



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 11:28 PM EST

PDB ID : 6B3M  
Title : The crystal structure of a broadly-reactive human anti-hemagglutinin stalk antibody (70-1F02) in complex with H5 hemagglutinin  
Authors : Shore, D.A.; Yang, H.; Stevens, J.  
Deposited on : 2017-09-22  
Resolution : 3.92 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.

The types of validation reports are described at

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

---

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                       |
| Xtriage (Phenix)               | : | 1.21   |
| EDS                            | : | 3.0  |
| Percentile statistics          | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4                           | : | 9.0.004 (Gargrove)   |
| Density-Fitness                | : | 1.0.11   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.40   |

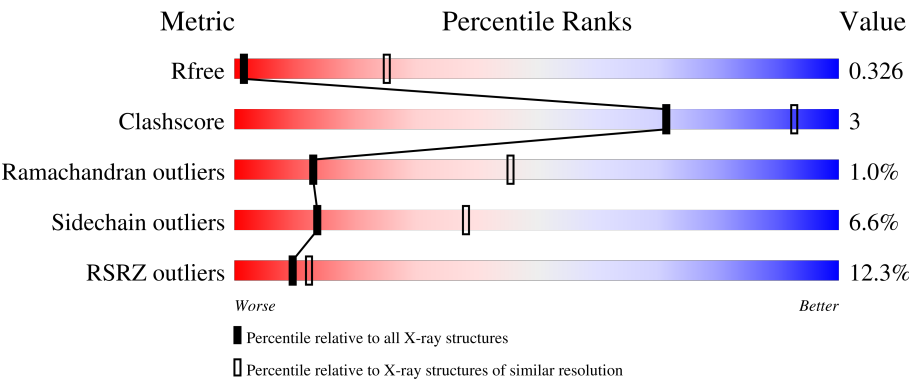
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.92 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 164625                      | 1175 (4.14-3.70)                                      |
| Clashscore            | 180529                      | 1045 (4.12-3.72)                                      |
| Ramachandran outliers | 177936                      | 1006 (4.12-3.72)                                      |
| Sidechain outliers    | 177891                      | 1185 (4.14-3.70)                                      |
| RSRZ outliers         | 164620                      | 1175 (4.14-3.70)                                      |

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 of 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>19%</div><div><div></div><div></div><div></div><div></div></div><div>82%</div><div>13%</div><div>..</div></div> |
| 1   | E     | 330    | <div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>83%</div><div>12%</div><div>..</div></div> |
| 1   | G     | 330    | <div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>84%</div><div>12%</div><div>..</div></div> |
| 1   | K     | 330    | <div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>82%</div><div>13%</div><div>..</div></div>  |
| 1   | Q     | 330    | <div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>82%</div><div>13%</div><div>..</div></div>  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | S     | 330    |                  |
| 2   | B     | 181    |                  |
| 2   | F     | 181    |                  |
| 2   | H     | 181    |                  |
| 2   | L     | 181    |                  |
| 2   | R     | 181    |                  |
| 2   | T     | 181    |                  |
| 3   | C     | 221    |                  |
| 3   | I     | 221    |                  |
| 3   | M     | 221    |                  |
| 3   | O     | 221    |                  |
| 3   | V     | 221    |                  |
| 3   | Y     | 221    |                  |
| 4   | D     | 215    |                  |
| 4   | J     | 215    |                  |
| 4   | N     | 215    |                  |
| 4   | P     | 215    |                  |
| 4   | U     | 215    |                  |
| 4   | W     | 215    |                  |
| 5   | X     | 4      |                  |
| 5   | k     | 4      |                  |
| 5   | o     | 4      |                  |
| 5   | p     | 4      |                  |
| 6   | Z     | 3      |                  |
| 7   | a     | 2      |                  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 7   | b     | 2      |  100%    |
| 7   | c     | 2      |  100%    |
| 7   | d     | 2      |  100%    |
| 7   | e     | 2      |  100%    |
| 7   | f     | 2      |  100%    |
| 7   | h     | 2      |  100%    |
| 7   | m     | 2      |  100%    |
| 7   | n     | 2      |  100%    |
| 8   | g     | 5      |  100%    |
| 9   | i     | 5      |  100%    |
| 9   | l     | 5      |  20% 80% |
| 10  | j     | 4      |  100%    |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | NAG  | F     | 201 | X         | -        | -       | -                |
| 11  | NAG  | G     | 401 | X         | -        | -       | -                |
| 6   | NAG  | Z     | 1   | X         | -        | -       | -                |
| 7   | NAG  | b     | 1   | X         | -        | -       | -                |
| 7   | NAG  | e     | 1   | X         | -        | -       | -                |
| 7   | NAG  | f     | 1   | X         | -        | -       | -                |
| 9   | BMA  | i     | 5   | X         | -        | -       | -                |
| 9   | NAG  | l     | 1   | X         | -        | -       | -                |

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 44024 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.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |         |       |
| 1   | E     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |         |       |
| 1   | G     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |         |       |
| 1   | K     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |         |       |
| 1   | Q     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |         |       |
| 1   | S     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |         |       |

- Molecule 2 is a protein called Hemagglutinin HA2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1412  | 878 | 245 | 281 | 8 |         |         |       |
| 2   | F     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 880 | 246 | 282 | 8 |         |         |       |
| 2   | H     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 880 | 246 | 282 | 8 |         |         |       |
| 2   | L     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 880 | 246 | 282 | 8 |         |         |       |
| 2   | R     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 880 | 246 | 282 | 8 |         |         |       |
| 2   | T     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1416  | 880 | 246 | 282 | 8 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| B     | 147     | GLU      | LYS    | conflict | UNP A0A182DWE1 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| F     | 147     | GLU      | LYS    | conflict | UNP A0A182DWE1 |
| H     | 147     | GLU      | LYS    | conflict | UNP A0A182DWE1 |
| L     | 147     | GLU      | LYS    | conflict | UNP A0A182DWE1 |
| R     | 147     | GLU      | LYS    | conflict | UNP A0A182DWE1 |
| T     | 147     | GLU      | LYS    | conflict | UNP A0A182DWE1 |

- Molecule 3 is a protein called 70-1F02 Fab Heavy Chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1006 | 270 | 313 | 7 |         |         |       |
| 3   | I     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1006 | 270 | 313 | 7 |         |         |       |
| 3   | M     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1006 | 270 | 313 | 7 |         |         |       |
| 3   | O     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1006 | 270 | 313 | 7 |         |         |       |
| 3   | V     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1006 | 270 | 313 | 7 |         |         |       |
| 3   | Y     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1006 | 270 | 313 | 7 |         |         |       |

- Molecule 4 is a protein called 70-1F02 Fab Light Chain.

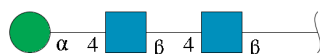
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | P     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1626  | 1016 | 278 | 327 | 5 |         |         |       |
| 4   | U     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1021 | 279 | 330 | 5 |         |         |       |
| 4   | J     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1021 | 279 | 330 | 5 |         |         |       |
| 4   | D     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1021 | 279 | 330 | 5 |         |         |       |
| 4   | W     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1021 | 279 | 330 | 5 |         |         |       |
| 4   | N     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1021 | 279 | 330 | 5 |         |         |       |

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-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   | X     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | k     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | o     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |
| 5   | p     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |

- Molecule 6 is an oligosaccharide called alpha-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   | Z     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



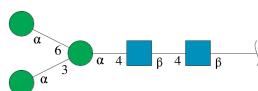
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 7   | a     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | b     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | c     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | d     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | e     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

*Continued on next page...*

Continued from previous page...

