



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 12:17 PM JST

PDB ID : 6LKS  
Title : Effects of zinc ion on oligomerization and pH stability of influenza virus hemagglutinin  
Authors : Seok, J.; Kim, K.  
Deposited on : 2019-12-20  
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

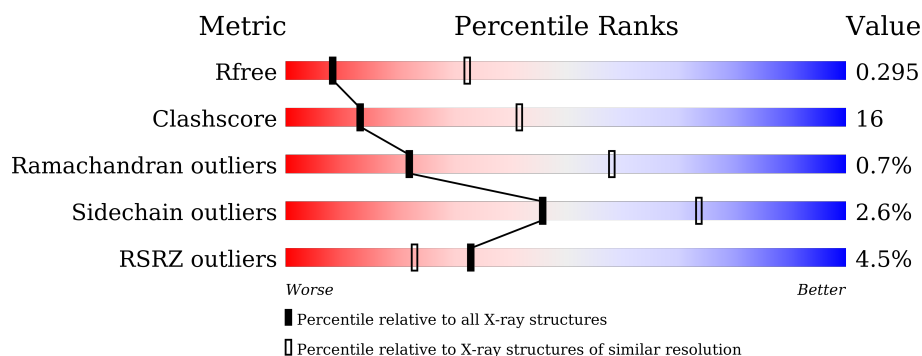
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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.



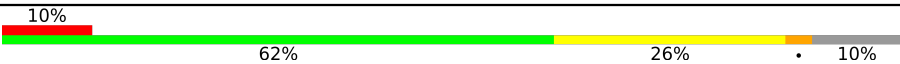

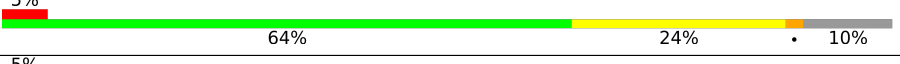
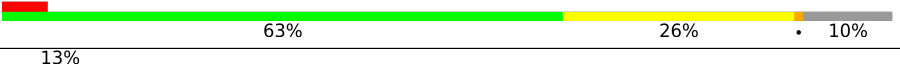
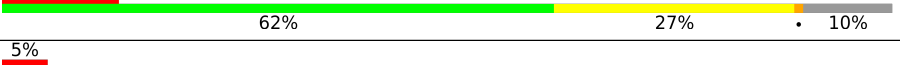

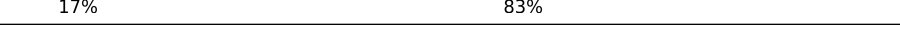



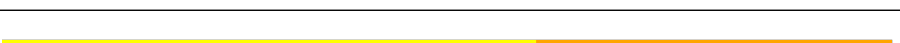
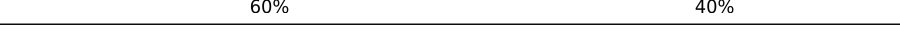
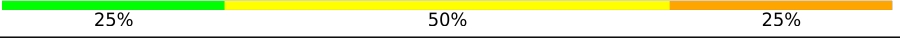





| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1619 (3.28-3.20)                                      |
| Clashscore            | 141614                      | 1755 (3.28-3.20)                                      |
| Ramachandran outliers | 138981                      | 1728 (3.28-3.20)                                      |
| Sidechain outliers    | 138945                      | 1727 (3.28-3.20)                                      |
| RSRZ outliers         | 127900                      | 1567 (3.28-3.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 330    | <div> <div>2%</div> <div>58%</div> <div>37%</div> <div>..</div> </div> |
| 1   | C     | 330    | <div> <div>2%</div> <div>66%</div> <div>29%</div> <div>..</div> </div> |
| 1   | E     | 330    | <div> <div>61%</div> <div>35%</div> <div>..</div> </div>               |
| 1   | G     | 330    | <div> <div>62%</div> <div>33%</div> <div>..</div> </div>               |
| 1   | I     | 330    | <div> <div>3%</div> <div>61%</div> <div>33%</div> <div>..</div> </div> |
| 1   | K     | 330    | <div> <div>2%</div> <div>64%</div> <div>31%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | B     | 183    |    |
| 2   | D     | 183    |    |
| 2   | F     | 183    |    |
| 2   | H     | 183    |    |
| 2   | J     | 183    |    |
| 2   | L     | 183    |    |
| 3   | M     | 6      |    |
| 3   | S     | 6      |    |
| 3   | V     | 6      |    |
| 4   | N     | 5      |    |
| 4   | P     | 5      |    |
| 5   | O     | 4      |    |
| 5   | Q     | 4      |   |
| 5   | R     | 4      |  |
| 5   | T     | 4      |  |
| 5   | U     | 4      |  |
| 5   | X     | 4      |  |
| 6   | W     | 3      |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NAG  | M     | 5   | -         | -        | -       | X                |
| 3   | MAN  | S     | 4   | -         | -        | -       | X                |
| 3   | NAG  | V     | 5   | -         | -        | -       | X                |
| 7   | NAG  | A     | 412 | -         | -        | -       | X                |
| 7   | NAG  | I     | 410 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 24413 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Hemagglutinin HA1 chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | K     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2515  | 1591 | 436 | 477 | 11 |         |         |       |
| 1   | A     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2515  | 1591 | 436 | 477 | 11 |         |         |       |
| 1   | C     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2515  | 1591 | 436 | 477 | 11 |         |         |       |
| 1   | E     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2515  | 1591 | 436 | 477 | 11 |         |         |       |
| 1   | G     | 320      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2507  | 1585 | 435 | 476 | 11 |         |         |       |
| 1   | I     | 320      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2507  | 1585 | 435 | 476 | 11 |         |         |       |

There are 30 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -3      | ALA      | -      | expression tag | UNP A7LI25 |
| K     | -2      | ASP      | -      | expression tag | UNP A7LI25 |
| K     | -1      | PRO      | -      | expression tag | UNP A7LI25 |
| K     | 0       | GLY      | -      | expression tag | UNP A7LI25 |
| K     | 116     | ILE      | MET    | conflict       | UNP A7LI25 |
| A     | -3      | ALA      | -      | expression tag | UNP A7LI25 |
| A     | -2      | ASP      | -      | expression tag | UNP A7LI25 |
| A     | -1      | PRO      | -      | expression tag | UNP A7LI25 |
| A     | 0       | GLY      | -      | expression tag | UNP A7LI25 |
| A     | 116     | ILE      | MET    | conflict       | UNP A7LI25 |
| C     | -3      | ALA      | -      | expression tag | UNP A7LI25 |
| C     | -2      | ASP      | -      | expression tag | UNP A7LI25 |
| C     | -1      | PRO      | -      | expression tag | UNP A7LI25 |
| C     | 0       | GLY      | -      | expression tag | UNP A7LI25 |
| C     | 116     | ILE      | MET    | conflict       | UNP A7LI25 |
| E     | -3      | ALA      | -      | expression tag | UNP A7LI25 |
| E     | -2      | ASP      | -      | expression tag | UNP A7LI25 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | -1      | PRO      | -      | expression tag | UNP A7LI25 |
| E     | 0       | GLY      | -      | expression tag | UNP A7LI25 |
| E     | 116     | ILE      | MET    | conflict       | UNP A7LI25 |
| G     | -3      | ALA      | -      | expression tag | UNP A7LI25 |
| G     | -2      | ASP      | -      | expression tag | UNP A7LI25 |
| G     | -1      | PRO      | -      | expression tag | UNP A7LI25 |
| G     | 0       | GLY      | -      | expression tag | UNP A7LI25 |
| G     | 116     | ILE      | MET    | conflict       | UNP A7LI25 |
| I     | -3      | ALA      | -      | expression tag | UNP A7LI25 |
| I     | -2      | ASP      | -      | expression tag | UNP A7LI25 |
| I     | -1      | PRO      | -      | expression tag | UNP A7LI25 |
| I     | 0       | GLY      | -      | expression tag | UNP A7LI25 |
| I     | 116     | ILE      | MET    | conflict       | UNP A7LI25 |

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | L     | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1325  | 831 | 224 | 263 | 7 |         |         |       |
| 2   | B     | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1325  | 831 | 224 | 263 | 7 |         |         |       |
| 2   | D     | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1325  | 831 | 224 | 263 | 7 |         |         |       |
| 2   | F     | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1325  | 831 | 224 | 263 | 7 |         |         |       |
| 2   | H     | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1325  | 831 | 224 | 263 | 7 |         |         |       |
| 2   | J     | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1325  | 831 | 224 | 263 | 7 |         |         |       |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| L     | 91      | VAL      | ILE    | conflict       | UNP A7LI25 |
| L     | 169     | SER      | ASN    | conflict       | UNP A7LI25 |
| L     | 177     | SER      | -      | expression tag | UNP A7LI25 |
| L     | 178     | GLY      | -      | expression tag | UNP A7LI25 |
| L     | 179     | ARG      | -      | expression tag | UNP A7LI25 |
| L     | 180     | LEU      | -      | expression tag | UNP A7LI25 |
| L     | 181     | VAL      | -      | expression tag | UNP A7LI25 |
| L     | 182     | PRO      | -      | expression tag | UNP A7LI25 |
| L     | 183     | ARG      | -      | expression tag | UNP A7LI25 |

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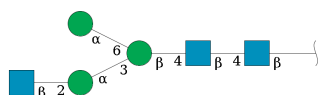
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 91      | VAL      | ILE    | conflict       | UNP A7LI25 |
| B     | 169     | SER      | ASN    | conflict       | UNP A7LI25 |
| B     | 177     | SER      | -      | expression tag | UNP A7LI25 |
| B     | 178     | GLY      | -      | expression tag | UNP A7LI25 |
| B     | 179     | ARG      | -      | expression tag | UNP A7LI25 |
| B     | 180     | LEU      | -      | expression tag | UNP A7LI25 |
| B     | 181     | VAL      | -      | expression tag | UNP A7LI25 |
| B     | 182     | PRO      | -      | expression tag | UNP A7LI25 |
| B     | 183     | ARG      | -      | expression tag | UNP A7LI25 |
| D     | 91      | VAL      | ILE    | conflict       | UNP A7LI25 |
| D     | 169     | SER      | ASN    | conflict       | UNP A7LI25 |
| D     | 177     | SER      | -      | expression tag | UNP A7LI25 |
| D     | 178     | GLY      | -      | expression tag | UNP A7LI25 |
| D     | 179     | ARG      | -      | expression tag | UNP A7LI25 |
| D     | 180     | LEU      | -      | expression tag | UNP A7LI25 |
| D     | 181     | VAL      | -      | expression tag | UNP A7LI25 |
| D     | 182     | PRO      | -      | expression tag | UNP A7LI25 |
| D     | 183     | ARG      | -      | expression tag | UNP A7LI25 |
| F     | 91      | VAL      | ILE    | conflict       | UNP A7LI25 |
| F     | 169     | SER      | ASN    | conflict       | UNP A7LI25 |
| F     | 177     | SER      | -      | expression tag | UNP A7LI25 |
| F     | 178     | GLY      | -      | expression tag | UNP A7LI25 |
| F     | 179     | ARG      | -      | expression tag | UNP A7LI25 |
| F     | 180     | LEU      | -      | expression tag | UNP A7LI25 |
| F     | 181     | VAL      | -      | expression tag | UNP A7LI25 |
| F     | 182     | PRO      | -      | expression tag | UNP A7LI25 |
| F     | 183     | ARG      | -      | expression tag | UNP A7LI25 |
| H     | 91      | VAL      | ILE    | conflict       | UNP A7LI25 |
| H     | 169     | SER      | ASN    | conflict       | UNP A7LI25 |
| H     | 177     | SER      | -      | expression tag | UNP A7LI25 |
| H     | 178     | GLY      | -      | expression tag | UNP A7LI25 |
| H     | 179     | ARG      | -      | expression tag | UNP A7LI25 |
| H     | 180     | LEU      | -      | expression tag | UNP A7LI25 |
| H     | 181     | VAL      | -      | expression tag | UNP A7LI25 |
| H     | 182     | PRO      | -      | expression tag | UNP A7LI25 |
| H     | 183     | ARG      | -      | expression tag | UNP A7LI25 |
| J     | 91      | VAL      | ILE    | conflict       | UNP A7LI25 |
| J     | 169     | SER      | ASN    | conflict       | UNP A7LI25 |
| J     | 177     | SER      | -      | expression tag | UNP A7LI25 |
| J     | 178     | GLY      | -      | expression tag | UNP A7LI25 |
| J     | 179     | ARG      | -      | expression tag | UNP A7LI25 |
| J     | 180     | LEU      | -      | expression tag | UNP A7LI25 |

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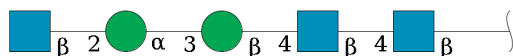
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 181     | VAL      | -      | expression tag | UNP A7LI25 |
| J     | 182     | PRO      | -      | expression tag | UNP A7LI25 |
| J     | 183     | ARG      | -      | expression tag | UNP A7LI25 |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 3   | M     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 75    | 42 | 3 | 30 |         |         |       |
| 3   | S     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 75    | 42 | 3 | 30 |         |         |       |
| 3   | V     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 75    | 42 | 3 | 30 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4   | N     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 64    | 36 | 3 | 25 |         |         |       |
| 4   | P     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 64    | 36 | 3 | 25 |         |         |       |

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



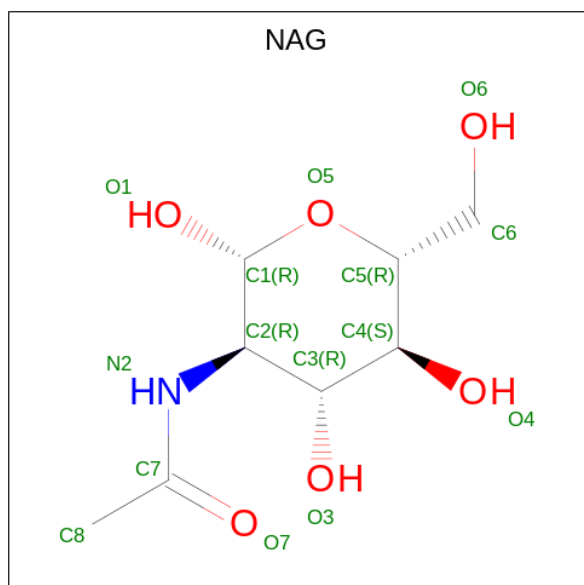
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5   | O     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | Q     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | R     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | T     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | U     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | X     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6   | W     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by author).





| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 7   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | G     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 8   | I     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 8   | K     | 1        | Total Zn<br>1 1 | 0       | 0       |

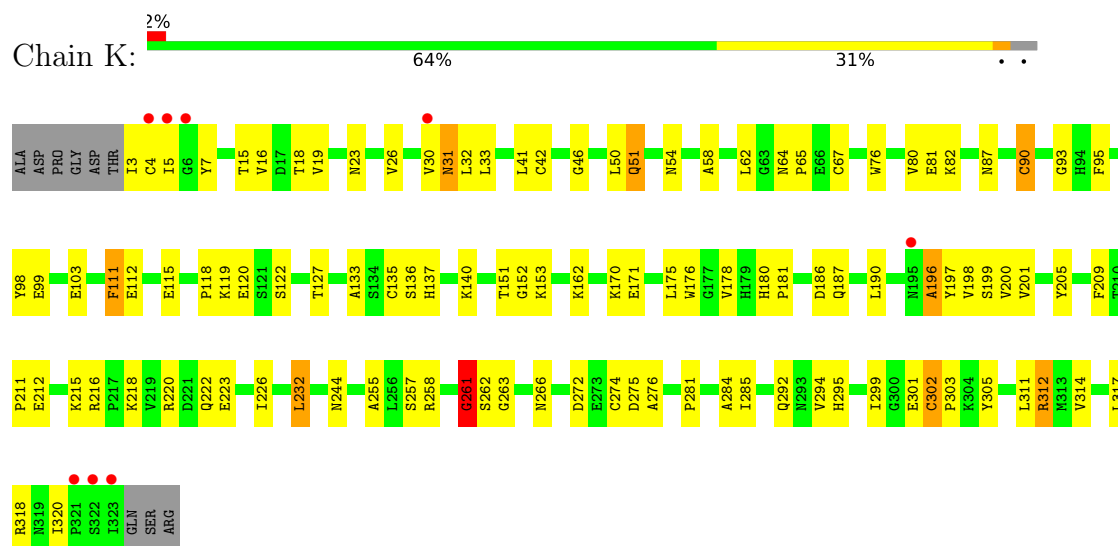
- Molecule 9 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 9   | K     | 61       | Total O<br>61 61 | 0       | 0       |
| 9   | L     | 19       | Total O<br>19 19 | 0       | 0       |
| 9   | A     | 71       | Total O<br>71 71 | 0       | 0       |
| 9   | B     | 7        | Total O<br>7 7   | 0       | 0       |
| 9   | C     | 61       | Total O<br>61 61 | 0       | 0       |
| 9   | D     | 13       | Total O<br>13 13 | 0       | 0       |
| 9   | E     | 42       | Total O<br>42 42 | 0       | 0       |
| 9   | F     | 17       | Total O<br>17 17 | 0       | 0       |
| 9   | G     | 44       | Total O<br>44 44 | 0       | 0       |
| 9   | H     | 16       | Total O<br>16 16 | 0       | 0       |
| 9   | I     | 61       | Total O<br>61 61 | 0       | 0       |
| 9   | J     | 16       | Total O<br>16 16 | 0       | 0       |

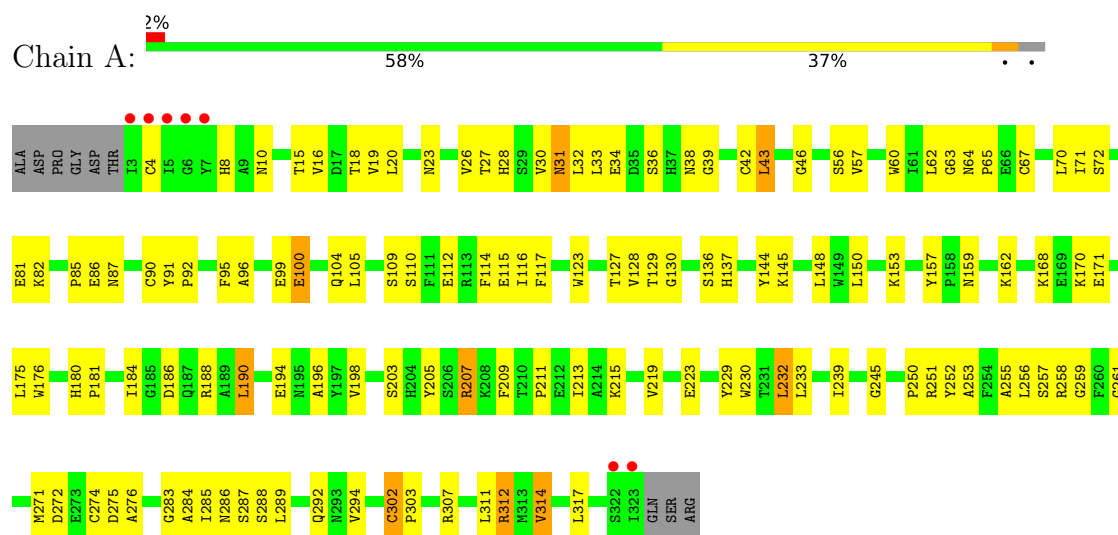
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Hemagglutinin HA1 chain

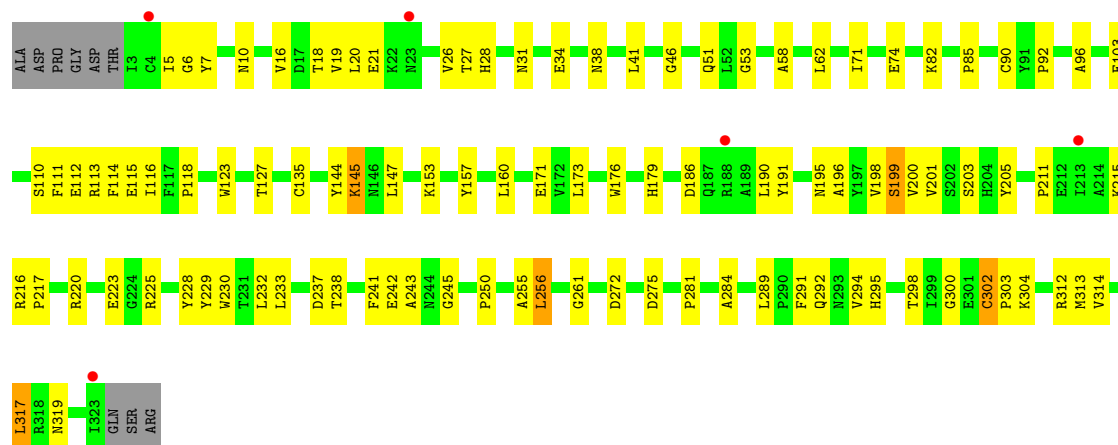


#### • Molecule 1: Hemagglutinin HA1 chain

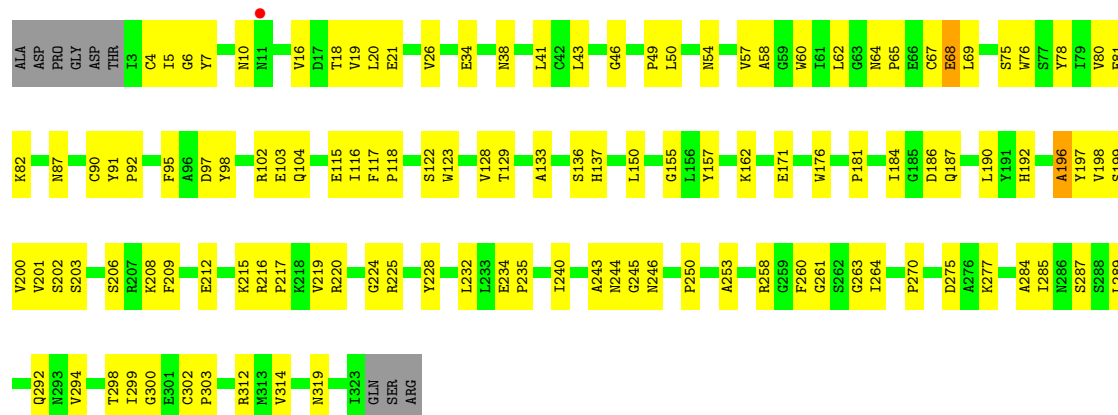


#### • Molecule 1: Hemagglutinin HA1 chain

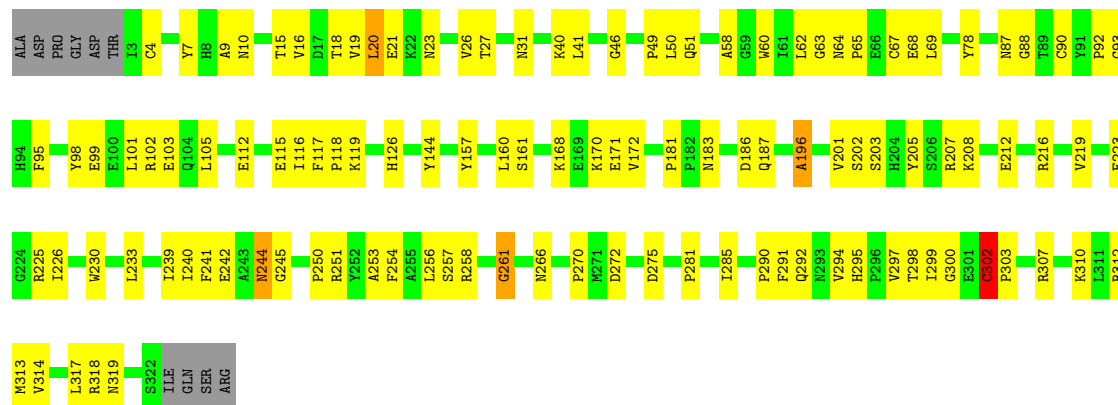




- Molecule 1: Hemagglutinin HA1 chain

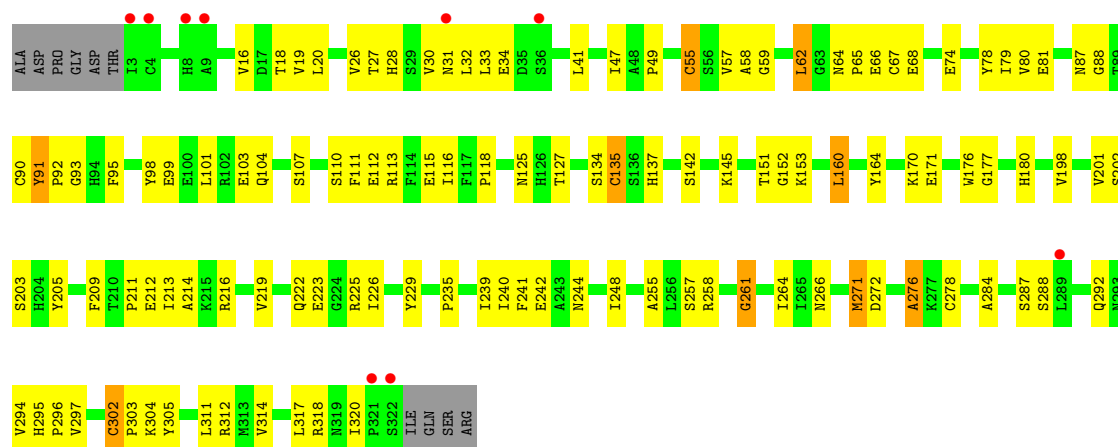


- Molecule 1: Hemagglutinin HA1 chain

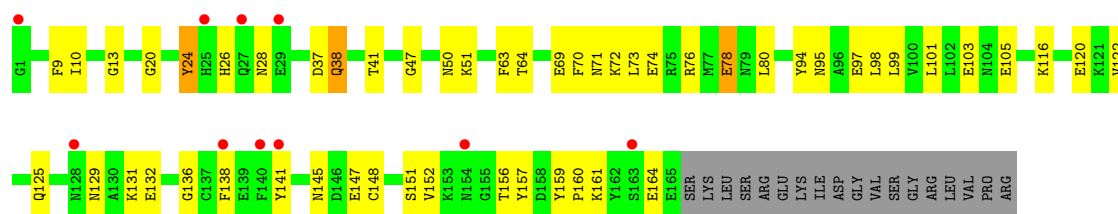


- Molecule 1: Hemagglutinin HA1 chain

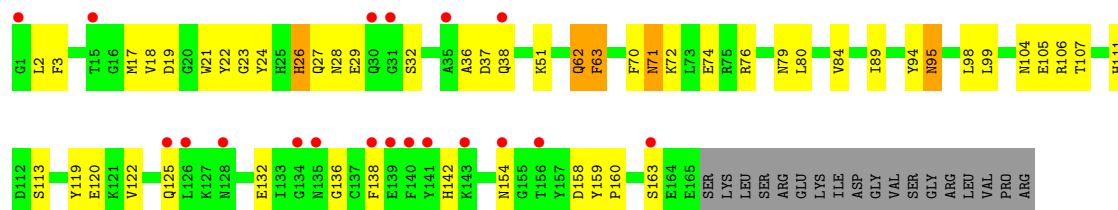




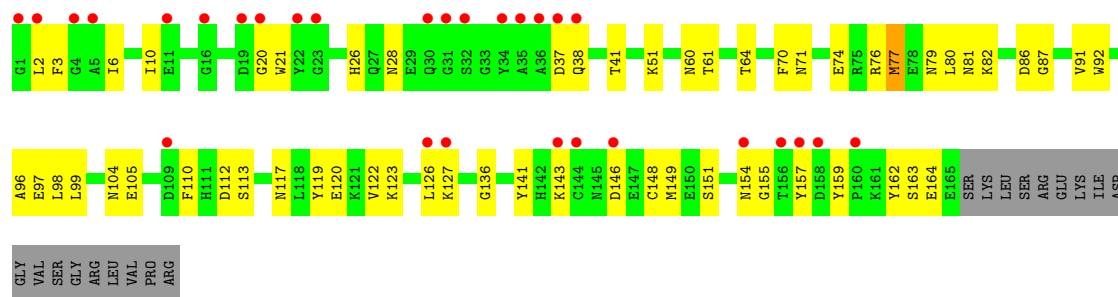
• Molecule 2: Hemagglutinin HA2 chain



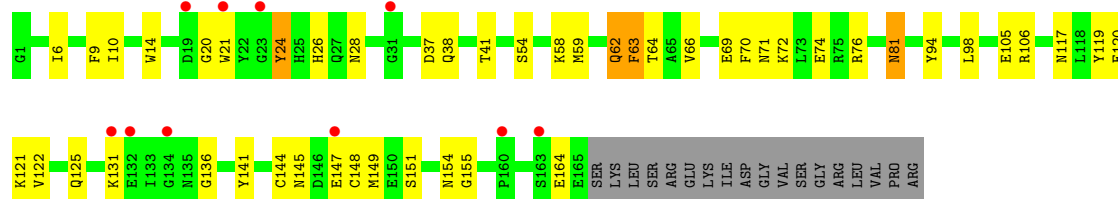
• Molecule 2: Hemagglutinin HA2 chain



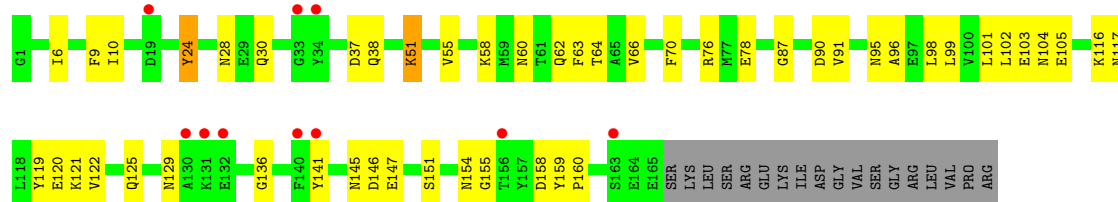
• Molecule 2: Hemagglutinin HA2 chain



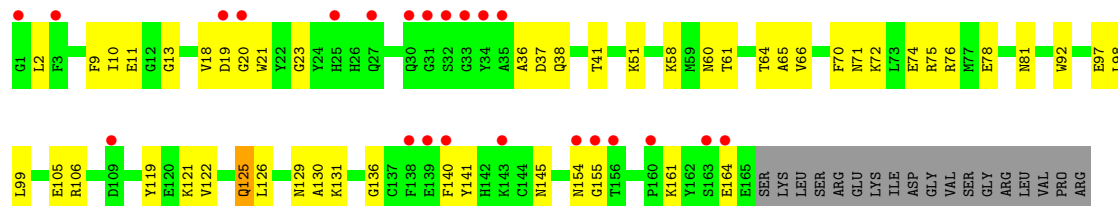
• Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



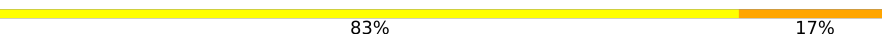
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain V:  83% 17%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
MAN6

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

Chain N:  40% 60%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5

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

Chain P:  60% 40%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  25% 50% 25%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

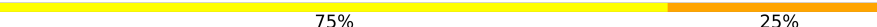
NAG1  
NAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  75% 25%

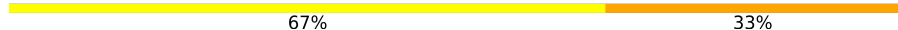


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  25% 50% 25%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  67% 33%





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 215.71Å 124.27Å 214.53Å<br>90.00° 102.91° 90.00°            | Depositor        |
| Resolution (Å)  | 48.75 – 3.24<br>48.75 – 3.24                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (48.75-3.24)<br>94.7 (48.75-3.24)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.03 (at 3.25Å)   | Xtrriage         |
| Refinement program  | PHENIX 1.17.1 _3660   | Depositor        |
| R, $R_{free}$   | 0.265 , 0.295<br>0.265 , 0.295                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1999 reflections (2.27%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.5  | Xtrriage         |
| Anisotropy  | 0.550   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 62.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.86  | EDS              |
| Total number of atoms   | 24413   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 74.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6117e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.66         | 3/2581 (0.1%)   | 0.90        | 4/3512 (0.1%)   |
| 1   | C     | 0.65         | 0/2581          | 0.85        | 2/3512 (0.1%)   |
| 1   | E     | 0.63         | 1/2581 (0.0%)   | 0.88        | 3/3512 (0.1%)   |
| 1   | G     | 0.64         | 1/2573 (0.0%)   | 0.86        | 2/3501 (0.1%)   |
| 1   | I     | 0.66         | 3/2573 (0.1%)   | 0.89        | 4/3501 (0.1%)   |
| 1   | K     | 0.63         | 1/2581 (0.0%)   | 0.86        | 3/3512 (0.1%)   |
| 2   | B     | 0.46         | 0/1352          | 0.75        | 0/1819          |
| 2   | D     | 0.43         | 0/1352          | 0.74        | 0/1819          |
| 2   | F     | 0.52         | 0/1352          | 0.76        | 0/1819          |
| 2   | H     | 0.53         | 0/1352          | 0.79        | 0/1819          |
| 2   | J     | 0.49         | 0/1352          | 0.78        | 0/1819          |
| 2   | L     | 0.55         | 1/1352 (0.1%)   | 0.80        | 1/1819 (0.1%)   |
| All | All   | 0.60         | 10/23582 (0.0%) | 0.84        | 19/31964 (0.1%) |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 302 | CYS  | CB-SG  | -7.29 | 1.69        | 1.82     |
| 1   | A     | 100 | GLU  | CG-CD  | 6.17  | 1.61        | 1.51     |
| 1   | I     | 47  | ILE  | C-N    | 5.49  | 1.46        | 1.34     |
| 1   | A     | 100 | GLU  | CD-OE1 | 5.45  | 1.31        | 1.25     |
| 1   | E     | 68  | GLU  | CG-CD  | 5.42  | 1.60        | 1.51     |
| 1   | I     | 55  | CYS  | CB-SG  | -5.17 | 1.73        | 1.81     |
| 1   | A     | 314 | VAL  | CB-CG1 | -5.16 | 1.42        | 1.52     |
| 2   | L     | 78  | GLU  | CG-CD  | 5.10  | 1.59        | 1.51     |
| 1   | I     | 135 | CYS  | CB-SG  | 5.09  | 1.91        | 1.82     |
| 1   | K     | 135 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 69  | LEU  | CA-CB-CG  | -7.17 | 98.82       | 115.30   |
| 1   | G     | 20  | LEU  | CA-CB-CG  | 6.96  | 131.31      | 115.30   |
| 1   | C     | 256 | LEU  | CA-CB-CG  | 6.26  | 129.69      | 115.30   |
| 1   | E     | 90  | CYS  | CA-CB-SG  | 6.23  | 125.21      | 114.00   |
| 1   | A     | 190 | LEU  | CA-CB-CG  | 6.12  | 129.36      | 115.30   |
| 1   | E     | 67  | CYS  | CA-CB-SG  | -5.96 | 103.27      | 114.00   |
| 1   | G     | 261 | GLY  | N-CA-C    | 5.90  | 127.84      | 113.10   |
| 1   | I     | 160 | LEU  | CB-CG-CD1 | -5.89 | 100.99      | 111.00   |
| 1   | K     | 261 | GLY  | N-CA-C    | 5.53  | 126.91      | 113.10   |
| 1   | K     | 111 | PHE  | CB-CA-C   | -5.45 | 99.49       | 110.40   |
| 1   | K     | 111 | PHE  | CB-CG-CD2 | -5.45 | 116.98      | 120.80   |
| 1   | I     | 111 | PHE  | CB-CA-C   | -5.36 | 99.68       | 110.40   |
| 1   | I     | 62  | LEU  | CB-CG-CD1 | -5.29 | 102.00      | 111.00   |
| 1   | I     | 278 | CYS  | CA-CB-SG  | -5.26 | 104.53      | 114.00   |
| 1   | C     | 111 | PHE  | CB-CG-CD2 | -5.21 | 117.15      | 120.80   |
| 1   | A     | 207 | ARG  | CA-CB-CG  | 5.21  | 124.86      | 113.40   |
| 1   | A     | 43  | LEU  | CA-CB-CG  | 5.17  | 127.20      | 115.30   |
| 2   | L     | 156 | THR  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | A     | 256 | LEU  | CA-CB-CG  | 5.00  | 126.81      | 115.30   |

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     | 2515  | 0        | 2435     | 106     | 0            |
| 1   | C     | 2515  | 0        | 2440     | 85      | 0            |
| 1   | E     | 2515  | 0        | 2437     | 105     | 1            |
| 1   | G     | 2507  | 0        | 2427     | 105     | 0            |
| 1   | I     | 2507  | 0        | 2427     | 100     | 1            |
| 1   | K     | 2515  | 0        | 2439     | 89      | 0            |
| 2   | B     | 1325  | 0        | 1246     | 47      | 0            |
| 2   | D     | 1325  | 0        | 1246     | 51      | 0            |
| 2   | F     | 1325  | 0        | 1246     | 52      | 0            |
| 2   | H     | 1325  | 0        | 1246     | 46      | 0            |
| 2   | J     | 1325  | 0        | 1246     | 50      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | L     | 1325  | 0        | 1246     | 49      | 0            |
| 3   | M     | 75    | 0        | 64       | 5       | 0            |
| 3   | S     | 75    | 0        | 64       | 2       | 0            |
| 3   | V     | 75    | 0        | 64       | 5       | 0            |
| 4   | N     | 64    | 0        | 55       | 6       | 0            |
| 4   | P     | 64    | 0        | 55       | 4       | 0            |
| 5   | O     | 50    | 0        | 43       | 1       | 0            |
| 5   | Q     | 50    | 0        | 43       | 0       | 0            |
| 5   | R     | 50    | 0        | 43       | 3       | 0            |
| 5   | T     | 50    | 0        | 43       | 4       | 0            |
| 5   | U     | 50    | 0        | 43       | 1       | 0            |
| 5   | X     | 50    | 0        | 43       | 4       | 0            |
| 6   | W     | 39    | 0        | 34       | 1       | 0            |
| 7   | A     | 70    | 0        | 65       | 4       | 0            |
| 7   | C     | 14    | 0        | 13       | 1       | 0            |
| 7   | E     | 56    | 0        | 52       | 0       | 0            |
| 7   | G     | 42    | 0        | 39       | 1       | 0            |
| 7   | I     | 42    | 0        | 39       | 1       | 0            |
| 7   | K     | 42    | 0        | 39       | 1       | 0            |
| 8   | G     | 1     | 0        | 0        | 0       | 0            |
| 8   | I     | 1     | 0        | 0        | 0       | 0            |
| 8   | K     | 1     | 0        | 0        | 0       | 0            |
| 9   | A     | 71    | 0        | 0        | 4       | 0            |
| 9   | B     | 7     | 0        | 0        | 1       | 0            |
| 9   | C     | 61    | 0        | 0        | 4       | 0            |
| 9   | D     | 13    | 0        | 0        | 3       | 0            |
| 9   | E     | 42    | 0        | 0        | 3       | 0            |
| 9   | F     | 17    | 0        | 0        | 1       | 0            |
| 9   | G     | 44    | 0        | 0        | 1       | 0            |
| 9   | H     | 16    | 0        | 0        | 0       | 0            |
| 9   | I     | 61    | 0        | 0        | 3       | 0            |
| 9   | J     | 16    | 0        | 0        | 0       | 0            |
| 9   | K     | 61    | 0        | 0        | 4       | 0            |
| 9   | L     | 19    | 0        | 0        | 1       | 0            |
| All | All   | 24413 | 0        | 22922    | 759     | 1            |

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 16.

