    | 0.97                     | 1.13              |
| 1:C:335:LEU:HA   | 1:C:362:VAL:HG13 | 1.33                     | 1.11              |
| 2:H:51:ILE:HD11  | 2:H:69:ILE:HG22  | 1.33                     | 1.11              |
| 1:C:551:VAL:HB   | 1:C:588:THR:HG23 | 1.29                     | 1.10              |
| 1:A:523:THR:HG22 | 1:A:524:VAL:H    | 0.97                     | 1.10              |
| 2:J:154:PRO:CG   | 2:J:207:HIS:CE1  | 2.33                     | 1.10              |
| 1:A:230:PRO:HB3  | 1:C:521:PRO:HG2  | 1.17                     | 1.09              |
| 2:H:198:THR:HA   | 2:J:198:THR:HG21 | 1.34                     | 1.09              |
| 2:H:154:PRO:CG   | 2:H:207:HIS:CE1  | 2.33                     | 1.09              |
| 3:L:4:LEU:HD23   | 3:L:5:THR:H      | 1.11                     | 1.09              |
| 3:N:4:LEU:HD23   | 3:N:5:THR:H      | 1.11                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:520:ALA:HB1  | 1:A:521:PRO:HD2  | 1.35                     | 1.08              |
| 1:A:230:PRO:HB2  | 1:C:521:PRO:HG2  | 1.28                     | 1.08              |
| 1:A:335:LEU:HA   | 1:A:362:VAL:HG13 | 1.33                     | 1.07              |
| 1:C:449:TYR:OH   | 3:N:31:GLY:HA2   | 1.55                     | 1.07              |
| 1:C:520:ALA:HB1  | 1:C:521:PRO:HD2  | 1.35                     | 1.07              |
| 1:A:449:TYR:OH   | 3:L:31:GLY:HA2   | 1.56                     | 1.06              |
| 1:A:392:PHE:HB3  | 1:A:517:LEU:HD21 | 1.35                     | 1.06              |
| 1:A:335:LEU:HA   | 1:A:362:VAL:CG1  | 1.86                     | 1.05              |
| 2:H:52:TYR:CE1   | 2:H:53:TYR:CE2   | 2.45                     | 1.05              |
| 2:J:51:ILE:HD11  | 2:J:69:ILE:HG22  | 1.33                     | 1.05              |
| 2:J:52:TYR:CE1   | 2:J:53:TYR:CE2   | 2.45                     | 1.05              |
| 1:C:392:PHE:HB3  | 1:C:517:LEU:CD2  | 1.88                     | 1.04              |
| 1:C:392:PHE:HB3  | 1:C:517:LEU:HD21 | 1.35                     | 1.03              |
| 1:A:392:PHE:HB3  | 1:A:517:LEU:CD2  | 1.88                     | 1.03              |
| 1:C:335:LEU:HA   | 1:C:362:VAL:CG1  | 1.86                     | 1.03              |
| 2:J:154:PRO:HG3  | 2:J:207:HIS:NE2  | 1.74                     | 1.02              |
| 1:A:233:ILE:HG12 | 1:A:234:ASN:N    | 1.72                     | 1.02              |
| 2:H:51:ILE:CD1   | 2:H:69:ILE:HG22  | 1.89                     | 1.02              |
| 2:H:51:ILE:HD11  | 2:H:69:ILE:HB    | 1.40                     | 1.02              |
| 2:J:121:ALA:HB1  | 2:J:153:PHE:HE2  | 1.00                     | 1.01              |
| 2:J:51:ILE:CD1   | 2:J:69:ILE:HG22  | 1.89                     | 1.01              |
| 1:B:422:ASN:HD21 | 1:B:455:LEU:H    | 1.08                     | 1.01              |
| 5:B:1410:NAG:C4  | 5:B:1411:NAG:C1  | 2.38                     | 1.01              |
| 2:H:154:PRO:HG3  | 2:H:207:HIS:NE2  | 1.74                     | 1.01              |
| 1:C:392:PHE:CB   | 1:C:517:LEU:HD21 | 1.91                     | 1.00              |
| 2:H:121:ALA:HB1  | 2:H:153:PHE:HE2  | 1.00                     | 0.99              |
| 3:L:56:ARG:HE    | 3:L:62:ASN:HA    | 1.27                     | 0.99              |
| 1:A:392:PHE:CB   | 1:A:517:LEU:HD21 | 1.92                     | 0.99              |
| 1:A:523:THR:HG22 | 1:A:524:VAL:N    | 1.72                     | 0.99              |
| 1:C:523:THR:HG22 | 1:C:524:VAL:N    | 1.72                     | 0.99              |
| 2:J:51:ILE:HD11  | 2:J:69:ILE:HB    | 1.40                     | 0.99              |
| 1:C:811:LYS:HB2  | 1:C:812:PRO:CD   | 1.91                     | 0.98              |
| 1:A:523:THR:CG2  | 1:A:524:VAL:H    | 1.77                     | 0.98              |
| 1:C:551:VAL:HB   | 1:C:588:THR:CG2  | 1.93                     | 0.98              |
| 1:C:676:THR:HA   | 1:C:690:GLN:HB3  | 1.46                     | 0.98              |
| 3:N:56:ARG:HE    | 3:N:62:ASN:HA    | 1.27                     | 0.98              |
| 2:J:106:ALA:HB1  | 3:N:38:TYR:OH    | 1.63                     | 0.98              |
| 2:H:154:PRO:C    | 2:H:156:PRO:HD2  | 1.89                     | 0.98              |
| 2:H:52:TYR:CE1   | 2:H:53:TYR:CD2   | 2.52                     | 0.97              |
| 1:A:227:VAL:HG12 | 1:A:228:ASP:H    | 1.27                     | 0.97              |
| 1:C:320:VAL:CG2  | 1:C:591:SER:HB3  | 1.95                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:154:PRO:O    | 2:H:156:PRO:HD2  | 1.65                     | 0.97              |
| 1:C:346:ARG:NH2  | 1:C:347:PHE:O    | 1.98                     | 0.97              |
| 3:L:56:ARG:NH2   | 3:L:62:ASN:HB2   | 1.79                     | 0.97              |
| 3:N:56:ARG:NH2   | 3:N:62:ASN:HB2   | 1.79                     | 0.97              |
| 2:H:106:ALA:HB1  | 3:L:38:TYR:OH    | 1.63                     | 0.96              |
| 2:J:52:TYR:CE1   | 2:J:53:TYR:CD2   | 2.52                     | 0.96              |
| 2:J:152:TYR:C    | 2:J:154:PRO:HD2  | 1.90                     | 0.96              |
| 2:H:152:TYR:C    | 2:H:154:PRO:HD2  | 1.90                     | 0.96              |
| 1:C:675:GLN:HE21 | 1:C:675:GLN:HA   | 1.26                     | 0.96              |
| 1:C:523:THR:CG2  | 1:C:524:VAL:H    | 1.77                     | 0.96              |
| 2:J:154:PRO:O    | 2:J:156:PRO:HD2  | 1.65                     | 0.96              |
| 3:N:56:ARG:NH2   | 3:N:62:ASN:CB    | 2.29                     | 0.96              |
| 2:J:154:PRO:C    | 2:J:156:PRO:HD2  | 1.89                     | 0.95              |
| 1:A:346:ARG:NH2  | 1:A:347:PHE:O    | 1.98                     | 0.95              |
| 3:L:56:ARG:NH2   | 3:L:62:ASN:CB    | 2.29                     | 0.95              |
| 1:C:320:VAL:HG23 | 1:C:591:SER:HB3  | 1.49                     | 0.94              |
| 2:J:51:ILE:CD1   | 2:J:69:ILE:CG2   | 2.45                     | 0.94              |
| 3:N:56:ARG:HH21  | 3:N:62:ASN:HB2   | 1.32                     | 0.94              |
| 1:A:456:PHE:HE1  | 3:L:55:LYS:HD2   | 1.16                     | 0.94              |
| 1:B:577:ARG:HH11 | 1:B:582:LEU:HD13 | 1.32                     | 0.93              |
| 3:L:56:ARG:HH21  | 3:L:62:ASN:HB2   | 1.32                     | 0.92              |
| 2:H:51:ILE:CD1   | 2:H:69:ILE:CG2   | 2.45                     | 0.92              |
| 1:C:811:LYS:HB2  | 1:C:812:PRO:HD2  | 1.50                     | 0.92              |
| 1:A:227:VAL:CG1  | 1:A:229:LEU:HD23 | 2.00                     | 0.91              |
| 1:A:227:VAL:HG11 | 1:A:229:LEU:CD2  | 2.01                     | 0.91              |
| 1:C:456:PHE:HE1  | 3:N:55:LYS:HD2   | 1.15                     | 0.91              |
| 1:C:456:PHE:CZ   | 3:N:55:LYS:HD2   | 2.05                     | 0.91              |
| 1:C:456:PHE:CE1  | 3:N:55:LYS:CD    | 2.52                     | 0.90              |
| 1:A:233:ILE:HG12 | 1:A:234:ASN:H    | 1.28                     | 0.90              |
| 1:A:456:PHE:CZ   | 3:L:55:LYS:HD2   | 2.05                     | 0.90              |
| 1:A:229:LEU:HD12 | 1:A:231:ILE:CG1  | 2.02                     | 0.90              |
| 3:N:25:THR:HG23  | 3:N:27:SER:H     | 1.37                     | 0.90              |
| 3:L:56:ARG:NE    | 3:L:62:ASN:HA    | 1.88                     | 0.89              |
| 1:C:486:PHE:CD1  | 3:N:65:SER:OG    | 2.25                     | 0.89              |
| 1:A:230:PRO:HB2  | 1:C:521:PRO:CG   | 1.92                     | 0.89              |
| 1:A:456:PHE:CE1  | 3:L:55:LYS:CD    | 2.53                     | 0.88              |
| 3:N:56:ARG:NE    | 3:N:62:ASN:HA    | 1.88                     | 0.88              |
| 3:L:25:THR:HG23  | 3:L:27:SER:H     | 1.37                     | 0.88              |
| 2:J:100:ARG:HH21 | 2:J:100:ARG:HG3  | 1.39                     | 0.88              |
| 2:J:153:PHE:N    | 2:J:154:PRO:CD   | 2.36                     | 0.88              |
| 2:J:154:PRO:CG   | 2:J:207:HIS:NE2  | 2.35                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:486:PHE:CD1  | 3:L:65:SER:OG    | 2.26                     | 0.88              |
| 2:H:153:PHE:N    | 2:H:154:PRO:CD   | 2.36                     | 0.87              |
| 2:H:154:PRO:CG   | 2:H:207:HIS:NE2  | 2.35                     | 0.87              |
| 3:N:4:LEU:CD2    | 3:N:5:THR:H      | 1.87                     | 0.87              |
| 1:A:229:LEU:HD12 | 1:A:231:ILE:HG12 | 1.55                     | 0.86              |
| 3:L:4:LEU:CD2    | 3:L:5:THR:H      | 1.87                     | 0.86              |
| 2:J:152:TYR:HB2  | 2:J:207:HIS:HE1  | 1.41                     | 0.86              |
| 2:J:153:PHE:N    | 2:J:154:PRO:HD2  | 1.90                     | 0.86              |
| 2:J:52:TYR:CD1   | 2:J:53:TYR:CD2   | 2.64                     | 0.86              |
| 1:A:393:THR:O    | 1:A:523:THR:HG21 | 1.76                     | 0.86              |
| 1:A:392:PHE:CD2  | 1:A:517:LEU:HD21 | 2.11                     | 0.86              |
| 2:H:52:TYR:CD1   | 2:H:53:TYR:CD2   | 2.64                     | 0.86              |
| 2:H:153:PHE:N    | 2:H:154:PRO:HD2  | 1.90                     | 0.86              |
| 1:C:392:PHE:CD2  | 1:C:517:LEU:HD21 | 2.11                     | 0.85              |
| 1:C:520:ALA:HB1  | 1:C:521:PRO:CD   | 2.06                     | 0.85              |
| 2:J:52:TYR:HE1   | 2:J:53:TYR:HE2   | 1.21                     | 0.85              |
| 1:A:729:VAL:HG13 | 1:A:1059:GLY:HA2 | 1.57                     | 0.85              |
| 1:C:408:ARG:CB   | 1:C:408:ARG:HH21 | 1.90                     | 0.85              |
| 1:B:577:ARG:HD3  | 1:B:582:LEU:CD1  | 2.07                     | 0.85              |
| 2:J:121:ALA:CB   | 2:J:153:PHE:HE2  | 1.77                     | 0.85              |
| 2:H:152:TYR:HB2  | 2:H:207:HIS:HE1  | 1.41                     | 0.85              |
| 1:A:229:LEU:HD13 | 1:A:231:ILE:HD11 | 1.58                     | 0.84              |
| 1:A:43:PHE:HD1   | 1:C:563:GLN:OE1  | 1.60                     | 0.84              |
| 1:A:408:ARG:CB   | 1:A:408:ARG:HH21 | 1.90                     | 0.84              |
| 1:A:520:ALA:HB1  | 1:A:521:PRO:CD   | 2.06                     | 0.84              |
| 2:H:100:ARG:HH21 | 2:H:100:ARG:HG3  | 1.39                     | 0.84              |
| 1:A:43:PHE:CE1   | 1:C:559:PHE:HA   | 2.12                     | 0.84              |
| 1:C:393:THR:O    | 1:C:523:THR:HG21 | 1.76                     | 0.84              |
| 2:H:121:ALA:CB   | 2:H:153:PHE:HE2  | 1.77                     | 0.84              |
| 2:H:154:PRO:O    | 2:H:156:PRO:CD   | 2.25                     | 0.84              |
| 1:C:127:VAL:HG21 | 5:C:1402:NAG:H5  | 1.59                     | 0.83              |
| 2:J:154:PRO:O    | 2:J:156:PRO:CD   | 2.25                     | 0.83              |
| 1:C:516:GLU:O    | 1:C:517:LEU:HD22 | 1.78                     | 0.83              |
| 1:C:676:THR:C    | 1:C:690:GLN:HE21 | 1.86                     | 0.83              |
| 2:J:152:TYR:HD2  | 2:J:154:PRO:HG2  | 1.44                     | 0.83              |
| 1:A:516:GLU:O    | 1:A:517:LEU:HD22 | 1.78                     | 0.83              |
| 2:H:121:ALA:HB3  | 2:H:153:PHE:CE2  | 2.13                     | 0.83              |
| 1:C:408:ARG:HH21 | 1:C:408:ARG:HB2  | 1.44                     | 0.82              |
| 1:B:901:GLN:HE21 | 1:B:905:ARG:HE   | 1.26                     | 0.82              |
| 1:A:200:TYR:CZ   | 1:C:521:PRO:HB2  | 2.14                     | 0.82              |
| 1:A:964:LYS:HD2  | 1:C:570:ALA:HA   | 1.61                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:320:VAL:CG2  | 1:C:591:SER:CB   | 2.56                     | 0.82              |
| 2:H:152:TYR:HD2  | 2:H:154:PRO:HG2  | 1.44                     | 0.82              |
| 1:C:320:VAL:HG23 | 1:C:591:SER:CB   | 2.09                     | 0.81              |
| 1:A:362:VAL:CG2  | 1:A:527:PRO:HG3  | 2.10                     | 0.81              |
| 1:A:456:PHE:HE1  | 3:L:55:LYS:CD    | 1.92                     | 0.81              |
| 1:C:901:GLN:HE21 | 1:C:905:ARG:HE   | 1.27                     | 0.81              |
| 1:B:452:LEU:HG   | 1:B:492:LEU:HD22 | 1.63                     | 0.81              |
| 2:H:162:ASN:HD21 | 2:H:201:TYR:HA   | 1.45                     | 0.81              |
| 3:L:56:ARG:HH21  | 3:L:62:ASN:HB3   | 1.44                     | 0.81              |
| 2:J:162:ASN:HD21 | 2:J:201:TYR:HA   | 1.45                     | 0.81              |
| 1:C:362:VAL:CG2  | 1:C:527:PRO:HG3  | 2.10                     | 0.81              |
| 2:J:66:ARG:HH21  | 2:J:82:LEU:HD21  | 1.46                     | 0.81              |
| 1:B:577:ARG:HD3  | 1:B:582:LEU:HD13 | 1.61                     | 0.81              |
| 3:L:56:ARG:HH11  | 3:L:56:ARG:HG3   | 1.45                     | 0.81              |
| 3:N:56:ARG:HG3   | 3:N:56:ARG:HH11  | 1.45                     | 0.81              |
| 1:A:335:LEU:HD12 | 1:A:335:LEU:O    | 1.81                     | 0.81              |
| 1:C:456:PHE:HE1  | 3:N:55:LYS:CD    | 1.91                     | 0.81              |
| 2:J:121:ALA:HB3  | 2:J:153:PHE:CE2  | 2.13                     | 0.81              |
| 3:L:4:LEU:HD23   | 3:L:5:THR:N      | 1.94                     | 0.80              |
| 1:A:284:THR:HB   | 1:C:560:LEU:HD11 | 1.64                     | 0.80              |
| 1:B:214:ARG:H    | 1:B:214:ARG:HH21 | 1.30                     | 0.80              |
| 1:A:200:TYR:CE1  | 1:C:521:PRO:CB   | 2.62                     | 0.80              |
| 1:C:335:LEU:HD12 | 1:C:335:LEU:O    | 1.81                     | 0.80              |
| 2:H:13:LYS:CD    | 2:H:14:PRO:CD    | 2.24                     | 0.80              |
| 2:H:66:ARG:HH21  | 2:H:82:LEU:HD21  | 1.46                     | 0.80              |
| 1:A:408:ARG:HH21 | 1:A:408:ARG:HB2  | 1.44                     | 0.80              |
| 1:C:486:PHE:HE1  | 3:N:76:THR:HG21  | 1.47                     | 0.80              |
| 2:H:52:TYR:HE1   | 2:H:53:TYR:HE2   | 1.21                     | 0.80              |
| 3:N:56:ARG:HH21  | 3:N:62:ASN:HB3   | 1.44                     | 0.80              |
| 1:A:230:PRO:CA   | 1:C:521:PRO:HG3  | 2.13                     | 0.79              |
| 1:C:417:LYS:HE3  | 1:C:453:TYR:CE2  | 2.17                     | 0.79              |
| 1:A:417:LYS:HE3  | 1:A:453:TYR:CE2  | 2.17                     | 0.79              |
| 1:C:324:GLU:OE2  | 1:C:534:VAL:HG11 | 1.83                     | 0.79              |
| 3:N:4:LEU:HD23   | 3:N:5:THR:N      | 1.94                     | 0.79              |
| 2:J:13:LYS:CD    | 2:J:14:PRO:CD    | 2.24                     | 0.79              |
| 1:A:390:LEU:HD23 | 1:A:391:CYS:H    | 1.48                     | 0.78              |
| 1:A:486:PHE:HE1  | 3:L:76:THR:HG21  | 1.48                     | 0.78              |
| 1:A:230:PRO:HA   | 1:C:521:PRO:HG3  | 1.64                     | 0.78              |
| 1:A:486:PHE:CE1  | 3:L:76:THR:OG1   | 2.36                     | 0.78              |
| 1:A:422:ASN:HD21 | 1:A:454:ARG:H    | 1.32                     | 0.78              |
| 2:J:14:PRO:O     | 2:J:15:SER:OG    | 2.02                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:392:PHE:O    | 1:A:523:THR:HB    | 1.83                     | 0.77              |
| 2:H:198:THR:CA   | 2:J:198:THR:HG21  | 2.12                     | 0.77              |
| 1:C:486:PHE:CE1  | 3:N:76:THR:OG1    | 2.35                     | 0.77              |
| 2:J:57:THR:OG1   | 2:J:58:ASN:N      | 2.15                     | 0.77              |
| 1:C:390:LEU:HD23 | 1:C:391:CYS:H     | 1.48                     | 0.77              |
| 3:L:187:GLU:O    | 3:L:191:SER:HB2   | 1.84                     | 0.77              |
| 2:H:157:VAL:HB   | 2:H:207:HIS:CD2   | 2.20                     | 0.77              |
| 3:L:56:ARG:HG3   | 3:L:56:ARG:NH1    | 2.00                     | 0.77              |
| 2:J:152:TYR:HD2  | 2:J:207:HIS:HE2   | 1.32                     | 0.77              |
| 1:C:392:PHE:O    | 1:C:523:THR:HB    | 1.83                     | 0.77              |
| 3:N:187:GLU:O    | 3:N:191:SER:HB2   | 1.84                     | 0.77              |
| 2:J:157:VAL:HB   | 2:J:207:HIS:CD2   | 2.20                     | 0.76              |
| 1:A:229:LEU:CD1  | 1:A:231:ILE:HD11  | 2.15                     | 0.76              |
| 2:J:121:ALA:HB3  | 2:J:153:PHE:CZ    | 2.21                     | 0.76              |
| 1:C:422:ASN:HD21 | 1:C:454:ARG:H     | 1.32                     | 0.76              |
| 3:L:148:VAL:HG12 | 3:L:201:HIS:HB2   | 1.68                     | 0.76              |
| 1:A:1125:ASN:H   | 1:A:1125:ASN:HD22 | 1.33                     | 0.76              |
| 1:C:675:GLN:HA   | 1:C:675:GLN:NE2   | 1.99                     | 0.75              |
| 2:J:61:PRO:HA    | 2:J:64:LYS:HB2    | 1.68                     | 0.75              |
| 1:A:826:VAL:HG13 | 1:A:1057:PRO:HG2  | 1.68                     | 0.75              |
| 2:H:62:SER:HB3   | 3:L:1:GLN:CB      | 2.13                     | 0.75              |
| 2:H:121:ALA:HB3  | 2:H:153:PHE:CZ    | 2.21                     | 0.75              |
| 1:A:521:PRO:HB3  | 1:B:199:GLY:HA3   | 1.67                     | 0.75              |
| 2:H:14:PRO:O     | 2:H:15:SER:OG     | 2.02                     | 0.75              |
| 3:N:56:ARG:HG3   | 3:N:56:ARG:NH1    | 2.00                     | 0.75              |
| 2:H:15:SER:O     | 2:H:16:GLU:CD     | 2.29                     | 0.75              |
| 2:J:15:SER:O     | 2:J:16:GLU:CD     | 2.29                     | 0.75              |
| 2:J:79:SER:OG    | 2:J:81:LYS:NZ     | 2.20                     | 0.74              |
| 2:H:152:TYR:HD2  | 2:H:207:HIS:HE2   | 1.32                     | 0.74              |
| 3:N:148:VAL:HG12 | 3:N:201:HIS:HB2   | 1.68                     | 0.74              |
| 1:C:676:THR:C    | 1:C:690:GLN:NE2   | 2.45                     | 0.74              |
| 2:H:57:THR:OG1   | 2:H:58:ASN:N      | 2.15                     | 0.74              |
| 2:H:79:SER:OG    | 2:H:81:LYS:NZ     | 2.20                     | 0.74              |
| 1:A:230:PRO:CA   | 1:C:521:PRO:CG    | 2.66                     | 0.74              |
| 2:H:61:PRO:HA    | 2:H:64:LYS:HB2    | 1.68                     | 0.74              |
| 2:H:152:TYR:OH   | 2:H:185:LEU:HD23  | 1.88                     | 0.74              |
| 2:H:152:TYR:HB2  | 2:H:154:PRO:CD    | 2.18                     | 0.73              |
| 2:J:152:TYR:HB2  | 2:J:154:PRO:CD    | 2.18                     | 0.73              |
| 1:C:811:LYS:CB   | 1:C:812:PRO:CD    | 2.66                     | 0.73              |
| 2:J:152:TYR:CD2  | 2:J:154:PRO:HG2   | 2.23                     | 0.73              |
| 2:J:152:TYR:OH   | 2:J:185:LEU:HD23  | 1.88                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:577:ARG:HH11 | 1:B:582:LEU:CD1  | 2.01                     | 0.73              |
| 2:H:51:ILE:CD1   | 2:H:69:ILE:HB    | 2.17                     | 0.73              |
| 2:H:152:TYR:CD2  | 2:H:154:PRO:HG2  | 2.23                     | 0.73              |
| 2:J:62:SER:CB    | 3:N:1:GLN:HB2    | 2.13                     | 0.73              |
| 3:N:56:ARG:HH21  | 3:N:62:ASN:CA    | 2.02                     | 0.73              |
| 3:N:85:GLU:N     | 3:N:85:GLU:OE1   | 2.21                     | 0.73              |
| 1:B:1142:GLN:HG3 | 1:B:1143:PRO:HD3 | 1.71                     | 0.73              |
| 2:H:104:LEU:HA   | 3:L:51:TYR:CD2   | 2.24                     | 0.73              |
| 1:B:164:ASN:ND2  | 5:B:1403:NAG:O6  | 2.22                     | 0.72              |
| 3:L:85:GLU:N     | 3:L:85:GLU:OE1   | 2.21                     | 0.72              |
| 1:B:973:ILE:HG12 | 1:B:992:GLN:HE21 | 1.53                     | 0.72              |
| 2:J:157:VAL:HB   | 2:J:207:HIS:NE2  | 2.04                     | 0.72              |
| 2:H:62:SER:CB    | 3:L:1:GLN:HB2    | 2.13                     | 0.72              |
| 2:J:51:ILE:CD1   | 2:J:69:ILE:HB    | 2.17                     | 0.72              |
| 1:C:319:ARG:HA   | 1:C:591:SER:O    | 1.89                     | 0.72              |
| 1:A:230:PRO:HB3  | 1:C:521:PRO:CG   | 2.04                     | 0.72              |
| 2:J:104:LEU:HA   | 3:N:51:TYR:CD2   | 2.24                     | 0.72              |
| 3:L:56:ARG:HH21  | 3:L:62:ASN:CA    | 2.02                     | 0.72              |
| 2:H:157:VAL:HB   | 2:H:207:HIS:NE2  | 2.04                     | 0.71              |
| 1:B:124:THR:OG1  | 5:B:1402:NAG:N2  | 2.22                     | 0.71              |
| 2:J:62:SER:HB3   | 3:N:1:GLN:CB     | 2.13                     | 0.71              |
| 1:A:790:LYS:NZ   | 1:C:702:GLU:OE2  | 2.20                     | 0.71              |
| 1:C:392:PHE:HD2  | 1:C:517:LEU:HD21 | 1.53                     | 0.71              |
| 3:L:28:ASP:OD1   | 3:L:29:VAL:N     | 2.24                     | 0.71              |
| 1:A:359:SER:O    | 1:A:524:VAL:CG1  | 2.39                     | 0.71              |
| 3:L:153:LYS:HA   | 3:L:157:SER:O    | 1.90                     | 0.71              |
| 1:C:359:SER:O    | 1:C:524:VAL:CG1  | 2.39                     | 0.70              |
| 5:B:1410:NAG:H4  | 5:B:1411:NAG:C1  | 2.21                     | 0.70              |
| 2:H:152:TYR:HD2  | 2:H:207:HIS:NE2  | 1.88                     | 0.70              |
| 2:J:35:SER:HB3   | 2:J:50:TYR:HB3   | 1.72                     | 0.70              |
| 1:C:417:LYS:CE   | 1:C:453:TYR:CE2  | 2.74                     | 0.70              |
| 2:J:152:TYR:HD2  | 2:J:207:HIS:NE2  | 1.88                     | 0.70              |
| 2:H:35:SER:HB3   | 2:H:50:TYR:HB3   | 1.72                     | 0.70              |
| 3:L:6:GLN:NE2    | 3:L:90:CYS:SG    | 2.65                     | 0.70              |
| 1:A:227:VAL:HG12 | 1:A:228:ASP:N    | 2.04                     | 0.70              |
| 1:A:229:LEU:O    | 1:A:231:ILE:N    | 2.21                     | 0.70              |
| 1:B:153:MET:HE3  | 1:B:154:GLU:HG3  | 1.72                     | 0.70              |
| 1:C:340:GLU:OE2  | 1:C:356:LYS:CE   | 2.35                     | 0.70              |
| 2:H:61:PRO:HG3   | 4:c:1:NAG:H82    | 1.74                     | 0.70              |
| 2:J:102:TRP:CE3  | 2:J:104:LEU:HD12 | 2.26                     | 0.70              |
| 3:N:153:LYS:HA   | 3:N:157:SER:O    | 1.90                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:LYS:N    | 1:A:212:LEU:O    | 2.25                     | 0.70              |
| 1:A:417:LYS:CE   | 1:A:453:TYR:CE2  | 2.73                     | 0.70              |
| 1:A:124:THR:HG21 | 5:A:1402:NAG:HN2 | 1.56                     | 0.70              |
| 3:N:28:ASP:OD1   | 3:N:29:VAL:N     | 2.24                     | 0.70              |
| 1:C:945:LEU:HD12 | 1:C:948:LEU:HD12 | 1.74                     | 0.70              |
| 3:L:171:GLN:NE2  | 3:L:173:ASN:OD1  | 2.25                     | 0.70              |
| 1:B:391:CYS:HA   | 1:B:525:CYS:HB2  | 1.73                     | 0.69              |
| 3:N:171:GLN:NE2  | 3:N:173:ASN:OD1  | 2.25                     | 0.69              |
| 2:H:102:TRP:CE3  | 2:H:104:LEU:HD12 | 2.26                     | 0.69              |
| 3:N:6:GLN:NE2    | 3:N:90:CYS:SG    | 2.65                     | 0.69              |
| 1:B:577:ARG:NH1  | 1:B:582:LEU:HD13 | 2.07                     | 0.69              |
| 1:A:392:PHE:HD2  | 1:A:517:LEU:HD21 | 1.53                     | 0.69              |
| 1:C:233:ILE:HG12 | 1:C:234:ASN:H    | 1.58                     | 0.68              |
| 2:J:61:PRO:HG3   | 4:d:1:NAG:H82    | 1.74                     | 0.68              |
| 1:C:417:LYS:CD   | 1:C:453:TYR:CE2  | 2.76                     | 0.68              |
| 2:H:152:TYR:CB   | 2:H:207:HIS:HE1  | 2.07                     | 0.68              |
| 1:A:417:LYS:CD   | 1:A:453:TYR:CE2  | 2.76                     | 0.68              |
| 2:J:152:TYR:CB   | 2:J:207:HIS:HE1  | 2.07                     | 0.68              |
| 1:B:546:LEU:HD11 | 1:B:573:THR:HG21 | 1.74                     | 0.68              |
| 1:B:403:ARG:NH2  | 1:B:405:ASP:OD2  | 2.27                     | 0.68              |
| 1:C:323:THR:O    | 1:C:539:VAL:HG23 | 1.93                     | 0.68              |
| 1:B:406:GLU:HG3  | 1:B:418:ILE:HG13 | 1.75                     | 0.68              |
| 1:A:392:PHE:CG   | 1:A:517:LEU:HD21 | 2.29                     | 0.67              |
| 2:H:52:TYR:O     | 2:H:53:TYR:HB3   | 1.95                     | 0.67              |
| 3:N:49:MET:O     | 3:N:57:PRO:HD2   | 1.95                     | 0.67              |
| 1:A:284:THR:CA   | 1:C:560:LEU:HD11 | 2.23                     | 0.67              |
| 1:A:96:GLU:OE1   | 1:A:98:SER:N     | 2.28                     | 0.67              |
| 1:A:964:LYS:CD   | 1:C:570:ALA:HA   | 2.25                     | 0.67              |
| 3:L:49:MET:O     | 3:L:50:ILE:CG2   | 2.43                     | 0.67              |
| 3:L:49:MET:O     | 3:L:57:PRO:HD2   | 1.95                     | 0.67              |
| 2:J:101:ASP:N    | 2:J:101:ASP:OD1  | 2.28                     | 0.67              |
| 2:J:155:GLU:HB3  | 2:J:156:PRO:HD3  | 1.76                     | 0.67              |
| 4:c:1:NAG:O3     | 4:c:2:NAG:C7     | 2.43                     | 0.67              |
| 4:d:1:NAG:O3     | 4:d:2:NAG:C7     | 2.43                     | 0.67              |
| 1:B:97:LYS:HD3   | 1:B:97:LYS:H     | 1.60                     | 0.67              |
| 1:C:392:PHE:CG   | 1:C:517:LEU:HD21 | 2.29                     | 0.67              |
| 3:N:155:ASP:OD2  | 3:N:194:SER:N    | 2.27                     | 0.67              |
| 1:A:310:LYS:NZ   | 1:A:663:ASP:OD1  | 2.27                     | 0.66              |
| 1:A:187:LYS:HG2  | 1:A:213:VAL:HA   | 1.77                     | 0.66              |
| 1:B:1045:LYS:NZ  | 1:C:786:LYS:HE3  | 2.09                     | 0.66              |
| 2:H:155:GLU:HB3  | 2:H:156:PRO:HD3  | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:335:LEU:CA   | 1:A:362:VAL:HG13 | 2.19                     | 0.66              |
| 3:N:49:MET:O     | 3:N:50:ILE:CG2   | 2.43                     | 0.66              |
| 1:C:85:PRO:HA    | 1:C:237:ARG:HA   | 1.78                     | 0.66              |
| 1:B:83:VAL:HG11  | 1:B:237:ARG:HH21 | 1.59                     | 0.66              |
| 1:A:486:PHE:HD1  | 3:L:65:SER:OG    | 1.78                     | 0.66              |
| 1:B:577:ARG:NH1  | 1:B:582:LEU:CD1  | 2.58                     | 0.66              |
| 1:B:691:SER:O    | 1:B:692:ILE:HG13 | 1.96                     | 0.66              |
| 3:L:155:ASP:OD2  | 3:L:194:SER:N    | 2.27                     | 0.66              |
| 3:L:193:ARG:HH21 | 3:L:211:ALA:HB1  | 1.60                     | 0.66              |
| 2:J:154:PRO:C    | 2:J:156:PRO:CD   | 2.67                     | 0.66              |
| 1:A:522:ALA:O    | 1:A:523:THR:OG1  | 2.14                     | 0.66              |
| 2:H:154:PRO:C    | 2:H:156:PRO:CD   | 2.67                     | 0.66              |
| 1:C:111:ASP:OD1  | 1:C:134:GLN:NE2  | 2.28                     | 0.66              |
| 2:H:15:SER:O     | 2:H:16:GLU:OE2   | 2.13                     | 0.66              |
| 2:J:100:ARG:HG3  | 2:J:100:ARG:NH2  | 2.05                     | 0.66              |
| 1:C:189:LEU:HB2  | 1:C:210:ILE:HD13 | 1.78                     | 0.65              |
| 1:C:522:ALA:O    | 1:C:523:THR:OG1  | 2.14                     | 0.65              |
| 2:J:102:TRP:O    | 2:J:104:LEU:HD13 | 1.97                     | 0.65              |
| 1:B:719:THR:HA   | 1:B:926:GLN:HE22 | 1.60                     | 0.65              |
| 1:C:216:LEU:HD12 | 1:C:217:PRO:HD2  | 1.78                     | 0.65              |
| 2:J:210:SER:HG   | 2:J:212:THR:HG1  | 1.41                     | 0.65              |
| 1:A:284:THR:CB   | 1:C:560:LEU:HD11 | 2.25                     | 0.65              |
| 1:A:362:VAL:HG22 | 1:A:527:PRO:HG3  | 1.79                     | 0.65              |
| 1:C:662:CYS:HB2  | 1:C:697:MET:HE3  | 1.76                     | 0.65              |
| 1:C:392:PHE:HD2  | 1:C:517:LEU:CD2  | 2.09                     | 0.65              |
| 2:H:141:GLY:O    | 2:H:193:SER:N    | 2.25                     | 0.65              |
| 2:J:141:GLY:O    | 2:J:193:SER:N    | 2.25                     | 0.65              |
| 1:A:340:GLU:OE2  | 1:A:356:LYS:CE   | 2.35                     | 0.65              |
| 2:J:15:SER:O     | 2:J:16:GLU:OE2   | 2.13                     | 0.65              |
| 2:J:157:VAL:HG23 | 2:J:207:HIS:CD2  | 2.32                     | 0.65              |
| 1:A:569:ILE:HD12 | 1:A:569:ILE:H    | 1.60                     | 0.65              |
| 1:B:358:ILE:HB   | 1:B:395:VAL:HB   | 1.78                     | 0.65              |
| 3:N:54:SER:O     | 3:N:55:LYS:HB2   | 1.96                     | 0.65              |
| 1:A:705:VAL:HB   | 1:B:883:THR:HG21 | 1.78                     | 0.65              |
| 2:H:101:ASP:OD1  | 2:H:101:ASP:N    | 2.28                     | 0.65              |
| 3:L:49:MET:C     | 3:L:50:ILE:HG23  | 2.22                     | 0.65              |
| 3:L:54:SER:O     | 3:L:55:LYS:HB2   | 1.96                     | 0.65              |
| 2:J:52:TYR:O     | 2:J:53:TYR:HB3   | 1.95                     | 0.65              |
| 1:C:569:ILE:H    | 1:C:569:ILE:HD12 | 1.60                     | 0.65              |
| 3:N:49:MET:C     | 3:N:50:ILE:HG23  | 2.22                     | 0.65              |
| 3:N:193:ARG:HH21 | 3:N:211:ALA:HB1  | 1.60                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:455:LEU:HD21 | 1:B:457:ARG:HG3  | 1.78                     | 0.65              |
| 1:A:392:PHE:HD2  | 1:A:517:LEU:CD2  | 2.09                     | 0.64              |
| 2:H:102:TRP:O    | 2:H:104:LEU:HD13 | 1.96                     | 0.64              |
| 2:H:157:VAL:HG23 | 2:H:207:HIS:CD2  | 2.32                     | 0.64              |
| 3:L:52:ASP:O     | 3:L:54:SER:N     | 2.29                     | 0.64              |
| 3:N:52:ASP:O     | 3:N:54:SER:N     | 2.29                     | 0.64              |
| 1:B:108:THR:HA   | 1:B:236:THR:HG22 | 1.79                     | 0.64              |
| 1:C:335:LEU:CA   | 1:C:362:VAL:HG13 | 2.19                     | 0.64              |
| 1:B:350:VAL:HG22 | 1:B:453:TYR:HB2  | 1.79                     | 0.64              |
| 1:B:472:ILE:HD13 | 1:B:474:GLN:HB3  | 1.79                     | 0.64              |
| 1:C:417:LYS:HD2  | 1:C:453:TYR:CD2  | 2.33                     | 0.64              |
| 1:C:676:THR:HA   | 1:C:690:GLN:CB   | 2.25                     | 0.64              |
| 1:C:331:ASN:O    | 1:C:332:ILE:HG13 | 1.98                     | 0.64              |
| 1:C:486:PHE:HD1  | 3:N:65:SER:OG    | 1.77                     | 0.64              |
| 2:J:13:LYS:HD2   | 2:J:14:PRO:HD3   | 1.65                     | 0.64              |
| 1:B:607:GLN:O    | 1:B:608:VAL:HG23 | 1.98                     | 0.64              |
| 1:A:391:CYS:SG   | 1:A:523:THR:O    | 2.56                     | 0.63              |
| 1:C:391:CYS:SG   | 1:C:523:THR:O    | 2.56                     | 0.63              |
| 2:J:152:TYR:CD2  | 2:J:207:HIS:NE2  | 2.66                     | 0.63              |
| 2:H:100:ARG:HG3  | 2:H:100:ARG:NH2  | 2.05                     | 0.63              |
| 1:A:523:THR:HG22 | 1:A:524:VAL:HG22 | 1.79                     | 0.63              |
| 1:C:196:ASN:ND2  | 1:C:200:TYR:O    | 2.32                     | 0.63              |
| 1:C:362:VAL:HG22 | 1:C:527:PRO:HG3  | 1.79                     | 0.63              |
| 1:C:523:THR:HG22 | 1:C:524:VAL:HG22 | 1.79                     | 0.63              |
| 1:A:117:LEU:HD12 | 1:A:118:LEU:H    | 1.63                     | 0.63              |
| 1:A:230:PRO:HB2  | 1:C:521:PRO:CD   | 2.28                     | 0.63              |
| 2:H:13:LYS:CG    | 2:H:14:PRO:HD2   | 2.25                     | 0.63              |
| 3:N:96:ASN:N     | 3:N:96:ASN:OD1   | 2.31                     | 0.63              |
| 1:A:417:LYS:HD2  | 1:A:453:TYR:CD2  | 2.33                     | 0.62              |
| 2:J:99:GLU:HG2   | 2:J:104:LEU:HD22 | 1.81                     | 0.62              |
| 1:A:124:THR:OG1  | 1:A:125:ASN:N    | 2.32                     | 0.62              |
| 2:H:152:TYR:CD2  | 2:H:207:HIS:NE2  | 2.66                     | 0.62              |
| 1:A:808:ASP:HB3  | 1:A:811:LYS:HD2  | 1.82                     | 0.62              |
| 1:B:111:ASP:OD1  | 1:B:112:SER:N    | 2.31                     | 0.62              |
| 1:C:811:LYS:HB2  | 1:C:812:PRO:HD3  | 1.80                     | 0.62              |
| 2:H:157:VAL:CB   | 2:H:207:HIS:CD2  | 2.83                     | 0.62              |
| 3:L:95:SER:C     | 3:L:96:ASN:OD1   | 2.42                     | 0.62              |
| 1:C:320:VAL:HG21 | 1:C:591:SER:CB   | 2.28                     | 0.62              |
| 1:C:813:SER:O    | 1:C:814:LYS:HE2  | 2.00                     | 0.62              |
| 3:N:95:SER:C     | 3:N:96:ASN:OD1   | 2.42                     | 0.62              |
| 2:H:99:GLU:O     | 2:H:100:ARG:HD3  | 1.99                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:331:ASN:O     | 1:A:332:ILE:HG13 | 1.98                     | 0.62              |
| 1:B:454:ARG:HH21  | 1:B:493:GLN:HG3  | 1.63                     | 0.62              |
| 1:C:457:ARG:NH1   | 1:C:459:SER:O    | 2.33                     | 0.62              |
| 2:H:99:GLU:HG2    | 2:H:104:LEU:HD22 | 1.81                     | 0.62              |
| 1:B:560:LEU:H     | 1:B:563:GLN:HE21 | 1.45                     | 0.62              |
| 1:C:486:PHE:CE1   | 3:N:76:THR:HG21  | 2.32                     | 0.62              |
| 2:H:152:TYR:HD2   | 2:H:154:PRO:CG   | 2.12                     | 0.62              |
| 2:H:202:ILE:HG12  | 2:H:217:LYS:HA   | 1.82                     | 0.62              |
| 1:A:96:GLU:OE1    | 1:A:97:LYS:N     | 2.32                     | 0.61              |
| 2:H:13:LYS:HD2    | 2:H:14:PRO:HD3   | 1.65                     | 0.61              |
| 3:L:92:SER:OG     | 3:L:93:TYR:N     | 2.28                     | 0.61              |
| 1:A:457:ARG:NH1   | 1:A:459:SER:O    | 2.33                     | 0.61              |
| 1:A:516:GLU:O     | 1:A:517:LEU:CD2  | 2.48                     | 0.61              |
| 1:B:391:CYS:CA    | 1:B:525:CYS:HB2  | 2.30                     | 0.61              |
| 2:J:99:GLU:O      | 2:J:100:ARG:HD3  | 1.99                     | 0.61              |
| 1:C:320:VAL:HG21  | 1:C:591:SER:HB2  | 1.82                     | 0.61              |
| 2:J:157:VAL:CB    | 2:J:207:HIS:CD2  | 2.83                     | 0.61              |
| 1:A:43:PHE:HB2    | 1:C:563:GLN:HB3  | 1.81                     | 0.61              |
| 3:L:96:ASN:OD1    | 3:L:96:ASN:N     | 2.31                     | 0.61              |
| 2:H:11:LEU:HD12   | 2:H:11:LEU:O     | 2.00                     | 0.61              |
| 3:L:52:ASP:C      | 3:L:54:SER:H     | 2.09                     | 0.61              |
| 2:J:13:LYS:CG     | 2:J:14:PRO:HD2   | 2.25                     | 0.61              |
| 2:J:152:TYR:HD2   | 2:J:154:PRO:CG   | 2.11                     | 0.61              |
| 1:C:516:GLU:O     | 1:C:517:LEU:CD2  | 2.48                     | 0.61              |
| 1:A:1077:THR:HG22 | 1:A:1095:PHE:O   | 2.01                     | 0.61              |
| 3:N:52:ASP:C      | 3:N:54:SER:H     | 2.09                     | 0.61              |
| 2:H:103:PRO:O     | 2:H:105:ASP:N    | 2.34                     | 0.61              |
| 3:L:56:ARG:CZ     | 3:L:62:ASN:HA    | 2.31                     | 0.61              |
| 2:J:47:TRP:O      | 2:J:60:ASN:ND2   | 2.34                     | 0.61              |
| 2:J:202:ILE:HG12  | 2:J:217:LYS:HA   | 1.82                     | 0.61              |
| 3:L:112:GLN:CD    | 3:L:112:GLN:H    | 2.09                     | 0.61              |
| 1:C:520:ALA:CB    | 1:C:521:PRO:CD   | 2.79                     | 0.60              |
| 2:J:11:LEU:HD12   | 2:J:11:LEU:O     | 2.00                     | 0.60              |
| 1:A:617:CYS:H     | 1:A:644:GLN:HE22 | 1.49                     | 0.60              |
| 1:C:112:SER:HB2   | 1:C:113:LYS:HD3  | 1.83                     | 0.60              |
| 2:J:157:VAL:CG2   | 2:J:207:HIS:CD2  | 2.84                     | 0.60              |
| 1:B:395:VAL:HG23  | 1:B:524:VAL:HG11 | 1.84                     | 0.60              |
| 1:B:409:GLN:NE2   | 1:B:416:GLY:HA3  | 2.16                     | 0.60              |
| 1:C:357:ARG:HH12  | 1:C:394:ASN:HD21 | 1.49                     | 0.60              |
| 3:N:4:LEU:HD23    | 3:N:5:THR:O      | 2.02                     | 0.60              |
| 3:N:152:TRP:O     | 3:N:153:LYS:NZ   | 2.34                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:164:ASN:OD1  | 1:A:164:ASN:N    | 2.35                     | 0.60              |
| 1:A:964:LYS:CE   | 1:C:570:ALA:HA   | 2.32                     | 0.60              |
| 2:J:66:ARG:NH2   | 2:J:89:ASP:OD2   | 2.35                     | 0.60              |
| 1:A:556:ASN:HD22 | 1:A:556:ASN:H    | 1.50                     | 0.60              |
| 1:C:556:ASN:HD22 | 1:C:556:ASN:H    | 1.49                     | 0.60              |
| 2:H:157:VAL:CG2  | 2:H:207:HIS:CD2  | 2.85                     | 0.60              |
| 3:N:56:ARG:CZ    | 3:N:62:ASN:HA    | 2.31                     | 0.60              |
| 1:C:521:PRO:O    | 1:C:522:ALA:HB2  | 2.01                     | 0.60              |
| 2:J:103:PRO:O    | 2:J:105:ASP:N    | 2.34                     | 0.60              |
| 1:B:216:LEU:HD12 | 1:B:217:PRO:HD2  | 1.84                     | 0.59              |
| 2:J:121:ALA:CB   | 2:J:153:PHE:CZ   | 2.81                     | 0.59              |
| 1:A:233:ILE:CG1  | 1:A:234:ASN:H    | 2.08                     | 0.59              |
| 1:A:521:PRO:O    | 1:A:522:ALA:HB2  | 2.01                     | 0.59              |
| 1:B:206:LYS:HD2  | 1:B:207:HIS:H    | 1.68                     | 0.59              |
| 2:H:48:ILE:HG22  | 2:H:49:GLY:H     | 1.67                     | 0.59              |
| 2:H:139:SER:N    | 2:H:142:THR:O    | 2.31                     | 0.59              |
| 3:L:4:LEU:HD23   | 3:L:5:THR:O      | 2.02                     | 0.59              |
| 1:A:141:LEU:HB2  | 1:A:156:GLU:HB2  | 1.85                     | 0.59              |
| 1:C:408:ARG:HH21 | 1:C:408:ARG:CG   | 2.14                     | 0.59              |
| 3:N:112:GLN:CD   | 3:N:112:GLN:H    | 2.09                     | 0.59              |
| 1:C:95:THR:HG22  | 1:C:96:GLU:H     | 1.66                     | 0.59              |
| 2:H:66:ARG:NH2   | 2:H:89:ASP:OD2   | 2.35                     | 0.59              |
| 2:H:152:TYR:CE1  | 2:H:183:TYR:O    | 2.55                     | 0.59              |
| 3:N:51:TYR:H     | 3:N:51:TYR:HD1   | 1.50                     | 0.59              |
| 3:N:92:SER:OG    | 3:N:93:TYR:N     | 2.28                     | 0.59              |
| 1:A:645:THR:HG22 | 1:A:647:ALA:H    | 1.67                     | 0.59              |
| 2:H:157:VAL:HB   | 2:H:207:HIS:HE2  | 1.67                     | 0.59              |
| 1:A:408:ARG:HH21 | 1:A:408:ARG:CG   | 2.14                     | 0.59              |
| 2:H:152:TYR:HB2  | 2:H:154:PRO:HD2  | 1.83                     | 0.59              |
| 2:J:145:LEU:HD13 | 2:J:218:VAL:HG21 | 1.84                     | 0.59              |
| 1:A:233:ILE:CG1  | 1:A:234:ASN:N    | 2.56                     | 0.59              |
| 1:A:357:ARG:HH12 | 1:A:394:ASN:HD21 | 1.49                     | 0.59              |
| 2:H:47:TRP:O     | 2:H:60:ASN:ND2   | 2.34                     | 0.59              |
| 2:J:48:ILE:HG22  | 2:J:49:GLY:H     | 1.67                     | 0.59              |
| 2:J:152:TYR:CD1  | 2:J:183:TYR:O    | 2.56                     | 0.59              |
| 3:N:39:GLN:NE2   | 3:N:88:TYR:OH    | 2.36                     | 0.59              |
| 1:A:361:CYS:N    | 1:A:524:VAL:HG12 | 2.18                     | 0.58              |
| 1:A:722:VAL:HA   | 1:A:1064:HIS:O   | 2.03                     | 0.58              |
| 1:C:599:THR:HG22 | 1:C:601:GLY:H    | 1.66                     | 0.58              |
| 1:C:811:LYS:CB   | 1:C:812:PRO:HD2  | 2.28                     | 0.58              |
| 2:H:64:LYS:O     | 2:H:65:SER:OG    | 2.19                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:132:ASN:HD22 | 3:L:186:PRO:HG2  | 1.68                     | 0.58              |
| 2:J:152:TYR:HB2  | 2:J:154:PRO:HD2  | 1.83                     | 0.58              |
| 2:J:152:TYR:CE1  | 2:J:183:TYR:O    | 2.55                     | 0.58              |
| 3:L:56:ARG:HH11  | 3:L:56:ARG:CG    | 2.14                     | 0.58              |
| 1:A:438:SER:O    | 1:A:438:SER:OG   | 2.21                     | 0.58              |
| 2:H:134:SER:H    | 2:H:137:SER:HB2  | 1.68                     | 0.58              |
| 4:Z:2:NAG:H3     | 4:Z:2:NAG:H83    | 1.86                     | 0.58              |
| 1:A:206:LYS:NZ   | 1:A:221:SER:OG   | 2.35                     | 0.58              |
| 1:B:452:LEU:HD21 | 1:B:492:LEU:HD13 | 1.85                     | 0.58              |
| 3:L:39:GLN:NE2   | 3:L:88:TYR:OH    | 2.36                     | 0.58              |
| 3:N:201:HIS:O    | 3:N:204:SER:OG   | 2.21                     | 0.58              |
| 1:A:901:GLN:HE21 | 1:A:905:ARG:HE   | 1.50                     | 0.58              |
| 1:C:324:GLU:OE2  | 1:C:534:VAL:CG1  | 2.50                     | 0.58              |
| 1:C:361:CYS:N    | 1:C:524:VAL:HG12 | 2.18                     | 0.58              |
| 2:H:145:LEU:HD13 | 2:H:218:VAL:HG21 | 1.84                     | 0.58              |
| 3:L:51:TYR:H     | 3:L:51:TYR:HD1   | 1.51                     | 0.58              |
| 3:N:5:THR:HB     | 3:N:23:THR:O     | 2.03                     | 0.58              |
| 2:H:152:TYR:CD1  | 2:H:183:TYR:O    | 2.56                     | 0.58              |
| 3:L:50:ILE:HG22  | 3:L:56:ARG:HA    | 1.85                     | 0.58              |
| 2:J:134:SER:H    | 2:J:137:SER:HB2  | 1.68                     | 0.58              |
| 3:N:49:MET:O     | 3:N:50:ILE:HG23  | 2.04                     | 0.58              |
| 3:N:132:ASN:HD22 | 3:N:186:PRO:HG2  | 1.68                     | 0.58              |
| 1:B:214:ARG:HD3  | 1:B:214:ARG:N    | 2.18                     | 0.57              |
| 3:L:49:MET:O     | 3:L:50:ILE:HG23  | 2.04                     | 0.57              |
| 3:L:201:HIS:O    | 3:L:204:SER:OG   | 2.21                     | 0.57              |
| 2:J:173:PHE:CE2  | 3:N:139:LEU:HG   | 2.40                     | 0.57              |
| 1:A:813:SER:O    | 1:A:813:SER:OG   | 2.18                     | 0.57              |
| 5:A:1405:NAG:H3  | 5:A:1405:NAG:H83 | 1.86                     | 0.57              |
| 2:J:152:TYR:CD2  | 2:J:207:HIS:CE1  | 2.93                     | 0.57              |
| 1:C:390:LEU:HD23 | 1:C:391:CYS:N    | 2.19                     | 0.57              |
| 2:J:51:ILE:HD12  | 2:J:69:ILE:HG22  | 1.83                     | 0.57              |
| 2:J:152:TYR:HB2  | 2:J:207:HIS:CE1  | 2.31                     | 0.57              |
| 1:B:901:GLN:NE2  | 1:B:905:ARG:HE   | 1.99                     | 0.57              |
| 3:N:50:ILE:HG22  | 3:N:56:ARG:HA    | 1.85                     | 0.57              |
| 1:A:486:PHE:CE1  | 3:L:76:THR:HG21  | 2.34                     | 0.57              |
| 1:C:334:ASN:O    | 1:C:362:VAL:HG12 | 2.05                     | 0.57              |
| 2:H:53:TYR:CD1   | 2:H:54:SER:N     | 2.73                     | 0.57              |
| 2:J:53:TYR:CD1   | 2:J:54:SER:N     | 2.73                     | 0.57              |
| 3:N:51:TYR:CD1   | 3:N:51:TYR:N     | 2.73                     | 0.57              |
| 1:A:392:PHE:HB3  | 1:A:517:LEU:HD22 | 1.82                     | 0.57              |
| 1:C:519:HIS:O    | 1:C:519:HIS:ND1  | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:51:ILE:HD12  | 2:H:69:ILE:HG22  | 1.83                     | 0.57              |
| 3:L:5:THR:HB     | 3:L:23:THR:O     | 2.03                     | 0.57              |
| 2:J:157:VAL:HB   | 2:J:207:HIS:HE2  | 1.67                     | 0.57              |
| 1:A:227:VAL:O    | 1:A:228:ASP:HB2  | 2.04                     | 0.57              |
| 1:A:334:ASN:O    | 1:A:362:VAL:HG12 | 2.05                     | 0.57              |
| 1:A:390:LEU:HD23 | 1:A:391:CYS:N    | 2.19                     | 0.57              |
| 1:A:417:LYS:HD2  | 1:A:453:TYR:CE2  | 2.40                     | 0.57              |
| 5:B:1405:NAG:H83 | 5:B:1405:NAG:H3  | 1.87                     | 0.57              |
| 3:L:152:TRP:O    | 3:L:153:LYS:NZ   | 2.34                     | 0.57              |
| 2:J:152:TYR:CD1  | 2:J:152:TYR:N    | 2.73                     | 0.57              |
| 2:H:74:SER:OG    | 2:H:75:LYS:N     | 2.37                     | 0.57              |
| 2:H:104:LEU:O    | 2:H:105:ASP:HB2  | 2.04                     | 0.57              |
| 2:J:104:LEU:O    | 2:J:105:ASP:HB2  | 2.04                     | 0.57              |
| 1:A:29:THR:HG22  | 1:A:30:ASN:H     | 1.70                     | 0.56              |
| 1:C:804:GLN:HE21 | 1:C:935:GLN:HE22 | 1.52                     | 0.56              |
| 1:A:43:PHE:CD1   | 1:C:563:GLN:OE1  | 2.50                     | 0.56              |
| 1:C:563:GLN:O    | 1:C:577:ARG:NH1  | 2.38                     | 0.56              |
| 2:J:11:LEU:HD21  | 2:J:123:THR:N    | 2.20                     | 0.56              |
| 4:a:2:NAG:H3     | 4:a:2:NAG:H83    | 1.87                     | 0.56              |
| 1:A:335:LEU:CA   | 1:A:362:VAL:CG1  | 2.75                     | 0.56              |
| 1:A:519:HIS:O    | 1:A:519:HIS:ND1  | 2.38                     | 0.56              |
| 1:B:213:VAL:HB   | 1:B:214:ARG:HD3  | 1.87                     | 0.56              |
| 1:B:408:ARG:O    | 1:B:414:GLN:NE2  | 2.32                     | 0.56              |
| 1:C:438:SER:O    | 1:C:438:SER:OG   | 2.21                     | 0.56              |
| 1:C:417:LYS:HD2  | 1:C:453:TYR:CE2  | 2.40                     | 0.56              |
| 2:H:173:PHE:CE2  | 3:L:139:LEU:HG   | 2.40                     | 0.56              |
| 1:A:417:LYS:CD   | 1:A:453:TYR:HE2  | 2.19                     | 0.56              |
| 1:A:563:GLN:O    | 1:A:577:ARG:NH1  | 2.38                     | 0.56              |
| 2:H:152:TYR:CD1  | 2:H:152:TYR:N    | 2.73                     | 0.56              |
| 1:A:105:ILE:HG12 | 1:A:239:GLN:HB2  | 1.87                     | 0.56              |
| 1:A:353:TRP:CD1  | 1:A:353:TRP:H    | 2.23                     | 0.56              |
| 1:B:105:ILE:HG13 | 1:B:110:LEU:HD11 | 1.87                     | 0.56              |
| 1:C:391:CYS:SG   | 1:C:524:VAL:O    | 2.64                     | 0.56              |
| 3:L:152:TRP:NE1  | 3:L:182:LEU:HB2  | 2.21                     | 0.56              |
| 2:J:53:TYR:CG    | 2:J:54:SER:N     | 2.73                     | 0.56              |
| 2:H:53:TYR:CG    | 2:H:54:SER:N     | 2.73                     | 0.56              |
| 2:J:13:LYS:CB    | 2:J:14:PRO:HD2   | 2.35                     | 0.56              |
| 1:B:187:LYS:NZ   | 1:B:213:VAL:HG13 | 2.21                     | 0.56              |
| 1:C:331:ASN:C    | 1:C:332:ILE:HD12 | 2.31                     | 0.56              |
| 5:C:1405:NAG:H3  | 5:C:1405:NAG:H83 | 1.88                     | 0.56              |
| 2:H:11:LEU:HD21  | 2:H:123:THR:N    | 2.20                     | 0.56              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:J:154:PRO:HG2 | 2:J:207:HIS:NE2  | 2.20                     | 0.56              |
| 3:N:152:TRP:NE1 | 3:N:182:LEU:HB2  | 2.21                     | 0.56              |
| 2:H:16:GLU:O    | 2:H:84:SER:N     | 2.39                     | 0.56              |
| 2:H:152:TYR:CD2 | 2:H:207:HIS:CE1  | 2.93                     | 0.56              |
| 2:H:152:TYR:CE1 | 2:H:183:TYR:C    | 2.84                     | 0.56              |
| 1:A:359:SER:O   | 1:A:524:VAL:HG11 | 2.06                     | 0.56              |
| 1:C:502:GLY:N   | 3:N:97:ASN:OD1   | 2.39                     | 0.56              |
| 2:H:210:SER:OG  | 2:H:212:THR:OG1  | 2.22                     | 0.56              |
| 2:J:74:SER:OG   | 2:J:75:LYS:N     | 2.37                     | 0.56              |
| 1:A:391:CYS:SG  | 1:A:524:VAL:O    | 2.64                     | 0.55              |
| 2:H:89:ASP:OD1  | 2:H:89:ASP:N     | 2.38                     | 0.55              |
| 2:H:152:TYR:CB  | 2:H:154:PRO:HD2  | 2.37                     | 0.55              |
| 2:H:154:PRO:HG2 | 2:H:207:HIS:NE2  | 2.20                     | 0.55              |
| 2:J:16:GLU:O    | 2:J:84:SER:N     | 2.39                     | 0.55              |
| 4:I:2:NAG:H3    | 4:I:2:NAG:H83    | 1.87                     | 0.55              |
| 2:H:100:ARG:O   | 2:H:102:TRP:N    | 2.39                     | 0.55              |
| 3:L:2:SER:O     | 3:L:3:ALA:HB2    | 2.06                     | 0.55              |
| 2:J:100:ARG:O   | 2:J:102:TRP:N    | 2.39                     | 0.55              |
| 2:J:152:TYR:CB  | 2:J:154:PRO:HD2  | 2.37                     | 0.55              |
| 2:J:152:TYR:CE1 | 2:J:183:TYR:C    | 2.84                     | 0.55              |
| 2:H:13:LYS:CB   | 2:H:14:PRO:HD2   | 2.35                     | 0.55              |
| 3:N:2:SER:O     | 3:N:3:ALA:HB2    | 2.06                     | 0.55              |
| 1:B:577:ARG:CD  | 1:B:582:LEU:HD13 | 2.35                     | 0.55              |
| 1:C:113:LYS:HD2 | 1:C:164:ASN:HD21 | 1.71                     | 0.55              |
| 1:C:359:SER:O   | 1:C:524:VAL:HG11 | 2.06                     | 0.55              |
| 2:H:13:LYS:HD3  | 2:H:120:SER:OG   | 2.07                     | 0.55              |
| 2:H:152:TYR:HD2 | 2:H:207:HIS:CE1  | 2.25                     | 0.55              |
| 2:H:154:PRO:O   | 2:H:156:PRO:HD3  | 2.07                     | 0.55              |
| 1:A:331:ASN:C   | 1:A:332:ILE:HD12 | 2.31                     | 0.55              |
| 1:A:967:SER:O   | 1:A:967:SER:OG   | 2.24                     | 0.55              |
| 2:J:210:SER:OG  | 2:J:212:THR:OG1  | 2.22                     | 0.55              |
| 3:N:56:ARG:HH11 | 3:N:56:ARG:CG    | 2.14                     | 0.55              |
| 3:N:185:THR:N   | 3:N:188:GLN:OE1  | 2.31                     | 0.55              |
| 1:B:661:GLU:OE2 | 1:B:698:SER:OG   | 2.25                     | 0.55              |
| 1:C:318:PHE:O   | 1:C:319:ARG:HB3  | 2.06                     | 0.55              |
| 4:V:1:NAG:H61   | 4:V:2:NAG:HN2    | 1.71                     | 0.55              |
| 1:A:663:ASP:OD2 | 1:A:673:SER:OG   | 2.22                     | 0.55              |
| 1:C:347:PHE:CE1 | 1:C:509:ARG:HD3  | 2.42                     | 0.55              |
| 1:C:493:GLN:HG2 | 3:N:33:ASN:OD1   | 2.07                     | 0.55              |
| 2:J:13:LYS:HD3  | 2:J:120:SER:OG   | 2.07                     | 0.55              |
| 3:N:127:GLU:CD  | 3:N:127:GLU:H    | 2.15                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:129:LYS:HD3  | 1:C:131:CYS:SG   | 2.46                     | 0.55              |
| 1:C:417:LYS:CD   | 1:C:453:TYR:HE2  | 2.19                     | 0.55              |
| 2:J:152:TYR:HD2  | 2:J:207:HIS:CE1  | 2.25                     | 0.55              |
| 1:A:115:GLN:O    | 1:A:233:ILE:HD11 | 2.08                     | 0.54              |
| 1:A:347:PHE:CE1  | 1:A:509:ARG:HD3  | 2.42                     | 0.54              |
| 1:B:352:ALA:HB2  | 1:B:468:ILE:HD12 | 1.88                     | 0.54              |
| 1:C:353:TRP:CD1  | 1:C:353:TRP:H    | 2.24                     | 0.54              |
| 1:C:556:ASN:HD22 | 1:C:556:ASN:N    | 2.05                     | 0.54              |
| 3:L:53:VAL:HG12  | 3:L:53:VAL:O     | 2.08                     | 0.54              |
| 3:L:56:ARG:NH2   | 3:L:62:ASN:HA    | 2.22                     | 0.54              |
| 1:A:551:VAL:HB   | 1:A:588:THR:HG23 | 1.88                     | 0.54              |
| 1:A:886:TRP:HH2  | 1:A:904:TYR:HD2  | 1.56                     | 0.54              |
| 2:H:198:THR:HA   | 2:J:198:THR:CG2  | 2.24                     | 0.54              |
| 2:J:139:SER:N    | 2:J:142:THR:O    | 2.31                     | 0.54              |
| 2:J:201:TYR:HB2  | 2:J:218:VAL:HG12 | 1.90                     | 0.54              |
| 1:A:556:ASN:HD22 | 1:A:556:ASN:N    | 2.05                     | 0.54              |
| 1:A:707:TYR:HB3  | 1:B:792:PRO:HG3  | 1.90                     | 0.54              |
| 2:H:86:THR:O     | 2:H:86:THR:OG1   | 2.21                     | 0.54              |
| 2:J:154:PRO:O    | 2:J:155:GLU:HB2  | 2.08                     | 0.54              |
| 3:N:115:ALA:HB3  | 3:N:144:TYR:N    | 2.23                     | 0.54              |
| 3:N:117:PRO:HD3  | 3:N:201:HIS:HD2  | 1.71                     | 0.54              |
| 1:A:100:ILE:O    | 1:A:242:LEU:HA   | 2.08                     | 0.54              |
| 1:B:166:CYS:SG   | 1:B:167:THR:N    | 2.81                     | 0.54              |
| 1:C:392:PHE:HA   | 1:C:517:LEU:HD11 | 1.89                     | 0.54              |
| 3:L:49:MET:C     | 3:L:50:ILE:CG2   | 2.81                     | 0.54              |
| 3:L:51:TYR:CD1   | 3:L:51:TYR:N     | 2.73                     | 0.54              |
| 3:L:115:ALA:HB3  | 3:L:144:TYR:N    | 2.23                     | 0.54              |
| 3:N:56:ARG:NH2   | 3:N:62:ASN:HA    | 2.22                     | 0.54              |
| 1:A:111:ASP:OD1  | 1:A:134:GLN:NE2  | 2.41                     | 0.54              |
| 1:A:392:PHE:HA   | 1:A:517:LEU:HD11 | 1.89                     | 0.54              |
| 2:H:33:TYR:CZ    | 2:H:52:TYR:HD2   | 2.26                     | 0.54              |
| 2:H:52:TYR:CE1   | 2:H:53:TYR:HD2   | 2.21                     | 0.54              |
| 1:A:421:TYR:HA   | 1:A:461:LEU:HG   | 1.90                     | 0.54              |
| 1:B:1142:GLN:HG3 | 1:B:1143:PRO:CD  | 2.37                     | 0.54              |
| 2:H:154:PRO:O    | 2:H:155:GLU:CB   | 2.56                     | 0.54              |
| 1:C:392:PHE:HB3  | 1:C:517:LEU:HD22 | 1.82                     | 0.54              |
| 2:J:33:TYR:CZ    | 2:J:52:TYR:HD2   | 2.26                     | 0.54              |
| 2:J:89:ASP:OD1   | 2:J:89:ASP:N     | 2.38                     | 0.54              |
| 2:J:150:LYS:HB3  | 2:J:151:ASP:OD2  | 2.08                     | 0.54              |
| 1:C:449:TYR:OH   | 3:N:31:GLY:CA    | 2.44                     | 0.54              |
| 2:H:152:TYR:HB2  | 2:H:207:HIS:CE1  | 2.31                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:158:THR:HG23  | 2:H:206:ASN:HB3   | 1.89                     | 0.54              |
| 4:E:1:NAG:H61     | 4:E:2:NAG:HN2     | 1.71                     | 0.54              |
| 4:d:1:NAG:HO3     | 4:d:2:NAG:C7      | 2.20                     | 0.54              |
| 1:B:165:ASN:OD1   | 5:B:1403:NAG:N2   | 2.40                     | 0.53              |
| 2:H:154:PRO:O     | 2:H:155:GLU:HB2   | 2.08                     | 0.53              |
| 2:J:64:LYS:O      | 2:J:65:SER:OG     | 2.19                     | 0.53              |
| 1:A:493:GLN:HG2   | 3:L:33:ASN:OD1    | 2.09                     | 0.53              |
| 1:B:333:THR:OG1   | 1:B:334:ASN:N     | 2.41                     | 0.53              |
| 1:B:1045:LYS:HZ2  | 1:C:786:LYS:HE3   | 1.71                     | 0.53              |
| 1:C:97:LYS:HB3    | 1:C:187:LYS:HA    | 1.89                     | 0.53              |
| 1:C:544:ASN:ND2   | 1:C:544:ASN:O     | 2.41                     | 0.53              |
| 3:N:53:VAL:HG12   | 3:N:53:VAL:O      | 2.08                     | 0.53              |
| 1:A:229:LEU:CD1   | 1:A:231:ILE:CD1   | 2.85                     | 0.53              |
| 2:H:56:SER:C      | 2:H:57:THR:HG22   | 2.33                     | 0.53              |
| 3:L:65:SER:OG     | 3:L:76:THR:OG1    | 2.23                     | 0.53              |
| 3:L:143:PHE:HE2   | 3:L:146:GLY:HA2   | 1.73                     | 0.53              |
| 2:J:106:ALA:HB2   | 3:N:36:SER:CB     | 2.39                     | 0.53              |
| 4:G:2:NAG:H83     | 4:G:2:NAG:H3      | 1.90                     | 0.53              |
| 3:L:127:GLU:CD    | 3:L:127:GLU:H     | 2.15                     | 0.53              |
| 2:J:154:PRO:O     | 2:J:155:GLU:CB    | 2.56                     | 0.53              |
| 1:A:964:LYS:HE3   | 1:C:570:ALA:HA    | 1.89                     | 0.53              |
| 1:A:1141:LEU:HD12 | 1:C:1141:LEU:HD11 | 1.90                     | 0.53              |
| 3:L:93:TYR:CG     | 3:L:93:TYR:O      | 2.60                     | 0.53              |
| 3:L:117:PRO:HD3   | 3:L:201:HIS:HD2   | 1.71                     | 0.53              |
| 2:J:13:LYS:CB     | 2:J:14:PRO:CD     | 2.87                     | 0.53              |
| 2:J:158:THR:HG23  | 2:J:206:ASN:HB3   | 1.89                     | 0.53              |
| 3:N:49:MET:C      | 3:N:50:ILE:CG2    | 2.81                     | 0.53              |