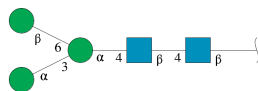
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 7   | f     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | h     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | m     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | n     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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 |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 8   | g     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |

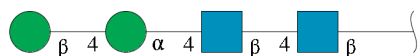
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 9   | i     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 9   | l     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |

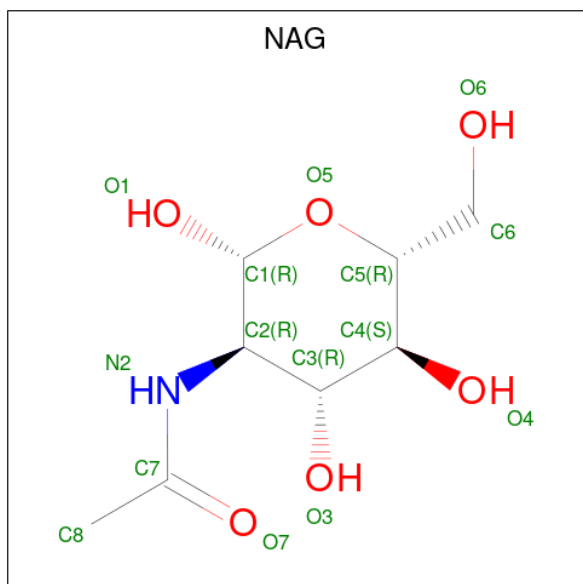
- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 10  | j     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |

- Molecule 11 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>).



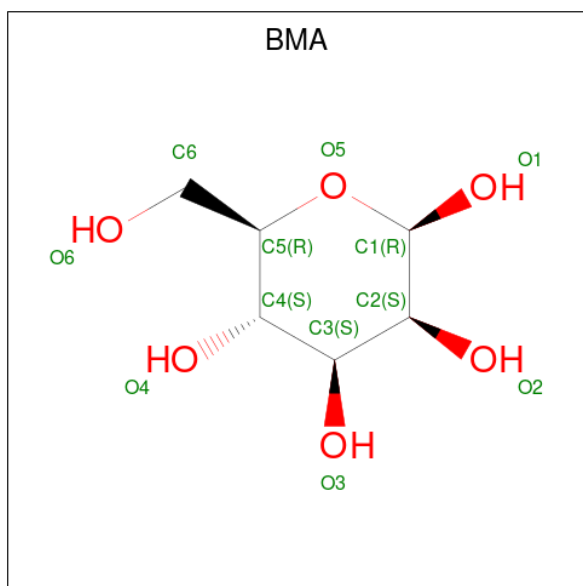
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 11  | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 11  | Q     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 11  | S     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 12 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

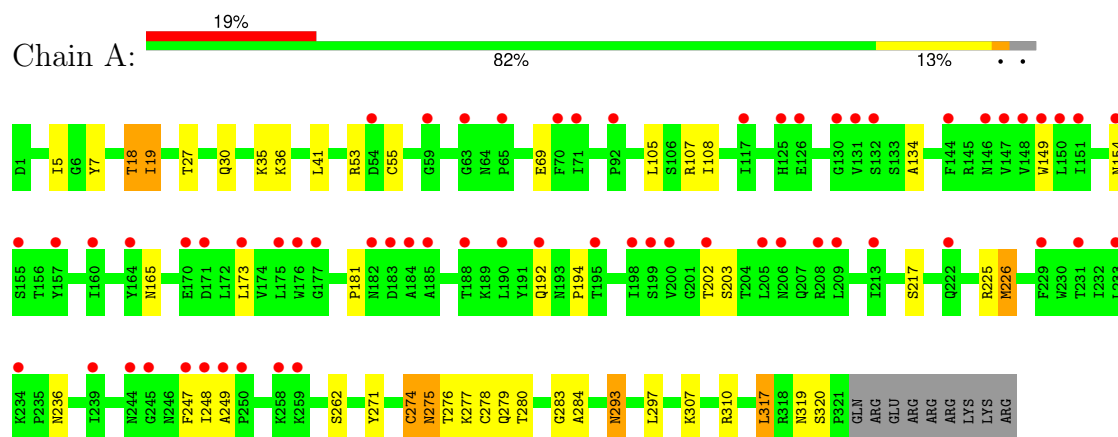


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 12  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

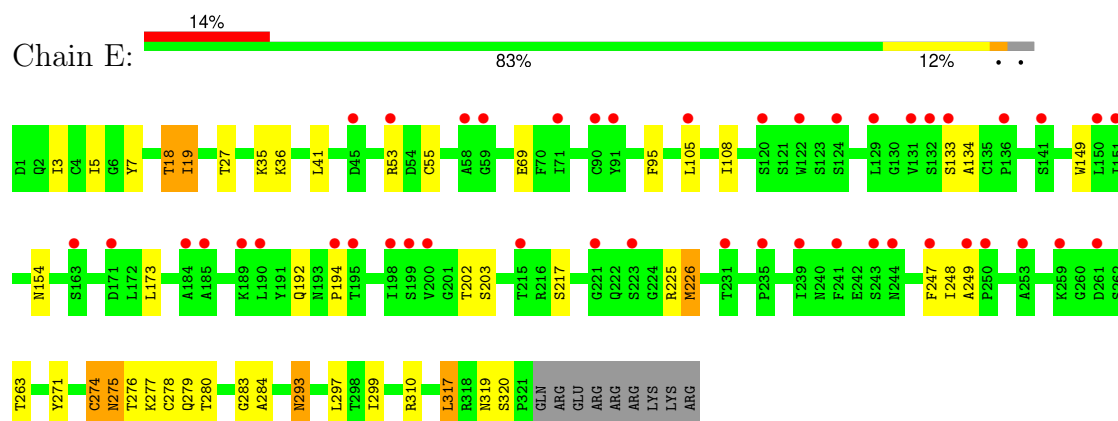
### 3 Residue-property plots [i](#)

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.