All (759) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:310:LYS:HB3 | 1:G:312:ARG:HD3  | 1.41                     | 1.02              |
| 1:E:19:VAL:HG12 | 2:F:105:GLU:HG3  | 1.36                     | 1.01              |
| 2:J:71:ASN:HB3  | 2:J:74:GLU:HG3   | 1.41                     | 1.00              |
| 1:K:87:ASN:HD22 | 4:N:1:NAG:H83    | 1.30                     | 0.96              |
| 1:I:202:SER:HB3 | 1:I:205:TYR:HB3  | 1.53                     | 0.88              |
| 1:K:19:VAL:HG12 | 2:L:105:GLU:HG3  | 1.56                     | 0.87              |
| 1:E:68:GLU:OE1  | 1:E:137:HIS:CE1  | 2.28                     | 0.86              |
| 1:C:300:GLY:H   | 2:D:64:THR:HG22  | 1.38                     | 0.86              |
| 1:I:292:GLN:HB3 | 1:I:303:PRO:HG2  | 1.56                     | 0.85              |
| 2:D:98:LEU:HD21 | 2:J:99:LEU:HD13  | 1.57                     | 0.84              |
| 1:E:19:VAL:HG12 | 2:F:105:GLU:CG   | 2.08                     | 0.83              |
| 2:L:71:ASN:OD1  | 2:L:72:LYS:N     | 2.13                     | 0.82              |
| 1:E:19:VAL:CG1  | 2:F:105:GLU:HG3  | 2.10                     | 0.82              |
| 1:E:68:GLU:OE1  | 1:E:137:HIS:NE2  | 2.13                     | 0.81              |
| 2:J:71:ASN:OD1  | 2:J:72:LYS:N     | 2.14                     | 0.81              |
| 5:R:1:NAG:H62   | 5:R:2:NAG:HN2    | 1.46                     | 0.80              |
| 1:I:87:ASN:HD22 | 5:X:1:NAG:H83    | 1.45                     | 0.80              |
| 1:A:16:VAL:HG21 | 1:A:314:VAL:HG13 | 1.62                     | 0.80              |
| 1:E:58:ALA:HB2  | 1:E:98:TYR:HE1   | 1.45                     | 0.80              |
| 2:F:76:ARG:HG3  | 1:G:103:GLU:HG3  | 1.64                     | 0.80              |
| 1:G:21:GLU:OE1  | 1:G:318:ARG:NH2  | 2.16                     | 0.79              |
| 1:A:26:VAL:HG21 | 1:A:314:VAL:HG11 | 1.63                     | 0.79              |
| 1:G:171:GLU:OE1 | 1:G:258:ARG:NH1  | 2.16                     | 0.79              |
| 1:A:65:PRO:HB2  | 1:A:137:HIS:HB2  | 1.63                     | 0.79              |
| 1:A:18:THR:OG1  | 2:B:105:GLU:HG2  | 1.83                     | 0.78              |
| 1:K:16:VAL:HG11 | 1:K:314:VAL:HG13 | 1.64                     | 0.78              |
| 1:E:64:ASN:HD22 | 1:E:87:ASN:HB3   | 1.49                     | 0.77              |
| 1:A:112:GLU:HB3 | 1:A:255:ALA:HB3  | 1.66                     | 0.76              |
| 1:G:95:PHE:HB3  | 1:G:98:TYR:HB2   | 1.68                     | 0.76              |
| 2:D:76:ARG:HG3  | 1:I:103:GLU:HG3  | 1.69                     | 0.75              |
| 1:K:103:GLU:HG3 | 2:H:76:ARG:HG3   | 1.68                     | 0.75              |
| 1:I:134:SER:OG  | 1:I:222:GLN:HG2  | 1.86                     | 0.75              |
| 1:A:198:VAL:HB  | 1:A:209:PHE:HB2  | 1.69                     | 0.74              |
| 1:C:176:TRP:HB3 | 1:C:250:PRO:HG3  | 1.67                     | 0.74              |
| 2:L:76:ARG:HG3  | 1:E:103:GLU:HG3  | 1.68                     | 0.74              |
| 1:K:42:CYS:SG   | 1:K:274:CYS:HB2  | 2.29                     | 0.73              |
| 1:G:212:GLU:O   | 1:G:216:ARG:NH2  | 2.21                     | 0.72              |
| 1:K:292:GLN:HB3 | 1:K:303:PRO:HG2  | 1.72                     | 0.72              |
| 1:K:54:ASN:OD1  | 1:K:82:LYS:NZ    | 2.21                     | 0.72              |
| 1:I:112:GLU:HB3 | 1:I:255:ALA:HB3  | 1.71                     | 0.72              |
| 1:E:299:ILE:HA  | 2:F:64:THR:HG22  | 1.72                     | 0.72              |
| 2:F:71:ASN:ND2  | 2:F:74:GLU:OE2   | 2.22                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:65:PRO:HB2   | 1:K:137:HIS:HB2  | 1.72                     | 0.71              |
| 2:F:72:LYS:HG3   | 9:F:209:HOH:O    | 1.91                     | 0.71              |
| 1:G:87:ASN:HD22  | 3:V:1:NAG:H83    | 1.56                     | 0.71              |
| 1:E:220:ARG:NH2  | 5:T:1:NAG:O7     | 2.24                     | 0.70              |
| 1:A:100:GLU:HG2  | 2:J:76:ARG:HE    | 1.56                     | 0.70              |
| 2:B:28:ASN:ND2   | 2:B:29:GLU:OE2   | 2.25                     | 0.70              |
| 1:K:93:GLY:HA3   | 1:K:226:ILE:O    | 1.92                     | 0.70              |
| 1:G:299:ILE:HA   | 2:H:64:THR:HG22  | 1.74                     | 0.70              |
| 3:S:5:NAG:O7     | 3:S:5:NAG:O3     | 2.07                     | 0.70              |
| 1:E:261:GLY:O    | 2:F:64:THR:HG21  | 1.91                     | 0.70              |
| 1:C:19:VAL:HG22  | 2:J:51:LYS:HG2   | 1.73                     | 0.69              |
| 1:E:171:GLU:OE1  | 1:E:258:ARG:NH1  | 2.25                     | 0.69              |
| 2:F:37:ASP:OD1   | 2:F:38:GLN:N     | 2.25                     | 0.69              |
| 1:I:16:VAL:HG22  | 1:I:312:ARG:HG2  | 1.75                     | 0.69              |
| 1:G:90:CYS:HB3   | 3:V:1:NAG:H81    | 1.75                     | 0.69              |
| 1:E:58:ALA:HB2   | 1:E:98:TYR:CE1   | 2.26                     | 0.68              |
| 1:I:59:GLY:HA3   | 1:I:88:GLY:HA2   | 1.75                     | 0.68              |
| 2:F:125:GLN:NE2  | 2:F:154:ASN:O    | 2.26                     | 0.68              |
| 1:C:123:TRP:HZ3  | 1:C:160:LEU:HD21 | 1.58                     | 0.68              |
| 1:C:304:LYS:HE2  | 2:D:92:TRP:CD1   | 2.29                     | 0.68              |
| 1:C:46:GLY:N     | 1:C:275:ASP:OD1  | 2.28                     | 0.67              |
| 1:K:302:CYS:SG   | 1:K:303:PRO:HD2  | 2.34                     | 0.67              |
| 1:E:298:THR:HG21 | 2:F:62:GLN:HG2   | 1.75                     | 0.67              |
| 1:E:298:THR:OG1  | 1:E:302:CYS:SG   | 2.52                     | 0.67              |
| 1:K:197:TYR:CD1  | 1:K:244:ASN:HB2  | 2.29                     | 0.67              |
| 1:G:93:GLY:HA3   | 1:G:226:ILE:O    | 1.94                     | 0.67              |
| 2:B:113:SER:OG   | 2:J:2:LEU:O      | 2.12                     | 0.67              |
| 1:G:307:ARG:NH2  | 2:H:90:ASP:OD1   | 2.20                     | 0.67              |
| 1:A:8:HIS:NE2    | 1:A:10:ASN:OD1   | 2.28                     | 0.67              |
| 1:E:18:THR:HG22  | 1:E:21:GLU:O     | 1.96                     | 0.66              |
| 1:A:116:ILE:HD13 | 1:A:253:ALA:HB2  | 1.76                     | 0.66              |
| 1:I:171:GLU:OE1  | 1:I:258:ARG:NH1  | 2.28                     | 0.66              |
| 2:L:141:TYR:HB2  | 2:L:164:GLU:HG3  | 1.78                     | 0.66              |
| 1:K:46:GLY:N     | 1:K:275:ASP:OD1  | 2.27                     | 0.66              |
| 2:D:71:ASN:HB3   | 2:D:74:GLU:HG3   | 1.75                     | 0.66              |
| 1:I:216:ARG:O    | 1:I:223:GLU:HG3  | 1.95                     | 0.66              |
| 1:C:19:VAL:HG12  | 2:D:105:GLU:HG3  | 1.77                     | 0.66              |
| 2:D:76:ARG:NH1   | 2:J:74:GLU:OE1   | 2.29                     | 0.65              |
| 1:I:18:THR:HG23  | 1:I:20:LEU:H     | 1.60                     | 0.65              |
| 2:B:76:ARG:CG    | 1:C:103:GLU:HG3  | 2.27                     | 0.65              |
| 2:B:99:LEU:HD13  | 2:J:98:LEU:HD21  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:171:GLU:OE1  | 1:K:258:ARG:NH1  | 2.29                     | 0.65              |
| 2:B:76:ARG:NH2   | 2:D:74:GLU:OE1   | 2.27                     | 0.65              |
| 1:E:128:VAL:HG12 | 1:E:150:LEU:HD22 | 1.78                     | 0.65              |
| 1:I:176:TRP:CE2  | 1:I:229:TYR:HB2  | 2.32                     | 0.65              |
| 1:A:100:GLU:OE2  | 2:J:75:ARG:N     | 2.30                     | 0.65              |
| 2:L:101:LEU:HD11 | 2:F:54:SER:OG    | 1.96                     | 0.65              |
| 1:K:26:VAL:HG21  | 1:K:314:VAL:HG11 | 1.79                     | 0.64              |
| 1:C:115:GLU:HG2  | 1:C:118:PRO:HA   | 1.79                     | 0.64              |
| 1:C:16:VAL:HG11  | 1:C:314:VAL:HG13 | 1.79                     | 0.64              |
| 1:I:65:PRO:HB2   | 1:I:137:HIS:HB2  | 1.79                     | 0.64              |
| 1:G:40:LYS:HD2   | 1:G:272:ASP:OD2  | 1.97                     | 0.64              |
| 1:I:104:GLN:OE1  | 1:I:258:ARG:NH2  | 2.31                     | 0.64              |
| 2:D:97:GLU:HB3   | 2:J:58:LYS:HE3   | 1.80                     | 0.64              |
| 1:G:302:CYS:SG   | 1:G:303:PRO:HD2  | 2.37                     | 0.64              |
| 2:B:2:LEU:O      | 2:D:113:SER:OG   | 2.08                     | 0.64              |
| 1:E:300:GLY:H    | 2:F:64:THR:HG23  | 1.63                     | 0.64              |
| 2:F:145:ASN:ND2  | 2:F:147:GLU:OE1  | 2.31                     | 0.64              |
| 1:K:299:ILE:HA   | 2:L:64:THR:HG22  | 1.80                     | 0.64              |
| 2:H:37:ASP:OD1   | 2:H:38:GLN:N     | 2.31                     | 0.64              |
| 1:G:16:VAL:HG11  | 1:G:314:VAL:HG13 | 1.80                     | 0.63              |
| 1:C:114:PHE:CE2  | 1:C:116:ILE:HG22 | 2.32                     | 0.63              |
| 2:L:28:ASN:HD21  | 2:L:145:ASN:HA   | 1.63                     | 0.63              |
| 1:E:16:VAL:HG11  | 1:E:314:VAL:HG13 | 1.80                     | 0.63              |
| 1:A:207:ARG:HG3  | 1:A:207:ARG:HH11 | 1.62                     | 0.63              |
| 2:H:121:LYS:O    | 2:H:125:GLN:HG3  | 1.98                     | 0.63              |
| 2:L:105:GLU:HB3  | 2:F:106:ARG:HH22 | 1.62                     | 0.63              |
| 1:G:202:SER:HB3  | 1:G:205:TYR:HB3  | 1.80                     | 0.63              |
| 1:G:64:ASN:HD22  | 1:G:87:ASN:HB3   | 1.62                     | 0.63              |
| 1:I:58:ALA:HB2   | 1:I:98:TYR:CE1   | 2.33                     | 0.63              |
| 1:C:18:THR:HG23  | 1:C:20:LEU:H     | 1.64                     | 0.62              |
| 2:B:29:GLU:OE2   | 2:B:29:GLU:N     | 2.30                     | 0.62              |
| 1:I:16:VAL:HG11  | 1:I:314:VAL:HG13 | 1.81                     | 0.62              |
| 1:A:19:VAL:HG12  | 2:B:105:GLU:HG3  | 1.81                     | 0.62              |
| 1:G:19:VAL:O     | 1:G:20:LEU:HG    | 1.99                     | 0.62              |
| 1:I:59:GLY:CA    | 1:I:88:GLY:HA2   | 2.30                     | 0.62              |
| 1:K:196:ALA:HA   | 1:K:244:ASN:HB3  | 1.81                     | 0.62              |
| 1:E:43:LEU:HD23  | 1:E:46:GLY:O     | 2.00                     | 0.62              |
| 1:E:197:TYR:CD1  | 1:E:244:ASN:HB2  | 2.34                     | 0.62              |
| 1:E:157:TYR:CZ   | 1:E:245:GLY:HA2  | 2.35                     | 0.62              |
| 1:K:103:GLU:HG3  | 2:H:76:ARG:CG    | 2.29                     | 0.62              |
| 2:F:20:GLY:HA2   | 2:F:41:THR:HG21  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:64:ASN:HD21  | 4:N:1:NAG:C8     | 2.13                     | 0.62              |
| 1:A:96:ALA:HB2   | 1:A:229:TYR:CD1  | 2.34                     | 0.61              |
| 1:A:100:GLU:HG2  | 2:J:76:ARG:NE    | 2.15                     | 0.61              |
| 6:W:2:NAG:O3     | 6:W:3:BMA:H61    | 1.99                     | 0.61              |
| 2:H:145:ASN:ND2  | 2:H:147:GLU:OE1  | 2.34                     | 0.61              |
| 1:K:212:GLU:O    | 1:K:216:ARG:NH2  | 2.33                     | 0.61              |
| 1:G:64:ASN:HD21  | 3:V:1:NAG:H83    | 1.66                     | 0.61              |
| 1:G:7:TYR:CZ     | 2:H:6:ILE:HG23   | 2.36                     | 0.61              |
| 1:A:203:SER:HB2  | 1:I:219:VAL:HG11 | 1.81                     | 0.61              |
| 1:G:207:ARG:NH2  | 9:G:503:HOH:O    | 2.34                     | 0.60              |
| 2:J:130:ALA:HB2  | 2:J:140:PHE:CD1  | 2.36                     | 0.60              |
| 2:J:18:VAL:HG12  | 2:J:19:ASP:H     | 1.64                     | 0.60              |
| 2:L:37:ASP:OD1   | 2:L:38:GLN:N     | 2.35                     | 0.60              |
| 1:E:116:ILE:HD13 | 1:E:253:ALA:HB2  | 1.83                     | 0.60              |
| 2:L:71:ASN:HB3   | 2:L:74:GLU:CD    | 2.21                     | 0.60              |
| 1:C:179:HIS:ND1  | 1:C:191:TYR:OH   | 2.30                     | 0.60              |
| 2:D:80:LEU:HD13  | 2:J:81:ASN:OD1   | 2.02                     | 0.60              |
| 1:I:18:THR:OG1   | 2:J:105:GLU:HG2  | 2.02                     | 0.60              |
| 2:L:70:PHE:CD2   | 2:L:78:GLU:HA    | 2.37                     | 0.60              |
| 1:A:87:ASN:ND2   | 4:P:1:NAG:O7     | 2.35                     | 0.60              |
| 1:E:186:ASP:O    | 1:E:190:LEU:HB2  | 2.02                     | 0.60              |
| 1:I:212:GLU:O    | 1:I:216:ARG:NH2  | 2.35                     | 0.60              |
| 2:B:76:ARG:HG2   | 1:C:103:GLU:HG3  | 1.83                     | 0.60              |
| 1:G:181:PRO:HG2  | 1:G:187:GLN:HB2  | 1.84                     | 0.60              |
| 1:K:281:PRO:HG2  | 1:K:295:HIS:CE1  | 2.36                     | 0.60              |
| 1:A:230:TRP:HZ3  | 1:A:232:LEU:HD12 | 1.66                     | 0.59              |
| 1:G:170:LYS:NZ   | 1:G:257:SER:OG   | 2.18                     | 0.59              |
| 1:I:115:GLU:CD   | 1:I:118:PRO:HA   | 2.22                     | 0.59              |
| 1:E:26:VAL:HG21  | 1:E:314:VAL:HG11 | 1.83                     | 0.59              |
| 1:I:49:PRO:HD2   | 1:I:271:MET:HE1  | 1.84                     | 0.59              |
| 1:K:212:GLU:HB3  | 1:E:208:LYS:HD3  | 1.85                     | 0.59              |
| 1:I:180:HIS:ND1  | 1:I:211:PRO:HA   | 2.18                     | 0.59              |
| 1:K:95:PHE:HB3   | 1:K:98:TYR:HB2   | 1.85                     | 0.59              |
| 2:L:51:LYS:HG2   | 1:G:19:VAL:HG22  | 1.84                     | 0.59              |
| 1:I:145:LYS:NZ   | 9:I:501:HOH:O    | 2.36                     | 0.59              |
| 1:I:292:GLN:OE1  | 1:I:294:VAL:N    | 2.36                     | 0.58              |
| 1:G:65:PRO:O     | 1:G:68:GLU:HG3   | 2.02                     | 0.58              |
| 2:F:125:GLN:HE22 | 2:F:155:GLY:HA3  | 1.68                     | 0.58              |
| 1:K:64:ASN:HB3   | 1:K:67:CYS:SG    | 2.44                     | 0.58              |
| 2:L:131:LYS:NZ   | 2:L:141:TYR:HB3  | 2.18                     | 0.58              |
| 1:I:180:HIS:CE1  | 1:I:211:PRO:HA   | 2.39                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:128:VAL:HG12 | 1:A:150:LEU:HD22 | 1.86                     | 0.57              |
| 1:E:16:VAL:HG21  | 1:E:314:VAL:HG12 | 1.85                     | 0.57              |
| 2:F:154:ASN:OD1  | 2:F:155:GLY:N    | 2.36                     | 0.57              |
| 1:C:10:ASN:O     | 1:C:319:ASN:ND2  | 2.30                     | 0.57              |
| 1:E:122:SER:O    | 1:E:162:LYS:HE2  | 2.04                     | 0.57              |
| 1:I:27:THR:HG22  | 1:I:317:LEU:O    | 2.04                     | 0.57              |
| 2:J:37:ASP:OD1   | 2:J:38:GLN:N     | 2.37                     | 0.57              |
| 1:K:261:GLY:O    | 2:L:64:THR:HG21  | 2.04                     | 0.57              |
| 1:K:119:LYS:NZ   | 9:K:504:HOH:O    | 2.37                     | 0.57              |
| 1:K:311:LEU:HD21 | 2:L:97:GLU:HG2   | 1.85                     | 0.57              |
| 1:A:170:LYS:HE3  | 1:A:257:SER:OG   | 2.04                     | 0.57              |
| 1:A:56:SER:HB3   | 1:A:85:PRO:HB2   | 1.85                     | 0.57              |
| 2:J:141:TYR:OH   | 2:J:161:LYS:HG3  | 2.05                     | 0.57              |
| 2:L:120:GLU:C    | 2:L:122:VAL:H    | 2.07                     | 0.57              |
| 1:A:15:THR:CG2   | 1:A:23:ASN:HA    | 2.35                     | 0.57              |
| 1:A:186:ASP:O    | 1:A:190:LEU:HB2  | 2.05                     | 0.57              |
| 2:L:50:ASN:HB3   | 1:G:20:LEU:HA    | 1.86                     | 0.57              |
| 1:C:196:ALA:HB1  | 1:C:211:PRO:HG2  | 1.87                     | 0.57              |
| 1:G:50:LEU:HD11  | 1:G:60:TRP:CZ2   | 2.39                     | 0.57              |
| 1:I:261:GLY:O    | 2:J:64:THR:HG21  | 2.05                     | 0.56              |
| 1:A:302:CYS:SG   | 1:A:303:PRO:HD2  | 2.45                     | 0.56              |
| 1:A:27:THR:HG22  | 1:A:317:LEU:O    | 2.05                     | 0.56              |
| 1:E:300:GLY:O    | 2:F:63:PHE:HA    | 2.04                     | 0.56              |
| 2:H:154:ASN:OD1  | 2:H:155:GLY:N    | 2.36                     | 0.56              |
| 1:I:127:THR:OG1  | 1:I:152:GLY:O    | 2.22                     | 0.56              |
| 2:H:129:ASN:HA   | 2:H:141:TYR:CE2  | 2.40                     | 0.56              |
| 1:A:117:PHE:CD1  | 1:A:162:LYS:HG2  | 2.41                     | 0.56              |
| 1:A:157:TYR:CZ   | 1:A:245:GLY:HA2  | 2.40                     | 0.56              |
| 1:C:82:LYS:HG3   | 9:C:512:HOH:O    | 2.05                     | 0.56              |
| 2:B:51:LYS:HG2   | 1:I:19:VAL:O     | 2.06                     | 0.56              |
| 2:J:119:TYR:CE1  | 2:J:136:GLY:HA2  | 2.41                     | 0.56              |
| 1:K:127:THR:HG23 | 1:K:153:LYS:HB2  | 1.87                     | 0.56              |
| 2:J:125:GLN:HE22 | 2:J:155:GLY:HA3  | 1.69                     | 0.56              |
| 1:C:18:THR:HG22  | 1:C:21:GLU:O     | 2.05                     | 0.56              |
| 2:D:37:ASP:OD1   | 2:D:38:GLN:N     | 2.38                     | 0.56              |
| 1:G:27:THR:HG22  | 1:G:317:LEU:O    | 2.05                     | 0.56              |
| 1:K:198:VAL:HB   | 1:K:209:PHE:HB2  | 1.88                     | 0.56              |
| 1:K:31:ASN:O     | 1:K:31:ASN:ND2   | 2.38                     | 0.56              |
| 1:C:96:ALA:HB2   | 1:C:229:TYR:CD1  | 2.40                     | 0.55              |
| 2:B:98:LEU:HD21  | 2:D:99:LEU:HD13  | 1.89                     | 0.55              |
| 1:A:114:PHE:CE2  | 1:A:116:ILE:HG23 | 2.41                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:201:VAL:HG11 | 1:G:216:ARG:HB3  | 1.89                     | 0.55              |
| 1:G:302:CYS:O    | 2:H:62:GLN:N     | 2.39                     | 0.55              |
| 2:J:130:ALA:HB2  | 2:J:140:PHE:HD1  | 1.70                     | 0.55              |
| 2:L:145:ASN:ND2  | 2:L:147:GLU:OE1  | 2.39                     | 0.55              |
| 2:B:37:ASP:OD1   | 2:B:38:GLN:N     | 2.39                     | 0.55              |
| 1:C:28:HIS:CE1   | 2:D:21:TRP:HE1   | 2.25                     | 0.55              |
| 1:G:18:THR:OG1   | 2:H:105:GLU:HG2  | 2.06                     | 0.55              |
| 1:I:170:LYS:N    | 1:I:235:PRO:HG3  | 2.21                     | 0.55              |
| 1:K:90:CYS:O     | 1:K:220:ARG:HD3  | 2.07                     | 0.55              |
| 1:C:233:LEU:HG   | 1:C:237:ASP:HB3  | 1.88                     | 0.55              |
| 1:G:161:SER:HA   | 1:G:241:PHE:O    | 2.06                     | 0.55              |
| 2:D:28:ASN:ND2   | 2:D:146:ASP:OD1  | 2.35                     | 0.55              |
| 2:B:27:GLN:HA    | 2:B:32:SER:HB2   | 1.89                     | 0.55              |
| 1:C:291:PHE:CE2  | 2:D:96:ALA:HB2   | 2.42                     | 0.55              |
| 1:C:34:GLU:HG2   | 1:C:289:LEU:HD12 | 1.89                     | 0.55              |
| 2:H:119:TYR:CE1  | 2:H:136:GLY:HA2  | 2.41                     | 0.55              |
| 1:E:54:ASN:OD1   | 1:E:82:LYS:NZ    | 2.28                     | 0.55              |
| 1:E:62:LEU:HD21  | 1:E:228:TYR:CD1  | 2.42                     | 0.55              |
| 2:J:9:PHE:CD1    | 2:J:10:ILE:HG13  | 2.42                     | 0.55              |
| 1:A:203:SER:HB2  | 1:I:219:VAL:CG1  | 2.37                     | 0.54              |
| 1:E:260:PHE:H    | 1:E:260:PHE:HD1  | 1.54                     | 0.54              |
| 2:H:28:ASN:ND2   | 2:H:146:ASP:OD1  | 2.27                     | 0.54              |
| 1:C:27:THR:HG22  | 1:C:317:LEU:O    | 2.06                     | 0.54              |
| 2:L:148:CYS:HA   | 2:L:151:SER:HB3  | 1.89                     | 0.54              |
| 1:E:16:VAL:HG21  | 1:E:314:VAL:CG1  | 2.37                     | 0.54              |
| 1:E:6:GLY:HA3    | 2:F:14:TRP:CZ2   | 2.42                     | 0.54              |
| 2:D:141:TYR:HE2  | 2:D:162:TYR:H    | 1.54                     | 0.54              |
| 1:E:64:ASN:ND2   | 1:E:87:ASN:HB3   | 2.18                     | 0.54              |
| 1:G:172:VAL:HA   | 1:G:254:PHE:O    | 2.07                     | 0.54              |
| 1:C:16:VAL:HG22  | 1:C:312:ARG:HB3  | 1.89                     | 0.54              |
| 1:I:16:VAL:HG21  | 1:I:314:VAL:HG12 | 1.90                     | 0.54              |
| 1:I:292:GLN:NE2  | 1:I:295:HIS:O    | 2.32                     | 0.54              |
| 2:D:127:LYS:HD3  | 2:D:159:TYR:OH   | 2.08                     | 0.54              |
| 1:C:302:CYS:SG   | 1:C:303:PRO:HD2  | 2.48                     | 0.54              |
| 1:G:297:VAL:HG13 | 2:H:66:VAL:HG12  | 1.90                     | 0.54              |
| 1:K:87:ASN:HA    | 4:N:1:NAG:H83    | 1.90                     | 0.54              |
| 1:A:233:LEU:HD13 | 1:A:239:ILE:HB   | 1.90                     | 0.53              |
| 2:B:132:GLU:HG3  | 2:B:138:PHE:HE1  | 1.73                     | 0.53              |
| 1:G:64:ASN:HD21  | 3:V:1:NAG:C8     | 2.21                     | 0.53              |
| 1:E:133:ALA:O    | 1:E:136:SER:OG   | 2.21                     | 0.53              |
| 1:I:304:LYS:HE2  | 2:J:92:TRP:CD1   | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:SER:HB3  | 1:A:259:GLY:HA3  | 1.90                     | 0.53              |
| 1:E:287:SER:HB2  | 1:E:303:PRO:HD3  | 1.90                     | 0.53              |
| 1:G:16:VAL:HG22  | 1:G:312:ARG:HB3  | 1.90                     | 0.53              |
| 2:B:51:LYS:HG2   | 1:I:19:VAL:HG22  | 1.90                     | 0.53              |
| 1:I:296:PRO:HG3  | 1:I:305:TYR:CE2  | 2.44                     | 0.53              |
| 1:A:91:TYR:CD1   | 1:A:92:PRO:HD2   | 2.44                     | 0.53              |
| 2:F:81:ASN:C     | 2:F:81:ASN:HD22  | 2.10                     | 0.53              |
| 1:A:115:GLU:OE2  | 1:A:251:ARG:NE   | 2.33                     | 0.53              |
| 1:G:116:ILE:HG22 | 1:G:117:PHE:CG   | 2.44                     | 0.53              |
| 1:E:176:TRP:NE1  | 1:E:200:VAL:HG21 | 2.23                     | 0.53              |
| 2:B:76:ARG:HG3   | 1:C:103:GLU:HG3  | 1.90                     | 0.53              |
| 1:E:234:GLU:N    | 9:E:502:HOH:O    | 2.27                     | 0.53              |
| 1:E:197:TYR:CE1  | 1:E:244:ASN:HB2  | 2.44                     | 0.53              |
| 1:A:100:GLU:HG3  | 2:J:76:ARG:HH21  | 1.72                     | 0.53              |
| 1:A:307:ARG:CZ   | 2:B:89:ILE:HG21  | 2.39                     | 0.52              |
| 1:C:157:TYR:CE1  | 1:C:245:GLY:HA2  | 2.45                     | 0.52              |
| 2:D:60:ASN:O     | 2:D:61:THR:HG23  | 2.08                     | 0.52              |
| 1:K:18:THR:HB    | 2:L:105:GLU:HG2  | 1.91                     | 0.52              |
| 1:C:5:ILE:O      | 2:D:10:ILE:HD13  | 2.09                     | 0.52              |
| 2:B:94:TYR:HD1   | 2:B:95:ASN:HD22  | 1.56                     | 0.52              |
| 1:E:202:SER:OG   | 1:E:203:SER:N    | 2.43                     | 0.52              |
| 1:E:92:PRO:HB2   | 1:E:225:ARG:HD3  | 1.91                     | 0.52              |
| 1:E:184:ILE:H    | 1:E:184:ILE:HD12 | 1.75                     | 0.52              |
| 1:E:104:GLN:NE2  | 9:E:503:HOH:O    | 2.30                     | 0.52              |
| 1:E:263:GLY:HA3  | 2:F:66:VAL:HG11  | 1.92                     | 0.52              |
| 1:A:127:THR:HG23 | 1:A:153:LYS:HB2  | 1.91                     | 0.52              |
| 1:C:62:LEU:HD21  | 1:C:228:TYR:CD1  | 2.45                     | 0.52              |
| 1:E:292:GLN:HG2  | 1:E:303:PRO:HG2  | 1.91                     | 0.52              |
| 4:P:5:NAG:O3     | 4:P:5:NAG:O7     | 2.23                     | 0.52              |
| 1:A:100:GLU:O    | 1:A:104:GLN:HG2  | 2.09                     | 0.52              |
| 1:E:116:ILE:HD11 | 1:E:250:PRO:HB2  | 1.92                     | 0.52              |
| 1:G:26:VAL:HG21  | 1:G:314:VAL:HG11 | 1.92                     | 0.52              |
| 1:I:112:GLU:HG3  | 9:I:544:HOH:O    | 2.10                     | 0.52              |
| 2:L:20:GLY:HA2   | 2:L:41:THR:HG21  | 1.92                     | 0.52              |
| 1:C:96:ALA:HB3   | 1:C:229:TYR:HA   | 1.92                     | 0.51              |
| 2:D:119:TYR:CE1  | 2:D:136:GLY:HA2  | 2.46                     | 0.51              |
| 1:G:310:LYS:HG2  | 1:G:312:ARG:NH1  | 2.25                     | 0.51              |
| 2:F:28:ASN:HD21  | 2:F:145:ASN:HA   | 1.75                     | 0.51              |
| 1:I:214:ALA:O    | 1:I:216:ARG:NH1  | 2.43                     | 0.51              |
| 1:I:64:ASN:HD21  | 5:X:1:NAG:C8     | 2.23                     | 0.51              |
| 1:I:87:ASN:HA    | 5:X:1:NAG:H83    | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:292:GLN:HG2  | 1:G:303:PRO:HG2  | 1.93                     | 0.51              |
| 2:J:119:TYR:HE1  | 2:J:136:GLY:HA2  | 1.75                     | 0.51              |
| 1:K:216:ARG:O    | 1:K:223:GLU:HG3  | 2.09                     | 0.51              |
| 1:E:16:VAL:HG22  | 1:E:312:ARG:HG2  | 1.92                     | 0.51              |
| 2:B:71:ASN:ND2   | 2:B:74:GLU:HG3   | 2.26                     | 0.51              |
| 2:F:26:HIS:HB2   | 2:F:149:MET:SD   | 2.50                     | 0.51              |
| 1:A:38:ASN:HB3   | 1:A:284:ALA:N    | 2.25                     | 0.51              |
| 1:C:112:GLU:HB3  | 1:C:255:ALA:HB3  | 1.93                     | 0.51              |
| 1:E:292:GLN:HB3  | 1:E:303:PRO:HG2  | 1.91                     | 0.51              |
| 1:E:57:VAL:HG23  | 1:E:81:GLU:OE2   | 2.11                     | 0.51              |
| 1:A:128:VAL:HB   | 1:A:148:LEU:HD21 | 1.93                     | 0.51              |
| 2:F:28:ASN:ND2   | 2:F:144:CYS:O    | 2.43                     | 0.51              |
| 1:I:135:CYS:O    | 1:I:142:SER:HB3  | 2.11                     | 0.51              |
| 2:B:74:GLU:OE1   | 2:J:76:ARG:NH1   | 2.43                     | 0.51              |
| 1:K:133:ALA:O    | 1:K:136:SER:OG   | 2.23                     | 0.51              |
| 1:A:63:GLY:O     | 1:A:145:LYS:N    | 2.43                     | 0.51              |
| 1:C:7:TYR:CE2    | 2:D:6:ILE:HA     | 2.45                     | 0.51              |
| 1:G:58:ALA:HB2   | 1:G:98:TYR:CE2   | 2.46                     | 0.51              |
| 2:H:129:ASN:HA   | 2:H:141:TYR:HE2  | 1.76                     | 0.51              |
| 1:C:96:ALA:O     | 1:C:230:TRP:NE1  | 2.40                     | 0.51              |
| 1:I:302:CYS:SG   | 1:I:303:PRO:HD2  | 2.51                     | 0.51              |
| 2:L:125:GLN:NE2  | 2:L:152:VAL:O    | 2.44                     | 0.51              |
| 1:E:215:LYS:HG3  | 1:G:240:ILE:HD13 | 1.92                     | 0.51              |
| 1:I:28:HIS:CE1   | 2:J:21:TRP:HE1   | 2.29                     | 0.51              |
| 2:J:23:GLY:HA3   | 2:J:36:ALA:HA    | 1.93                     | 0.51              |
| 1:K:276:ALA:HB2  | 1:K:284:ALA:HB1  | 1.92                     | 0.51              |
| 1:K:58:ALA:HB2   | 1:K:98:TYR:CE1   | 2.46                     | 0.51              |
| 2:B:3:PHE:CZ     | 2:B:113:SER:HB2  | 2.46                     | 0.50              |
| 1:I:213:ILE:HD12 | 9:I:539:HOH:O    | 2.10                     | 0.50              |
| 1:K:33:LEU:HD12  | 1:K:311:LEU:HD12 | 1.93                     | 0.50              |
| 1:K:23:ASN:CG    | 7:K:401:NAG:H83  | 2.32                     | 0.50              |
| 1:A:205:TYR:OH   | 1:A:207:ARG:HD3  | 2.11                     | 0.50              |
| 1:A:4:CYS:O      | 2:B:24:TYR:HA    | 2.11                     | 0.50              |
| 1:G:300:GLY:O    | 2:H:63:PHE:HA    | 2.11                     | 0.50              |
| 1:C:157:TYR:CZ   | 1:C:245:GLY:HA2  | 2.46                     | 0.50              |
| 1:C:298:THR:O    | 2:D:64:THR:HA    | 2.11                     | 0.50              |
| 1:G:49:PRO:HB3   | 1:G:78:TYR:CZ    | 2.45                     | 0.50              |
| 2:J:121:LYS:O    | 2:J:125:GLN:HG3  | 2.11                     | 0.50              |
| 1:K:87:ASN:ND2   | 4:N:1:NAG:H83    | 2.13                     | 0.50              |
| 2:F:76:ARG:CG    | 1:G:103:GLU:HG3  | 2.39                     | 0.50              |
| 1:K:276:ALA:CB   | 1:K:284:ALA:HB1  | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:28:ASN:HD21  | 2:H:145:ASN:C    | 2.14                     | 0.50              |
| 1:K:58:ALA:O     | 1:K:62:LEU:HB2   | 2.11                     | 0.50              |
| 3:M:1:NAG:H4     | 3:M:2:NAG:H61    | 1.92                     | 0.50              |
| 1:E:299:ILE:HA   | 2:F:64:THR:CG2   | 2.40                     | 0.50              |
| 1:C:292:GLN:OE1  | 1:C:294:VAL:HG22 | 2.12                     | 0.50              |
| 2:J:141:TYR:HB2  | 2:J:164:GLU:HG3  | 1.92                     | 0.50              |
| 1:C:71:ILE:HD13  | 1:C:145:LYS:HD3  | 1.93                     | 0.49              |
| 1:G:112:GLU:OE2  | 1:G:168:LYS:NZ   | 2.45                     | 0.49              |
| 1:G:41:LEU:N     | 1:G:270:PRO:O    | 2.31                     | 0.49              |
| 1:E:116:ILE:CD1  | 1:E:250:PRO:HB2  | 2.42                     | 0.49              |
| 2:F:9:PHE:CD1    | 2:F:10:ILE:HG13  | 2.47                     | 0.49              |
| 2:L:9:PHE:CD1    | 2:L:10:ILE:HG13  | 2.47                     | 0.49              |
| 1:A:219:VAL:HG11 | 1:C:203:SER:HB3  | 1.93                     | 0.49              |
| 1:A:286:ASN:OD1  | 7:A:413:NAG:H4   | 2.12                     | 0.49              |
| 7:A:414:NAG:H3   | 9:A:533:HOH:O    | 2.12                     | 0.49              |
| 1:E:91:TYR:HB3   | 1:E:228:TYR:OH   | 2.11                     | 0.49              |
| 1:E:98:TYR:HE2   | 1:E:102:ARG:HD2  | 1.77                     | 0.49              |
| 1:E:18:THR:OG1   | 2:F:105:GLU:HG2  | 2.12                     | 0.49              |
| 1:A:16:VAL:HG22  | 2:B:104:ASN:ND2  | 2.28                     | 0.49              |
| 1:G:95:PHE:HE1   | 1:G:230:TRP:CD1  | 2.30                     | 0.49              |
| 1:G:4:CYS:O      | 2:H:24:TYR:HA    | 2.12                     | 0.49              |
| 1:K:41:LEU:HD13  | 1:K:80:VAL:HG21  | 1.94                     | 0.49              |
| 2:L:76:ARG:CG    | 1:E:103:GLU:HG3  | 2.39                     | 0.49              |
| 1:A:99:GLU:CD    | 1:A:99:GLU:H     | 2.16                     | 0.49              |
| 1:A:123:TRP:CZ3  | 1:A:162:LYS:HD3  | 2.47                     | 0.49              |
| 1:A:181:PRO:HG2  | 1:A:213:ILE:HG12 | 1.94                     | 0.49              |
| 2:H:28:ASN:HD21  | 2:H:145:ASN:HA   | 1.78                     | 0.49              |
| 1:I:201:VAL:HG12 | 1:I:202:SER:O    | 2.13                     | 0.49              |
| 1:K:115:GLU:CD   | 1:K:118:PRO:HA   | 2.33                     | 0.49              |
| 2:D:76:ARG:CG    | 1:I:103:GLU:HG3  | 2.41                     | 0.49              |
| 2:L:73:LEU:HD13  | 1:E:97:ASP:OD1   | 2.13                     | 0.49              |
| 1:C:123:TRP:CZ3  | 1:C:160:LEU:HD21 | 2.45                     | 0.48              |
| 1:G:196:ALA:HA   | 1:G:244:ASN:HB3  | 1.95                     | 0.48              |
| 1:I:16:VAL:HG22  | 1:I:312:ARG:CG   | 2.43                     | 0.48              |
| 1:C:216:ARG:HA   | 1:I:240:ILE:HD12 | 1.94                     | 0.48              |
| 2:H:122:VAL:HA   | 2:H:125:GLN:HB2  | 1.95                     | 0.48              |
| 2:H:30:GLN:OE1   | 2:H:145:ASN:HB2  | 2.13                     | 0.48              |
| 1:C:123:TRP:CZ3  | 1:C:160:LEU:HD11 | 2.49                     | 0.48              |
| 1:C:7:TYR:CD2    | 2:D:6:ILE:HG22   | 2.48                     | 0.48              |
| 1:I:49:PRO:HB3   | 1:I:78:TYR:CZ    | 2.48                     | 0.48              |
| 5:U:4:MAN:H61    | 5:U:4:MAN:O2     | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:19:VAL:CG2   | 2:J:51:LYS:HG2   | 2.41                     | 0.48              |
| 2:L:131:LYS:HZ2  | 2:L:141:TYR:HB3  | 1.78                     | 0.48              |
| 1:E:64:ASN:OD1   | 1:E:65:PRO:HD2   | 2.13                     | 0.48              |
| 1:A:72:SER:OG    | 9:A:501:HOH:O    | 2.20                     | 0.48              |
| 1:C:38:ASN:HB3   | 1:C:284:ALA:HB3  | 1.95                     | 0.48              |
| 1:E:234:GLU:OE1  | 1:E:235:PRO:HD2  | 2.13                     | 0.48              |
| 5:T:1:NAG:H62    | 5:T:2:NAG:O7     | 2.14                     | 0.48              |
| 1:A:171:GLU:OE1  | 1:A:258:ARG:NH1  | 2.46                     | 0.48              |
| 1:I:57:VAL:HG21  | 1:I:264:ILE:HD13 | 1.94                     | 0.48              |
| 1:I:16:VAL:HG21  | 1:I:314:VAL:CG1  | 2.44                     | 0.48              |
| 1:A:71:ILE:CD1   | 1:A:145:LYS:HD3  | 2.43                     | 0.48              |
| 2:B:18:VAL:O     | 2:B:19:ASP:OD1   | 2.31                     | 0.48              |
| 1:I:115:GLU:OE2  | 1:I:118:PRO:HA   | 2.13                     | 0.48              |
| 1:I:79:ILE:HB    | 1:I:264:ILE:HG12 | 1.95                     | 0.48              |
| 1:C:292:GLN:HG2  | 1:C:303:PRO:HG2  | 1.94                     | 0.48              |
| 1:G:116:ILE:HG13 | 1:G:253:ALA:HB3  | 1.96                     | 0.48              |
| 1:G:291:PHE:CE1  | 2:H:96:ALA:HB2   | 2.49                     | 0.48              |
| 1:C:74:GLU:OE2   | 1:C:113:ARG:HB3  | 2.13                     | 0.47              |
| 2:B:80:LEU:HD13  | 2:D:81:ASN:OD1   | 2.12                     | 0.47              |
| 1:E:224:GLY:O    | 1:E:225:ARG:NH1  | 2.46                     | 0.47              |
| 1:A:64:ASN:OD1   | 1:A:65:PRO:HD2   | 2.14                     | 0.47              |
| 1:K:285:ILE:HD11 | 1:K:294:VAL:CG2  | 2.44                     | 0.47              |
| 1:A:30:VAL:O     | 1:A:312:ARG:O    | 2.32                     | 0.47              |
| 1:K:7:TYR:HE1    | 1:K:320:ILE:HD13 | 1.79                     | 0.47              |
| 2:L:145:ASN:OD1  | 2:L:145:ASN:N    | 2.42                     | 0.47              |
| 1:A:46:GLY:N     | 1:A:275:ASP:OD1  | 2.47                     | 0.47              |
| 1:K:197:TYR:CE1  | 1:K:244:ASN:HB2  | 2.49                     | 0.47              |
| 2:L:69:GLU:HA    | 9:L:202:HOH:O    | 2.15                     | 0.47              |
| 2:B:125:GLN:NE2  | 2:B:154:ASN:O    | 2.42                     | 0.47              |
| 1:E:212:GLU:HB3  | 1:G:208:LYS:HD3  | 1.95                     | 0.47              |
| 1:G:292:GLN:HB3  | 1:G:303:PRO:HG2  | 1.96                     | 0.47              |
| 1:I:320:ILE:O    | 2:J:13:GLY:N     | 2.38                     | 0.47              |
| 1:I:91:TYR:CD1   | 1:I:92:PRO:HD2   | 2.49                     | 0.47              |
| 1:K:215:LYS:HE3  | 1:E:240:ILE:HG21 | 1.95                     | 0.47              |
| 2:D:126:LEU:HD23 | 2:D:157:TYR:CE2  | 2.49                     | 0.47              |
| 1:E:41:LEU:N     | 1:E:270:PRO:O    | 2.34                     | 0.47              |
| 2:F:21:TRP:H     | 2:F:41:THR:HG23  | 1.80                     | 0.47              |
| 1:G:23:ASN:OD1   | 7:G:402:NAG:O6   | 2.33                     | 0.47              |
| 1:I:276:ALA:HB1  | 1:I:284:ALA:HB1  | 1.97                     | 0.47              |
| 2:D:3:PHE:HB2    | 2:D:112:ASP:CG   | 2.35                     | 0.47              |
| 1:E:46:GLY:N     | 1:E:275:ASP:OD1  | 2.41                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:281:PRO:HG2 | 1:G:295:HIS:CE1  | 2.48                     | 0.47              |
| 1:G:19:VAL:HB   | 2:H:101:LEU:HD23 | 1.96                     | 0.47              |
| 2:F:98:LEU:HD21 | 2:H:99:LEU:HD13  | 1.96                     | 0.47              |
| 1:K:180:HIS:ND1 | 1:K:211:PRO:HA   | 2.30                     | 0.47              |
| 1:E:289:LEU:O   | 1:E:303:PRO:HB3  | 2.15                     | 0.47              |
| 1:E:10:ASN:O    | 1:E:319:ASN:ND2  | 2.47                     | 0.47              |
| 1:E:4:CYS:O     | 2:F:24:TYR:HA    | 2.14                     | 0.47              |
| 2:F:131:LYS:HG3 | 2:F:141:TYR:CE1  | 2.50                     | 0.47              |
| 1:I:302:CYS:SG  | 1:I:303:PRO:CD   | 3.03                     | 0.47              |
| 1:I:55:CYS:HA   | 1:I:87:ASN:O     | 2.14                     | 0.47              |
| 2:J:60:ASN:O    | 2:J:61:THR:OG1   | 2.31                     | 0.47              |
| 1:G:115:GLU:OE2 | 1:G:118:PRO:HA   | 2.15                     | 0.47              |
| 1:G:16:VAL:HG22 | 1:G:312:ARG:CB   | 2.44                     | 0.47              |
| 1:C:6:GLY:HA2   | 2:D:10:ILE:HG21  | 1.97                     | 0.47              |
| 2:D:148:CYS:O   | 2:D:151:SER:HB3  | 2.15                     | 0.47              |
| 1:I:64:ASN:HB3  | 1:I:67:CYS:SG    | 2.55                     | 0.47              |
| 1:I:81:GLU:O    | 1:I:266:ASN:HA   | 2.15                     | 0.47              |
| 1:K:15:THR:CG2  | 1:K:23:ASN:HA    | 2.44                     | 0.47              |
| 1:C:7:TYR:CE2   | 2:D:6:ILE:HG22   | 2.50                     | 0.46              |
| 1:G:63:GLY:O    | 1:G:144:TYR:HA   | 2.15                     | 0.46              |
| 1:G:157:TYR:CE1 | 1:G:245:GLY:HA2  | 2.50                     | 0.46              |
| 1:A:180:HIS:CE1 | 1:A:211:PRO:HA   | 2.50                     | 0.46              |
| 1:A:26:VAL:HG21 | 1:A:314:VAL:CG1  | 2.40                     | 0.46              |
| 1:C:216:ARG:O   | 1:C:223:GLU:HG3  | 2.15                     | 0.46              |
| 2:D:82:LYS:HE2  | 2:D:86:ASP:OD2   | 2.15                     | 0.46              |
| 2:H:55:VAL:HG13 | 2:H:99:LEU:HD21  | 1.98                     | 0.46              |
| 2:B:160:PRO:O   | 9:B:201:HOH:O    | 2.20                     | 0.46              |
| 2:D:20:GLY:HA2  | 2:D:41:THR:HG21  | 1.97                     | 0.46              |
| 1:G:46:GLY:N    | 1:G:275:ASP:OD1  | 2.48                     | 0.46              |
| 1:G:313:MET:HA  | 2:H:104:ASN:OD1  | 2.16                     | 0.46              |
| 4:N:3:BMA:H3    | 4:N:4:MAN:H3     | 1.98                     | 0.46              |
| 2:B:23:GLY:HA3  | 2:B:36:ALA:HA    | 1.96                     | 0.46              |
| 2:J:18:VAL:HG12 | 2:J:19:ASP:N     | 2.30                     | 0.46              |
| 1:K:7:TYR:CE1   | 1:K:320:ILE:HD13 | 2.50                     | 0.46              |
| 3:S:3:BMA:H61   | 3:S:6:MAN:H2     | 1.73                     | 0.46              |
| 1:A:19:VAL:HG12 | 2:B:105:GLU:CG   | 2.45                     | 0.46              |
| 1:A:116:ILE:CD1 | 1:A:253:ALA:HB2  | 2.44                     | 0.46              |
| 1:A:31:ASN:O    | 1:A:33:LEU:N     | 2.48                     | 0.46              |
| 1:A:159:ASN:ND2 | 7:A:414:NAG:H83  | 2.31                     | 0.46              |
| 1:C:314:VAL:N   | 2:D:104:ASN:OD1  | 2.48                     | 0.46              |
| 1:E:7:TYR:CE2   | 2:F:6:ILE:HG22   | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:300:GLY:H    | 2:H:64:THR:HG23  | 1.80                     | 0.46              |
| 1:A:184:ILE:H    | 1:A:184:ILE:HD12 | 1.80                     | 0.46              |
| 1:A:18:THR:HG23  | 1:A:20:LEU:H     | 1.80                     | 0.46              |
| 1:A:36:SER:HB3   | 9:A:550:HOH:O    | 2.15                     | 0.46              |
| 1:C:171:GLU:HG2  | 1:C:171:GLU:H    | 1.36                     | 0.46              |
| 1:C:92:PRO:HB2   | 1:C:225:ARG:HD3  | 1.97                     | 0.46              |
| 1:K:215:LYS:HG3  | 1:K:215:LYS:O    | 2.15                     | 0.46              |
| 1:C:232:LEU:HD12 | 9:C:548:HOH:O    | 2.15                     | 0.46              |
| 1:G:101:LEU:HB2  | 1:G:230:TRP:CZ2  | 2.51                     | 0.46              |
| 1:I:95:PHE:HB3   | 1:I:98:TYR:HB2   | 1.98                     | 0.46              |
| 1:C:238:THR:HG21 | 9:C:531:HOH:O    | 2.16                     | 0.46              |
| 1:G:58:ALA:O     | 1:G:62:LEU:HB2   | 2.15                     | 0.46              |
| 2:H:116:LYS:O    | 2:H:120:GLU:HG2  | 2.16                     | 0.46              |
| 2:H:51:LYS:NZ    | 2:H:103:GLU:HB3  | 2.31                     | 0.46              |
| 1:A:64:ASN:HB3   | 1:A:67:CYS:SG    | 2.55                     | 0.46              |
| 1:A:96:ALA:HB2   | 1:A:229:TYR:HD1  | 1.77                     | 0.46              |
| 2:D:126:LEU:HD23 | 2:D:157:TYR:HE2  | 1.81                     | 0.46              |
| 1:I:93:GLY:HA3   | 1:I:226:ILE:O    | 2.15                     | 0.46              |
| 1:I:311:LEU:HD21 | 2:J:97:GLU:HG2   | 1.98                     | 0.46              |
| 1:E:299:ILE:HA   | 2:F:64:THR:HA    | 1.98                     | 0.46              |
| 1:E:19:VAL:HG22  | 2:H:51:LYS:HG2   | 1.97                     | 0.46              |
| 2:J:122:VAL:O    | 2:J:126:LEU:N    | 2.40                     | 0.46              |
| 2:J:20:GLY:HA2   | 2:J:41:THR:HG21  | 1.98                     | 0.46              |
| 1:A:28:HIS:CD2   | 2:B:21:TRP:HE1   | 2.35                     | 0.45              |
| 1:G:170:LYS:HZ2  | 1:G:257:SER:HG   | 1.54                     | 0.45              |
| 1:K:170:LYS:HD2  | 1:K:257:SER:OG   | 2.17                     | 0.45              |
| 1:A:16:VAL:CG2   | 1:A:314:VAL:HG13 | 2.40                     | 0.45              |
| 1:A:317:LEU:HB3  | 2:B:111:HIS:ND1  | 2.31                     | 0.45              |
| 1:G:64:ASN:HB3   | 1:G:67:CYS:SG    | 2.56                     | 0.45              |
| 1:I:99:GLU:CD    | 2:J:71:ASN:HB2   | 2.37                     | 0.45              |
| 5:T:1:NAG:HO3    | 5:T:1:NAG:C7     | 2.29                     | 0.45              |
| 1:E:38:ASN:HB3   | 1:E:284:ALA:N    | 2.31                     | 0.45              |
| 1:G:160:LEU:O    | 1:G:242:GLU:HA   | 2.15                     | 0.45              |
| 1:I:64:ASN:O     | 1:I:66:GLU:N     | 2.50                     | 0.45              |
| 2:J:129:ASN:HA   | 2:J:141:TYR:CE2  | 2.51                     | 0.45              |
| 1:C:220:ARG:NH2  | 5:R:1:NAG:O3     | 2.42                     | 0.45              |
| 9:K:508:HOH:O    | 1:E:201:VAL:HB   | 2.15                     | 0.45              |
| 1:I:74:GLU:OE2   | 1:I:113:ARG:HB3  | 2.17                     | 0.45              |
| 1:I:177:GLY:CA   | 1:I:248:ILE:HB   | 2.46                     | 0.45              |
| 1:I:26:VAL:HG21  | 1:I:314:VAL:HG11 | 1.98                     | 0.45              |
| 1:K:99:GLU:CD    | 1:K:99:GLU:H     | 2.20                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:3:BMA:H3     | 3:M:4:MAN:H5     | 1.98                     | 0.45              |
| 1:C:198:VAL:HG22 | 1:C:243:ALA:HB1  | 1.98                     | 0.45              |
| 1:E:115:GLU:HG2  | 1:E:118:PRO:HA   | 1.98                     | 0.45              |
| 1:G:16:VAL:HG21  | 1:G:314:VAL:HG12 | 1.99                     | 0.45              |
| 1:C:215:LYS:HG2  | 1:I:242:GLU:OE2  | 2.17                     | 0.45              |
| 1:K:151:THR:HG22 | 1:K:152:GLY:N    | 2.32                     | 0.45              |
| 1:K:205:TYR:CD1  | 1:K:205:TYR:C    | 2.89                     | 0.45              |
| 2:L:94:TYR:CZ    | 2:L:98:LEU:HD22  | 2.52                     | 0.45              |
| 1:A:209:PHE:CE2  | 1:A:229:TYR:CD2  | 3.04                     | 0.45              |
| 1:C:16:VAL:HG21  | 1:C:314:VAL:HG12 | 1.97                     | 0.45              |
| 1:C:173:LEU:HB2  | 1:C:256:LEU:HD21 | 1.98                     | 0.45              |
| 1:E:220:ARG:HH22 | 5:T:1:NAG:HO3    | 1.64                     | 0.45              |
| 1:G:19:VAL:CG1   | 2:H:105:GLU:HG3  | 2.45                     | 0.45              |
| 1:I:116:ILE:HG13 | 1:I:164:TYR:CD1  | 2.52                     | 0.45              |
| 1:I:20:LEU:HD12  | 2:J:105:GLU:HG3  | 1.99                     | 0.45              |
| 1:K:42:CYS:HB3   | 1:K:274:CYS:O    | 2.17                     | 0.45              |
| 1:E:215:LYS:HG2  | 1:G:242:GLU:OE2  | 2.17                     | 0.45              |
| 1:G:310:LYS:CB   | 1:G:312:ARG:HD3  | 2.29                     | 0.45              |
| 1:G:92:PRO:HB3   | 1:G:219:VAL:HG13 | 1.98                     | 0.45              |
| 1:I:198:VAL:O    | 1:I:209:PHE:HD1  | 2.00                     | 0.45              |
| 1:I:287:SER:OG   | 1:I:288:SER:N    | 2.50                     | 0.45              |
| 2:L:132:GLU:HG3  | 2:L:138:PHE:HE1  | 1.82                     | 0.45              |
| 1:K:140:LYS:HG2  | 5:O:2:NAG:H62    | 1.98                     | 0.45              |
| 1:C:123:TRP:CE3  | 1:C:160:LEU:HD11 | 2.52                     | 0.45              |
| 1:C:18:THR:OG1   | 2:D:105:GLU:HG2  | 2.16                     | 0.45              |
| 1:K:16:VAL:HG22  | 1:K:312:ARG:HB3  | 1.99                     | 0.45              |
| 2:L:129:ASN:HA   | 2:L:141:TYR:CE2  | 2.52                     | 0.45              |
| 2:B:51:LYS:NZ    | 2:B:107:THR:HG23 | 2.32                     | 0.45              |
| 1:K:186:ASP:O    | 1:K:190:LEU:HB2  | 2.17                     | 0.44              |
| 1:G:88:GLY:O     | 1:G:90:CYS:N     | 2.50                     | 0.44              |
| 1:K:292:GLN:HG3  | 1:K:305:TYR:HA   | 1.98                     | 0.44              |
| 1:E:123:TRP:CD2  | 1:E:150:LEU:HD11 | 2.53                     | 0.44              |
| 2:F:70:PHE:HZ    | 2:F:81:ASN:OD1   | 2.00                     | 0.44              |
| 1:G:216:ARG:O    | 1:G:223:GLU:HG3  | 2.17                     | 0.44              |
| 2:H:28:ASN:HD21  | 2:H:145:ASN:CA   | 2.30                     | 0.44              |
| 3:M:3:BMA:H62    | 3:M:6:MAN:H2     | 1.77                     | 0.44              |
| 1:A:215:LYS:HG2  | 1:A:223:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:8:HIS:ND1    | 2:B:17:MET:O     | 2.50                     | 0.44              |
| 1:G:290:PRO:HG2  | 1:G:291:PHE:CD2  | 2.53                     | 0.44              |
| 1:K:262:SER:OG   | 1:K:263:GLY:N    | 2.50                     | 0.44              |
| 1:K:81:GLU:O     | 1:K:266:ASN:HA   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:80:LEU:HD12  | 2:L:80:LEU:O     | 2.17                     | 0.44              |
| 1:C:127:THR:N    | 1:C:153:LYS:HB2  | 2.33                     | 0.44              |
| 1:C:281:PRO:HG2  | 1:C:295:HIS:CE1  | 2.51                     | 0.44              |
| 1:E:34:GLU:HG2   | 1:E:289:LEU:HD12 | 2.00                     | 0.44              |
| 1:G:183:ASN:HB2  | 1:G:186:ASP:H    | 1.83                     | 0.44              |
| 1:E:216:ARG:HB3  | 1:G:201:VAL:HG11 | 1.98                     | 0.44              |
| 1:G:310:LYS:HD3  | 1:G:312:ARG:HD3  | 1.99                     | 0.44              |
| 1:I:239:ILE:HG12 | 1:I:241:PHE:CE1  | 2.53                     | 0.44              |
| 2:L:159:TYR:N    | 2:L:160:PRO:HD2  | 2.33                     | 0.44              |
| 1:I:19:VAL:HG12  | 2:J:105:GLU:HG3  | 1.99                     | 0.44              |
| 2:J:131:LYS:NZ   | 2:J:141:TYR:HB3  | 2.31                     | 0.44              |
| 1:K:50:LEU:HD12  | 1:K:76:TRP:CE3   | 2.53                     | 0.44              |
| 1:K:301:GLU:HG2  | 2:L:63:PHE:CE1   | 2.53                     | 0.44              |
| 1:E:49:PRO:HG3   | 1:E:78:TYR:CZ    | 2.53                     | 0.44              |
| 2:H:120:GLU:C    | 2:H:122:VAL:H    | 2.21                     | 0.44              |
| 1:I:92:PRO:HB3   | 1:I:219:VAL:CG2  | 2.47                     | 0.44              |
| 1:E:198:VAL:HB   | 1:E:209:PHE:HB2  | 1.99                     | 0.44              |
| 1:E:5:ILE:HG13   | 2:F:119:TYR:HA   | 1.99                     | 0.44              |
| 2:H:87:GLY:O     | 2:H:91:VAL:HG23  | 2.18                     | 0.44              |
| 1:I:127:THR:HG23 | 1:I:153:LYS:HB2  | 2.00                     | 0.44              |
| 1:I:297:VAL:HG13 | 2:J:66:VAL:HG12  | 1.99                     | 0.44              |
| 1:A:285:ILE:HD11 | 1:A:294:VAL:HG21 | 1.99                     | 0.44              |
| 1:E:98:TYR:CE2   | 1:E:102:ARG:HD2  | 2.53                     | 0.44              |
| 2:H:70:PHE:CE1   | 2:H:78:GLU:HA    | 2.53                     | 0.44              |
| 1:I:226:ILE:HD13 | 1:I:226:ILE:HG21 | 1.82                     | 0.44              |
| 2:B:3:PHE:CE1    | 2:B:113:SER:HB2  | 2.53                     | 0.43              |
| 2:D:141:TYR:HB2  | 2:D:164:GLU:HG3  | 1.99                     | 0.43              |
| 1:E:129:THR:HG23 | 1:E:129:THR:O    | 2.18                     | 0.43              |
| 1:G:116:ILE:HG22 | 1:G:117:PHE:CD2  | 2.53                     | 0.43              |
| 1:G:15:THR:HB    | 1:G:312:ARG:HH21 | 1.82                     | 0.43              |
| 1:G:26:VAL:HG21  | 1:G:314:VAL:CG1  | 2.48                     | 0.43              |
| 1:I:320:ILE:HG21 | 2:J:11:GLU:O     | 2.18                     | 0.43              |
| 2:B:26:HIS:O     | 2:B:26:HIS:HD2   | 2.01                     | 0.43              |
| 1:C:147:LEU:HD22 | 1:C:176:TRP:HA   | 2.00                     | 0.43              |
| 1:C:201:VAL:HA   | 1:C:205:TYR:O    | 2.18                     | 0.43              |
| 1:G:19:VAL:HG12  | 2:H:105:GLU:HG3  | 2.00                     | 0.43              |
| 1:G:298:THR:O    | 2:H:64:THR:HA    | 2.18                     | 0.43              |
| 1:I:88:GLY:O     | 1:I:90:CYS:N     | 2.49                     | 0.43              |
| 2:L:116:LYS:O    | 2:L:120:GLU:HG2  | 2.18                     | 0.43              |
| 1:A:104:GLN:OE1  | 1:A:258:ARG:NH2  | 2.51                     | 0.43              |
| 1:I:41:LEU:HD11  | 1:I:80:VAL:HG11  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:181:PRO:HG2  | 1:K:187:GLN:HB2  | 1.99                     | 0.43              |
| 1:A:129:THR:OG1  | 1:A:130:GLY:N    | 2.50                     | 0.43              |
| 1:C:186:ASP:O    | 1:C:190:LEU:HB2  | 2.18                     | 0.43              |
| 1:G:51:GLN:HB2   | 1:G:51:GLN:HE21  | 1.48                     | 0.43              |
| 1:A:203:SER:HA   | 1:I:225:ARG:HH21 | 1.84                     | 0.43              |
| 1:I:30:VAL:O     | 1:I:312:ARG:O    | 2.37                     | 0.43              |
| 3:M:6:MAN:HO6    | 3:M:6:MAN:HO3    | 1.65                     | 0.43              |
| 2:B:72:LYS:HA    | 2:B:72:LYS:HD3   | 1.81                     | 0.43              |
| 2:B:79:ASN:ND2   | 1:C:103:GLU:OE1  | 2.52                     | 0.43              |
| 2:H:158:ASP:C    | 2:H:160:PRO:HD2  | 2.38                     | 0.43              |
| 2:F:94:TYR:HD2   | 2:H:58:LYS:O     | 2.01                     | 0.43              |
| 1:K:3:ILE:HD12   | 2:L:26:HIS:HB3   | 2.00                     | 0.43              |
| 1:A:136:SER:OG   | 3:M:6:MAN:H4     | 2.18                     | 0.43              |
| 1:A:188:ARG:HH21 | 1:A:194:GLU:CD   | 2.22                     | 0.43              |
| 1:C:199:SER:N    | 1:C:242:GLU:O    | 2.38                     | 0.43              |
| 2:D:2:LEU:HD23   | 2:D:3:PHE:CE1    | 2.53                     | 0.43              |
| 2:L:103:GLU:OE1  | 2:H:102:LEU:HD11 | 2.19                     | 0.43              |
| 1:I:151:THR:OG1  | 1:I:152:GLY:N    | 2.51                     | 0.43              |
| 1:K:176:TRP:CE2  | 1:K:200:VAL:HG21 | 2.53                     | 0.43              |
| 1:K:292:GLN:HB3  | 1:K:303:PRO:CG   | 2.46                     | 0.43              |
| 2:B:62:GLN:O     | 2:B:63:PHE:CD2   | 2.72                     | 0.43              |
| 1:G:256:LEU:HD23 | 1:G:258:ARG:NH2  | 2.33                     | 0.43              |
| 1:K:120:GLU:HB2  | 9:K:556:HOH:O    | 2.18                     | 0.43              |
| 2:L:132:GLU:HG3  | 2:L:138:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:220:ARG:NH2  | 5:R:1:NAG:H82    | 2.34                     | 0.43              |
| 1:A:289:LEU:O    | 1:A:303:PRO:HB3  | 2.18                     | 0.43              |
| 1:I:101:LEU:HA   | 1:I:101:LEU:HD12 | 1.69                     | 0.43              |
| 1:I:125:ASN:OD1  | 7:I:409:NAG:H83  | 2.19                     | 0.43              |
| 2:J:70:PHE:CD1   | 2:J:78:GLU:HA    | 2.54                     | 0.43              |
| 1:K:112:GLU:HB3  | 1:K:255:ALA:HB3  | 2.00                     | 0.43              |
| 2:D:120:GLU:C    | 2:D:122:VAL:H    | 2.22                     | 0.43              |
| 2:F:119:TYR:CE1  | 2:F:136:GLY:HA2  | 2.54                     | 0.43              |
| 1:A:90:CYS:HB3   | 4:P:1:NAG:H81    | 2.01                     | 0.43              |
| 1:C:313:MET:HA   | 2:D:104:ASN:OD1  | 2.19                     | 0.42              |
| 2:D:71:ASN:CB    | 2:D:74:GLU:HG3   | 2.45                     | 0.42              |
| 1:G:69:LEU:HD12  | 1:G:69:LEU:H     | 1.84                     | 0.42              |
| 1:K:171:GLU:OE2  | 1:K:232:LEU:HD22 | 2.19                     | 0.42              |
| 1:E:38:ASN:HB3   | 1:E:284:ALA:H    | 1.84                     | 0.42              |
| 1:I:317:LEU:HD12 | 1:I:318:ARG:O    | 2.19                     | 0.42              |
| 1:A:15:THR:HG23  | 1:A:23:ASN:HA    | 2.01                     | 0.42              |
| 1:E:201:VAL:HG13 | 1:E:206:SER:HB2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:58:ALA:O     | 1:I:62:LEU:HB2   | 2.19                     | 0.42              |
| 1:K:320:ILE:HB   | 2:L:13:GLY:H     | 1.83                     | 0.42              |
| 2:L:141:TYR:OH   | 2:L:161:LYS:HG3  | 2.20                     | 0.42              |
| 2:L:47:GLY:CA    | 1:G:20:LEU:HB2   | 2.49                     | 0.42              |
| 2:F:120:GLU:C    | 2:F:122:VAL:H    | 2.22                     | 0.42              |
| 2:F:20:GLY:CA    | 2:F:41:THR:HG21  | 2.48                     | 0.42              |
| 1:G:119:LYS:HD2  | 1:G:251:ARG:CZ   | 2.49                     | 0.42              |
| 2:H:60:ASN:OD1   | 2:H:60:ASN:N     | 2.51                     | 0.42              |
| 1:I:33:LEU:HD12  | 1:I:311:LEU:HD12 | 2.02                     | 0.42              |
| 1:K:16:VAL:HG22  | 1:K:312:ARG:CB   | 2.50                     | 0.42              |
| 2:B:120:GLU:C    | 2:B:122:VAL:H    | 2.22                     | 0.42              |
| 1:C:292:GLN:HB3  | 1:C:303:PRO:HG2  | 2.02                     | 0.42              |
| 2:D:51:LYS:HB3   | 2:D:51:LYS:HE3   | 1.89                     | 0.42              |
| 1:E:264:ILE:HG21 | 1:E:264:ILE:HD13 | 1.81                     | 0.42              |
| 1:G:285:ILE:HD11 | 1:G:294:VAL:CG2  | 2.50                     | 0.42              |
| 2:J:23:GLY:HA2   | 2:J:37:ASP:H     | 1.84                     | 0.42              |
| 1:A:114:PHE:CE2  | 1:A:168:LYS:HE3  | 2.55                     | 0.42              |
| 1:A:38:ASN:HB3   | 1:A:284:ALA:H    | 1.84                     | 0.42              |
| 1:A:86:GLU:HB3   | 4:P:1:NAG:H62    | 2.02                     | 0.42              |
| 2:B:119:TYR:CD1  | 2:B:136:GLY:HA2  | 2.54                     | 0.42              |
| 1:A:203:SER:HA   | 1:I:225:ARG:NH2  | 2.34                     | 0.42              |
| 2:D:77:MET:HB3   | 2:D:77:MET:HE3   | 1.86                     | 0.42              |
| 1:E:176:TRP:HB3  | 1:E:250:PRO:HG3  | 2.01                     | 0.42              |
| 1:E:92:PRO:HB3   | 1:E:219:VAL:HG13 | 2.02                     | 0.42              |
| 1:E:62:LEU:HD13  | 1:E:95:PHE:HE2   | 1.84                     | 0.42              |
| 1:G:92:PRO:HB2   | 1:G:225:ARG:HD3  | 2.01                     | 0.42              |
| 1:K:19:VAL:HA    | 2:L:101:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:60:TRP:CZ3   | 1:A:105:LEU:HD13 | 2.54                     | 0.42              |
| 9:E:533:HOH:O    | 2:F:69:GLU:HG3   | 2.19                     | 0.42              |
| 1:G:18:THR:OG1   | 1:G:19:VAL:N     | 2.53                     | 0.42              |
| 1:G:241:PHE:CZ   | 1:G:250:PRO:HG2  | 2.54                     | 0.42              |
| 2:H:154:ASN:CG   | 2:H:155:GLY:H    | 2.18                     | 0.42              |
| 1:C:62:LEU:HB3   | 1:C:144:TYR:CD2  | 2.55                     | 0.42              |
| 2:D:26:HIS:HB2   | 2:D:149:MET:SD   | 2.60                     | 0.42              |
| 2:F:120:GLU:OE1  | 2:F:121:LYS:N    | 2.53                     | 0.42              |
| 1:G:10:ASN:O     | 1:G:319:ASN:ND2  | 2.50                     | 0.42              |
| 1:G:15:THR:CG2   | 1:G:23:ASN:HA    | 2.50                     | 0.42              |
| 2:J:154:ASN:OD1  | 2:J:155:GLY:N    | 2.43                     | 0.42              |
| 1:A:18:THR:OG1   | 1:A:19:VAL:N     | 2.53                     | 0.42              |
| 1:C:261:GLY:HA2  | 2:D:64:THR:HG21  | 2.02                     | 0.42              |
| 2:J:145:ASN:N    | 2:J:145:ASN:OD1  | 2.43                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:19:VAL:O     | 2:D:51:LYS:HG2   | 2.19                     | 0.41              |
| 1:E:285:ILE:HD11 | 1:E:294:VAL:CG2  | 2.50                     | 0.41              |
| 2:F:154:ASN:CG   | 2:F:155:GLY:H    | 2.20                     | 0.41              |
| 2:H:159:TYR:N    | 2:H:160:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:63:GLY:O     | 1:A:144:TYR:HA   | 2.19                     | 0.41              |
| 1:A:82:LYS:HG3   | 9:A:561:HOH:O    | 2.19                     | 0.41              |
| 2:D:70:PHE:CD1   | 2:D:70:PHE:N     | 2.87                     | 0.41              |
| 1:E:118:PRO:O    | 1:E:122:SER:HB2  | 2.20                     | 0.41              |
| 1:E:217:PRO:HG2  | 1:G:203:SER:HA   | 2.02                     | 0.41              |
| 1:I:209:PHE:HE2  | 1:I:229:TYR:CE1  | 2.38                     | 0.41              |
| 1:K:178:VAL:O    | 1:K:226:ILE:HA   | 2.20                     | 0.41              |
| 1:K:209:PHE:CD1  | 1:K:209:PHE:N    | 2.88                     | 0.41              |
| 1:C:41:LEU:HD23  | 1:C:41:LEU:HA    | 1.83                     | 0.41              |
| 1:K:5:ILE:HG13   | 2:L:24:TYR:CD2   | 2.55                     | 0.41              |
| 1:A:207:ARG:HG2  | 1:A:209:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:87:ASN:HD22  | 1:A:87:ASN:HA    | 1.67                     | 0.41              |
| 1:C:217:PRO:HG2  | 1:I:203:SER:HA   | 2.02                     | 0.41              |
| 1:E:198:VAL:HG22 | 1:E:243:ALA:HB1  | 2.03                     | 0.41              |
| 1:G:90:CYS:CB    | 3:V:1:NAG:H81    | 2.47                     | 0.41              |
| 1:C:103:GLU:HG2  | 9:D:202:HOH:O    | 2.20                     | 0.41              |
| 1:C:127:THR:HG23 | 1:C:153:LYS:HB2  | 2.03                     | 0.41              |
| 1:C:26:VAL:HG21  | 1:C:314:VAL:HG11 | 2.03                     | 0.41              |
| 1:C:51:GLN:HE21  | 1:C:53:GLY:H     | 1.69                     | 0.41              |
| 1:E:196:ALA:HB1  | 1:E:246:ASN:OD1  | 2.21                     | 0.41              |
| 1:E:117:PHE:HB2  | 1:E:250:PRO:O    | 2.20                     | 0.41              |
| 1:K:30:VAL:O     | 1:K:312:ARG:O    | 2.38                     | 0.41              |
| 1:K:31:ASN:O     | 1:K:33:LEU:N     | 2.54                     | 0.41              |
| 1:K:87:ASN:HD22  | 4:N:1:NAG:C8     | 2.15                     | 0.41              |
| 2:B:142:HIS:HE2  | 2:B:158:ASP:CG   | 2.24                     | 0.41              |
| 2:B:80:LEU:O     | 2:B:84:VAL:HG23  | 2.20                     | 0.41              |
| 2:F:62:GLN:O     | 2:F:63:PHE:CD2   | 2.74                     | 0.41              |
| 1:G:266:ASN:O    | 1:G:281:PRO:HB3  | 2.20                     | 0.41              |
| 1:A:287:SER:OG   | 1:A:288:SER:N    | 2.53                     | 0.41              |
| 1:A:33:LEU:HD12  | 1:A:311:LEU:HD12 | 2.02                     | 0.41              |
| 7:A:402:NAG:H83  | 7:A:402:NAG:H3   | 2.02                     | 0.41              |
| 2:B:70:PHE:CD1   | 2:B:70:PHE:N     | 2.88                     | 0.41              |
| 1:C:96:ALA:HB2   | 1:C:229:TYR:HD1  | 1.81                     | 0.41              |
| 1:E:75:SER:O     | 1:E:76:TRP:HB3   | 2.20                     | 0.41              |
| 1:G:105:LEU:HA   | 1:G:105:LEU:HD23 | 1.78                     | 0.41              |
| 1:A:176:TRP:CZ3  | 1:A:230:TRP:HA   | 2.55                     | 0.41              |
| 1:A:38:ASN:HD22  | 1:A:284:ALA:H    | 1.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:70:LEU:HA    | 1:A:70:LEU:HD23  | 1.88                     | 0.41              |
| 1:C:58:ALA:O     | 1:C:62:LEU:HB2   | 2.21                     | 0.41              |
| 1:E:155:GLY:HA2  | 1:E:192:HIS:CE1  | 2.56                     | 0.41              |
| 1:E:5:ILE:O      | 2:F:10:ILE:HD13  | 2.21                     | 0.41              |
| 1:G:126:HIS:HE1  | 1:G:157:TYR:CD1  | 2.39                     | 0.41              |
| 2:L:99:LEU:HD13  | 2:H:98:LEU:HD21  | 2.02                     | 0.41              |
| 1:I:49:PRO:HB3   | 1:I:78:TYR:CE2   | 2.56                     | 0.41              |
| 1:A:62:LEU:HD13  | 1:A:95:PHE:HE2   | 1.86                     | 0.41              |
| 1:E:50:LEU:HD11  | 1:E:60:TRP:CZ2   | 2.56                     | 0.41              |
| 1:G:9:ALA:HA     | 1:G:319:ASN:OD1  | 2.21                     | 0.41              |
| 2:H:9:PHE:CD1    | 2:H:10:ILE:HG13  | 2.55                     | 0.41              |
| 1:K:122:SER:HA   | 1:K:162:LYS:NZ   | 2.35                     | 0.41              |
| 2:L:157:TYR:C    | 2:L:159:TYR:N    | 2.74                     | 0.41              |
| 1:A:115:GLU:HA   | 1:A:252:TYR:HA   | 2.03                     | 0.41              |
| 1:A:285:ILE:HD11 | 1:A:294:VAL:CG2  | 2.51                     | 0.41              |
| 1:A:292:GLN:HG2  | 1:A:303:PRO:HG2  | 2.02                     | 0.41              |
| 1:A:39:GLY:H     | 1:A:283:GLY:HA3  | 1.86                     | 0.41              |
| 1:C:200:VAL:HG22 | 1:C:241:PHE:CD1  | 2.56                     | 0.41              |
| 2:D:87:GLY:O     | 2:D:91:VAL:HG23  | 2.20                     | 0.41              |
| 1:E:41:LEU:HA    | 1:E:41:LEU:HD23  | 1.87                     | 0.41              |
| 2:L:101:LEU:HD13 | 2:F:58:LYS:HE2   | 2.02                     | 0.41              |
| 1:G:310:LYS:HB3  | 1:G:312:ARG:CD   | 2.29                     | 0.41              |
| 9:D:209:HOH:O    | 2:J:65:ALA:HB1   | 2.20                     | 0.41              |
| 1:A:292:GLN:HB3  | 1:A:303:PRO:HG2  | 2.03                     | 0.41              |
| 2:B:23:GLY:HA2   | 2:B:37:ASP:H     | 1.86                     | 0.41              |
| 2:F:148:CYS:O    | 2:F:151:SER:HB3  | 2.21                     | 0.41              |
| 1:G:62:LEU:O     | 1:G:144:TYR:HB3  | 2.21                     | 0.41              |
| 1:I:57:VAL:HG21  | 1:I:264:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:10:ASN:ND2   | 1:A:28:HIS:CE1   | 2.89                     | 0.40              |
| 1:A:38:ASN:ND2   | 1:A:42:CYS:SG    | 2.94                     | 0.40              |
| 1:C:173:LEU:CB   | 1:C:256:LEU:HD21 | 2.50                     | 0.40              |
| 2:D:110:PHE:HB2  | 9:D:205:HOH:O    | 2.20                     | 0.40              |
| 1:E:181:PRO:HG2  | 1:E:187:GLN:HB2  | 2.02                     | 0.40              |
| 1:E:41:LEU:HD13  | 1:E:80:VAL:HG21  | 2.03                     | 0.40              |
| 2:F:59:MET:HB3   | 2:F:59:MET:HE2   | 1.93                     | 0.40              |
| 1:G:233:LEU:HD13 | 1:G:239:ILE:HB   | 2.03                     | 0.40              |
| 1:K:285:ILE:HD11 | 1:K:294:VAL:HG22 | 2.02                     | 0.40              |
| 1:K:317:LEU:HD12 | 1:K:318:ARG:O    | 2.20                     | 0.40              |
| 1:K:62:LEU:HD12  | 1:K:175:LEU:HD22 | 2.03                     | 0.40              |
| 1:A:57:VAL:HG23  | 1:A:81:GLU:OE2   | 2.21                     | 0.40              |
| 2:B:23:GLY:CA    | 2:B:37:ASP:H     | 2.35                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:D:154:ASN:OD1 | 2:D:155:GLY:N   | 2.46                     | 0.40              |
| 1:G:99:GLU:O    | 1:G:102:ARG:HB2 | 2.22                     | 0.40              |
| 1:I:160:LEU:O   | 1:I:242:GLU:HA  | 2.21                     | 0.40              |
| 2:B:106:ARG:NH1 | 2:J:106:ARG:HG2 | 2.36                     | 0.40              |
| 1:K:218:LYS:HA  | 1:K:222:GLN:O   | 2.21                     | 0.40              |
| 2:L:10:ILE:HG12 | 2:L:136:GLY:HA3 | 2.03                     | 0.40              |
| 1:A:43:LEU:HD23 | 1:A:46:GLY:O    | 2.21                     | 0.40              |
| 1:C:216:ARG:HB3 | 1:C:217:PRO:HD2 | 2.04                     | 0.40              |
| 2:F:141:TYR:CG  | 2:F:164:GLU:HG3 | 2.57                     | 0.40              |
| 1:I:90:CYS:HB3  | 5:X:1:NAG:H81   | 2.02                     | 0.40              |
| 7:C:409:NAG:H83 | 9:C:544:HOH:O   | 2.22                     | 0.40              |
| 2:D:79:ASN:ND2  | 1:I:103:GLU:OE1 | 2.55                     | 0.40              |
| 1:K:51:GLN:HG2  | 9:K:536:HOH:O   | 2.21                     | 0.40              |
| 1:K:5:ILE:HG13  | 2:L:24:TYR:HD2  | 1.86                     | 0.40              |
| 1:K:4:CYS:O     | 2:L:24:TYR:HA   | 2.21                     | 0.40              |
| 1:A:175:LEU:O   | 1:A:250:PRO:HB3 | 2.21                     | 0.40              |
| 1:E:277:LYS:HD3 | 1:E:287:SER:HB3 | 2.03                     | 0.40              |
| 2:F:125:GLN:NE2 | 2:F:155:GLY:HA3 | 2.33                     | 0.40              |
| 1:E:299:ILE:CA  | 2:F:64:THR:HG22 | 2.47                     | 0.40              |
| 1:I:112:GLU:CB  | 1:I:255:ALA:HB3 | 2.44                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:E:68:GLU:OE2 | 1:I:68:GLU:OE2[3_555] | 2.09                     | 0.11              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 319/330 (97%) | 291 (91%) | 24 (8%) | 4 (1%)   | 12 44       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | C     | 319/330 (97%)   | 290 (91%)  | 28 (9%)  | 1 (0%)   | 41          | 73  |
| 1   | E     | 319/330 (97%)   | 291 (91%)  | 27 (8%)  | 1 (0%)   | 41          | 73  |
| 1   | G     | 318/330 (96%)   | 289 (91%)  | 27 (8%)  | 2 (1%)   | 25          | 61  |
| 1   | I     | 318/330 (96%)   | 288 (91%)  | 27 (8%)  | 3 (1%)   | 17          | 52  |
| 1   | K     | 319/330 (97%)   | 290 (91%)  | 25 (8%)  | 4 (1%)   | 12          | 44  |
| 2   | B     | 163/183 (89%)   | 143 (88%)  | 18 (11%) | 2 (1%)   | 13          | 46  |
| 2   | D     | 163/183 (89%)   | 146 (90%)  | 17 (10%) | 0        | 100         | 100 |
| 2   | F     | 163/183 (89%)   | 145 (89%)  | 16 (10%) | 2 (1%)   | 13          | 46  |
| 2   | H     | 163/183 (89%)   | 149 (91%)  | 14 (9%)  | 0        | 100         | 100 |
| 2   | J     | 163/183 (89%)   | 146 (90%)  | 17 (10%) | 0        | 100         | 100 |
| 2   | L     | 163/183 (89%)   | 147 (90%)  | 16 (10%) | 0        | 100         | 100 |
| All | All   | 2890/3078 (94%) | 2615 (90%) | 256 (9%) | 19 (1%)  | 22          | 58  |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 32  | LEU  |
| 1   | A     | 32  | LEU  |
| 2   | B     | 62  | GLN  |
| 2   | B     | 63  | PHE  |
| 2   | F     | 62  | GLN  |
| 2   | F     | 63  | PHE  |
| 1   | K     | 261 | GLY  |
| 1   | E     | 196 | ALA  |
| 1   | I     | 261 | GLY  |
| 1   | A     | 261 | GLY  |
| 1   | K     | 90  | CYS  |
| 1   | A     | 196 | ALA  |
| 1   | G     | 196 | ALA  |
| 1   | G     | 261 | GLY  |
| 1   | I     | 276 | ALA  |
| 1   | K     | 196 | ALA  |
| 1   | A     | 276 | ALA  |
| 1   | C     | 90  | CYS  |
| 1   | I     | 32  | LEU  |



### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 281/288 (98%)   | 272 (97%)  | 9 (3%)   | 39          | 69 |
| 1   | C     | 281/288 (98%)   | 271 (96%)  | 10 (4%)  | 35          | 66 |
| 1   | E     | 281/288 (98%)   | 278 (99%)  | 3 (1%)   | 73          | 87 |
| 1   | G     | 280/288 (97%)   | 277 (99%)  | 3 (1%)   | 73          | 87 |
| 1   | I     | 280/288 (97%)   | 270 (96%)  | 10 (4%)  | 35          | 66 |
| 1   | K     | 281/288 (98%)   | 273 (97%)  | 8 (3%)   | 43          | 72 |
| 2   | B     | 141/157 (90%)   | 135 (96%)  | 6 (4%)   | 29          | 62 |
| 2   | D     | 141/157 (90%)   | 136 (96%)  | 5 (4%)   | 36          | 67 |
| 2   | F     | 141/157 (90%)   | 138 (98%)  | 3 (2%)   | 53          | 77 |
| 2   | H     | 141/157 (90%)   | 136 (96%)  | 5 (4%)   | 36          | 67 |
| 2   | J     | 141/157 (90%)   | 140 (99%)  | 1 (1%)   | 84          | 92 |
| 2   | L     | 141/157 (90%)   | 138 (98%)  | 3 (2%)   | 53          | 77 |
| All | All   | 2530/2670 (95%) | 2464 (97%) | 66 (3%)  | 46          | 74 |

All (66) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 31  | ASN  |
| 1   | K     | 51  | GLN  |
| 1   | K     | 111 | PHE  |
| 1   | K     | 199 | SER  |
| 1   | K     | 232 | LEU  |
| 1   | K     | 272 | ASP  |
| 1   | K     | 302 | CYS  |
| 1   | K     | 312 | ARG  |
| 2   | L     | 24  | TYR  |
| 2   | L     | 38  | GLN  |
| 2   | L     | 95  | ASN  |
| 1   | A     | 31  | ASN  |
| 1   | A     | 34  | GLU  |
| 1   | A     | 110 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 232 | LEU  |
| 1   | A     | 271 | MET  |
| 1   | A     | 272 | ASP  |
| 1   | A     | 274 | CYS  |
| 1   | A     | 302 | CYS  |
| 1   | A     | 312 | ARG  |
| 2   | B     | 22  | TYR  |
| 2   | B     | 26  | HIS  |
| 2   | B     | 71  | ASN  |
| 2   | B     | 95  | ASN  |
| 2   | B     | 159 | TYR  |
| 2   | B     | 163 | SER  |
| 1   | C     | 31  | ASN  |
| 1   | C     | 85  | PRO  |
| 1   | C     | 110 | SER  |
| 1   | C     | 135 | CYS  |
| 1   | C     | 145 | LYS  |
| 1   | C     | 195 | ASN  |
| 1   | C     | 199 | SER  |
| 1   | C     | 272 | ASP  |
| 1   | C     | 302 | CYS  |
| 1   | C     | 317 | LEU  |
| 2   | D     | 77  | MET  |
| 2   | D     | 117 | ASN  |
| 2   | D     | 123 | LYS  |
| 2   | D     | 143 | LYS  |
| 2   | D     | 163 | SER  |
| 1   | E     | 20  | LEU  |
| 1   | E     | 199 | SER  |
| 1   | E     | 232 | LEU  |
| 2   | F     | 24  | TYR  |
| 2   | F     | 81  | ASN  |
| 2   | F     | 117 | ASN  |
| 1   | G     | 31  | ASN  |
| 1   | G     | 244 | ASN  |
| 1   | G     | 302 | CYS  |
| 2   | H     | 24  | TYR  |
| 2   | H     | 51  | LYS  |
| 2   | H     | 95  | ASN  |
| 2   | H     | 117 | ASN  |
| 2   | H     | 151 | SER  |
| 1   | I     | 31  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 34  | GLU  |
| 1   | I     | 91  | TYR  |
| 1   | I     | 107 | SER  |
| 1   | I     | 110 | SER  |
| 1   | I     | 244 | ASN  |
| 1   | I     | 257 | SER  |
| 1   | I     | 271 | MET  |
| 1   | I     | 272 | ASP  |
| 1   | I     | 302 | CYS  |
| 2   | J     | 125 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 64  | ASN  |
| 2   | L     | 28  | ASN  |
| 2   | L     | 53  | ASN  |
| 2   | L     | 60  | ASN  |
| 2   | L     | 95  | ASN  |
| 2   | L     | 129 | ASN  |
| 1   | A     | 28  | HIS  |
| 1   | A     | 38  | ASN  |
| 1   | A     | 279 | GLN  |
| 2   | B     | 28  | ASN  |
| 2   | B     | 53  | ASN  |
| 2   | B     | 95  | ASN  |
| 1   | C     | 28  | HIS  |
| 1   | C     | 31  | ASN  |
| 1   | C     | 51  | GLN  |
| 2   | D     | 25  | HIS  |
| 1   | E     | 28  | HIS  |
| 2   | F     | 26  | HIS  |
| 2   | F     | 117 | ASN  |
| 1   | G     | 31  | ASN  |
| 1   | G     | 51  | GLN  |
| 1   | G     | 64  | ASN  |
| 1   | G     | 126 | HIS  |
| 2   | H     | 26  | HIS  |
| 2   | H     | 95  | ASN  |
| 2   | H     | 129 | ASN  |
| 2   | H     | 142 | HIS  |
| 1   | I     | 31  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 53  | ASN  |
| 2   | J     | 125 | GLN  |
| 2   | J     | 128 | ASN  |
| 2   | J     | 142 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

55 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$ |
| 3   | NAG  | M     | 1   | 1,3  | 14,14,15     | 0.40 | 0           | 17,19,21    | 2.46 | 3 (17%)     |
| 3   | NAG  | M     | 2   | 3    | 14,14,15     | 1.25 | 1 (7%)      | 17,19,21    | 1.58 | 2 (11%)     |
| 3   | BMA  | M     | 3   | 3    | 11,11,12     | 2.19 | 4 (36%)     | 15,15,17    | 1.78 | 3 (20%)     |
| 3   | MAN  | M     | 4   | 3    | 11,11,12     | 2.60 | 3 (27%)     | 15,15,17    | 1.82 | 3 (20%)     |
| 3   | NAG  | M     | 5   | 3    | 14,14,15     | 0.87 | 2 (14%)     | 17,19,21    | 0.69 | 0           |
| 3   | MAN  | M     | 6   | 3    | 11,11,12     | 1.85 | 3 (27%)     | 15,15,17    | 1.66 | 3 (20%)     |
| 4   | NAG  | N     | 1   | 1,4  | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.92 | 1 (5%)      |
| 4   | NAG  | N     | 2   | 4    | 14,14,15     | 0.82 | 1 (7%)      | 17,19,21    | 1.58 | 1 (5%)      |
| 4   | BMA  | N     | 3   | 4    | 11,11,12     | 1.75 | 3 (27%)     | 15,15,17    | 1.40 | 1 (6%)      |
| 4   | MAN  | N     | 4   | 4    | 11,11,12     | 2.19 | 4 (36%)     | 15,15,17    | 2.50 | 5 (33%)     |
| 4   | NAG  | N     | 5   | 4    | 14,14,15     | 0.76 | 0           | 17,19,21    | 0.89 | 1 (5%)      |
| 5   | NAG  | O     | 1   | 1,5  | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.94 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | NAG  | O     | 2   | 5    | 14,14,15     | 0.86 | 1 (7%)   | 17,19,21    | 1.68 | 3 (17%)  |
| 5   | BMA  | O     | 3   | 5    | 11,11,12     | 2.17 | 3 (27%)  | 15,15,17    | 2.18 | 3 (20%)  |
| 5   | MAN  | O     | 4   | 5    | 11,11,12     | 2.00 | 4 (36%)  | 15,15,17    | 1.93 | 5 (33%)  |
| 4   | NAG  | P     | 1   | 1,4  | 14,14,15     | 0.97 | 1 (7%)   | 17,19,21    | 0.87 | 1 (5%)   |
| 4   | NAG  | P     | 2   | 4    | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.93 | 1 (5%)   |
| 4   | BMA  | P     | 3   | 4    | 11,11,12     | 2.66 | 3 (27%)  | 15,15,17    | 1.87 | 2 (13%)  |
| 4   | MAN  | P     | 4   | 4    | 11,11,12     | 4.00 | 7 (63%)  | 15,15,17    | 2.74 | 8 (53%)  |
| 4   | NAG  | P     | 5   | 4    | 14,14,15     | 1.00 | 1 (7%)   | 17,19,21    | 1.40 | 3 (17%)  |
| 5   | NAG  | Q     | 1   | 1,5  | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.80 | 0        |
| 5   | NAG  | Q     | 2   | 5    | 14,14,15     | 0.36 | 0        | 17,19,21    | 1.23 | 0        |
| 5   | BMA  | Q     | 3   | 5    | 11,11,12     | 2.40 | 4 (36%)  | 15,15,17    | 2.23 | 5 (33%)  |
| 5   | MAN  | Q     | 4   | 5    | 11,11,12     | 1.86 | 3 (27%)  | 15,15,17    | 1.34 | 3 (20%)  |
| 5   | NAG  | R     | 1   | 1,5  | 14,14,15     | 0.93 | 1 (7%)   | 17,19,21    | 0.92 | 1 (5%)   |
| 5   | NAG  | R     | 2   | 5    | 14,14,15     | 0.90 | 2 (14%)  | 17,19,21    | 1.10 | 1 (5%)   |
| 5   | BMA  | R     | 3   | 5    | 11,11,12     | 1.93 | 2 (18%)  | 15,15,17    | 2.19 | 6 (40%)  |
| 5   | MAN  | R     | 4   | 5    | 11,11,12     | 2.29 | 4 (36%)  | 15,15,17    | 1.50 | 3 (20%)  |
| 3   | NAG  | S     | 1   | 1,3  | 14,14,15     | 0.51 | 0        | 17,19,21    | 2.38 | 2 (11%)  |
| 3   | NAG  | S     | 2   | 3    | 14,14,15     | 0.91 | 1 (7%)   | 17,19,21    | 1.44 | 3 (17%)  |
| 3   | BMA  | S     | 3   | 3    | 11,11,12     | 3.49 | 7 (63%)  | 15,15,17    | 1.92 | 5 (33%)  |
| 3   | MAN  | S     | 4   | 3    | 11,11,12     | 3.00 | 6 (54%)  | 15,15,17    | 2.97 | 5 (33%)  |
| 3   | NAG  | S     | 5   | 3    | 14,14,15     | 2.78 | 2 (14%)  | 17,19,21    | 3.07 | 3 (17%)  |
| 3   | MAN  | S     | 6   | 3    | 11,11,12     | 2.84 | 7 (63%)  | 15,15,17    | 1.84 | 3 (20%)  |
| 5   | NAG  | T     | 1   | 1,5  | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 5   | NAG  | T     | 2   | 5    | 14,14,15     | 0.69 | 1 (7%)   | 17,19,21    | 1.64 | 2 (11%)  |
| 5   | BMA  | T     | 3   | 5    | 11,11,12     | 2.35 | 4 (36%)  | 15,15,17    | 2.59 | 6 (40%)  |
| 5   | MAN  | T     | 4   | 5    | 11,11,12     | 2.31 | 3 (27%)  | 15,15,17    | 1.52 | 4 (26%)  |
| 5   | NAG  | U     | 1   | 1,5  | 14,14,15     | 1.10 | 2 (14%)  | 17,19,21    | 1.53 | 2 (11%)  |
| 5   | NAG  | U     | 2   | 5    | 14,14,15     | 0.72 | 0        | 17,19,21    | 1.28 | 2 (11%)  |
| 5   | BMA  | U     | 3   | 5    | 11,11,12     | 2.26 | 5 (45%)  | 15,15,17    | 1.97 | 4 (26%)  |
| 5   | MAN  | U     | 4   | 5    | 11,11,12     | 2.33 | 5 (45%)  | 15,15,17    | 2.37 | 4 (26%)  |
| 3   | NAG  | V     | 1   | 1,3  | 14,14,15     | 0.35 | 0        | 17,19,21    | 1.13 | 2 (11%)  |
| 3   | NAG  | V     | 2   | 3    | 14,14,15     | 0.49 | 0        | 17,19,21    | 1.02 | 2 (11%)  |
| 3   | BMA  | V     | 3   | 3    | 11,11,12     | 1.73 | 1 (9%)   | 15,15,17    | 1.52 | 2 (13%)  |
| 3   | MAN  | V     | 4   | 3    | 11,11,12     | 3.40 | 5 (45%)  | 15,15,17    | 2.58 | 7 (46%)  |
| 3   | NAG  | V     | 5   | 3    | 14,14,15     | 1.90 | 2 (14%)  | 17,19,21    | 1.51 | 1 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | MAN  | V     | 6   | 3    | 11,11,12     | 1.93 | 3 (27%)  | 15,15,17    | 1.26 | 2 (13%)  |
| 6   | NAG  | W     | 1   | 1,6  | 14,14,15     | 0.71 | 1 (7%)   | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | W     | 2   | 6    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.69 | 0        |
| 6   | BMA  | W     | 3   | 6    | 11,11,12     | 2.08 | 3 (27%)  | 15,15,17    | 2.03 | 5 (33%)  |
| 5   | NAG  | X     | 1   | 1,5  | 14,14,15     | 1.15 | 1 (7%)   | 17,19,21    | 1.05 | 2 (11%)  |
| 5   | NAG  | X     | 2   | 5    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.85 | 0        |
| 5   | BMA  | X     | 3   | 5    | 11,11,12     | 2.23 | 3 (27%)  | 15,15,17    | 1.74 | 3 (20%)  |
| 5   | MAN  | X     | 4   | 5    | 11,11,12     | 1.56 | 2 (18%)  | 15,15,17    | 1.45 | 2 (13%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | M     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | M     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | M     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | M     | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | M     | 5   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | MAN  | M     | 6   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | NAG  | N     | 1   | 1,4  | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | N     | 2   | 4    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | BMA  | N     | 3   | 4    | -       | 1/2/19/22 | 1/1/1/1 |
| 4   | MAN  | N     | 4   | 4    | -       | 2/2/19/22 | 0/1/1/1 |
| 4   | NAG  | N     | 5   | 4    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | O     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | O     | 2   | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | BMA  | O     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | O     | 4   | 5    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | NAG  | P     | 1   | 1,4  | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | P     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | BMA  | P     | 3   | 4    | -       | 2/2/19/22 | 0/1/1/1 |
| 4   | MAN  | P     | 4   | 4    | -       | 2/2/19/22 | 0/1/1/1 |
| 4   | NAG  | P     | 5   | 4    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | Q     | 1   | 1,5  | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | Q     | 2   | 5    | -       | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | BMA  | Q     | 3   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 5   | MAN  | Q     | 4   | 5    | -       | 2/2/19/22 | 1/1/1/1 |
| 5   | NAG  | R     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | R     | 2   | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | BMA  | R     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | R     | 4   | 5    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | S     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | S     | 2   | 3    | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | BMA  | S     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | S     | 4   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | S     | 5   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | MAN  | S     | 6   | 3    | -       | 2/2/19/22 | 1/1/1/1 |
| 5   | NAG  | T     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | T     | 2   | 5    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | BMA  | T     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | T     | 4   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 5   | NAG  | U     | 1   | 1,5  | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | U     | 2   | 5    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | BMA  | U     | 3   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 5   | MAN  | U     | 4   | 5    | -       | 1/2/19/22 | 1/1/1/1 |
| 3   | NAG  | V     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | V     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | BMA  | V     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | V     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | V     | 5   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | MAN  | V     | 6   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | W     | 1   | 1,6  | -       | 4/6/23/26 | 0/1/1/1 |
| 6   | NAG  | W     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | W     | 3   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | NAG  | X     | 1   | 1,5  | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | NAG  | X     | 2   | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | BMA  | X     | 3   | 5    | -       | 1/2/19/22 | 1/1/1/1 |
| 5   | MAN  | X     | 4   | 5    | -       | 1/2/19/22 | 1/1/1/1 |