| 3:N:143:PHE:HE2   | 3:N:146:GLY:HA2   | 1.73                     | 0.53              |
| 1:C:319:ARG:HB2   | 1:C:592:PHE:HB3   | 1.91                     | 0.53              |
| 1:C:421:TYR:HA    | 1:C:461:LEU:HG    | 1.90                     | 0.53              |
| 2:H:201:TYR:HB2   | 2:H:218:VAL:HG12  | 1.90                     | 0.53              |
| 1:C:105:ILE:HG23  | 1:C:241:LEU:HD11  | 1.91                     | 0.53              |
| 1:C:476:GLY:H     | 1:C:487:ASN:HB3   | 1.74                     | 0.53              |
| 1:B:402:ILE:O     | 1:B:507:PRO:HA    | 2.09                     | 0.53              |
| 2:H:33:TYR:CZ     | 2:H:52:TYR:CD2    | 2.96                     | 0.53              |
| 1:A:516:GLU:C     | 1:A:517:LEU:CD2   | 2.82                     | 0.53              |
| 3:L:154:ALA:O     | 3:L:156:SER:N     | 2.42                     | 0.53              |
| 4:c:1:NAG:HO3     | 4:c:2:NAG:C7      | 2.22                     | 0.53              |
| 1:A:43:PHE:CD1    | 1:C:559:PHE:HA    | 2.44                     | 0.53              |
| 1:B:1104:VAL:HG22 | 1:B:1115:ILE:HG12 | 1.91                     | 0.53              |
| 2:J:33:TYR:CZ     | 2:J:52:TYR:CD2    | 2.96                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:154:ALA:O    | 3:N:156:SER:N    | 2.42                     | 0.53              |
| 1:A:57:PRO:O     | 1:A:60:SER:OG    | 2.24                     | 0.52              |
| 1:C:319:ARG:HA   | 1:C:592:PHE:HA   | 1.91                     | 0.52              |
| 1:C:320:VAL:HG23 | 1:C:591:SER:O    | 2.09                     | 0.52              |
| 2:H:52:TYR:CD1   | 2:H:53:TYR:HD2   | 2.25                     | 0.52              |
| 2:H:82:LEU:HD22  | 2:H:85:VAL:HG12  | 1.91                     | 0.52              |
| 1:A:476:GLY:H    | 1:A:487:ASN:HB3  | 1.74                     | 0.52              |
| 1:A:544:ASN:O    | 1:A:544:ASN:ND2  | 2.41                     | 0.52              |
| 2:H:106:ALA:HB2  | 3:L:36:SER:CB    | 2.39                     | 0.52              |
| 2:H:162:ASN:ND2  | 2:H:201:TYR:HA   | 2.20                     | 0.52              |
| 1:A:486:PHE:HE1  | 3:L:76:THR:CG2   | 2.21                     | 0.52              |
| 2:J:56:SER:C     | 2:J:57:THR:HG22  | 2.33                     | 0.52              |
| 3:L:4:LEU:CG     | 3:L:5:THR:H      | 2.23                     | 0.52              |
| 3:L:39:GLN:HB3   | 3:L:49:MET:HE3   | 1.91                     | 0.52              |
| 1:A:894:LEU:HB3  | 1:C:713:ALA:HB3  | 1.90                     | 0.52              |
| 1:B:112:SER:O    | 1:B:113:LYS:HB2  | 2.10                     | 0.52              |
| 2:H:150:LYS:HB3  | 2:H:151:ASP:OD2  | 2.08                     | 0.52              |
| 3:N:115:ALA:HB3  | 3:N:144:TYR:H    | 1.75                     | 0.52              |
| 1:A:230:PRO:HB2  | 1:C:521:PRO:HD2  | 1.90                     | 0.52              |
| 1:B:424:LYS:HB3  | 1:B:463:PRO:HA   | 1.92                     | 0.52              |
| 1:C:392:PHE:CD2  | 1:C:517:LEU:CD2  | 2.85                     | 0.52              |
| 1:C:516:GLU:C    | 1:C:517:LEU:CD2  | 2.82                     | 0.52              |
| 2:J:58:ASN:HB3   | 2:J:64:LYS:HZ1   | 1.75                     | 0.52              |
| 2:J:162:ASN:ND2  | 2:J:201:TYR:HA   | 2.20                     | 0.52              |
| 1:B:403:ARG:HA   | 1:B:495:TYR:OH   | 2.10                     | 0.52              |
| 1:B:457:ARG:NH2  | 1:B:469:SER:O    | 2.43                     | 0.52              |
| 3:N:117:PRO:HD3  | 3:N:201:HIS:CD2  | 2.45                     | 0.52              |
| 1:C:113:LYS:HD3  | 1:C:113:LYS:N    | 2.25                     | 0.52              |
| 1:C:1101:HIS:CD2 | 4:a:1:NAG:H5     | 2.45                     | 0.52              |
| 3:L:185:THR:N    | 3:L:188:GLN:OE1  | 2.31                     | 0.52              |
| 1:B:555:SER:OG   | 1:B:584:ILE:O    | 2.28                     | 0.52              |
| 1:C:193:VAL:HG23 | 1:C:223:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:329:PHE:CE1  | 1:C:544:ASN:HA   | 2.45                     | 0.52              |
| 3:L:117:PRO:HD3  | 3:L:201:HIS:CD2  | 2.45                     | 0.52              |
| 2:J:154:PRO:O    | 2:J:156:PRO:HD3  | 2.07                     | 0.52              |
| 1:B:353:TRP:CZ2  | 1:B:466:ARG:HB3  | 2.45                     | 0.52              |
| 2:J:82:LEU:HD22  | 2:J:85:VAL:HG12  | 1.91                     | 0.52              |
| 1:A:348:ALA:HB2  | 1:A:354:ASN:ND2  | 2.26                     | 0.51              |
| 1:C:715:PRO:HA   | 1:C:1072:GLU:HA  | 1.92                     | 0.51              |
| 3:L:115:ALA:HB3  | 3:L:144:TYR:H    | 1.75                     | 0.51              |
| 1:B:380:TYR:O    | 1:B:430:THR:HA   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:64:TRP:HD1   | 1:A:65:PHE:N     | 2.07                     | 0.51              |
| 1:A:379:CYS:HB3  | 1:A:382:VAL:O    | 2.10                     | 0.51              |
| 1:A:901:GLN:NE2  | 1:A:905:ARG:HH21 | 2.07                     | 0.51              |
| 1:B:560:LEU:H    | 1:B:563:GLN:NE2  | 2.08                     | 0.51              |
| 1:C:83:VAL:HG22  | 1:C:237:ARG:HD2  | 1.92                     | 0.51              |
| 2:H:13:LYS:CD    | 2:H:14:PRO:HD3   | 2.32                     | 0.51              |
| 3:N:39:GLN:HB3   | 3:N:49:MET:HE3   | 1.91                     | 0.51              |
| 3:N:93:TYR:O     | 3:N:93:TYR:CG    | 2.60                     | 0.51              |
| 3:L:152:TRP:CE2  | 3:L:182:LEU:HB2  | 2.46                     | 0.51              |
| 3:L:193:ARG:NH2  | 3:L:212:PRO:O    | 2.25                     | 0.51              |
| 1:A:502:GLY:N    | 3:L:97:ASN:OD1   | 2.41                     | 0.51              |
| 2:H:13:LYS:CB    | 2:H:14:PRO:CD    | 2.87                     | 0.51              |
| 2:H:14:PRO:O     | 2:H:15:SER:CB    | 2.59                     | 0.51              |
| 2:H:58:ASN:HD21  | 2:H:67:VAL:HG22  | 1.76                     | 0.51              |
| 1:C:348:ALA:HB2  | 1:C:354:ASN:ND2  | 2.26                     | 0.51              |
| 2:H:104:LEU:HA   | 3:L:51:TYR:HD2   | 1.75                     | 0.51              |
| 2:J:47:TRP:C     | 2:J:48:ILE:HG13  | 2.36                     | 0.51              |
| 1:A:130:VAL:HB   | 1:A:168:PHE:HB3  | 1.93                     | 0.51              |
| 1:A:329:PHE:CE1  | 1:A:544:ASN:HA   | 2.45                     | 0.51              |
| 2:H:186:SER:HG   | 3:L:181:TYR:HH   | 1.58                     | 0.51              |
| 3:N:84:ASP:OD1   | 3:N:84:ASP:N     | 2.43                     | 0.51              |
| 3:N:193:ARG:NH2  | 3:N:212:PRO:O    | 2.26                     | 0.51              |
| 1:C:97:LYS:HD3   | 1:C:187:LYS:HA   | 1.93                     | 0.51              |
| 1:C:379:CYS:HB3  | 1:C:382:VAL:O    | 2.10                     | 0.51              |
| 1:C:502:GLY:HA3  | 3:N:97:ASN:OD1   | 2.11                     | 0.51              |
| 2:H:162:ASN:HD22 | 2:H:166:LEU:HD11 | 1.76                     | 0.51              |
| 2:J:106:ALA:HB2  | 3:N:36:SER:OG    | 2.11                     | 0.51              |
| 1:A:408:ARG:CG   | 1:A:408:ARG:NH2  | 2.73                     | 0.51              |
| 1:A:521:PRO:HG3  | 1:B:199:GLY:O    | 2.11                     | 0.51              |
| 1:C:113:LYS:H    | 1:C:132:GLU:HB3  | 1.76                     | 0.51              |
| 1:A:502:GLY:HA3  | 3:L:97:ASN:OD1   | 2.11                     | 0.50              |
| 2:H:47:TRP:C     | 2:H:48:ILE:HG13  | 2.36                     | 0.50              |
| 1:A:129:LYS:HG2  | 1:A:133:PHE:HZ   | 1.76                     | 0.50              |
| 1:C:401:VAL:HG22 | 1:C:509:ARG:HG2  | 1.93                     | 0.50              |
| 2:J:58:ASN:HD21  | 2:J:67:VAL:HG22  | 1.76                     | 0.50              |
| 2:J:13:LYS:CD    | 2:J:14:PRO:HD3   | 2.32                     | 0.50              |
| 3:N:49:MET:O     | 3:N:50:ILE:HG22  | 2.11                     | 0.50              |
| 1:C:804:GLN:HE21 | 1:C:935:GLN:NE2  | 2.08                     | 0.50              |
| 1:A:401:VAL:HG22 | 1:A:509:ARG:HG2  | 1.93                     | 0.50              |
| 1:B:675:GLN:HA   | 1:B:690:GLN:HG3  | 1.93                     | 0.50              |
| 1:C:493:GLN:CG   | 3:N:33:ASN:OD1   | 2.60                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:58:ASN:OD1   | 2:H:59:TYR:N     | 2.45                     | 0.50              |
| 3:N:56:ARG:NH2   | 3:N:62:ASN:CA    | 2.70                     | 0.50              |
| 3:N:65:SER:OG    | 3:N:76:THR:OG1   | 2.23                     | 0.50              |
| 3:L:49:MET:O     | 3:L:50:ILE:HG22  | 2.11                     | 0.50              |
| 2:J:52:TYR:CD1   | 2:J:53:TYR:HD2   | 2.25                     | 0.50              |
| 2:J:58:ASN:OD1   | 2:J:59:TYR:N     | 2.45                     | 0.50              |
| 2:J:104:LEU:O    | 2:J:105:ASP:CB   | 2.60                     | 0.50              |
| 2:J:162:ASN:HD22 | 2:J:166:LEU:HD11 | 1.76                     | 0.50              |
| 1:B:616:ASN:HB3  | 1:B:618:THR:HG22 | 1.94                     | 0.50              |
| 1:C:1032:CYS:O   | 1:C:1051:SER:HB2 | 2.12                     | 0.50              |
| 1:C:1090:PRO:HD3 | 1:C:1095:PHE:CE2 | 2.47                     | 0.50              |
| 4:S:1:NAG:H62    | 4:S:2:NAG:H2     | 1.93                     | 0.50              |
| 1:A:106:PHE:HB3  | 1:A:235:ILE:HD13 | 1.93                     | 0.50              |
| 3:L:16:GLN:O     | 3:L:79:GLY:N     | 2.45                     | 0.50              |
| 3:L:187:GLU:HA   | 3:L:190:LYS:HG2  | 1.94                     | 0.50              |
| 2:J:52:TYR:CE1   | 2:J:53:TYR:HE2   | 2.08                     | 0.50              |
| 3:N:152:TRP:CE2  | 3:N:182:LEU:HB2  | 2.46                     | 0.50              |
| 1:A:431:GLY:HA3  | 1:A:513:LEU:O    | 2.12                     | 0.49              |
| 1:A:735:SER:HB3  | 1:A:859:THR:HG22 | 1.94                     | 0.49              |
| 1:B:112:SER:N    | 1:B:133:PHE:O    | 2.45                     | 0.49              |
| 1:B:350:VAL:HG23 | 1:B:422:ASN:HD22 | 1.77                     | 0.49              |
| 1:C:807:PRO:O    | 1:C:809:PRO:HD3  | 2.12                     | 0.49              |
| 2:H:104:LEU:O    | 2:H:105:ASP:CB   | 2.60                     | 0.49              |
| 2:H:115:MET:HE2  | 2:H:155:GLU:OE2  | 2.12                     | 0.49              |
| 3:L:84:ASP:OD1   | 3:L:84:ASP:N     | 2.43                     | 0.49              |
| 2:J:115:MET:HE2  | 2:J:155:GLU:OE2  | 2.12                     | 0.49              |
| 3:N:69:SER:OG    | 3:N:70:GLY:N     | 2.45                     | 0.49              |
| 1:B:31:SER:O     | 1:B:59:PHE:HA    | 2.10                     | 0.49              |
| 1:C:576:VAL:HG22 | 1:C:587:ILE:HD11 | 1.94                     | 0.49              |
| 2:H:21:THR:HA    | 2:H:78:PHE:O     | 2.13                     | 0.49              |
| 2:H:106:ALA:HB2  | 3:L:36:SER:OG    | 2.11                     | 0.49              |
| 3:L:56:ARG:NH2   | 3:L:62:ASN:CA    | 2.70                     | 0.49              |
| 1:C:363:ALA:O    | 1:C:527:PRO:HD3  | 2.12                     | 0.49              |
| 2:H:157:VAL:HG22 | 2:H:158:THR:N    | 2.27                     | 0.49              |
| 1:A:131:CYS:H    | 1:A:133:PHE:HE1  | 1.59                     | 0.49              |
| 1:A:363:ALA:O    | 1:A:527:PRO:HD3  | 2.12                     | 0.49              |
| 1:C:321:GLN:O    | 1:C:538:CYS:HB3  | 2.13                     | 0.49              |
| 1:A:229:LEU:CD1  | 1:A:231:ILE:CG1  | 2.86                     | 0.49              |
| 1:C:322:PRO:C    | 1:C:323:THR:CG2  | 2.86                     | 0.49              |
| 2:H:39:GLN:O     | 2:H:91:ALA:HB1   | 2.13                     | 0.49              |
| 2:J:14:PRO:O     | 2:J:15:SER:CB    | 2.59                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:187:GLU:HA   | 3:N:190:LYS:HG2  | 1.94                     | 0.49              |
| 1:A:530:SER:C    | 1:A:531:THR:CG2  | 2.86                     | 0.49              |
| 1:B:331:ASN:HD22 | 4:O:1:NAG:H83    | 1.78                     | 0.49              |
| 1:A:437:ASN:OD1  | 1:A:438:SER:N    | 2.46                     | 0.49              |
| 1:C:117:LEU:HB2  | 1:C:130:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:200:TYR:HB3  | 1:C:228:ASP:OD1  | 2.13                     | 0.49              |
| 1:C:530:SER:C    | 1:C:531:THR:CG2  | 2.86                     | 0.49              |
| 3:N:61:SER:OG    | 3:N:62:ASN:N     | 2.46                     | 0.49              |
| 1:C:408:ARG:CG   | 1:C:408:ARG:NH2  | 2.73                     | 0.49              |
| 3:L:152:TRP:HA   | 3:L:152:TRP:CE3  | 2.48                     | 0.49              |
| 1:A:171:VAL:HG12 | 1:A:172:SER:H    | 1.78                     | 0.49              |
| 1:A:229:LEU:HD12 | 1:A:231:ILE:CD1  | 2.42                     | 0.49              |
| 1:C:335:LEU:O    | 1:C:362:VAL:O    | 2.30                     | 0.49              |
| 2:J:13:LYS:HD2   | 2:J:14:PRO:CG    | 2.28                     | 0.49              |
| 2:J:100:ARG:O    | 2:J:101:ASP:C    | 2.55                     | 0.49              |
| 3:N:25:THR:HG23  | 3:N:27:SER:N     | 2.18                     | 0.49              |
| 3:N:152:TRP:HA   | 3:N:152:TRP:CE3  | 2.48                     | 0.49              |
| 1:A:122:ASN:OD1  | 1:A:122:ASN:N    | 2.46                     | 0.48              |
| 1:B:396:TYR:HB2  | 1:B:514:SER:HB2  | 1.95                     | 0.48              |
| 2:J:21:THR:HA    | 2:J:78:PHE:O     | 2.13                     | 0.48              |
| 1:A:493:GLN:CG   | 3:L:33:ASN:OD1   | 2.62                     | 0.48              |
| 1:A:896:ILE:HG13 | 1:A:897:PRO:HD2  | 1.96                     | 0.48              |
| 1:C:322:PRO:O    | 1:C:323:THR:HG22 | 2.13                     | 0.48              |
| 2:H:58:ASN:HB3   | 2:H:64:LYS:HZ1   | 1.78                     | 0.48              |
| 2:J:157:VAL:HG22 | 2:J:158:THR:N    | 2.27                     | 0.48              |
| 1:B:457:ARG:NH1  | 1:B:467:ASP:HB3  | 2.28                     | 0.48              |
| 1:C:437:ASN:OD1  | 1:C:438:SER:N    | 2.46                     | 0.48              |
| 2:H:152:TYR:N    | 2:H:152:TYR:HD1  | 2.10                     | 0.48              |
| 2:J:86:THR:O     | 2:J:86:THR:OG1   | 2.21                     | 0.48              |
| 2:J:100:ARG:C    | 2:J:101:ASP:OD1  | 2.56                     | 0.48              |
| 1:A:335:LEU:O    | 1:A:362:VAL:O    | 2.30                     | 0.48              |
| 1:C:320:VAL:HG12 | 1:C:321:GLN:H    | 1.77                     | 0.48              |
| 3:L:155:ASP:OD1  | 3:L:192:HIS:HB3  | 2.14                     | 0.48              |
| 2:J:39:GLN:O     | 2:J:91:ALA:HB1   | 2.13                     | 0.48              |
| 1:C:417:LYS:NZ   | 2:J:103:PRO:HG2  | 2.29                     | 0.48              |
| 1:C:675:GLN:NE2  | 1:C:675:GLN:CA   | 2.73                     | 0.48              |
| 2:H:100:ARG:C    | 2:H:101:ASP:OD1  | 2.56                     | 0.48              |
| 3:L:97:ASN:C     | 3:L:98:THR:CG2   | 2.86                     | 0.48              |
| 1:A:707:TYR:HB2  | 1:B:883:THR:HG23 | 1.94                     | 0.48              |
| 1:B:281:GLU:OE2  | 5:B:1405:NAG:H81 | 2.14                     | 0.48              |
| 1:B:327:VAL:HG22 | 1:B:542:ASN:HB3  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1104:VAL:HG22 | 1:C:1115:ILE:HG12 | 1.95                     | 0.48              |
| 2:H:100:ARG:O     | 2:H:101:ASP:C     | 2.55                     | 0.48              |
| 1:A:935:GLN:O     | 1:A:939:SER:HB3   | 2.14                     | 0.48              |
| 1:C:118:LEU:O     | 1:C:128:ILE:HA    | 2.14                     | 0.48              |
| 2:H:84:SER:O      | 2:H:84:SER:OG     | 2.28                     | 0.48              |
| 3:L:61:SER:OG     | 3:L:62:ASN:N      | 2.46                     | 0.48              |
| 1:A:361:CYS:H     | 1:A:524:VAL:HG12  | 1.79                     | 0.48              |
| 1:A:662:CYS:HB2   | 1:A:697:MET:HE3   | 1.95                     | 0.48              |
| 2:H:106:ALA:CB    | 3:L:38:TYR:OH     | 2.50                     | 0.48              |
| 2:H:193:SER:O     | 2:H:196:LEU:HD22  | 2.14                     | 0.48              |
| 2:J:152:TYR:N     | 2:J:152:TYR:HD1   | 2.10                     | 0.48              |
| 1:C:197:ILE:HG22  | 1:C:198:ASP:H     | 1.78                     | 0.48              |
| 3:L:69:SER:OG     | 3:L:70:GLY:N      | 2.45                     | 0.48              |
| 2:J:78:PHE:CD1    | 2:J:78:PHE:N      | 2.82                     | 0.47              |
| 3:N:97:ASN:C      | 3:N:98:THR:CG2    | 2.86                     | 0.47              |
| 1:A:232:GLY:O     | 1:A:233:ILE:HB    | 2.13                     | 0.47              |
| 1:B:459:SER:C     | 1:B:461:LEU:H     | 2.22                     | 0.47              |
| 1:B:557:LYS:NZ    | 1:B:575:ALA:HB2   | 2.29                     | 0.47              |
| 1:C:431:GLY:HA3   | 1:C:513:LEU:O     | 2.12                     | 0.47              |
| 1:C:486:PHE:CE1   | 3:N:76:THR:CB     | 2.97                     | 0.47              |
| 1:C:560:LEU:O     | 1:C:562:PHE:N     | 2.47                     | 0.47              |
| 2:J:52:TYR:CE1    | 2:J:53:TYR:HD2    | 2.21                     | 0.47              |
| 3:N:16:GLN:O      | 3:N:79:GLY:N      | 2.45                     | 0.47              |
| 1:B:576:VAL:O     | 1:B:584:ILE:HA    | 2.13                     | 0.47              |
| 1:B:710:ASN:N     | 1:B:710:ASN:HD22  | 2.11                     | 0.47              |
| 1:C:140:PHE:CE2   | 1:C:244:LEU:HB2   | 2.49                     | 0.47              |
| 2:H:101:ASP:O     | 2:H:103:PRO:HD3   | 2.14                     | 0.47              |
| 3:L:95:SER:C      | 3:L:97:ASN:H      | 2.21                     | 0.47              |
| 3:L:145:PRO:HD2   | 3:L:201:HIS:CE1   | 2.50                     | 0.47              |
| 2:J:49:GLY:HA2    | 2:J:59:TYR:HB2    | 1.96                     | 0.47              |
| 2:J:52:TYR:HD1    | 2:J:53:TYR:CD2    | 2.30                     | 0.47              |
| 2:J:102:TRP:HB3   | 2:J:104:LEU:HD13  | 1.96                     | 0.47              |
| 3:N:145:PRO:HD2   | 3:N:201:HIS:CE1   | 2.50                     | 0.47              |
| 1:A:200:TYR:CZ    | 1:C:521:PRO:CB    | 2.92                     | 0.47              |
| 1:A:886:TRP:CH2   | 1:A:904:TYR:HD2   | 2.31                     | 0.47              |
| 1:C:456:PHE:CE1   | 3:N:55:LYS:CE     | 2.97                     | 0.47              |
| 2:H:50:TYR:O      | 2:H:57:THR:HG23   | 2.14                     | 0.47              |
| 2:H:54:SER:OG     | 2:H:55:GLY:N      | 2.46                     | 0.47              |
| 2:H:134:SER:HB3   | 2:H:221:LYS:HD3   | 1.97                     | 0.47              |
| 2:J:152:TYR:CD2   | 2:J:154:PRO:CG    | 2.94                     | 0.47              |
| 1:A:45:SER:O      | 1:A:47:VAL:HG22   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:284:THR:HA   | 1:C:560:LEU:HD11  | 1.96                     | 0.47              |
| 1:B:748:GLU:CD   | 1:B:981:LEU:HD21  | 2.39                     | 0.47              |
| 1:C:278:LYS:HB2  | 1:C:306:PHE:CZ    | 2.50                     | 0.47              |
| 1:C:530:SER:O    | 1:C:531:THR:HG22  | 2.15                     | 0.47              |
| 3:N:95:SER:C     | 3:N:97:ASN:H      | 2.21                     | 0.47              |
| 3:N:155:ASP:OD1  | 3:N:192:HIS:HB3   | 2.14                     | 0.47              |
| 1:A:369:TYR:CE2  | 1:A:384:PRO:HB2   | 2.50                     | 0.47              |
| 1:A:417:LYS:NZ   | 2:H:103:PRO:HG2   | 2.30                     | 0.47              |
| 1:B:577:ARG:HD3  | 1:B:582:LEU:HD11  | 1.92                     | 0.47              |
| 1:B:1045:LYS:HZ1 | 1:C:786:LYS:HE3   | 1.78                     | 0.47              |
| 1:C:66:HIS:CE1   | 1:C:214:ARG:HH22  | 2.32                     | 0.47              |
| 1:C:143:VAL:C    | 1:C:154:GLU:HA    | 2.38                     | 0.47              |
| 1:C:361:CYS:H    | 1:C:524:VAL:HG12  | 1.79                     | 0.47              |
| 1:C:605:SER:OG   | 1:C:606:ASN:N     | 2.47                     | 0.47              |
| 1:C:973:ILE:HG12 | 1:C:992:GLN:HE21  | 1.79                     | 0.47              |
| 3:L:25:THR:HG22  | 3:L:28:ASP:OD2    | 2.15                     | 0.47              |
| 2:J:50:TYR:O     | 2:J:57:THR:HG23   | 2.14                     | 0.47              |
| 2:J:54:SER:OG    | 2:J:55:GLY:N      | 2.46                     | 0.47              |
| 3:N:25:THR:HG22  | 3:N:28:ASP:OD2    | 2.15                     | 0.47              |
| 3:N:52:ASP:C     | 3:N:54:SER:N      | 2.73                     | 0.47              |
| 3:N:143:PHE:CE2  | 3:N:146:GLY:HA2   | 2.49                     | 0.47              |
| 1:C:369:TYR:CE2  | 1:C:384:PRO:HB2   | 2.50                     | 0.47              |
| 2:H:53:TYR:CE1   | 2:H:54:SER:HB3    | 2.50                     | 0.47              |
| 2:J:84:SER:O     | 2:J:84:SER:OG     | 2.28                     | 0.47              |
| 2:J:193:SER:O    | 2:J:196:LEU:HD22  | 2.14                     | 0.47              |
| 3:N:95:SER:C     | 3:N:97:ASN:N      | 2.73                     | 0.47              |
| 3:N:201:HIS:CE1  | 3:N:202:GLU:HG2   | 2.50                     | 0.47              |
| 1:A:516:GLU:C    | 1:A:517:LEU:HD23  | 2.39                     | 0.47              |
| 1:B:729:VAL:HG13 | 1:B:1059:GLY:HA2  | 1.97                     | 0.47              |
| 1:C:726:ILE:HG12 | 1:C:1061:VAL:HG22 | 1.97                     | 0.47              |
| 3:L:97:ASN:O     | 3:L:98:THR:HG22   | 2.15                     | 0.47              |
| 3:L:143:PHE:CE2  | 3:L:146:GLY:HA2   | 2.49                     | 0.47              |
| 1:A:229:LEU:C    | 1:A:231:ILE:N     | 2.73                     | 0.47              |
| 1:B:403:ARG:NH2  | 1:B:504:GLY:O     | 2.47                     | 0.47              |
| 1:C:393:THR:HA   | 1:C:523:THR:HB    | 1.97                     | 0.47              |
| 2:J:104:LEU:HA   | 3:N:51:TYR:HD2    | 1.75                     | 0.47              |
| 1:A:212:LEU:HD23 | 1:A:215:ASP:HB2   | 1.95                     | 0.46              |
| 1:C:66:HIS:HE1   | 1:C:214:ARG:HH22  | 1.62                     | 0.46              |
| 1:C:364:ASP:O    | 1:C:367:VAL:HG12  | 2.15                     | 0.46              |
| 1:C:804:GLN:HG3  | 1:C:935:GLN:HE22  | 1.80                     | 0.46              |
| 2:H:102:TRP:HB3  | 2:H:104:LEU:HD13  | 1.96                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:152:TYR:HE1   | 2:H:183:TYR:C    | 2.23                     | 0.46              |
| 3:N:97:ASN:O      | 3:N:98:THR:HG22  | 2.15                     | 0.46              |
| 1:A:334:ASN:HB3   | 1:A:361:CYS:HA   | 1.97                     | 0.46              |
| 1:A:1105:THR:HG22 | 1:A:1111:GLU:H   | 1.80                     | 0.46              |
| 1:C:486:PHE:HE1   | 3:N:76:THR:CG2   | 2.20                     | 0.46              |
| 2:H:52:TYR:CE1    | 2:H:53:TYR:HE2   | 2.08                     | 0.46              |
| 1:A:117:LEU:HD12  | 1:A:118:LEU:N    | 2.30                     | 0.46              |
| 1:A:229:LEU:HB2   | 1:A:231:ILE:CD1  | 2.45                     | 0.46              |
| 1:A:456:PHE:CE1   | 3:L:55:LYS:CE    | 2.98                     | 0.46              |
| 2:H:64:LYS:HD2    | 2:H:65:SER:H     | 1.80                     | 0.46              |
| 2:J:33:TYR:CE2    | 2:J:52:TYR:HD2   | 2.33                     | 0.46              |
| 2:J:53:TYR:CE1    | 2:J:54:SER:HB3   | 2.50                     | 0.46              |
| 2:J:64:LYS:HD2    | 2:J:65:SER:H     | 1.80                     | 0.46              |
| 2:J:118:VAL:O     | 2:J:119:SER:OG   | 2.30                     | 0.46              |
| 2:J:152:TYR:HE1   | 2:J:183:TYR:C    | 2.23                     | 0.46              |
| 3:N:117:PRO:HA    | 3:N:143:PHE:HB3  | 1.98                     | 0.46              |
| 1:A:985:ASP:OD1   | 1:A:985:ASP:N    | 2.46                     | 0.46              |
| 1:B:603:ASN:OD1   | 5:B:1407:NAG:N2  | 2.49                     | 0.46              |
| 1:B:713:ALA:HB3   | 1:C:894:LEU:HB3  | 1.97                     | 0.46              |
| 2:J:13:LYS:HB3    | 2:J:14:PRO:HD2   | 1.98                     | 0.46              |
| 2:J:101:ASP:O     | 2:J:103:PRO:HD3  | 2.14                     | 0.46              |
| 2:J:104:LEU:C     | 2:J:105:ASP:OD1  | 2.59                     | 0.46              |
| 1:A:530:SER:O     | 1:A:531:THR:HG22 | 2.15                     | 0.46              |
| 1:A:912:THR:OG1   | 1:A:914:ASN:ND2  | 2.48                     | 0.46              |
| 1:C:516:GLU:C     | 1:C:517:LEU:HD23 | 2.40                     | 0.46              |
| 1:C:977:LEU:HD12  | 1:C:996:LEU:HD12 | 1.98                     | 0.46              |
| 2:H:33:TYR:CE2    | 2:H:52:TYR:HD2   | 2.33                     | 0.46              |
| 3:L:201:HIS:CE1   | 3:L:202:GLU:HG2  | 2.50                     | 0.46              |
| 1:A:500:THR:O     | 1:A:500:THR:OG1  | 2.31                     | 0.46              |
| 1:C:447:GLY:HA2   | 1:C:497:PHE:O    | 2.16                     | 0.46              |
| 2:H:49:GLY:HA2    | 2:H:59:TYR:HB2   | 1.96                     | 0.46              |
| 2:H:78:PHE:N      | 2:H:78:PHE:CD1   | 2.82                     | 0.46              |
| 1:A:449:TYR:OH    | 3:L:31:GLY:CA    | 2.45                     | 0.46              |
| 1:C:334:ASN:HB3   | 1:C:361:CYS:HA   | 1.97                     | 0.46              |
| 1:C:335:LEU:CA    | 1:C:362:VAL:CG1  | 2.75                     | 0.46              |
| 3:L:7:PRO:O       | 3:L:105:THR:OG1  | 2.31                     | 0.46              |
| 3:L:25:THR:HG23   | 3:L:27:SER:N     | 2.18                     | 0.46              |
| 2:J:134:SER:HB3   | 2:J:221:LYS:HD3  | 1.97                     | 0.46              |
| 1:B:532:ASN:ND2   | 1:B:533:LEU:H    | 2.14                     | 0.46              |
| 1:C:53:ASP:HB3    | 1:C:55:PHE:CE2   | 2.51                     | 0.46              |
| 3:L:24:GLY:O      | 3:L:71:ASN:HB2   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:24:GLY:O      | 3:N:71:ASN:HB2   | 2.16                     | 0.46              |
| 1:A:127:VAL:HG11  | 5:A:1402:NAG:H61 | 1.98                     | 0.46              |
| 1:B:710:ASN:HD22  | 1:B:710:ASN:H    | 1.62                     | 0.46              |
| 1:B:722:VAL:HA    | 1:B:1064:HIS:O   | 2.16                     | 0.46              |
| 2:J:33:TYR:HB2    | 2:J:98:LEU:HB3   | 1.98                     | 0.46              |
| 3:N:81:GLN:NE2    | 3:N:83:GLU:OE1   | 2.49                     | 0.46              |
| 1:A:486:PHE:CE1   | 3:L:76:THR:CB    | 2.98                     | 0.46              |
| 1:B:825:LYS:HB3   | 1:B:825:LYS:HE2  | 1.79                     | 0.46              |
| 1:B:1032:CYS:O    | 1:B:1051:SER:HB2 | 2.16                     | 0.46              |
| 1:C:523:THR:CG2   | 1:C:524:VAL:N    | 2.45                     | 0.46              |
| 1:C:703:ASN:C     | 1:C:703:ASN:HD22 | 2.24                     | 0.46              |
| 2:H:13:LYS:HD2    | 2:H:14:PRO:CG    | 2.28                     | 0.46              |
| 2:H:104:LEU:C     | 2:H:105:ASP:OD1  | 2.58                     | 0.46              |
| 2:H:151:ASP:HB3   | 2:H:182:LEU:HD12 | 1.97                     | 0.46              |
| 3:L:95:SER:C      | 3:L:97:ASN:N     | 2.73                     | 0.46              |
| 1:B:424:LYS:HG3   | 1:B:461:LEU:O    | 2.17                     | 0.45              |
| 1:B:437:ASN:HD21  | 1:B:506:GLN:HE21 | 1.64                     | 0.45              |
| 1:B:758:SER:O     | 1:B:762:GLN:HG3  | 2.16                     | 0.45              |
| 1:C:318:PHE:CG    | 1:C:319:ARG:N    | 2.83                     | 0.45              |
| 3:L:84:ASP:N      | 3:L:85:GLU:OE1   | 2.49                     | 0.45              |
| 3:L:154:ALA:HA    | 3:L:195:TYR:CD1  | 2.51                     | 0.45              |
| 2:J:151:ASP:HB3   | 2:J:182:LEU:HD12 | 1.97                     | 0.45              |
| 3:N:84:ASP:N      | 3:N:85:GLU:OE1   | 2.50                     | 0.45              |
| 1:C:314:GLN:HE21  | 1:C:314:GLN:HB2  | 1.56                     | 0.45              |
| 1:C:417:LYS:NZ    | 2:J:103:PRO:CG   | 2.79                     | 0.45              |
| 1:C:456:PHE:HE1   | 3:N:55:LYS:CE    | 2.29                     | 0.45              |
| 1:A:29:THR:HG22   | 1:A:30:ASN:N     | 2.31                     | 0.45              |
| 1:A:393:THR:HA    | 1:A:523:THR:HB   | 1.97                     | 0.45              |
| 1:A:456:PHE:HE1   | 3:L:55:LYS:CE    | 2.30                     | 0.45              |
| 1:A:1094:VAL:HG22 | 1:A:1107:ARG:HG2 | 1.98                     | 0.45              |
| 1:B:130:VAL:HG21  | 1:B:231:ILE:HD12 | 1.99                     | 0.45              |
| 1:B:567:ARG:HE    | 1:B:567:ARG:HB3  | 1.48                     | 0.45              |
| 1:C:319:ARG:O     | 1:C:319:ARG:HG2  | 2.16                     | 0.45              |
| 2:H:25:SER:OG     | 2:H:26:GLY:N     | 2.49                     | 0.45              |
| 2:J:75:LYS:HG3    | 2:J:77:GLN:HG2   | 1.98                     | 0.45              |
| 3:N:154:ALA:HA    | 3:N:195:TYR:CD1  | 2.51                     | 0.45              |
| 3:N:189:TRP:CZ2   | 3:N:212:PRO:HA   | 2.51                     | 0.45              |
| 1:A:227:VAL:CG1   | 1:A:228:ASP:H    | 2.05                     | 0.45              |
| 1:A:903:ALA:HB1   | 1:A:913:GLN:HG2  | 1.98                     | 0.45              |
| 3:L:189:TRP:CZ2   | 3:L:212:PRO:HA   | 2.51                     | 0.45              |
| 1:A:153:MET:SD    | 1:A:153:MET:N    | 2.90                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:364:ASP:O    | 1:A:367:VAL:HG12  | 2.15                     | 0.45              |
| 1:A:578:ASP:OD2  | 1:A:581:THR:HG22  | 2.16                     | 0.45              |
| 1:C:37:TYR:HA    | 1:C:223:LEU:H     | 1.81                     | 0.45              |
| 1:C:377:PHE:CD2  | 1:C:434:ILE:HG12  | 2.51                     | 0.45              |
| 2:H:29:ILE:HD12  | 2:H:29:ILE:HA     | 1.78                     | 0.45              |
| 2:H:93:TYR:O     | 2:H:113:GLY:HA2   | 2.17                     | 0.45              |
| 2:J:25:SER:OG    | 2:J:26:GLY:N      | 2.49                     | 0.45              |
| 1:A:560:LEU:O    | 1:A:562:PHE:N     | 2.47                     | 0.45              |
| 2:H:75:LYS:HG3   | 2:H:77:GLN:HG2    | 1.98                     | 0.45              |
| 2:J:13:LYS:HD2   | 2:J:14:PRO:HD2    | 0.51                     | 0.45              |
| 1:C:676:THR:CA   | 1:C:690:GLN:HE21  | 2.29                     | 0.45              |
| 3:N:154:ALA:O    | 3:N:155:ASP:C     | 2.60                     | 0.45              |
| 1:A:377:PHE:CD2  | 1:A:434:ILE:HG12  | 2.51                     | 0.45              |
| 1:B:353:TRP:CD1  | 1:B:353:TRP:H     | 2.34                     | 0.45              |
| 2:H:70:SER:OG    | 2:H:79:SER:HB3    | 2.17                     | 0.45              |
| 3:L:154:ALA:O    | 3:L:155:ASP:C     | 2.60                     | 0.45              |
| 1:A:447:GLY:HA2  | 1:A:497:PHE:O     | 2.16                     | 0.45              |
| 1:A:617:CYS:HB2  | 1:A:649:CYS:HB2   | 1.87                     | 0.45              |
| 1:A:1090:PRO:HD3 | 1:A:1095:PHE:CE2  | 2.51                     | 0.45              |
| 1:B:521:PRO:HG3  | 1:B:564:GLN:HE21  | 1.81                     | 0.45              |
| 2:H:210:SER:OG   | 2:H:211:ASN:N     | 2.49                     | 0.45              |
| 3:L:81:GLN:NE2   | 3:L:83:GLU:OE1    | 2.49                     | 0.45              |
| 1:A:187:LYS:HE3  | 1:A:213:VAL:HG12  | 1.99                     | 0.45              |
| 1:A:417:LYS:NZ   | 2:H:103:PRO:CG    | 2.80                     | 0.45              |
| 1:A:676:THR:HB   | 1:A:693:ILE:HG21  | 1.98                     | 0.45              |
| 1:C:486:PHE:CE1  | 3:N:76:THR:CG2    | 2.97                     | 0.45              |
| 3:L:117:PRO:HA   | 3:L:143:PHE:HB3   | 1.98                     | 0.45              |
| 1:B:437:ASN:OD1  | 1:B:438:SER:N     | 2.51                     | 0.44              |
| 1:B:521:PRO:HG3  | 1:B:564:GLN:NE2   | 2.32                     | 0.44              |
| 1:C:335:LEU:HD12 | 1:C:335:LEU:C     | 2.42                     | 0.44              |
| 1:C:1141:LEU:O   | 1:C:1145:LEU:HD12 | 2.16                     | 0.44              |
| 3:L:192:HIS:HB2  | 3:L:195:TYR:CE2   | 2.52                     | 0.44              |
| 2:J:121:ALA:O    | 2:J:153:PHE:CD2   | 2.69                     | 0.44              |
| 1:B:350:VAL:HG11 | 1:B:402:ILE:HG23  | 2.00                     | 0.44              |
| 3:L:154:ALA:HB3  | 3:L:157:SER:OG    | 2.18                     | 0.44              |
| 2:J:72:ASP:OD2   | 2:J:75:LYS:NZ     | 2.31                     | 0.44              |
| 3:N:192:HIS:HB2  | 3:N:195:TYR:CE2   | 2.52                     | 0.44              |
| 2:H:13:LYS:HG2   | 2:H:120:SER:HA    | 1.99                     | 0.44              |
| 2:H:33:TYR:HB2   | 2:H:98:LEU:HB3    | 1.98                     | 0.44              |
| 2:H:121:ALA:O    | 2:H:153:PHE:CD2   | 2.69                     | 0.44              |
| 2:J:70:SER:OG    | 2:J:79:SER:HB3    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:J:106:ALA:O     | 2:J:107:PHE:CD2   | 2.70                     | 0.44              |
| 1:A:134:GLN:HB3   | 1:A:162:SER:HB2   | 2.00                     | 0.44              |
| 1:A:440:ASN:ND2   | 1:A:441:LEU:HG    | 2.32                     | 0.44              |
| 1:A:486:PHE:CE1   | 3:L:76:THR:CG2    | 2.99                     | 0.44              |
| 1:B:472:ILE:H     | 1:B:472:ILE:HG13  | 1.56                     | 0.44              |
| 1:B:1045:LYS:NZ   | 1:C:786:LYS:CE    | 2.79                     | 0.44              |
| 2:H:13:LYS:HB3    | 2:H:14:PRO:HD2    | 1.98                     | 0.44              |
| 1:A:43:PHE:CD2    | 1:C:559:PHE:CE1   | 3.05                     | 0.44              |
| 1:A:521:PRO:O     | 1:A:522:ALA:CB    | 2.66                     | 0.44              |
| 1:B:376:THR:CG2   | 1:B:378:LYS:HG3   | 2.48                     | 0.44              |
| 1:C:142:GLY:H     | 1:C:243:ALA:HA    | 1.83                     | 0.44              |
| 1:C:320:VAL:HG12  | 1:C:321:GLN:N     | 2.33                     | 0.44              |
| 1:C:322:PRO:C     | 1:C:323:THR:HG23  | 2.43                     | 0.44              |
| 3:L:51:TYR:CD2    | 3:L:52:ASP:OD1    | 2.70                     | 0.44              |
| 2:J:106:ALA:O     | 2:J:107:PHE:CG    | 2.70                     | 0.44              |
| 1:A:392:PHE:CD2   | 1:A:517:LEU:CD2   | 2.85                     | 0.44              |
| 1:B:453:TYR:HD1   | 1:B:453:TYR:H     | 1.64                     | 0.44              |
| 1:B:454:ARG:NH2   | 1:B:456:PHE:HZ    | 2.16                     | 0.44              |
| 1:C:338:PHE:C     | 1:C:340:GLU:H     | 2.26                     | 0.44              |
| 2:J:186:SER:HG    | 3:N:181:TYR:HH    | 1.65                     | 0.44              |
| 3:N:51:TYR:CD2    | 3:N:52:ASP:OD1    | 2.71                     | 0.44              |
| 1:C:440:ASN:ND2   | 1:C:441:LEU:HG    | 2.32                     | 0.44              |
| 1:C:530:SER:C     | 1:C:531:THR:HG23  | 2.42                     | 0.44              |
| 1:C:578:ASP:OD2   | 1:C:581:THR:HG22  | 2.16                     | 0.44              |
| 2:H:106:ALA:O     | 2:H:107:PHE:CG    | 2.70                     | 0.44              |
| 2:J:108:ASP:O     | 2:J:110:TRP:CD1   | 2.71                     | 0.44              |
| 1:A:140:PHE:CG    | 1:A:244:LEU:HD11  | 2.53                     | 0.44              |
| 1:A:393:THR:O     | 1:A:523:THR:CG2   | 2.58                     | 0.44              |
| 1:C:212:LEU:HD12  | 1:C:212:LEU:HA    | 1.77                     | 0.44              |
| 1:C:417:LYS:HG2   | 2:J:103:PRO:HG2   | 1.99                     | 0.44              |
| 1:C:1040:VAL:O    | 1:C:1041:ASP:HB2  | 2.17                     | 0.44              |
| 2:H:108:ASP:O     | 2:H:110:TRP:CD1   | 2.71                     | 0.44              |
| 2:H:177:LEU:HB2   | 2:H:183:TYR:CE1   | 2.52                     | 0.44              |
| 3:N:4:LEU:CG      | 3:N:5:THR:H       | 2.23                     | 0.44              |
| 3:N:112:GLN:CD    | 3:N:113:PRO:HD3   | 2.43                     | 0.44              |
| 4:V:1:NAG:H61     | 4:V:2:NAG:N2      | 2.33                     | 0.44              |
| 1:A:502:GLY:CA    | 3:L:97:ASN:OD1    | 2.66                     | 0.44              |
| 1:A:546:LEU:HD11  | 1:A:565:PHE:CG    | 2.53                     | 0.44              |
| 1:A:959:LEU:HD23  | 1:A:959:LEU:HA    | 1.78                     | 0.44              |
| 3:L:112:GLN:CD    | 3:L:113:PRO:HD3   | 2.43                     | 0.44              |
| 1:A:1104:VAL:HG22 | 1:A:1115:ILE:HG12 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:167:THR:HG22  | 1:B:168:PHE:H    | 1.82                     | 0.43              |
| 1:C:1081:ILE:HG12 | 1:C:1095:PHE:CE2 | 2.53                     | 0.43              |
| 1:A:646:ARG:O     | 1:A:646:ARG:HG3  | 2.17                     | 0.43              |
| 1:B:439:ASN:HB3   | 1:B:506:GLN:HB2  | 1.99                     | 0.43              |
| 1:B:461:LEU:HD12  | 1:B:461:LEU:HA   | 1.85                     | 0.43              |
| 1:C:502:GLY:CA    | 3:N:97:ASN:OD1   | 2.66                     | 0.43              |
| 2:H:108:ASP:O     | 2:H:109:ILE:C    | 2.61                     | 0.43              |
| 2:J:93:TYR:O      | 2:J:113:GLY:HA2  | 2.17                     | 0.43              |
| 2:J:106:ALA:HB1   | 3:N:38:TYR:HH    | 1.74                     | 0.43              |
| 1:A:964:LYS:HE3   | 1:C:570:ALA:H    | 1.84                     | 0.43              |
| 1:B:187:LYS:HZ3   | 1:B:213:VAL:HG13 | 1.83                     | 0.43              |
| 1:C:84:LEU:HD13   | 1:C:238:PHE:CE1  | 2.52                     | 0.43              |
| 1:C:995:ARG:HE    | 1:C:995:ARG:HB3  | 1.66                     | 0.43              |
| 3:L:151:ALA:HB1   | 3:L:153:LYS:NZ   | 2.33                     | 0.43              |
| 3:N:2:SER:OG      | 3:N:3:ALA:N      | 2.50                     | 0.43              |
| 1:A:338:PHE:C     | 1:A:340:GLU:H    | 2.26                     | 0.43              |
| 1:A:612:TYR:HE1   | 1:A:651:ILE:HD12 | 1.84                     | 0.43              |
| 1:C:132:GLU:CD    | 1:C:165:ASN:HB2  | 2.43                     | 0.43              |
| 1:C:546:LEU:HD11  | 1:C:565:PHE:CG   | 2.53                     | 0.43              |
| 2:H:106:ALA:O     | 2:H:107:PHE:CD2  | 2.71                     | 0.43              |
| 2:H:198:THR:HB    | 2:J:198:THR:OG1  | 2.18                     | 0.43              |
| 2:J:177:LEU:HB2   | 2:J:183:TYR:CE1  | 2.52                     | 0.43              |
| 2:J:210:SER:OG    | 2:J:211:ASN:N    | 2.49                     | 0.43              |
| 1:A:530:SER:C     | 1:A:531:THR:HG23 | 2.43                     | 0.43              |
| 1:A:640:SER:OG    | 1:A:641:ASN:N    | 2.48                     | 0.43              |
| 1:A:1097:SER:HA   | 1:A:1101:HIS:O   | 2.19                     | 0.43              |
| 1:B:121:ASN:O     | 1:B:121:ASN:ND2  | 2.49                     | 0.43              |
| 1:C:521:PRO:O     | 1:C:522:ALA:CB   | 2.66                     | 0.43              |
| 2:H:31:SER:HB2    | 2:H:32:TYR:CD1   | 2.54                     | 0.43              |
| 2:J:31:SER:HB2    | 2:J:32:TYR:CD1   | 2.54                     | 0.43              |
| 2:J:126:PRO:HD3   | 2:J:207:HIS:ND1  | 2.34                     | 0.43              |
| 2:J:198:THR:HG23  | 2:J:199:GLN:HG2  | 2.00                     | 0.43              |
| 1:A:417:LYS:HG2   | 2:H:103:PRO:HG2  | 2.00                     | 0.43              |
| 1:B:364:ASP:OD1   | 1:B:364:ASP:N    | 2.50                     | 0.43              |
| 1:C:119:ILE:HG13  | 1:C:128:ILE:HG23 | 2.01                     | 0.43              |
| 2:H:126:PRO:HD3   | 2:H:207:HIS:ND1  | 2.34                     | 0.43              |
| 3:L:56:ARG:HH21   | 3:L:62:ASN:HA    | 1.75                     | 0.43              |
| 1:A:795:LYS:HB3   | 1:A:797:PHE:CE2  | 2.54                     | 0.43              |
| 1:B:559:PHE:O     | 1:B:560:LEU:HD13 | 2.18                     | 0.43              |
| 1:C:393:THR:O     | 1:C:523:THR:CG2  | 2.58                     | 0.43              |
| 2:H:82:LEU:HD23   | 2:H:83:SER:N     | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:198:THR:HG23 | 2:H:199:GLN:HG2  | 2.00                     | 0.43              |
| 3:L:2:SER:OG     | 3:L:3:ALA:N      | 2.50                     | 0.43              |
| 4:E:1:NAG:H61    | 4:E:2:NAG:N2     | 2.33                     | 0.43              |
| 1:A:1032:CYS:O   | 1:A:1051:SER:HB2 | 2.18                     | 0.43              |
| 1:A:113:LYS:O    | 1:A:113:LYS:NZ   | 2.31                     | 0.43              |
| 1:A:131:CYS:HB3  | 1:A:164:ASN:O    | 2.19                     | 0.43              |
| 1:B:462:LYS:H    | 1:B:462:LYS:HD3  | 1.84                     | 0.43              |
| 1:C:569:ILE:O    | 1:C:570:ALA:HB3  | 2.19                     | 0.43              |
| 2:J:13:LYS:HG2   | 2:J:120:SER:HA   | 1.99                     | 0.43              |
| 3:N:154:ALA:HB3  | 3:N:157:SER:OG   | 2.17                     | 0.43              |
| 1:A:294:ASP:OD1  | 1:A:294:ASP:N    | 2.50                     | 0.43              |
| 1:B:91:TYR:OH    | 1:B:191:GLU:HG2  | 2.19                     | 0.43              |
| 1:B:600:PRO:HB3  | 1:B:674:TYR:HB2  | 2.00                     | 0.43              |
| 2:H:196:LEU:HD23 | 2:H:197:GLY:H    | 1.84                     | 0.43              |
| 2:J:82:LEU:HD23  | 2:J:83:SER:N     | 2.34                     | 0.43              |
| 3:N:56:ARG:HH21  | 3:N:62:ASN:HA    | 1.75                     | 0.43              |
| 1:A:27:ALA:HB3   | 1:A:64:TRP:HB3   | 2.01                     | 0.42              |
| 1:A:569:ILE:O    | 1:A:570:ALA:HB3  | 2.19                     | 0.42              |
| 1:C:722:VAL:HA   | 1:C:1064:HIS:O   | 2.19                     | 0.42              |
| 2:J:29:ILE:O     | 2:J:30:SER:OG    | 2.28                     | 0.42              |
| 2:J:152:TYR:CE2  | 2:J:157:VAL:CG1  | 3.02                     | 0.42              |
| 3:N:151:ALA:HB1  | 3:N:153:LYS:NZ   | 2.33                     | 0.42              |
| 1:A:141:LEU:O    | 1:A:243:ALA:HA   | 2.18                     | 0.42              |
| 1:C:784:GLN:HE21 | 1:C:784:GLN:HB3  | 1.63                     | 0.42              |
| 1:C:912:THR:OG1  | 1:C:914:ASN:ND2  | 2.51                     | 0.42              |
| 1:A:112:SER:O    | 1:A:113:LYS:HB3  | 2.20                     | 0.42              |
| 1:A:127:VAL:HG21 | 5:A:1402:NAG:H5  | 2.01                     | 0.42              |
| 1:A:869:MET:HE1  | 1:C:697:MET:HG3  | 2.00                     | 0.42              |
| 1:C:334:ASN:C    | 1:C:336:CYS:N    | 2.77                     | 0.42              |
| 1:C:740:MET:HE2  | 1:C:740:MET:HB2  | 1.91                     | 0.42              |
| 2:H:86:THR:C     | 2:H:88:ALA:H     | 2.27                     | 0.42              |
| 2:H:152:TYR:CE2  | 2:H:157:VAL:CG1  | 3.02                     | 0.42              |
| 2:J:86:THR:C     | 2:J:88:ALA:H     | 2.27                     | 0.42              |
| 3:N:144:TYR:HB3  | 3:N:145:PRO:HD3  | 1.99                     | 0.42              |
| 1:B:472:ILE:CD1  | 1:B:474:GLN:HB3  | 2.47                     | 0.42              |
| 5:B:1410:NAG:O4  | 5:B:1411:NAG:O5  | 2.28                     | 0.42              |
| 1:C:505:TYR:OH   | 2:J:100:ARG:NH1  | 2.52                     | 0.42              |
| 1:C:793:PRO:HG2  | 1:C:794:ILE:HD12 | 2.00                     | 0.42              |
| 2:H:53:TYR:CD1   | 2:H:53:TYR:C     | 2.97                     | 0.42              |
| 2:H:169:GLY:O    | 2:H:189:VAL:HA   | 2.20                     | 0.42              |
| 3:L:144:TYR:HB3  | 3:L:145:PRO:HD3  | 1.99                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:J:53:TYR:CD1    | 2:J:53:TYR:C     | 2.97                     | 0.42              |
| 2:J:63:LEU:HD23   | 2:J:63:LEU:HA    | 1.75                     | 0.42              |
| 3:N:151:ALA:HB1   | 3:N:153:LYS:HZ3  | 1.84                     | 0.42              |
| 1:A:408:ARG:HD2   | 1:A:409:GLN:HG2  | 2.01                     | 0.42              |
| 1:B:29:THR:OG1    | 1:B:30:ASN:N     | 2.50                     | 0.42              |
| 1:C:1027:THR:HG22 | 1:C:1042:PHE:HZ  | 1.83                     | 0.42              |
| 2:J:108:ASP:O     | 2:J:109:ILE:C    | 2.61                     | 0.42              |
| 1:A:417:LYS:HZ3   | 2:H:103:PRO:HG2  | 1.85                     | 0.42              |
| 1:C:233:ILE:HG12  | 1:C:234:ASN:N    | 2.28                     | 0.42              |
| 1:C:792:PRO:O     | 1:C:795:LYS:NZ   | 2.52                     | 0.42              |
| 2:J:106:ALA:CB    | 3:N:38:TYR:OH    | 2.50                     | 0.42              |
| 3:N:152:TRP:C     | 3:N:153:LYS:HG2  | 2.45                     | 0.42              |
| 1:B:567:ARG:HG2   | 1:C:42:VAL:HG11  | 2.02                     | 0.42              |
| 1:C:408:ARG:HD2   | 1:C:409:GLN:HG2  | 2.01                     | 0.42              |
| 3:L:154:ALA:HB1   | 3:L:192:HIS:HD2  | 1.85                     | 0.42              |
| 1:C:736:VAL:HG23  | 1:C:858:LEU:HD23 | 2.02                     | 0.42              |
| 2:H:51:ILE:HD11   | 2:H:69:ILE:C     | 2.44                     | 0.42              |
| 2:H:87:ALA:HA     | 2:H:118:VAL:HB   | 2.01                     | 0.42              |
| 2:H:152:TYR:CD2   | 2:H:154:PRO:CG   | 2.94                     | 0.42              |
| 2:J:169:GLY:O     | 2:J:189:VAL:HA   | 2.20                     | 0.42              |
| 1:A:973:ILE:HG23  | 1:A:992:GLN:NE2  | 2.35                     | 0.42              |
| 1:B:341:VAL:HG23  | 1:B:342:PHE:HD1  | 1.84                     | 0.42              |
| 1:C:320:VAL:HG23  | 1:C:591:SER:CA   | 2.49                     | 0.42              |
| 2:H:121:ALA:CB    | 2:H:153:PHE:CZ   | 2.82                     | 0.42              |
| 2:J:51:ILE:HD11   | 2:J:69:ILE:C     | 2.44                     | 0.42              |
| 1:A:333:THR:C     | 1:A:335:LEU:H    | 2.28                     | 0.42              |
| 1:B:376:THR:O     | 1:B:434:ILE:HA   | 2.20                     | 0.42              |
| 1:B:495:TYR:CZ    | 1:B:507:PRO:HG3  | 2.55                     | 0.42              |
| 2:H:13:LYS:HD2    | 2:H:14:PRO:HD2   | 0.51                     | 0.42              |
| 2:J:124:LYS:HD3   | 2:J:182:LEU:HD11 | 2.02                     | 0.42              |
| 3:N:120:THR:HG23  | 3:N:139:LEU:HB2  | 2.02                     | 0.42              |
| 1:A:99:ASN:O      | 1:A:102:ARG:NE   | 2.35                     | 0.41              |
| 1:A:334:ASN:C     | 1:A:336:CYS:N    | 2.77                     | 0.41              |
| 1:A:933:LYS:HB2   | 1:A:933:LYS:HE3  | 1.86                     | 0.41              |
| 1:B:110:LEU:HD12  | 1:B:110:LEU:HA   | 1.71                     | 0.41              |
| 1:C:333:THR:C     | 1:C:335:LEU:H    | 2.28                     | 0.41              |
| 2:H:55:GLY:C      | 2:H:56:SER:HG    | 2.27                     | 0.41              |
| 2:H:124:LYS:HD3   | 2:H:182:LEU:HD11 | 2.02                     | 0.41              |
| 2:J:152:TYR:HE1   | 2:J:184:SER:HA   | 1.85                     | 0.41              |
| 2:J:152:TYR:HE2   | 2:J:157:VAL:HG12 | 1.85                     | 0.41              |
| 1:A:758:SER:O     | 1:A:762:GLN:HG3  | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:122:ASN:ND2  | 1:C:125:ASN:HB2  | 2.35                     | 0.41              |
| 3:N:193:ARG:NH1  | 3:N:212:PRO:HG2  | 2.35                     | 0.41              |
| 4:W:1:NAG:H83    | 4:W:1:NAG:H3     | 2.02                     | 0.41              |
| 1:B:81:ASN:O     | 1:B:239:GLN:NE2  | 2.54                     | 0.41              |
| 1:B:379:CYS:HA   | 1:B:432:CYS:HA   | 2.02                     | 0.41              |
| 1:C:117:LEU:HD22 | 1:C:231:ILE:HD12 | 2.03                     | 0.41              |
| 1:C:393:THR:H    | 1:C:517:LEU:HD22 | 1.85                     | 0.41              |
| 3:L:93:TYR:OH    | 3:L:97:ASN:OD1   | 2.38                     | 0.41              |
| 2:J:154:PRO:HG2  | 2:J:207:HIS:HE2  | 1.83                     | 0.41              |
| 1:A:886:TRP:HH2  | 1:A:904:TYR:CD2  | 2.35                     | 0.41              |
| 1:B:142:GLY:O    | 1:B:156:GLU:HG3  | 2.20                     | 0.41              |
| 1:C:856:ASN:O    | 1:C:856:ASN:ND2  | 2.48                     | 0.41              |
| 3:N:193:ARG:HH22 | 3:N:212:PRO:C    | 2.21                     | 0.41              |
| 1:C:392:PHE:CA   | 1:C:517:LEU:HD21 | 2.49                     | 0.41              |
| 1:C:460:ASN:OD1  | 1:C:460:ASN:N    | 2.53                     | 0.41              |
| 1:C:542:ASN:HA   | 1:C:546:LEU:O    | 2.21                     | 0.41              |
| 1:C:931:ILE:HD13 | 1:C:931:ILE:HA   | 1.86                     | 0.41              |
| 1:A:295:PRO:HB2  | 1:A:608:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:335:LEU:HD12 | 1:A:335:LEU:C    | 2.42                     | 0.41              |
| 1:B:187:LYS:HG2  | 1:B:212:LEU:O    | 2.21                     | 0.41              |
| 1:C:111:ASP:CG   | 1:C:112:SER:H    | 2.28                     | 0.41              |
| 1:C:973:ILE:HG23 | 1:C:992:GLN:NE2  | 2.34                     | 0.41              |
| 2:H:52:TYR:HD1   | 2:H:53:TYR:CD2   | 2.30                     | 0.41              |
| 3:L:120:THR:HG23 | 3:L:139:LEU:HB2  | 2.02                     | 0.41              |
| 3:L:152:TRP:C    | 3:L:153:LYS:HG2  | 2.45                     | 0.41              |
| 2:J:157:VAL:HG23 | 2:J:207:HIS:HD2  | 1.85                     | 0.41              |
| 2:H:154:PRO:HG2  | 2:H:207:HIS:HE2  | 1.83                     | 0.41              |
| 3:L:153:LYS:HB2  | 3:L:196:SER:OG   | 2.20                     | 0.41              |
| 2:J:196:LEU:HD23 | 2:J:197:GLY:H    | 1.84                     | 0.41              |
| 3:N:7:PRO:O      | 3:N:105:THR:OG1  | 2.31                     | 0.41              |
| 3:N:153:LYS:HB2  | 3:N:196:SER:OG   | 2.20                     | 0.41              |
| 1:A:193:VAL:HG23 | 1:A:223:LEU:CD2  | 2.51                     | 0.41              |
| 1:A:280:ASN:OD1  | 1:A:281:GLU:N    | 2.51                     | 0.41              |
| 1:A:392:PHE:CA   | 1:A:517:LEU:HD21 | 2.49                     | 0.41              |
| 1:A:393:THR:H    | 1:A:517:LEU:HD22 | 1.85                     | 0.41              |
| 1:A:1123:SER:O   | 1:A:1123:SER:OG  | 2.39                     | 0.41              |
| 1:B:273:ARG:HA   | 1:B:273:ARG:HD3  | 1.70                     | 0.41              |
| 1:B:458:LYS:HE2  | 1:B:458:LYS:HB2  | 1.78                     | 0.41              |
| 1:B:776:LYS:HE3  | 1:B:776:LYS:HB3  | 1.65                     | 0.41              |
| 3:L:68:LYS:HB3   | 3:L:68:LYS:HE3   | 1.81                     | 0.41              |
| 2:J:30:SER:HA    | 2:J:53:TYR:CG    | 2.56                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:J:87:ALA:HA     | 2:J:118:VAL:HB   | 2.01                     | 0.41              |
| 3:N:93:TYR:OH     | 3:N:97:ASN:OD1   | 2.38                     | 0.41              |
| 1:A:309:GLU:H     | 1:A:309:GLU:HG2  | 1.71                     | 0.41              |
| 1:A:460:ASN:OD1   | 1:A:460:ASN:N    | 2.53                     | 0.41              |
| 1:A:505:TYR:OH    | 2:H:100:ARG:NH1  | 2.54                     | 0.41              |
| 1:B:403:ARG:NE    | 1:B:505:TYR:HD1  | 2.19                     | 0.41              |
| 1:B:541:PHE:O     | 1:B:547:THR:HA   | 2.20                     | 0.41              |
| 1:C:188:ASN:HB2   | 1:C:190:ARG:HH11 | 1.86                     | 0.41              |
| 1:C:985:ASP:OD1   | 1:C:985:ASP:N    | 2.46                     | 0.41              |
| 2:H:38:ARG:NE     | 2:H:46:GLU:OE1   | 2.52                     | 0.41              |
| 3:L:166:THR:CG2   | 3:L:179:SER:H    | 2.34                     | 0.41              |
| 2:J:106:ALA:CB    | 3:N:36:SER:OG    | 2.69                     | 0.41              |
| 3:N:154:ALA:HB1   | 3:N:192:HIS:CD2  | 2.56                     | 0.41              |
| 3:N:166:THR:CG2   | 3:N:179:SER:H    | 2.34                     | 0.41              |
| 1:B:132:GLU:HG3   | 1:B:165:ASN:HB2  | 2.02                     | 0.41              |
| 2:H:30:SER:HA     | 2:H:53:TYR:CG    | 2.56                     | 0.41              |
| 2:H:152:TYR:HE1   | 2:H:184:SER:HA   | 1.85                     | 0.41              |
| 2:H:155:GLU:CB    | 2:H:156:PRO:HD3  | 2.48                     | 0.41              |
| 3:L:97:ASN:C      | 3:L:98:THR:HG23  | 2.46                     | 0.41              |
| 2:J:102:TRP:CE3   | 2:J:104:LEU:CD1  | 3.02                     | 0.41              |
| 1:B:794:ILE:H     | 1:B:794:ILE:HG13 | 1.69                     | 0.40              |
| 1:B:1040:VAL:O    | 1:B:1041:ASP:HB2 | 2.21                     | 0.40              |
| 1:C:467:ASP:OD1   | 1:C:469:SER:OG   | 2.40                     | 0.40              |
| 1:C:854:LYS:HE2   | 1:C:854:LYS:HB3  | 1.88                     | 0.40              |
| 1:C:870:ILE:O     | 1:C:874:THR:HG23 | 2.21                     | 0.40              |
| 2:H:152:TYR:HE2   | 2:H:157:VAL:HG12 | 1.86                     | 0.40              |
| 1:A:166:CYS:HB3   | 1:A:169:GLU:OE1  | 2.21                     | 0.40              |
| 1:C:371:SER:C     | 1:C:373:SER:H    | 2.30                     | 0.40              |
| 1:C:821:LEU:HD22  | 1:C:939:SER:HB3  | 2.03                     | 0.40              |
| 2:H:106:ALA:CB    | 3:L:36:SER:OG    | 2.69                     | 0.40              |
| 3:L:193:ARG:NH1   | 3:L:212:PRO:HG2  | 2.35                     | 0.40              |
| 2:J:152:TYR:HB2   | 2:J:154:PRO:CG   | 2.52                     | 0.40              |
| 3:N:97:ASN:C      | 3:N:98:THR:HG23  | 2.46                     | 0.40              |
| 1:A:227:VAL:CG1   | 1:A:228:ASP:N    | 2.73                     | 0.40              |
| 1:A:347:PHE:CD1   | 1:A:509:ARG:HD3  | 2.56                     | 0.40              |
| 1:A:1051:SER:OG   | 1:A:1064:HIS:ND1 | 2.46                     | 0.40              |
| 1:A:1105:THR:HG21 | 1:A:1110:TYR:CD1 | 2.57                     | 0.40              |
| 1:B:135:PHE:HE1   | 1:B:159:VAL:HG12 | 1.86                     | 0.40              |
| 1:B:646:ARG:O     | 1:B:646:ARG:HG3  | 2.22                     | 0.40              |
| 2:H:118:VAL:O     | 2:H:119:SER:OG   | 2.30                     | 0.40              |
| 1:A:369:TYR:CZ    | 1:A:384:PRO:HB2  | 2.57                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:770:ILE:O    | 1:C:774:GLN:HG2  | 2.21                     | 0.40              |
| 2:H:63:LEU:HA    | 2:H:63:LEU:HD23  | 1.75                     | 0.40              |
| 3:L:18:ILE:HD12  | 3:L:19:THR:H     | 1.87                     | 0.40              |
| 3:N:18:ILE:HG22  | 3:N:80:LEU:HD11  | 2.04                     | 0.40              |
| 3:N:193:ARG:NH2  | 3:N:211:ALA:HB1  | 2.33                     | 0.40              |
| 1:A:703:ASN:O    | 1:B:789:TYR:HA   | 2.22                     | 0.40              |
| 1:A:879:ALA:O    | 1:A:883:THR:HB   | 2.22                     | 0.40              |
| 1:B:116:SER:HA   | 1:B:233:ILE:HD11 | 2.03                     | 0.40              |
| 1:B:578:ASP:N    | 1:B:583:GLU:O    | 2.37                     | 0.40              |
| 1:B:984:LEU:HD23 | 1:B:988:GLU:HB3  | 2.03                     | 0.40              |
| 1:C:456:PHE:CE1  | 3:N:55:LYS:HE2   | 2.57                     | 0.40              |
| 1:C:615:VAL:HG12 | 1:C:616:ASN:O    | 2.20                     | 0.40              |
| 1:C:959:LEU:HD23 | 1:C:959: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     | 988/1283 (77%)  | 885 (90%)  | 92 (9%)   | 11 (1%)  | 11          | 43 |
| 1   | B     | 958/1283 (75%)  | 868 (91%)  | 89 (9%)   | 1 (0%)   | 48          | 80 |
| 1   | C     | 986/1283 (77%)  | 883 (90%)  | 90 (9%)   | 13 (1%)  | 9           | 38 |
| 2   | H     | 220/450 (49%)   | 159 (72%)  | 46 (21%)  | 15 (7%)  | 1           | 5  |
| 2   | J     | 220/450 (49%)   | 159 (72%)  | 46 (21%)  | 15 (7%)  | 1           | 5  |
| 3   | L     | 211/216 (98%)   | 168 (80%)  | 35 (17%)  | 8 (4%)   | 2           | 15 |
| 3   | N     | 211/216 (98%)   | 168 (80%)  | 35 (17%)  | 8 (4%)   | 2           | 15 |
| All | All   | 3794/5181 (73%) | 3290 (87%) | 433 (11%) | 71 (2%)  | 8           | 30 |