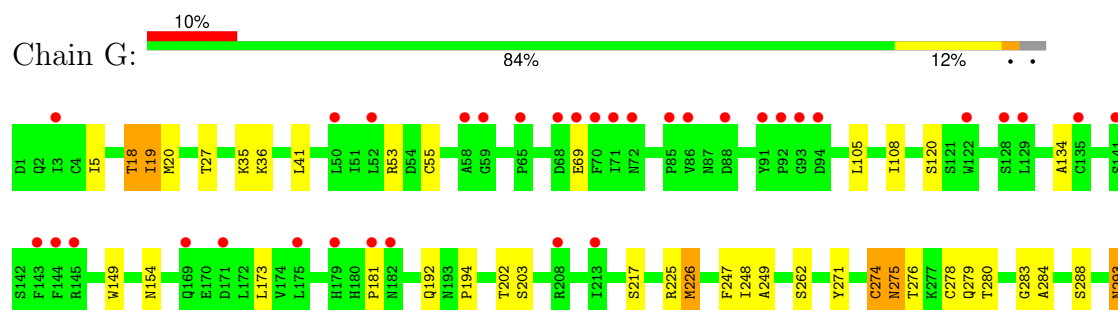
#### • Molecule 1: Hemagglutinin HA1



#### • Molecule 1: Hemagglutinin HA1

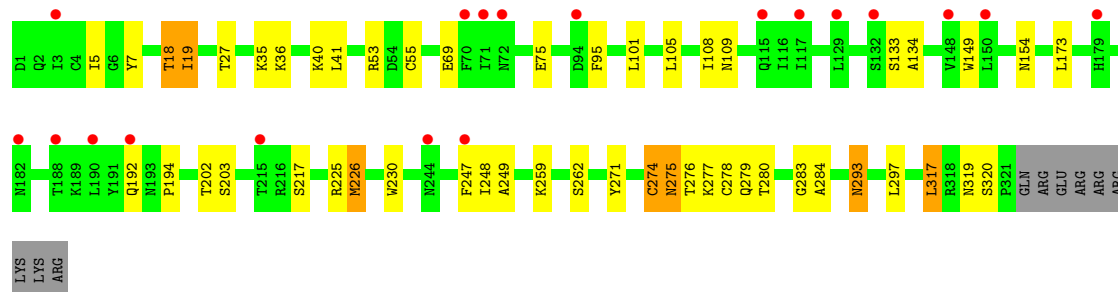
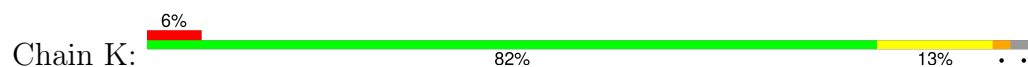


#### • Molecule 1: Hemagglutinin HA1

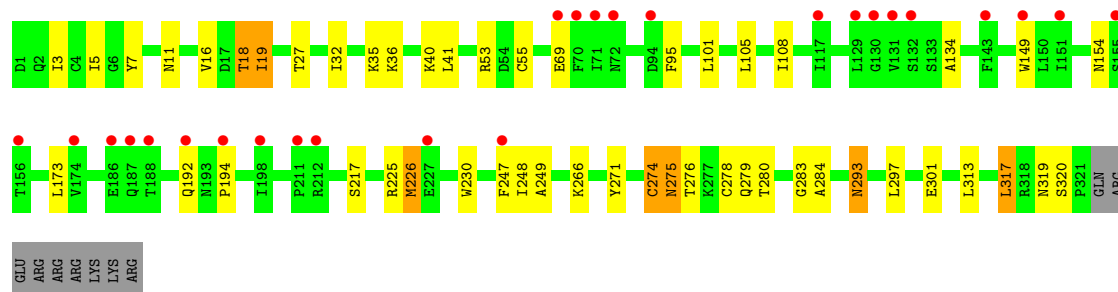
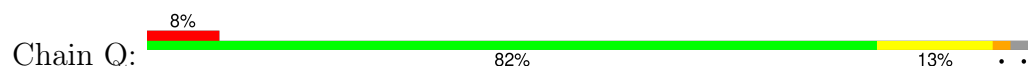




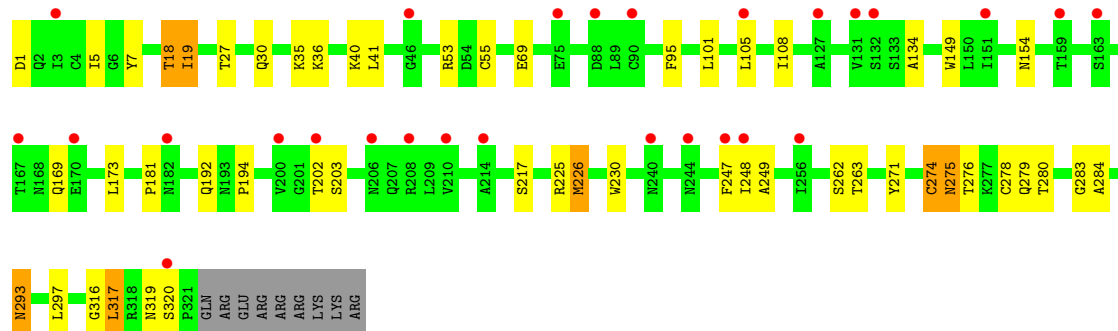
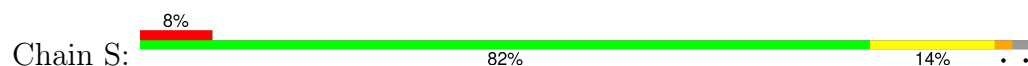
• Molecule 1: Hemagglutinin HA1



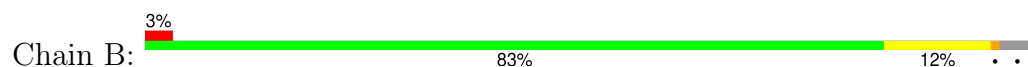
• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1

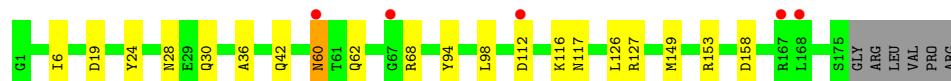
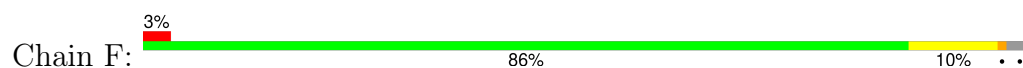


• Molecule 2: Hemagglutinin HA2

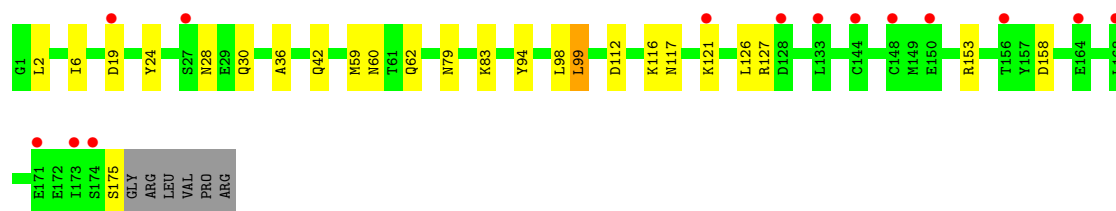
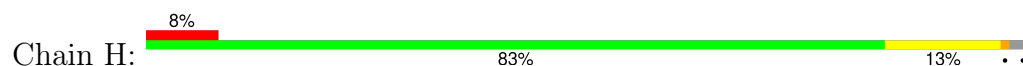




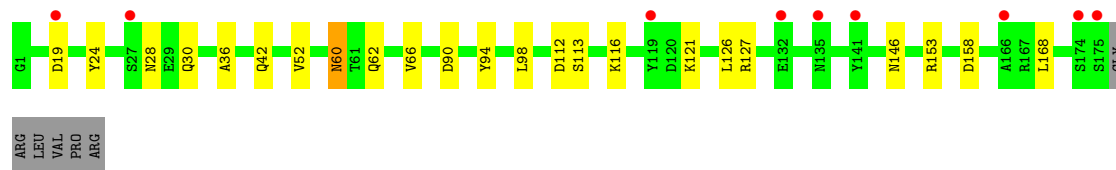
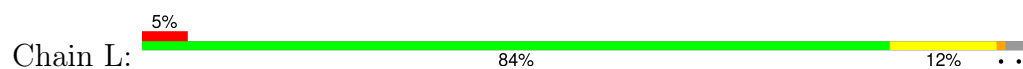
• Molecule 2: Hemagglutinin HA2