All (121) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | S     | 5   | NAG  | O5-C1 | 9.78 | 1.59        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | P     | 4   | MAN  | C2-C3 | 8.04  | 1.64        | 1.52     |
| 4   | P     | 4   | MAN  | O2-C2 | 6.77  | 1.57        | 1.43     |
| 3   | S     | 3   | BMA  | C4-C5 | 6.67  | 1.67        | 1.53     |
| 3   | V     | 4   | MAN  | O2-C2 | 6.34  | 1.56        | 1.43     |
| 4   | P     | 3   | BMA  | C2-C3 | -6.02 | 1.43        | 1.52     |
| 3   | M     | 4   | MAN  | C1-C2 | 6.00  | 1.65        | 1.52     |
| 5   | T     | 4   | MAN  | C2-C3 | 5.99  | 1.61        | 1.52     |
| 3   | V     | 4   | MAN  | O5-C5 | 5.80  | 1.55        | 1.43     |
| 3   | V     | 5   | NAG  | O5-C1 | 5.73  | 1.52        | 1.43     |
| 3   | S     | 4   | MAN  | O5-C5 | 5.72  | 1.55        | 1.43     |
| 5   | X     | 3   | BMA  | C2-C3 | 5.48  | 1.60        | 1.52     |
| 3   | S     | 6   | MAN  | C1-C2 | 5.14  | 1.63        | 1.52     |
| 3   | V     | 4   | MAN  | O5-C1 | 5.05  | 1.51        | 1.43     |
| 3   | M     | 4   | MAN  | C2-C3 | 5.00  | 1.59        | 1.52     |
| 4   | P     | 4   | MAN  | C4-C3 | 4.93  | 1.64        | 1.52     |
| 3   | S     | 4   | MAN  | C1-C2 | 4.91  | 1.63        | 1.52     |
| 5   | Q     | 3   | BMA  | O5-C1 | 4.80  | 1.51        | 1.43     |
| 5   | U     | 3   | BMA  | C4-C5 | 4.76  | 1.63        | 1.53     |
| 5   | U     | 4   | MAN  | O5-C5 | 4.72  | 1.53        | 1.43     |
| 6   | W     | 3   | BMA  | C2-C3 | 4.69  | 1.59        | 1.52     |
| 3   | S     | 4   | MAN  | O5-C1 | 4.65  | 1.51        | 1.43     |
| 3   | S     | 3   | BMA  | O5-C5 | 4.63  | 1.52        | 1.43     |
| 5   | R     | 4   | MAN  | O5-C5 | 4.62  | 1.52        | 1.43     |
| 3   | S     | 3   | BMA  | O3-C3 | 4.57  | 1.53        | 1.43     |
| 3   | M     | 2   | NAG  | O5-C1 | 4.50  | 1.50        | 1.43     |
| 5   | O     | 3   | BMA  | C4-C3 | 4.48  | 1.63        | 1.52     |
| 5   | R     | 3   | BMA  | C4-C5 | 4.41  | 1.62        | 1.53     |
| 4   | P     | 3   | BMA  | C4-C5 | 4.33  | 1.62        | 1.53     |
| 3   | M     | 3   | BMA  | C4-C3 | 4.32  | 1.63        | 1.52     |
| 4   | N     | 4   | MAN  | O5-C5 | 4.30  | 1.52        | 1.43     |
| 5   | T     | 3   | BMA  | C4-C5 | 4.29  | 1.62        | 1.53     |
| 3   | V     | 5   | NAG  | C1-C2 | 4.18  | 1.58        | 1.52     |
| 5   | O     | 3   | BMA  | C4-C5 | 4.17  | 1.61        | 1.53     |
| 5   | T     | 3   | BMA  | C4-C3 | 4.10  | 1.62        | 1.52     |
| 5   | R     | 4   | MAN  | C4-C5 | 4.07  | 1.61        | 1.53     |
| 5   | Q     | 4   | MAN  | C1-C2 | 4.05  | 1.61        | 1.52     |
| 5   | T     | 3   | BMA  | C1-C2 | 4.04  | 1.61        | 1.52     |
| 5   | R     | 3   | BMA  | C4-C3 | 3.92  | 1.62        | 1.52     |
| 5   | X     | 1   | NAG  | O5-C1 | -3.90 | 1.37        | 1.43     |
| 3   | V     | 4   | MAN  | C4-C5 | 3.84  | 1.61        | 1.53     |
| 3   | S     | 6   | MAN  | O5-C5 | 3.81  | 1.51        | 1.43     |
| 5   | U     | 4   | MAN  | O5-C1 | 3.80  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | S     | 3   | BMA  | C4-C3 | 3.78  | 1.61        | 1.52     |
| 5   | O     | 4   | MAN  | C4-C5 | 3.75  | 1.60        | 1.53     |
| 5   | Q     | 3   | BMA  | C2-C3 | 3.72  | 1.58        | 1.52     |
| 3   | S     | 3   | BMA  | C2-C3 | -3.71 | 1.47        | 1.52     |
| 3   | V     | 6   | MAN  | C4-C3 | 3.62  | 1.61        | 1.52     |
| 4   | P     | 4   | MAN  | O5-C1 | 3.48  | 1.49        | 1.43     |
| 4   | P     | 1   | NAG  | O5-C1 | -3.46 | 1.38        | 1.43     |
| 3   | M     | 3   | BMA  | O3-C3 | 3.44  | 1.51        | 1.43     |
| 5   | Q     | 3   | BMA  | C1-C2 | 3.43  | 1.60        | 1.52     |
| 3   | M     | 6   | MAN  | O5-C5 | 3.42  | 1.50        | 1.43     |
| 3   | V     | 3   | BMA  | C4-C3 | 3.37  | 1.60        | 1.52     |
| 3   | S     | 5   | NAG  | C1-C2 | 3.33  | 1.57        | 1.52     |
| 5   | O     | 4   | MAN  | O5-C5 | 3.33  | 1.50        | 1.43     |
| 5   | T     | 4   | MAN  | C1-C2 | 3.31  | 1.59        | 1.52     |
| 4   | P     | 4   | MAN  | C1-C2 | 3.31  | 1.59        | 1.52     |
| 4   | N     | 4   | MAN  | O5-C1 | 3.30  | 1.49        | 1.43     |
| 5   | X     | 4   | MAN  | C1-C2 | 3.30  | 1.59        | 1.52     |
| 4   | P     | 5   | NAG  | O5-C1 | 3.30  | 1.49        | 1.43     |
| 6   | W     | 3   | BMA  | O5-C5 | 3.30  | 1.50        | 1.43     |
| 3   | S     | 6   | MAN  | O2-C2 | 3.29  | 1.50        | 1.43     |
| 5   | U     | 1   | NAG  | O5-C1 | -3.27 | 1.38        | 1.43     |
| 3   | S     | 6   | MAN  | C6-C5 | 3.26  | 1.62        | 1.51     |
| 4   | N     | 4   | MAN  | C1-C2 | 3.25  | 1.59        | 1.52     |
| 3   | S     | 3   | BMA  | O5-C1 | 3.21  | 1.48        | 1.43     |
| 3   | S     | 6   | MAN  | C2-C3 | 3.18  | 1.57        | 1.52     |
| 4   | P     | 3   | BMA  | C4-C3 | 3.18  | 1.60        | 1.52     |
| 3   | M     | 6   | MAN  | C1-C2 | 3.18  | 1.59        | 1.52     |
| 4   | N     | 3   | BMA  | O5-C1 | 3.11  | 1.48        | 1.43     |
| 5   | X     | 3   | BMA  | C1-C2 | 3.06  | 1.59        | 1.52     |
| 3   | S     | 2   | NAG  | O5-C1 | -3.01 | 1.38        | 1.43     |
| 5   | O     | 4   | MAN  | C1-C2 | 2.96  | 1.59        | 1.52     |
| 4   | P     | 4   | MAN  | O5-C5 | 2.93  | 1.49        | 1.43     |
| 5   | O     | 2   | NAG  | O5-C1 | -2.82 | 1.39        | 1.43     |
| 4   | N     | 3   | BMA  | O5-C5 | 2.81  | 1.49        | 1.43     |
| 5   | O     | 3   | BMA  | C1-C2 | 2.80  | 1.58        | 1.52     |
| 5   | U     | 3   | BMA  | O4-C4 | 2.79  | 1.49        | 1.43     |
| 5   | U     | 4   | MAN  | C6-C5 | 2.76  | 1.61        | 1.51     |
| 3   | V     | 6   | MAN  | O5-C5 | 2.74  | 1.49        | 1.43     |
| 3   | V     | 6   | MAN  | O5-C1 | 2.72  | 1.48        | 1.43     |
| 5   | U     | 3   | BMA  | O5-C5 | 2.71  | 1.48        | 1.43     |
| 4   | N     | 2   | NAG  | O5-C1 | 2.69  | 1.48        | 1.43     |
| 4   | N     | 4   | MAN  | O2-C2 | 2.66  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | T     | 4   | MAN  | C4-C3 | 2.65  | 1.59        | 1.52     |
| 3   | M     | 6   | MAN  | O5-C1 | 2.60  | 1.47        | 1.43     |
| 5   | R     | 4   | MAN  | C4-C3 | 2.58  | 1.58        | 1.52     |
| 5   | R     | 4   | MAN  | O5-C1 | 2.56  | 1.47        | 1.43     |
| 3   | S     | 4   | MAN  | C4-C5 | 2.51  | 1.58        | 1.53     |
| 5   | X     | 3   | BMA  | O3-C3 | 2.51  | 1.48        | 1.43     |
| 5   | U     | 3   | BMA  | C2-C3 | 2.48  | 1.56        | 1.52     |
| 5   | R     | 1   | NAG  | O5-C1 | -2.45 | 1.39        | 1.43     |
| 3   | M     | 3   | BMA  | O5-C5 | 2.41  | 1.48        | 1.43     |
| 5   | R     | 2   | NAG  | O5-C1 | -2.39 | 1.39        | 1.43     |
| 3   | M     | 3   | BMA  | O5-C1 | 2.39  | 1.47        | 1.43     |
| 5   | Q     | 4   | MAN  | C2-C3 | 2.37  | 1.56        | 1.52     |
| 3   | S     | 4   | MAN  | O2-C2 | 2.36  | 1.48        | 1.43     |
| 3   | M     | 4   | MAN  | O2-C2 | 2.33  | 1.48        | 1.43     |
| 6   | W     | 1   | NAG  | O5-C1 | 2.31  | 1.47        | 1.43     |
| 3   | S     | 3   | BMA  | O2-C2 | 2.27  | 1.48        | 1.43     |
| 6   | W     | 3   | BMA  | C6-C5 | 2.26  | 1.59        | 1.51     |
| 4   | N     | 3   | BMA  | C4-C3 | 2.26  | 1.58        | 1.52     |
| 5   | T     | 2   | NAG  | O5-C1 | -2.25 | 1.40        | 1.43     |
| 5   | U     | 4   | MAN  | C4-C3 | 2.24  | 1.58        | 1.52     |
| 3   | M     | 5   | NAG  | C1-C2 | 2.21  | 1.55        | 1.52     |
| 3   | S     | 6   | MAN  | C4-C3 | 2.20  | 1.57        | 1.52     |
| 5   | O     | 4   | MAN  | C2-C3 | 2.19  | 1.55        | 1.52     |
| 5   | X     | 4   | MAN  | O5-C5 | 2.17  | 1.47        | 1.43     |
| 3   | V     | 4   | MAN  | C2-C3 | 2.16  | 1.55        | 1.52     |
| 5   | Q     | 4   | MAN  | O3-C3 | 2.16  | 1.48        | 1.43     |
| 5   | U     | 1   | NAG  | C1-C2 | -2.12 | 1.49        | 1.52     |
| 5   | U     | 3   | BMA  | C1-C2 | 2.12  | 1.57        | 1.52     |
| 5   | U     | 4   | MAN  | O2-C2 | 2.07  | 1.47        | 1.43     |
| 5   | T     | 3   | BMA  | O5-C1 | 2.06  | 1.47        | 1.43     |
| 5   | Q     | 3   | BMA  | C6-C5 | 2.06  | 1.58        | 1.51     |
| 4   | P     | 4   | MAN  | C6-C5 | 2.02  | 1.58        | 1.51     |
| 5   | R     | 2   | NAG  | C1-C2 | -2.02 | 1.49        | 1.52     |
| 3   | M     | 5   | NAG  | O5-C1 | 2.01  | 1.46        | 1.43     |
| 3   | S     | 6   | MAN  | C4-C5 | 2.00  | 1.57        | 1.53     |
| 3   | S     | 4   | MAN  | C6-C5 | 2.00  | 1.58        | 1.51     |

All (142) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | S     | 5   | NAG  | C1-O5-C5 | 10.99 | 127.09      | 112.19   |
| 3   | M     | 1   | NAG  | C1-O5-C5 | 8.25  | 123.37      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | S     | 1   | NAG  | C1-O5-C5 | 8.19  | 123.29      | 112.19   |
| 3   | S     | 4   | MAN  | C1-O5-C5 | 8.10  | 123.16      | 112.19   |
| 3   | V     | 4   | MAN  | C1-O5-C5 | 6.35  | 120.79      | 112.19   |
| 4   | P     | 4   | MAN  | C1-O5-C5 | 6.30  | 120.73      | 112.19   |
| 5   | T     | 3   | BMA  | C1-O5-C5 | -6.13 | 103.89      | 112.19   |
| 4   | N     | 4   | MAN  | C1-O5-C5 | 5.96  | 120.27      | 112.19   |
| 3   | V     | 5   | NAG  | C1-O5-C5 | 5.89  | 120.17      | 112.19   |
| 4   | N     | 2   | NAG  | C1-O5-C5 | 5.83  | 120.10      | 112.19   |
| 5   | O     | 3   | BMA  | C1-O5-C5 | -5.76 | 104.39      | 112.19   |
| 5   | R     | 3   | BMA  | C1-C2-C3 | -5.75 | 102.60      | 109.67   |
| 3   | S     | 4   | MAN  | O2-C2-C3 | -5.53 | 99.06       | 110.14   |
| 5   | U     | 4   | MAN  | C1-O5-C5 | 5.51  | 119.66      | 112.19   |
| 5   | U     | 4   | MAN  | O5-C5-C6 | 5.43  | 115.71      | 107.20   |
| 5   | Q     | 3   | BMA  | O5-C5-C6 | 4.80  | 114.73      | 107.20   |
| 5   | U     | 3   | BMA  | O5-C1-C2 | -4.75 | 103.44      | 110.77   |
| 3   | M     | 3   | BMA  | O5-C1-C2 | -4.69 | 103.52      | 110.77   |
| 4   | P     | 3   | BMA  | C3-C4-C5 | 4.64  | 118.52      | 110.24   |
| 5   | T     | 2   | NAG  | C1-O5-C5 | 4.58  | 118.40      | 112.19   |
| 4   | P     | 4   | MAN  | C2-C3-C4 | 4.57  | 118.80      | 110.89   |
| 5   | O     | 2   | NAG  | C3-C4-C5 | 4.55  | 118.35      | 110.24   |
| 3   | S     | 5   | NAG  | C2-N2-C7 | 4.52  | 129.34      | 122.90   |
| 5   | X     | 3   | BMA  | C1-O5-C5 | 4.47  | 118.25      | 112.19   |
| 3   | M     | 2   | NAG  | C1-O5-C5 | 4.47  | 118.25      | 112.19   |
| 3   | S     | 1   | NAG  | O4-C4-C3 | -4.47 | 100.03      | 110.35   |
| 5   | U     | 1   | NAG  | C1-O5-C5 | 4.46  | 118.24      | 112.19   |
| 3   | S     | 3   | BMA  | C2-C3-C4 | -4.43 | 103.22      | 110.89   |
| 3   | V     | 4   | MAN  | O2-C2-C1 | 4.35  | 118.06      | 109.15   |
| 3   | M     | 4   | MAN  | C1-C2-C3 | 4.34  | 115.00      | 109.67   |
| 5   | O     | 4   | MAN  | C1-O5-C5 | 4.29  | 118.00      | 112.19   |
| 5   | T     | 3   | BMA  | C3-C4-C5 | 4.28  | 117.88      | 110.24   |
| 5   | Q     | 3   | BMA  | C1-O5-C5 | 4.28  | 117.99      | 112.19   |
| 5   | T     | 3   | BMA  | C1-C2-C3 | -4.26 | 104.43      | 109.67   |
| 4   | N     | 3   | BMA  | C1-O5-C5 | 4.26  | 117.96      | 112.19   |
| 3   | M     | 6   | MAN  | C1-O5-C5 | 4.24  | 117.94      | 112.19   |
| 3   | S     | 6   | MAN  | C1-O5-C5 | 4.20  | 117.89      | 112.19   |
| 4   | P     | 5   | NAG  | C1-O5-C5 | 4.16  | 117.83      | 112.19   |
| 6   | W     | 3   | BMA  | C1-O5-C5 | 4.10  | 117.75      | 112.19   |
| 3   | M     | 2   | NAG  | O4-C4-C5 | 3.92  | 119.04      | 109.30   |
| 3   | S     | 6   | MAN  | O5-C5-C6 | 3.89  | 113.30      | 107.20   |
| 5   | R     | 4   | MAN  | C1-C2-C3 | -3.88 | 104.90      | 109.67   |
| 5   | R     | 3   | BMA  | C3-C4-C5 | 3.72  | 116.88      | 110.24   |
| 3   | V     | 3   | BMA  | C3-C4-C5 | 3.69  | 116.82      | 110.24   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | M     | 4   | MAN  | C1-O5-C5 | 3.68  | 117.18      | 112.19   |
| 6   | W     | 3   | BMA  | O5-C5-C6 | 3.66  | 112.94      | 107.20   |
| 4   | N     | 4   | MAN  | O2-C2-C3 | -3.63 | 102.87      | 110.14   |
| 4   | P     | 3   | BMA  | C1-O5-C5 | 3.62  | 117.10      | 112.19   |
| 4   | N     | 4   | MAN  | C1-C2-C3 | -3.59 | 105.25      | 109.67   |
| 6   | W     | 3   | BMA  | C1-C2-C3 | 3.58  | 114.06      | 109.67   |
| 5   | O     | 3   | BMA  | O3-C3-C4 | 3.55  | 118.55      | 110.35   |
| 5   | X     | 4   | MAN  | O2-C2-C1 | 3.54  | 116.40      | 109.15   |
| 5   | T     | 4   | MAN  | O5-C1-C2 | -3.51 | 105.36      | 110.77   |
| 3   | M     | 1   | NAG  | O5-C5-C6 | -3.50 | 101.72      | 107.20   |
| 4   | P     | 4   | MAN  | C1-C2-C3 | 3.41  | 113.86      | 109.67   |
| 5   | O     | 2   | NAG  | C1-O5-C5 | -3.37 | 107.63      | 112.19   |
| 5   | Q     | 3   | BMA  | C2-C3-C4 | 3.29  | 116.59      | 110.89   |
| 4   | P     | 4   | MAN  | O2-C2-C1 | 3.28  | 115.87      | 109.15   |
| 5   | U     | 1   | NAG  | C3-C4-C5 | 3.27  | 116.06      | 110.24   |
| 3   | V     | 3   | BMA  | O5-C5-C6 | 3.21  | 112.24      | 107.20   |
| 4   | N     | 4   | MAN  | C2-C3-C4 | -3.18 | 105.39      | 110.89   |
| 4   | N     | 4   | MAN  | O3-C3-C2 | 3.17  | 116.07      | 109.99   |
| 3   | S     | 4   | MAN  | O5-C5-C6 | 3.17  | 112.17      | 107.20   |
| 5   | U     | 2   | NAG  | C3-C4-C5 | 3.14  | 115.84      | 110.24   |
| 4   | P     | 4   | MAN  | C3-C4-C5 | 3.14  | 115.83      | 110.24   |
| 3   | M     | 6   | MAN  | O2-C2-C1 | 3.14  | 115.57      | 109.15   |
| 3   | V     | 4   | MAN  | O5-C5-C6 | 3.10  | 112.06      | 107.20   |
| 3   | S     | 4   | MAN  | O3-C3-C4 | -3.09 | 103.22      | 110.35   |
| 3   | M     | 3   | BMA  | O5-C5-C6 | 3.06  | 112.01      | 107.20   |
| 5   | U     | 3   | BMA  | C1-C2-C3 | -3.05 | 105.92      | 109.67   |
| 5   | O     | 2   | NAG  | C4-C3-C2 | 3.04  | 115.47      | 111.02   |
| 3   | S     | 2   | NAG  | C3-C4-C5 | 3.03  | 115.64      | 110.24   |
| 5   | U     | 3   | BMA  | O3-C3-C2 | 3.00  | 115.74      | 109.99   |
| 3   | S     | 2   | NAG  | C1-O5-C5 | -2.98 | 108.16      | 112.19   |
| 3   | V     | 1   | NAG  | O4-C4-C3 | -2.94 | 103.55      | 110.35   |
| 5   | T     | 3   | BMA  | O5-C5-C6 | 2.93  | 111.79      | 107.20   |
| 5   | T     | 2   | NAG  | C3-C4-C5 | 2.92  | 115.45      | 110.24   |
| 6   | W     | 3   | BMA  | C2-C3-C4 | 2.90  | 115.91      | 110.89   |
| 5   | X     | 3   | BMA  | O3-C3-C2 | 2.89  | 115.52      | 109.99   |
| 5   | O     | 4   | MAN  | C1-C2-C3 | 2.89  | 113.22      | 109.67   |
| 5   | R     | 4   | MAN  | O5-C1-C2 | -2.88 | 106.32      | 110.77   |
| 3   | S     | 3   | BMA  | C1-C2-C3 | -2.81 | 106.21      | 109.67   |
| 5   | R     | 1   | NAG  | O4-C4-C3 | -2.80 | 103.87      | 110.35   |
| 5   | O     | 3   | BMA  | C6-C5-C4 | 2.78  | 119.51      | 113.00   |
| 4   | P     | 4   | MAN  | O2-C2-C3 | 2.76  | 115.67      | 110.14   |
| 3   | S     | 3   | BMA  | O3-C3-C4 | 2.74  | 116.68      | 110.35   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | V     | 4   | MAN  | O3-C3-C2 | 2.72  | 115.21      | 109.99   |
| 3   | V     | 4   | MAN  | C2-C3-C4 | -2.72 | 106.19      | 110.89   |
| 5   | R     | 2   | NAG  | C3-C4-C5 | 2.71  | 115.07      | 110.24   |
| 5   | Q     | 4   | MAN  | C1-O5-C5 | 2.70  | 115.85      | 112.19   |
| 4   | P     | 5   | NAG  | C3-C4-C5 | 2.68  | 115.02      | 110.24   |
| 5   | U     | 4   | MAN  | O2-C2-C1 | 2.66  | 114.59      | 109.15   |
| 5   | X     | 3   | BMA  | C1-C2-C3 | 2.63  | 112.89      | 109.67   |
| 3   | V     | 6   | MAN  | C1-O5-C5 | 2.61  | 115.73      | 112.19   |
| 3   | M     | 3   | BMA  | C1-C2-C3 | -2.60 | 106.47      | 109.67   |
| 5   | U     | 2   | NAG  | C1-O5-C5 | 2.60  | 115.71      | 112.19   |
| 4   | P     | 2   | NAG  | O4-C4-C3 | -2.57 | 104.42      | 110.35   |
| 5   | Q     | 4   | MAN  | O2-C2-C1 | 2.56  | 114.39      | 109.15   |
| 5   | Q     | 3   | BMA  | C1-C2-C3 | 2.54  | 112.79      | 109.67   |
| 5   | T     | 3   | BMA  | O5-C1-C2 | -2.52 | 106.89      | 110.77   |
| 4   | N     | 5   | NAG  | C3-C4-C5 | 2.51  | 114.71      | 110.24   |
| 5   | O     | 4   | MAN  | O5-C1-C2 | 2.50  | 114.62      | 110.77   |
| 3   | M     | 1   | NAG  | O4-C4-C3 | -2.49 | 104.60      | 110.35   |
| 3   | S     | 6   | MAN  | O2-C2-C1 | 2.48  | 114.23      | 109.15   |
| 3   | S     | 3   | BMA  | C3-C4-C5 | 2.46  | 114.62      | 110.24   |
| 5   | X     | 1   | NAG  | O4-C4-C5 | -2.44 | 103.23      | 109.30   |
| 3   | M     | 6   | MAN  | C1-C2-C3 | -2.42 | 106.69      | 109.67   |
| 5   | R     | 3   | BMA  | O6-C6-C5 | -2.39 | 103.08      | 111.29   |
| 5   | O     | 4   | MAN  | O2-C2-C1 | 2.39  | 114.04      | 109.15   |
| 5   | T     | 4   | MAN  | C2-C3-C4 | 2.35  | 114.97      | 110.89   |
| 5   | T     | 1   | NAG  | C1-O5-C5 | 2.35  | 115.37      | 112.19   |
| 4   | N     | 1   | NAG  | C1-O5-C5 | 2.30  | 115.30      | 112.19   |
| 5   | X     | 4   | MAN  | C1-O5-C5 | 2.29  | 115.30      | 112.19   |
| 3   | V     | 2   | NAG  | C2-N2-C7 | 2.29  | 126.17      | 122.90   |
| 5   | Q     | 3   | BMA  | C3-C4-C5 | 2.29  | 114.33      | 110.24   |
| 5   | X     | 1   | NAG  | C1-O5-C5 | -2.28 | 109.10      | 112.19   |
| 5   | R     | 3   | BMA  | O5-C5-C6 | -2.25 | 103.67      | 107.20   |
| 5   | U     | 3   | BMA  | O5-C5-C6 | 2.25  | 110.73      | 107.20   |
| 3   | S     | 5   | NAG  | C1-C2-N2 | -2.23 | 106.68      | 110.49   |
| 6   | W     | 3   | BMA  | O5-C1-C2 | 2.21  | 114.18      | 110.77   |
| 5   | R     | 3   | BMA  | C1-O5-C5 | 2.19  | 115.15      | 112.19   |
| 3   | S     | 3   | BMA  | O5-C1-C2 | -2.18 | 107.41      | 110.77   |
| 3   | V     | 4   | MAN  | O5-C5-C4 | 2.18  | 116.12      | 110.83   |
| 3   | S     | 2   | NAG  | O4-C4-C5 | -2.18 | 103.89      | 109.30   |
| 3   | V     | 4   | MAN  | O2-C2-C3 | 2.17  | 114.48      | 110.14   |
| 5   | R     | 4   | MAN  | O2-C2-C1 | 2.16  | 113.58      | 109.15   |
| 4   | P     | 4   | MAN  | O3-C3-C2 | 2.16  | 114.14      | 109.99   |
| 5   | T     | 4   | MAN  | O3-C3-C2 | 2.15  | 114.11      | 109.99   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | T     | 3   | BMA  | O2-C2-C1 | 2.14  | 113.53      | 109.15   |
| 3   | S     | 4   | MAN  | C3-C4-C5 | 2.13  | 114.04      | 110.24   |
| 5   | Q     | 4   | MAN  | O3-C3-C2 | 2.09  | 114.00      | 109.99   |
| 4   | P     | 4   | MAN  | O5-C1-C2 | 2.09  | 114.00      | 110.77   |
| 3   | M     | 4   | MAN  | O3-C3-C2 | 2.09  | 113.99      | 109.99   |
| 3   | V     | 2   | NAG  | C3-C4-C5 | 2.07  | 113.93      | 110.24   |
| 4   | P     | 1   | NAG  | O4-C4-C3 | -2.06 | 105.58      | 110.35   |
| 5   | T     | 4   | MAN  | O2-C2-C3 | -2.06 | 106.00      | 110.14   |
| 5   | R     | 3   | BMA  | O5-C1-C2 | 2.04  | 113.92      | 110.77   |
| 4   | P     | 5   | NAG  | C1-C2-N2 | 2.04  | 113.97      | 110.49   |
| 3   | V     | 6   | MAN  | C1-C2-C3 | -2.03 | 107.17      | 109.67   |
| 5   | U     | 4   | MAN  | C2-C3-C4 | 2.03  | 114.41      | 110.89   |
| 3   | V     | 1   | NAG  | C1-O5-C5 | 2.01  | 114.92      | 112.19   |
| 5   | O     | 4   | MAN  | C3-C4-C5 | 2.01  | 113.82      | 110.24   |

There are no chirality outliers.

All (111) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | P     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | S     | 5   | NAG  | C3-C2-N2-C7 |
| 4   | P     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | M     | 5   | NAG  | C4-C5-C6-O6 |
| 5   | Q     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | V     | 4   | MAN  | O5-C5-C6-O6 |
| 6   | W     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | U     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | Q     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | S     | 3   | BMA  | C4-C5-C6-O6 |
| 4   | P     | 5   | NAG  | C1-C2-N2-C7 |
| 3   | M     | 5   | NAG  | O5-C5-C6-O6 |
| 5   | R     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | X     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | S     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | T     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | P     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | O     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | N     | 4   | MAN  | C4-C5-C6-O6 |
| 5   | X     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | V     | 5   | NAG  | C4-C5-C6-O6 |
| 5   | O     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | U     | 1   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | V     | 5   | NAG  | O5-C5-C6-O6 |
| 4   | P     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | P     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | R     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | N     | 5   | NAG  | O5-C5-C6-O6 |
| 4   | P     | 4   | MAN  | O5-C5-C6-O6 |
| 4   | P     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | P     | 5   | NAG  | O5-C5-C6-O6 |
| 4   | N     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | V     | 4   | MAN  | C4-C5-C6-O6 |
| 4   | N     | 5   | NAG  | C1-C2-N2-C7 |
| 6   | W     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | T     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | U     | 2   | NAG  | C8-C7-N2-C2 |
| 5   | U     | 2   | NAG  | O7-C7-N2-C2 |
| 5   | Q     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | Q     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | O     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | O     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | W     | 1   | NAG  | C8-C7-N2-C2 |
| 6   | W     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | R     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | R     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | V     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | V     | 1   | NAG  | O7-C7-N2-C2 |
| 4   | N     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | N     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | U     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | U     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | X     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | X     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | S     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | S     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | M     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | M     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | X     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | N     | 5   | NAG  | C4-C5-C6-O6 |
| 4   | P     | 5   | NAG  | C4-C5-C6-O6 |
| 4   | P     | 4   | MAN  | C4-C5-C6-O6 |
| 5   | X     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | M     | 3   | BMA  | O5-C5-C6-O6 |
| 6   | W     | 2   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | Q     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | U     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | W     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | Q     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | U     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | S     | 6   | MAN  | C4-C5-C6-O6 |
| 4   | N     | 2   | NAG  | C1-C2-N2-C7 |
| 3   | V     | 3   | BMA  | C4-C5-C6-O6 |
| 4   | N     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | M     | 5   | NAG  | C1-C2-N2-C7 |
| 6   | W     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | R     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | X     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | S     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | O     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | V     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | S     | 4   | MAN  | O5-C5-C6-O6 |
| 5   | T     | 1   | NAG  | C1-C2-N2-C7 |
| 5   | R     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | M     | 5   | NAG  | C3-C2-N2-C7 |
| 3   | V     | 2   | NAG  | C3-C2-N2-C7 |
| 5   | R     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | V     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | T     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | M     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | M     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | S     | 6   | MAN  | O5-C5-C6-O6 |
| 5   | Q     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | S     | 2   | NAG  | C1-C2-N2-C7 |
| 4   | N     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | P     | 5   | NAG  | C3-C2-N2-C7 |
| 3   | S     | 2   | NAG  | C3-C2-N2-C7 |
| 4   | N     | 5   | NAG  | C3-C2-N2-C7 |
| 5   | Q     | 2   | NAG  | C3-C2-N2-C7 |
| 5   | O     | 2   | NAG  | C3-C2-N2-C7 |
| 5   | X     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | M     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | P     | 1   | NAG  | C1-C2-N2-C7 |
| 5   | T     | 2   | NAG  | C1-C2-N2-C7 |
| 3   | V     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | O     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | U     | 4   | MAN  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | T     | 1   | NAG  | C3-C2-N2-C7 |
| 5   | T     | 2   | NAG  | C3-C2-N2-C7 |
| 5   | T     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | P     | 3   | BMA  | C4-C5-C6-O6 |

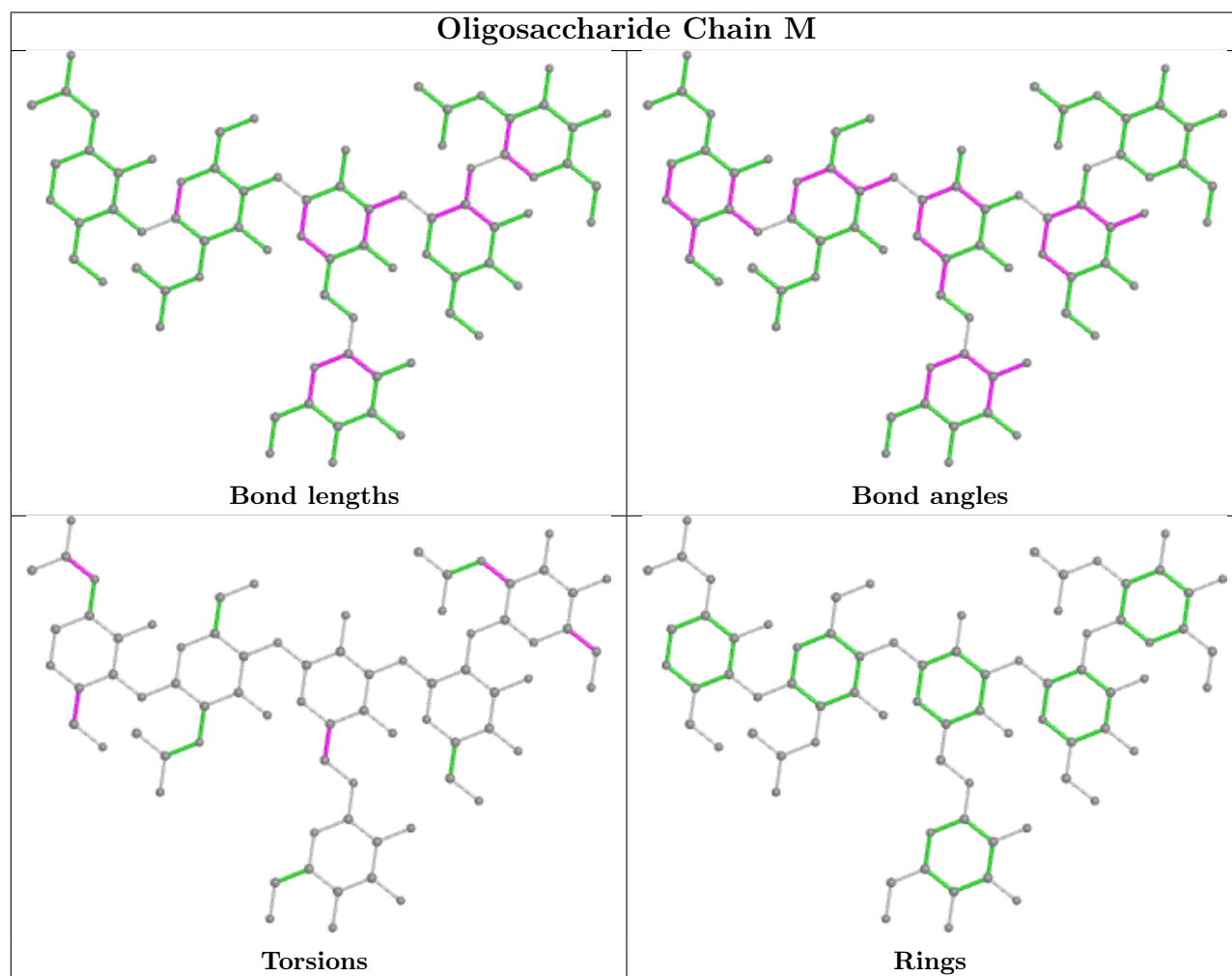
All (6) ring outliers are listed below:

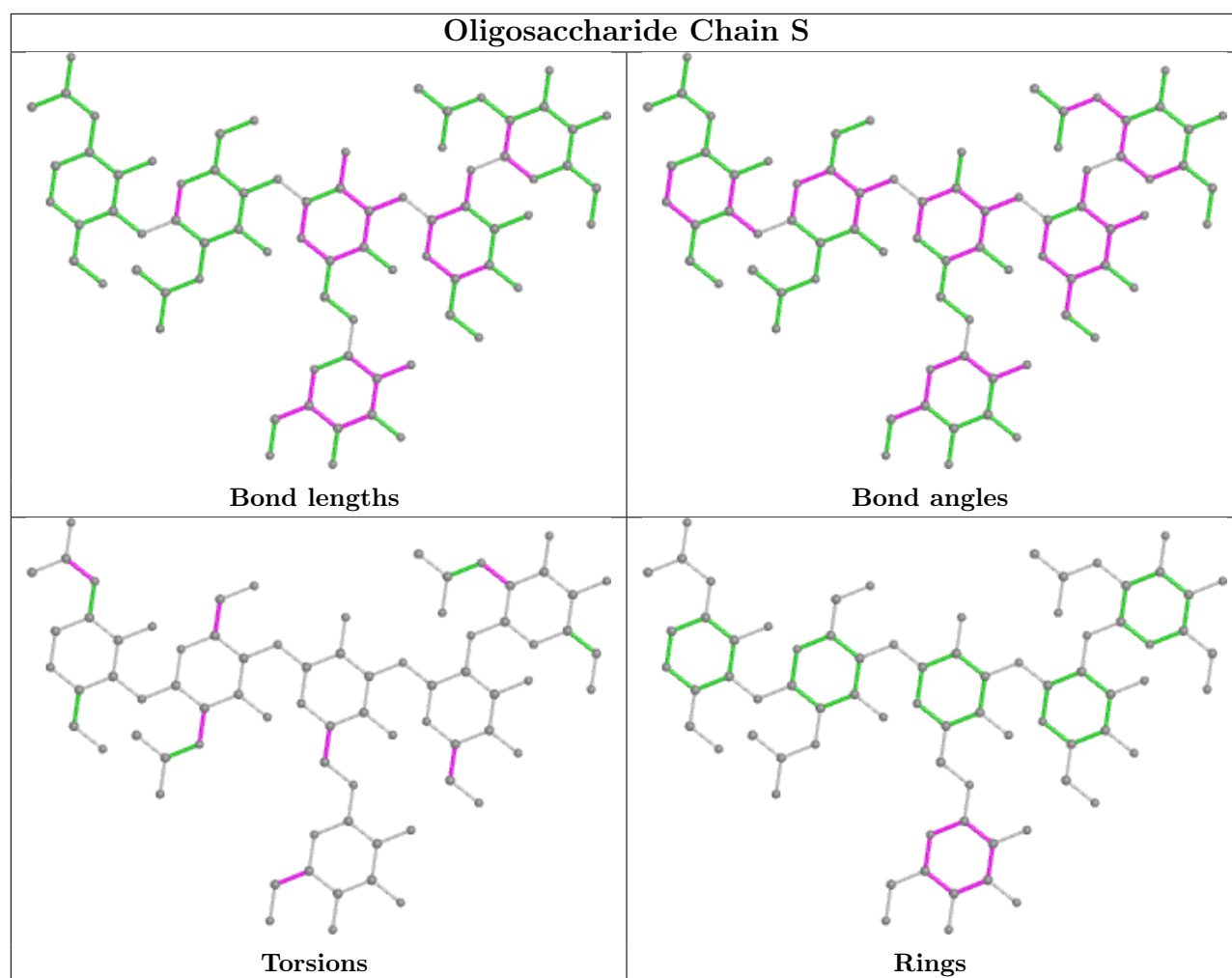
| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 5   | X     | 3   | BMA  | C1-C2-C3-C4-C5-O5 |
| 3   | S     | 6   | MAN  | C1-C2-C3-C4-C5-O5 |
| 5   | U     | 4   | MAN  | C1-C2-C3-C4-C5-O5 |
| 5   | Q     | 4   | MAN  | C1-C2-C3-C4-C5-O5 |
| 5   | X     | 4   | MAN  | C1-C2-C3-C4-C5-O5 |
| 4   | N     | 3   | BMA  | C1-C2-C3-C4-C5-O5 |

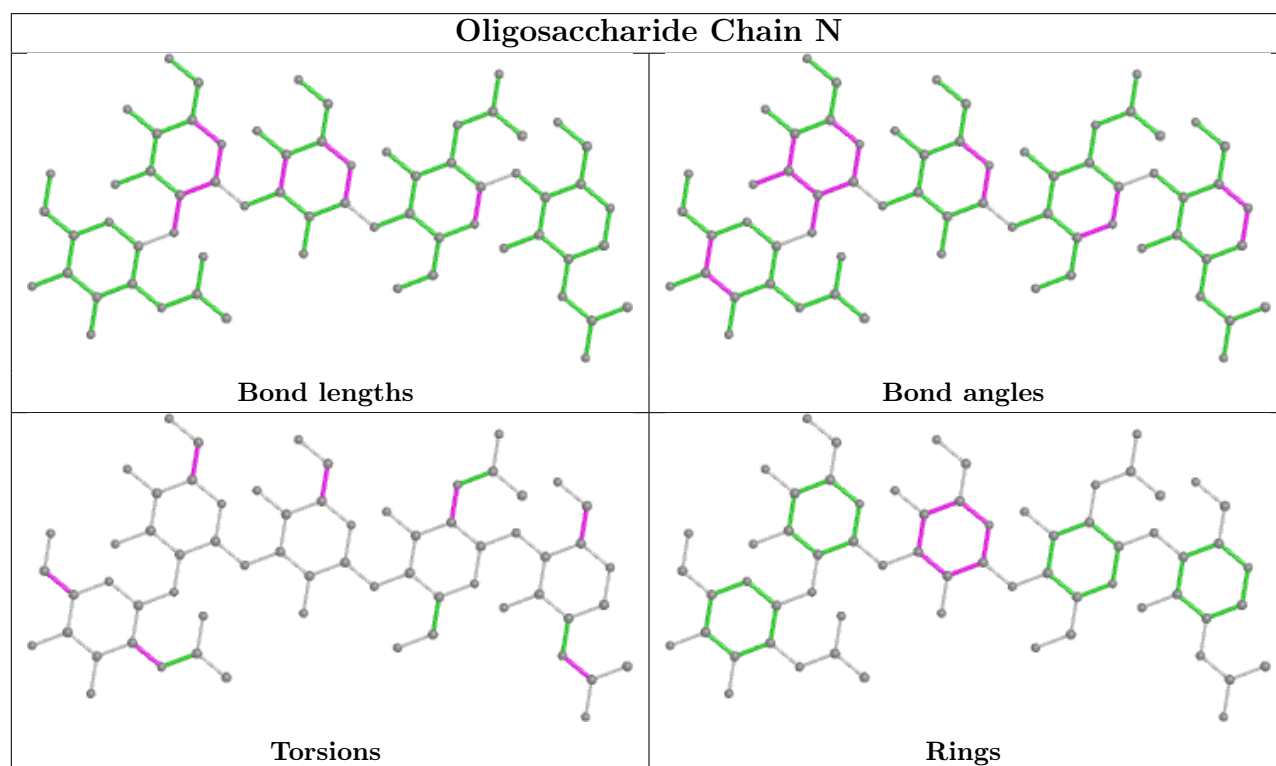
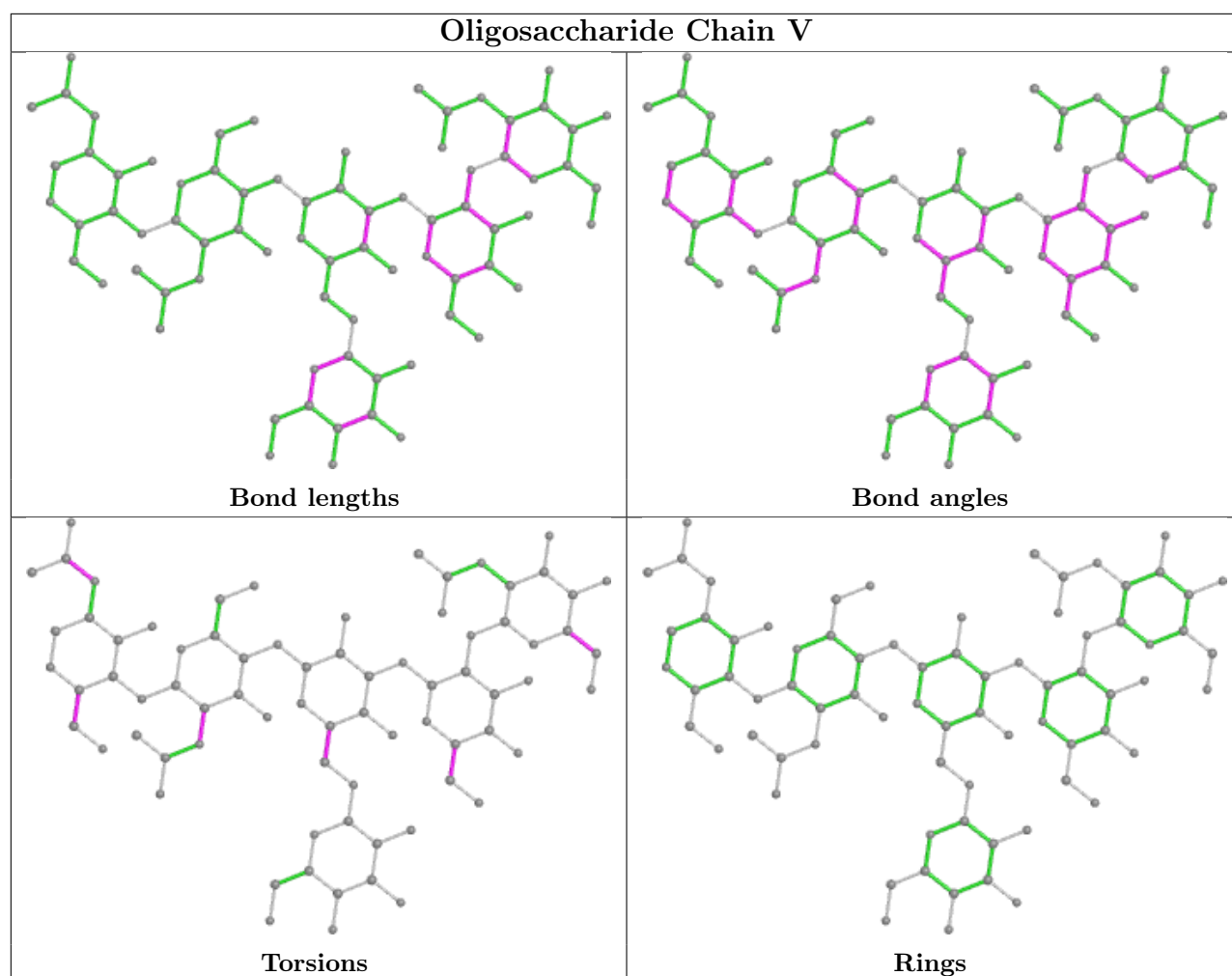
23 monomers are involved in 36 short contacts:

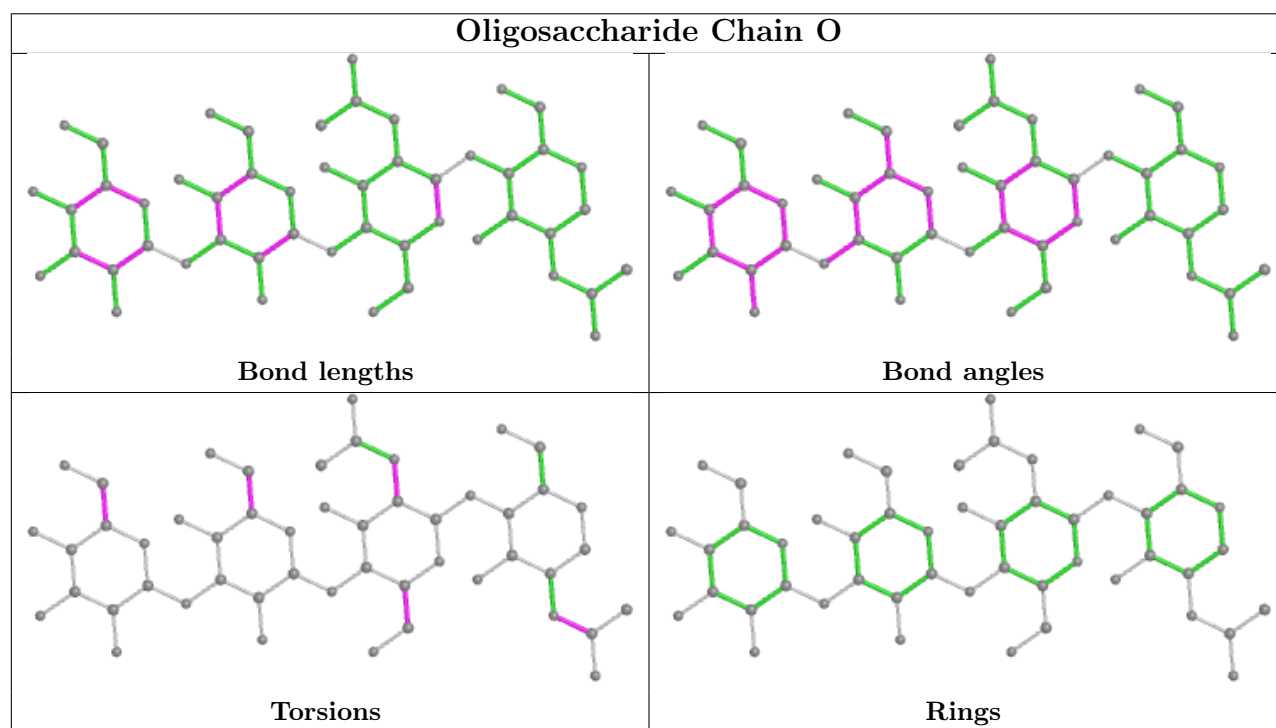
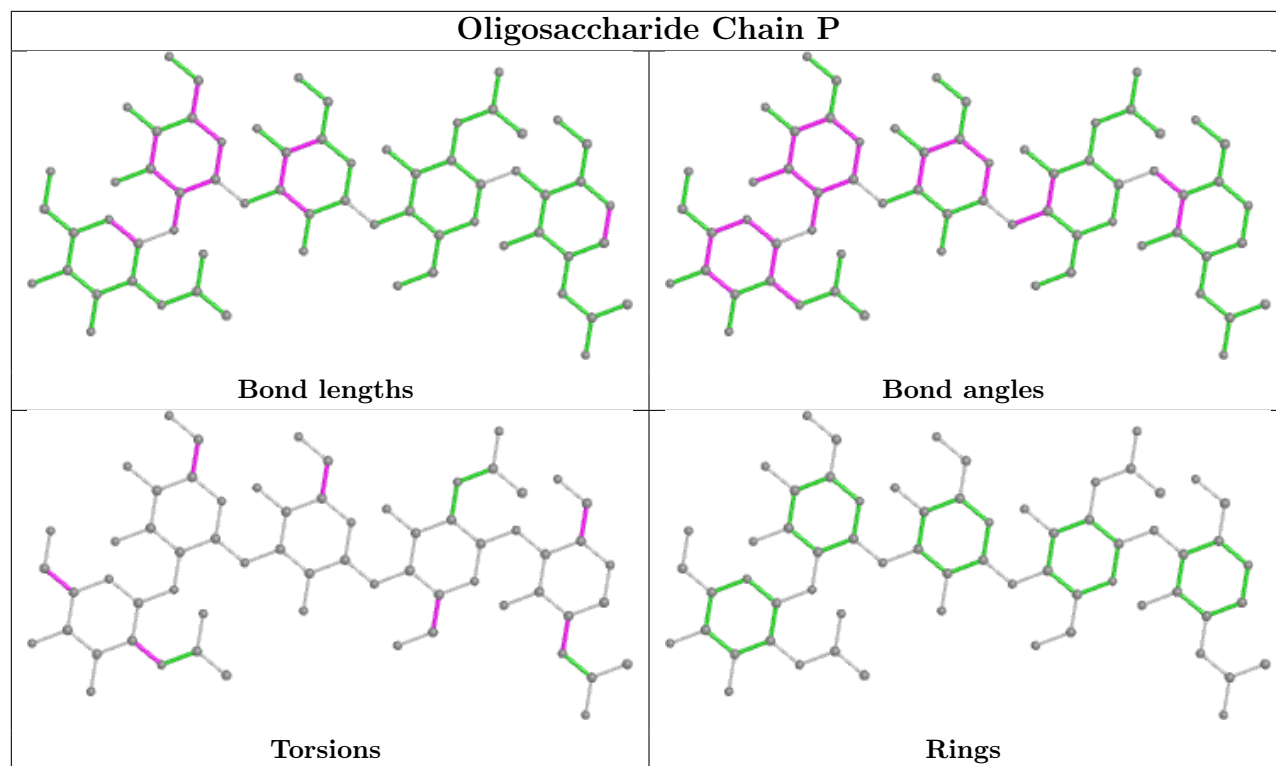
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | S     | 6   | MAN  | 1       | 0            |
| 6   | W     | 2   | NAG  | 1       | 0            |
| 3   | M     | 2   | NAG  | 1       | 0            |
| 3   | M     | 6   | MAN  | 3       | 0            |
| 4   | P     | 5   | NAG  | 1       | 0            |
| 3   | M     | 4   | MAN  | 1       | 0            |
| 5   | U     | 4   | MAN  | 1       | 0            |
| 5   | T     | 2   | NAG  | 1       | 0            |
| 5   | R     | 2   | NAG  | 1       | 0            |
| 6   | W     | 3   | BMA  | 1       | 0            |
| 5   | R     | 1   | NAG  | 3       | 0            |
| 3   | V     | 1   | NAG  | 5       | 0            |
| 4   | N     | 1   | NAG  | 5       | 0            |
| 5   | T     | 1   | NAG  | 4       | 0            |
| 3   | M     | 3   | BMA  | 2       | 0            |
| 5   | X     | 1   | NAG  | 4       | 0            |
| 3   | S     | 3   | BMA  | 1       | 0            |
| 4   | N     | 4   | MAN  | 1       | 0            |
| 4   | N     | 3   | BMA  | 1       | 0            |
| 3   | M     | 1   | NAG  | 1       | 0            |
| 5   | O     | 2   | NAG  | 1       | 0            |
| 4   | P     | 1   | NAG  | 3       | 0            |
| 3   | S     | 5   | NAG  | 1       | 0            |

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

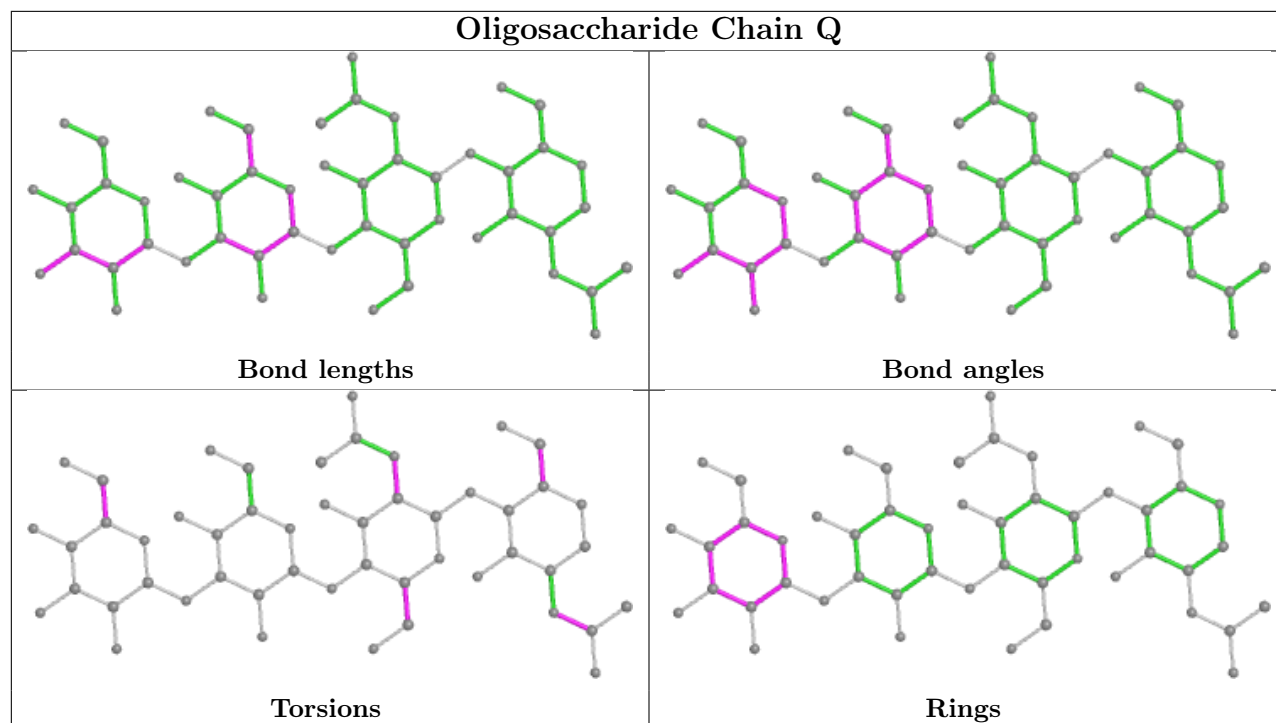




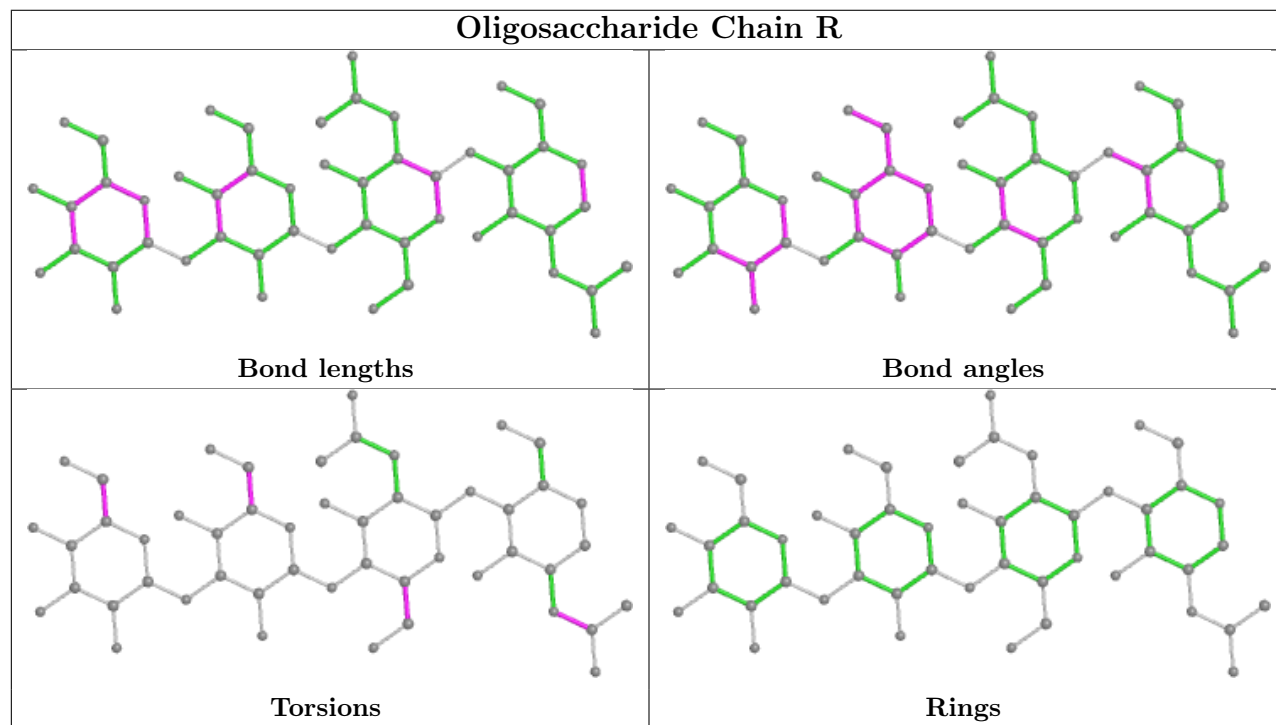




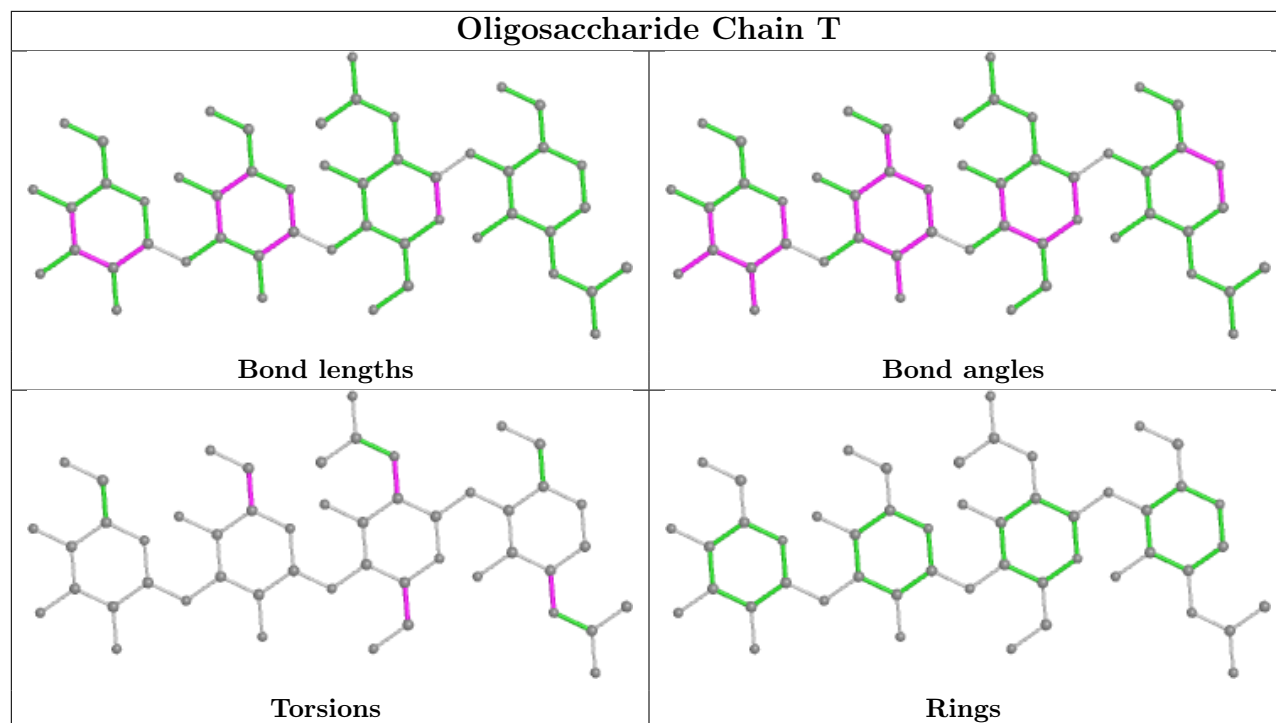
## Oligosaccharide Chain Q



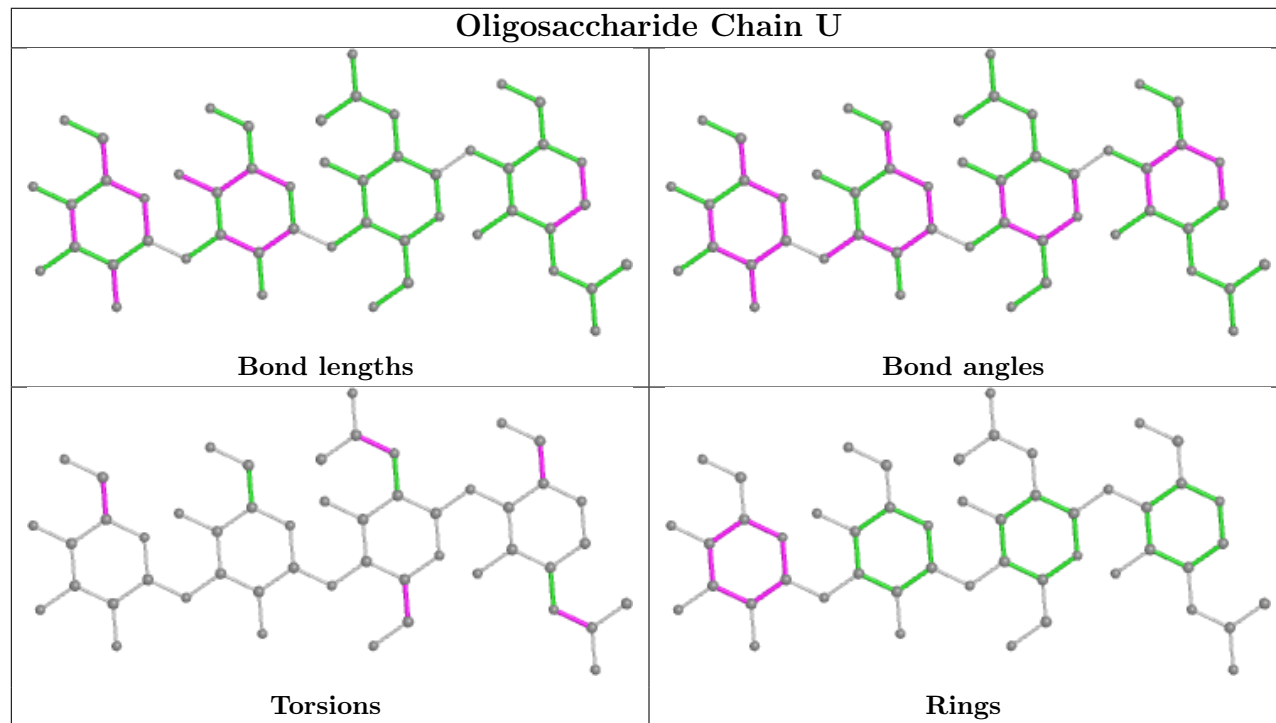
## Oligosaccharide Chain R

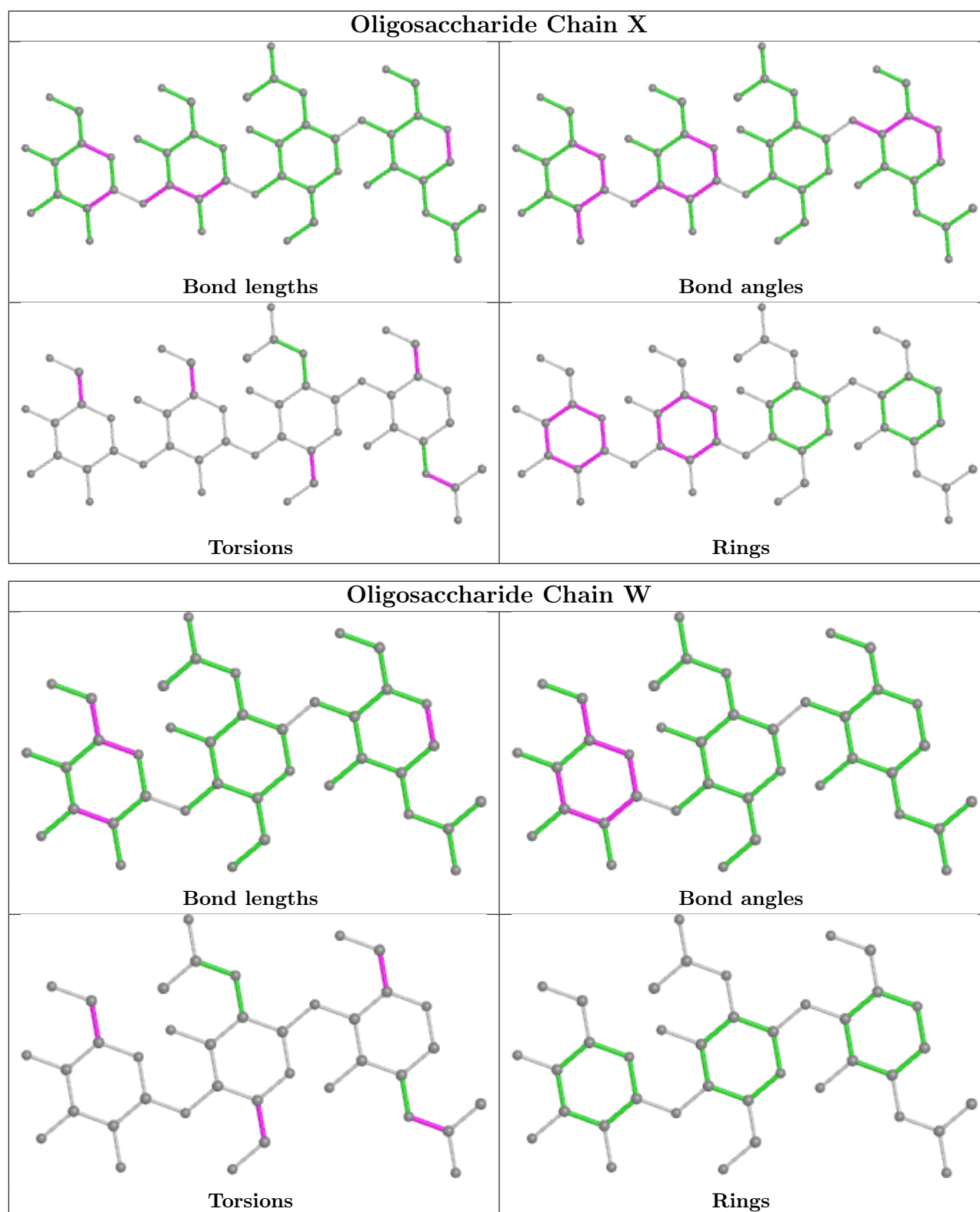


## Oligosaccharide Chain T



## Oligosaccharide Chain U





## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 for Mogul analysis.

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$ |
| 7   | NAG  | G     | 401 | 1    | 14,14,15     | 1.58 | 1 (7%)      | 17,19,21    | 1.87 | 1 (5%)      |
| 7   | NAG  | E     | 401 | 1    | 14,14,15     | 1.12 | 1 (7%)      | 17,19,21    | 0.75 | 0           |
| 7   | NAG  | G     | 402 | 1    | 14,14,15     | 0.96 | 1 (7%)      | 17,19,21    | 1.73 | 1 (5%)      |
| 7   | NAG  | A     | 402 | 1    | 14,14,15     | 0.78 | 1 (7%)      | 17,19,21    | 2.32 | 3 (17%)     |
| 7   | NAG  | E     | 412 | 1    | 14,14,15     | 1.16 | 1 (7%)      | 17,19,21    | 1.04 | 2 (11%)     |
| 7   | NAG  | I     | 410 | 1    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.82 | 0           |
| 7   | NAG  | K     | 401 | 1    | 14,14,15     | 0.70 | 1 (7%)      | 17,19,21    | 0.65 | 0           |
| 7   | NAG  | A     | 414 | 1    | 14,14,15     | 0.80 | 1 (7%)      | 17,19,21    | 0.64 | 0           |
| 7   | NAG  | K     | 413 | 1    | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.66 | 0           |
| 7   | NAG  | K     | 414 | 1    | 14,14,15     | 1.08 | 2 (14%)     | 17,19,21    | 1.51 | 1 (5%)      |
| 7   | NAG  | A     | 401 | 1    | 14,14,15     | 0.85 | 1 (7%)      | 17,19,21    | 1.30 | 1 (5%)      |
| 7   | NAG  | E     | 414 | 1    | 14,14,15     | 2.00 | 2 (14%)     | 17,19,21    | 1.92 | 1 (5%)      |
| 7   | NAG  | G     | 413 | 1    | 14,14,15     | 2.14 | 2 (14%)     | 17,19,21    | 2.71 | 1 (5%)      |
| 7   | NAG  | I     | 401 | 1    | 14,14,15     | 0.49 | 0           | 17,19,21    | 0.47 | 0           |
| 7   | NAG  | E     | 413 | 1    | 14,14,15     | 0.63 | 1 (7%)      | 17,19,21    | 0.86 | 1 (5%)      |
| 7   | NAG  | A     | 412 | 1    | 14,14,15     | 1.81 | 2 (14%)     | 17,19,21    | 1.40 | 1 (5%)      |
| 7   | NAG  | A     | 413 | 1    | 14,14,15     | 1.72 | 2 (14%)     | 17,19,21    | 1.25 | 1 (5%)      |
| 7   | NAG  | C     | 409 | 1    | 14,14,15     | 0.63 | 0           | 17,19,21    | 0.64 | 0           |
| 7   | NAG  | I     | 409 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 1.18 | 1 (5%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7   | NAG  | G     | 401 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | E     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | G     | 402 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | A     | 402 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | E     | 412 | 1    | -       | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7   | NAG  | I     | 410 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | K     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | A     | 414 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | K     | 413 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | K     | 414 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | A     | 401 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | E     | 414 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | G     | 413 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | I     | 401 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | E     | 413 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | A     | 412 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | A     | 413 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | C     | 409 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | I     | 409 | 1    | -       | 4/6/23/26 | 0/1/1/1 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | G     | 413 | NAG  | O5-C1 | 7.43  | 1.55        | 1.43     |
| 7   | E     | 414 | NAG  | O5-C1 | 6.54  | 1.54        | 1.43     |
| 7   | G     | 401 | NAG  | O5-C1 | 5.68  | 1.52        | 1.43     |
| 7   | A     | 412 | NAG  | O5-C1 | 5.62  | 1.52        | 1.43     |
| 7   | A     | 413 | NAG  | C1-C2 | 4.67  | 1.59        | 1.52     |
| 7   | A     | 413 | NAG  | O5-C1 | 4.21  | 1.50        | 1.43     |
| 7   | E     | 401 | NAG  | O5-C1 | -4.09 | 1.37        | 1.43     |
| 7   | E     | 412 | NAG  | C1-C2 | 3.68  | 1.57        | 1.52     |
| 7   | A     | 412 | NAG  | C1-C2 | 3.64  | 1.57        | 1.52     |
| 7   | E     | 414 | NAG  | C1-C2 | 3.48  | 1.57        | 1.52     |
| 7   | K     | 414 | NAG  | O5-C1 | 3.29  | 1.49        | 1.43     |
| 7   | G     | 413 | NAG  | C1-C2 | 2.89  | 1.56        | 1.52     |
| 7   | G     | 402 | NAG  | O5-C1 | 2.81  | 1.48        | 1.43     |
| 7   | A     | 401 | NAG  | O5-C1 | 2.79  | 1.48        | 1.43     |
| 7   | A     | 402 | NAG  | O5-C1 | 2.62  | 1.47        | 1.43     |
| 7   | K     | 414 | NAG  | C1-C2 | 2.27  | 1.55        | 1.52     |
| 7   | A     | 414 | NAG  | C1-C2 | 2.17  | 1.55        | 1.52     |
| 7   | E     | 413 | NAG  | O5-C1 | 2.13  | 1.47        | 1.43     |
| 7   | K     | 401 | NAG  | O5-C1 | -2.02 | 1.40        | 1.43     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | G     | 413 | NAG  | C1-O5-C5 | 11.06 | 127.17      | 112.19   |
| 7   | E     | 414 | NAG  | C1-O5-C5 | 7.55  | 122.42      | 112.19   |
| 7   | A     | 402 | NAG  | C1-O5-C5 | 7.29  | 122.07      | 112.19   |
| 7   | G     | 401 | NAG  | C1-O5-C5 | 6.97  | 121.64      | 112.19   |
| 7   | G     | 402 | NAG  | C1-O5-C5 | 6.57  | 121.09      | 112.19   |
| 7   | K     | 414 | NAG  | C1-O5-C5 | 6.13  | 120.50      | 112.19   |
| 7   | A     | 412 | NAG  | C1-O5-C5 | 4.87  | 118.79      | 112.19   |
| 7   | A     | 401 | NAG  | C1-O5-C5 | 4.86  | 118.77      | 112.19   |
| 7   | A     | 413 | NAG  | C1-O5-C5 | 4.54  | 118.34      | 112.19   |
| 7   | A     | 402 | NAG  | C2-N2-C7 | 4.47  | 129.26      | 122.90   |
| 7   | E     | 413 | NAG  | C1-O5-C5 | 2.89  | 116.11      | 112.19   |
| 7   | E     | 412 | NAG  | C1-O5-C5 | -2.88 | 108.29      | 112.19   |
| 7   | A     | 402 | NAG  | C1-C2-N2 | 2.61  | 114.94      | 110.49   |
| 7   | I     | 409 | NAG  | C1-O5-C5 | 2.58  | 115.68      | 112.19   |
| 7   | E     | 412 | NAG  | C4-C3-C2 | 2.21  | 114.25      | 111.02   |

There are no chirality outliers.

All (62) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 7   | A     | 412 | NAG  | C3-C2-N2-C7 |
| 7   | E     | 401 | NAG  | O5-C5-C6-O6 |
| 7   | I     | 410 | NAG  | O5-C5-C6-O6 |
| 7   | A     | 414 | NAG  | O5-C5-C6-O6 |
| 7   | E     | 413 | NAG  | O5-C5-C6-O6 |
| 7   | I     | 410 | NAG  | C4-C5-C6-O6 |
| 7   | E     | 413 | NAG  | C4-C5-C6-O6 |
| 7   | E     | 401 | NAG  | C4-C5-C6-O6 |
| 7   | A     | 412 | NAG  | O5-C5-C6-O6 |
| 7   | A     | 414 | NAG  | C4-C5-C6-O6 |
| 7   | G     | 402 | NAG  | C1-C2-N2-C7 |
| 7   | A     | 412 | NAG  | C4-C5-C6-O6 |
| 7   | A     | 402 | NAG  | C8-C7-N2-C2 |
| 7   | A     | 402 | NAG  | O7-C7-N2-C2 |
| 7   | K     | 413 | NAG  | C8-C7-N2-C2 |
| 7   | K     | 413 | NAG  | O7-C7-N2-C2 |
| 7   | K     | 401 | NAG  | C8-C7-N2-C2 |
| 7   | K     | 401 | NAG  | O7-C7-N2-C2 |
| 7   | A     | 401 | NAG  | C8-C7-N2-C2 |
| 7   | A     | 401 | NAG  | O7-C7-N2-C2 |
| 7   | E     | 401 | NAG  | C8-C7-N2-C2 |
| 7   | E     | 401 | NAG  | O7-C7-N2-C2 |
| 7   | K     | 414 | NAG  | C8-C7-N2-C2 |

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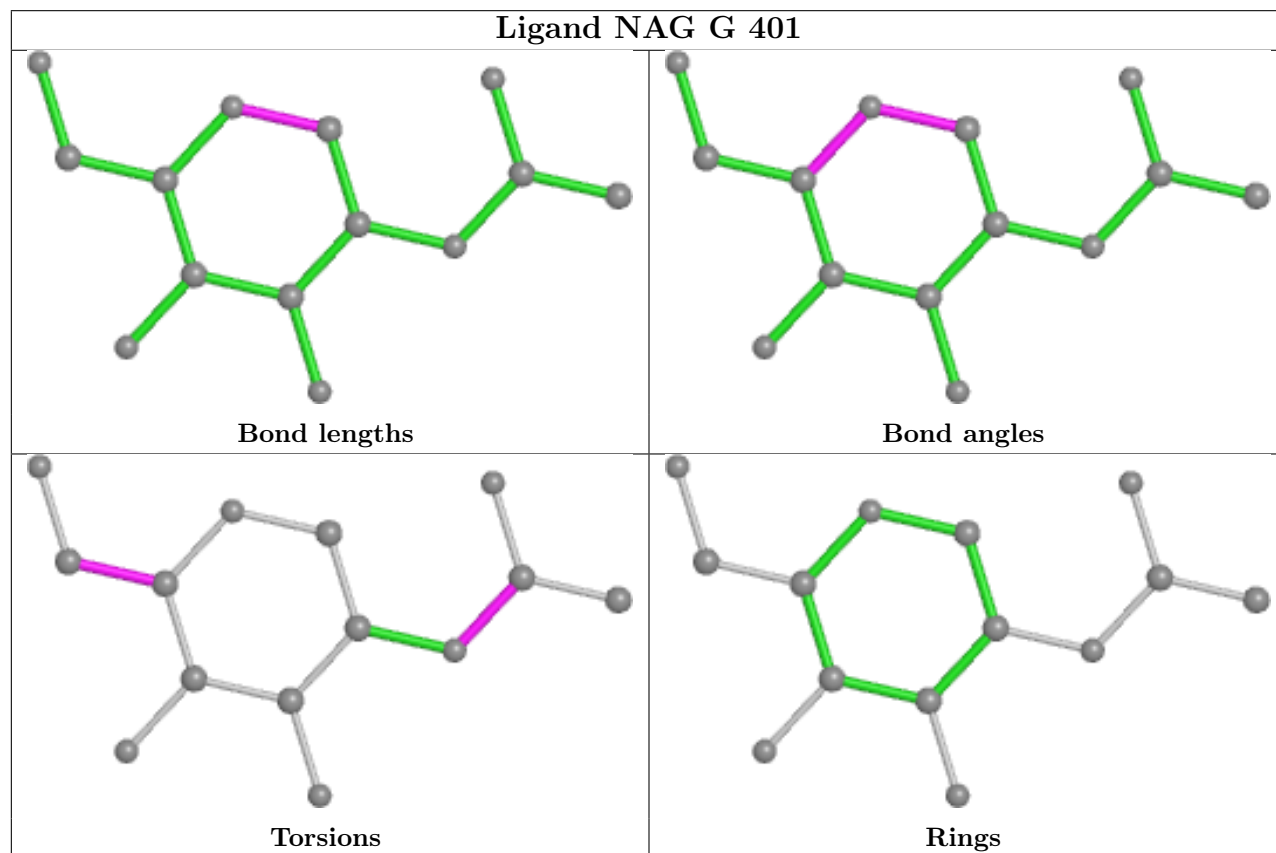
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 7   | K     | 414 | NAG  | O7-C7-N2-C2 |
| 7   | G     | 413 | NAG  | C8-C7-N2-C2 |
| 7   | G     | 413 | NAG  | O7-C7-N2-C2 |
| 7   | G     | 401 | NAG  | C8-C7-N2-C2 |
| 7   | G     | 401 | NAG  | O7-C7-N2-C2 |
| 7   | A     | 414 | NAG  | C8-C7-N2-C2 |
| 7   | A     | 414 | NAG  | O7-C7-N2-C2 |
| 7   | A     | 413 | NAG  | C8-C7-N2-C2 |
| 7   | A     | 413 | NAG  | O7-C7-N2-C2 |
| 7   | C     | 409 | NAG  | C8-C7-N2-C2 |
| 7   | C     | 409 | NAG  | O7-C7-N2-C2 |
| 7   | I     | 409 | NAG  | C8-C7-N2-C2 |
| 7   | I     | 409 | NAG  | O7-C7-N2-C2 |
| 7   | E     | 412 | NAG  | C8-C7-N2-C2 |
| 7   | E     | 412 | NAG  | O7-C7-N2-C2 |
| 7   | I     | 401 | NAG  | C8-C7-N2-C2 |
| 7   | I     | 401 | NAG  | O7-C7-N2-C2 |
| 7   | G     | 402 | NAG  | O5-C5-C6-O6 |
| 7   | I     | 409 | NAG  | O5-C5-C6-O6 |
| 7   | K     | 413 | NAG  | O5-C5-C6-O6 |
| 7   | I     | 409 | NAG  | C4-C5-C6-O6 |
| 7   | G     | 401 | NAG  | O5-C5-C6-O6 |
| 7   | E     | 412 | NAG  | O5-C5-C6-O6 |
| 7   | C     | 409 | NAG  | O5-C5-C6-O6 |
| 7   | A     | 401 | NAG  | O5-C5-C6-O6 |
| 7   | A     | 413 | NAG  | C4-C5-C6-O6 |
| 7   | K     | 413 | NAG  | C4-C5-C6-O6 |
| 7   | K     | 401 | NAG  | C4-C5-C6-O6 |
| 7   | K     | 401 | NAG  | O5-C5-C6-O6 |
| 7   | A     | 413 | NAG  | O5-C5-C6-O6 |
| 7   | E     | 414 | NAG  | C1-C2-N2-C7 |
| 7   | G     | 402 | NAG  | C3-C2-N2-C7 |
| 7   | A     | 402 | NAG  | C3-C2-N2-C7 |
| 7   | I     | 410 | NAG  | C3-C2-N2-C7 |
| 7   | G     | 402 | NAG  | C4-C5-C6-O6 |
| 7   | I     | 401 | NAG  | O5-C5-C6-O6 |
| 7   | E     | 414 | NAG  | C4-C5-C6-O6 |
| 7   | A     | 412 | NAG  | C1-C2-N2-C7 |
| 7   | E     | 414 | NAG  | O5-C5-C6-O6 |

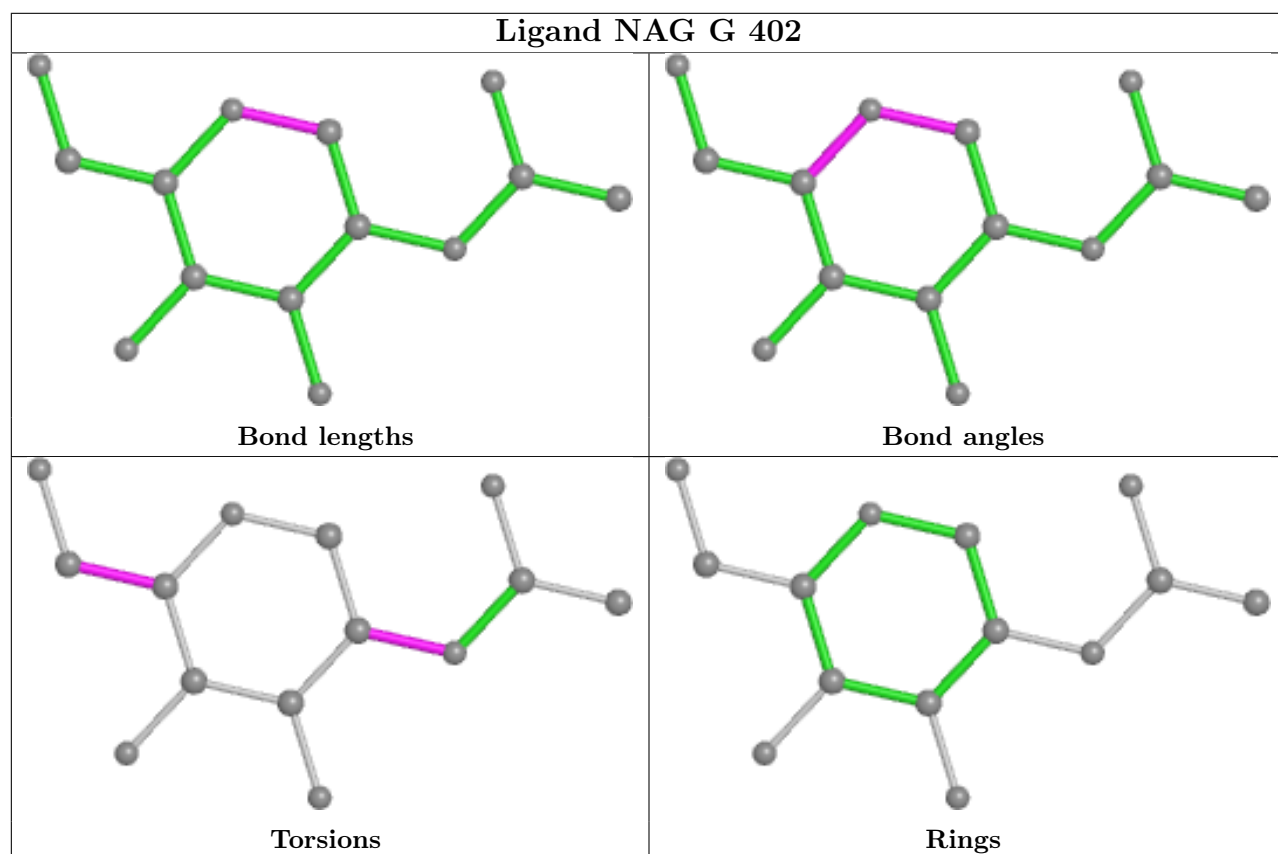
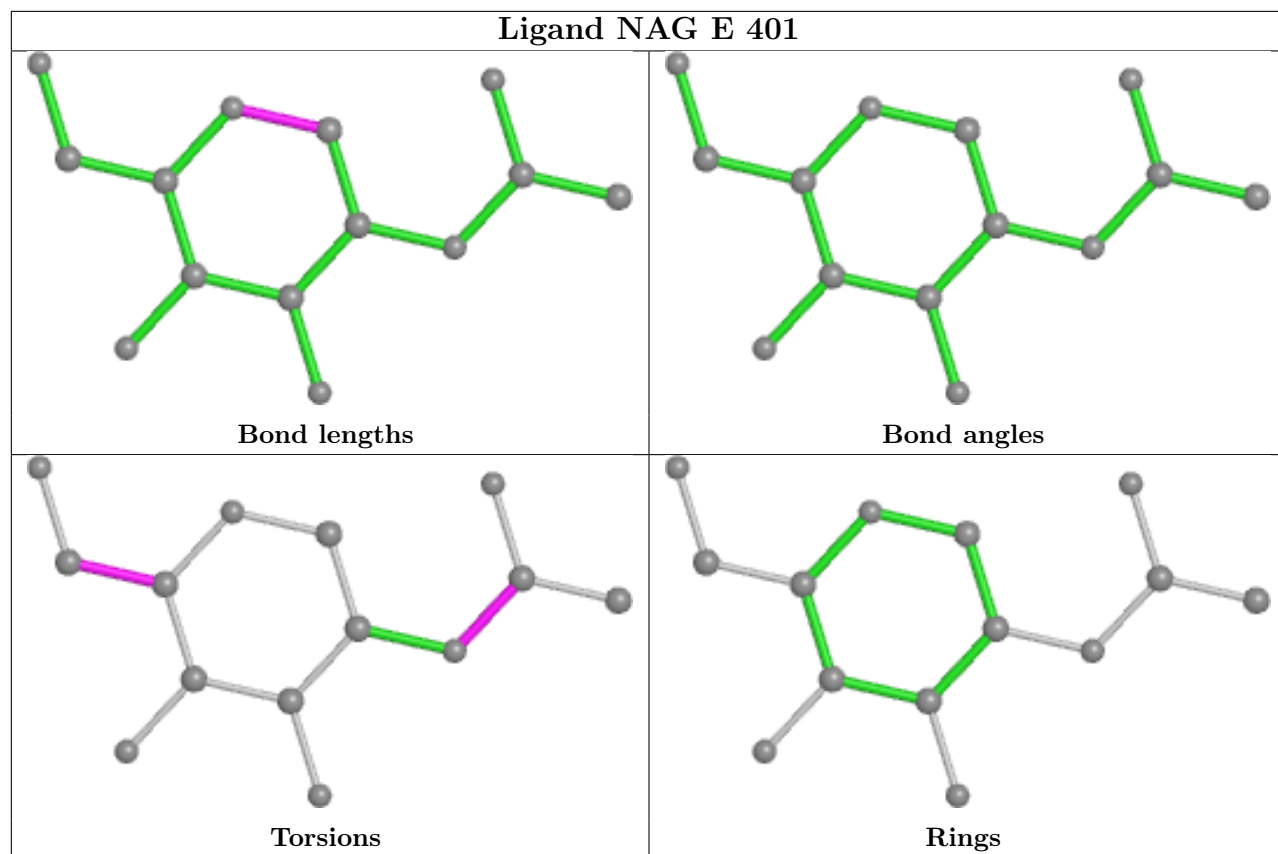
There are no ring outliers.