All (71) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 228 | ASP  |
| 1   | A     | 233 | ILE  |
| 1   | A     | 331 | ASN  |
| 1   | A     | 518 | LEU  |
| 1   | C     | 331 | ASN  |
| 1   | C     | 518 | LEU  |
| 1   | C     | 814 | LYS  |
| 2   | H     | 13  | LYS  |
| 2   | H     | 53  | TYR  |
| 2   | H     | 155 | GLU  |
| 3   | L     | 53  | VAL  |
| 3   | L     | 55  | LYS  |
| 2   | J     | 13  | LYS  |
| 2   | J     | 53  | TYR  |
| 2   | J     | 155 | GLU  |
| 3   | N     | 53  | VAL  |
| 3   | N     | 55  | LYS  |
| 1   | A     | 232 | GLY  |
| 1   | C     | 810 | SER  |
| 2   | H     | 11  | LEU  |
| 2   | H     | 15  | SER  |
| 2   | H     | 56  | SER  |
| 2   | H     | 97  | ARG  |
| 2   | H     | 98  | LEU  |
| 2   | H     | 104 | LEU  |
| 2   | H     | 105 | ASP  |
| 3   | L     | 54  | SER  |
| 3   | L     | 95  | SER  |
| 2   | J     | 11  | LEU  |
| 2   | J     | 15  | SER  |
| 2   | J     | 56  | SER  |
| 2   | J     | 97  | ARG  |
| 2   | J     | 98  | LEU  |
| 2   | J     | 104 | LEU  |
| 2   | J     | 105 | ASP  |
| 3   | N     | 54  | SER  |
| 3   | N     | 95  | SER  |
| 1   | A     | 522 | ALA  |
| 1   | C     | 522 | ALA  |
| 2   | H     | 52  | TYR  |
| 2   | H     | 57  | THR  |
| 2   | H     | 103 | PRO  |
| 2   | H     | 108 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 94  | THR  |
| 2   | J     | 52  | TYR  |
| 2   | J     | 57  | THR  |
| 2   | J     | 103 | PRO  |
| 2   | J     | 108 | ASP  |
| 3   | N     | 94  | THR  |
| 1   | A     | 336 | CYS  |
| 1   | A     | 349 | SER  |
| 1   | A     | 520 | ALA  |
| 1   | C     | 336 | CYS  |
| 1   | C     | 349 | SER  |
| 1   | C     | 520 | ALA  |
| 1   | C     | 813 | SER  |
| 3   | L     | 58  | SER  |
| 2   | J     | 156 | PRO  |
| 3   | N     | 58  | SER  |
| 1   | B     | 88  | ASP  |
| 1   | C     | 319 | ARG  |
| 2   | H     | 156 | PRO  |
| 3   | L     | 71  | ASN  |
| 3   | L     | 155 | ASP  |
| 3   | N     | 71  | ASN  |
| 3   | N     | 155 | ASP  |
| 1   | C     | 811 | LYS  |
| 1   | C     | 812 | PRO  |
| 1   | A     | 339 | GLY  |
| 1   | C     | 339 | GLY  |
| 1   | A     | 227 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 881/1122 (78%) | 766 (87%) | 115 (13%) | 4           | 19 |
| 1   | B     | 862/1122 (77%) | 757 (88%) | 105 (12%) | 5           | 21 |
| 1   | C     | 879/1122 (78%) | 770 (88%) | 109 (12%) | 4           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | H     | 193/404 (48%)   | 157 (81%)  | 36 (19%)  | 1           | 9  |
| 2   | J     | 193/404 (48%)   | 157 (81%)  | 36 (19%)  | 1           | 9  |
| 3   | L     | 178/181 (98%)   | 154 (86%)  | 24 (14%)  | 4           | 18 |
| 3   | N     | 178/181 (98%)   | 154 (86%)  | 24 (14%)  | 4           | 18 |
| All | All   | 3364/4536 (74%) | 2915 (87%) | 449 (13%) | 6           | 18 |