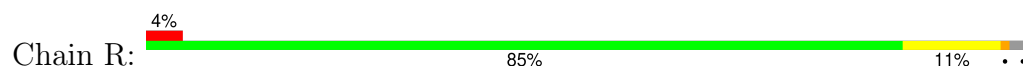
• Molecule 2: Hemagglutinin HA2



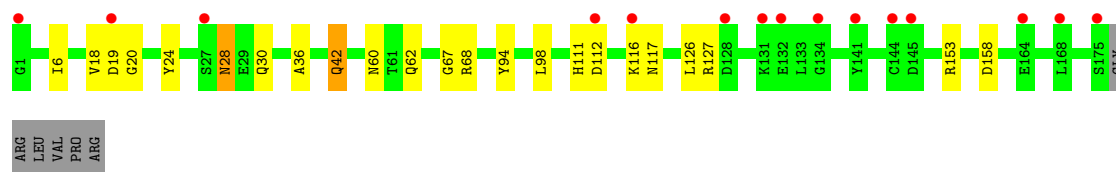
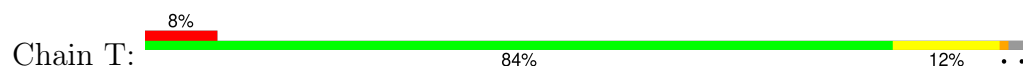
• Molecule 2: Hemagglutinin HA2



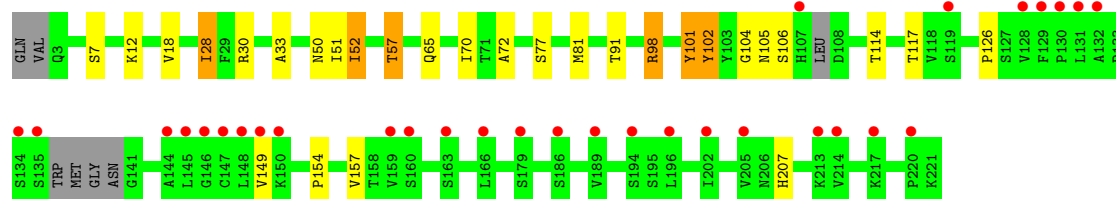
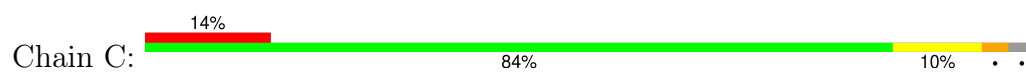
• Molecule 2: Hemagglutinin HA2



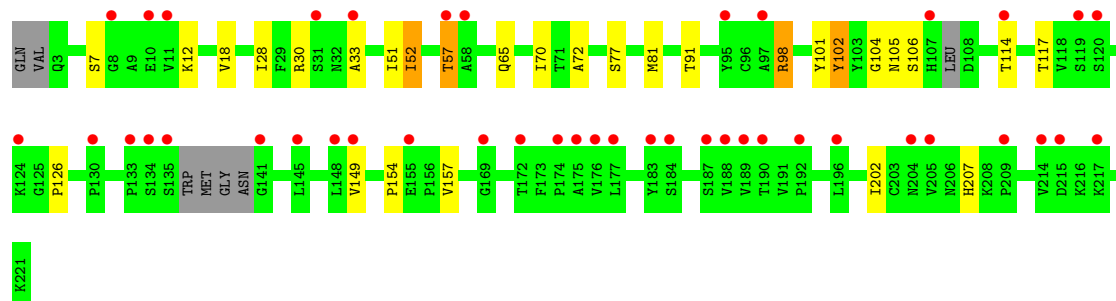
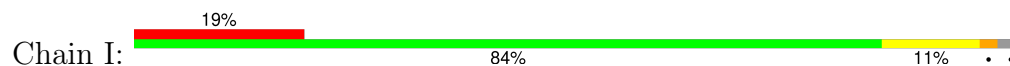
• Molecule 2: Hemagglutinin HA2



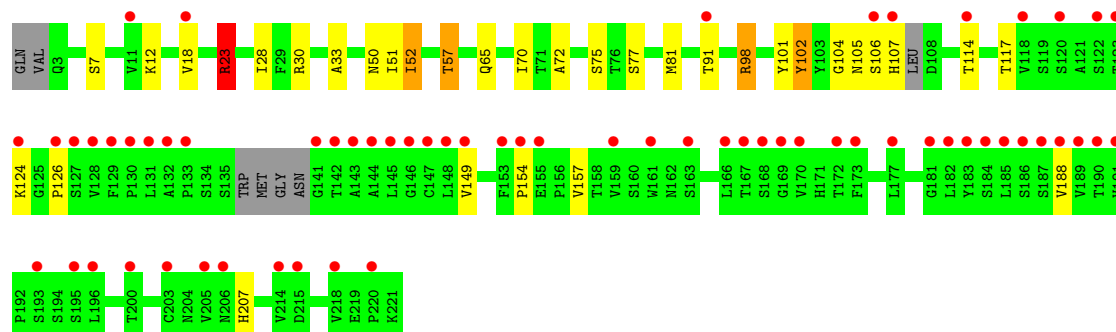
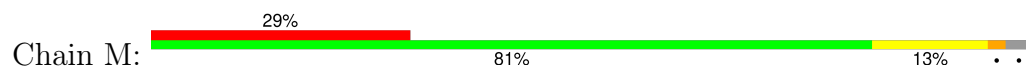
• Molecule 3: 70-1F02 Fab Heavy Chain



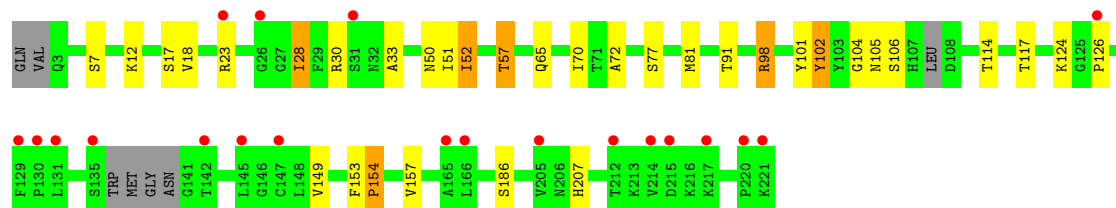
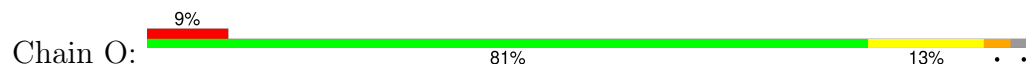
• Molecule 3: 70-1F02 Fab Heavy Chain