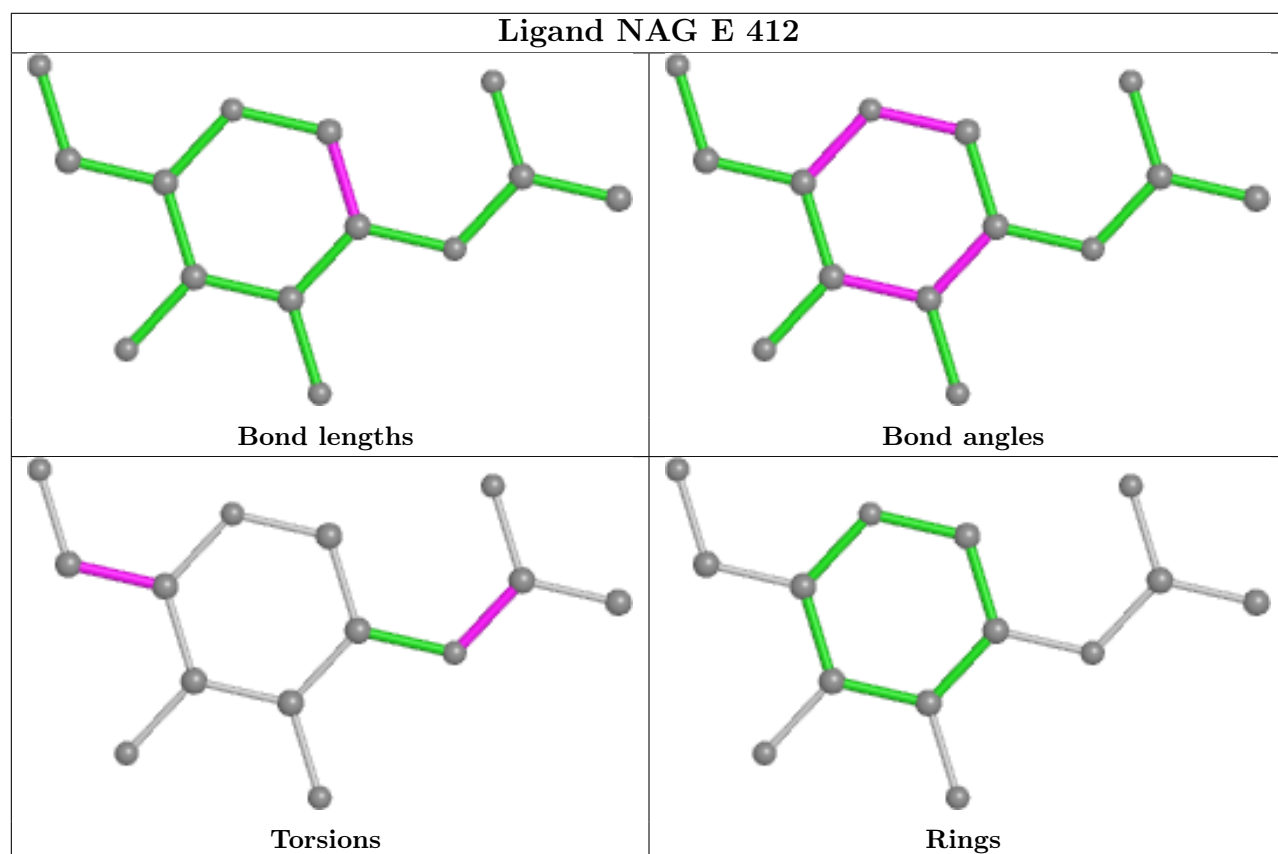
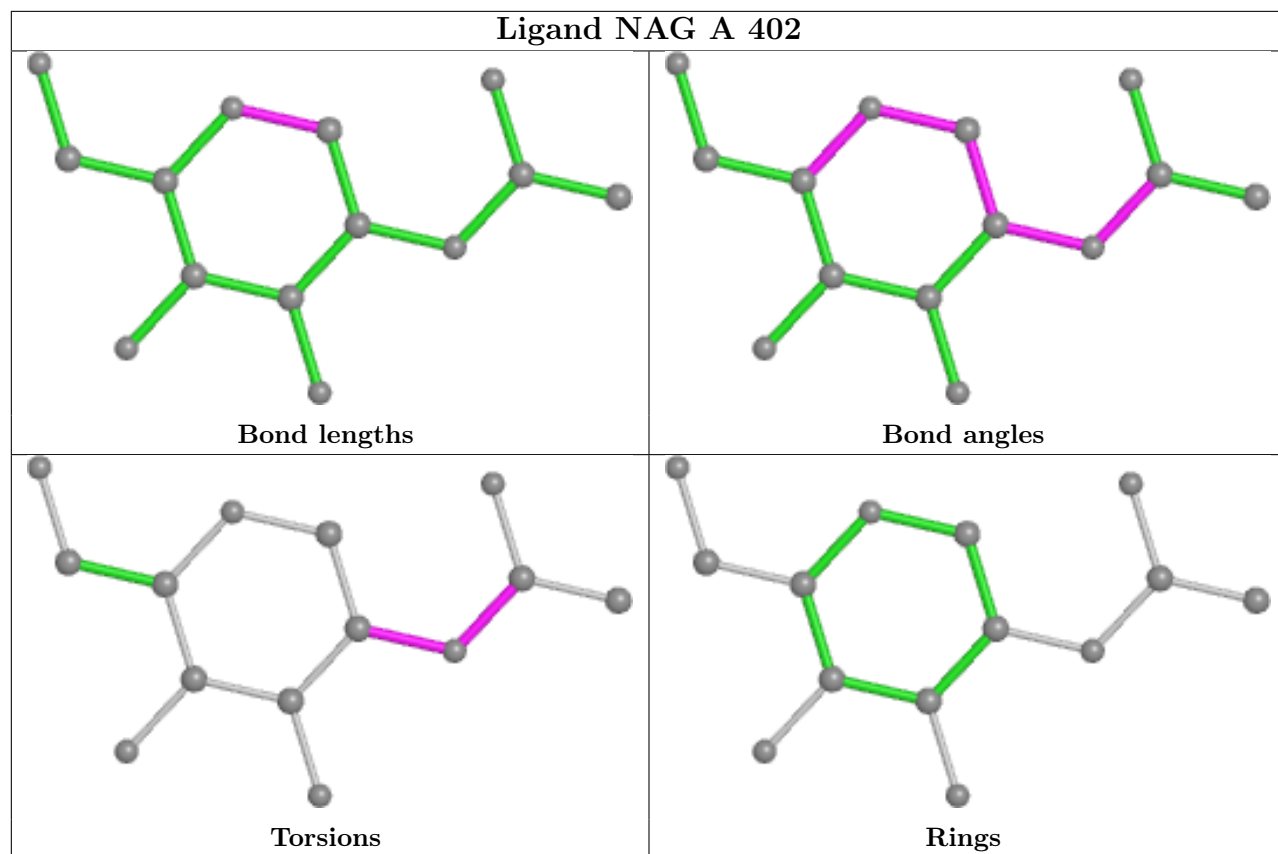
7 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | G     | 402 | NAG  | 1       | 0            |
| 7   | A     | 402 | NAG  | 1       | 0            |
| 7   | K     | 401 | NAG  | 1       | 0            |
| 7   | A     | 414 | NAG  | 2       | 0            |
| 7   | A     | 413 | NAG  | 1       | 0            |
| 7   | C     | 409 | NAG  | 1       | 0            |
| 7   | I     | 409 | NAG  | 1       | 0            |

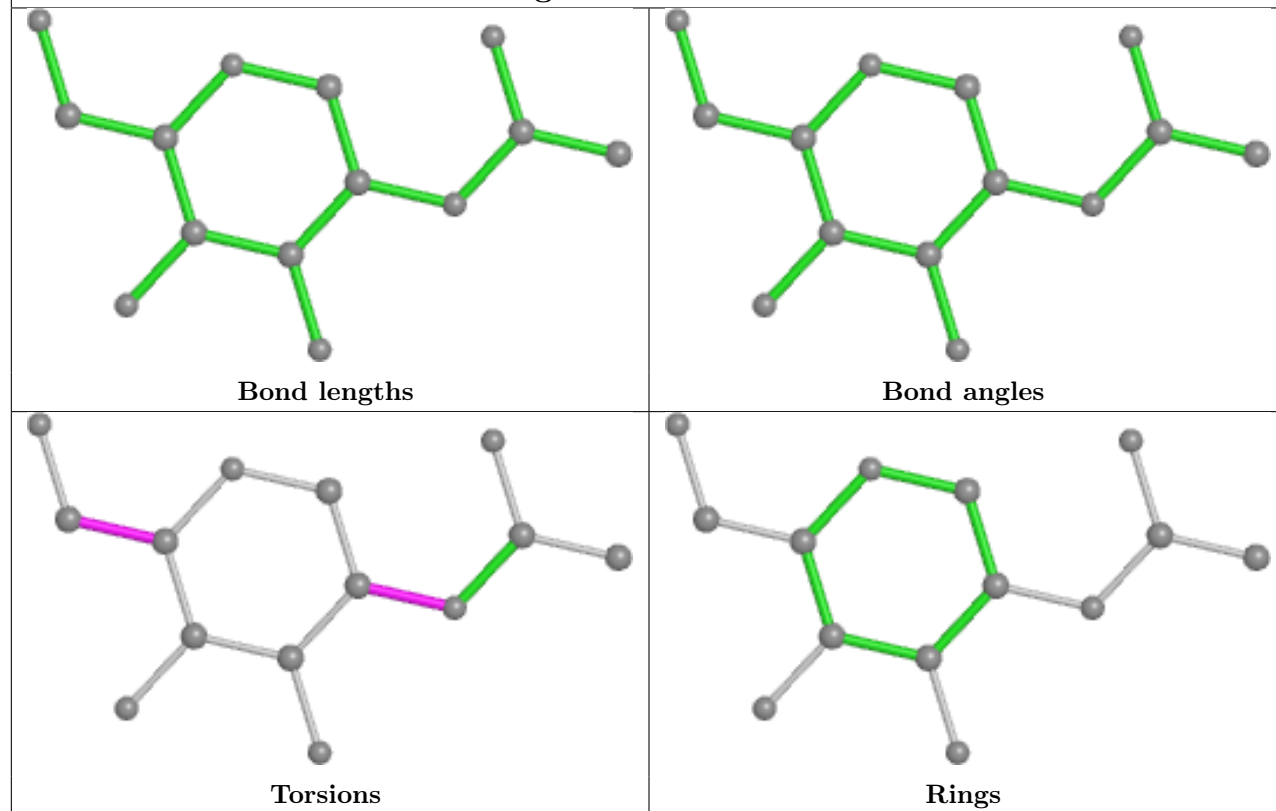
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



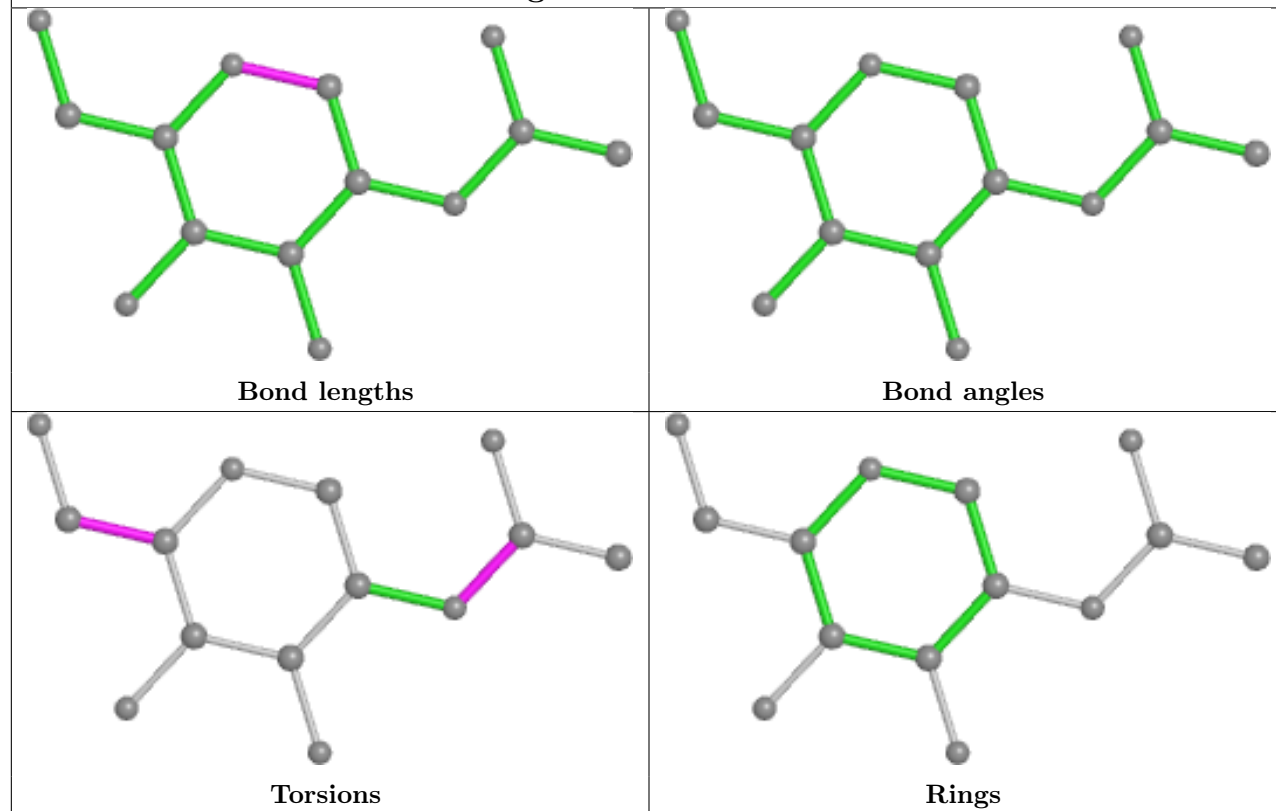




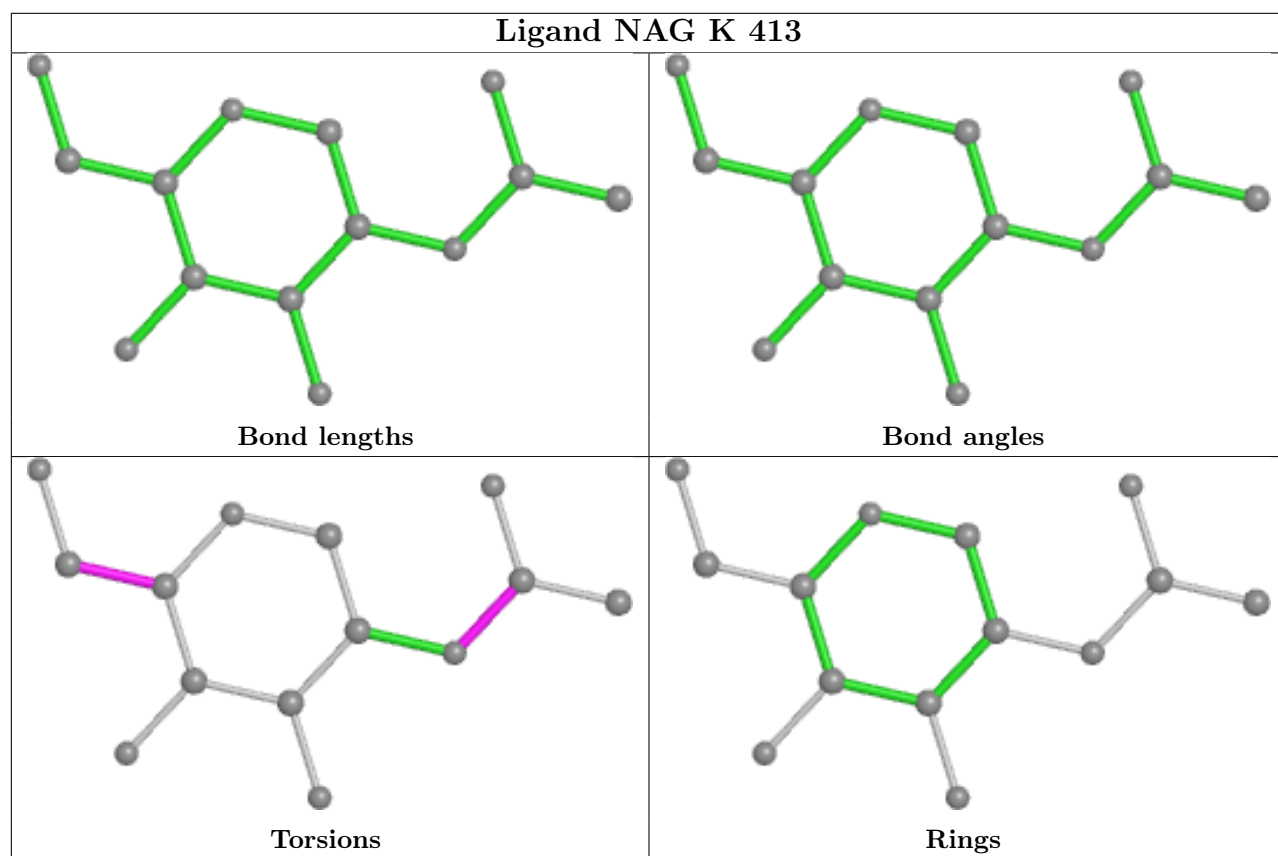
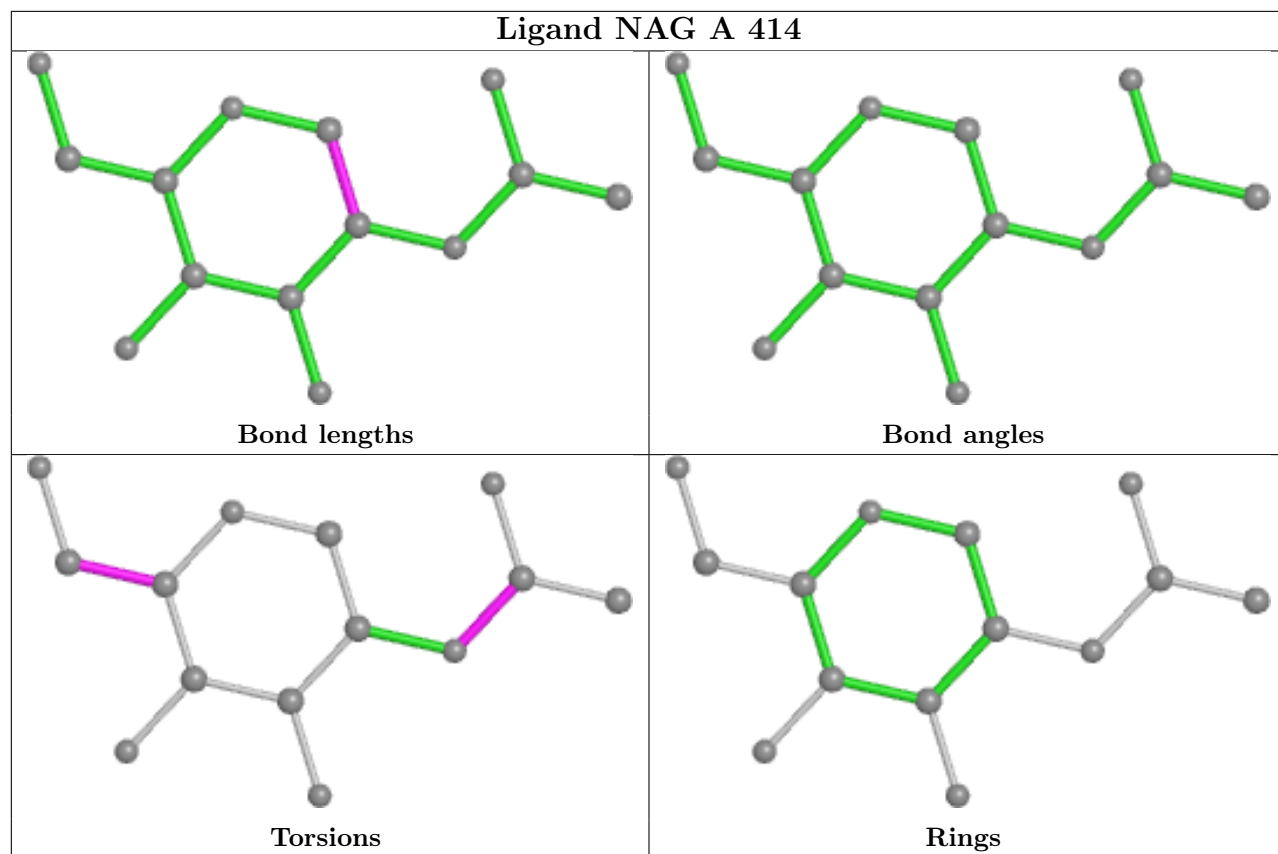
## Ligand NAG I 410

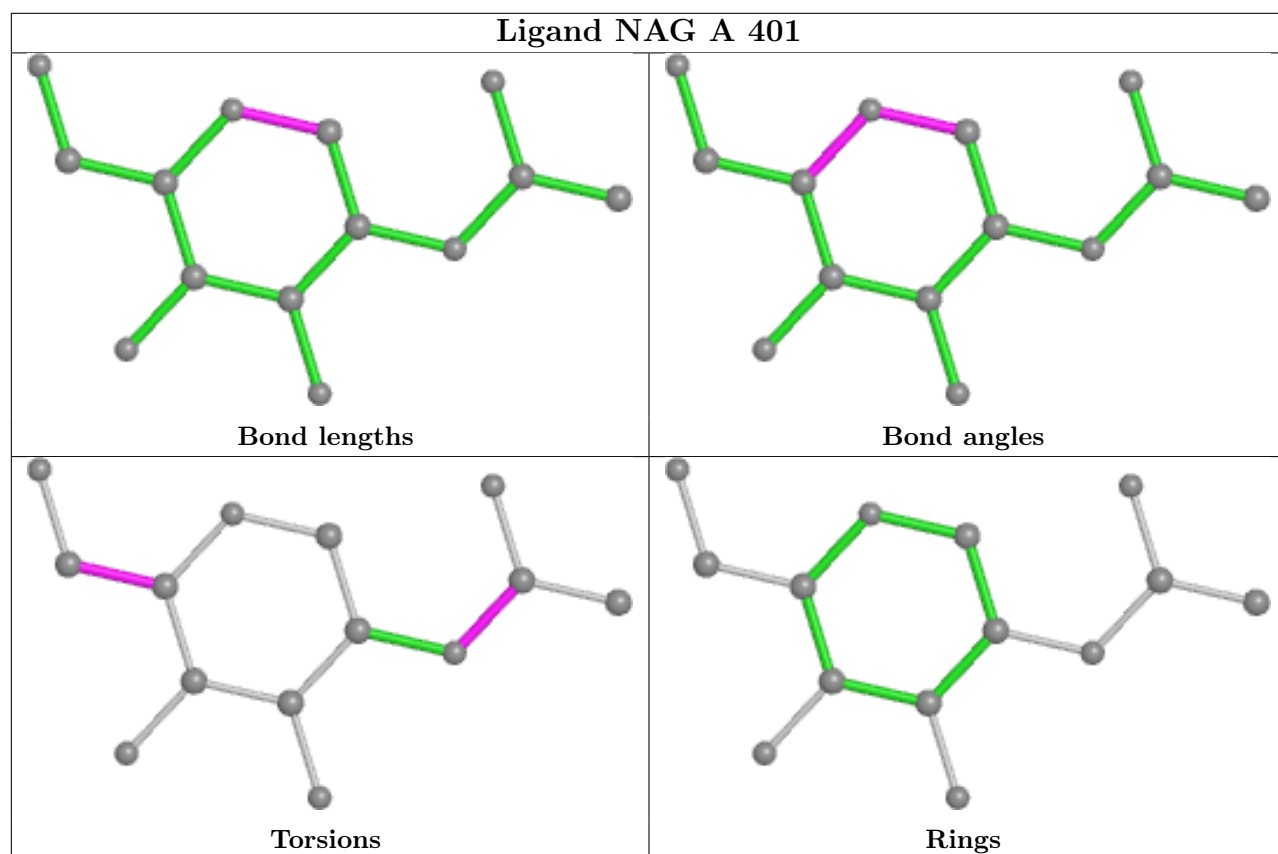
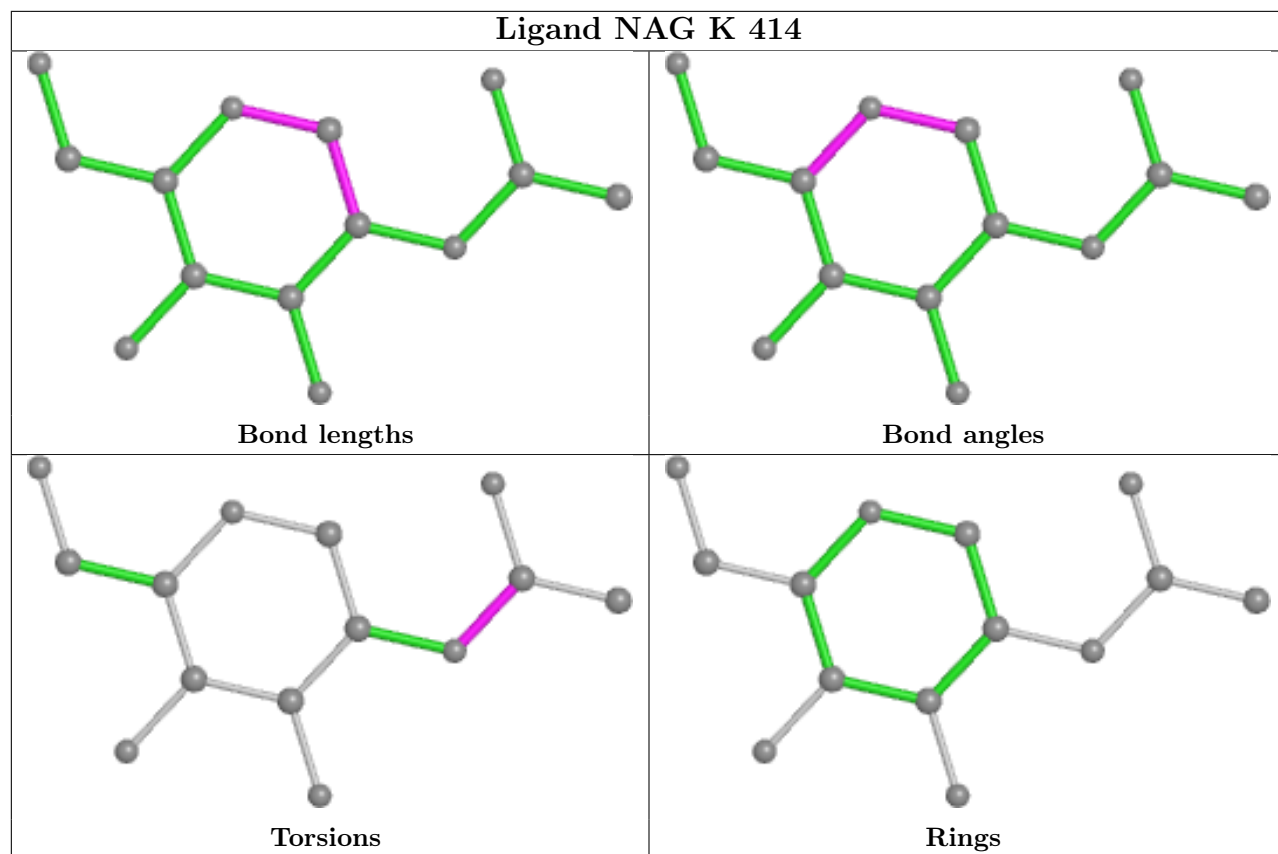


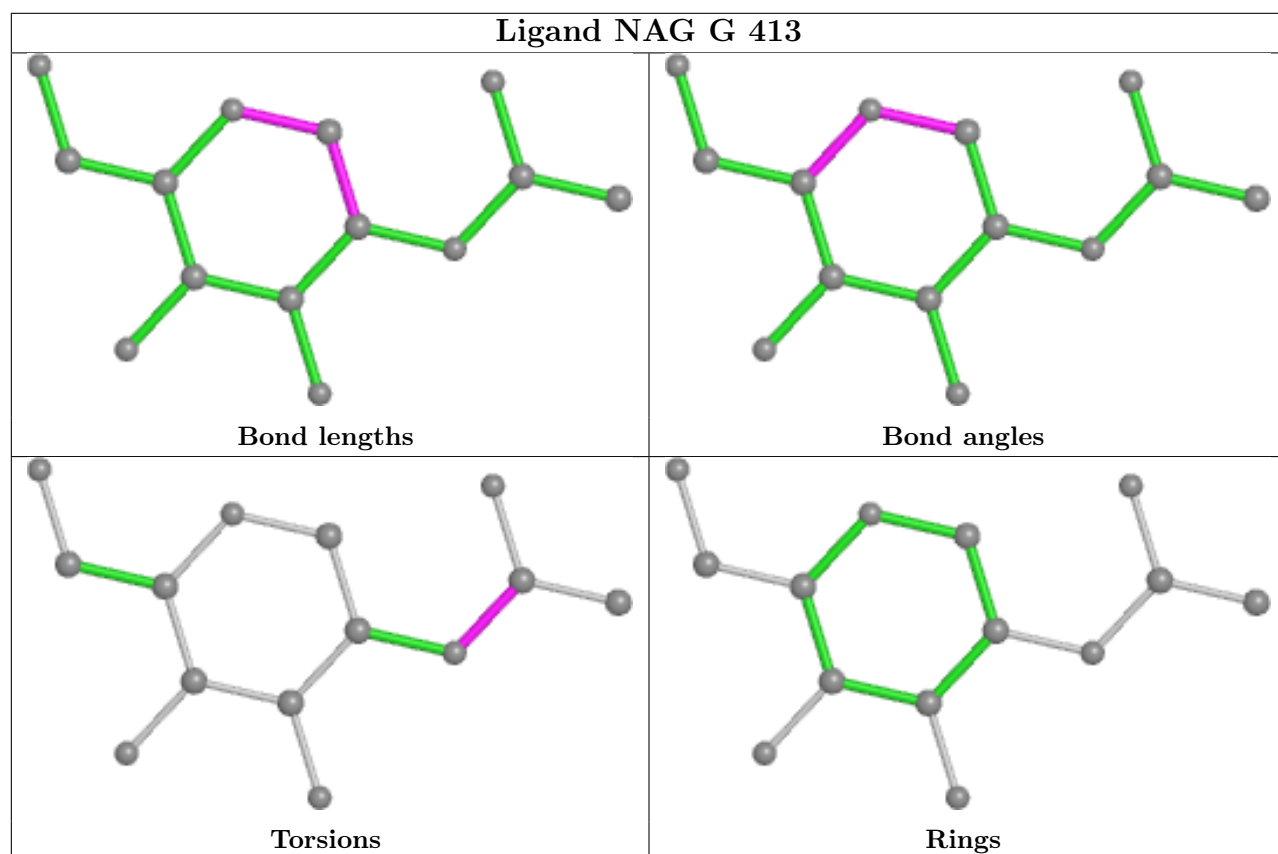
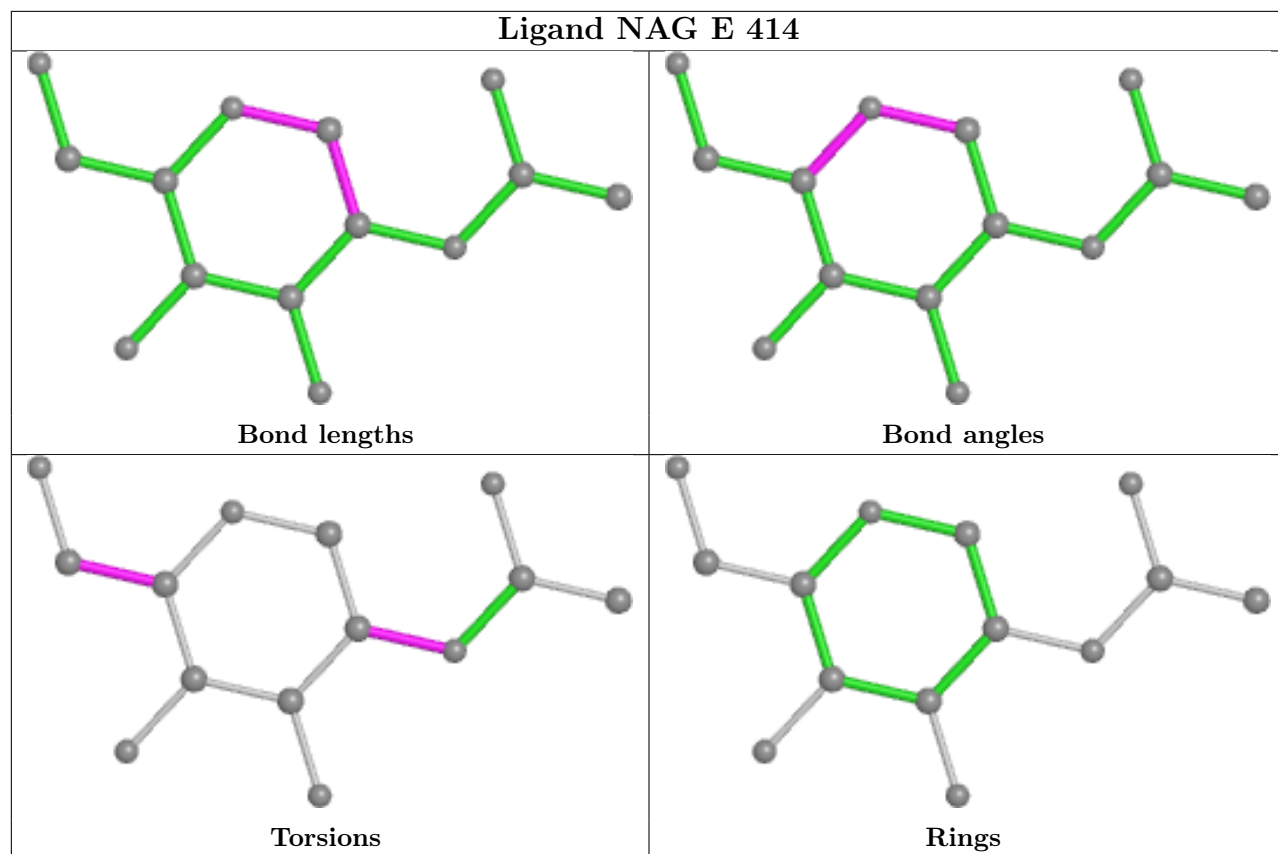
## Ligand NAG K 401



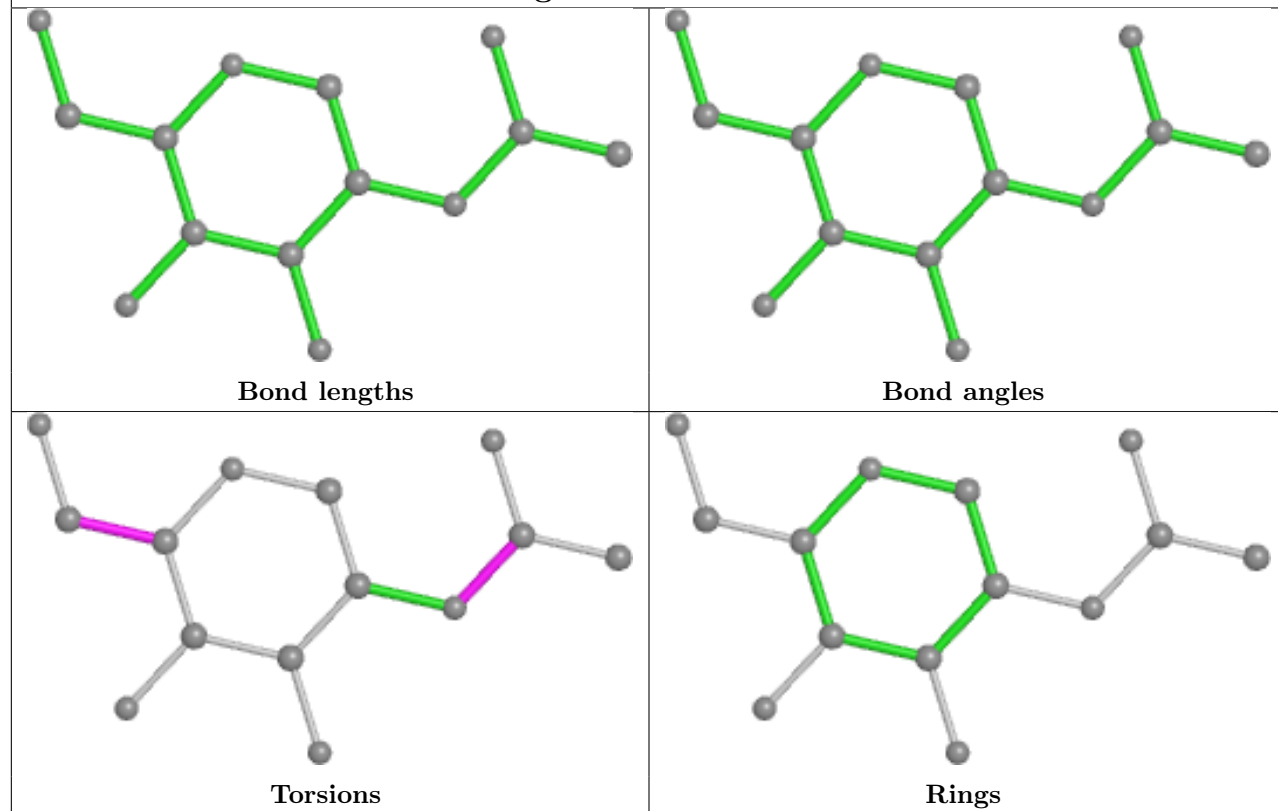




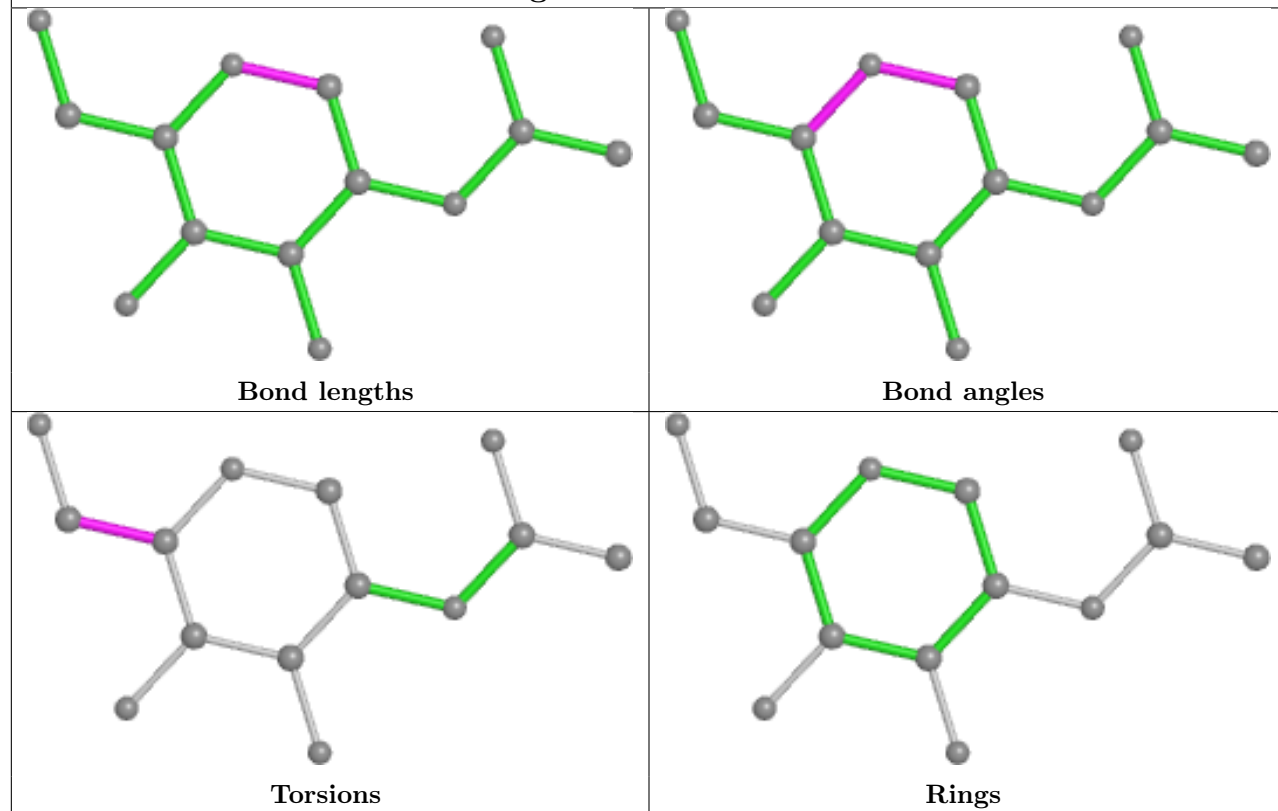


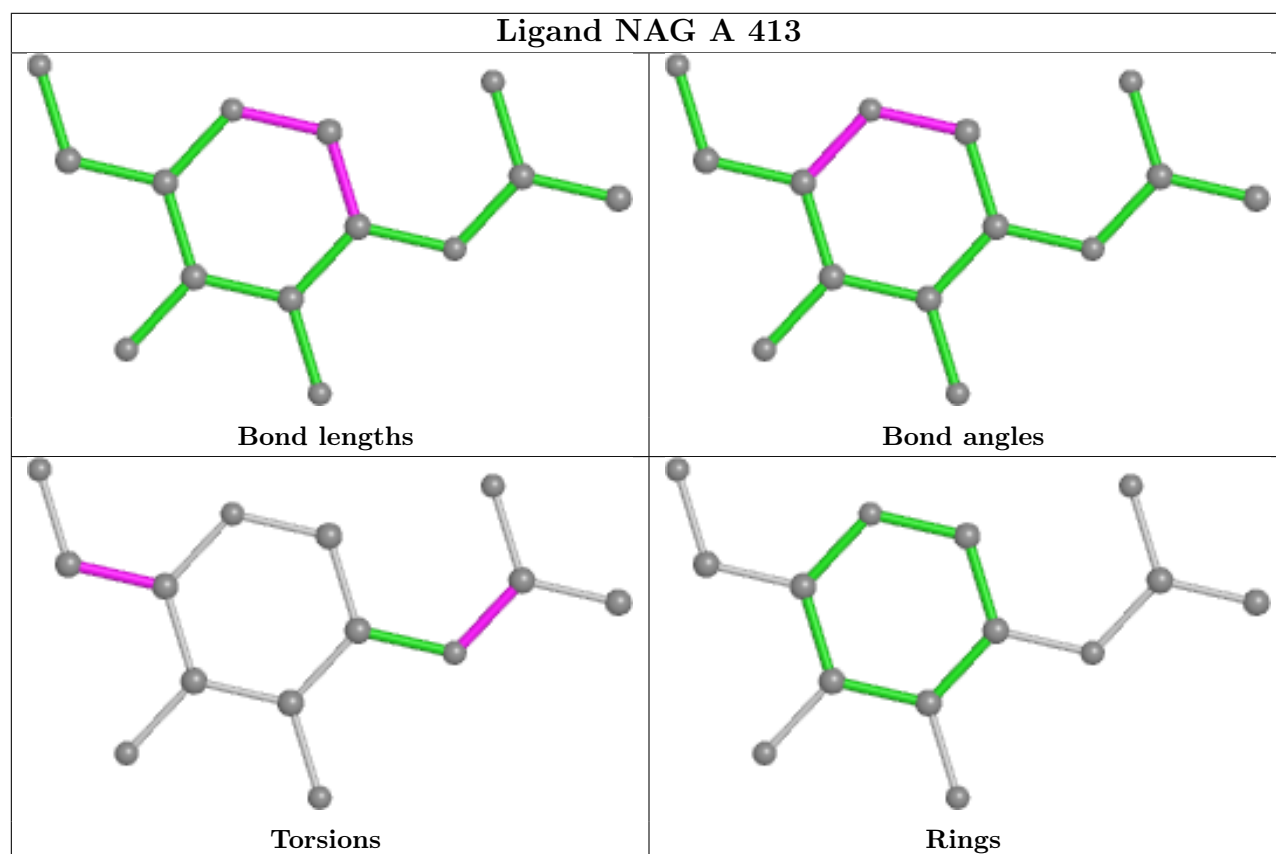
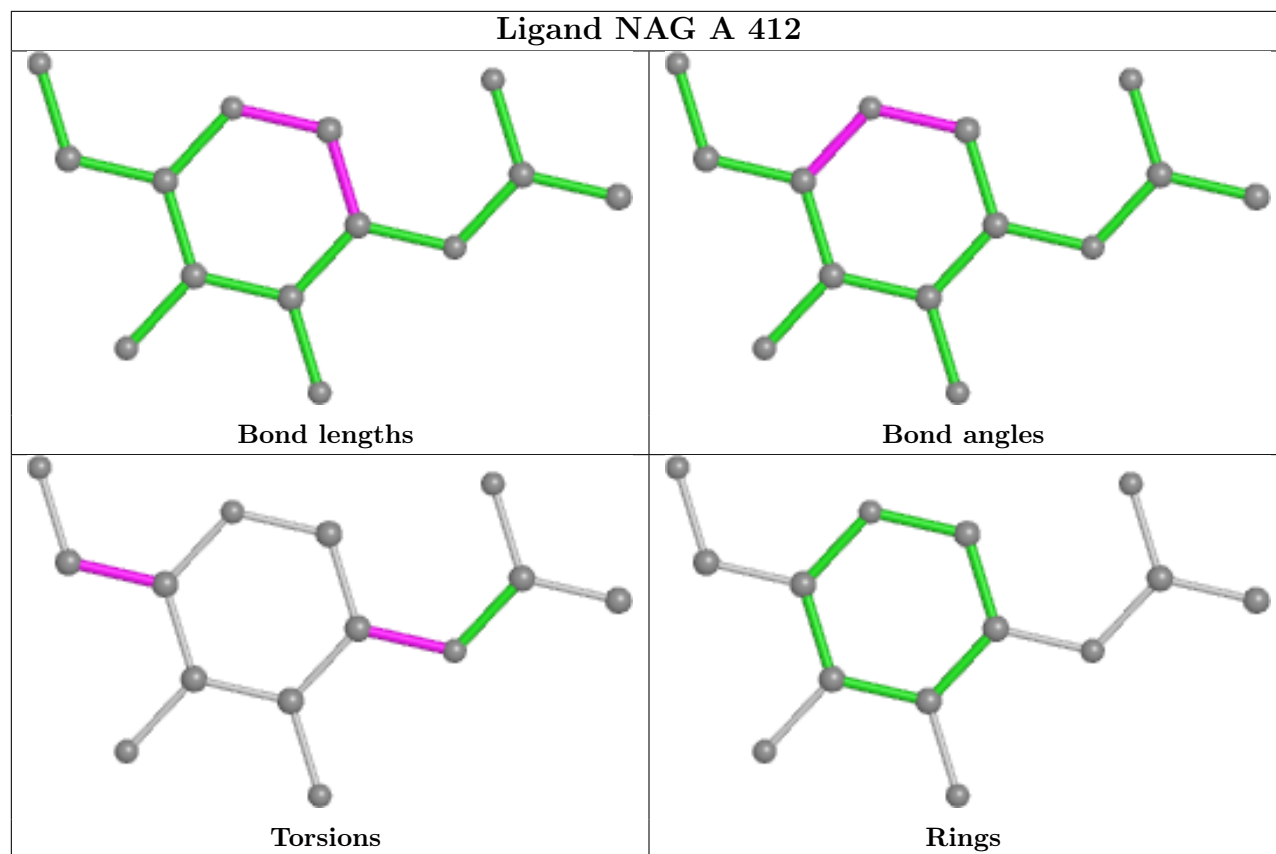