All (449) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 45  | SER  |
| 1   | A     | 66  | HIS  |
| 1   | A     | 81  | ASN  |
| 1   | A     | 97  | LYS  |
| 1   | A     | 109 | THR  |
| 1   | A     | 116 | SER  |
| 1   | A     | 118 | LEU  |
| 1   | A     | 122 | ASN  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 158 | ARG  |
| 1   | A     | 164 | ASN  |
| 1   | A     | 169 | GLU  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 195 | LYS  |
| 1   | A     | 205 | SER  |
| 1   | A     | 208 | THR  |
| 1   | A     | 221 | SER  |
| 1   | A     | 229 | LEU  |
| 1   | A     | 233 | ILE  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 289 | VAL  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 301 | CYS  |
| 1   | A     | 308 | VAL  |
| 1   | A     | 314 | GLN  |
| 1   | A     | 315 | THR  |
| 1   | A     | 318 | PHE  |
| 1   | A     | 324 | GLU  |
| 1   | A     | 325 | SER  |
| 1   | A     | 335 | LEU  |
| 1   | A     | 336 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 338 | PHE  |
| 1   | A     | 362 | VAL  |
| 1   | A     | 375 | SER  |
| 1   | A     | 382 | VAL  |
| 1   | A     | 383 | SER  |
| 1   | A     | 389 | ASP  |
| 1   | A     | 390 | LEU  |
| 1   | A     | 408 | ARG  |
| 1   | A     | 417 | LYS  |
| 1   | A     | 421 | TYR  |
| 1   | A     | 430 | THR  |
| 1   | A     | 438 | SER  |
| 1   | A     | 459 | SER  |
| 1   | A     | 469 | SER  |
| 1   | A     | 472 | ILE  |
| 1   | A     | 500 | THR  |
| 1   | A     | 514 | SER  |
| 1   | A     | 517 | LEU  |
| 1   | A     | 518 | LEU  |
| 1   | A     | 525 | CYS  |
| 1   | A     | 528 | LYS  |
| 1   | A     | 529 | LYS  |
| 1   | A     | 532 | ASN  |
| 1   | A     | 533 | LEU  |
| 1   | A     | 540 | ASN  |
| 1   | A     | 546 | LEU  |
| 1   | A     | 553 | THR  |
| 1   | A     | 554 | GLU  |
| 1   | A     | 556 | ASN  |
| 1   | A     | 576 | VAL  |
| 1   | A     | 583 | GLU  |
| 1   | A     | 585 | LEU  |
| 1   | A     | 588 | THR  |
| 1   | A     | 599 | THR  |
| 1   | A     | 602 | THR  |
| 1   | A     | 608 | VAL  |
| 1   | A     | 673 | SER  |
| 1   | A     | 692 | ILE  |
| 1   | A     | 698 | SER  |
| 1   | A     | 702 | GLU  |
| 1   | A     | 719 | THR  |
| 1   | A     | 722 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 729  | VAL  |
| 1   | A     | 730  | SER  |
| 1   | A     | 738  | CYS  |
| 1   | A     | 746  | SER  |
| 1   | A     | 772  | VAL  |
| 1   | A     | 773  | GLU  |
| 1   | A     | 785  | VAL  |
| 1   | A     | 787  | GLN  |
| 1   | A     | 791  | THR  |
| 1   | A     | 826  | VAL  |
| 1   | A     | 868  | GLU  |
| 1   | A     | 878  | LEU  |
| 1   | A     | 883  | THR  |
| 1   | A     | 902  | MET  |
| 1   | A     | 916  | LEU  |
| 1   | A     | 929  | SER  |
| 1   | A     | 939  | SER  |
| 1   | A     | 951  | VAL  |
| 1   | A     | 960  | ASN  |
| 1   | A     | 967  | SER  |
| 1   | A     | 973  | ILE  |
| 1   | A     | 976  | VAL  |
| 1   | A     | 991  | VAL  |
| 1   | A     | 994  | ASP  |
| 1   | A     | 998  | THR  |
| 1   | A     | 1005 | GLN  |
| 1   | A     | 1018 | ILE  |
| 1   | A     | 1039 | ARG  |
| 1   | A     | 1074 | ASN  |
| 1   | A     | 1076 | THR  |
| 1   | A     | 1077 | THR  |
| 1   | A     | 1092 | GLU  |
| 1   | A     | 1094 | VAL  |
| 1   | A     | 1100 | THR  |
| 1   | A     | 1104 | VAL  |
| 1   | A     | 1114 | ILE  |
| 1   | A     | 1123 | SER  |
| 1   | A     | 1125 | ASN  |
| 1   | A     | 1132 | ILE  |
| 1   | A     | 1142 | GLN  |
| 1   | A     | 1144 | GLU  |
| 1   | B     | 45   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 46  | SER  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 50  | SER  |
| 1   | B     | 51  | THR  |
| 1   | B     | 52  | GLN  |
| 1   | B     | 60  | SER  |
| 1   | B     | 62  | VAL  |
| 1   | B     | 66  | HIS  |
| 1   | B     | 87  | ASN  |
| 1   | B     | 95  | THR  |
| 1   | B     | 99  | ASN  |
| 1   | B     | 108 | THR  |
| 1   | B     | 109 | THR  |
| 1   | B     | 112 | SER  |
| 1   | B     | 116 | SER  |
| 1   | B     | 120 | VAL  |
| 1   | B     | 122 | ASN  |
| 1   | B     | 127 | VAL  |
| 1   | B     | 164 | ASN  |
| 1   | B     | 205 | SER  |
| 1   | B     | 208 | THR  |
| 1   | B     | 214 | ARG  |
| 1   | B     | 240 | THR  |
| 1   | B     | 277 | LEU  |
| 1   | B     | 278 | LYS  |
| 1   | B     | 284 | THR  |
| 1   | B     | 307 | THR  |
| 1   | B     | 324 | GLU  |
| 1   | B     | 327 | VAL  |
| 1   | B     | 345 | THR  |
| 1   | B     | 349 | SER  |
| 1   | B     | 359 | SER  |
| 1   | B     | 371 | SER  |
| 1   | B     | 373 | SER  |
| 1   | B     | 382 | VAL  |
| 1   | B     | 385 | THR  |
| 1   | B     | 401 | VAL  |
| 1   | B     | 402 | ILE  |
| 1   | B     | 409 | GLN  |
| 1   | B     | 417 | LYS  |
| 1   | B     | 418 | ILE  |
| 1   | B     | 430 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 441 | LEU  |
| 1   | B     | 453 | TYR  |
| 1   | B     | 462 | LYS  |
| 1   | B     | 464 | PHE  |
| 1   | B     | 465 | GLU  |
| 1   | B     | 472 | ILE  |
| 1   | B     | 473 | TYR  |
| 1   | B     | 494 | SER  |
| 1   | B     | 506 | GLN  |
| 1   | B     | 514 | SER  |
| 1   | B     | 524 | VAL  |
| 1   | B     | 525 | CYS  |
| 1   | B     | 528 | LYS  |
| 1   | B     | 531 | THR  |
| 1   | B     | 532 | ASN  |
| 1   | B     | 533 | LEU  |
| 1   | B     | 534 | VAL  |
| 1   | B     | 555 | SER  |
| 1   | B     | 567 | ARG  |
| 1   | B     | 569 | ILE  |
| 1   | B     | 576 | VAL  |
| 1   | B     | 582 | LEU  |
| 1   | B     | 597 | VAL  |
| 1   | B     | 606 | ASN  |
| 1   | B     | 607 | GLN  |
| 1   | B     | 608 | VAL  |
| 1   | B     | 615 | VAL  |
| 1   | B     | 617 | CYS  |
| 1   | B     | 619 | GLU  |
| 1   | B     | 640 | SER  |
| 1   | B     | 642 | VAL  |
| 1   | B     | 676 | THR  |
| 1   | B     | 710 | ASN  |
| 1   | B     | 729 | VAL  |
| 1   | B     | 772 | VAL  |
| 1   | B     | 779 | GLN  |
| 1   | B     | 787 | GLN  |
| 1   | B     | 791 | THR  |
| 1   | B     | 811 | LYS  |
| 1   | B     | 855 | PHE  |
| 1   | B     | 856 | ASN  |
| 1   | B     | 868 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 878  | LEU  |
| 1   | B     | 912  | THR  |
| 1   | B     | 916  | LEU  |
| 1   | B     | 935  | GLN  |
| 1   | B     | 968  | SER  |
| 1   | B     | 969  | ASN  |
| 1   | B     | 974  | SER  |
| 1   | B     | 976  | VAL  |
| 1   | B     | 991  | VAL  |
| 1   | B     | 1030 | SER  |
| 1   | B     | 1037 | SER  |
| 1   | B     | 1045 | LYS  |
| 1   | B     | 1074 | ASN  |
| 1   | B     | 1081 | ILE  |
| 1   | B     | 1094 | VAL  |
| 1   | B     | 1104 | VAL  |
| 1   | B     | 1114 | ILE  |
| 1   | B     | 1126 | CYS  |
| 1   | B     | 1133 | VAL  |
| 1   | B     | 1141 | LEU  |
| 1   | C     | 29   | THR  |
| 1   | C     | 50   | SER  |
| 1   | C     | 51   | THR  |
| 1   | C     | 60   | SER  |
| 1   | C     | 63   | THR  |
| 1   | C     | 84   | LEU  |
| 1   | C     | 86   | PHE  |
| 1   | C     | 90   | VAL  |
| 1   | C     | 114  | THR  |
| 1   | C     | 117  | LEU  |
| 1   | C     | 120  | VAL  |
| 1   | C     | 125  | ASN  |
| 1   | C     | 143  | VAL  |
| 1   | C     | 155  | SER  |
| 1   | C     | 172  | SER  |
| 1   | C     | 195  | LYS  |
| 1   | C     | 197  | ILE  |
| 1   | C     | 208  | THR  |
| 1   | C     | 212  | LEU  |
| 1   | C     | 215  | ASP  |
| 1   | C     | 216  | LEU  |
| 1   | C     | 221  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 224 | GLU  |
| 1   | C     | 233 | ILE  |
| 1   | C     | 234 | ASN  |
| 1   | C     | 271 | GLN  |
| 1   | C     | 277 | LEU  |
| 1   | C     | 301 | CYS  |
| 1   | C     | 305 | SER  |
| 1   | C     | 308 | VAL  |
| 1   | C     | 314 | GLN  |
| 1   | C     | 318 | PHE  |
| 1   | C     | 319 | ARG  |
| 1   | C     | 324 | GLU  |
| 1   | C     | 325 | SER  |
| 1   | C     | 335 | LEU  |
| 1   | C     | 336 | CYS  |
| 1   | C     | 338 | PHE  |
| 1   | C     | 362 | VAL  |
| 1   | C     | 375 | SER  |
| 1   | C     | 382 | VAL  |
| 1   | C     | 383 | SER  |
| 1   | C     | 389 | ASP  |
| 1   | C     | 390 | LEU  |
| 1   | C     | 408 | ARG  |
| 1   | C     | 417 | LYS  |
| 1   | C     | 421 | TYR  |
| 1   | C     | 430 | THR  |
| 1   | C     | 438 | SER  |
| 1   | C     | 459 | SER  |
| 1   | C     | 469 | SER  |
| 1   | C     | 472 | ILE  |
| 1   | C     | 500 | THR  |
| 1   | C     | 514 | SER  |
| 1   | C     | 517 | LEU  |
| 1   | C     | 518 | LEU  |
| 1   | C     | 525 | CYS  |
| 1   | C     | 528 | LYS  |
| 1   | C     | 529 | LYS  |
| 1   | C     | 532 | ASN  |
| 1   | C     | 533 | LEU  |
| 1   | C     | 540 | ASN  |
| 1   | C     | 546 | LEU  |
| 1   | C     | 553 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 554  | GLU  |
| 1   | C     | 556  | ASN  |
| 1   | C     | 576  | VAL  |
| 1   | C     | 583  | GLU  |
| 1   | C     | 585  | LEU  |
| 1   | C     | 591  | SER  |
| 1   | C     | 602  | THR  |
| 1   | C     | 620  | VAL  |
| 1   | C     | 658  | ASN  |
| 1   | C     | 675  | GLN  |
| 1   | C     | 693  | ILE  |
| 1   | C     | 697  | MET  |
| 1   | C     | 699  | LEU  |
| 1   | C     | 727  | LEU  |
| 1   | C     | 768  | THR  |
| 1   | C     | 770  | ILE  |
| 1   | C     | 778  | THR  |
| 1   | C     | 787  | GLN  |
| 1   | C     | 791  | THR  |
| 1   | C     | 814  | LYS  |
| 1   | C     | 856  | ASN  |
| 1   | C     | 859  | THR  |
| 1   | C     | 878  | LEU  |
| 1   | C     | 907  | ASN  |
| 1   | C     | 922  | LEU  |
| 1   | C     | 929  | SER  |
| 1   | C     | 931  | ILE  |
| 1   | C     | 934  | ILE  |
| 1   | C     | 937  | SER  |
| 1   | C     | 968  | SER  |
| 1   | C     | 975  | SER  |
| 1   | C     | 976  | VAL  |
| 1   | C     | 977  | LEU  |
| 1   | C     | 1018 | ILE  |
| 1   | C     | 1027 | THR  |
| 1   | C     | 1063 | LEU  |
| 1   | C     | 1077 | THR  |
| 1   | C     | 1092 | GLU  |
| 1   | C     | 1094 | VAL  |
| 1   | C     | 1104 | VAL  |
| 1   | C     | 1126 | CYS  |
| 1   | C     | 1129 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1132 | ILE  |
| 1   | C     | 1136 | THR  |
| 1   | C     | 1145 | LEU  |
| 2   | H     | 2    | VAL  |
| 2   | H     | 12   | VAL  |
| 2   | H     | 13   | LYS  |
| 2   | H     | 17   | THR  |
| 2   | H     | 18   | LEU  |
| 2   | H     | 23   | THR  |
| 2   | H     | 29   | ILE  |
| 2   | H     | 31   | SER  |
| 2   | H     | 48   | ILE  |
| 2   | H     | 51   | ILE  |
| 2   | H     | 56   | SER  |
| 2   | H     | 57   | THR  |
| 2   | H     | 67   | VAL  |
| 2   | H     | 68   | THR  |
| 2   | H     | 78   | PHE  |
| 2   | H     | 80   | LEU  |
| 2   | H     | 85   | VAL  |
| 2   | H     | 86   | THR  |
| 2   | H     | 89   | ASP  |
| 2   | H     | 100  | ARG  |
| 2   | H     | 101  | ASP  |
| 2   | H     | 102  | TRP  |
| 2   | H     | 109  | ILE  |
| 2   | H     | 117  | THR  |
| 2   | H     | 123  | THR  |
| 2   | H     | 142  | THR  |
| 2   | H     | 152  | TYR  |
| 2   | H     | 155  | GLU  |
| 2   | H     | 176  | VAL  |
| 2   | H     | 186  | SER  |
| 2   | H     | 191  | VAL  |
| 2   | H     | 204  | ASN  |
| 2   | H     | 205  | VAL  |
| 2   | H     | 207  | HIS  |
| 2   | H     | 210  | SER  |
| 2   | H     | 212  | THR  |
| 3   | L     | 1    | GLN  |
| 3   | L     | 20   | ILE  |
| 3   | L     | 23   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 35  | VAL  |
| 3   | L     | 40  | GLN  |
| 3   | L     | 51  | TYR  |
| 3   | L     | 54  | SER  |
| 3   | L     | 55  | LYS  |
| 3   | L     | 56  | ARG  |
| 3   | L     | 61  | SER  |
| 3   | L     | 68  | LYS  |
| 3   | L     | 77  | ILE  |
| 3   | L     | 83  | GLU  |
| 3   | L     | 90  | CYS  |
| 3   | L     | 96  | ASN  |
| 3   | L     | 118 | SER  |
| 3   | L     | 120 | THR  |
| 3   | L     | 135 | THR  |
| 3   | L     | 139 | LEU  |
| 3   | L     | 140 | ILE  |
| 3   | L     | 152 | TRP  |
| 3   | L     | 191 | SER  |
| 3   | L     | 199 | VAL  |
| 3   | L     | 200 | THR  |
| 2   | J     | 2   | VAL  |
| 2   | J     | 12  | VAL  |
| 2   | J     | 13  | LYS  |
| 2   | J     | 17  | THR  |
| 2   | J     | 18  | LEU  |
| 2   | J     | 23  | THR  |
| 2   | J     | 29  | ILE  |
| 2   | J     | 31  | SER  |
| 2   | J     | 48  | ILE  |
| 2   | J     | 51  | ILE  |
| 2   | J     | 56  | SER  |
| 2   | J     | 57  | THR  |
| 2   | J     | 67  | VAL  |
| 2   | J     | 68  | THR  |
| 2   | J     | 78  | PHE  |
| 2   | J     | 80  | LEU  |
| 2   | J     | 85  | VAL  |
| 2   | J     | 86  | THR  |
| 2   | J     | 89  | ASP  |
| 2   | J     | 100 | ARG  |
| 2   | J     | 101 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 102 | TRP  |
| 2   | J     | 109 | ILE  |
| 2   | J     | 117 | THR  |
| 2   | J     | 123 | THR  |
| 2   | J     | 142 | THR  |
| 2   | J     | 152 | TYR  |
| 2   | J     | 155 | GLU  |
| 2   | J     | 176 | VAL  |
| 2   | J     | 186 | SER  |
| 2   | J     | 191 | VAL  |
| 2   | J     | 204 | ASN  |
| 2   | J     | 205 | VAL  |
| 2   | J     | 207 | HIS  |
| 2   | J     | 210 | SER  |
| 2   | J     | 212 | THR  |
| 3   | N     | 1   | GLN  |
| 3   | N     | 20  | ILE  |
| 3   | N     | 23  | THR  |
| 3   | N     | 35  | VAL  |
| 3   | N     | 40  | GLN  |
| 3   | N     | 51  | TYR  |
| 3   | N     | 54  | SER  |
| 3   | N     | 55  | LYS  |
| 3   | N     | 56  | ARG  |
| 3   | N     | 61  | SER  |
| 3   | N     | 68  | LYS  |
| 3   | N     | 77  | ILE  |
| 3   | N     | 83  | GLU  |
| 3   | N     | 90  | CYS  |
| 3   | N     | 96  | ASN  |
| 3   | N     | 118 | SER  |
| 3   | N     | 120 | THR  |
| 3   | N     | 135 | THR  |
| 3   | N     | 139 | LEU  |
| 3   | N     | 140 | ILE  |
| 3   | N     | 152 | TRP  |
| 3   | N     | 191 | SER  |
| 3   | N     | 199 | VAL  |
| 3   | N     | 200 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 134  | GLN  |
| 1   | A     | 137  | ASN  |
| 1   | A     | 188  | ASN  |
| 1   | A     | 394  | ASN  |
| 1   | A     | 422  | ASN  |
| 1   | A     | 440  | ASN  |
| 1   | A     | 450  | ASN  |
| 1   | A     | 498  | GLN  |
| 1   | A     | 556  | ASN  |
| 1   | A     | 644  | GLN  |
| 1   | A     | 658  | ASN  |
| 1   | A     | 675  | GLN  |
| 1   | A     | 690  | GLN  |
| 1   | A     | 703  | ASN  |
| 1   | A     | 755  | GLN  |
| 1   | A     | 762  | GLN  |
| 1   | A     | 787  | GLN  |
| 1   | A     | 901  | GLN  |
| 1   | A     | 914  | ASN  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 949  | GLN  |
| 1   | A     | 955  | ASN  |
| 1   | A     | 969  | ASN  |
| 1   | A     | 992  | GLN  |
| 1   | A     | 1010 | GLN  |
| 1   | A     | 1054 | GLN  |
| 1   | A     | 1113 | GLN  |
| 1   | A     | 1125 | ASN  |
| 1   | B     | 52   | GLN  |
| 1   | B     | 164  | ASN  |
| 1   | B     | 188  | ASN  |
| 1   | B     | 245  | HIS  |
| 1   | B     | 334  | ASN  |
| 1   | B     | 422  | ASN  |
| 1   | B     | 460  | ASN  |
| 1   | B     | 487  | ASN  |
| 1   | B     | 506  | GLN  |
| 1   | B     | 532  | ASN  |
| 1   | B     | 540  | ASN  |
| 1   | B     | 563  | GLN  |
| 1   | B     | 607  | GLN  |
| 1   | B     | 613  | GLN  |
| 1   | B     | 675  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 690  | GLN  |
| 1   | B     | 703  | ASN  |
| 1   | B     | 710  | ASN  |
| 1   | B     | 804  | GLN  |
| 1   | B     | 901  | GLN  |
| 1   | B     | 914  | ASN  |
| 1   | B     | 920  | GLN  |
| 1   | B     | 926  | GLN  |
| 1   | B     | 949  | GLN  |
| 1   | B     | 957  | GLN  |
| 1   | B     | 960  | ASN  |
| 1   | B     | 992  | GLN  |
| 1   | B     | 1011 | GLN  |
| 1   | B     | 1083 | HIS  |
| 1   | B     | 1101 | HIS  |
| 1   | C     | 30   | ASN  |
| 1   | C     | 188  | ASN  |
| 1   | C     | 207  | HIS  |
| 1   | C     | 271  | GLN  |
| 1   | C     | 314  | GLN  |
| 1   | C     | 394  | ASN  |
| 1   | C     | 422  | ASN  |
| 1   | C     | 440  | ASN  |
| 1   | C     | 498  | GLN  |
| 1   | C     | 542  | ASN  |
| 1   | C     | 556  | ASN  |
| 1   | C     | 606  | ASN  |
| 1   | C     | 641  | ASN  |
| 1   | C     | 675  | GLN  |
| 1   | C     | 690  | GLN  |
| 1   | C     | 703  | ASN  |
| 1   | C     | 764  | ASN  |
| 1   | C     | 779  | GLN  |
| 1   | C     | 784  | GLN  |
| 1   | C     | 804  | GLN  |
| 1   | C     | 901  | GLN  |
| 1   | C     | 907  | ASN  |
| 1   | C     | 914  | ASN  |
| 1   | C     | 926  | GLN  |
| 1   | C     | 935  | GLN  |
| 1   | C     | 992  | GLN  |
| 1   | C     | 1010 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1011 | GLN  |
| 1   | C     | 1071 | GLN  |
| 1   | C     | 1101 | HIS  |
| 1   | C     | 1106 | GLN  |
| 1   | C     | 1125 | ASN  |
| 2   | H     | 199  | GLN  |
| 2   | H     | 207  | HIS  |
| 3   | L     | 39   | GLN  |
| 3   | L     | 132  | ASN  |
| 3   | L     | 174  | ASN  |
| 3   | L     | 201  | HIS  |
| 3   | N     | 39   | GLN  |
| 3   | N     | 132  | ASN  |
| 3   | N     | 174  | ASN  |
| 3   | N     | 198  | GLN  |
| 3   | N     | 201  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