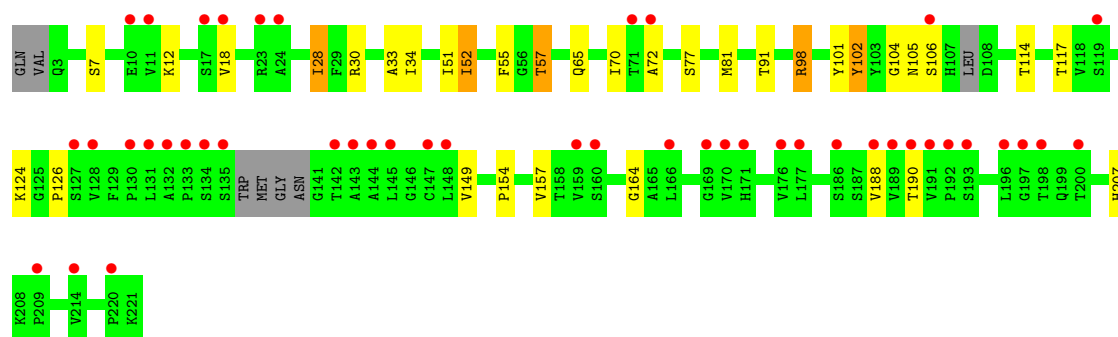
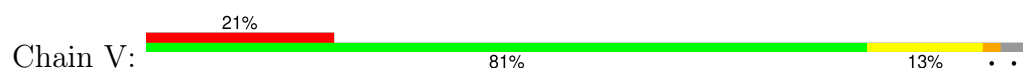
• Molecule 3: 70-1F02 Fab Heavy Chain



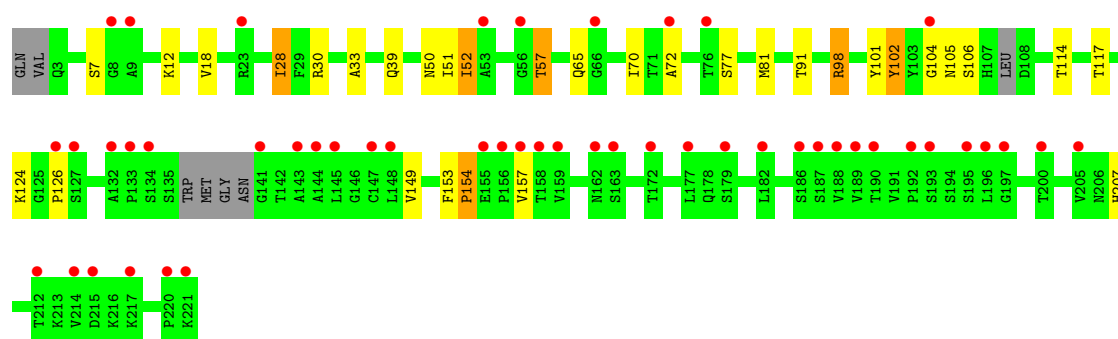
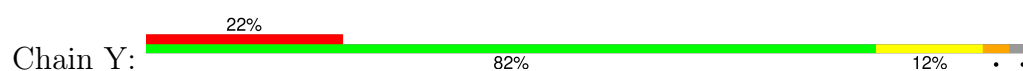
• Molecule 3: 70-1F02 Fab Heavy Chain



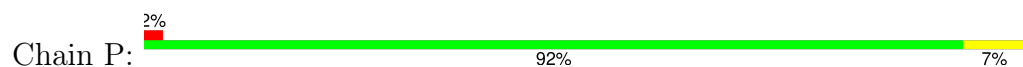
• Molecule 3: 70-1F02 Fab Heavy Chain



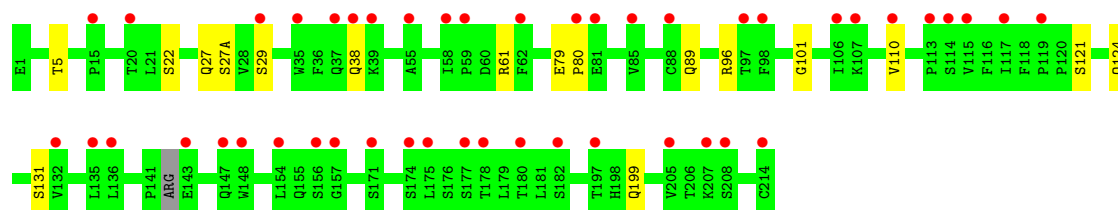
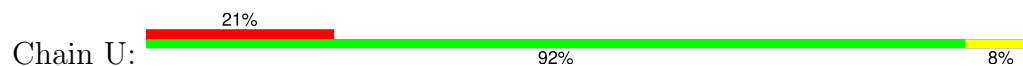
• Molecule 3: 70-1F02 Fab Heavy Chain



• Molecule 4: 70-1F02 Fab Light Chain

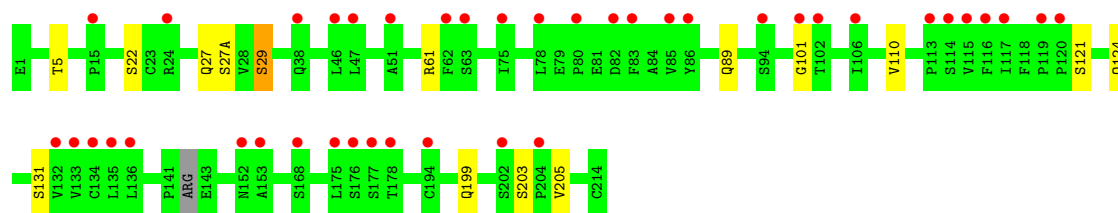


• Molecule 4: 70-1F02 Fab Light Chain

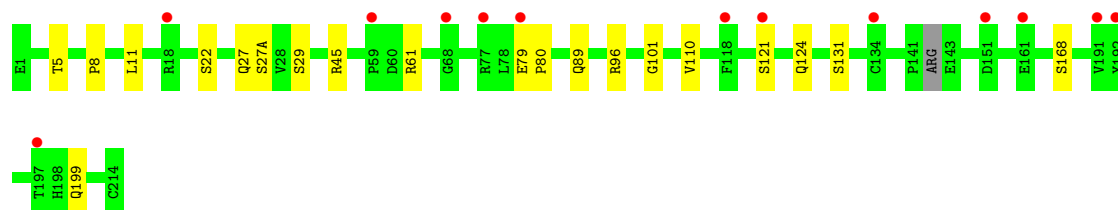
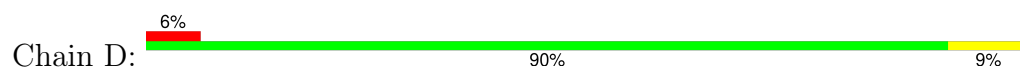


• Molecule 4: 70-1F02 Fab Light Chain

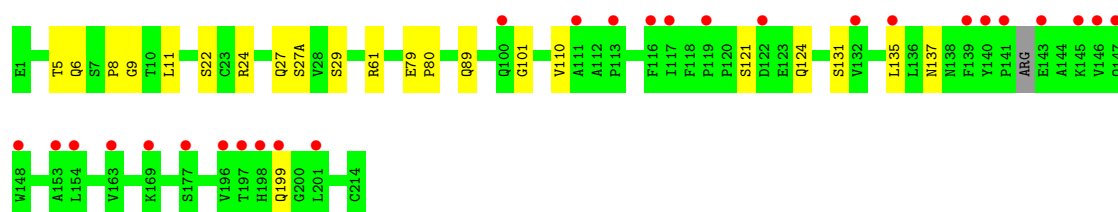
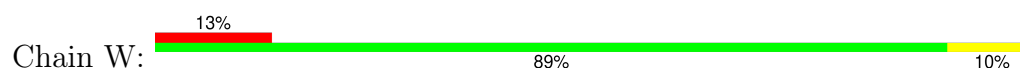