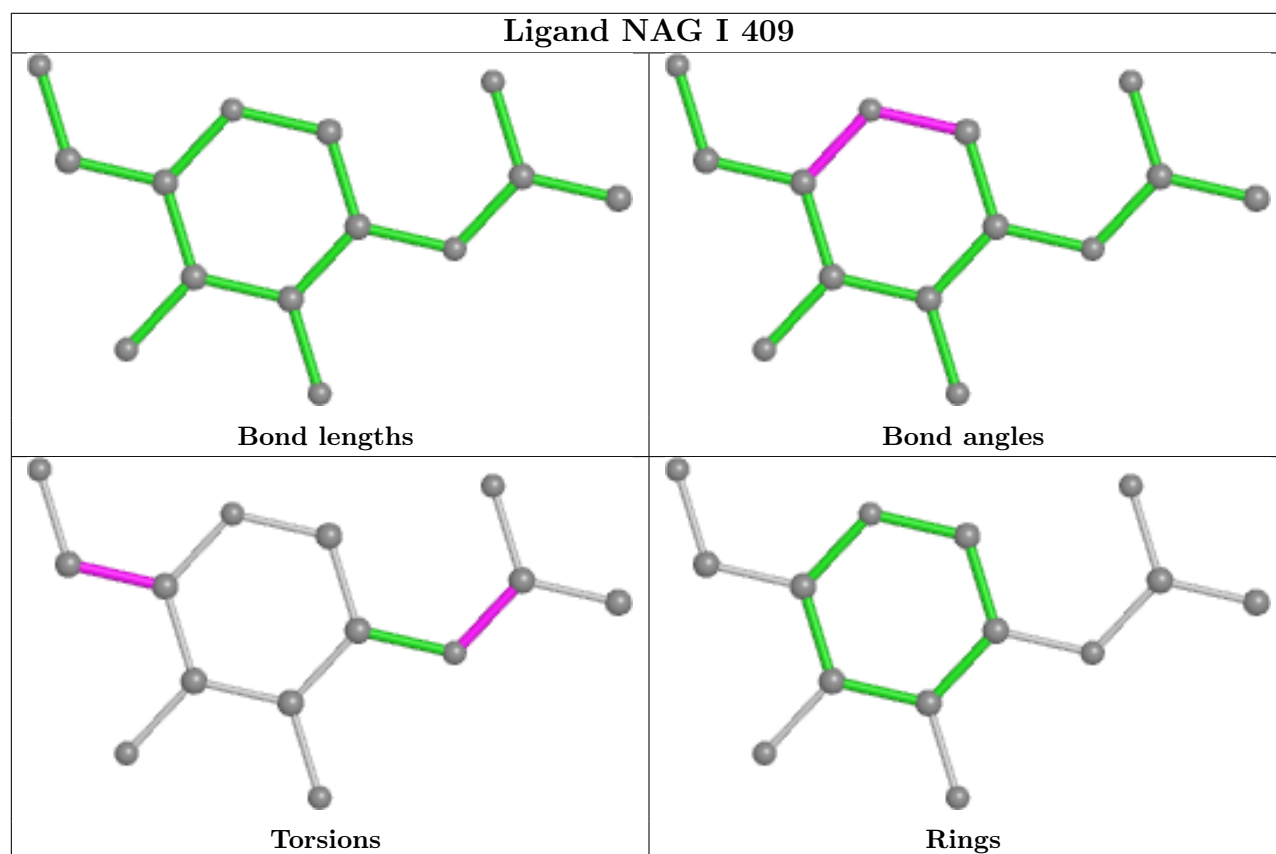
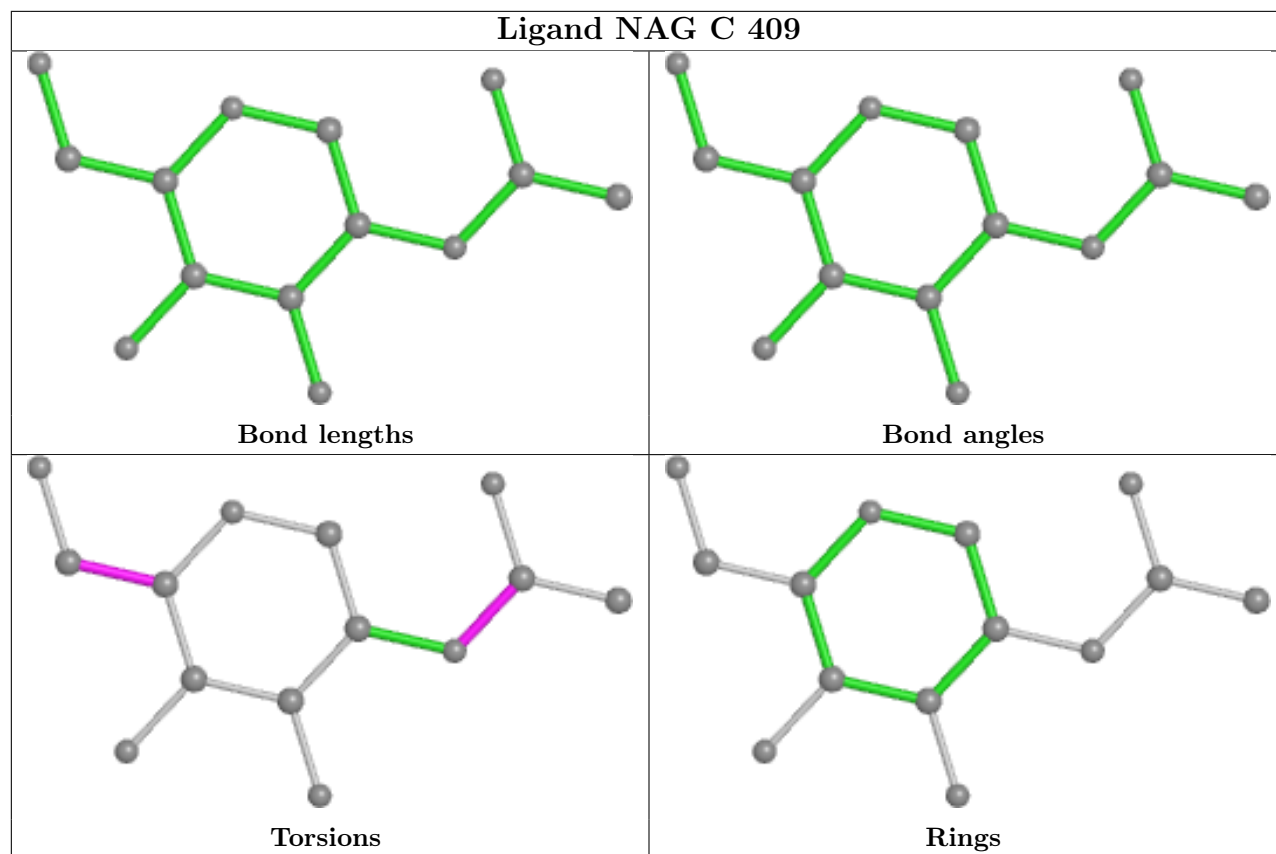
## Ligand NAG I 401



## Ligand NAG E 413







## 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 321/330 (97%)   | -0.16  | 7 (2%) 62 52   | 20, 54, 117, 244      | 0     |
| 1   | C     | 321/330 (97%)   | -0.17  | 5 (1%) 72 63   | 26, 54, 108, 183      | 0     |
| 1   | E     | 321/330 (97%)   | -0.29  | 1 (0%) 94 93   | 19, 57, 93, 133       | 0     |
| 1   | G     | 320/330 (96%)   | -0.26  | 0 100 100      | 28, 56, 92, 143       | 0     |
| 1   | I     | 320/330 (96%)   | -0.13  | 9 (2%) 53 41   | 25, 58, 122, 170      | 0     |
| 1   | K     | 321/330 (97%)   | -0.23  | 8 (2%) 57 46   | 26, 54, 103, 176      | 0     |
| 2   | B     | 165/183 (90%)   | 0.48   | 19 (11%) 4 4   | 37, 117, 172, 201     | 0     |
| 2   | D     | 165/183 (90%)   | 0.79   | 29 (17%) 1 1   | 35, 121, 195, 238     | 0     |
| 2   | F     | 165/183 (90%)   | 0.21   | 10 (6%) 21 14  | 31, 94, 155, 206      | 0     |
| 2   | H     | 165/183 (90%)   | 0.23   | 10 (6%) 21 14  | 31, 82, 131, 177      | 0     |
| 2   | J     | 165/183 (90%)   | 0.78   | 23 (13%) 2 2   | 34, 112, 180, 205     | 0     |
| 2   | L     | 165/183 (90%)   | 0.34   | 10 (6%) 21 14  | 34, 95, 153, 186      | 0     |
| All | All   | 2914/3078 (94%) | 0.02   | 131 (4%) 33 23 | 19, 65, 150, 244      | 0     |

All (131) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 6   | GLY  | 9.5  |
| 2   | J     | 156 | THR  | 8.7  |
| 2   | J     | 163 | SER  | 8.4  |
| 2   | B     | 134 | GLY  | 8.0  |
| 2   | B     | 143 | LYS  | 7.3  |
| 2   | H     | 156 | THR  | 7.0  |
| 1   | A     | 323 | ILE  | 6.9  |
| 2   | D     | 156 | THR  | 6.5  |
| 1   | C     | 323 | ILE  | 6.0  |
| 2   | B     | 156 | THR  | 5.3  |
| 2   | D     | 34  | TYR  | 5.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 23  | GLY  | 4.6  |
| 2   | D     | 23  | GLY  | 4.6  |
| 1   | K     | 5   | ILE  | 4.3  |
| 1   | A     | 4   | CYS  | 4.2  |
| 2   | L     | 138 | PHE  | 4.2  |
| 2   | F     | 147 | GLU  | 4.2  |
| 2   | F     | 160 | PRO  | 4.2  |
| 1   | K     | 323 | ILE  | 4.1  |
| 2   | D     | 35  | ALA  | 4.1  |
| 1   | I     | 31  | ASN  | 4.1  |
| 2   | J     | 154 | ASN  | 4.1  |
| 2   | J     | 138 | PHE  | 4.0  |
| 2   | D     | 4   | GLY  | 3.9  |
| 1   | E     | 11  | ASN  | 3.8  |
| 2   | D     | 30  | GLN  | 3.8  |
| 1   | K     | 6   | GLY  | 3.7  |
| 2   | F     | 131 | LYS  | 3.7  |
| 2   | H     | 163 | SER  | 3.7  |
| 2   | D     | 160 | PRO  | 3.6  |
| 2   | J     | 155 | GLY  | 3.6  |
| 2   | B     | 139 | GLU  | 3.6  |
| 2   | L     | 1   | GLY  | 3.6  |
| 2   | J     | 109 | ASP  | 3.6  |
| 2   | J     | 1   | GLY  | 3.6  |
| 2   | D     | 22  | TYR  | 3.6  |
| 2   | D     | 31  | GLY  | 3.6  |
| 2   | D     | 2   | LEU  | 3.6  |
| 2   | L     | 154 | ASN  | 3.5  |
| 2   | J     | 164 | GLU  | 3.4  |
| 2   | J     | 19  | ASP  | 3.4  |
| 2   | J     | 31  | GLY  | 3.4  |
| 2   | D     | 144 | CYS  | 3.4  |
| 2   | D     | 19  | ASP  | 3.4  |
| 2   | J     | 32  | SER  | 3.4  |
| 1   | A     | 5   | ILE  | 3.3  |
| 1   | I     | 3   | ILE  | 3.3  |
| 2   | B     | 135 | ASN  | 3.3  |
| 1   | K     | 322 | SER  | 3.3  |
| 2   | D     | 36  | ALA  | 3.3  |
| 1   | C     | 23  | ASN  | 3.3  |
| 2   | B     | 15  | THR  | 3.2  |
| 2   | B     | 138 | PHE  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 126 | LEU  | 3.2  |
| 1   | I     | 322 | SER  | 3.1  |
| 2   | J     | 139 | GLU  | 3.1  |
| 2   | B     | 141 | TYR  | 3.1  |
| 2   | H     | 33  | GLY  | 3.0  |
| 2   | D     | 157 | TYR  | 3.0  |
| 1   | A     | 7   | TYR  | 3.0  |
| 2   | L     | 163 | SER  | 3.0  |
| 2   | D     | 143 | LYS  | 2.9  |
| 1   | A     | 3   | ILE  | 2.9  |
| 2   | F     | 21  | TRP  | 2.9  |
| 2   | J     | 140 | PHE  | 2.9  |
| 2   | J     | 30  | GLN  | 2.9  |
| 2   | J     | 35  | ALA  | 2.9  |
| 2   | J     | 20  | GLY  | 2.9  |
| 2   | D     | 158 | ASP  | 2.8  |
| 2   | B     | 30  | GLN  | 2.8  |
| 1   | K     | 4   | CYS  | 2.8  |
| 2   | J     | 33  | GLY  | 2.7  |
| 2   | H     | 140 | PHE  | 2.7  |
| 2   | B     | 38  | GLN  | 2.7  |
| 2   | D     | 1   | GLY  | 2.7  |
| 2   | L     | 25  | HIS  | 2.7  |
| 1   | I     | 9   | ALA  | 2.7  |
| 2   | B     | 163 | SER  | 2.7  |
| 2   | H     | 131 | LYS  | 2.6  |
| 2   | D     | 38  | GLN  | 2.6  |
| 2   | J     | 160 | PRO  | 2.6  |
| 2   | B     | 154 | ASN  | 2.6  |
| 2   | B     | 126 | LEU  | 2.6  |
| 1   | I     | 321 | PRO  | 2.6  |
| 1   | I     | 4   | CYS  | 2.6  |
| 1   | I     | 289 | LEU  | 2.6  |
| 2   | B     | 31  | GLY  | 2.5  |
| 2   | H     | 141 | TYR  | 2.5  |
| 2   | J     | 27  | GLN  | 2.5  |
| 2   | J     | 34  | TYR  | 2.5  |
| 1   | K     | 321 | PRO  | 2.5  |
| 1   | A     | 322 | SER  | 2.5  |
| 2   | D     | 127 | LYS  | 2.5  |
| 2   | J     | 143 | LYS  | 2.5  |
| 1   | C     | 213 | ILE  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 25  | HIS  | 2.4  |
| 1   | C     | 188 | ARG  | 2.4  |
| 1   | C     | 4   | CYS  | 2.4  |
| 1   | I     | 8   | HIS  | 2.4  |
| 2   | L     | 141 | TYR  | 2.3  |
| 2   | L     | 140 | PHE  | 2.3  |
| 2   | D     | 20  | GLY  | 2.3  |
| 2   | L     | 29  | GLU  | 2.3  |
| 2   | B     | 35  | ALA  | 2.3  |
| 2   | F     | 19  | ASP  | 2.3  |
| 2   | F     | 31  | GLY  | 2.3  |
| 2   | D     | 146 | ASP  | 2.2  |
| 1   | I     | 36  | SER  | 2.2  |
| 2   | L     | 128 | ASN  | 2.2  |
| 2   | D     | 32  | SER  | 2.2  |
| 2   | B     | 1   | GLY  | 2.2  |
| 2   | H     | 19  | ASP  | 2.2  |
| 2   | L     | 27  | GLN  | 2.2  |
| 1   | K     | 30  | VAL  | 2.2  |
| 2   | D     | 11  | GLU  | 2.2  |
| 2   | H     | 132 | GLU  | 2.1  |
| 2   | B     | 128 | ASN  | 2.1  |
| 2   | B     | 125 | GLN  | 2.1  |
| 2   | B     | 140 | PHE  | 2.1  |
| 2   | D     | 109 | ASP  | 2.1  |
| 2   | F     | 134 | GLY  | 2.1  |
| 2   | D     | 154 | ASN  | 2.1  |
| 1   | K     | 195 | ASN  | 2.1  |
| 2   | H     | 130 | ALA  | 2.0  |
| 2   | F     | 132 | GLU  | 2.0  |
| 2   | D     | 5   | ALA  | 2.0  |
| 2   | J     | 3   | PHE  | 2.0  |
| 2   | H     | 34  | TYR  | 2.0  |
| 2   | D     | 37  | ASP  | 2.0  |
| 2   | F     | 163 | SER  | 2.0  |
| 2   | D     | 16  | GLY  | 2.0  |

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

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

### 6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | MAN  | S     | 4   | 11/12 | 0.66 | 0.47 | 75,91,111,113              | 0     |
| 3   | MAN  | V     | 4   | 11/12 | 0.72 | 0.26 | 78,108,117,120             | 0     |
| 4   | MAN  | N     | 4   | 11/12 | 0.72 | 0.21 | 82,115,129,130             | 0     |
| 3   | MAN  | M     | 4   | 11/12 | 0.74 | 0.26 | 59,104,113,116             | 0     |
| 3   | NAG  | V     | 5   | 14/15 | 0.74 | 0.45 | 87,108,116,123             | 0     |
| 3   | MAN  | V     | 6   | 11/12 | 0.74 | 0.21 | 56,76,83,86                | 0     |
| 5   | BMA  | X     | 3   | 11/12 | 0.75 | 0.30 | 101,108,114,116            | 0     |
| 3   | NAG  | M     | 5   | 14/15 | 0.76 | 0.41 | 76,102,119,119             | 0     |
| 4   | NAG  | N     | 5   | 14/15 | 0.78 | 0.22 | 73,91,104,110              | 0     |
| 3   | BMA  | V     | 3   | 11/12 | 0.78 | 0.23 | 91,99,104,114              | 0     |
| 5   | MAN  | T     | 4   | 11/12 | 0.79 | 0.17 | 87,109,122,125             | 0     |
| 5   | BMA  | O     | 3   | 11/12 | 0.79 | 0.27 | 85,115,121,131             | 0     |
| 5   | MAN  | O     | 4   | 11/12 | 0.80 | 0.29 | 85,94,108,121              | 0     |
| 4   | BMA  | N     | 3   | 11/12 | 0.80 | 0.28 | 64,92,108,124              | 0     |
| 3   | NAG  | S     | 5   | 14/15 | 0.80 | 0.38 | 58,94,100,100              | 0     |
| 5   | NAG  | U     | 2   | 14/15 | 0.82 | 0.33 | 73,94,99,100               | 0     |
| 3   | MAN  | M     | 6   | 11/12 | 0.83 | 0.27 | 47,69,82,83                | 0     |
| 5   | MAN  | Q     | 4   | 11/12 | 0.84 | 0.40 | 67,80,105,112              | 0     |
| 3   | NAG  | V     | 2   | 14/15 | 0.84 | 0.21 | 46,65,70,71                | 0     |
| 3   | BMA  | M     | 3   | 11/12 | 0.84 | 0.23 | 75,82,103,119              | 0     |
| 5   | MAN  | R     | 4   | 11/12 | 0.84 | 0.26 | 74,98,103,107              | 0     |
| 5   | BMA  | Q     | 3   | 11/12 | 0.85 | 0.22 | 78,91,103,104              | 0     |
| 6   | BMA  | W     | 3   | 11/12 | 0.85 | 0.23 | 79,86,95,97                | 0     |
| 5   | BMA  | T     | 3   | 11/12 | 0.86 | 0.20 | 70,80,86,89                | 0     |
| 3   | NAG  | S     | 2   | 14/15 | 0.86 | 0.29 | 61,83,87,93                | 0     |
| 5   | NAG  | Q     | 2   | 14/15 | 0.86 | 0.26 | 73,83,91,98                | 0     |
| 5   | NAG  | X     | 2   | 14/15 | 0.87 | 0.22 | 68,80,92,98                | 0     |
| 4   | MAN  | P     | 4   | 11/12 | 0.87 | 0.23 | 72,91,95,108               | 0     |
| 5   | NAG  | U     | 1   | 14/15 | 0.87 | 0.24 | 61,71,92,93                | 0     |
| 6   | NAG  | W     | 2   | 14/15 | 0.88 | 0.23 | 53,92,106,115              | 0     |
| 3   | BMA  | S     | 3   | 11/12 | 0.88 | 0.42 | 60,82,98,107               | 0     |
| 5   | BMA  | U     | 3   | 11/12 | 0.88 | 0.21 | 59,68,74,78                | 0     |
| 3   | MAN  | S     | 6   | 11/12 | 0.88 | 0.21 | 35,45,52,52                | 0     |
| 3   | NAG  | M     | 2   | 14/15 | 0.88 | 0.28 | 83,94,106,108              | 0     |
| 5   | NAG  | O     | 2   | 14/15 | 0.89 | 0.22 | 60,84,97,104               | 0     |
| 4   | NAG  | N     | 2   | 14/15 | 0.89 | 0.23 | 47,61,75,88                | 0     |
| 5   | NAG  | T     | 2   | 14/15 | 0.89 | 0.23 | 52,66,72,82                | 0     |

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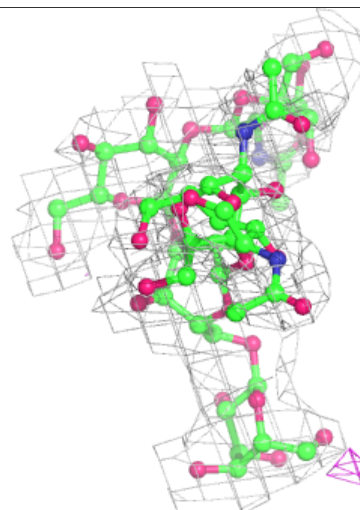
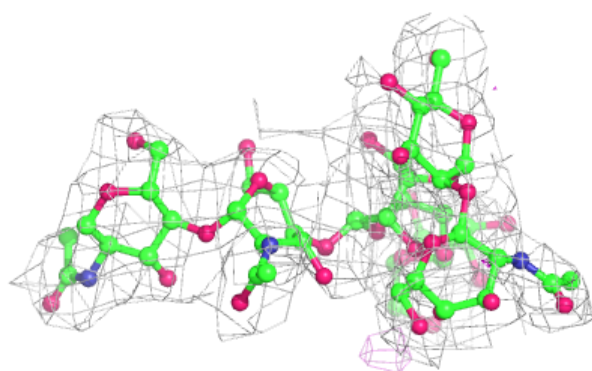
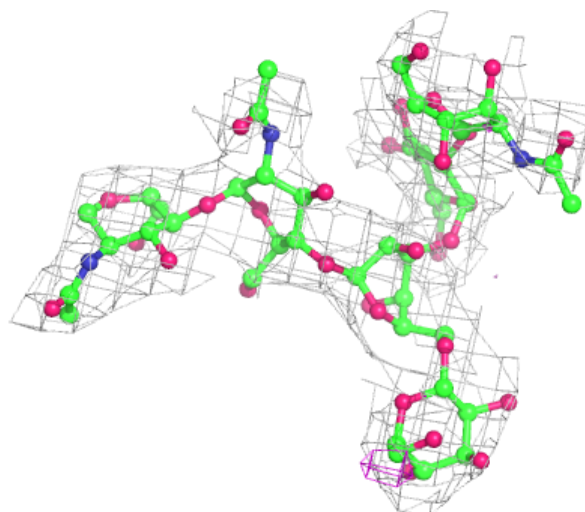
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | NAG  | Q     | 1   | 14/15 | 0.89 | 0.21 | 36,50,56,71                 | 0     |
| 4   | NAG  | P     | 2   | 14/15 | 0.90 | 0.20 | 44,52,68,69                 | 0     |
| 5   | NAG  | R     | 2   | 14/15 | 0.90 | 0.22 | 57,74,95,102                | 0     |
| 4   | BMA  | P     | 3   | 11/12 | 0.91 | 0.21 | 70,88,95,96                 | 0     |
| 3   | NAG  | S     | 1   | 14/15 | 0.91 | 0.22 | 33,62,74,79                 | 0     |
| 5   | MAN  | X     | 4   | 11/12 | 0.92 | 0.12 | 56,67,76,78                 | 0     |
| 4   | NAG  | P     | 5   | 14/15 | 0.92 | 0.16 | 55,72,77,83                 | 0     |
| 5   | BMA  | R     | 3   | 11/12 | 0.93 | 0.16 | 67,73,78,81                 | 0     |
| 5   | NAG  | T     | 1   | 14/15 | 0.93 | 0.18 | 34,49,57,63                 | 0     |
| 5   | MAN  | U     | 4   | 11/12 | 0.93 | 0.20 | 39,59,70,73                 | 0     |
| 5   | NAG  | R     | 1   | 14/15 | 0.93 | 0.16 | 37,40,44,46                 | 0     |
| 4   | NAG  | P     | 1   | 14/15 | 0.93 | 0.17 | 34,45,58,67                 | 0     |
| 5   | NAG  | O     | 1   | 14/15 | 0.93 | 0.22 | 31,52,63,73                 | 0     |
| 3   | NAG  | V     | 1   | 14/15 | 0.94 | 0.17 | 32,37,40,42                 | 0     |
| 6   | NAG  | W     | 1   | 14/15 | 0.94 | 0.15 | 53,56,60,65                 | 0     |
| 4   | NAG  | N     | 1   | 14/15 | 0.95 | 0.18 | 32,34,36,46                 | 0     |
| 3   | NAG  | M     | 1   | 14/15 | 0.95 | 0.12 | 51,54,59,59                 | 0     |
| 5   | NAG  | X     | 1   | 14/15 | 0.95 | 0.13 | 32,39,55,58                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

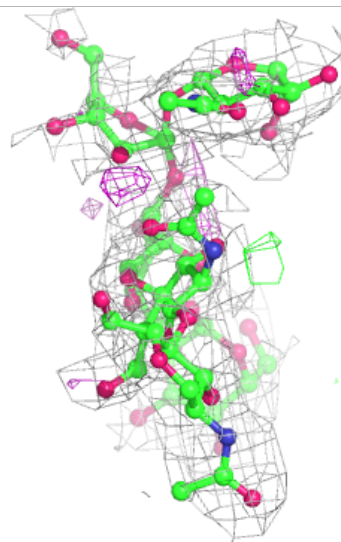
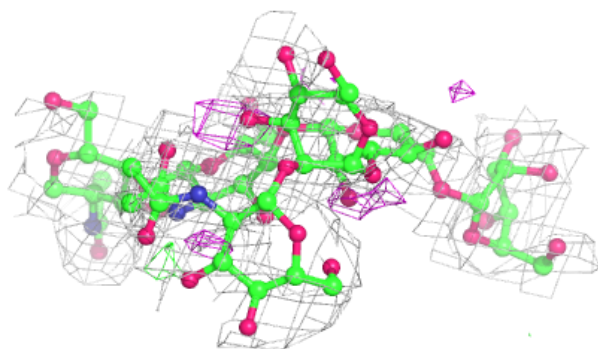
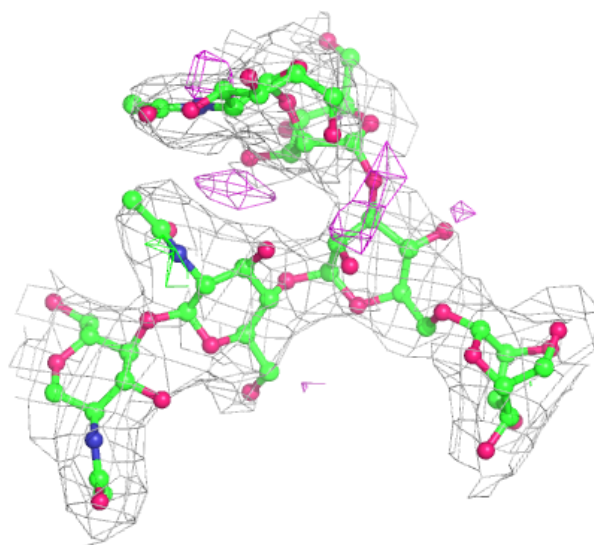
**Electron density around Chain M:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



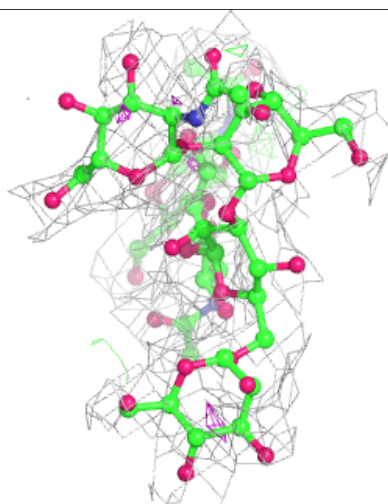
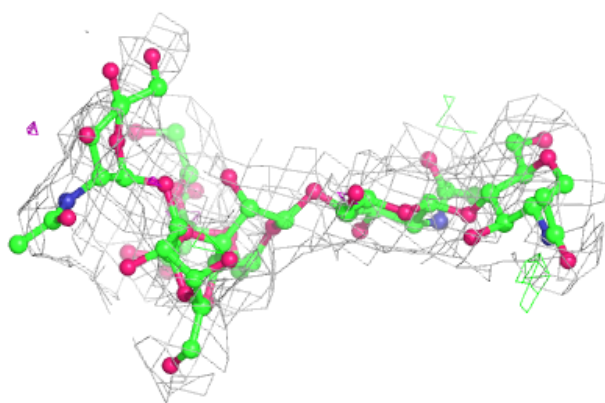
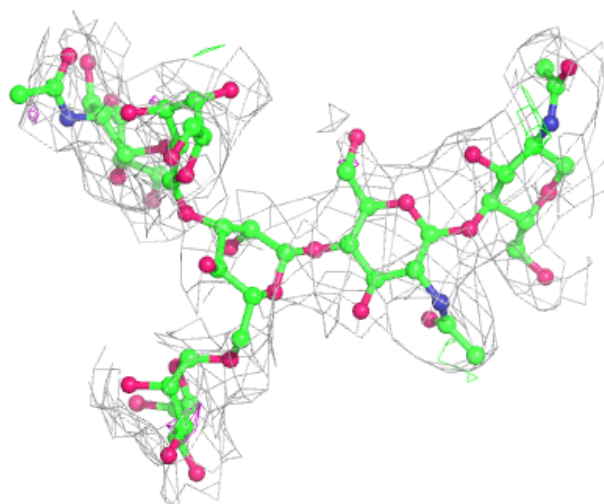
**Electron density around Chain S:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain V:**

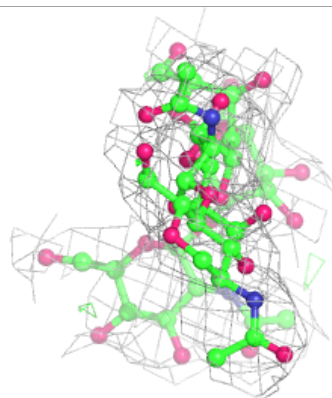
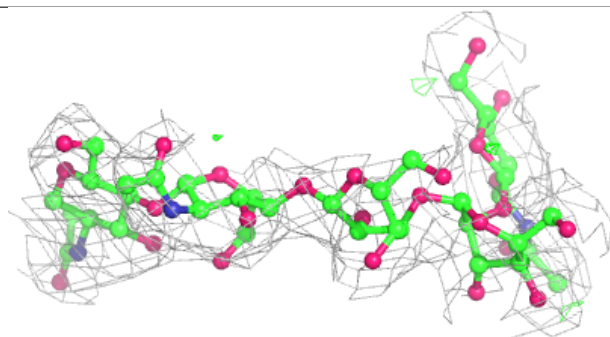
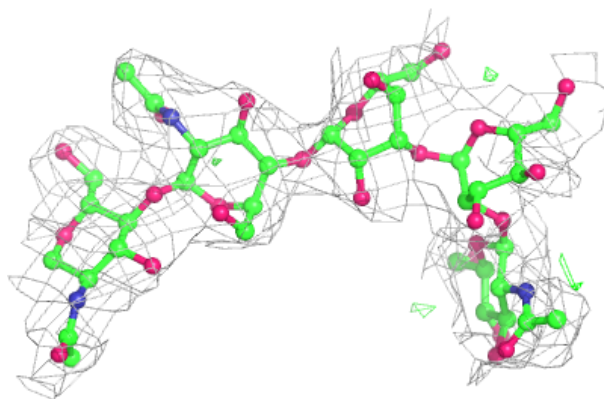
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



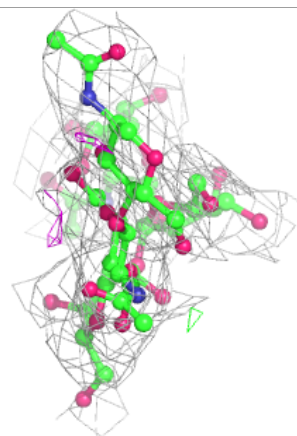
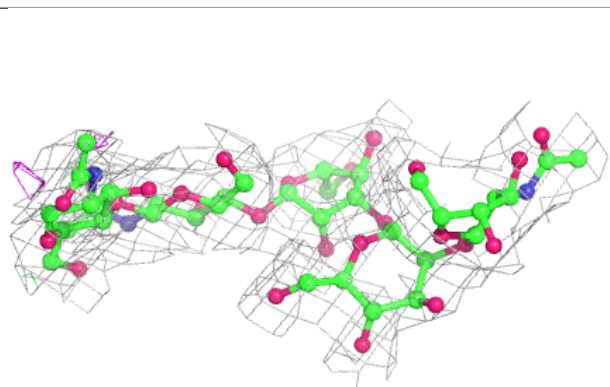
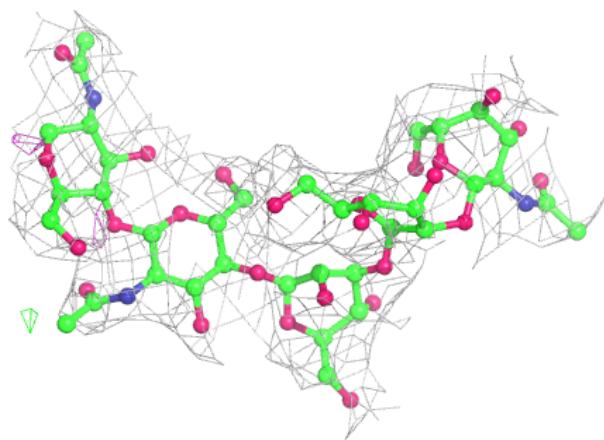


**Electron density around Chain N:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

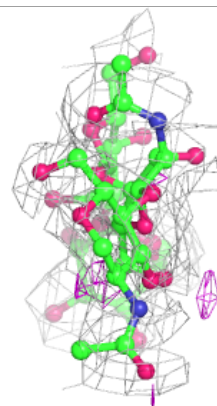
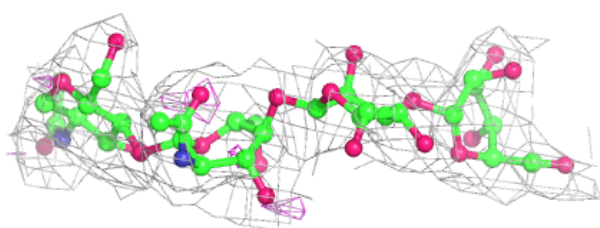
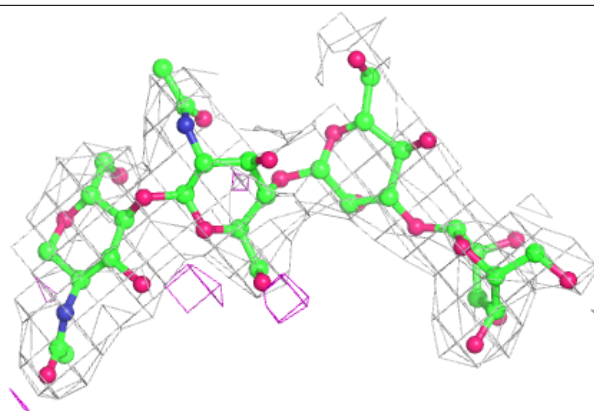
**Electron density around Chain P:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

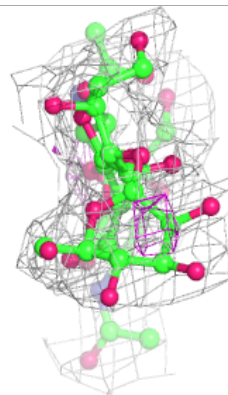
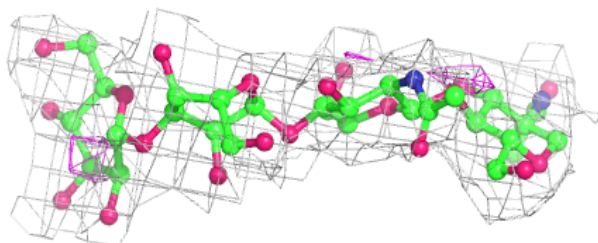
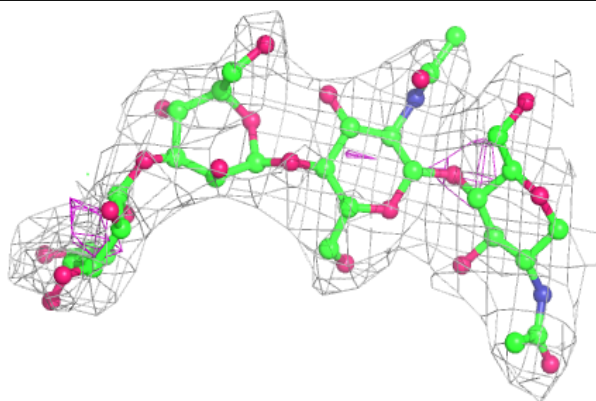


**Electron density around Chain O:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

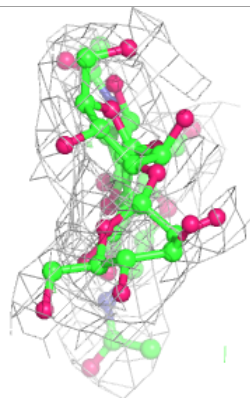
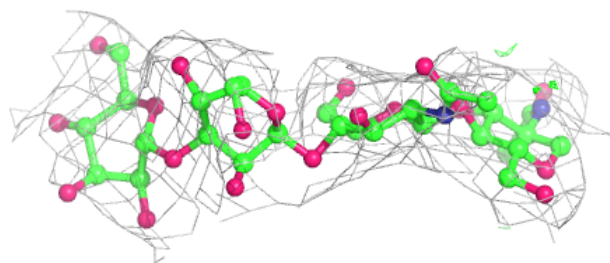
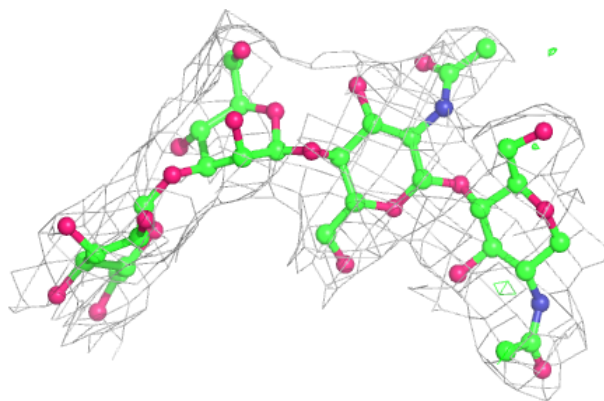
**Electron density around Chain Q:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

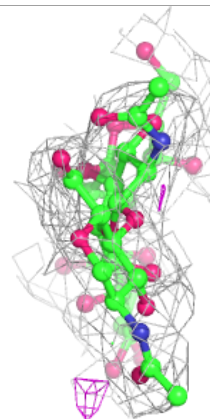
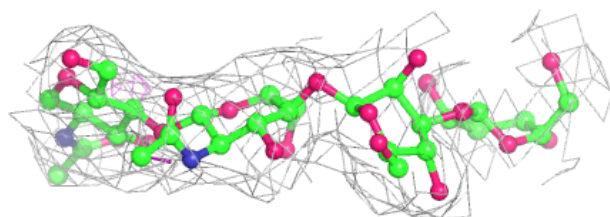
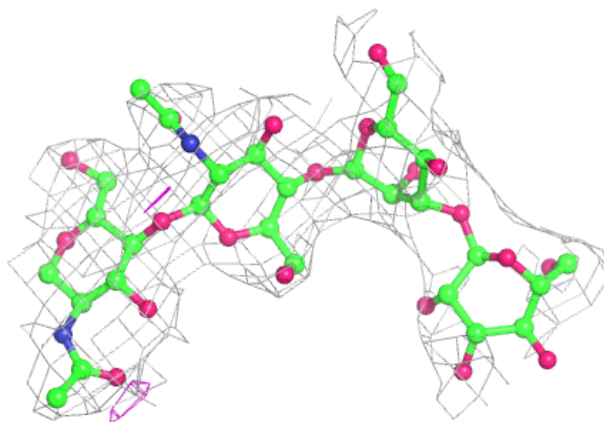


**Electron density around Chain R:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

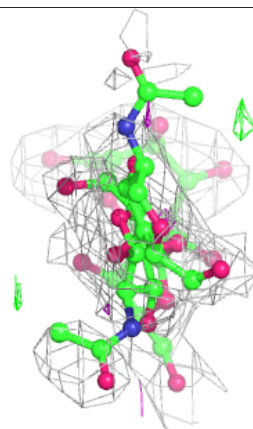
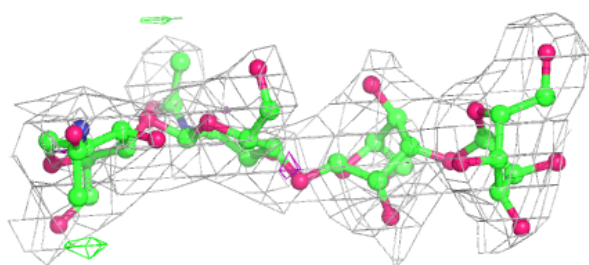
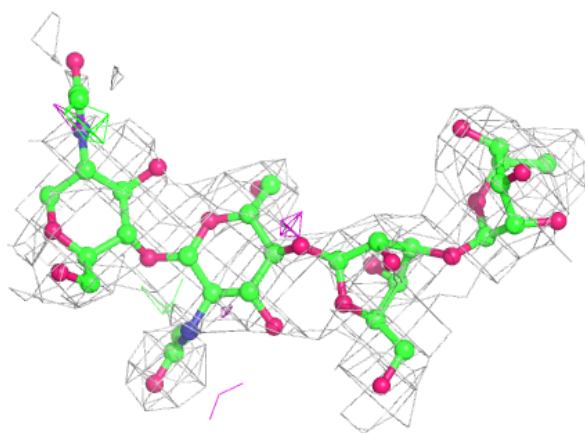
**Electron density around Chain T:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

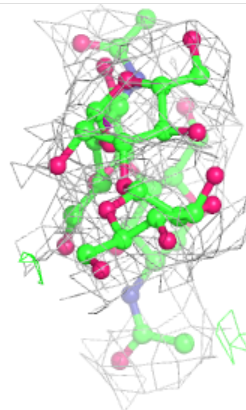
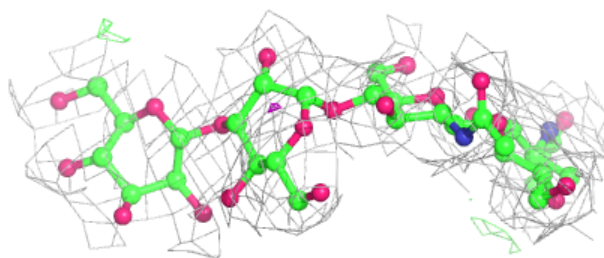
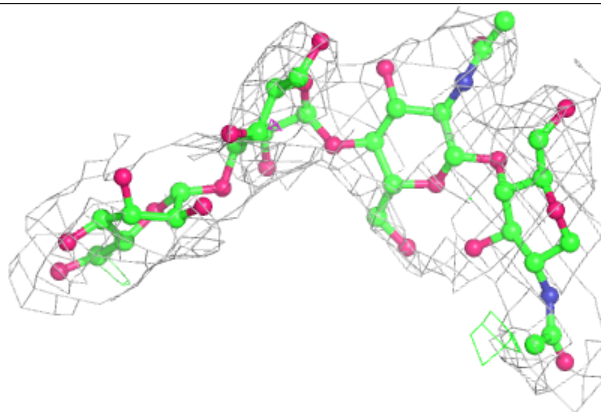


**Electron density around Chain U:**

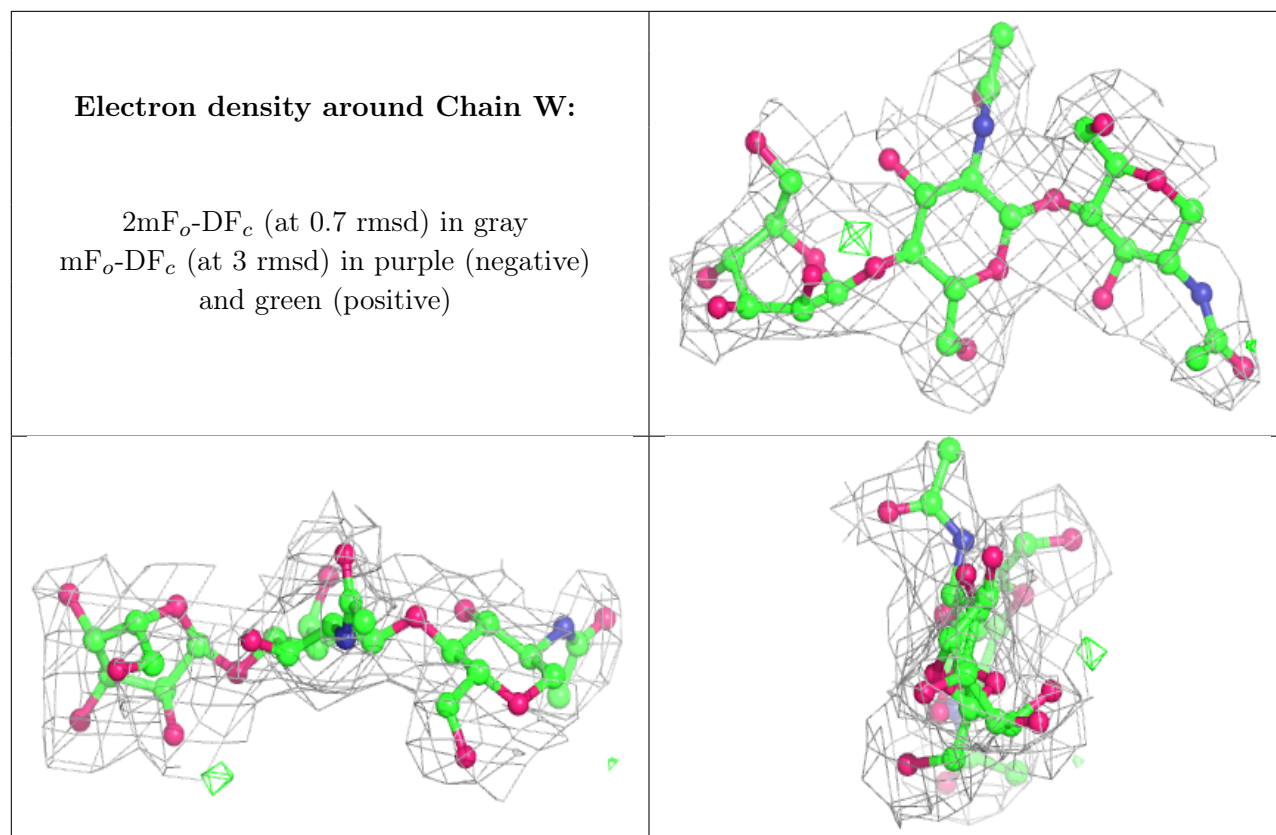
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain X:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