46 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 | $\# Z  > 2$ |
| 4   | NAG  | D     | 1   | 4    | 14,14,15     | 0.49 | 0           | 17,19,21    | 0.53 | 0           |
| 4   | NAG  | D     | 2   | 4    | 14,14,15     | 0.27 | 0           | 17,19,21    | 0.61 | 0           |
| 4   | NAG  | E     | 1   | 4,1  | 14,14,15     | 0.54 | 0           | 17,19,21    | 0.58 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | E     | 2   | 4    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.48 | 0        |
| 4   | NAG  | F     | 1   | 4,1  | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.66 | 1 (5%)   |
| 4   | NAG  | F     | 2   | 4    | 14,14,15     | 0.53 | 0        | 17,19,21    | 0.49 | 0        |
| 4   | NAG  | G     | 1   | 4,1  | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.74 | 0        |
| 4   | NAG  | G     | 2   | 4    | 14,14,15     | 0.31 | 0        | 17,19,21    | 1.40 | 2 (11%)  |
| 4   | NAG  | I     | 1   | 4,1  | 14,14,15     | 0.67 | 1 (7%)   | 17,19,21    | 0.71 | 0        |
| 4   | NAG  | I     | 2   | 4    | 14,14,15     | 0.45 | 0        | 17,19,21    | 1.49 | 3 (17%)  |
| 4   | NAG  | K     | 1   | 4,1  | 14,14,15     | 0.68 | 1 (7%)   | 17,19,21    | 0.68 | 0        |
| 4   | NAG  | K     | 2   | 4    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.67 | 0        |
| 4   | NAG  | M     | 1   | 4,1  | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.71 | 1 (5%)   |
| 4   | NAG  | M     | 2   | 4    | 14,14,15     | 0.16 | 0        | 17,19,21    | 0.48 | 0        |
| 4   | NAG  | O     | 1   | 4,1  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.43 | 0        |
| 4   | NAG  | O     | 2   | 4    | 14,14,15     | 0.15 | 0        | 17,19,21    | 0.49 | 0        |
| 4   | NAG  | P     | 1   | 4,1  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.41 | 0        |
| 4   | NAG  | P     | 2   | 4    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.39 | 0        |
| 4   | NAG  | Q     | 1   | 4,1  | 14,14,15     | 0.35 | 0        | 17,19,21    | 1.15 | 1 (5%)   |
| 4   | NAG  | Q     | 2   | 4    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | R     | 1   | 4,1  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.71 | 1 (5%)   |
| 4   | NAG  | R     | 2   | 4    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.42 | 0        |
| 4   | NAG  | S     | 1   | 4,1  | 14,14,15     | 0.71 | 1 (7%)   | 17,19,21    | 0.91 | 1 (5%)   |
| 4   | NAG  | S     | 2   | 4    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 4   | NAG  | T     | 1   | 4,1  | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.46 | 0        |
| 4   | NAG  | T     | 2   | 4    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.40 | 0        |
| 4   | NAG  | U     | 1   | 4,1  | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.59 | 0        |
| 4   | NAG  | U     | 2   | 4    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.63 | 1 (5%)   |
| 4   | NAG  | V     | 1   | 4,1  | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.58 | 0        |
| 4   | NAG  | V     | 2   | 4    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.46 | 0        |
| 4   | NAG  | W     | 1   | 4,1  | 14,14,15     | 0.23 | 0        | 17,19,21    | 1.43 | 2 (11%)  |
| 4   | NAG  | W     | 2   | 4    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.52 | 0        |
| 4   | NAG  | X     | 1   | 4,1  | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 4   | NAG  | X     | 2   | 4    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | Y     | 1   | 4,1  | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.42 | 0        |
| 4   | NAG  | Y     | 2   | 4    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.75 | 0        |
| 4   | NAG  | Z     | 1   | 4,1  | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.49 | 0        |
| 4   | NAG  | Z     | 2   | 4    | 14,14,15     | 0.60 | 1 (7%)   | 17,19,21    | 1.40 | 2 (11%)  |
| 4   | NAG  | a     | 1   | 4,1  | 14,14,15     | 0.63 | 1 (7%)   | 17,19,21    | 0.46 | 0        |
| 4   | NAG  | a     | 2   | 4    | 14,14,15     | 0.32 | 0        | 17,19,21    | 1.44 | 2 (11%)  |
| 4   | NAG  | b     | 1   | 4,1  | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.45 | 0        |
| 4   | NAG  | b     | 2   | 4    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.50 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | c     | 1   | 4,3  | 14,14,15     | 0.43 | 0        | 17,19,21    | 1.16 | 2 (11%)  |
| 4   | NAG  | c     | 2   | 4    | 14,14,15     | 0.42 | 0        | 17,19,21    | 1.15 | 2 (11%)  |
| 4   | NAG  | d     | 1   | 4,3  | 14,14,15     | 0.44 | 0        | 17,19,21    | 1.16 | 2 (11%)  |
| 4   | NAG  | d     | 2   | 4    | 14,14,15     | 0.42 | 0        | 17,19,21    | 1.16 | 2 (11%)  |

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  | D     | 1   | 4    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | D     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 1   | 4,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 2   | 4    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | F     | 1   | 4,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | F     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 2   | 4    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | I     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | I     | 2   | 4    | -       | 6/6/23/26 | 0/1/1/1 |
| 4   | NAG  | K     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | K     | 2   | 4    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | M     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | M     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | O     | 1   | 4,1  | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | O     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | P     | 1   | 4,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | P     | 2   | 4    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Q     | 1   | 4,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Q     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | R     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | R     | 2   | 4    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | S     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | S     | 2   | 4    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | T     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | T     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | U     | 1   | 4,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | U     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | V     | 1   | 4,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | V     | 2   | 4    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | W     | 1   | 4,1  | -       | 6/6/23/26 | 0/1/1/1 |
| 4   | NAG  | W     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | X     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | X     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Y     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Y     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Z     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Z     | 2   | 4    | -       | 6/6/23/26 | 0/1/1/1 |
| 4   | NAG  | a     | 1   | 4,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | a     | 2   | 4    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | b     | 1   | 4,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | b     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | c     | 1   | 4,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | c     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | d     | 1   | 4,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | d     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | S     | 1   | NAG  | O5-C1 | -2.56 | 1.39        | 1.43     |
| 4   | K     | 1   | NAG  | O5-C1 | -2.45 | 1.39        | 1.43     |
| 4   | I     | 1   | NAG  | O5-C1 | -2.23 | 1.39        | 1.43     |
| 4   | a     | 1   | NAG  | O5-C1 | -2.07 | 1.40        | 1.43     |
| 4   | Z     | 2   | NAG  | C1-C2 | 2.05  | 1.55        | 1.52     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4   | W     | 1   | NAG  | C2-N2-C7 | 4.96 | 129.55      | 122.90   |
| 4   | I     | 2   | NAG  | C2-N2-C7 | 4.68 | 129.17      | 122.90   |
| 4   | Z     | 2   | NAG  | C2-N2-C7 | 4.63 | 129.11      | 122.90   |
| 4   | a     | 2   | NAG  | C2-N2-C7 | 4.62 | 129.09      | 122.90   |
| 4   | G     | 2   | NAG  | C2-N2-C7 | 4.56 | 129.01      | 122.90   |
| 4   | Q     | 1   | NAG  | C1-O5-C5 | 3.27 | 116.57      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | I     | 2   | NAG  | C1-C2-N2 | 2.61  | 114.54      | 110.43   |
| 4   | G     | 2   | NAG  | C1-C2-N2 | 2.51  | 114.39      | 110.43   |
| 4   | a     | 2   | NAG  | C1-C2-N2 | 2.50  | 114.37      | 110.43   |
| 4   | d     | 2   | NAG  | C8-C7-N2 | 2.40  | 120.10      | 116.12   |
| 4   | d     | 1   | NAG  | C8-C7-N2 | 2.37  | 120.05      | 116.12   |
| 4   | S     | 1   | NAG  | O4-C4-C3 | -2.37 | 104.79      | 110.38   |
| 4   | c     | 2   | NAG  | C8-C7-N2 | 2.36  | 120.03      | 116.12   |
| 4   | c     | 1   | NAG  | C8-C7-N2 | 2.34  | 120.00      | 116.12   |
| 4   | X     | 1   | NAG  | C1-O5-C5 | 2.30  | 115.26      | 112.19   |
| 4   | R     | 1   | NAG  | C1-O5-C5 | 2.30  | 115.26      | 112.19   |
| 4   | M     | 1   | NAG  | C1-O5-C5 | 2.18  | 115.10      | 112.19   |
| 4   | c     | 1   | NAG  | C2-N2-C7 | -2.14 | 120.03      | 122.90   |
| 4   | I     | 2   | NAG  | C1-O5-C5 | 2.14  | 115.05      | 112.19   |
| 4   | c     | 2   | NAG  | C2-N2-C7 | -2.12 | 120.06      | 122.90   |
| 4   | d     | 1   | NAG  | C2-N2-C7 | -2.12 | 120.06      | 122.90   |
| 4   | F     | 1   | NAG  | C1-O5-C5 | 2.11  | 115.02      | 112.19   |
| 4   | W     | 1   | NAG  | C1-C2-N2 | 2.10  | 113.74      | 110.43   |
| 4   | U     | 2   | NAG  | C1-O5-C5 | 2.08  | 114.98      | 112.19   |
| 4   | d     | 2   | NAG  | C2-N2-C7 | -2.08 | 120.11      | 122.90   |
| 4   | S     | 2   | NAG  | C1-O5-C5 | 2.05  | 114.93      | 112.19   |
| 4   | Z     | 2   | NAG  | C1-C2-N2 | 2.04  | 113.64      | 110.43   |

There are no chirality outliers.

All (90) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | W     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | X     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | Y     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | D     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | K     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | S     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | O     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | D     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | S     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | X     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | S     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | K     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | X     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | Y     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | X     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | O     | 1   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | T     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | Z     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | O     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | W     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | O     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | S     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | Z     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | T     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | W     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | W     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | G     | 2   | NAG  | C8-C7-N2-C2 |
| 4   | G     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | I     | 2   | NAG  | C8-C7-N2-C2 |
| 4   | I     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | O     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | O     | 1   | NAG  | O7-C7-N2-C2 |
| 4   | R     | 2   | NAG  | C8-C7-N2-C2 |
| 4   | R     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | W     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | W     | 1   | NAG  | O7-C7-N2-C2 |
| 4   | Z     | 2   | NAG  | C8-C7-N2-C2 |
| 4   | Z     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | a     | 2   | NAG  | C8-C7-N2-C2 |
| 4   | a     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | G     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | I     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | T     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | T     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | U     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | G     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | I     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | K     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | K     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | a     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | a     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | M     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | M     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | U     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | a     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | R     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | W     | 1   | NAG  | C1-C2-N2-C7 |
| 4   | D     | 1   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | R     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | F     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | F     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | b     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | Z     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | K     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | Q     | 1   | NAG  | C3-C2-N2-C7 |
| 4   | S     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | Y     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | b     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | P     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | I     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | Z     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | I     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | G     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | I     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | K     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | Y     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | Z     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | a     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | V     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | E     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | G     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | I     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | V     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | W     | 1   | NAG  | C3-C2-N2-C7 |
| 4   | Z     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | a     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | R     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | V     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | E     | 2   | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

17 monomers are involved in 18 short contacts:

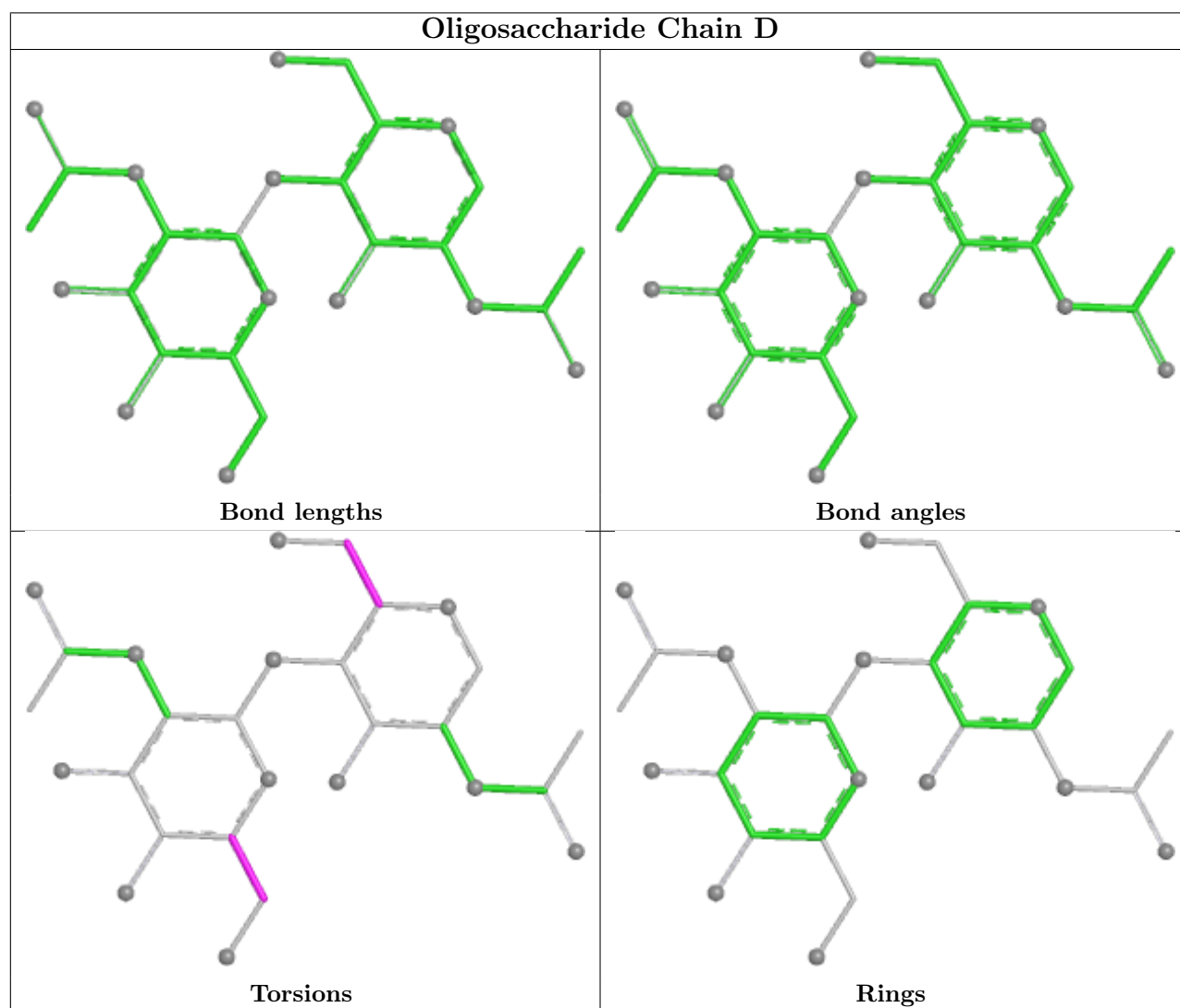
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | E     | 2   | NAG  | 2       | 0            |
| 4   | c     | 1   | NAG  | 3       | 0            |
| 4   | S     | 1   | NAG  | 1       | 0            |
| 4   | V     | 2   | NAG  | 2       | 0            |
| 4   | W     | 1   | NAG  | 1       | 0            |

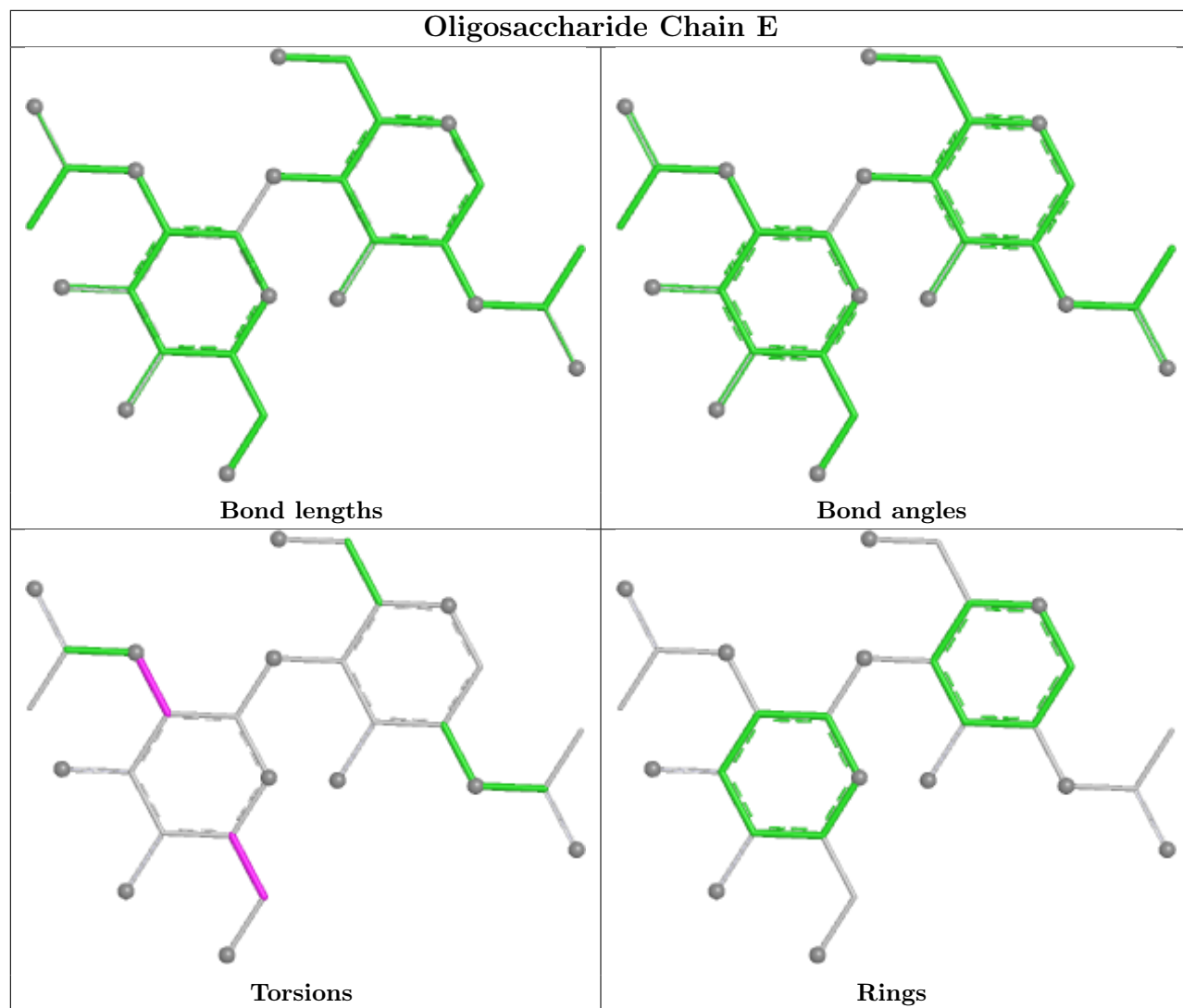
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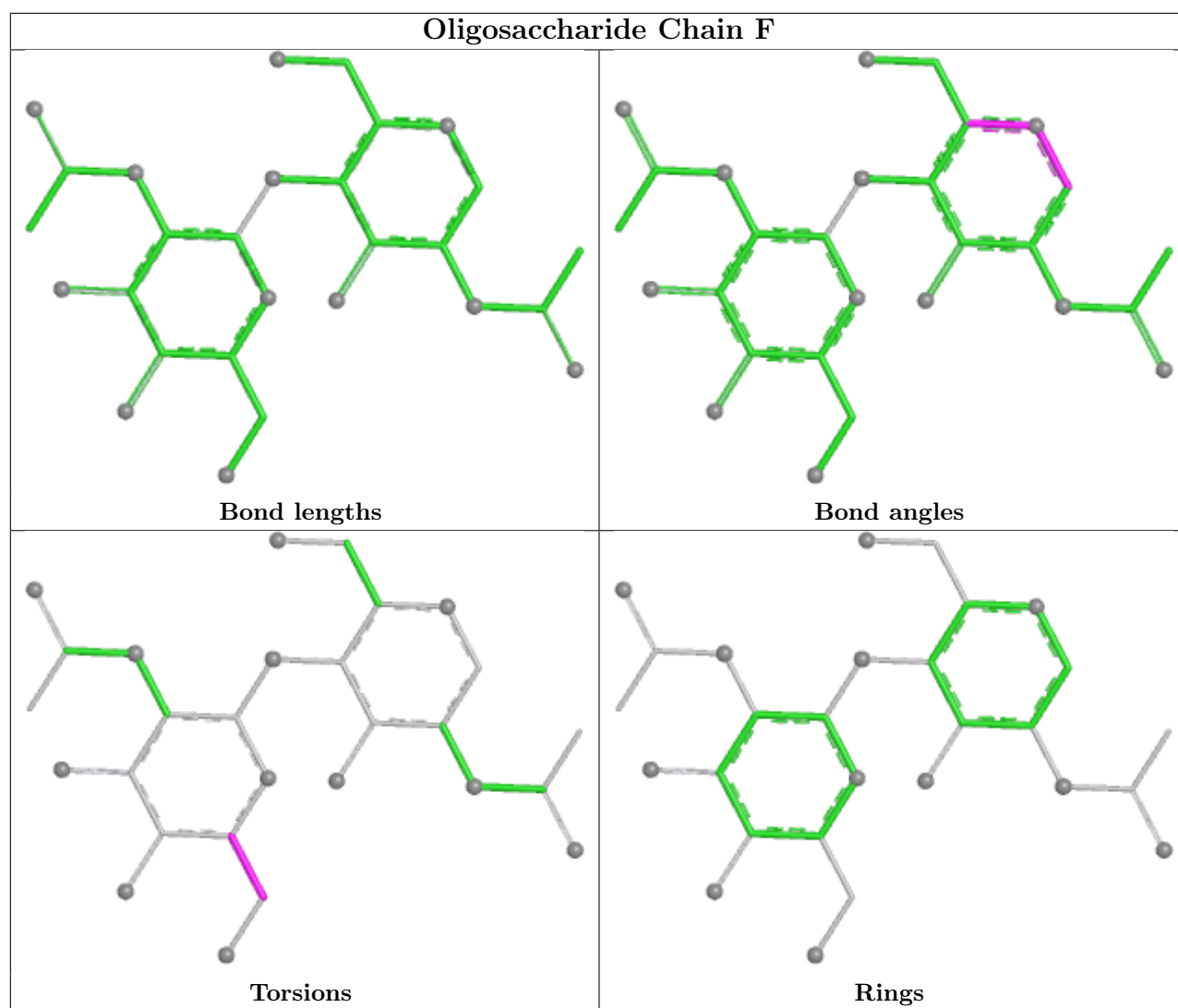
Continued from previous page...

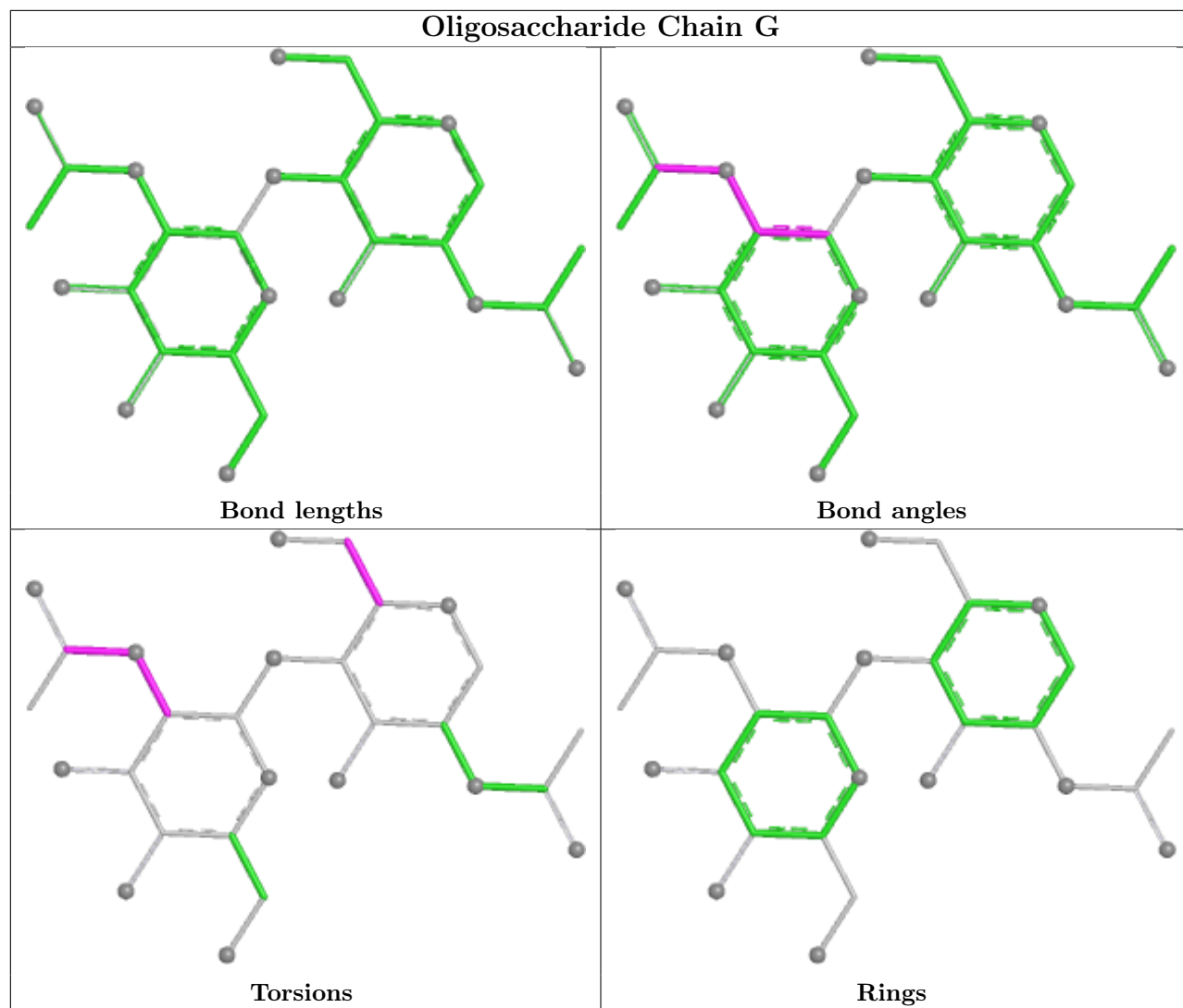
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | d     | 2   | NAG  | 2       | 0            |
| 4   | d     | 1   | NAG  | 3       | 0            |
| 4   | Z     | 2   | NAG  | 1       | 0            |
| 4   | I     | 2   | NAG  | 1       | 0            |
| 4   | E     | 1   | NAG  | 2       | 0            |
| 4   | V     | 1   | NAG  | 2       | 0            |
| 4   | a     | 2   | NAG  | 1       | 0            |
| 4   | S     | 2   | NAG  | 1       | 0            |
| 4   | G     | 2   | NAG  | 1       | 0            |
| 4   | a     | 1   | NAG  | 1       | 0            |
| 4   | O     | 1   | NAG  | 1       | 0            |
| 4   | c     | 2   | NAG  | 2       | 0            |

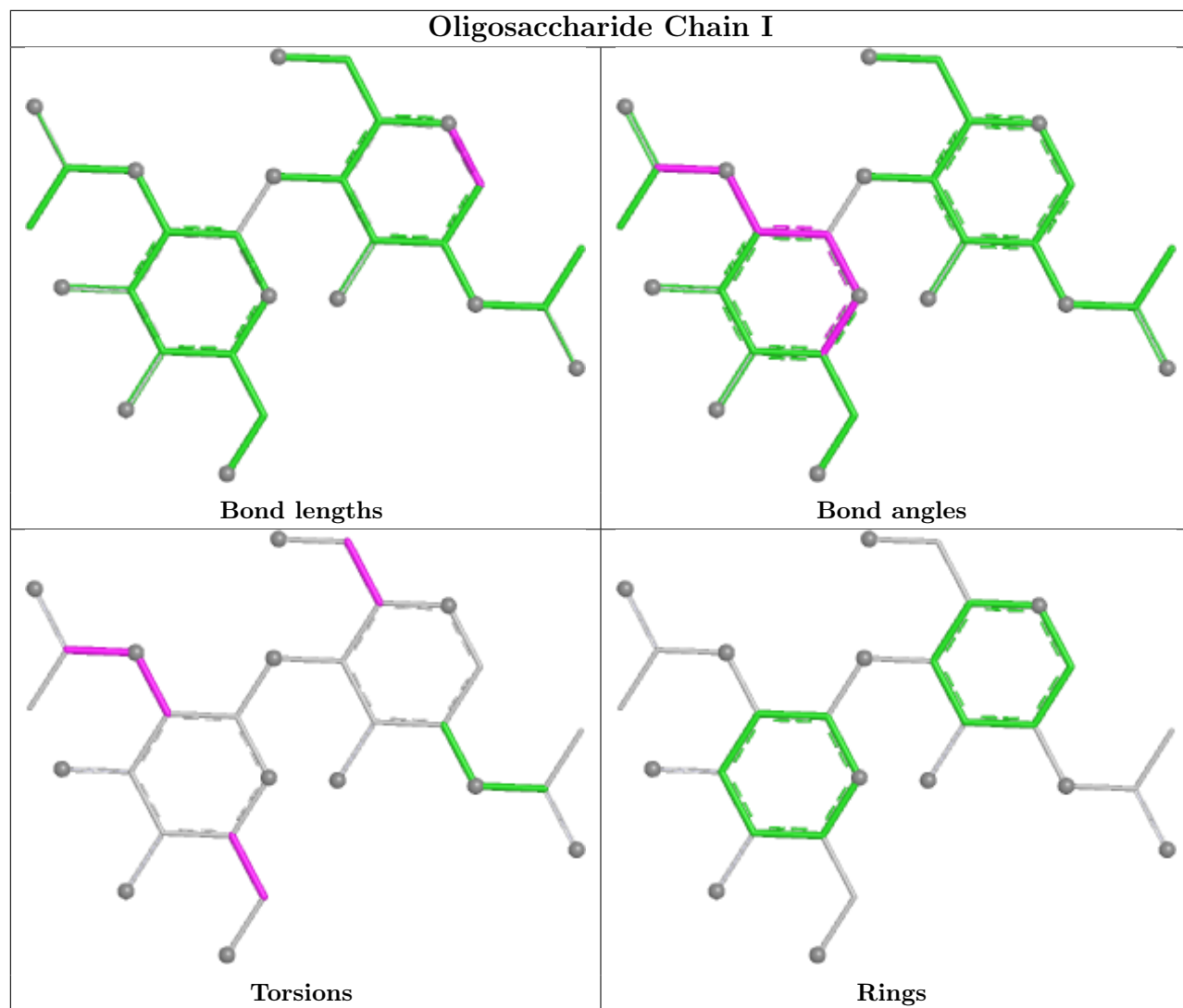
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