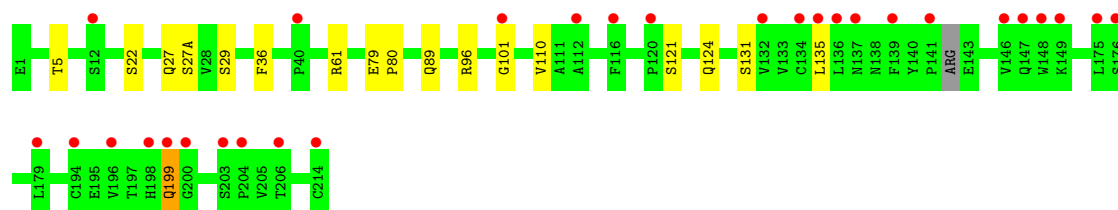
• Molecule 4: 70-1F02 Fab Light Chain



• Molecule 4: 70-1F02 Fab Light Chain



• Molecule 4: 70-1F02 Fab Light Chain



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



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



Chain k:  100%

MAG1  
MAG2  
MAN3  
MAN4

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

Chain o:  100%

MAG1  
MAG2  
MAN3  
MAN4

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

Chain p:  100%

MAG1  
MAG2  
MAN3  
MAN4

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

Chain Z:  67% 33%

MAG1  
MAG2  
MAN3

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%


MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%

MAG1  
MAG2

- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%

NAG1  
NAG2  
MAN3  
MAN4  
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%

NAG1  
NAG2  
MAN3  
MAN4  
BMA5

- Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  20% 80%

NAG1  
NAG2  
MAN3  
MAN4  
BMA5

- Molecule 10: beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%

NAG1  
NAG2  
MAN3  
BMA4

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 174.58Å 205.37Å 222.26Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 50.01 – 3.92<br>50.01 – 3.92                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.7 (50.01-3.92)<br>93.7 (50.01-3.92)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.86 (at 3.88Å)   | Xtriage          |
| Refinement program  | REFMAC 5.8.0158   | Depositor        |
| R, $R_{free}$   | 0.286 , 0.329<br>0.285 , 0.326                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3659 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.6  | Xtriage          |
| Anisotropy  | 0.350   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 27.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.77  | EDS              |
| Total number of atoms   | 44024   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MAN, BMA, NAG

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.56         | 0/2611         | 0.71        | 2/3546 (0.1%)   |
| 1   | E     | 0.53         | 0/2611         | 0.69        | 1/3546 (0.0%)   |
| 1   | G     | 0.55         | 0/2611         | 0.73        | 0/3546          |
| 1   | K     | 0.53         | 0/2611         | 0.72        | 0/3546          |
| 1   | Q     | 0.57         | 1/2611 (0.0%)  | 0.73        | 1/3546 (0.0%)   |
| 1   | S     | 0.53         | 0/2611         | 0.70        | 0/3546          |
| 2   | B     | 0.66         | 0/1439         | 0.72        | 0/1934          |
| 2   | F     | 0.69         | 0/1443         | 0.75        | 0/1939          |
| 2   | H     | 0.65         | 0/1443         | 0.73        | 0/1939          |
| 2   | L     | 0.65         | 0/1443         | 0.71        | 0/1939          |
| 2   | R     | 0.64         | 0/1443         | 0.72        | 1/1939 (0.1%)   |
| 2   | T     | 0.67         | 0/1443         | 0.73        | 0/1939          |
| 3   | C     | 0.57         | 0/1634         | 0.71        | 0/2224          |
| 3   | I     | 0.52         | 0/1634         | 0.68        | 0/2224          |
| 3   | M     | 0.61         | 2/1634 (0.1%)  | 0.84        | 5/2224 (0.2%)   |
| 3   | O     | 0.58         | 0/1634         | 0.72        | 1/2224 (0.0%)   |
| 3   | V     | 0.56         | 0/1634         | 0.70        | 0/2224          |
| 3   | Y     | 0.53         | 0/1634         | 0.68        | 0/2224          |
| 4   | D     | 0.50         | 0/1668         | 0.67        | 1/2261 (0.0%)   |
| 4   | J     | 0.48         | 0/1668         | 0.64        | 0/2261          |
| 4   | N     | 0.53         | 0/1668         | 0.66        | 0/2261          |
| 4   | P     | 0.51         | 0/1659         | 0.68        | 0/2249          |
| 4   | U     | 0.48         | 0/1668         | 0.63        | 0/2261          |
| 4   | W     | 0.50         | 0/1668         | 0.65        | 0/2261          |
| All | All   | 0.56         | 3/44123 (0.0%) | 0.71        | 12/59803 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| 2   | R     | 0                   | 1                   |
| 2   | T     | 0                   | 1                   |
| 3   | M     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | M     | 23  | ARG  | CZ-NH1 | -7.07 | 1.23        | 1.33     |
| 1   | Q     | 301 | GLU  | CG-CD  | 5.63  | 1.60        | 1.51     |
| 3   | M     | 23  | ARG  | CD-NE  | 5.06  | 1.55        | 1.46     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3   | M     | 23  | ARG  | NE-CZ-NH1  | -20.07 | 110.26      | 120.30   |
| 3   | O     | 23  | ARG  | NE-CZ-NH2  | -7.31  | 116.65      | 120.30   |
| 4   | D     | 45  | ARG  | NE-CZ-NH1  | 6.22   | 123.41      | 120.30   |
| 3   | M     | 23  | ARG  | NH1-CZ-NH2 | -6.15  | 112.64      | 119.40   |
| 1   | Q     | 266 | LYS  | CD-CE-NZ   | 5.66   | 124.72      | 111.70   |
| 3   | M     | 23  | ARG  | CG-CD-NE   | 5.66   | 123.68      | 111.80   |
| 3   | M     | 23  | ARG  | NE-CZ-NH2  | -5.65  | 117.47      | 120.30   |
| 1   | E     | 310 | ARG  | NE-CZ-NH1  | 5.49   | 123.05      | 120.30   |
| 3   | M     | 23  | ARG  | CD-NE-CZ   | 5.44   | 131.21      | 123.60   |
| 1   | A     | 107 | ARG  | NE-CZ-NH2  | -5.38  | 117.61      | 120.30   |
| 2   | R     | 68  | ARG  | NE-CZ-NH1  | 5.31   | 122.96      | 120.30   |
| 1   | A     | 310 | ARG  | NE-CZ-NH1  | 5.11   | 122.85      | 120.30   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 68  | ARG  | Peptide   |
| 2   | F     | 68  | ARG  | Peptide   |
| 3   | M     | 23  | ARG  | Sidechain |
| 2   | R     | 68  | ARG  | Peptide   |
| 2   | T     | 68  | ARG  | Peptide   |