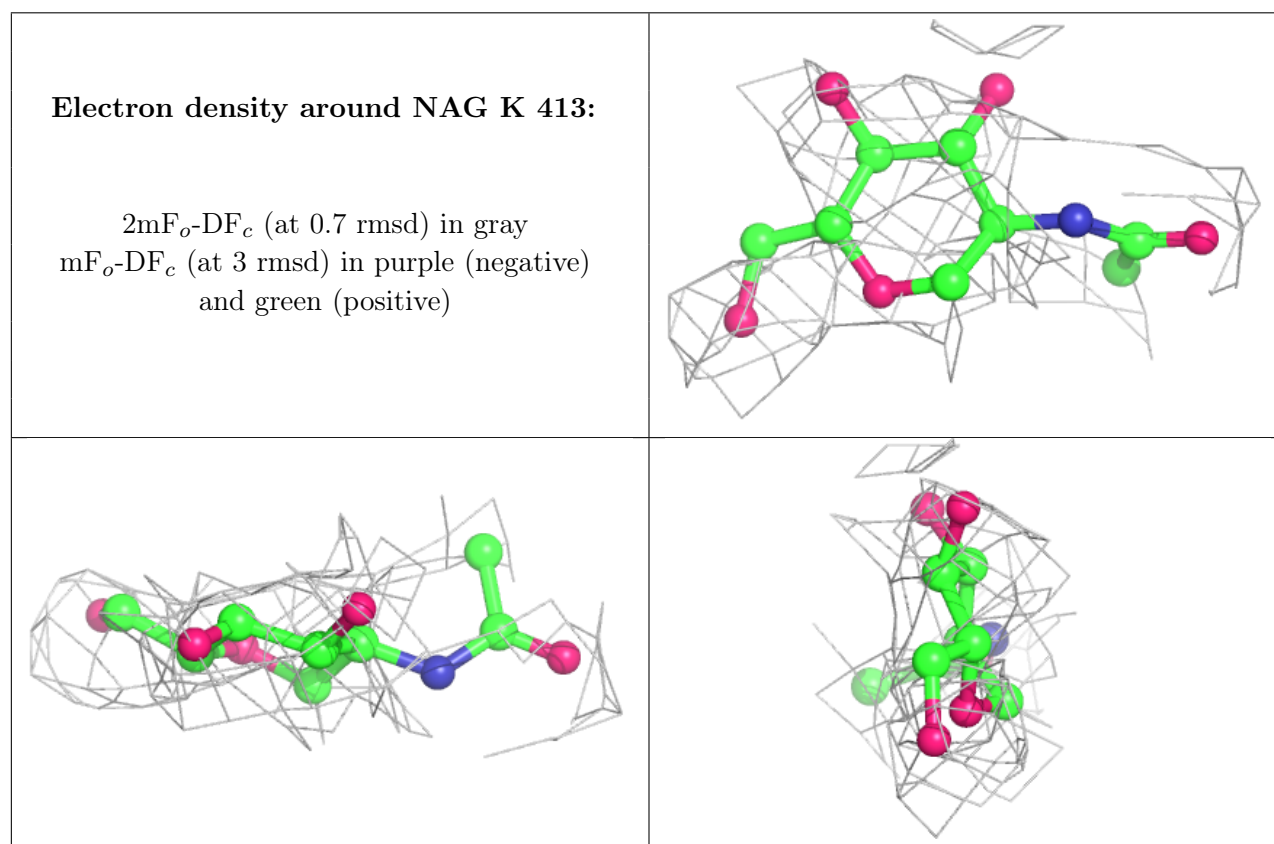
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 7   | NAG  | K     | 413 | 14/15 | 0.63 | 0.33 | 79,112,140,143              | 0     |
| 7   | NAG  | A     | 401 | 14/15 | 0.69 | 0.29 | 108,129,155,157             | 0     |
| 7   | NAG  | A     | 413 | 14/15 | 0.69 | 0.32 | 80,93,100,101               | 0     |
| 7   | NAG  | E     | 412 | 14/15 | 0.70 | 0.30 | 98,123,129,130              | 0     |
| 7   | NAG  | A     | 402 | 14/15 | 0.71 | 0.33 | 118,155,164,170             | 0     |
| 7   | NAG  | I     | 410 | 14/15 | 0.71 | 0.44 | 100,131,137,147             | 0     |
| 7   | NAG  | I     | 409 | 14/15 | 0.72 | 0.25 | 75,90,97,99                 | 0     |
| 7   | NAG  | K     | 401 | 14/15 | 0.72 | 0.39 | 102,134,139,140             | 0     |
| 7   | NAG  | E     | 414 | 14/15 | 0.73 | 0.34 | 103,124,132,137             | 0     |
| 7   | NAG  | A     | 412 | 14/15 | 0.74 | 0.64 | 60,112,127,129              | 0     |
| 7   | NAG  | G     | 401 | 14/15 | 0.76 | 0.20 | 71,80,91,92                 | 0     |
| 7   | NAG  | I     | 401 | 14/15 | 0.76 | 0.28 | 118,132,146,152             | 0     |
| 7   | NAG  | G     | 402 | 14/15 | 0.77 | 0.16 | 82,107,120,120              | 0     |
| 7   | NAG  | K     | 414 | 14/15 | 0.81 | 0.29 | 103,115,122,122             | 0     |

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*Continued from previous page...*

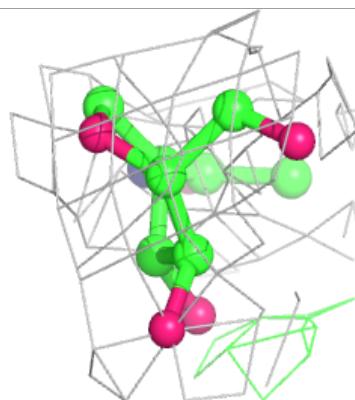
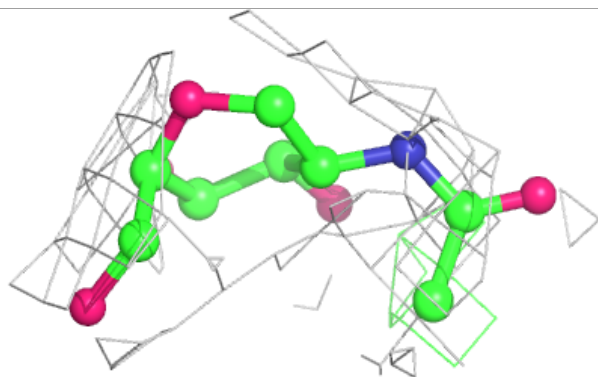
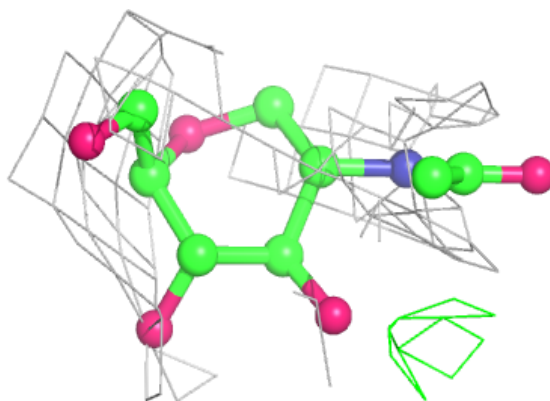
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 7   | NAG  | C     | 409 | 14/15 | 0.82 | 0.27 | 84,91,98,101                | 0     |
| 7   | NAG  | E     | 413 | 14/15 | 0.82 | 0.50 | 75,88,96,98                 | 0     |
| 7   | NAG  | E     | 401 | 14/15 | 0.84 | 0.22 | 66,91,109,110               | 0     |
| 7   | NAG  | A     | 414 | 14/15 | 0.88 | 0.25 | 62,80,86,88                 | 0     |
| 7   | NAG  | G     | 413 | 14/15 | 0.88 | 0.20 | 57,80,96,97                 | 0     |
| 8   | ZN   | G     | 414 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 8   | ZN   | I     | 411 | 1/1   | 0.99 | 0.04 | 43,43,43,43                 | 0     |
| 8   | ZN   | K     | 415 | 1/1   | 0.99 | 0.06 | 47,47,47,47                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

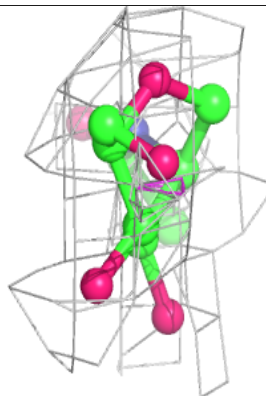
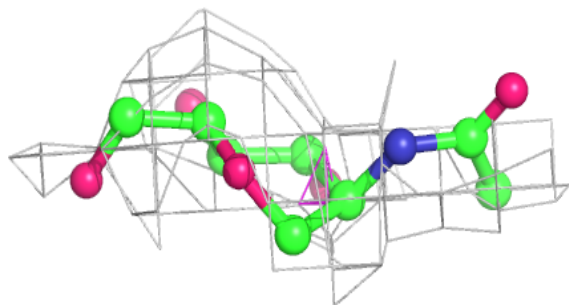
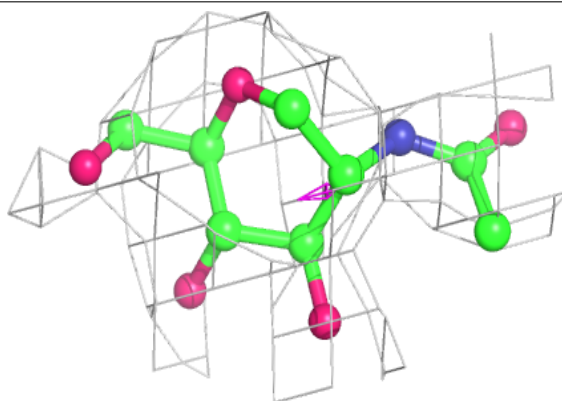


**Electron density around NAG A 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

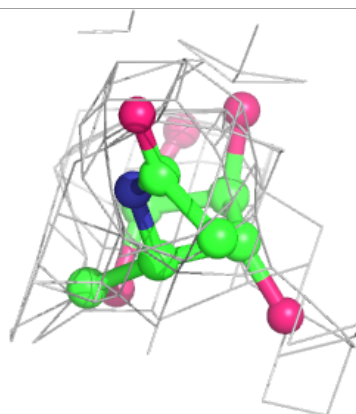
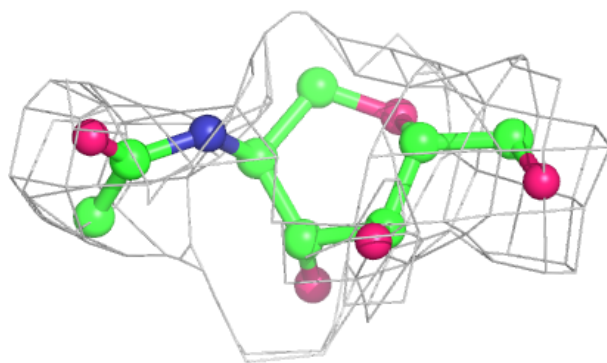
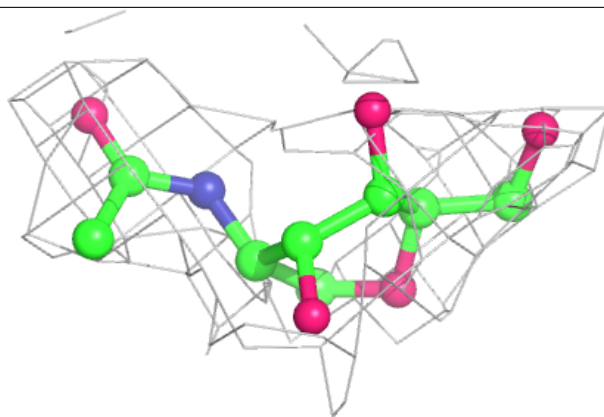
**Electron density around NAG A 413:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

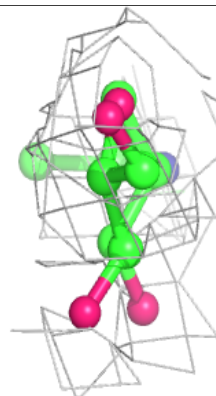
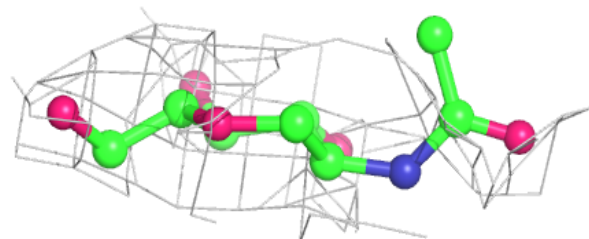
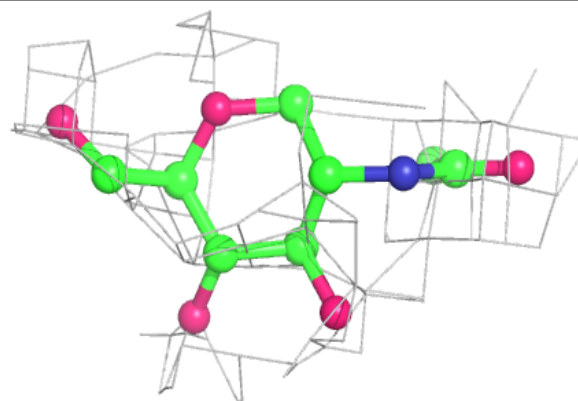


**Electron density around NAG E 412:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAG A 402:**

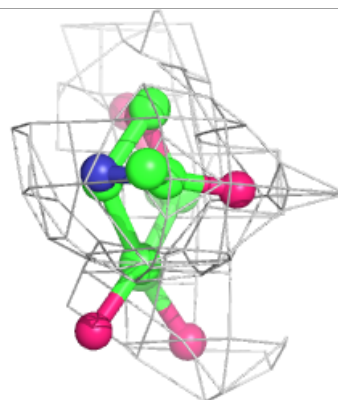
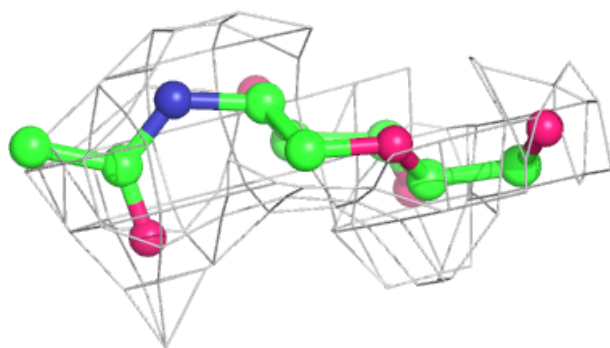
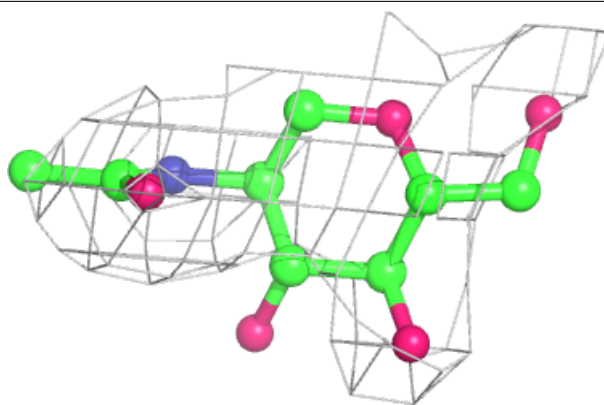
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



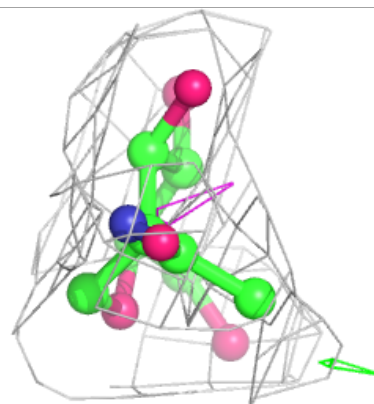
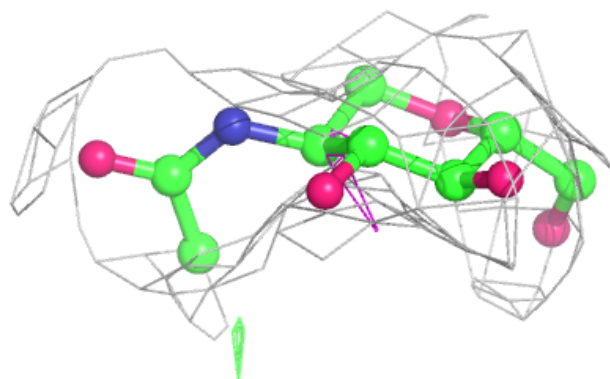
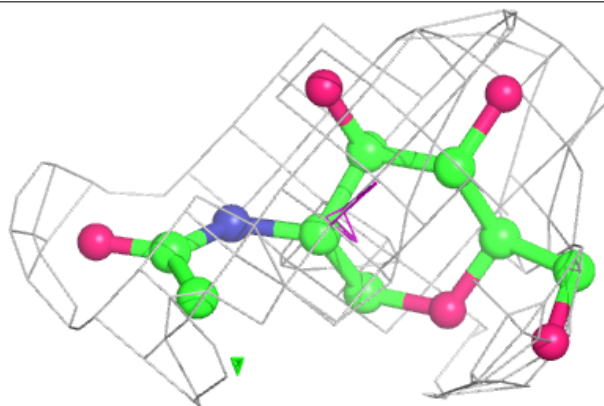


**Electron density around NAG I 410:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

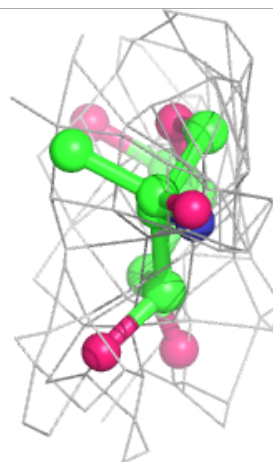
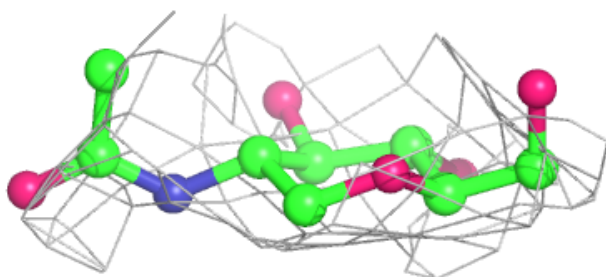
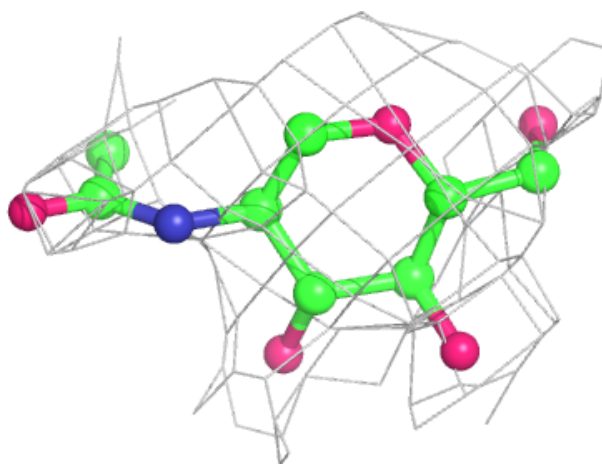
**Electron density around NAG I 409:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



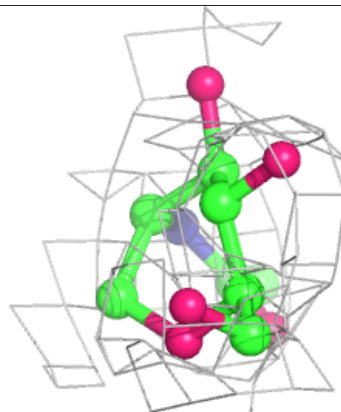
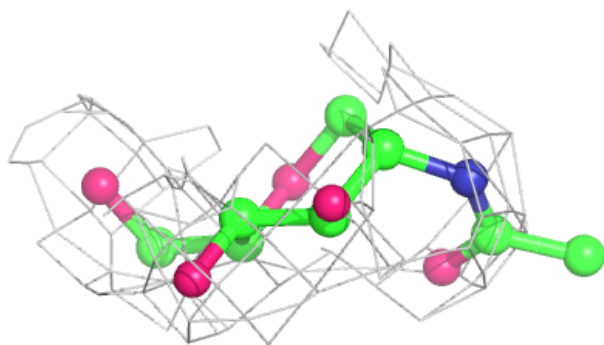
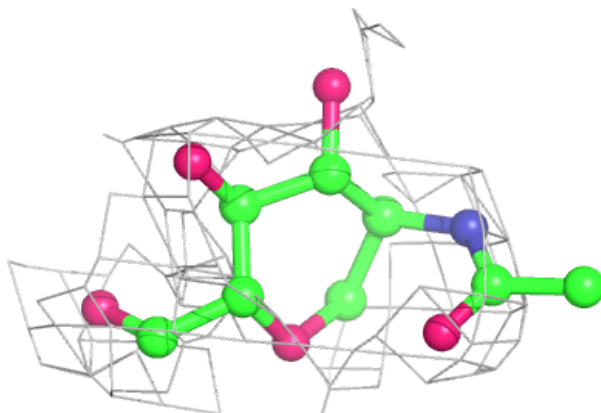
**Electron density around NAG K 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

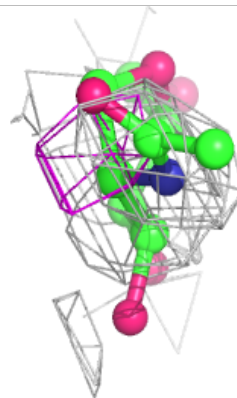
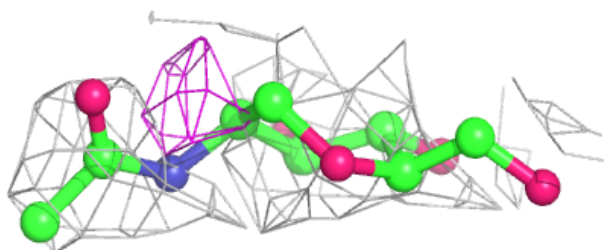
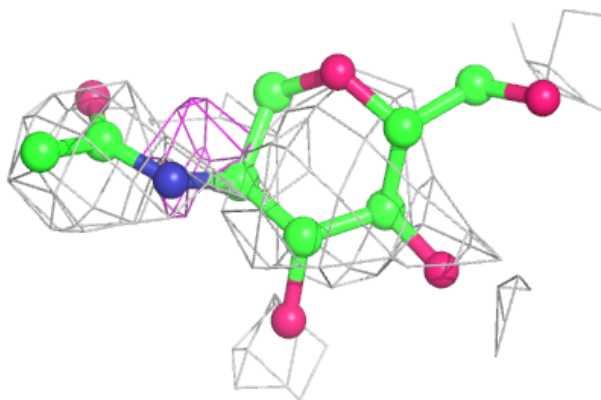


**Electron density around NAG E 414:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

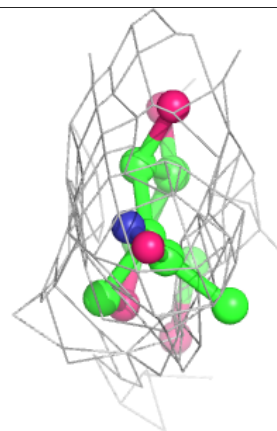
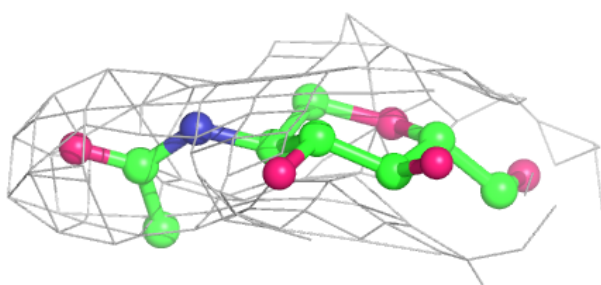
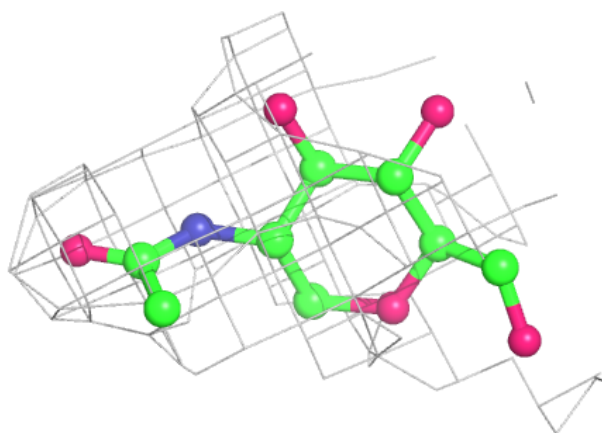
**Electron density around NAG A 412:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

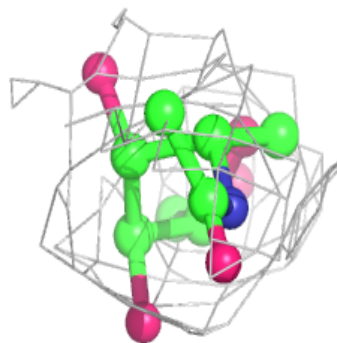
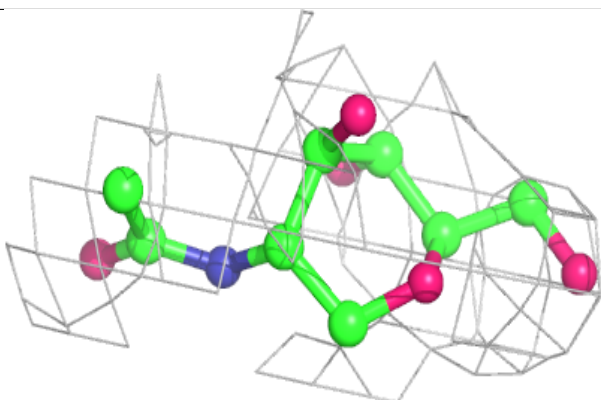
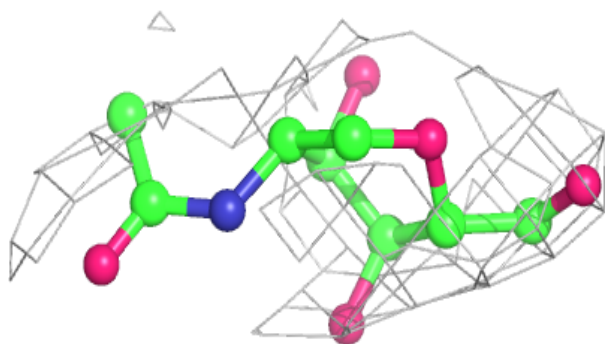


**Electron density around NAG G 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

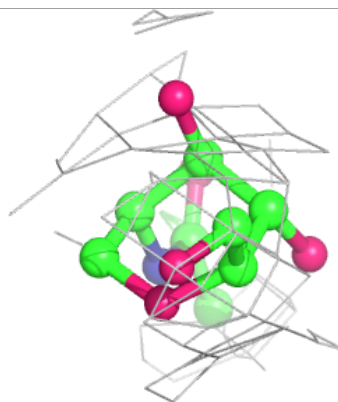
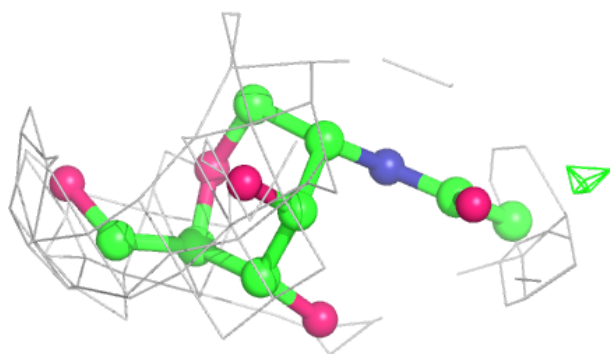
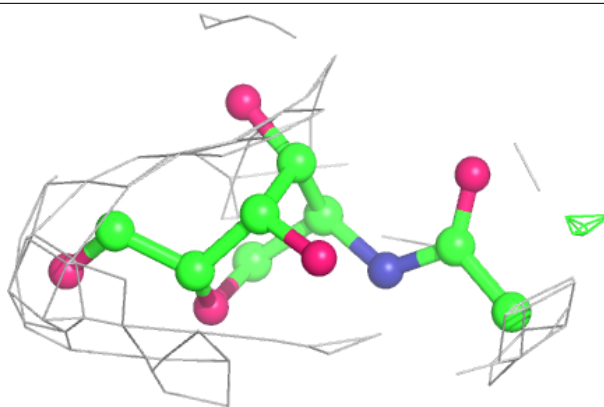
**Electron density around NAG I 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

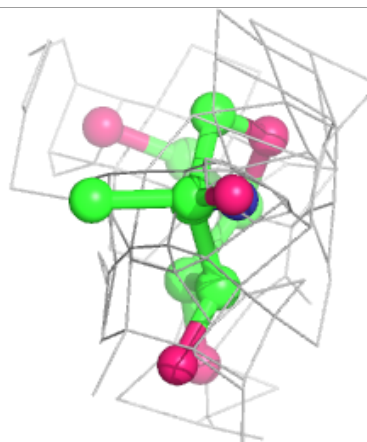
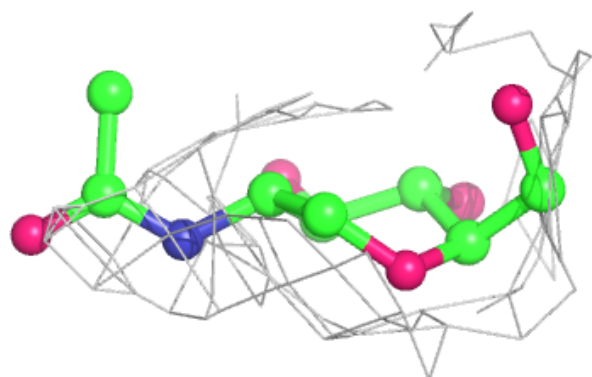
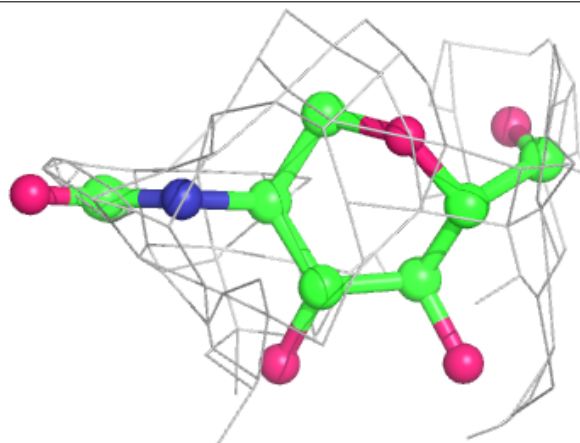


**Electron density around NAG G 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAG K 414:**

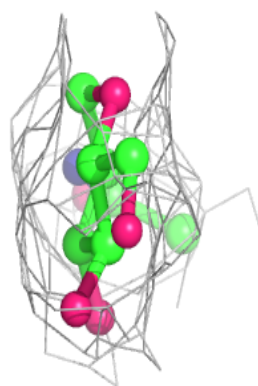
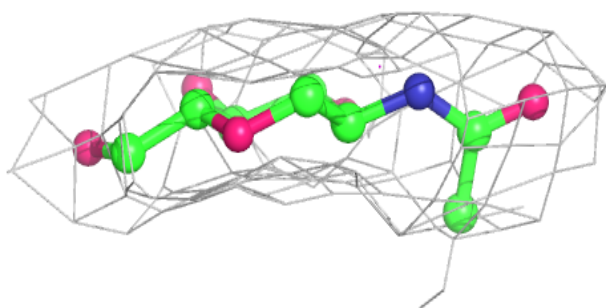
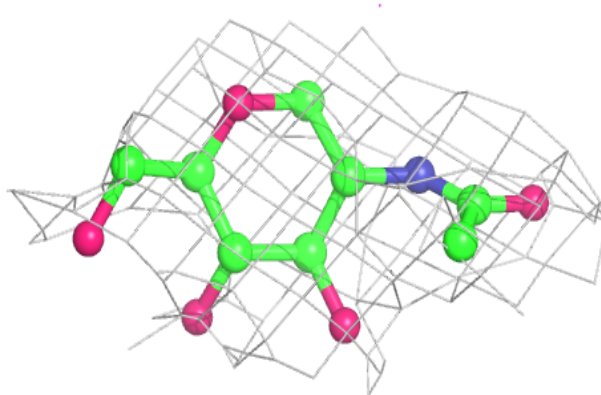
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



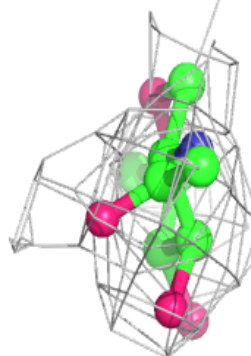
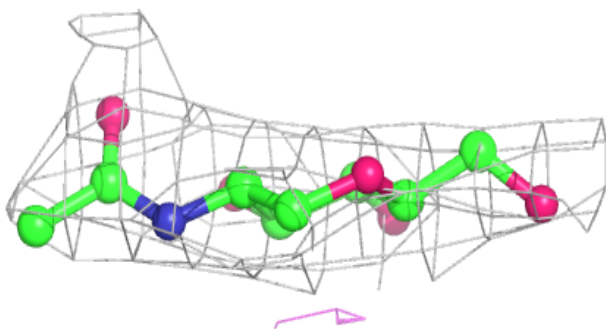
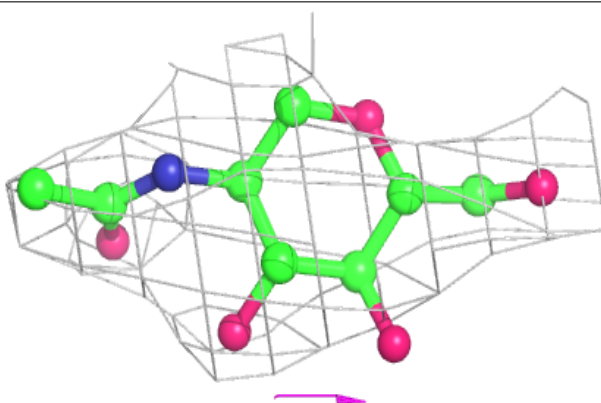


**Electron density around NAG C 409:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

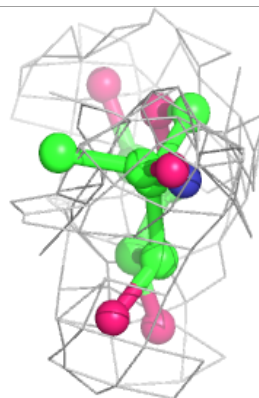
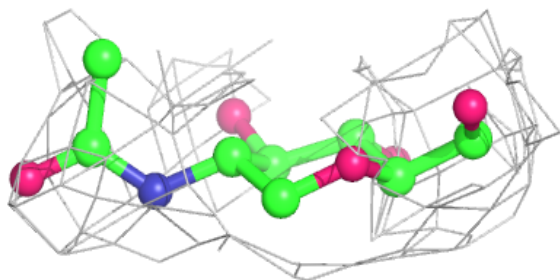
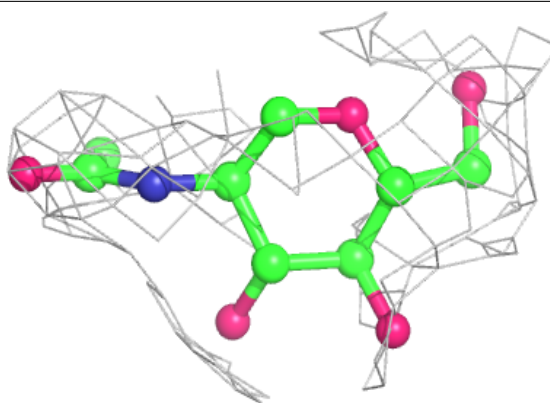
**Electron density around NAG E 413:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

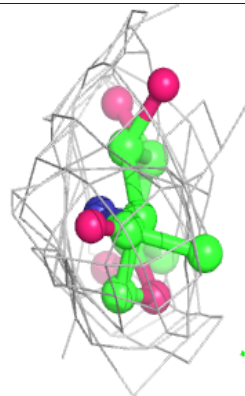
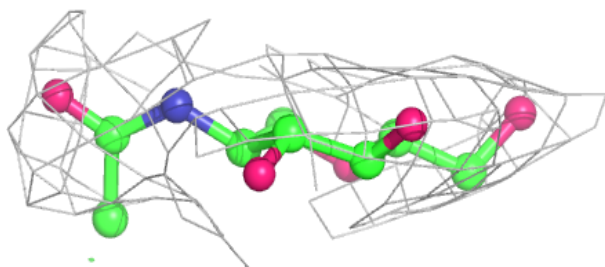
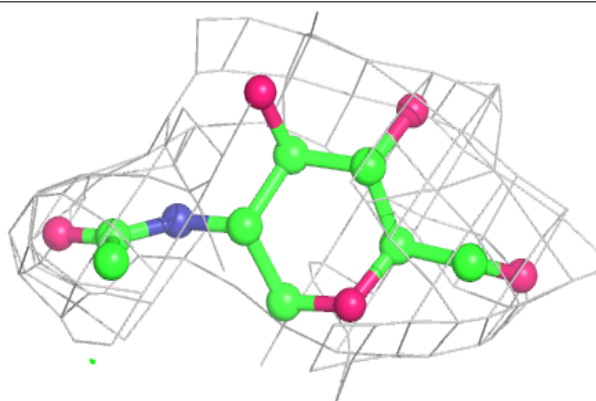


**Electron density around NAG E 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

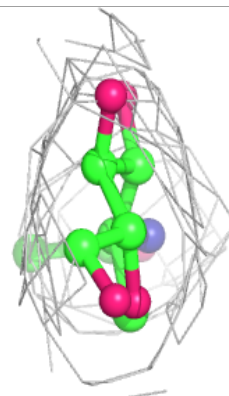
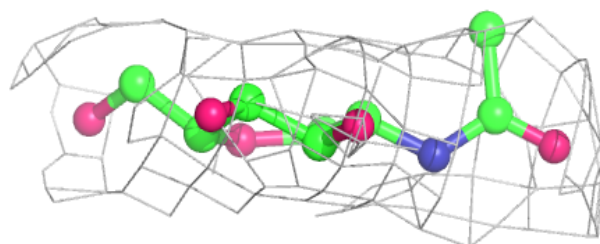
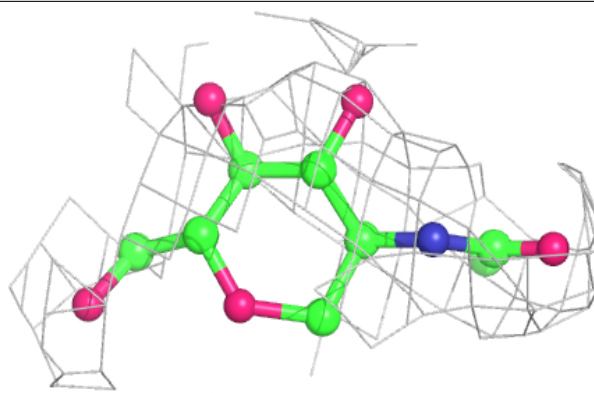
**Electron density around NAG A 414:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAG G 413:**

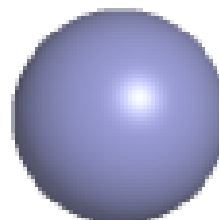
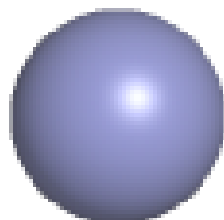
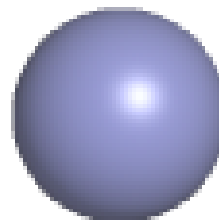
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





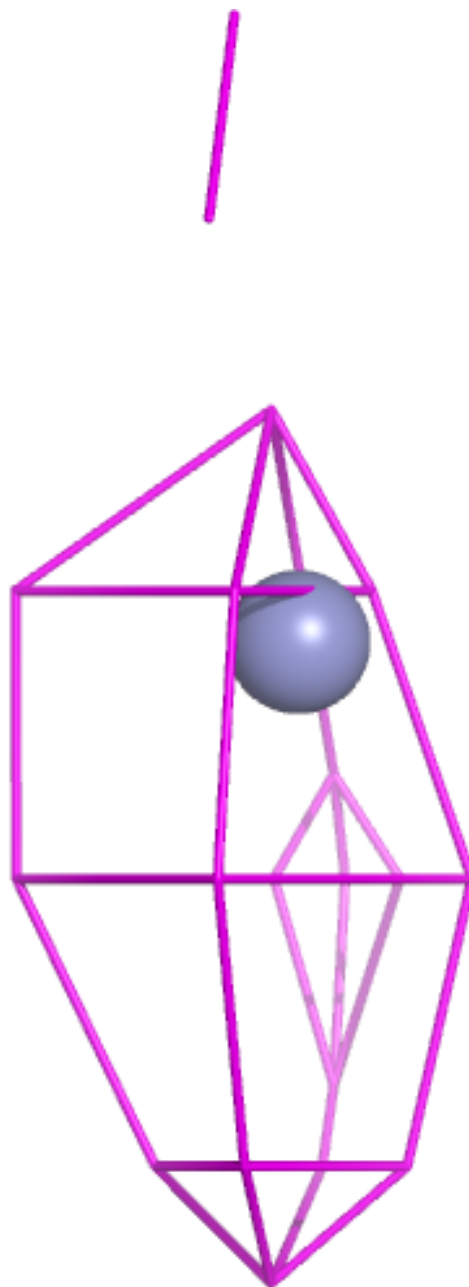
**Electron density around ZN G 414:**

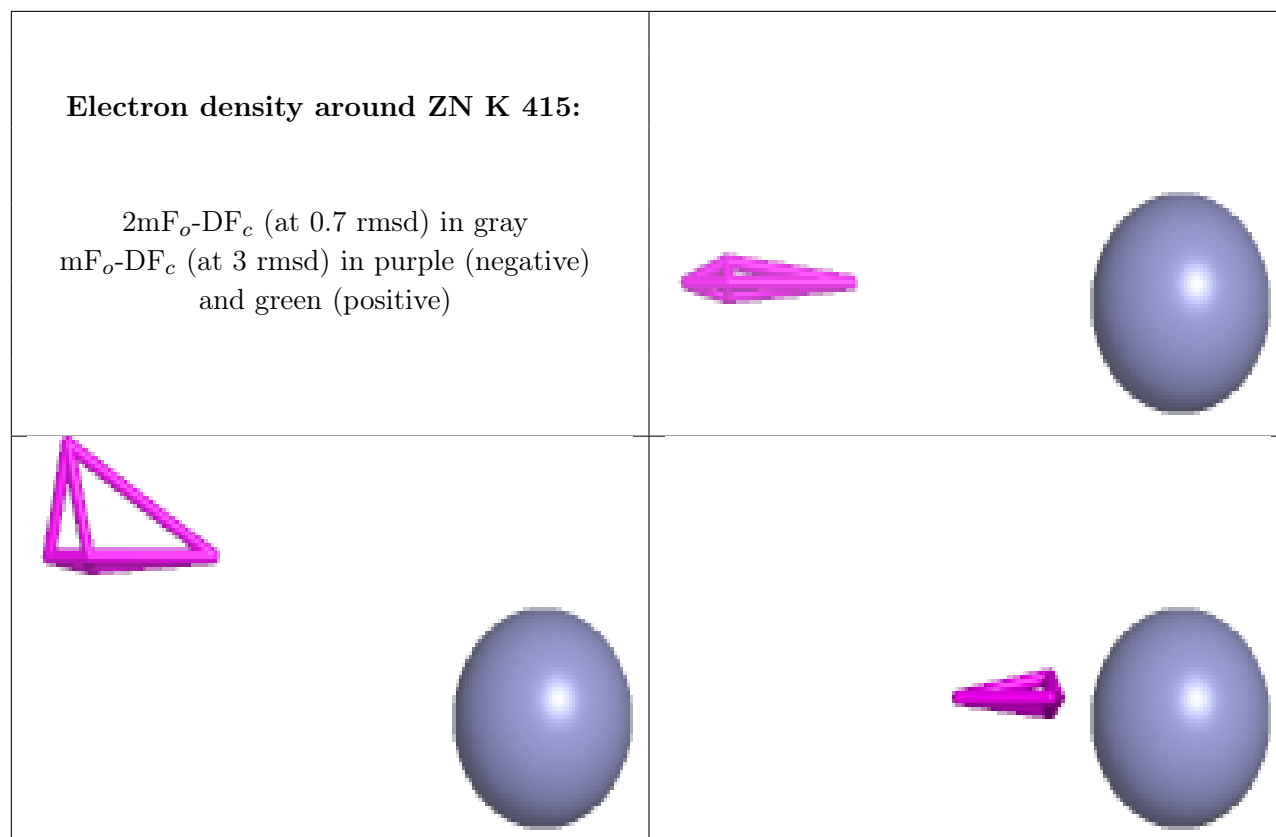
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN I 411:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.