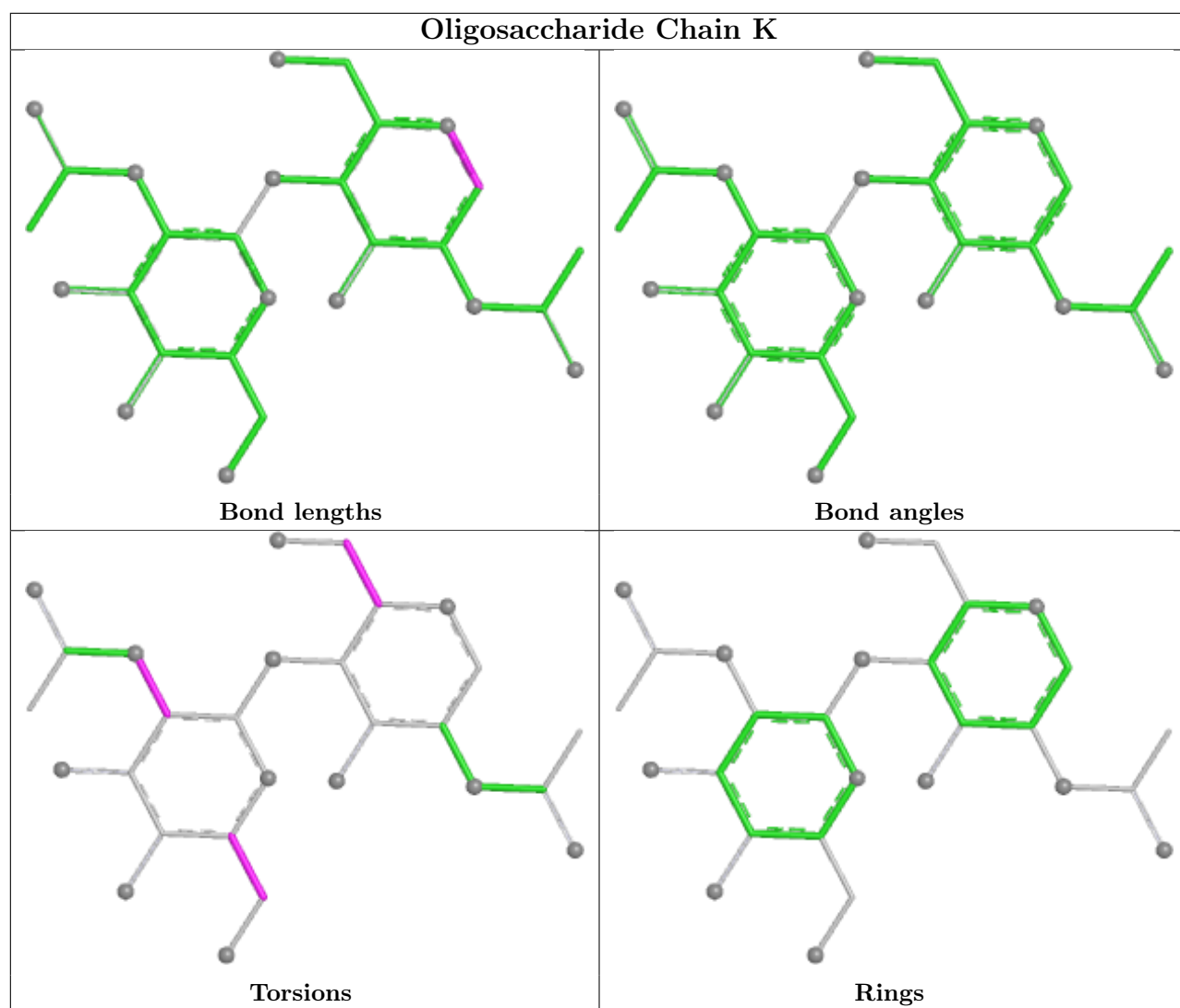


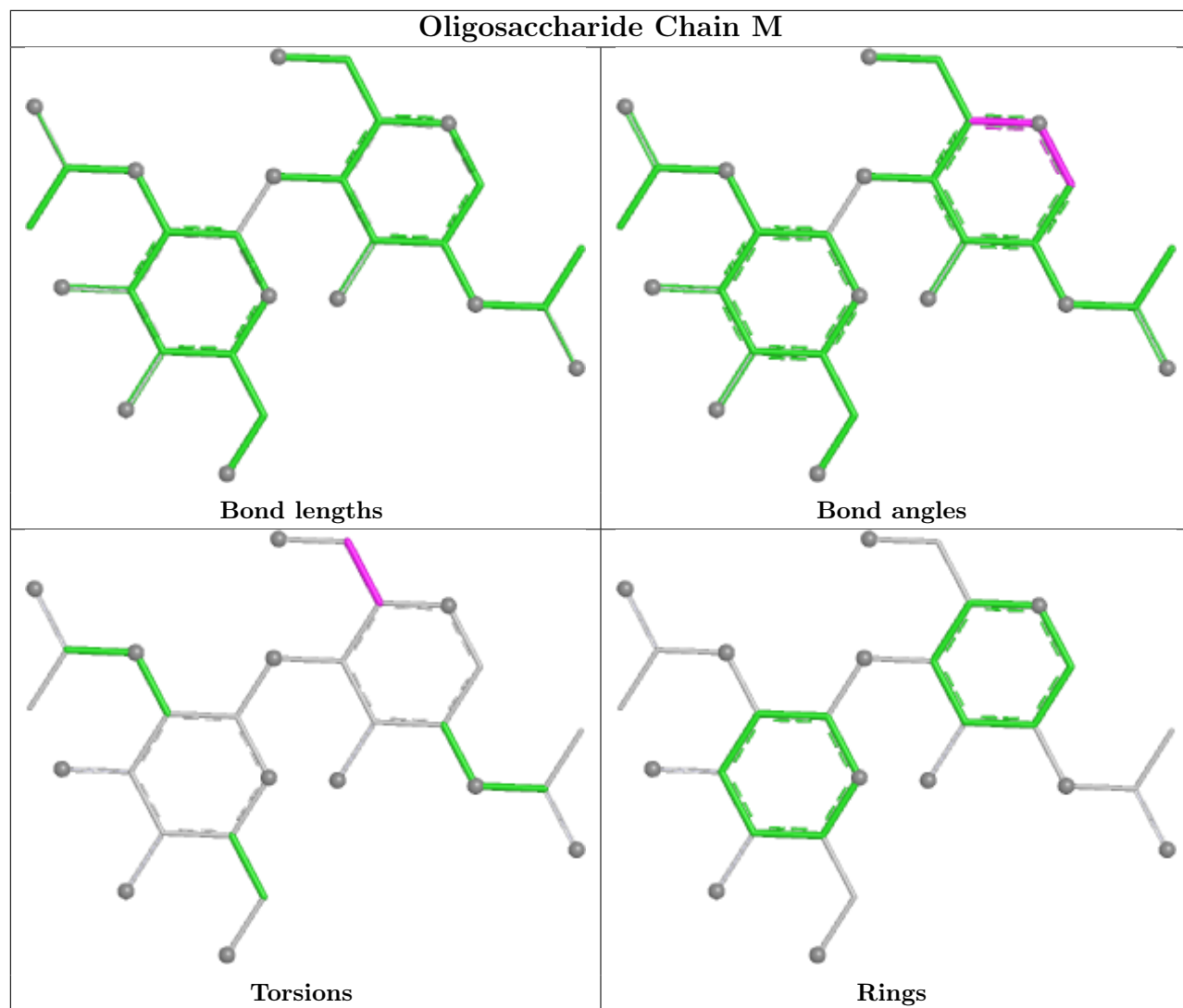


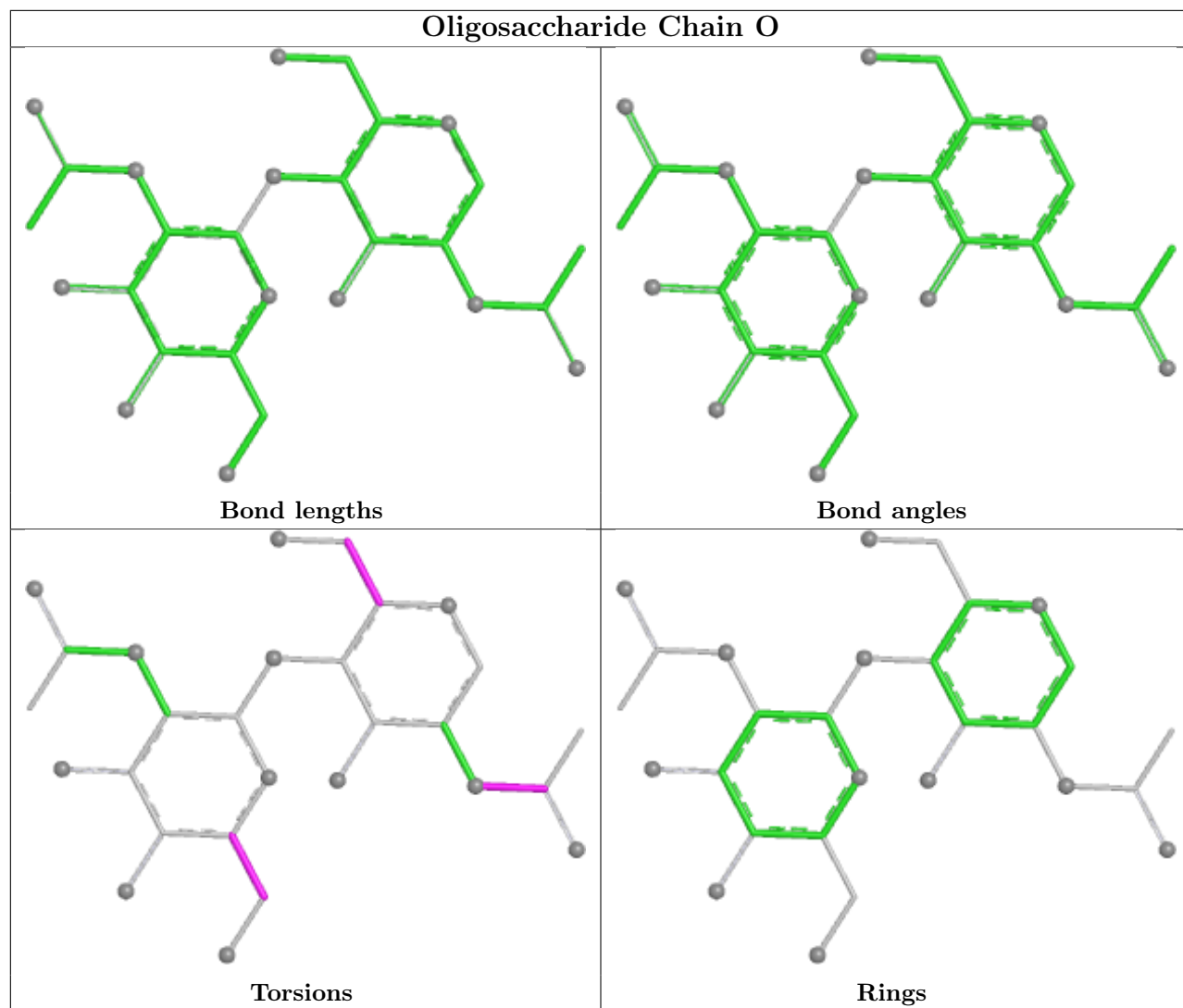


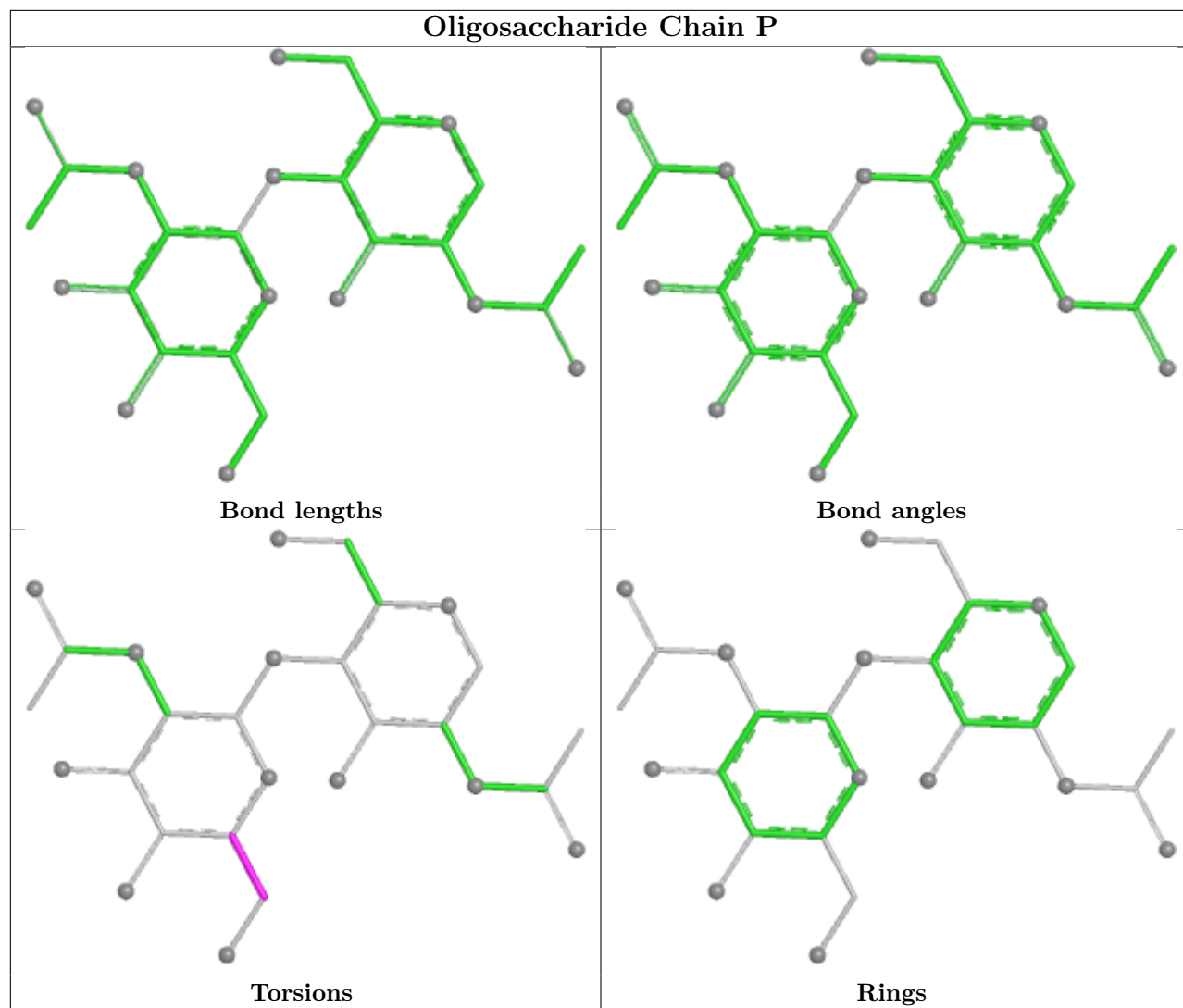


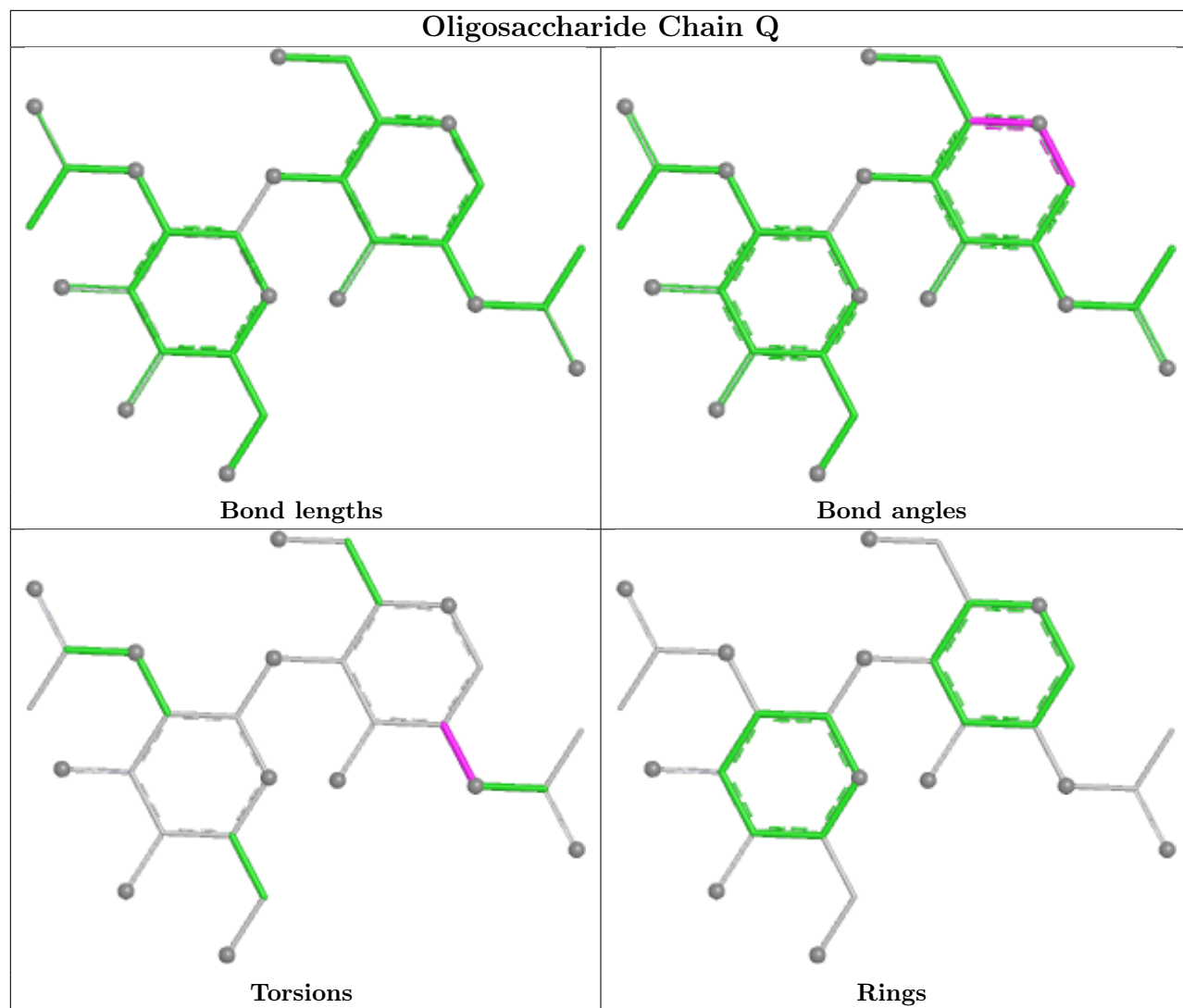


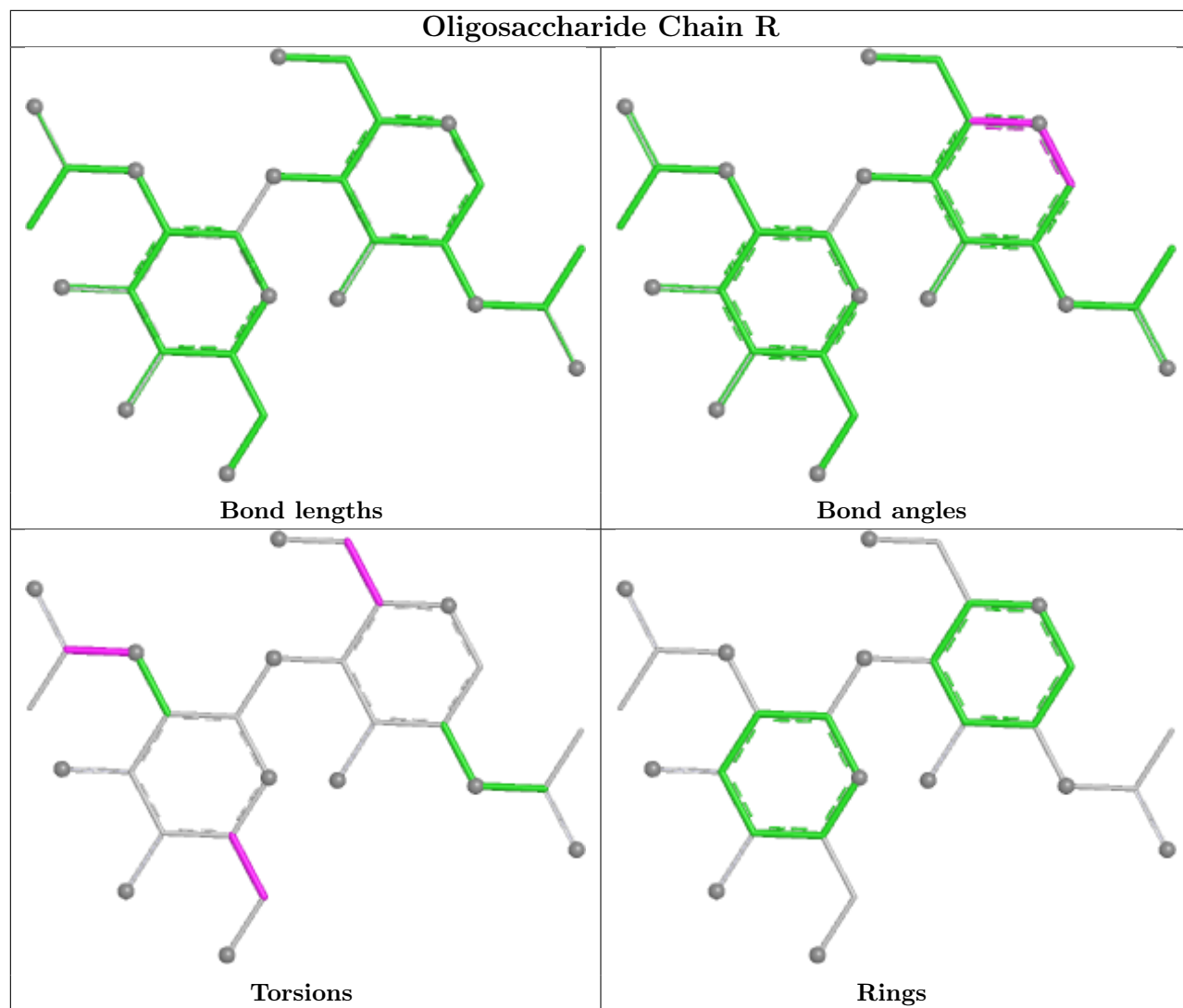


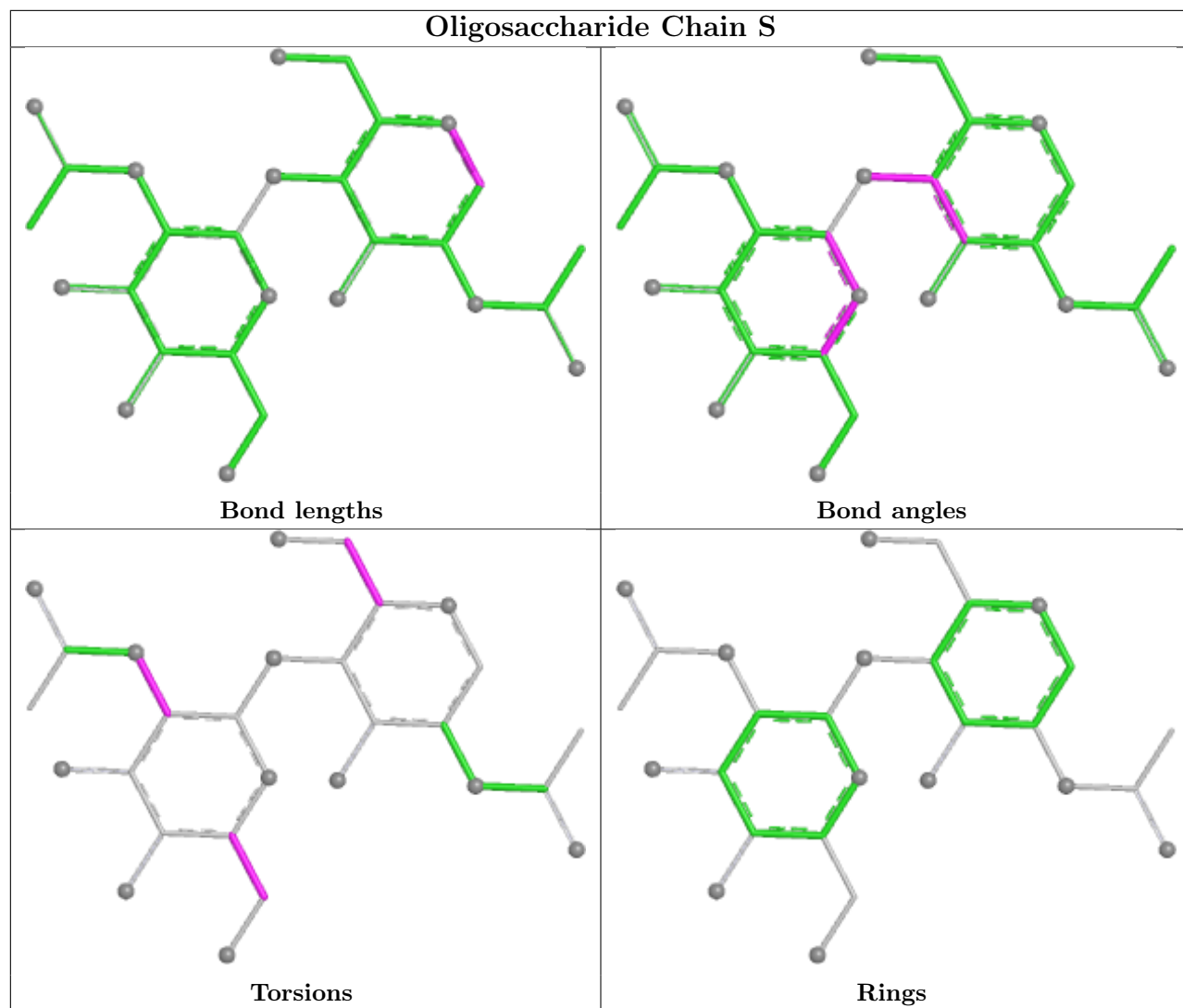


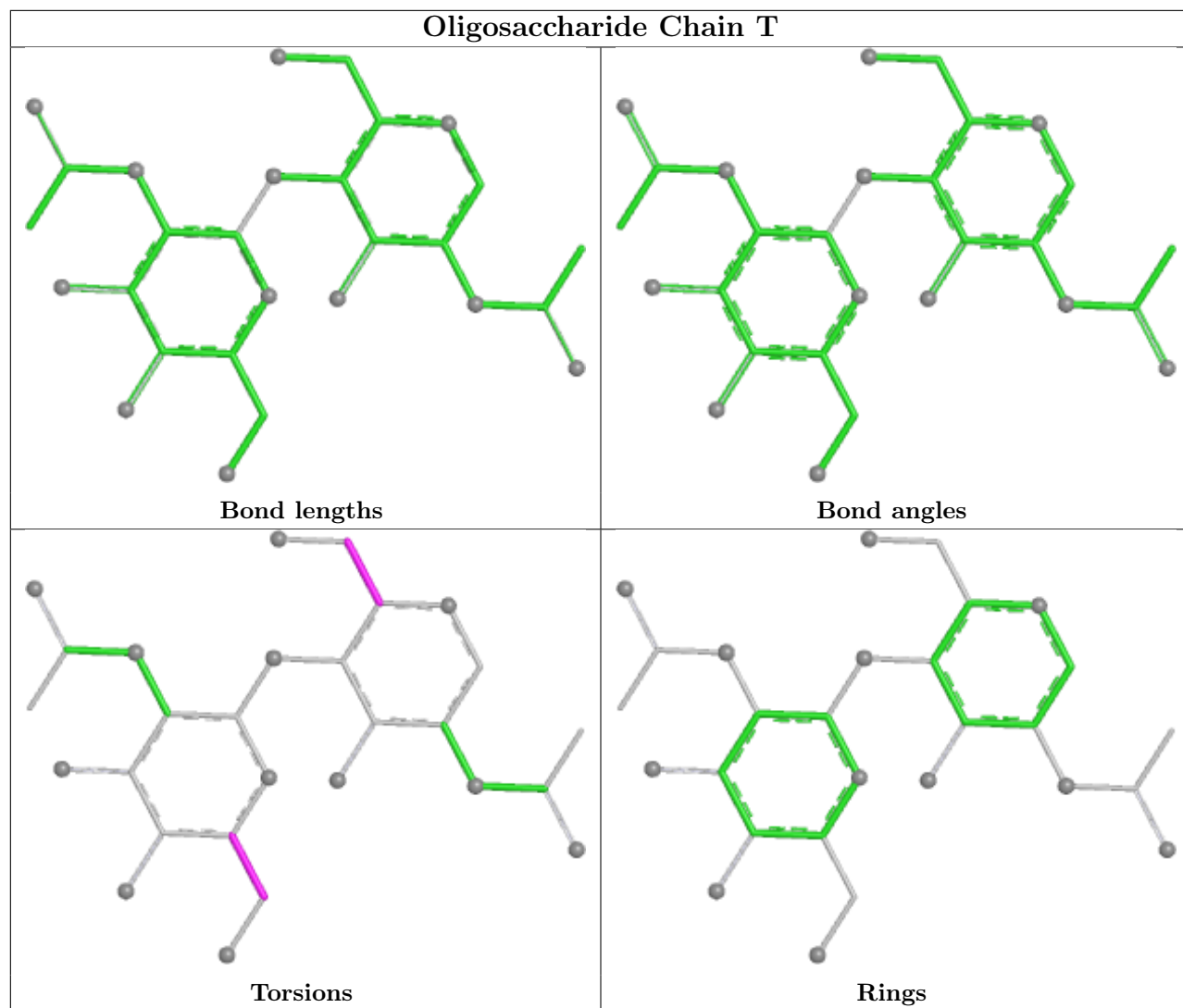


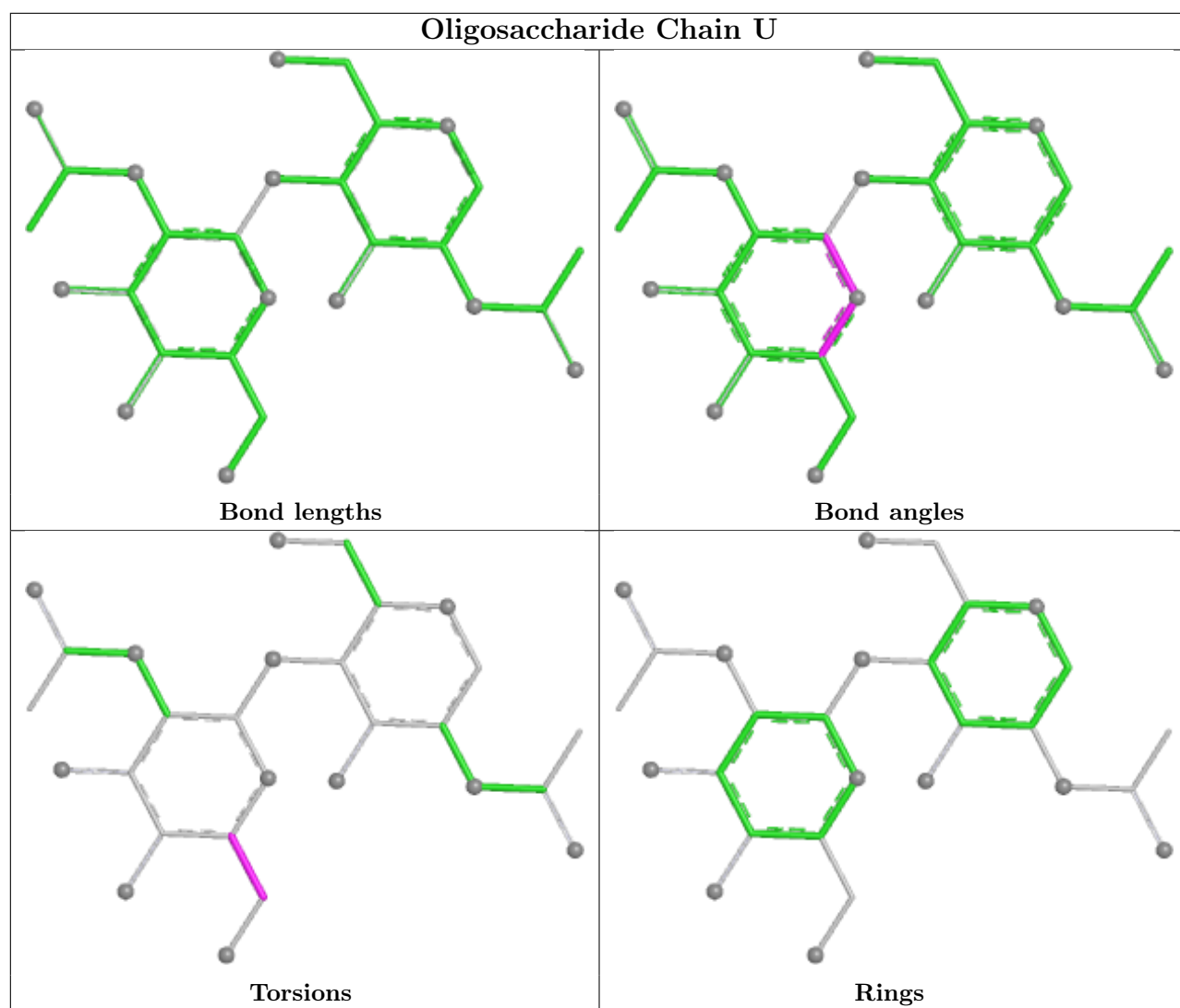


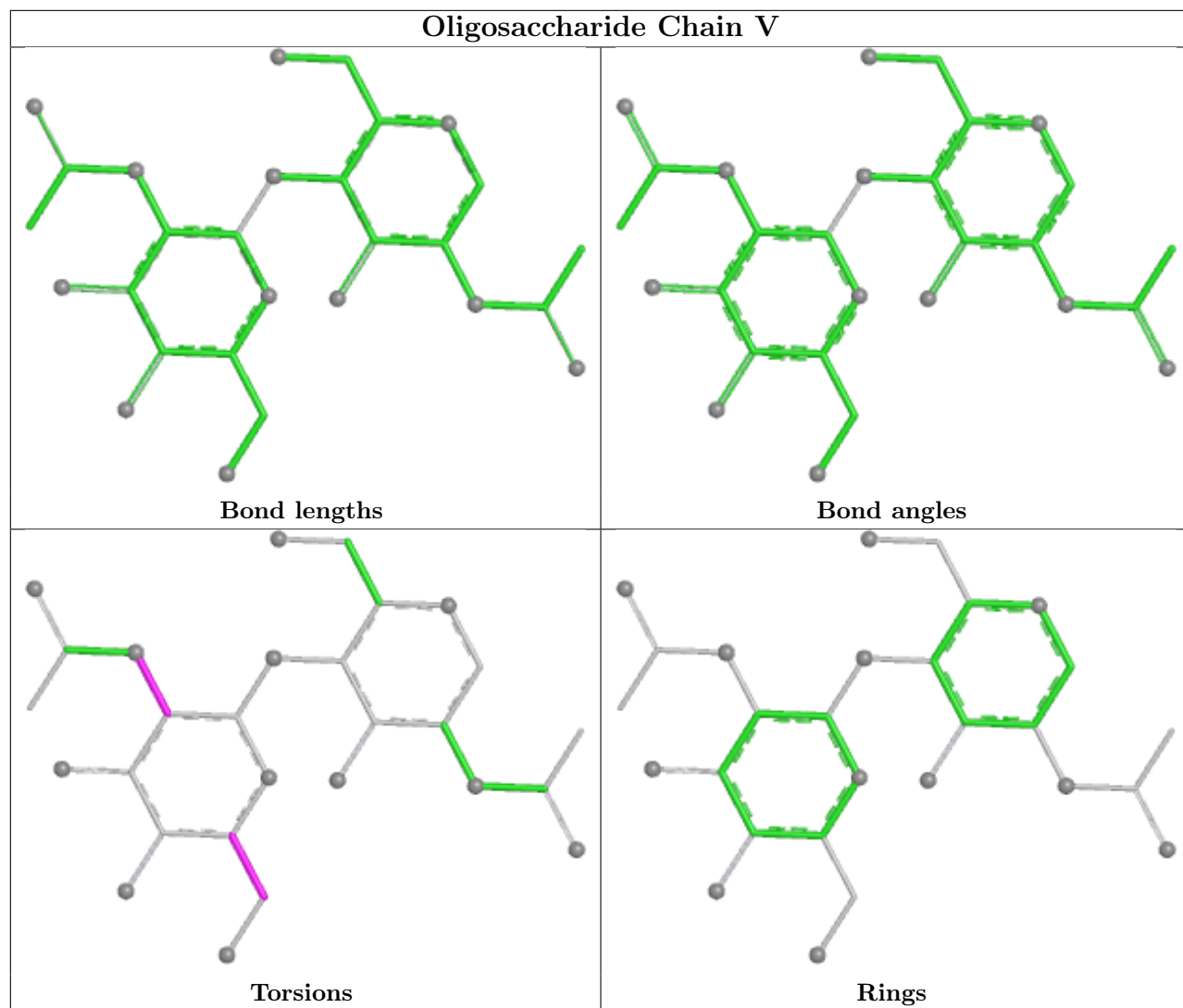


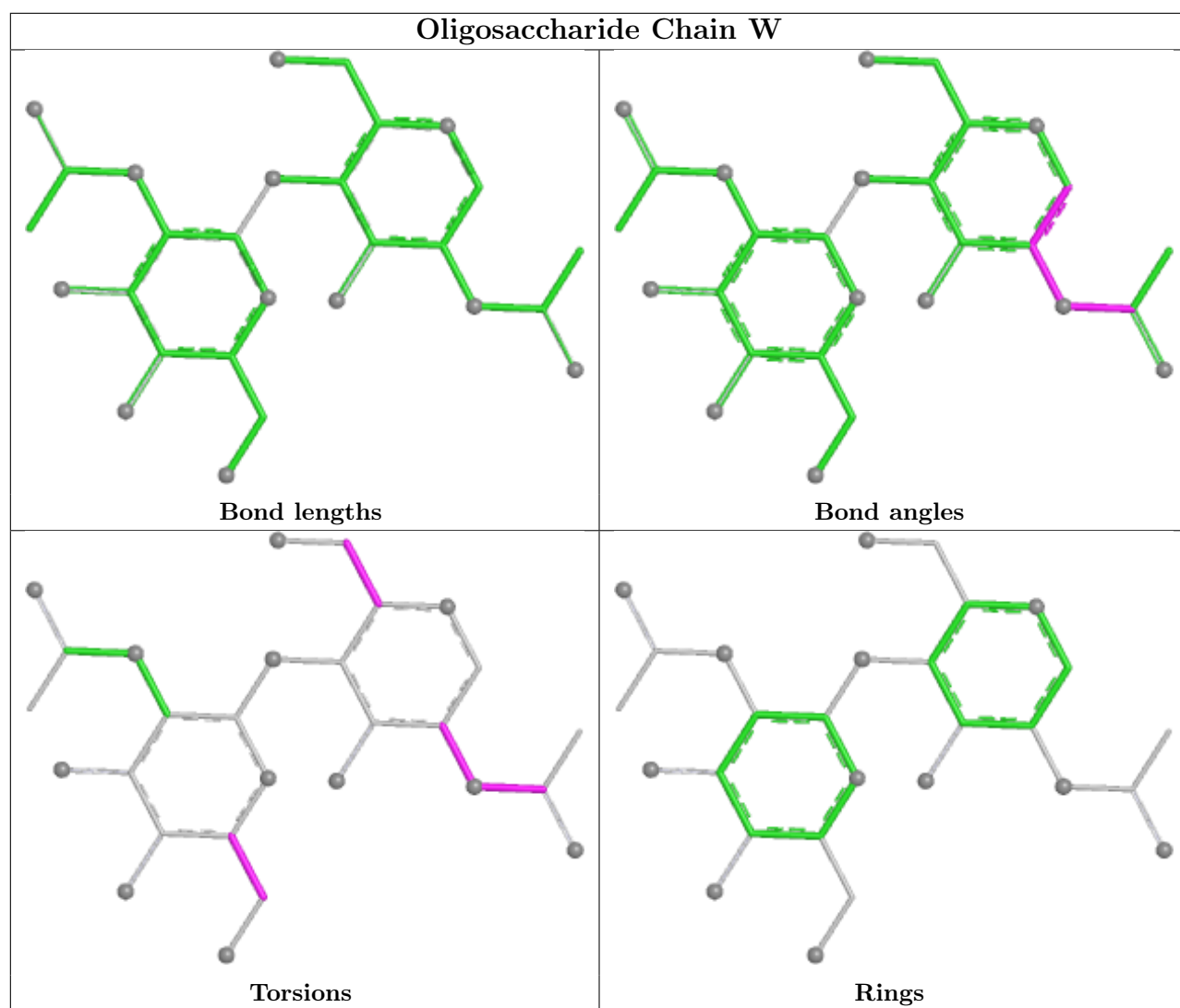


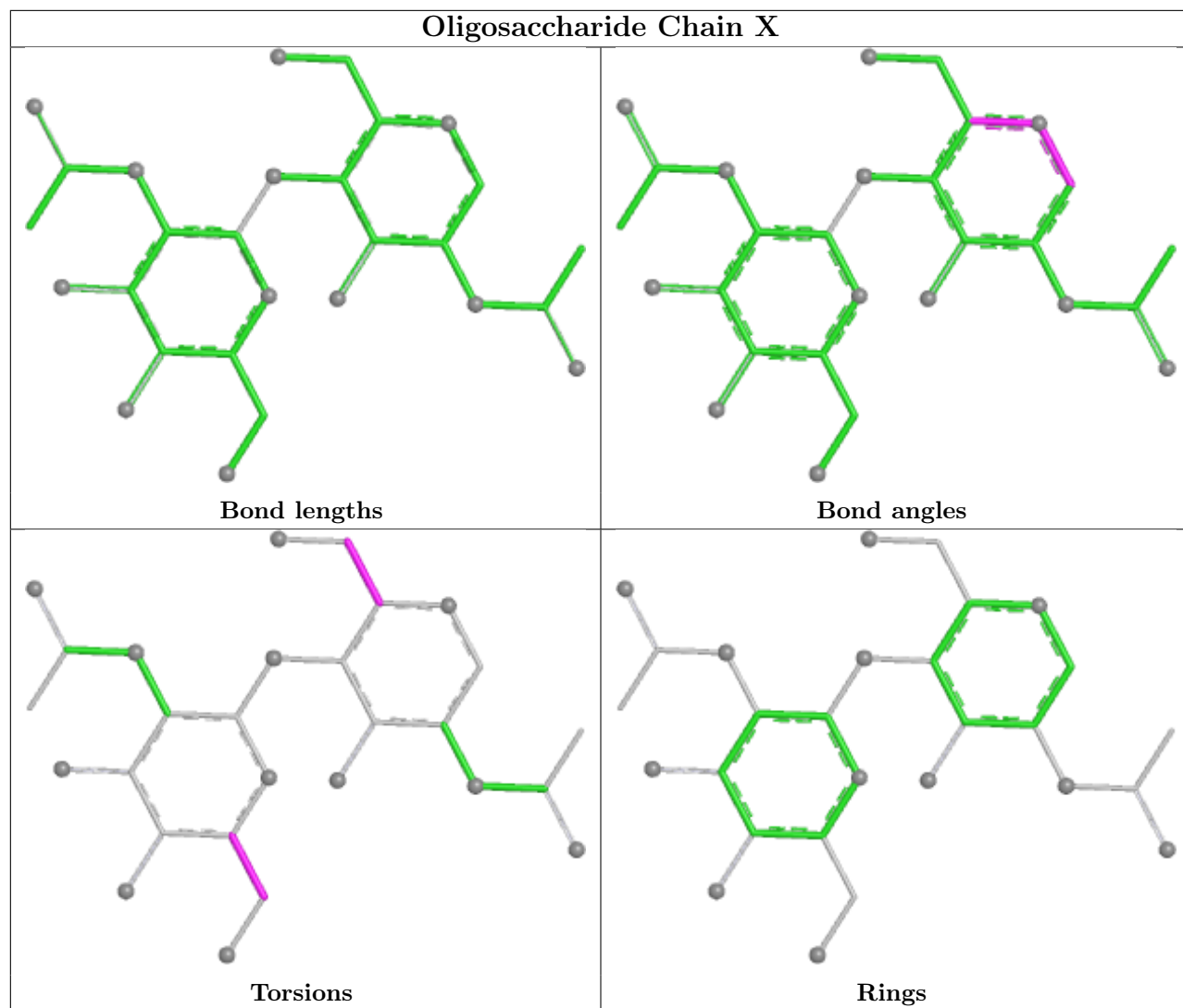


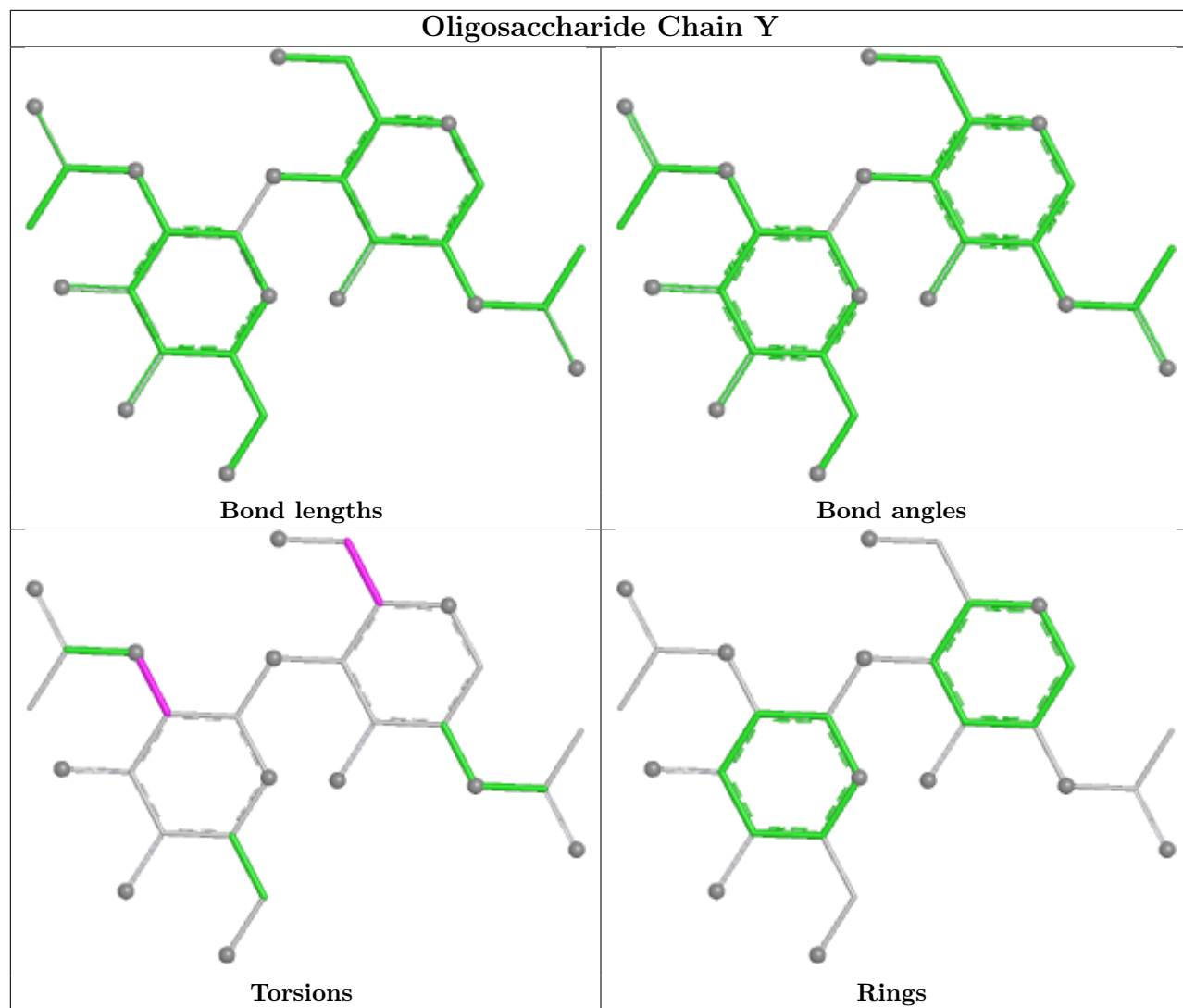


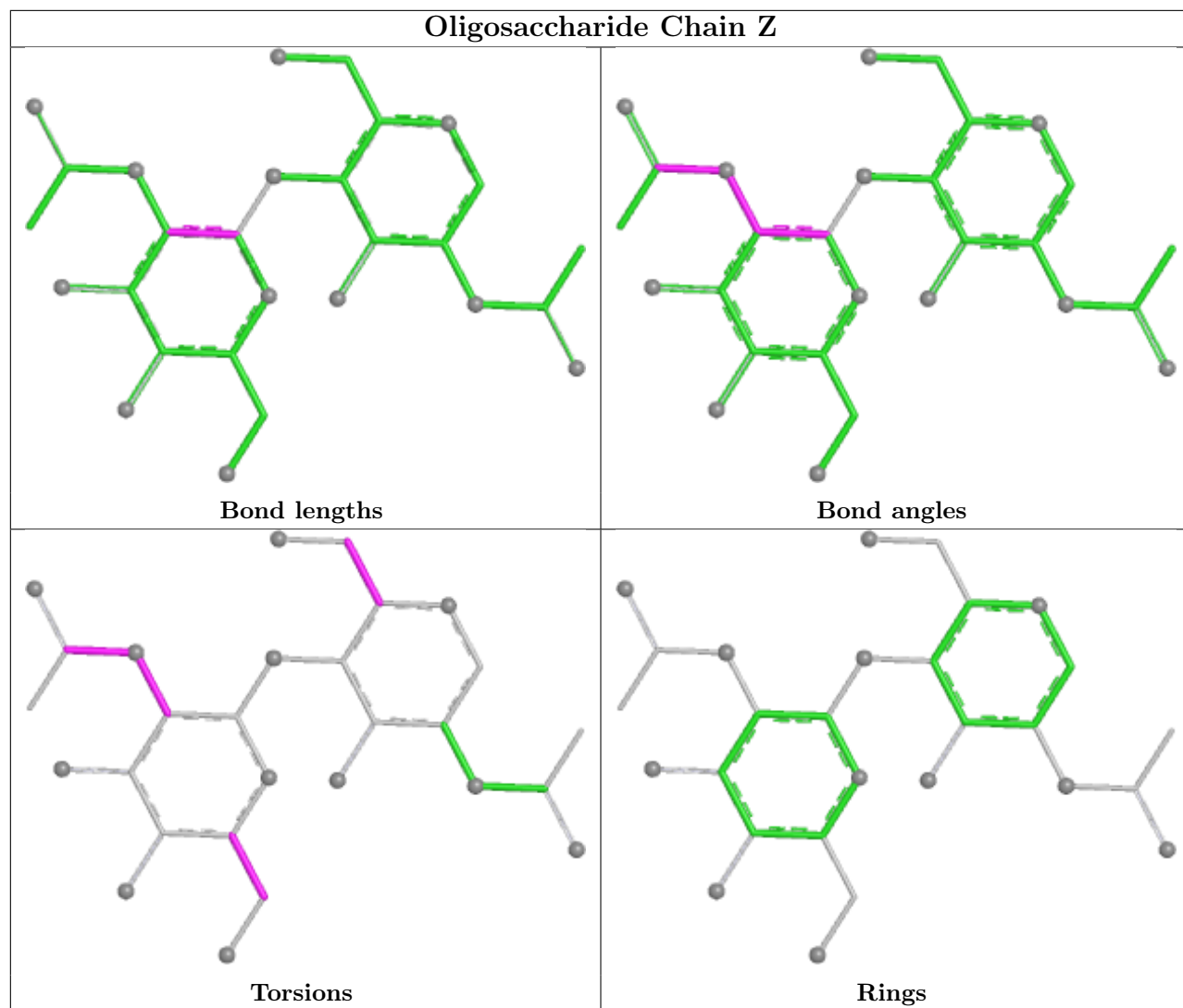


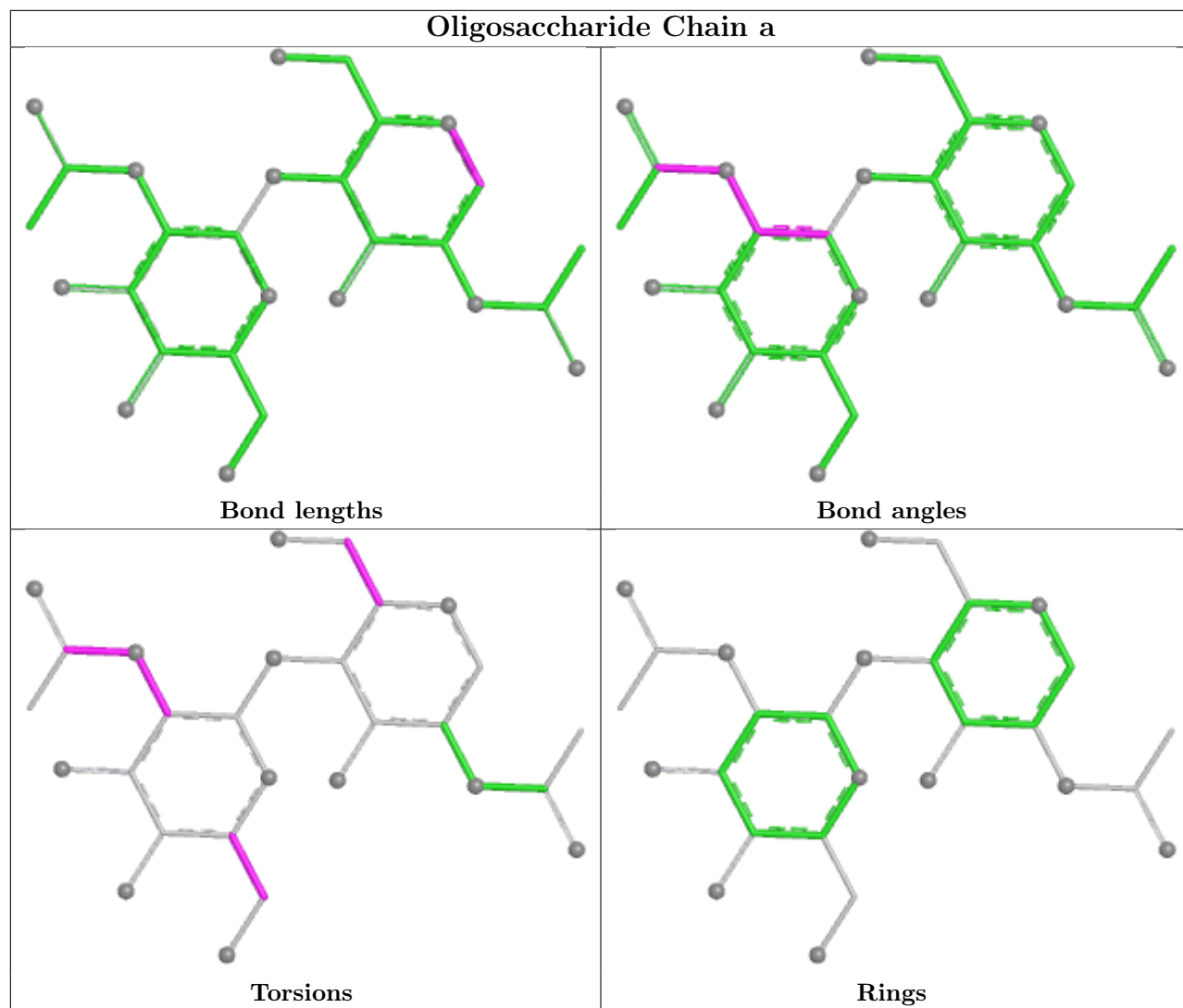


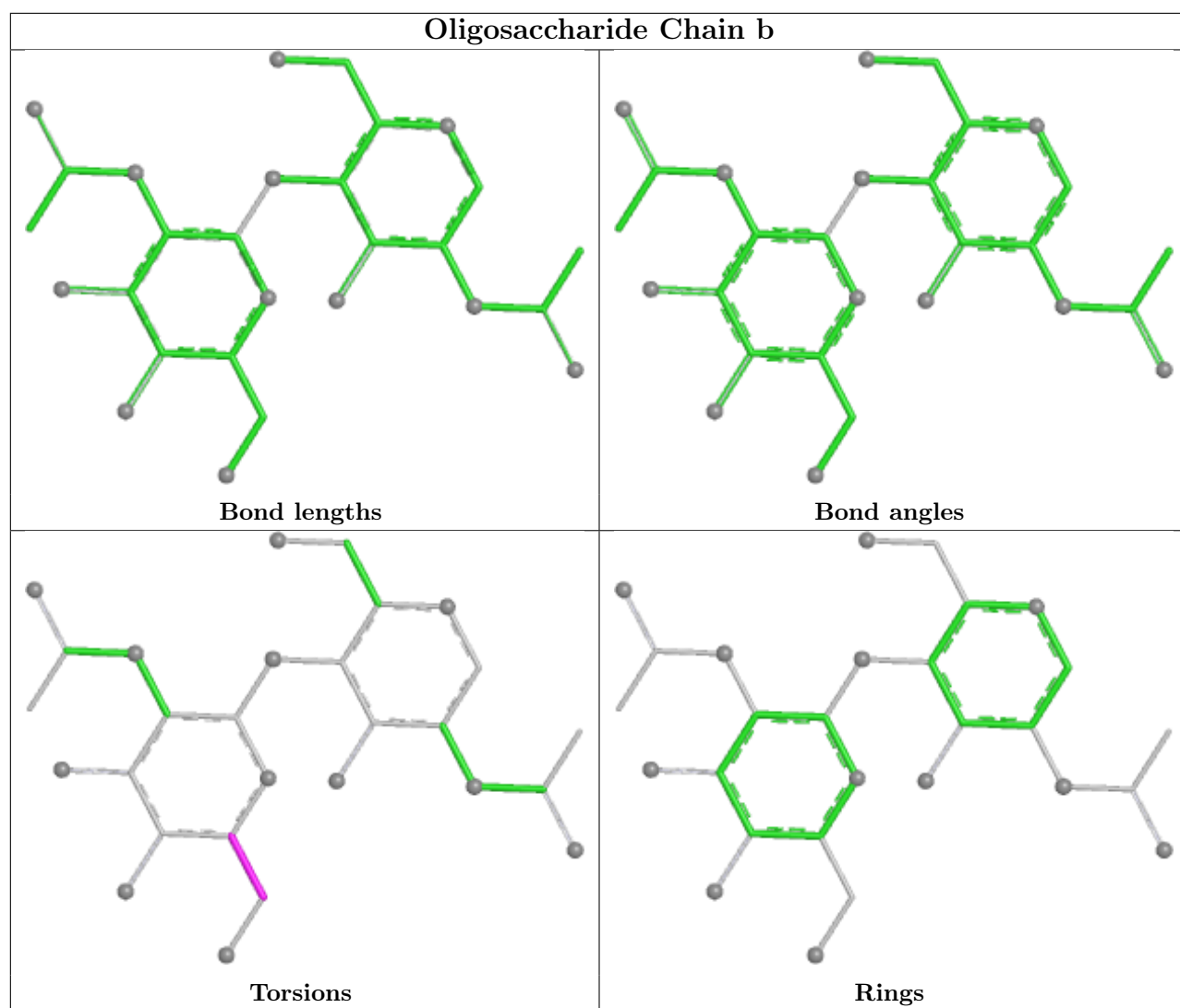


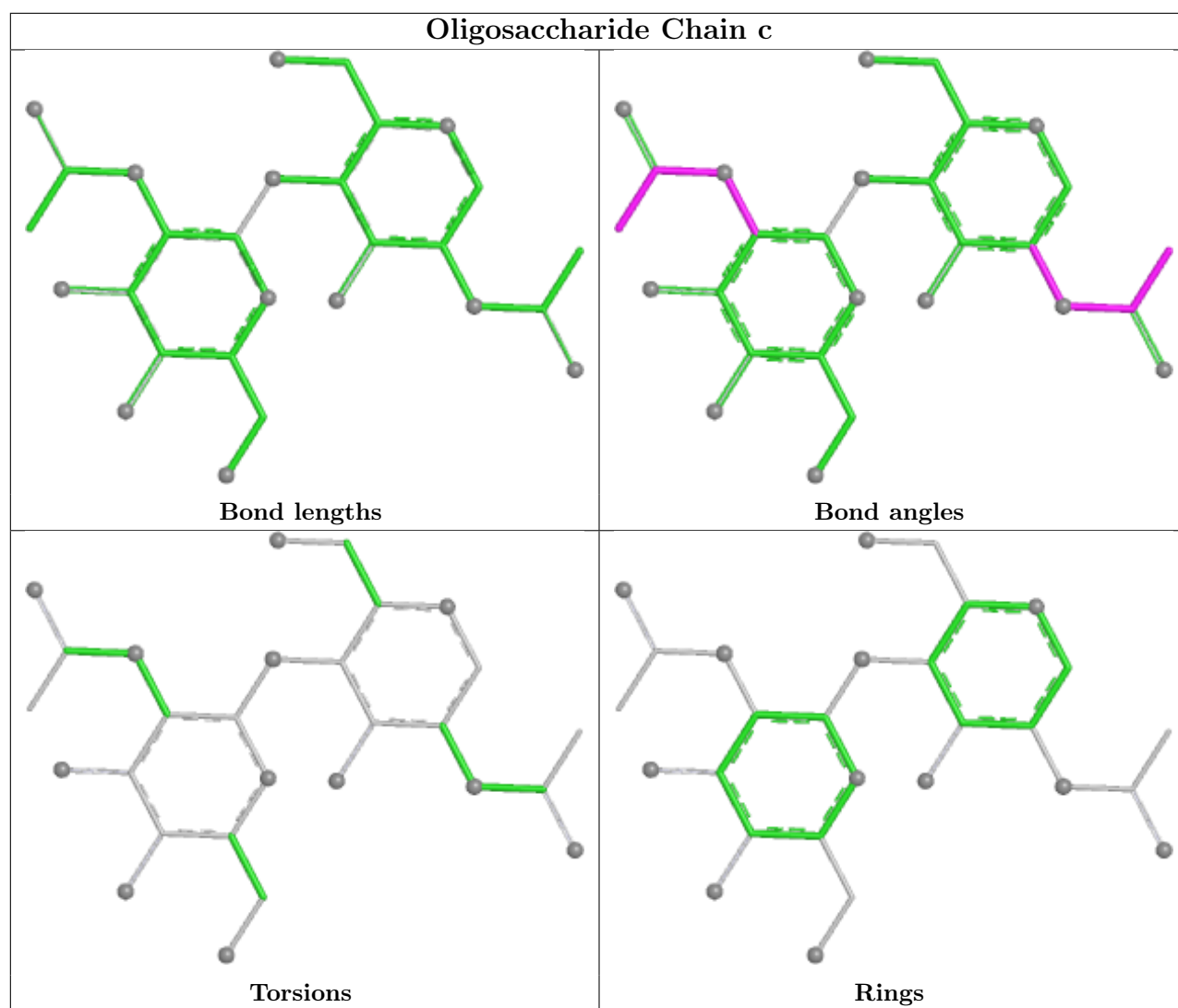


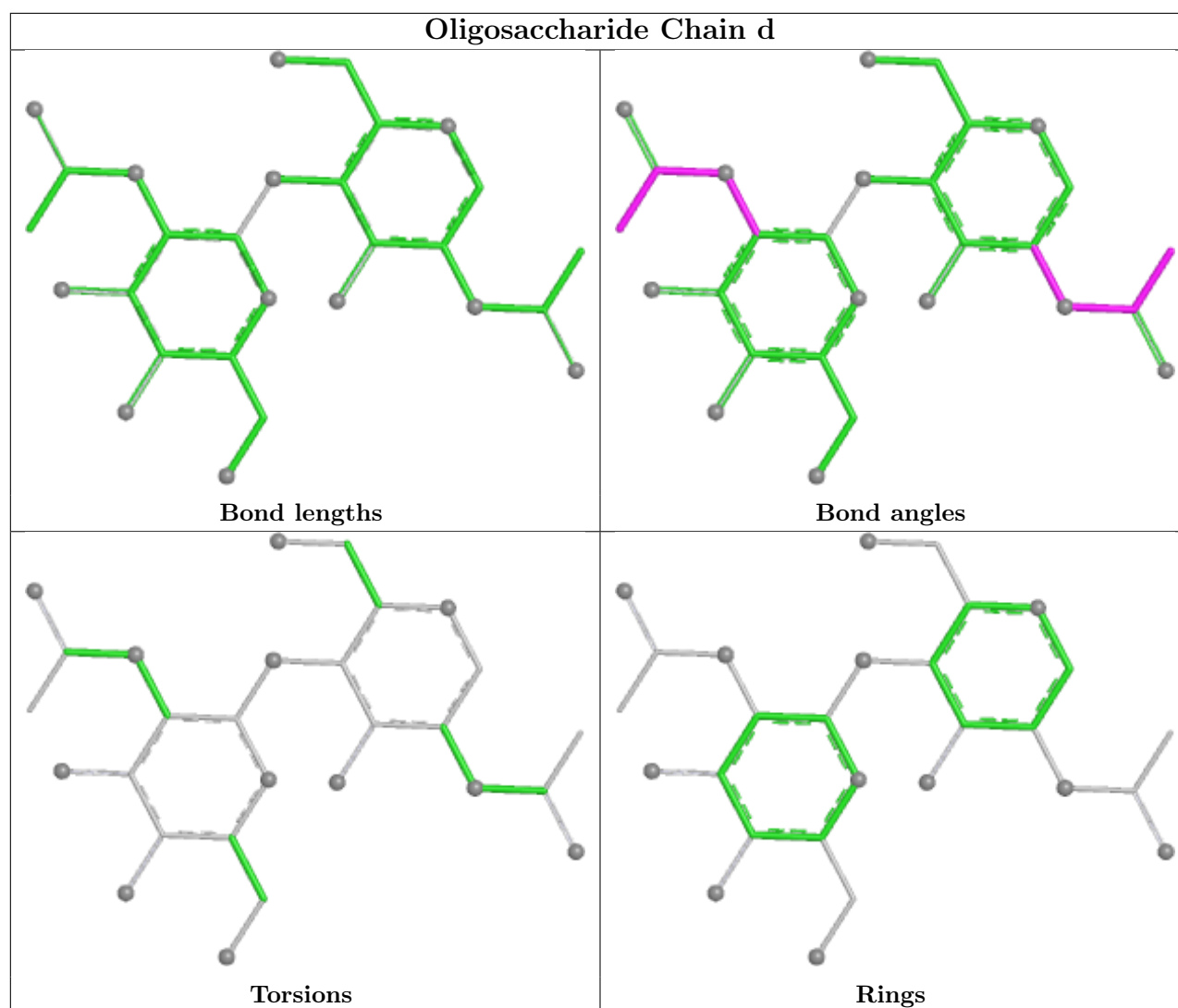












## 5.6 Ligand geometry [i](#)

28 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 | $\# Z  > 2$ |
| 5   | NAG  | C     | 1402 | 1    | 14,14,15     | 0.45 | 0           | 17,19,21    | 0.58 | 0           |
| 5   | NAG  | C     | 1403 | 1    | 14,14,15     | 0.52 | 0           | 17,19,21    | 0.47 | 0           |
| 5   | NAG  | B     | 1401 | 1    | 14,14,15     | 0.33 | 0           | 17,19,21    | 0.57 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | NAG  | A     | 1401 | 1    | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.36 | 0        |
| 5   | NAG  | B     | 1409 | 1    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.42 | 0        |
| 5   | NAG  | B     | 1404 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.61 | 1 (5%)   |
| 5   | NAG  | C     | 1408 | 1    | 14,14,15     | 0.17 | 0        | 17,19,21    | 0.58 | 0        |
| 5   | NAG  | C     | 1401 | 1    | 14,14,15     | 0.46 | 0        | 17,19,21    | 0.80 | 1 (5%)   |
| 5   | NAG  | C     | 1406 | 1    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.39 | 0        |
| 5   | NAG  | B     | 1405 | 1    | 14,14,15     | 0.41 | 0        | 17,19,21    | 1.36 | 2 (11%)  |
| 5   | NAG  | C     | 1405 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 1.38 | 2 (11%)  |
| 5   | NAG  | B     | 1406 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.84 | 1 (5%)   |
| 5   | NAG  | A     | 1407 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.51 | 0        |
| 5   | NAG  | B     | 1407 | 1    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.77 | 1 (5%)   |
| 5   | NAG  | A     | 1406 | 1    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.39 | 0        |
| 5   | NAG  | B     | 1410 | 1    | 14,14,15     | 0.42 | 0        | 17,19,21    | 1.14 | 2 (11%)  |
| 5   | NAG  | B     | 1411 | -    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.43 | 0        |
| 5   | NAG  | A     | 1403 | 1    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.44 | 0        |
| 5   | NAG  | A     | 1402 | 1    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.66 | 0        |
| 5   | NAG  | A     | 1405 | 1    | 14,14,15     | 0.59 | 0        | 17,19,21    | 1.34 | 2 (11%)  |
| 5   | NAG  | C     | 1404 | 1    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.39 | 0        |
| 5   | NAG  | B     | 1402 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.66 | 0        |
| 5   | NAG  | A     | 1404 | 1    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.55 | 0        |
| 5   | NAG  | B     | 1408 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.43 | 0        |
| 5   | NAG  | B     | 1403 | 1    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.42 | 0        |
| 5   | NAG  | C     | 1407 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.65 | 0        |
| 5   | NAG  | A     | 1408 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.39 | 0        |
| 5   | NAG  | A     | 1409 | 1    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.36 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 5   | NAG  | C     | 1402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 1403 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1401 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1401 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1409 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1404 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 1408 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 5   | NAG  | C     | 1401 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 1406 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1405 | 1    | -       | 6/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 1405 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1406 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1407 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1407 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1406 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1410 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1411 | -    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1403 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1402 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1405 | 1    | -       | 6/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 1404 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1402 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1404 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1408 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | B     | 1403 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 1407 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1408 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | A     | 1409 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5   | C     | 1405 | NAG  | C2-N2-C7 | 4.58  | 129.04      | 122.90   |
| 5   | A     | 1405 | NAG  | C2-N2-C7 | 4.57  | 129.02      | 122.90   |
| 5   | B     | 1405 | NAG  | C2-N2-C7 | 4.39  | 128.79      | 122.90   |
| 5   | C     | 1401 | NAG  | C1-O5-C5 | 2.88  | 116.05      | 112.19   |
| 5   | B     | 1406 | NAG  | C1-O5-C5 | 2.61  | 115.69      | 112.19   |
| 5   | C     | 1405 | NAG  | C1-C2-N2 | 2.46  | 114.32      | 110.43   |
| 5   | B     | 1407 | NAG  | C1-O5-C5 | 2.44  | 115.46      | 112.19   |
| 5   | B     | 1410 | NAG  | C8-C7-N2 | 2.33  | 119.99      | 116.12   |
| 5   | B     | 1405 | NAG  | C1-C2-N2 | 2.32  | 114.09      | 110.43   |
| 5   | B     | 1410 | NAG  | C2-N2-C7 | -2.14 | 120.03      | 122.90   |
| 5   | A     | 1405 | NAG  | C1-C2-N2 | 2.12  | 113.78      | 110.43   |
| 5   | B     | 1404 | NAG  | C1-O5-C5 | 2.03  | 114.90      | 112.19   |

There are no chirality outliers.

All (63) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 5   | B     | 1408 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1401 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1406 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1402 | NAG  | O5-C5-C6-O6 |
| 5   | C     | 1408 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1402 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1404 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1401 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1401 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1402 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1405 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1404 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1408 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1405 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1409 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1407 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1408 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1402 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1404 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1409 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1406 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1405 | NAG  | C8-C7-N2-C2 |
| 5   | A     | 1405 | NAG  | O7-C7-N2-C2 |
| 5   | B     | 1405 | NAG  | C8-C7-N2-C2 |
| 5   | B     | 1405 | NAG  | O7-C7-N2-C2 |
| 5   | C     | 1405 | NAG  | C8-C7-N2-C2 |
| 5   | C     | 1405 | NAG  | O7-C7-N2-C2 |
| 5   | C     | 1406 | NAG  | C8-C7-N2-C2 |
| 5   | C     | 1406 | NAG  | O7-C7-N2-C2 |
| 5   | B     | 1407 | NAG  | C4-C5-C6-O6 |
| 5   | C     | 1401 | NAG  | O5-C5-C6-O6 |
| 5   | C     | 1408 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1405 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1404 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1403 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1403 | NAG  | O5-C5-C6-O6 |
| 5   | C     | 1403 | NAG  | O5-C5-C6-O6 |
| 5   | C     | 1407 | NAG  | C4-C5-C6-O6 |
| 5   | C     | 1403 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1409 | NAG  | C4-C5-C6-O6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 5   | A     | 1408 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1406 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1403 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1403 | NAG  | C4-C5-C6-O6 |
| 5   | C     | 1404 | NAG  | O5-C5-C6-O6 |
| 5   | C     | 1407 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1409 | NAG  | O5-C5-C6-O6 |
| 5   | A     | 1401 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1405 | NAG  | C4-C5-C6-O6 |
| 5   | B     | 1406 | NAG  | O5-C5-C6-O6 |
| 5   | B     | 1406 | NAG  | C3-C2-N2-C7 |
| 5   | B     | 1407 | NAG  | C3-C2-N2-C7 |
| 5   | C     | 1407 | NAG  | C3-C2-N2-C7 |
| 5   | A     | 1405 | NAG  | C1-C2-N2-C7 |
| 5   | B     | 1405 | NAG  | C1-C2-N2-C7 |
| 5   | B     | 1406 | NAG  | C1-C2-N2-C7 |
| 5   | B     | 1407 | NAG  | C1-C2-N2-C7 |
| 5   | C     | 1405 | NAG  | C1-C2-N2-C7 |
| 5   | C     | 1407 | NAG  | C1-C2-N2-C7 |
| 5   | A     | 1405 | NAG  | C3-C2-N2-C7 |
| 5   | B     | 1405 | NAG  | C3-C2-N2-C7 |
| 5   | C     | 1403 | NAG  | C3-C2-N2-C7 |
| 5   | C     | 1405 | NAG  | C3-C2-N2-C7 |

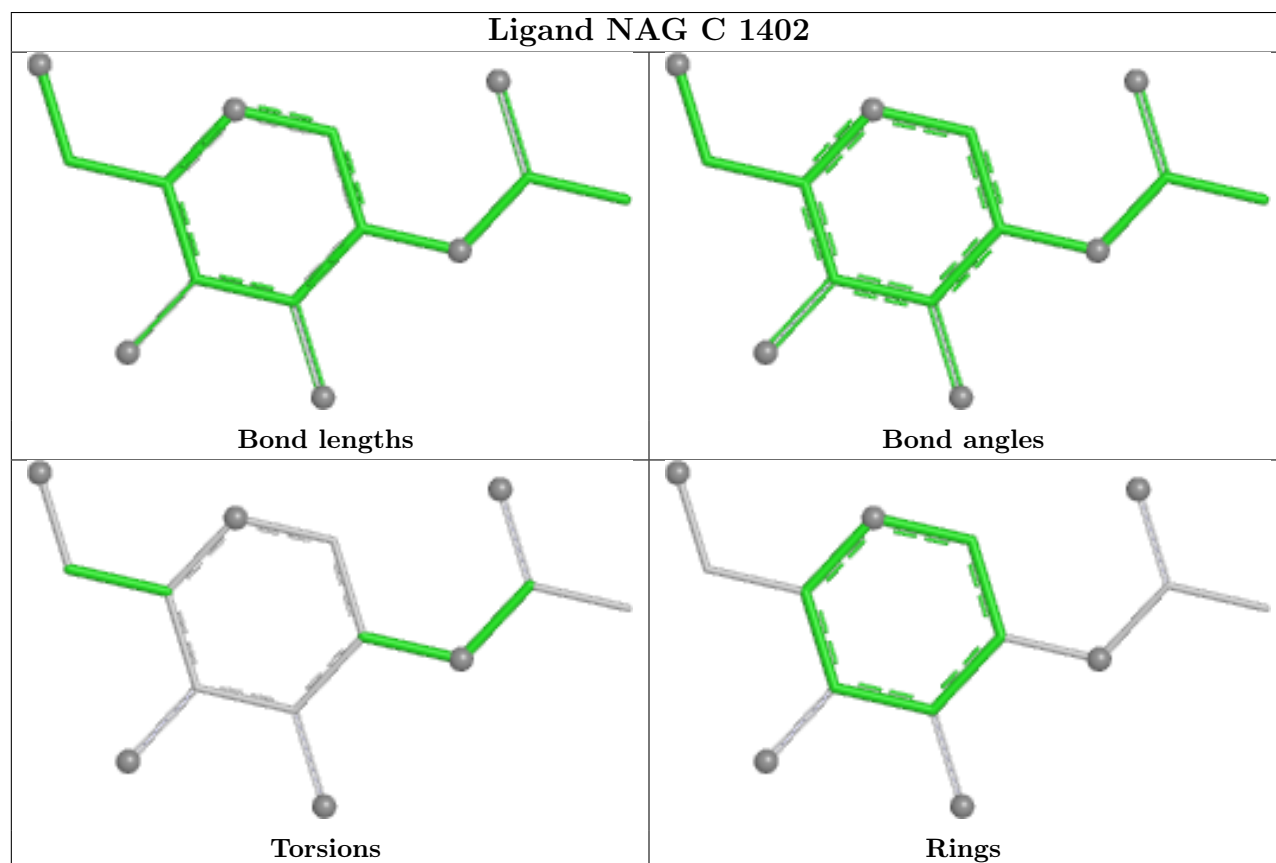
There are no ring outliers.

10 monomers are involved in 16 short contacts:

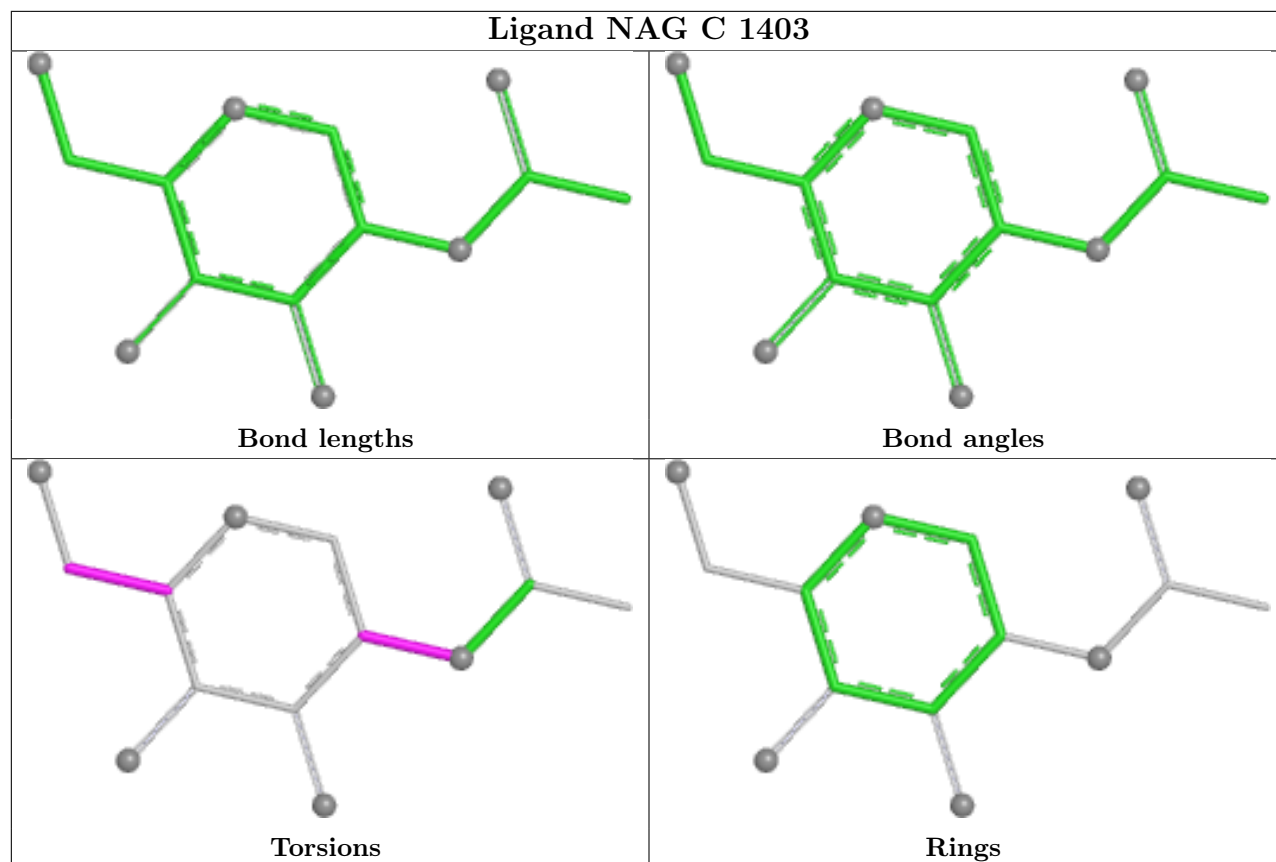
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | C     | 1402 | NAG  | 1       | 0            |
| 5   | B     | 1405 | NAG  | 2       | 0            |
| 5   | C     | 1405 | NAG  | 1       | 0            |
| 5   | B     | 1407 | NAG  | 1       | 0            |
| 5   | B     | 1410 | NAG  | 4       | 0            |
| 5   | B     | 1411 | NAG  | 4       | 0            |
| 5   | A     | 1402 | NAG  | 3       | 0            |
| 5   | A     | 1405 | NAG  | 1       | 0            |
| 5   | B     | 1402 | NAG  | 1       | 0            |
| 5   | B     | 1403 | NAG  | 2       | 0            |

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

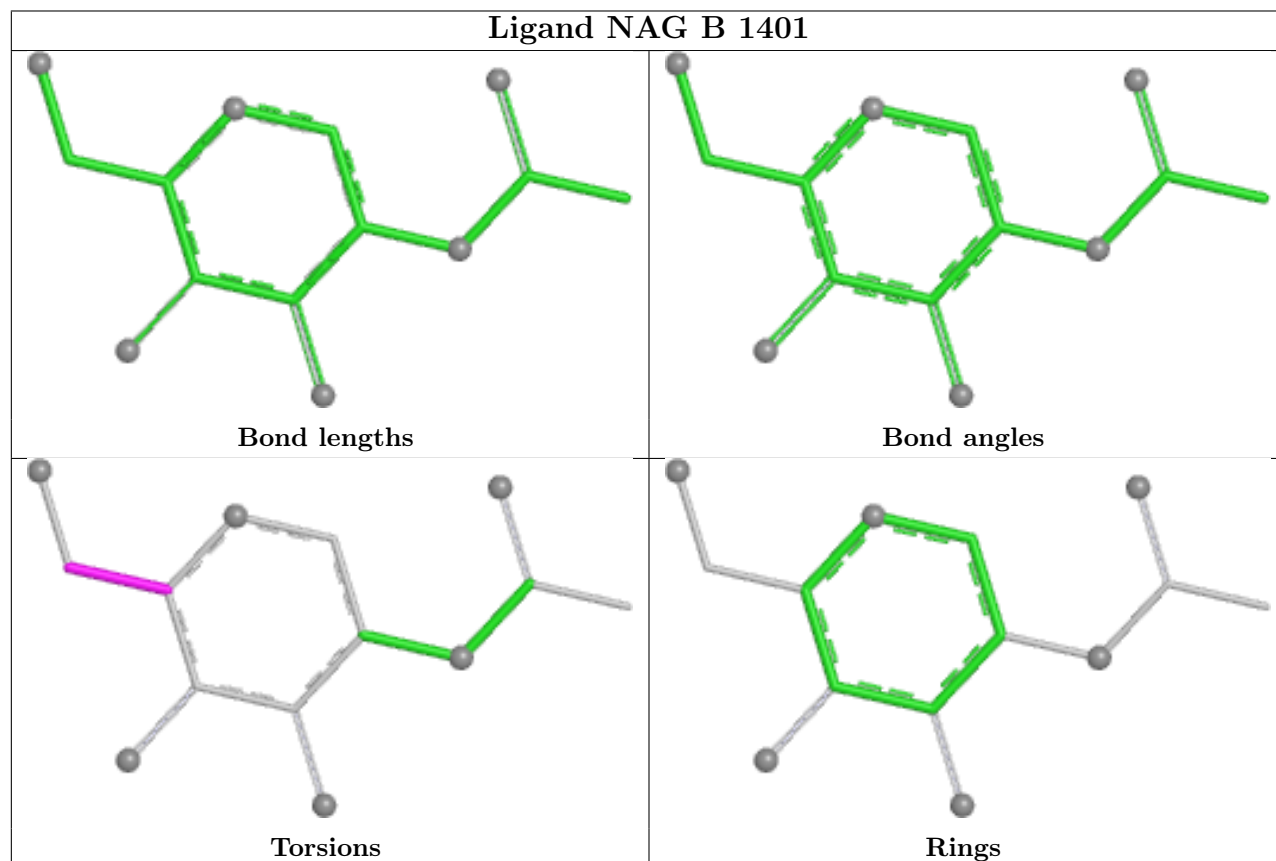
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



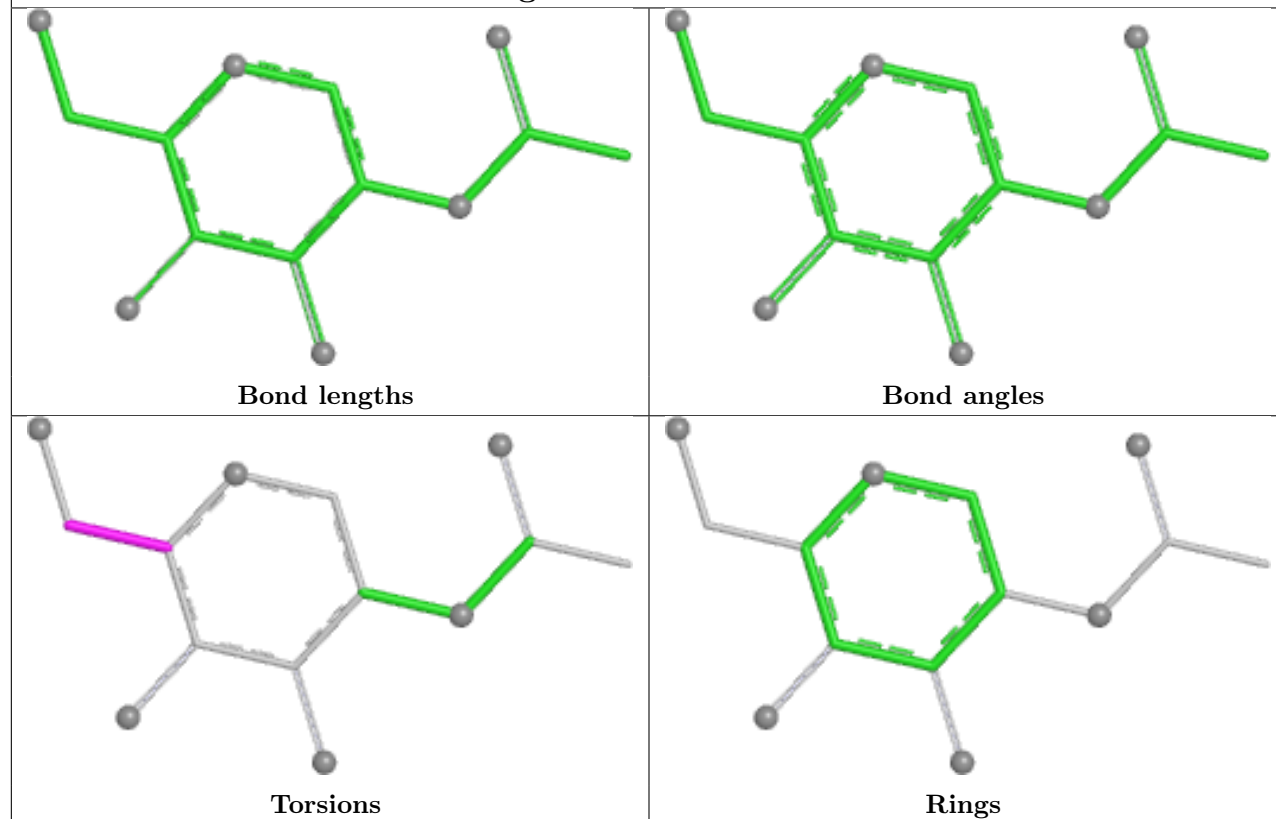
## Ligand NAG C 1403



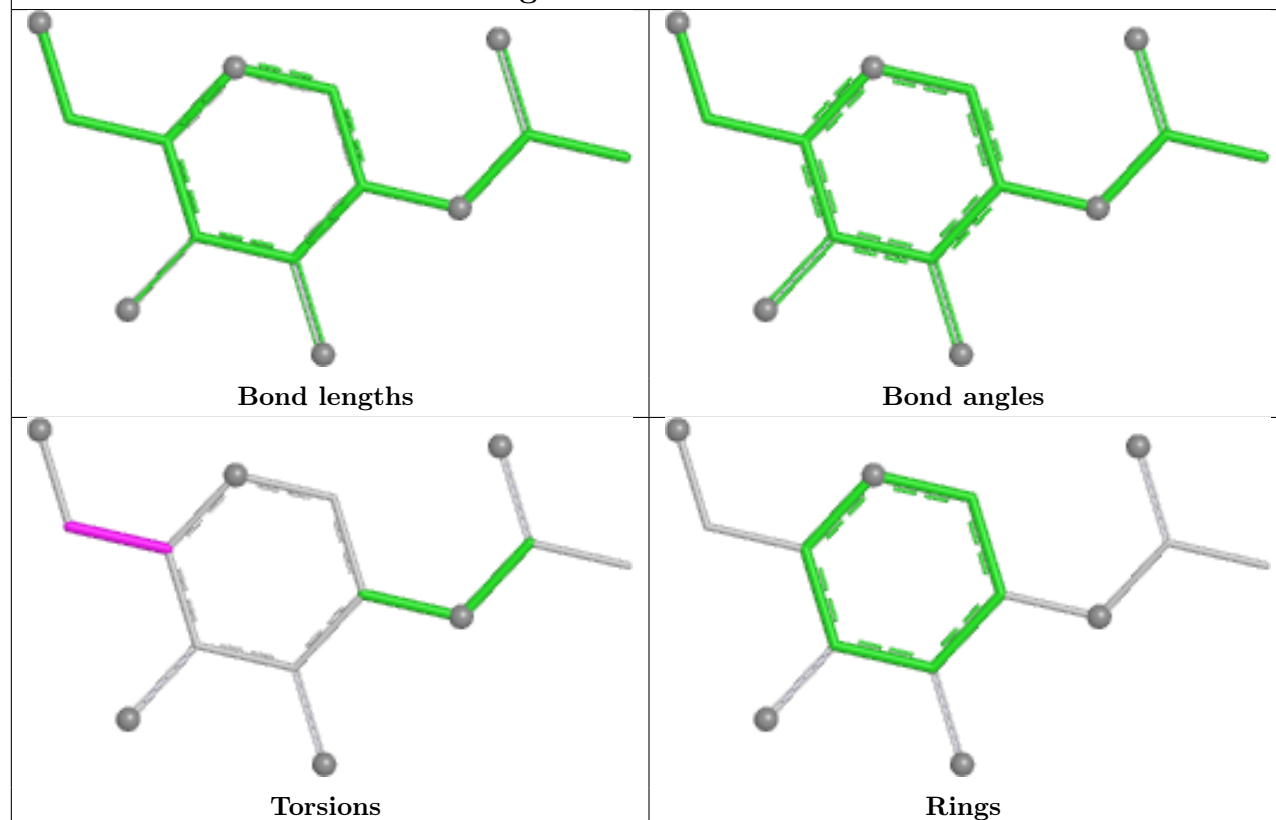
## Ligand NAG B 1401

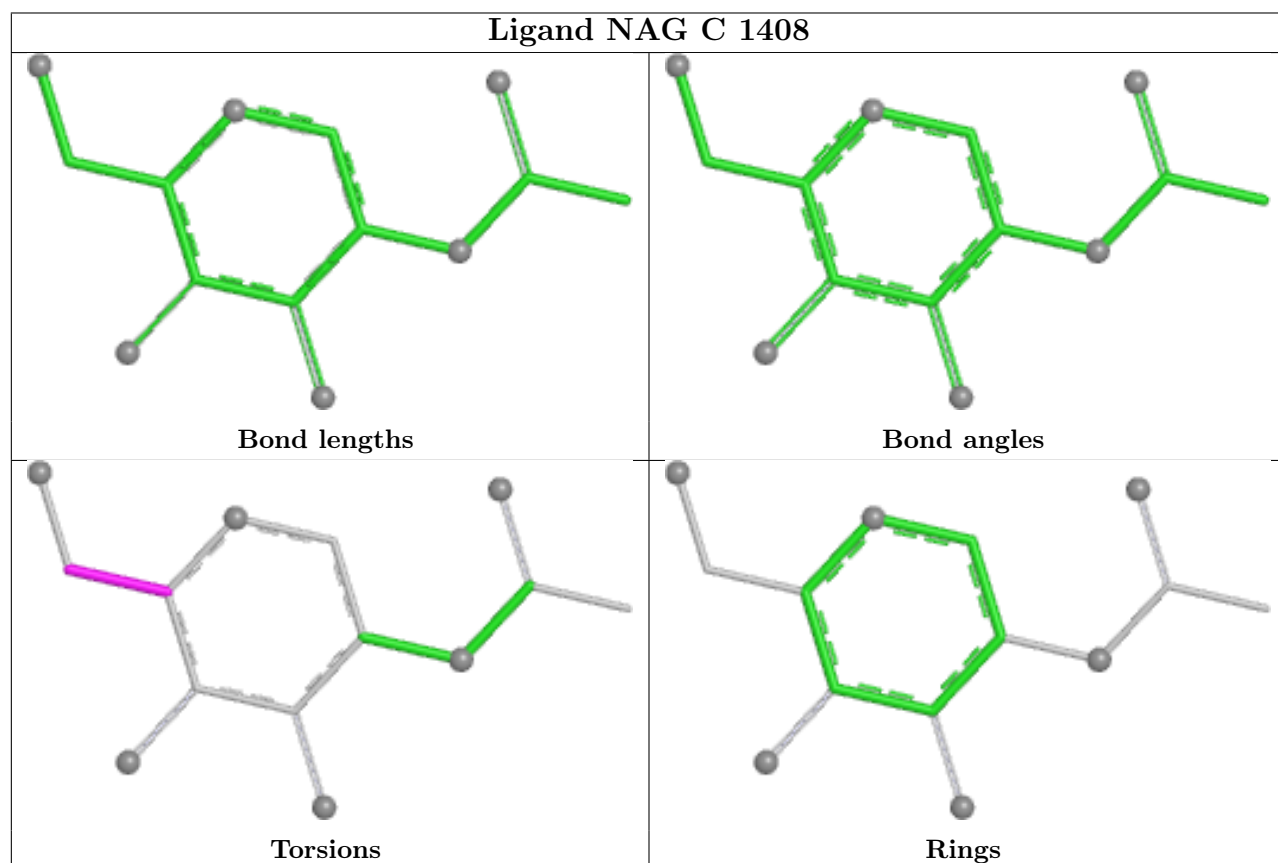
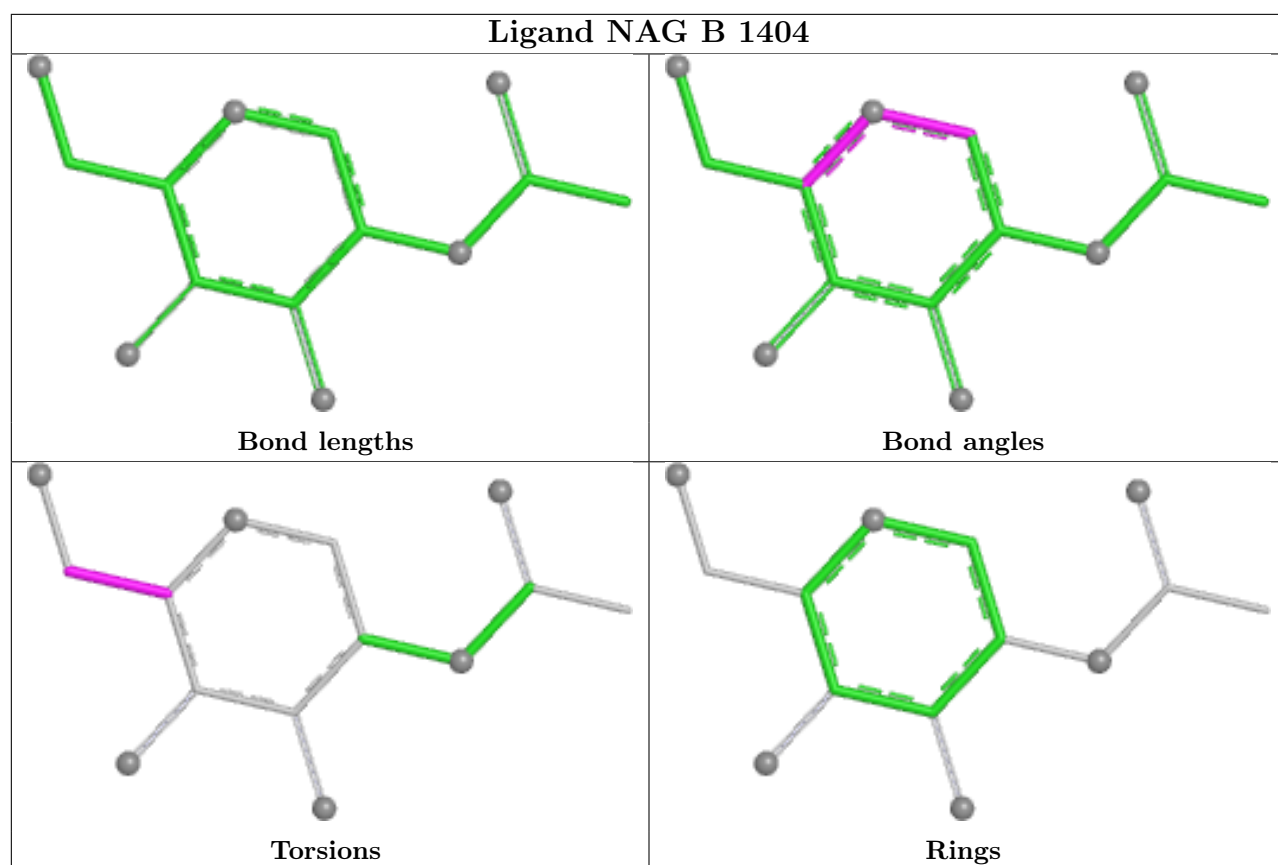