## 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     | 2549  | 0        | 2493     | 19      | 0            |
| 1   | E     | 2549  | 0        | 2493     | 16      | 0            |
| 1   | G     | 2549  | 0        | 2493     | 15      | 0            |
| 1   | K     | 2549  | 0        | 2494     | 20      | 0            |
| 1   | Q     | 2549  | 0        | 2495     | 19      | 0            |
| 1   | S     | 2549  | 0        | 2495     | 23      | 0            |
| 2   | B     | 1412  | 0        | 1317     | 11      | 0            |
| 2   | F     | 1416  | 0        | 1318     | 6       | 0            |
| 2   | H     | 1416  | 0        | 1320     | 12      | 0            |
| 2   | L     | 1416  | 0        | 1320     | 14      | 0            |
| 2   | R     | 1416  | 0        | 1319     | 8       | 0            |
| 2   | T     | 1416  | 0        | 1320     | 11      | 0            |
| 3   | C     | 1596  | 0        | 1557     | 15      | 0            |
| 3   | I     | 1596  | 0        | 1557     | 14      | 0            |
| 3   | M     | 1596  | 0        | 1550     | 15      | 0            |
| 3   | O     | 1596  | 0        | 1555     | 17      | 0            |
| 3   | V     | 1596  | 0        | 1557     | 23      | 0            |
| 3   | Y     | 1596  | 0        | 1556     | 16      | 0            |
| 4   | D     | 1635  | 0        | 1582     | 6       | 0            |
| 4   | J     | 1635  | 0        | 1582     | 7       | 0            |
| 4   | N     | 1635  | 0        | 1582     | 7       | 0            |
| 4   | P     | 1626  | 0        | 1573     | 5       | 0            |
| 4   | U     | 1635  | 0        | 1582     | 6       | 0            |
| 4   | W     | 1635  | 0        | 1582     | 13      | 0            |
| 5   | X     | 50    | 0        | 41       | 0       | 0            |
| 5   | k     | 50    | 0        | 41       | 0       | 0            |
| 5   | o     | 50    | 0        | 43       | 0       | 0            |
| 5   | p     | 50    | 0        | 43       | 0       | 0            |
| 6   | Z     | 39    | 0        | 34       | 3       | 0            |
| 7   | a     | 28    | 0        | 25       | 0       | 0            |
| 7   | b     | 28    | 0        | 25       | 0       | 0            |
| 7   | c     | 28    | 0        | 25       | 0       | 0            |
| 7   | d     | 28    | 0        | 25       | 0       | 0            |
| 7   | e     | 28    | 0        | 25       | 0       | 0            |
| 7   | f     | 28    | 0        | 25       | 0       | 0            |
| 7   | h     | 28    | 0        | 25       | 0       | 0            |
| 7   | m     | 28    | 0        | 25       | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | n     | 28    | 0        | 25       | 0       | 0            |
| 8   | g     | 61    | 0        | 50       | 0       | 0            |
| 9   | i     | 61    | 0        | 49       | 0       | 0            |
| 9   | l     | 61    | 0        | 51       | 0       | 0            |
| 10  | j     | 50    | 0        | 39       | 0       | 0            |
| 11  | A     | 14    | 0        | 13       | 0       | 0            |
| 11  | E     | 14    | 0        | 13       | 0       | 0            |
| 11  | F     | 14    | 0        | 13       | 0       | 0            |
| 11  | G     | 28    | 0        | 26       | 0       | 0            |
| 11  | K     | 28    | 0        | 26       | 0       | 0            |
| 11  | Q     | 14    | 0        | 13       | 1       | 0            |
| 11  | S     | 14    | 0        | 13       | 0       | 0            |
| 12  | C     | 11    | 0        | 10       | 0       | 0            |
| All | All   | 44024 | 0        | 42435    | 264     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (264) 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:S:169:GLN:NE2  | 4:J:203:SER:O    | 2.25                     | 0.70              |
| 1:A:236:ASN:HA   | 6:Z:1:NAG:H81    | 1.73                     | 0.69              |
| 1:S:169:GLN:NE2  | 4:J:205:VAL:HG23 | 2.10                     | 0.67              |
| 2:L:52:VAL:HG11  | 3:O:28:ILE:HG21  | 1.76                     | 0.66              |
| 1:S:169:GLN:NE2  | 4:J:205:VAL:CG2  | 2.61                     | 0.64              |
| 3:M:50:ASN:HD21  | 4:N:96:ARG:NH1   | 1.97                     | 0.63              |
| 3:I:30:ARG:HB3   | 3:I:77:SER:HB2   | 1.81                     | 0.62              |
| 1:Q:276:THR:HG21 | 1:Q:284:ALA:HB1  | 1.81                     | 0.62              |
| 3:V:30:ARG:HB3   | 3:V:77:SER:HB2   | 1.82                     | 0.62              |
| 1:K:279:GLN:NE2  | 1:K:283:GLY:O    | 2.33                     | 0.62              |
| 3:O:30:ARG:HB3   | 3:O:77:SER:HB2   | 1.82                     | 0.61              |
| 1:A:279:GLN:NE2  | 1:A:283:GLY:O    | 2.33                     | 0.61              |
| 1:S:276:THR:HG21 | 1:S:284:ALA:HB1  | 1.82                     | 0.61              |
| 1:E:279:GLN:NE2  | 1:E:283:GLY:O    | 2.33                     | 0.61              |
| 3:C:30:ARG:HB3   | 3:C:77:SER:HB2   | 1.82                     | 0.60              |
| 1:Q:279:GLN:NE2  | 1:Q:283:GLY:O    | 2.34                     | 0.60              |
| 1:K:276:THR:HG21 | 1:K:284:ALA:HB1  | 1.82                     | 0.60              |
| 1:E:276:THR:HG21 | 1:E:284:ALA:HB1  | 1.82                     | 0.60              |
| 1:G:279:GLN:NE2  | 1:G:283:GLY:O    | 2.33                     | 0.60              |
| 1:S:279:GLN:NE2  | 1:S:283:GLY:O    | 2.34                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:276:THR:HG21 | 1:A:284:ALA:HB1  | 1.83                     | 0.59              |
| 3:M:30:ARG:HB3   | 3:M:77:SER:HB2   | 1.82                     | 0.59              |
| 3:O:50:ASN:HD21  | 4:P:96:ARG:NH1   | 2.00                     | 0.59              |
| 1:G:276:THR:HG21 | 1:G:284:ALA:HB1  | 1.83                     | 0.58              |
| 3:Y:30:ARG:HB3   | 3:Y:77:SER:HB2   | 1.83                     | 0.58              |
| 3:M:52:ILE:HD11  | 3:M:57:THR:HG23  | 1.88                     | 0.56              |