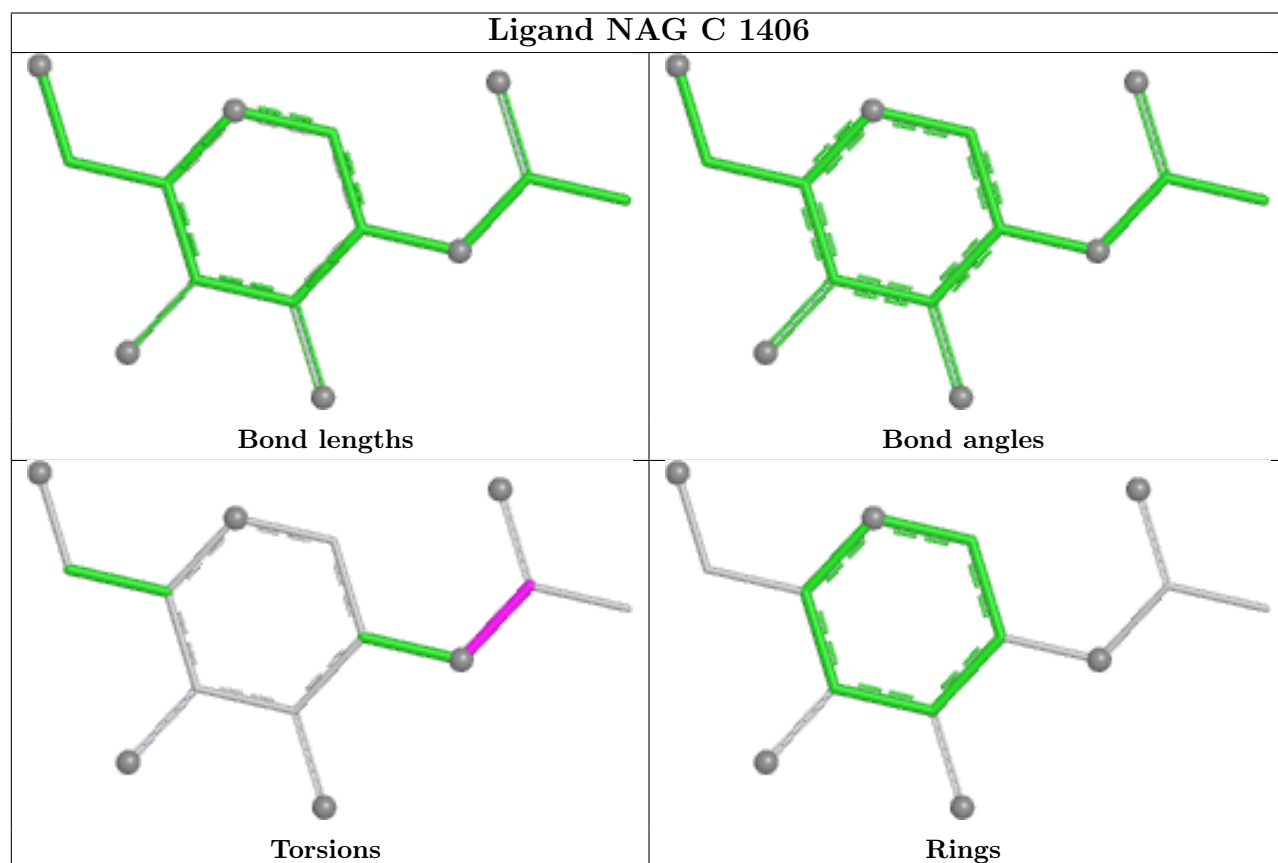
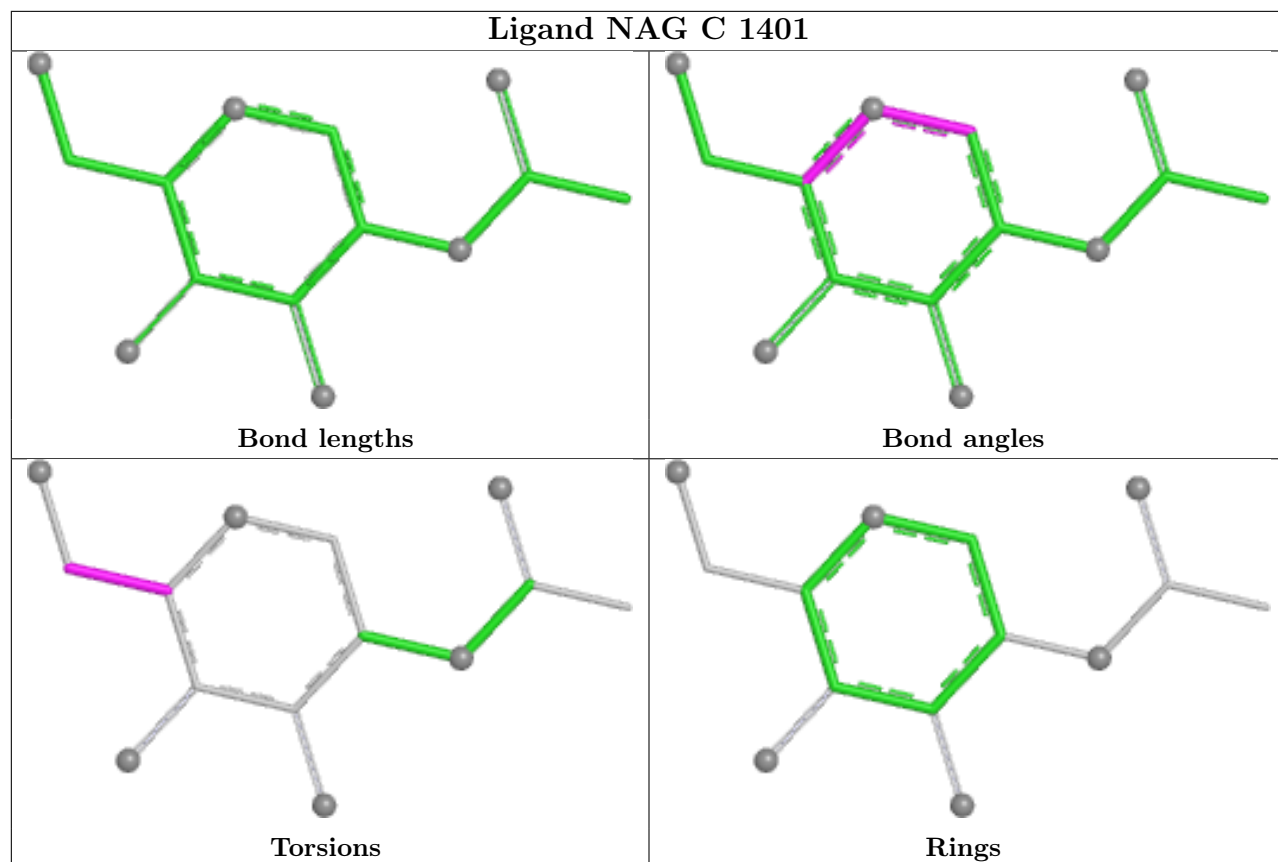
## Ligand NAG A 1401



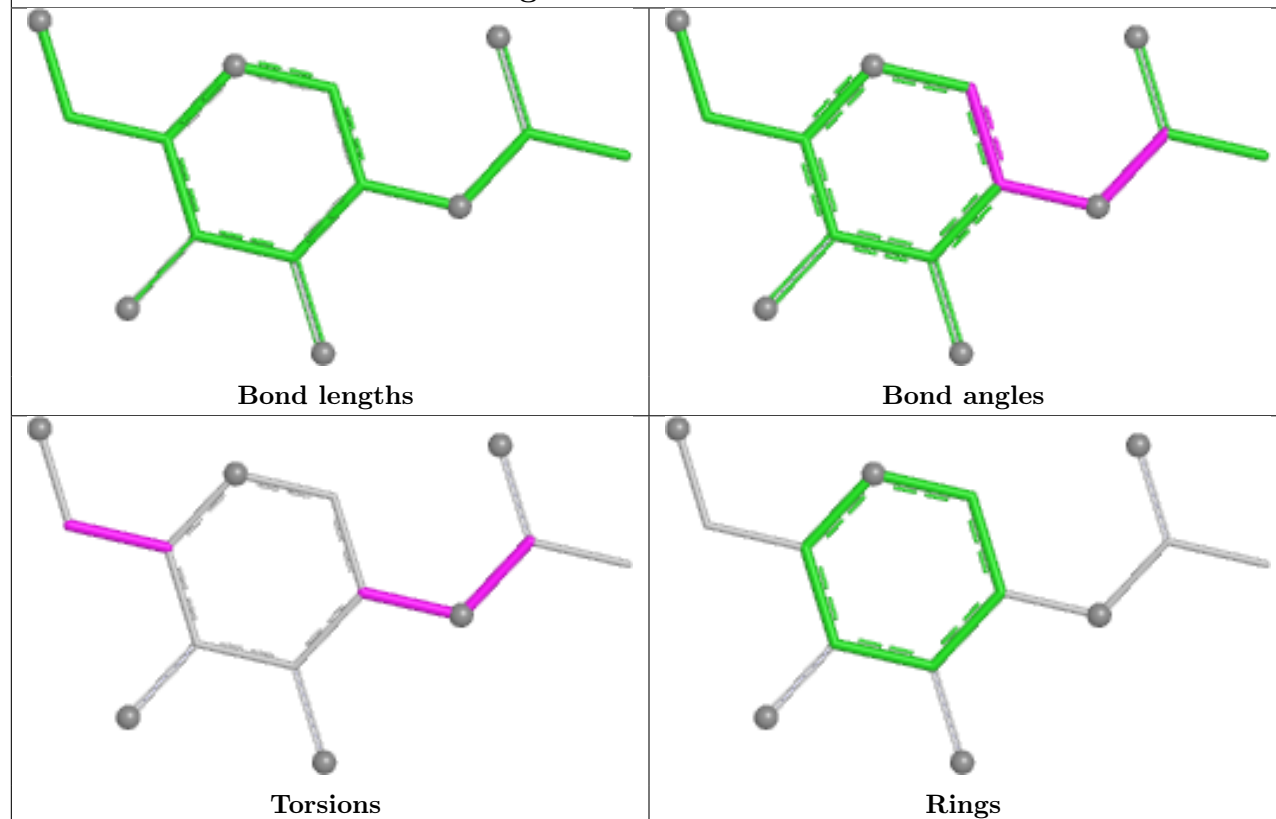
## Ligand NAG B 1409



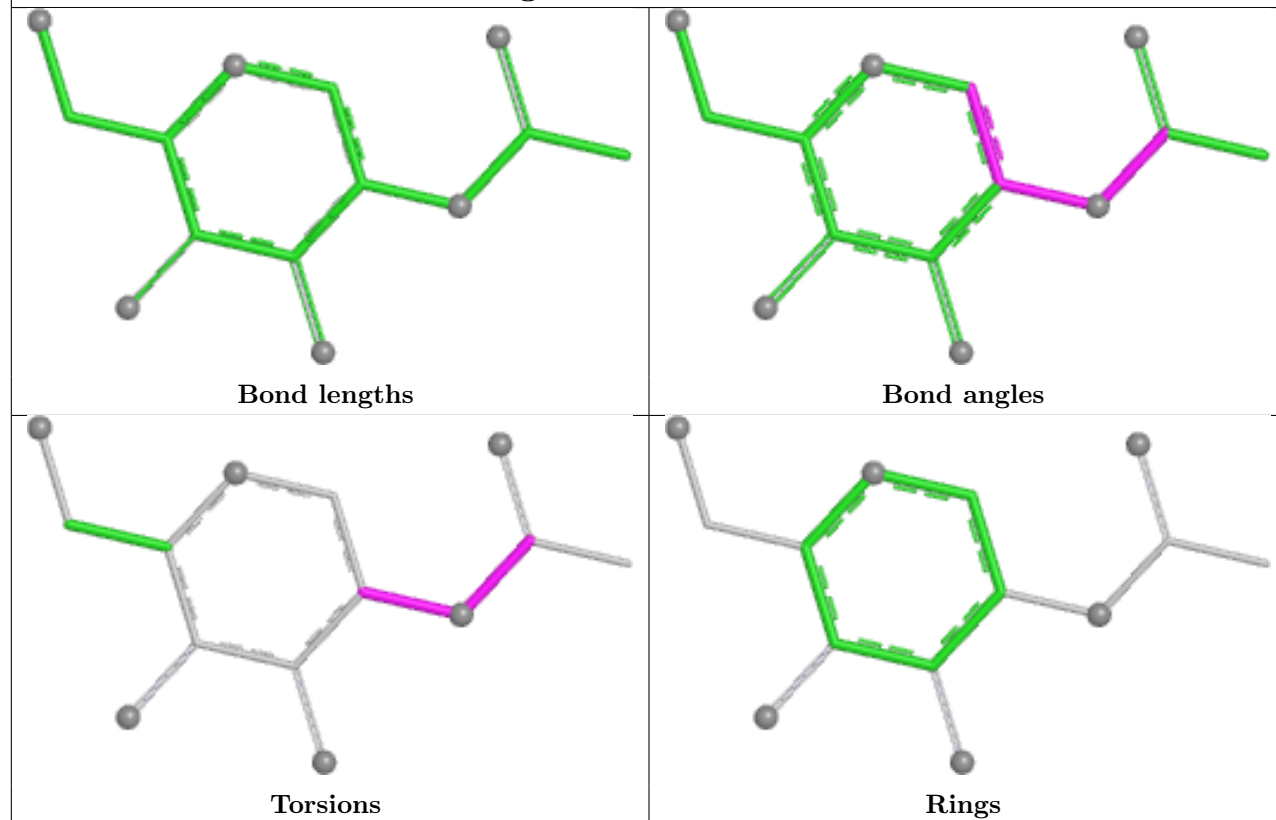




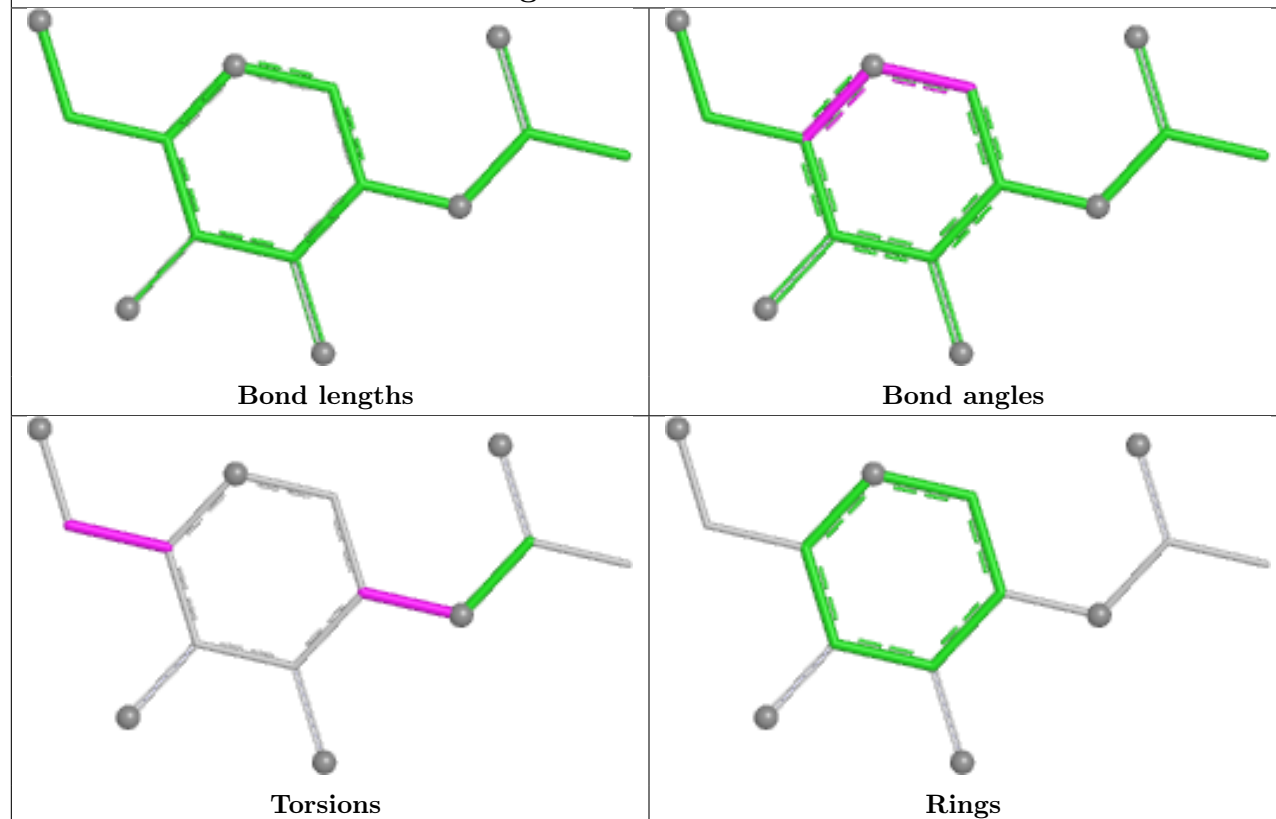
## Ligand NAG B 1405



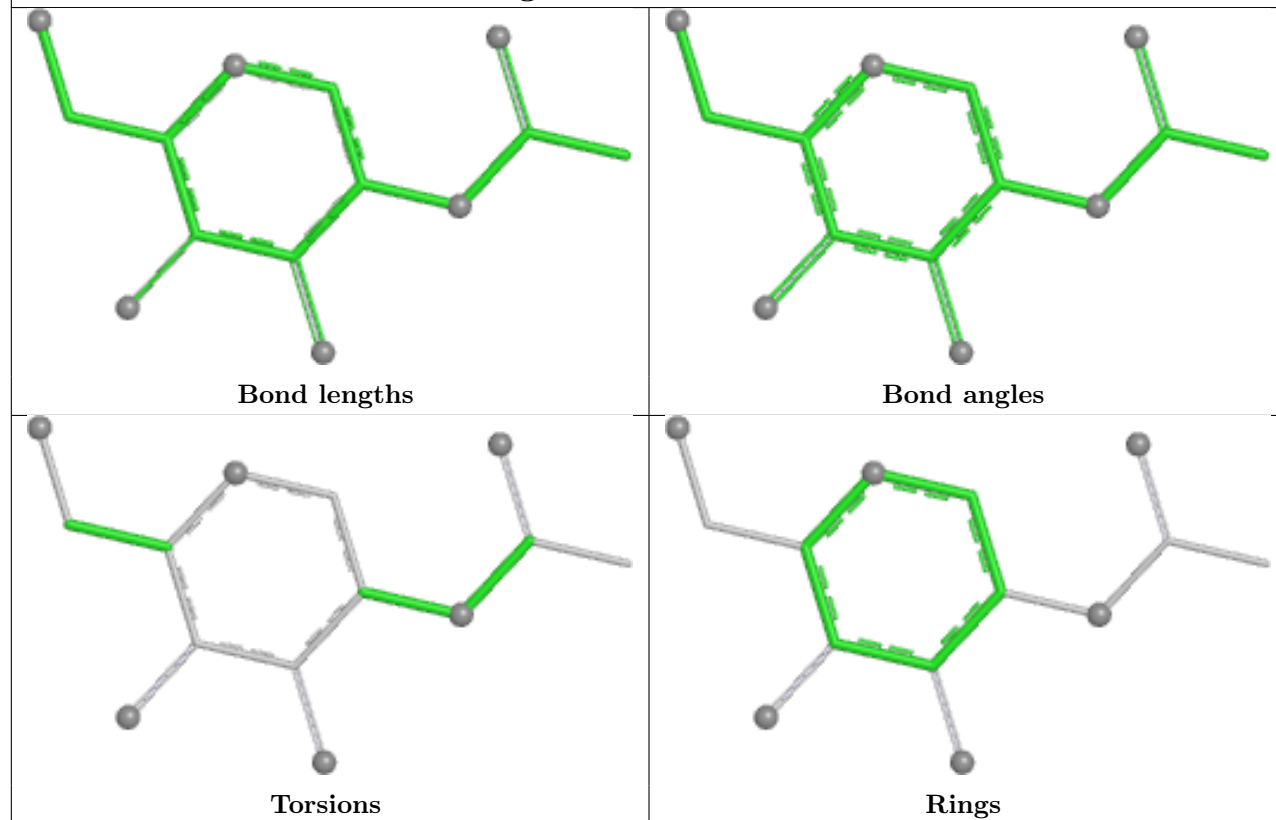
## Ligand NAG C 1405



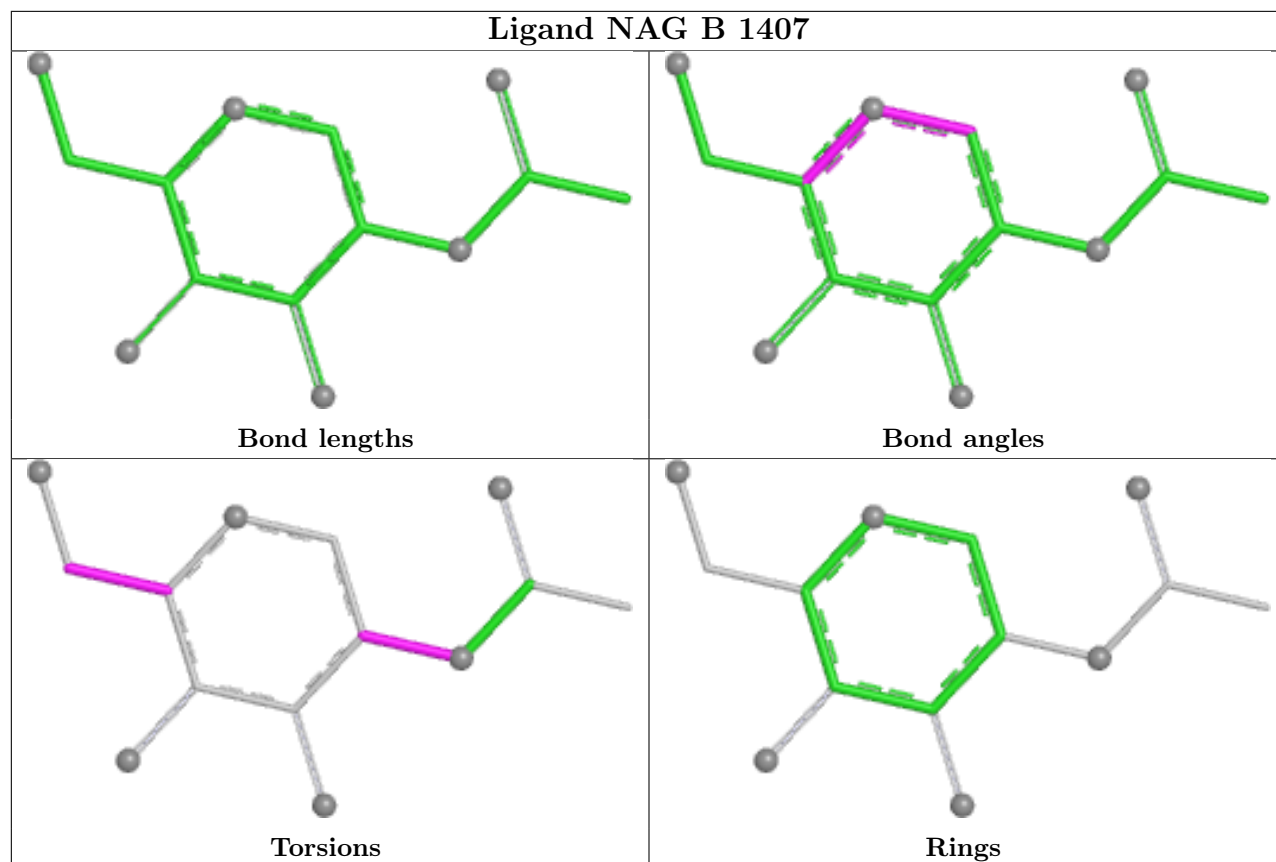
## Ligand NAG B 1406



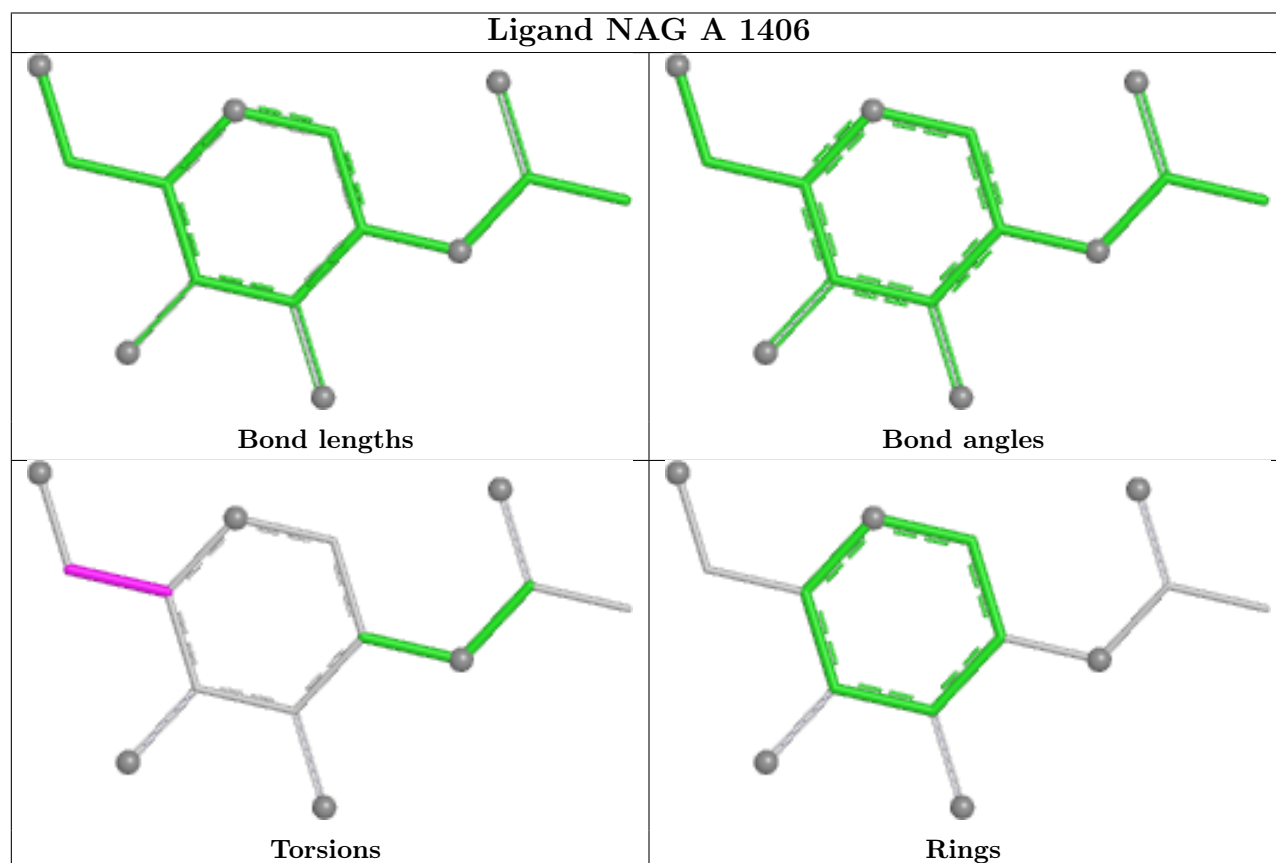
## Ligand NAG A 1407

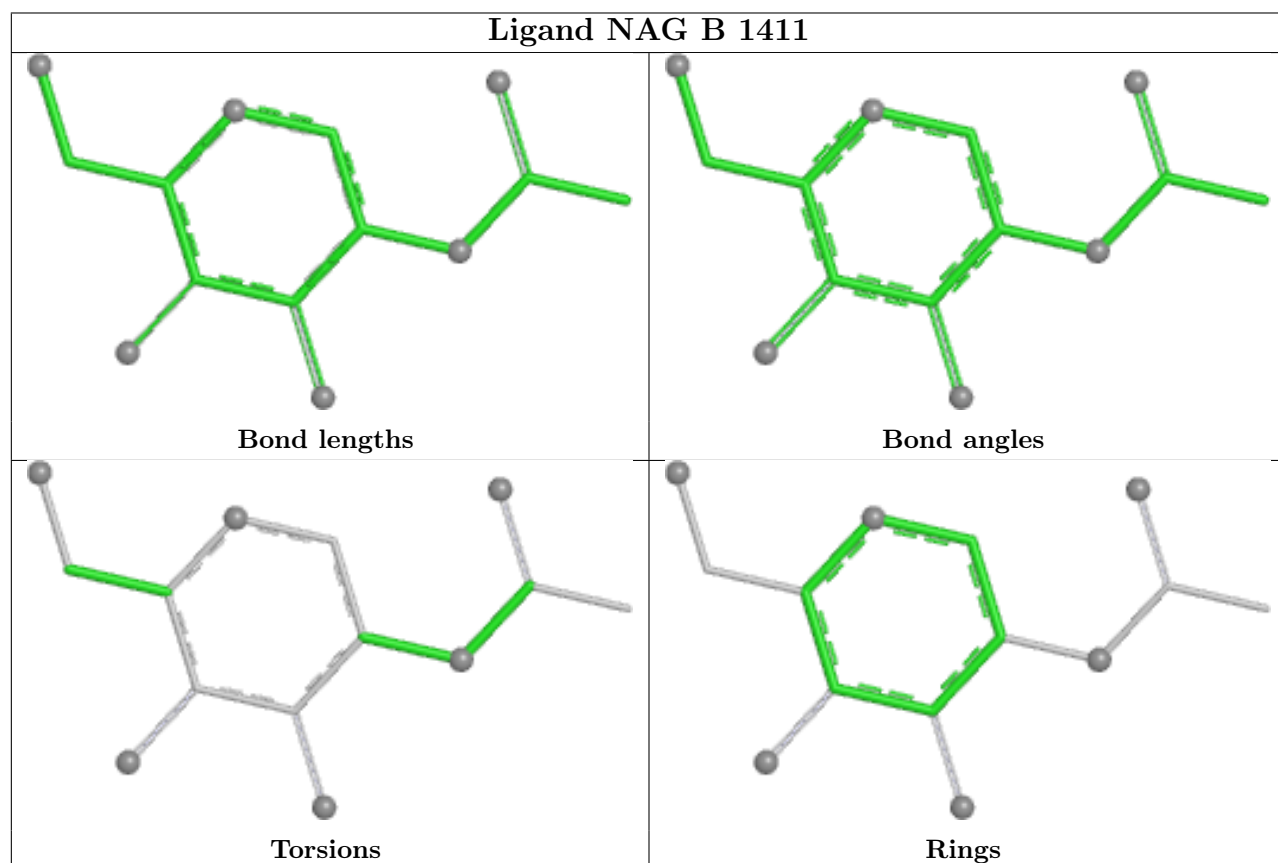
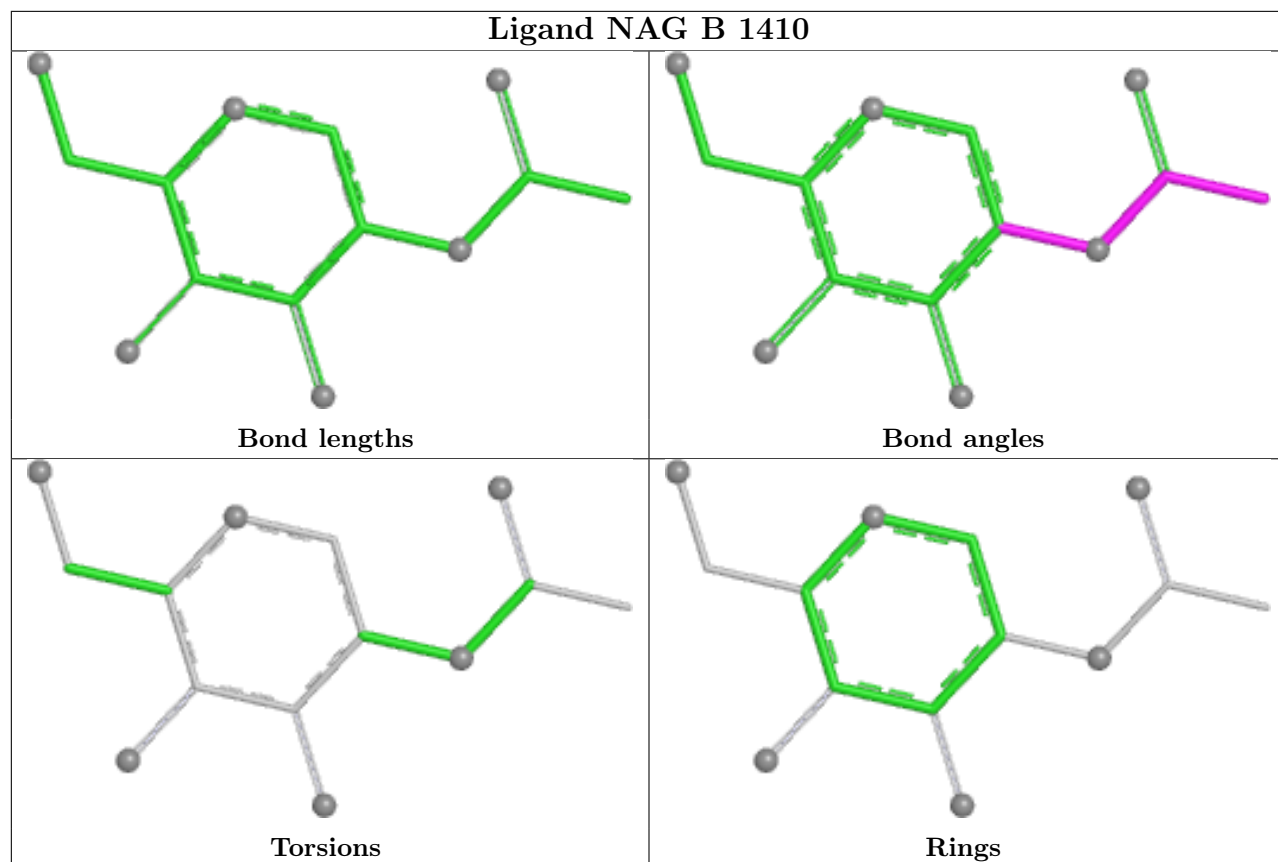


## Ligand NAG B 1407

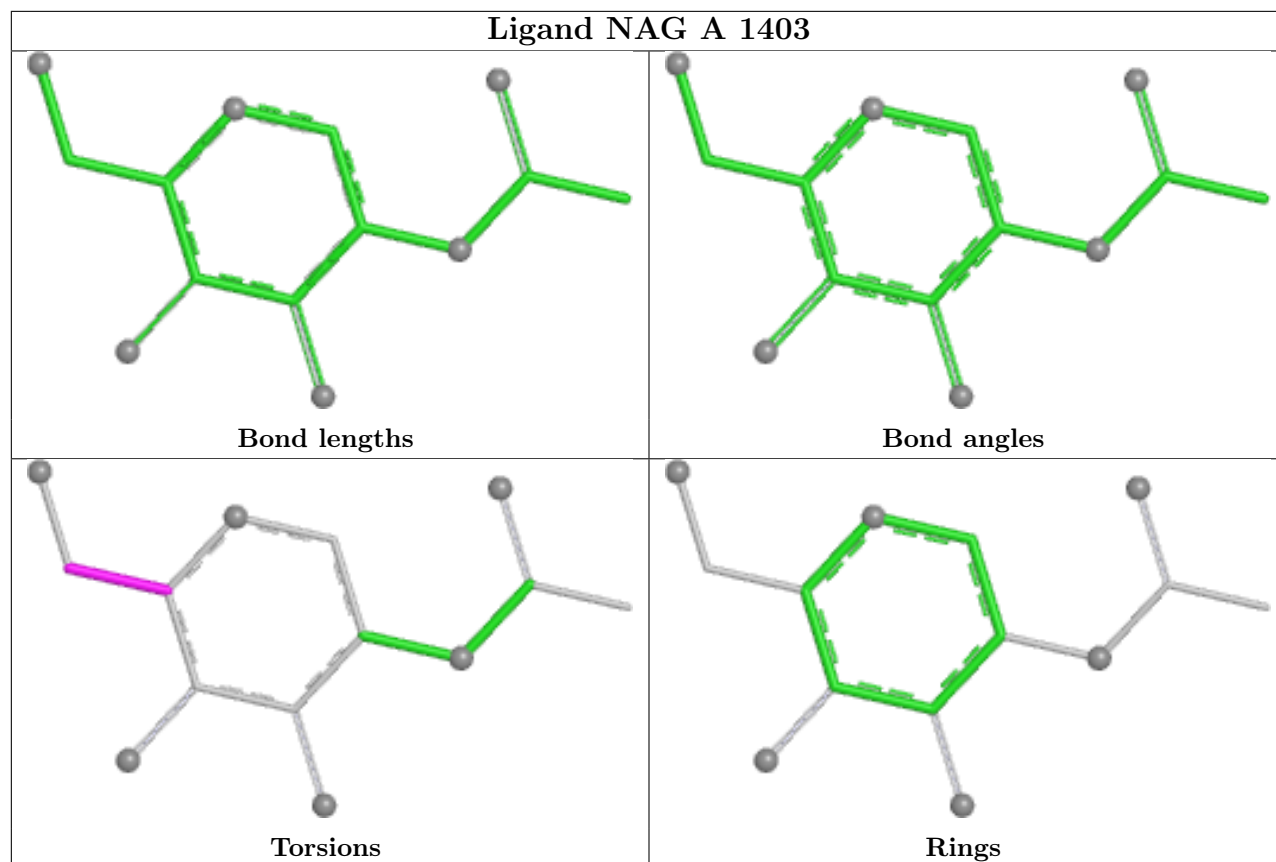


## Ligand NAG A 1406

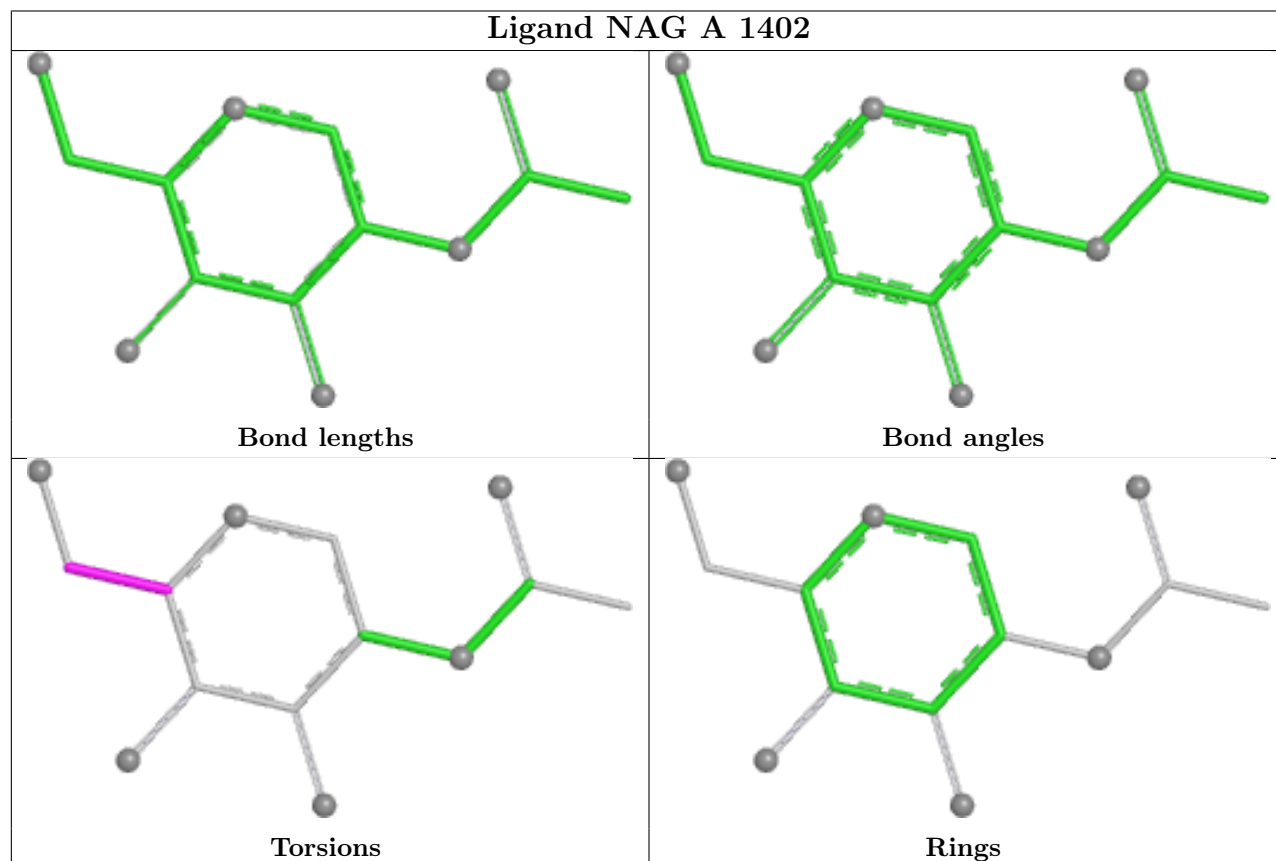




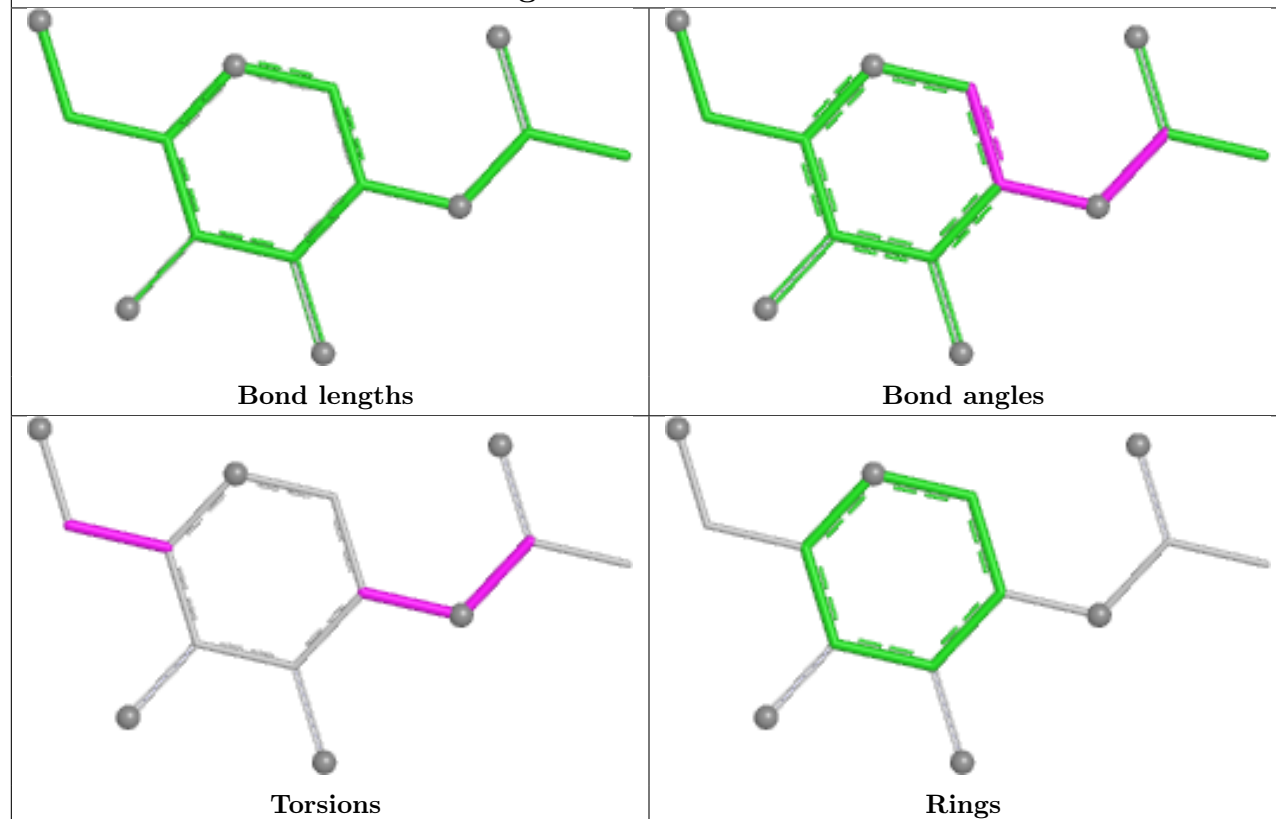
## Ligand NAG A 1403



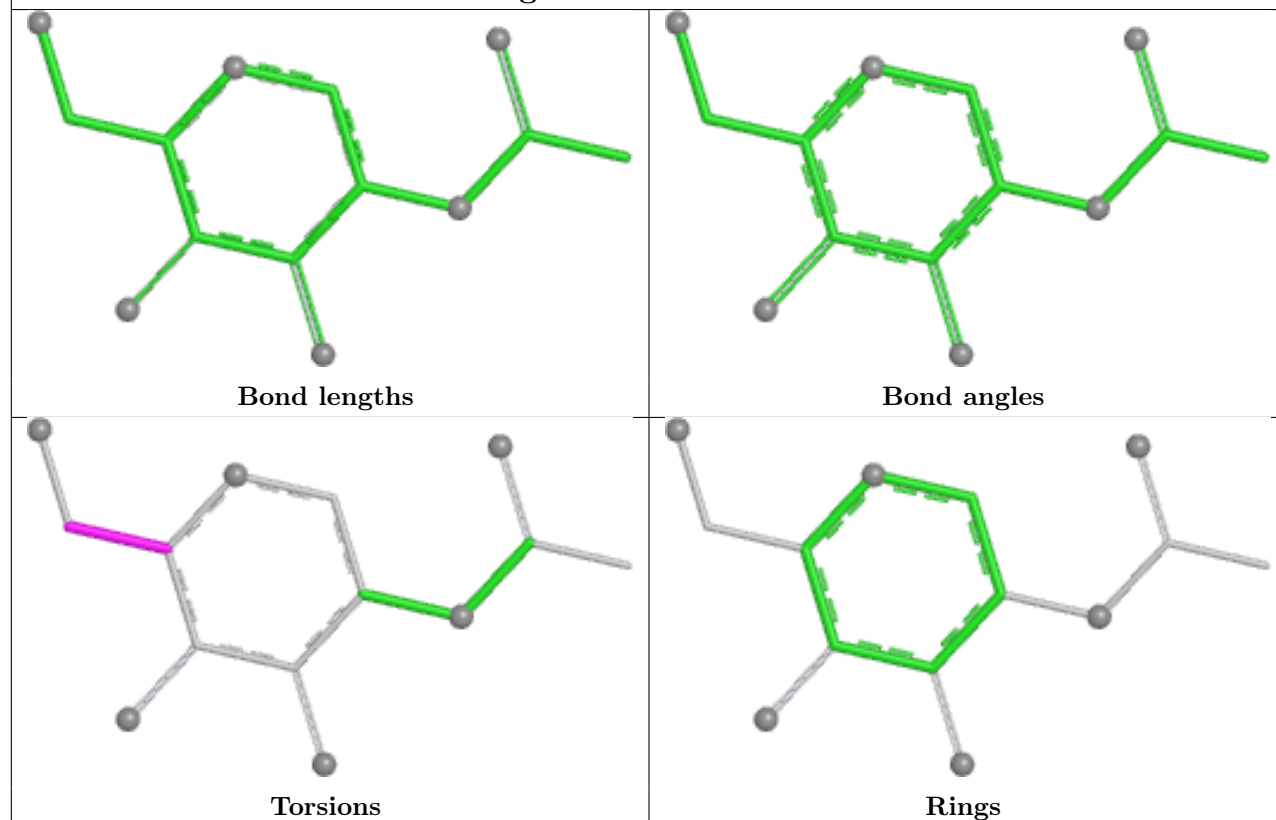
## Ligand NAG A 1402



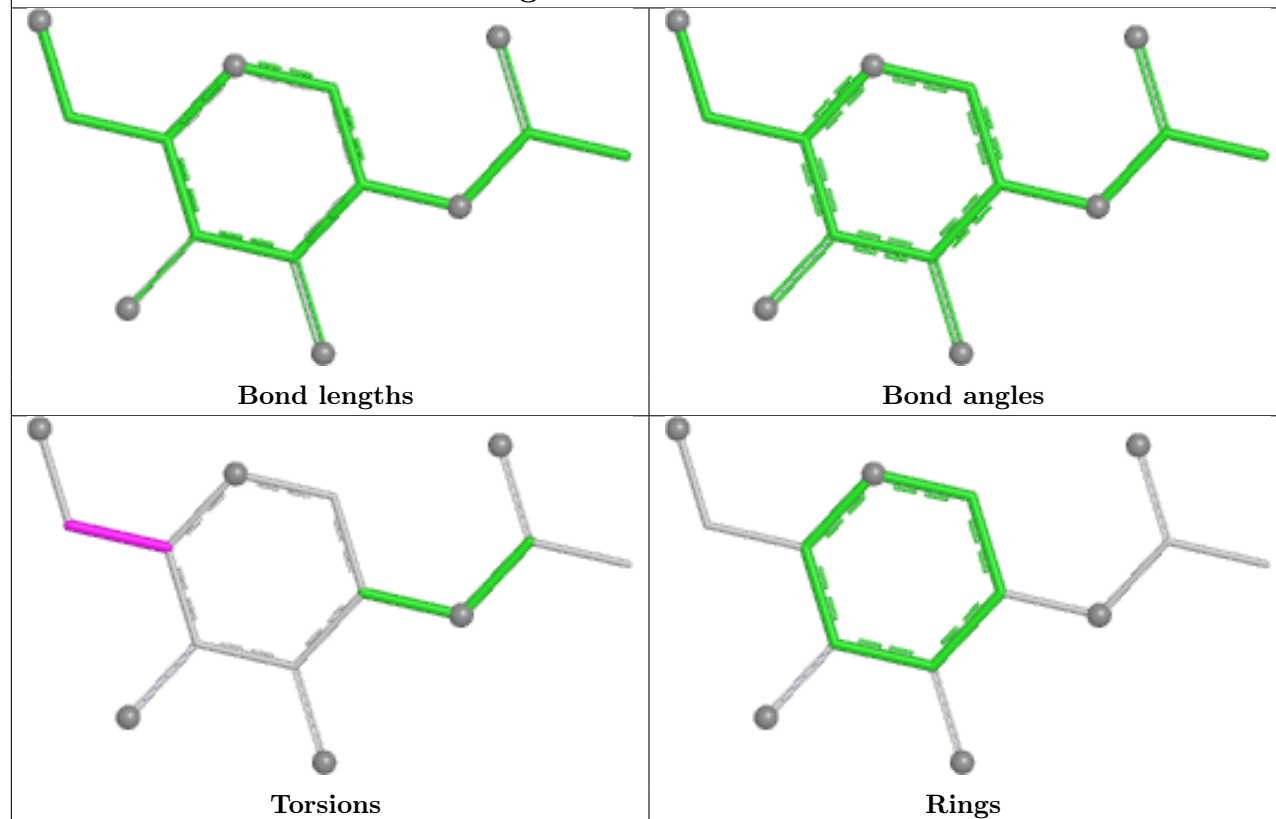
## Ligand NAG A 1405



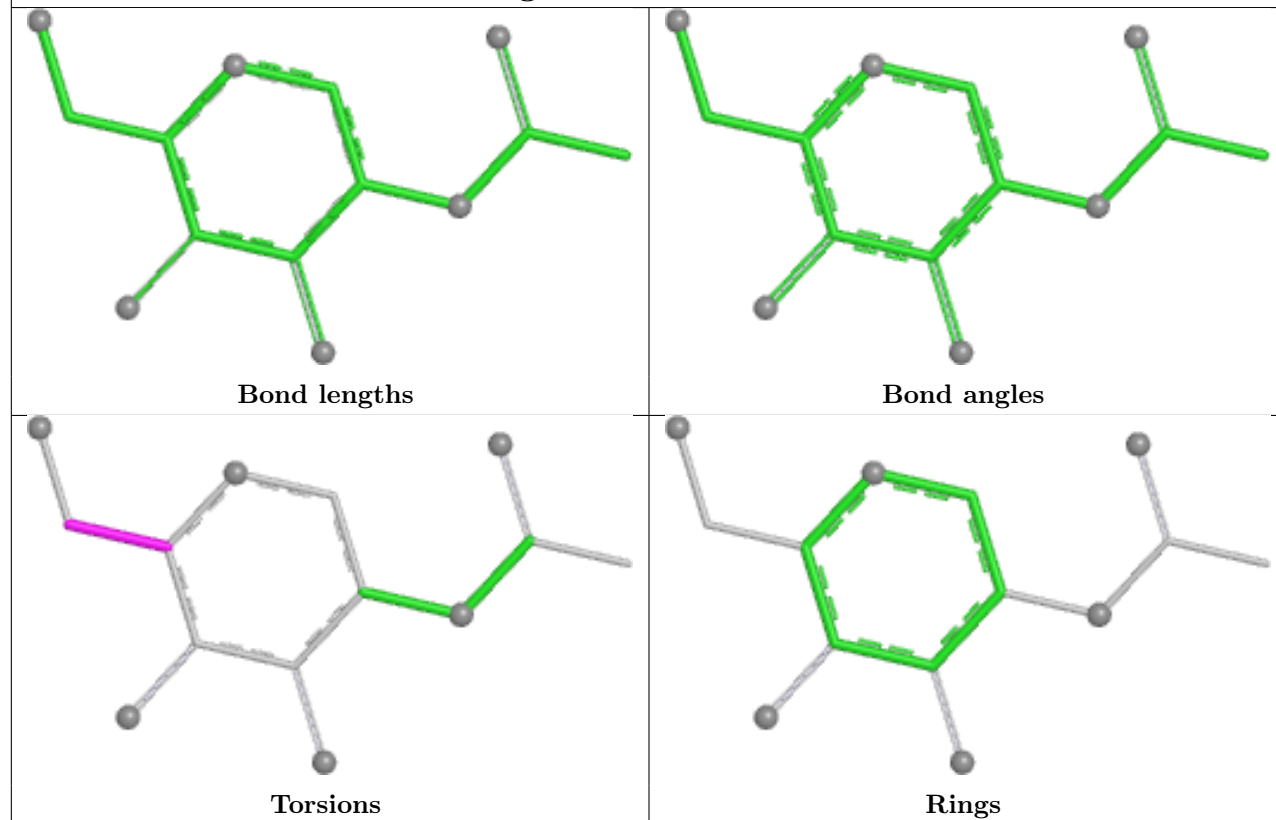
## Ligand NAG C 1404



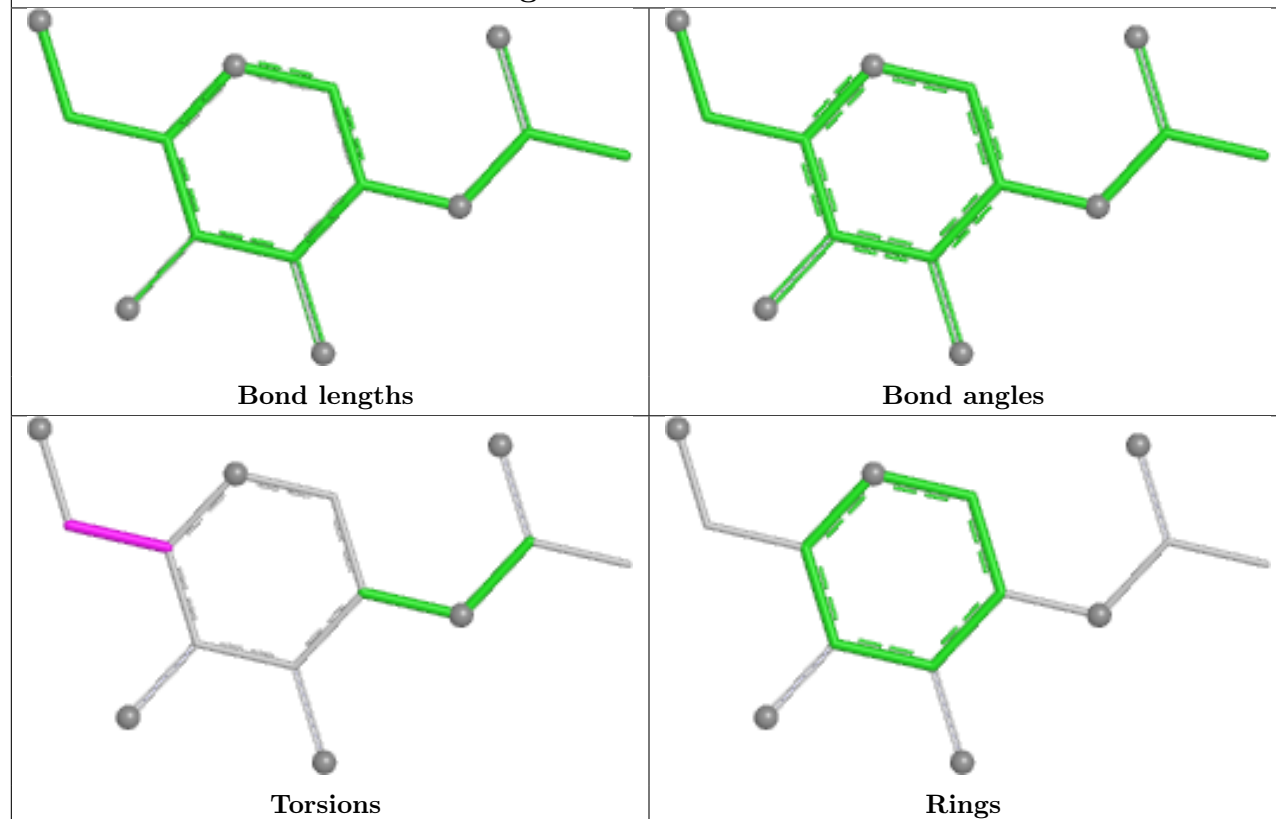
## Ligand NAG B 1402



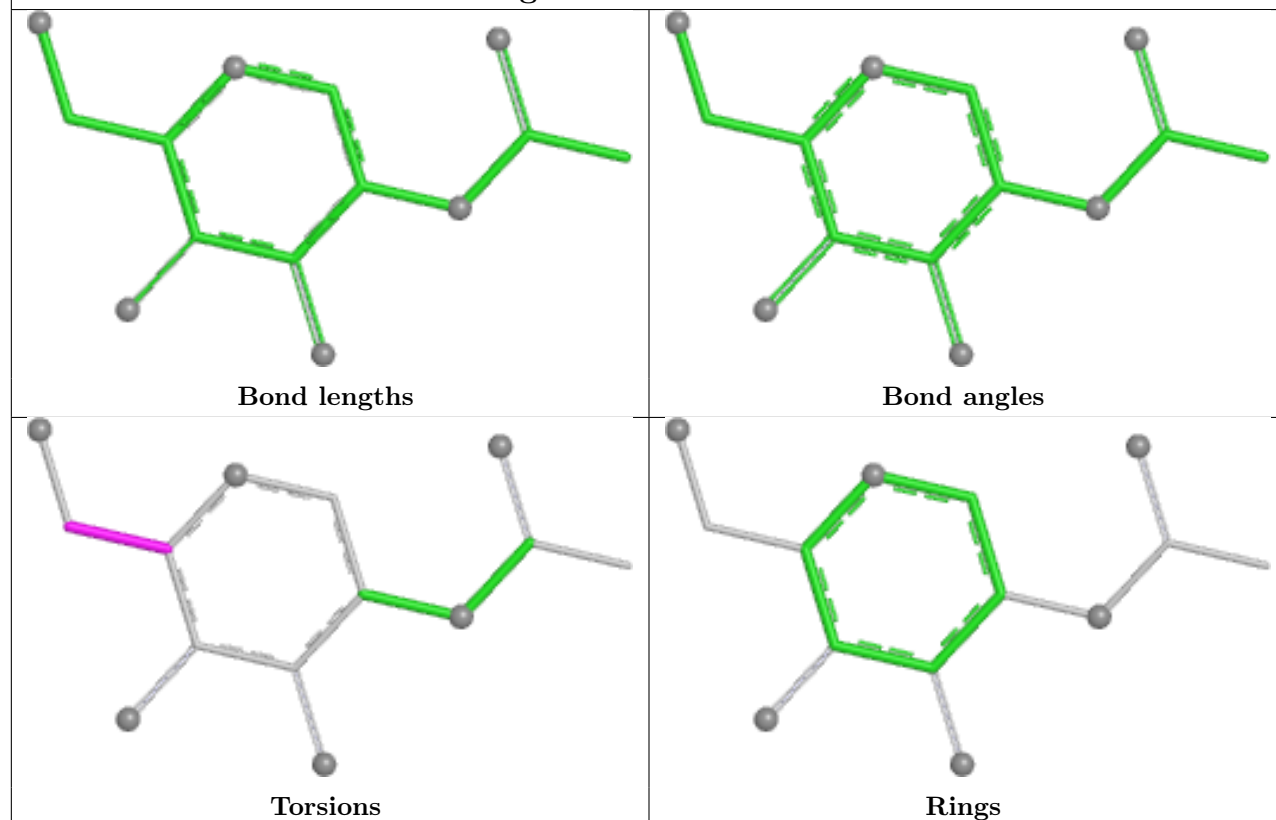
## Ligand NAG A 1404



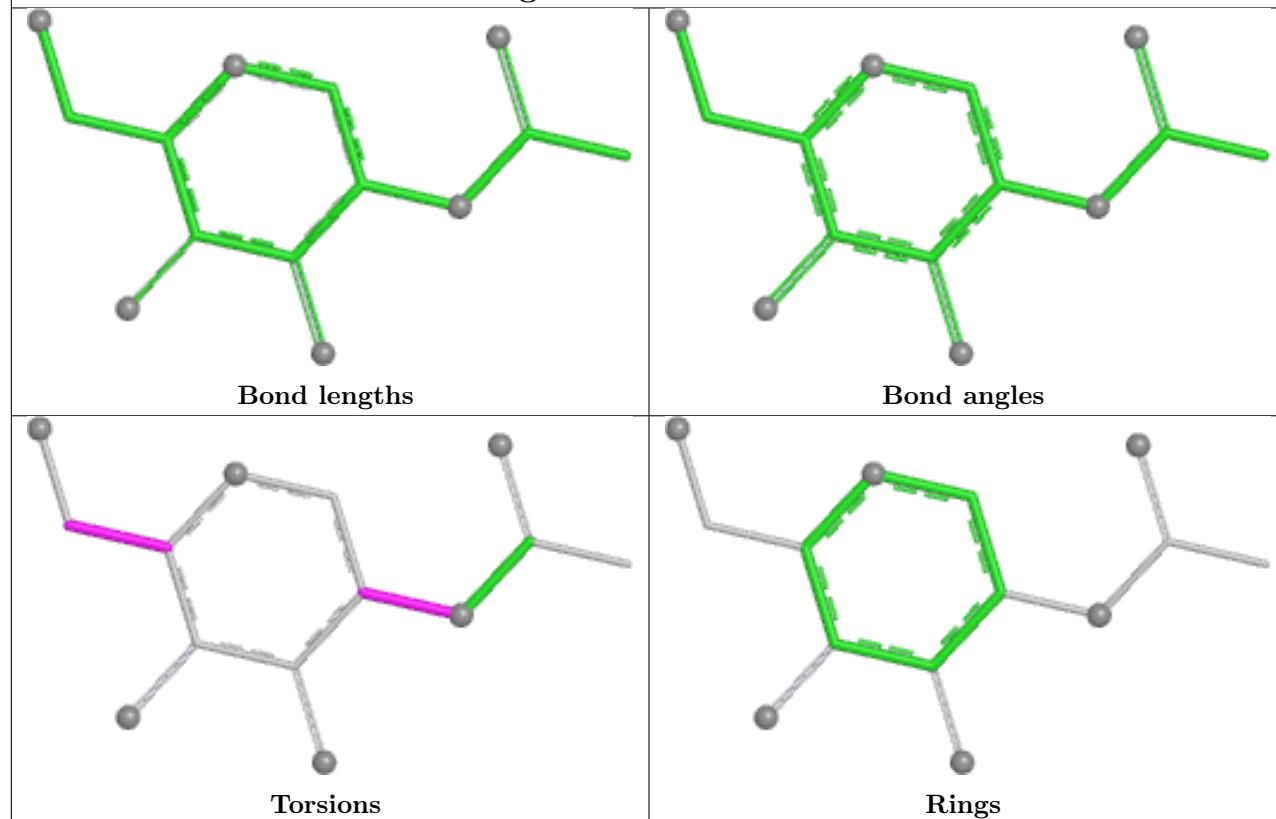
## Ligand NAG B 1408



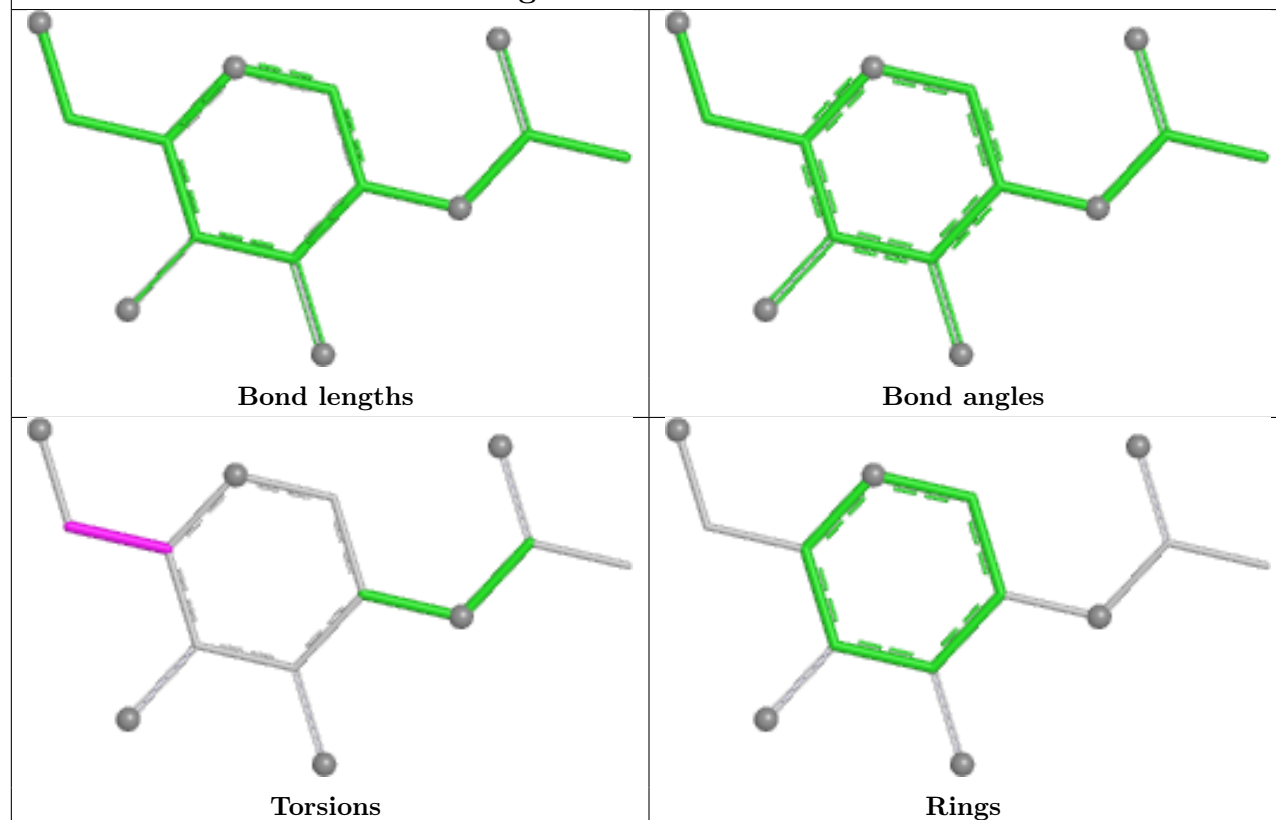
## Ligand NAG B 1403

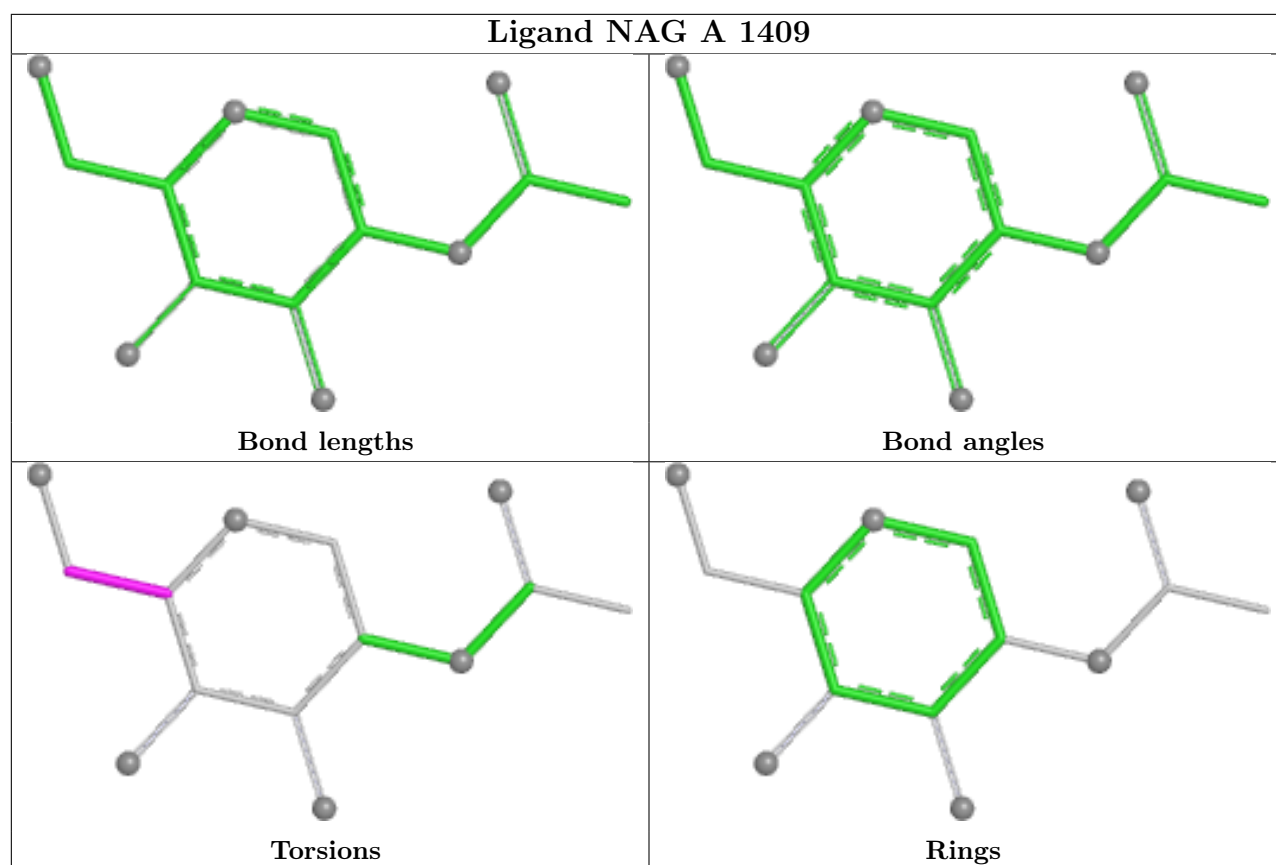


## Ligand NAG C 1407



## Ligand NAG A 1408





## 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.

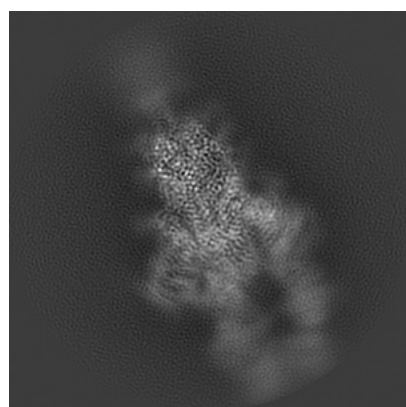
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30512. These allow visual inspection of the internal detail of the map and identification of artifacts.

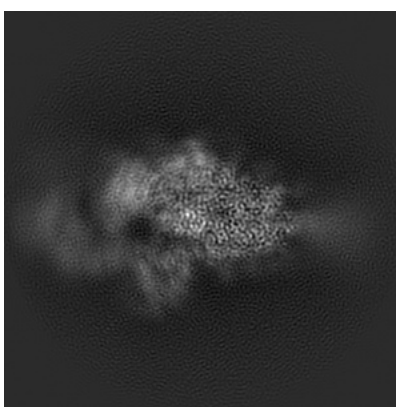
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

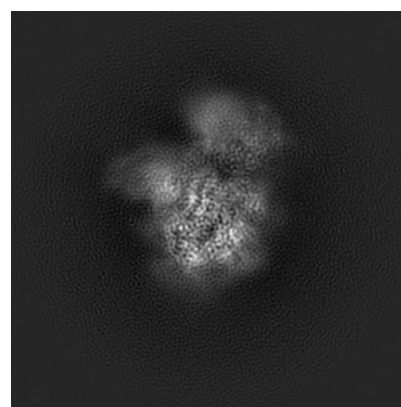
#### 6.1.1 Primary map



X



Y

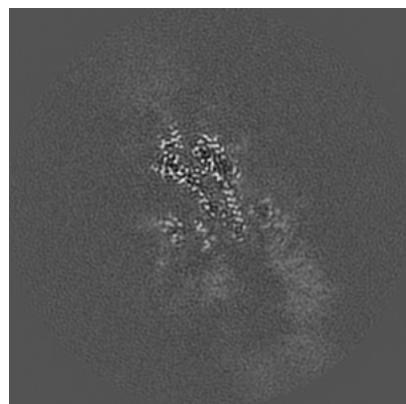


Z

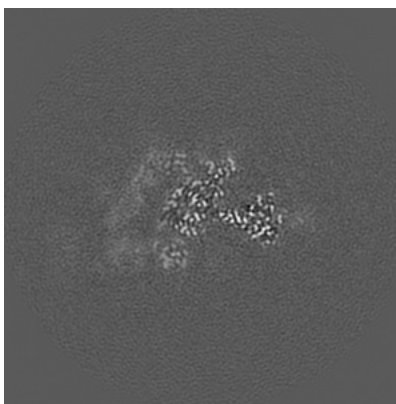
The images above show the map projected in three orthogonal directions.

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

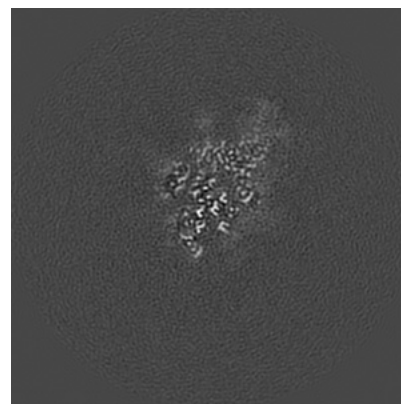
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

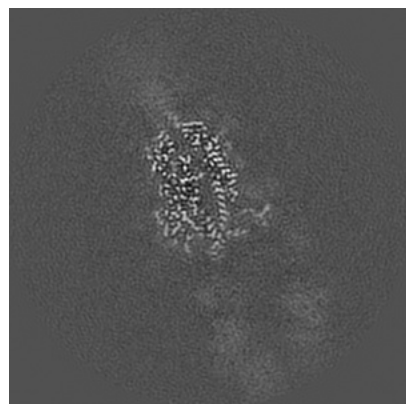


Z Index: 144

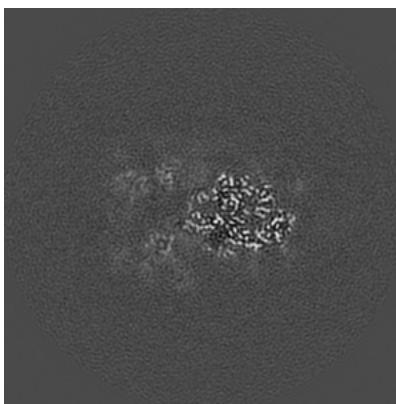
The images above show central slices of the map in three orthogonal directions.

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

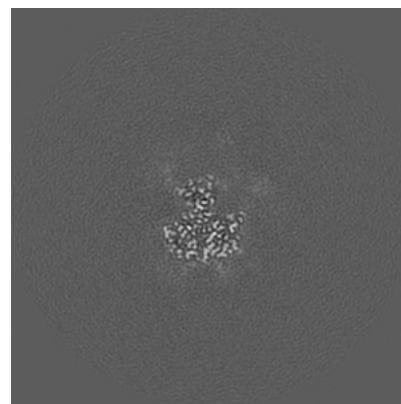
### 6.3.1 Primary map



X Index: 129



Y Index: 133

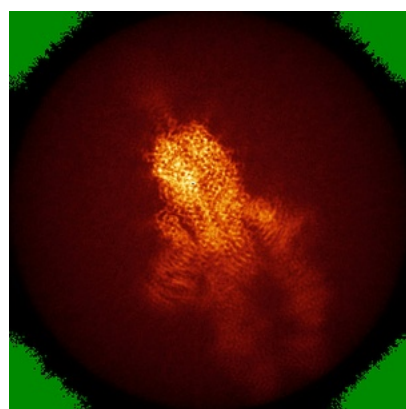


Z Index: 168

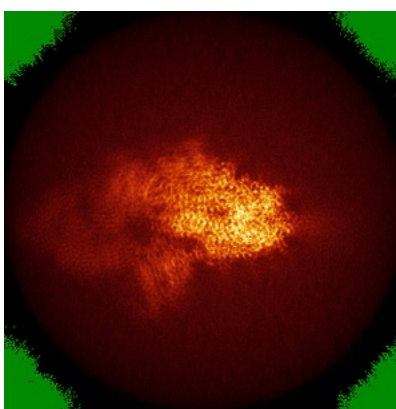
The images above show the largest variance slices of the map in three orthogonal directions.

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

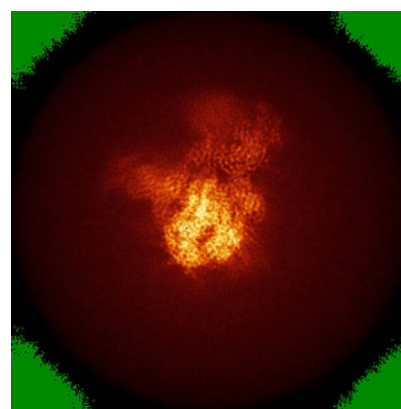
### 6.4.1 Primary map



X



Y

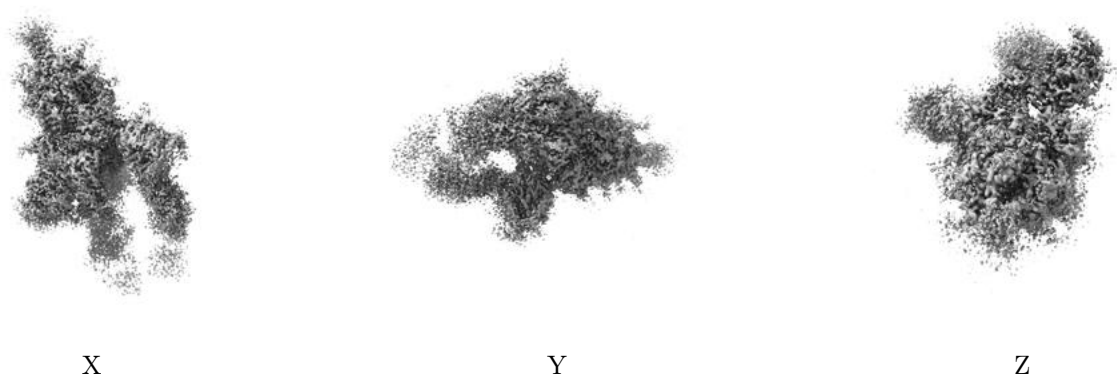


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

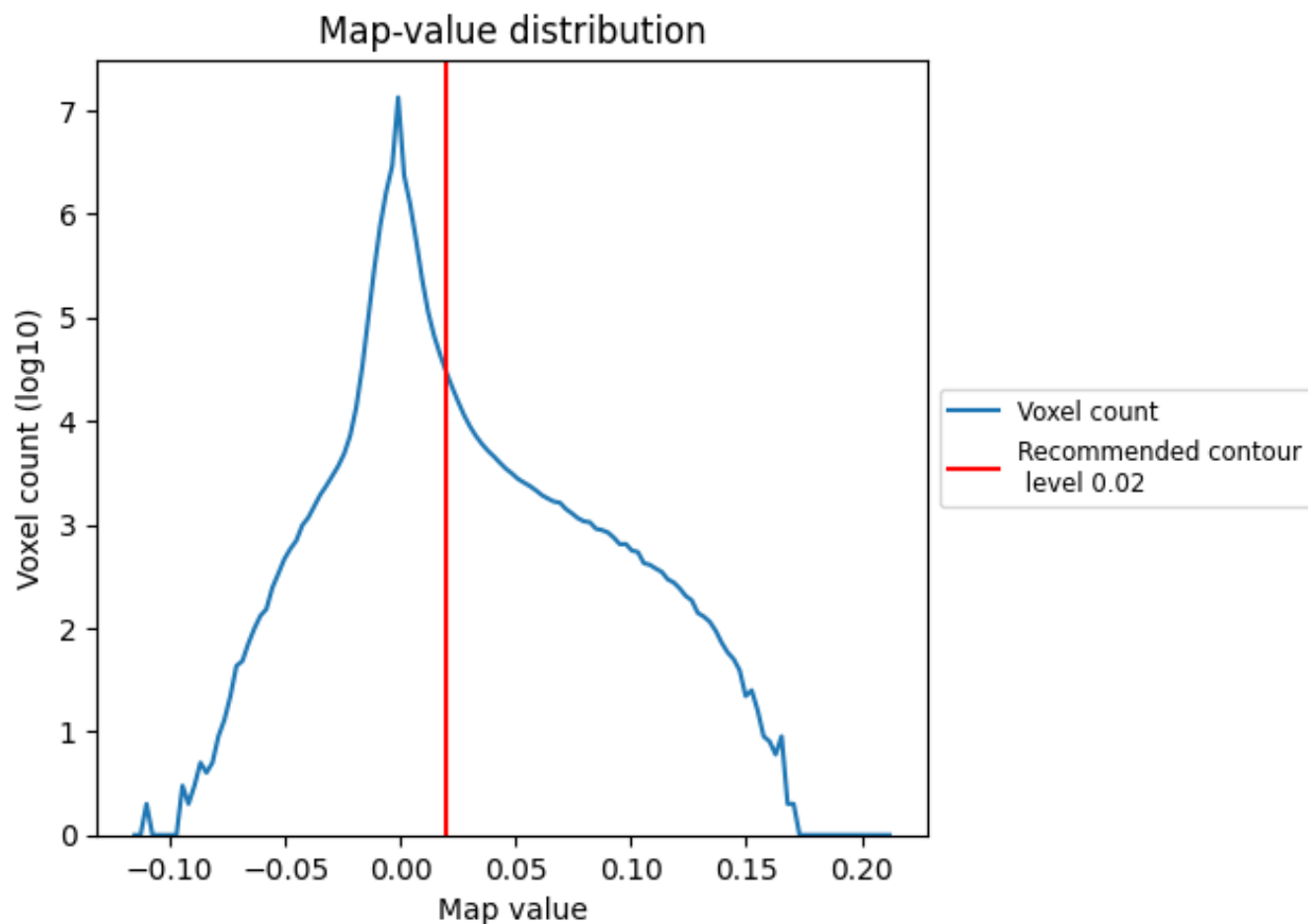
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

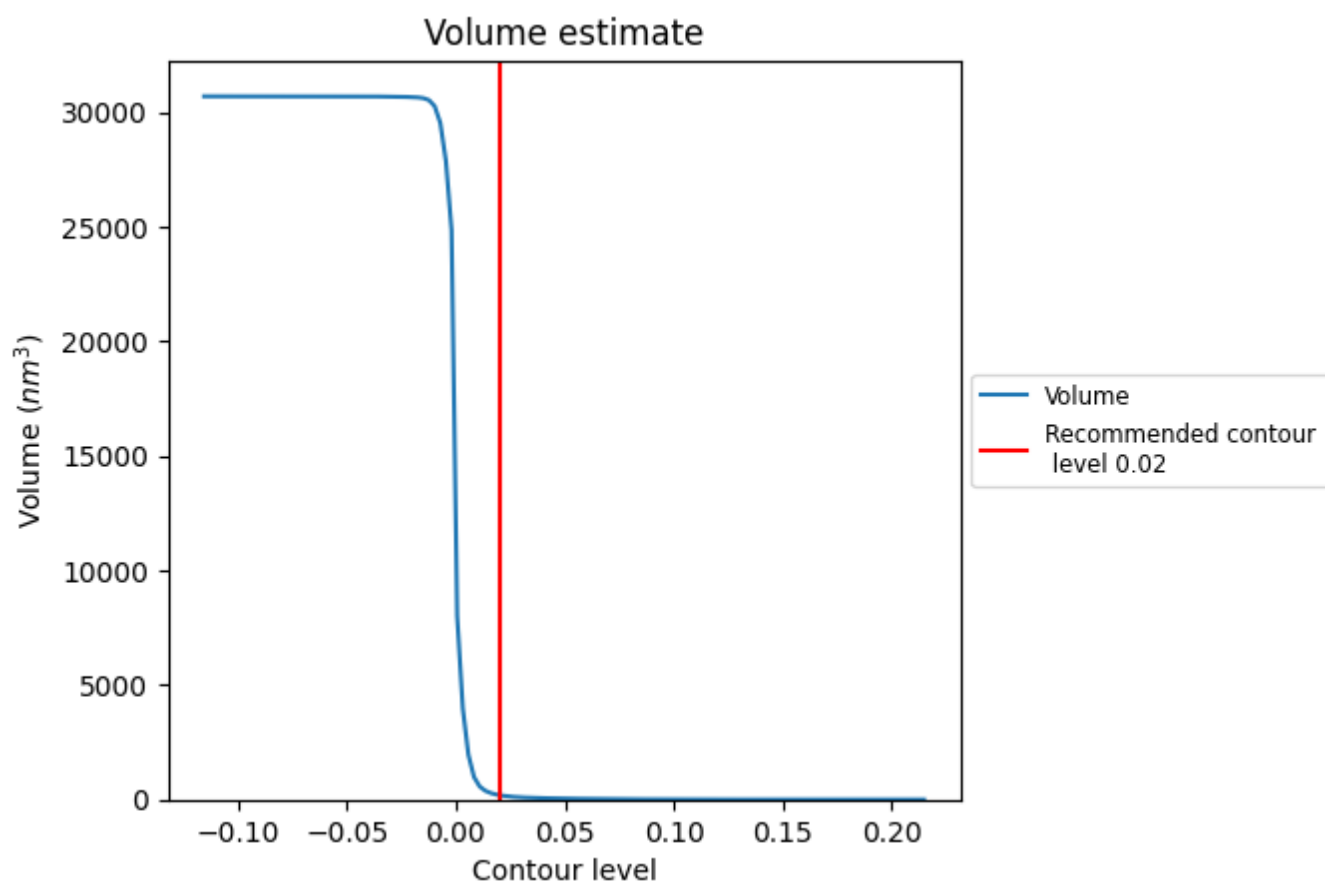
This section contains the results of statistical analysis of the map.

### 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.

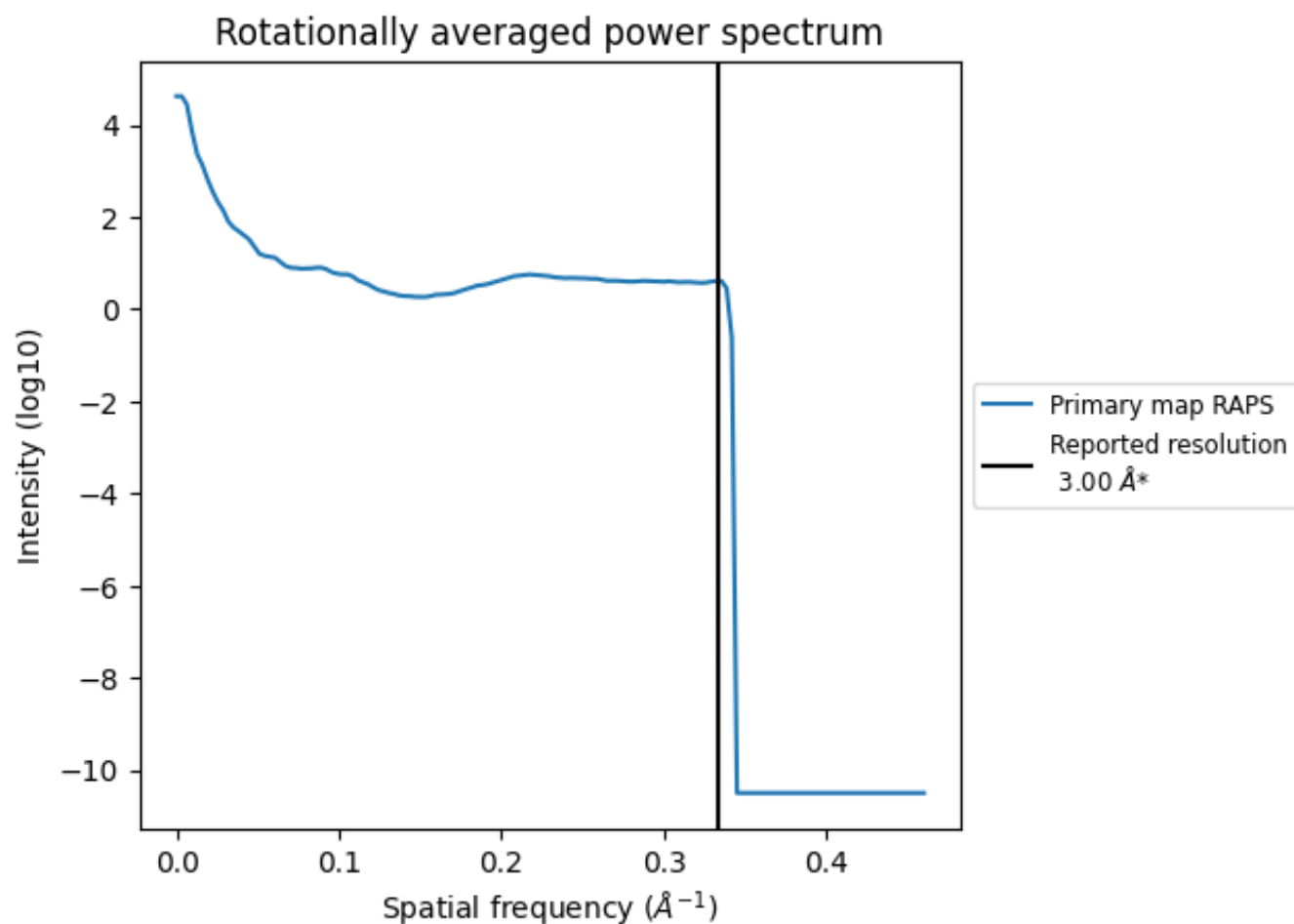
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193  $\text{nm}^3$ ; this corresponds to an approximate mass of 175 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 0.333 Å<sup>-1</sup>

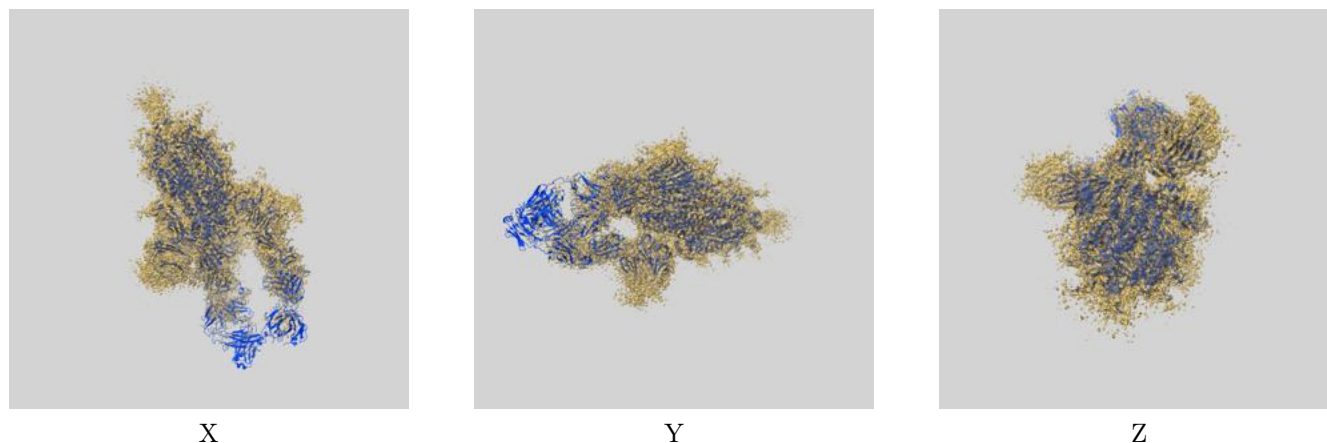
## 8 Fourier-Shell correlation ⓘ

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

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

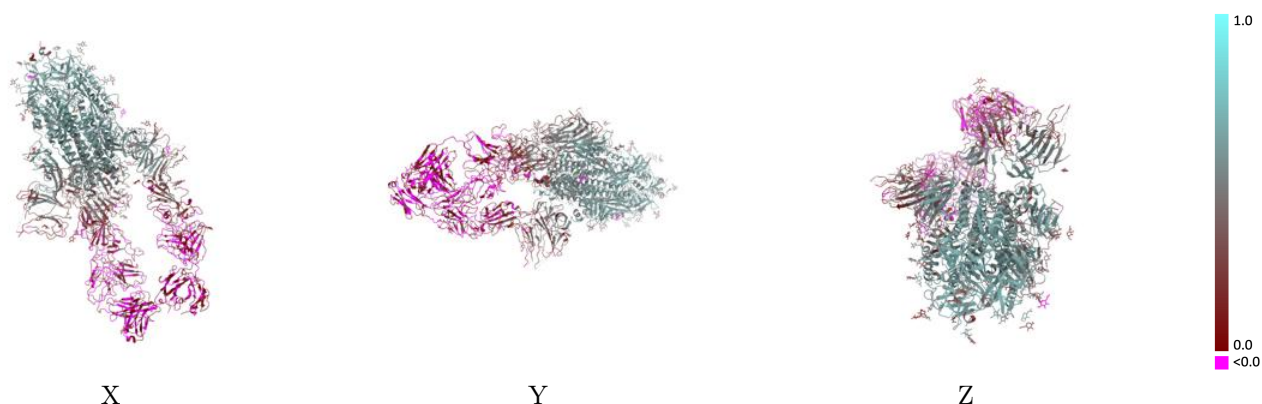
This section contains information regarding the fit between EMDB map EMD-30512 and PDB model 7CZP. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

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



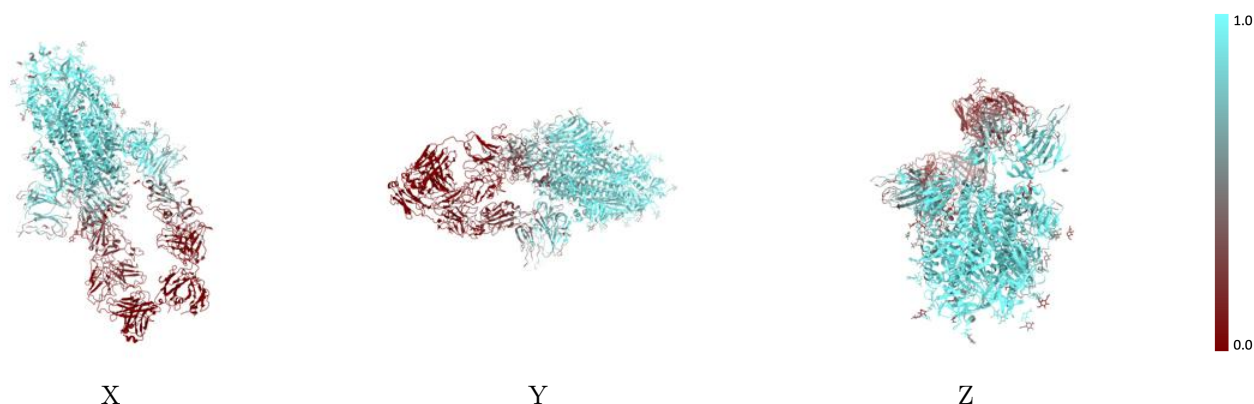
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



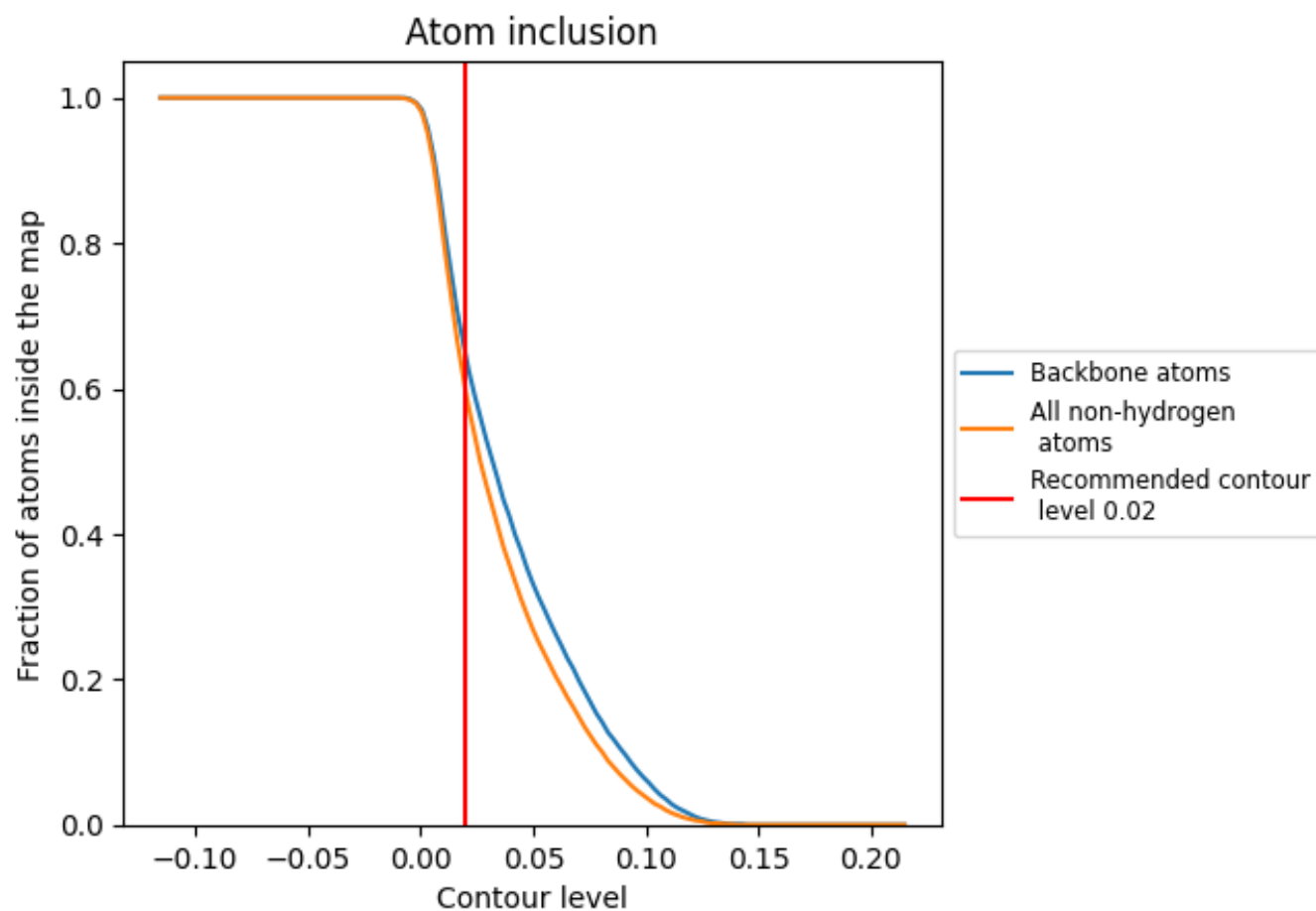
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                       |
|-------|--------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| All   |  0.5960   |  0.3590      |
| A     |  0.7370   |  0.4360      |
| B     |  0.7970   |  0.4860      |
| C     |  0.7170   |  0.4280      |
| D     |  0.5000   |  0.1570      |
| E     |  0.1430   |  0.1650      |
| F     |  0.8570   |  0.5080      |
| G     |  0.8570   |  0.4710      |
| H     |  0.0340   |  0.0220      |
| I     |  0.6070   |  0.4970      |
| J     |  0.0240   |  0.0180      |
| K     |  0.7140   |  0.3980      |
| L     |  0.0540   |  0.0510      |
| M     |  0.7140   |  0.4360      |
| N     |  0.0310  |  0.0170     |
| O     |  0.3570 |  0.1930    |
| P     |  0.4290 |  0.1470    |
| Q     |  0.8930 |  0.4620    |
| R     |  0.7140 |  0.4480    |
| S     |  0.8930 |  0.4920    |
| T     |  0.6430 |  0.4190    |
| U     |  0.5000 |  0.3580    |
| V     |  0.0000 |  -0.1820 |
| W     |  0.4640 |  0.2730    |
| X     |  0.8210 |  0.5000    |
| Y     |  0.6790 |  0.3940    |
| Z     |  0.5710 |  0.3700    |
| a     |  0.7500 |  0.4580    |
| b     |  0.6430 |  0.3830    |
| c     |  0.0000 |  0.1240    |
| d     |  0.0000 |  0.1290    |