| 3:V:104:GLY:C    | 3:V:105:ASN:HD22 | 2.10                     | 0.55              |
| 4:N:27:GLN:C     | 4:N:27(A):SER:N  | 2.61                     | 0.55              |
| 1:A:7:TYR:CZ     | 2:B:6:ILE:HG23   | 2.42                     | 0.55              |
| 4:W:110:VAL:HG21 | 4:W:199:GLN:HE22 | 1.70                     | 0.54              |
| 2:B:52:VAL:HG11  | 3:C:28:ILE:HG21  | 1.89                     | 0.54              |
| 3:O:52:ILE:HD11  | 3:O:57:THR:HG23  | 1.90                     | 0.54              |
| 3:Y:52:ILE:HD11  | 3:Y:57:THR:HG23  | 1.89                     | 0.54              |
| 4:P:27:GLN:C     | 4:P:27(A):SER:N  | 2.61                     | 0.54              |
| 4:U:27:GLN:C     | 4:U:27(A):SER:N  | 2.62                     | 0.54              |
| 4:J:27:GLN:C     | 4:J:27(A):SER:N  | 2.61                     | 0.54              |
| 4:W:27:GLN:C     | 4:W:27(A):SER:N  | 2.61                     | 0.53              |
| 4:D:27:GLN:C     | 4:D:27(A):SER:N  | 2.61                     | 0.53              |
| 3:V:190:THR:HG21 | 4:W:137:ASN:ND2  | 2.24                     | 0.53              |
| 3:C:52:ILE:HD11  | 3:C:57:THR:HG23  | 1.90                     | 0.53              |
| 3:I:52:ILE:HD11  | 3:I:57:THR:HG23  | 1.90                     | 0.53              |
| 1:S:7:TYR:CZ     | 2:T:6:ILE:HG23   | 2.43                     | 0.53              |
| 3:I:104:GLY:C    | 3:I:105:ASN:HD22 | 2.10                     | 0.52              |
| 4:D:110:VAL:HG21 | 4:D:199:GLN:HE22 | 1.74                     | 0.52              |
| 1:E:7:TYR:CZ     | 2:F:6:ILE:HG23   | 2.45                     | 0.52              |
| 3:V:52:ILE:HD11  | 3:V:57:THR:HG23  | 1.91                     | 0.51              |
| 4:N:110:VAL:HG21 | 4:N:199:GLN:HE22 | 1.76                     | 0.51              |
| 3:I:202:ILE:HD13 | 3:V:164:GLY:HA3  | 1.91                     | 0.51              |
| 2:L:30:GLN:NE2   | 2:L:146:ASN:ND2  | 2.59                     | 0.51              |
| 1:Q:3:ILE:HD11   | 2:R:149:MET:SD   | 2.50                     | 0.51              |
| 3:Y:50:ASN:HD21  | 4:U:96:ARG:NH1   | 2.09                     | 0.51              |
| 1:K:109:ASN:ND2  | 4:W:6:GLN:O      | 2.44                     | 0.51              |
| 1:K:109:ASN:OD1  | 4:W:8:PRO:HA     | 2.11                     | 0.50              |
| 1:A:165:ASN:OD1  | 6:Z:1:NAG:C7     | 2.59                     | 0.50              |
| 3:O:104:GLY:C    | 3:O:105:ASN:HD22 | 2.15                     | 0.50              |
| 2:T:20:GLY:HA2   | 3:V:55:PHE:CZ    | 2.46                     | 0.50              |
| 2:H:94:TYR:CZ    | 2:H:98:LEU:HD11  | 2.47                     | 0.50              |
| 2:R:94:TYR:CZ    | 2:R:98:LEU:HD11  | 2.47                     | 0.49              |
| 1:S:149:TRP:HA   | 1:S:248:ILE:HG22 | 1.94                     | 0.49              |
| 4:U:110:VAL:HG21 | 4:U:199:GLN:HE22 | 1.77                     | 0.49              |
| 3:M:104:GLY:C    | 3:M:105:ASN:HD22 | 2.15                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:317:LEU:HD13 | 1:A:317:LEU:N    | 2.27                     | 0.49              |
| 1:E:149:TRP:HA   | 1:E:248:ILE:HG22 | 1.95                     | 0.49              |
| 1:G:317:LEU:N    | 1:G:317:LEU:HD13 | 2.28                     | 0.49              |
| 2:L:94:TYR:CZ    | 2:L:98:LEU:HD11  | 2.47                     | 0.49              |
| 3:C:12:LYS:HG3   | 3:C:18:VAL:HG22  | 1.94                     | 0.49              |
| 1:K:317:LEU:HD13 | 1:K:317:LEU:N    | 2.28                     | 0.49              |
| 1:Q:35:LYS:HA    | 1:Q:293:ASN:HD21 | 1.77                     | 0.49              |
| 2:F:19:ASP:HB2   | 2:F:36:ALA:HB3   | 1.95                     | 0.49              |
| 1:E:317:LEU:N    | 1:E:317:LEU:HD13 | 2.28                     | 0.49              |
| 2:F:24:TYR:CE1   | 2:F:153:ARG:HG2  | 2.47                     | 0.49              |
| 2:H:19:ASP:HB2   | 2:H:36:ALA:HB3   | 1.94                     | 0.49              |
| 1:S:105:LEU:HA   | 1:S:108:ILE:HD11 | 1.95                     | 0.49              |
| 1:G:35:LYS:HA    | 1:G:293:ASN:HD21 | 1.78                     | 0.49              |
| 1:S:317:LEU:N    | 1:S:317:LEU:HD13 | 2.27                     | 0.49              |
| 1:S:30:GLN:OE1   | 3:V:28:ILE:HG22  | 2.12                     | 0.48              |
| 1:E:105:LEU:HA   | 1:E:108:ILE:HD11 | 1.95                     | 0.48              |
| 2:H:6:ILE:HG23   | 1:K:7:TYR:CZ     | 2.48                     | 0.48              |
| 1:K:35:LYS:HA    | 1:K:293:ASN:HD21 | 1.77                     | 0.48              |
| 1:K:105:LEU:HA   | 1:K:108:ILE:HD11 | 1.94                     | 0.48              |
| 2:L:30:GLN:NE2   | 2:L:146:ASN:HD22 | 2.12                     | 0.48              |
| 1:E:35:LYS:HA    | 1:E:293:ASN:HD21 | 1.77                     | 0.48              |
| 1:G:105:LEU:HA   | 1:G:108:ILE:HD11 | 1.95                     | 0.48              |
| 1:G:247:PHE:CE2  | 1:G:249:ALA:HB2  | 2.48                     | 0.48              |
| 1:Q:317:LEU:N    | 1:Q:317:LEU:HD13 | 2.28                     | 0.48              |
| 1:A:247:PHE:CE2  | 1:A:249:ALA:HB2  | 2.49                     | 0.48              |
| 1:K:149:TRP:HA   | 1:K:248:ILE:HG22 | 1.95                     | 0.48              |
| 4:J:110:VAL:HG21 | 4:J:199:GLN:HE22 | 1.79                     | 0.48              |
| 1:G:149:TRP:HA   | 1:G:248:ILE:HG22 | 1.95                     | 0.48              |
| 1:A:149:TRP:HA   | 1:A:248:ILE:HG22 | 1.96                     | 0.48              |
| 1:Q:149:TRP:HA   | 1:Q:248:ILE:HG22 | 1.95                     | 0.48              |
| 1:S:35:LYS:HA    | 1:S:293:ASN:HD21 | 1.78                     | 0.48              |
| 1:Q:105:LEU:HA   | 1:Q:108:ILE:HD11 | 1.96                     | 0.47              |
| 1:Q:247:PHE:CE2  | 1:Q:249:ALA:HB2  | 2.48                     | 0.47              |
| 1:A:35:LYS:HA    | 1:A:293:ASN:HD21 | 1.78                     | 0.47              |
| 2:B:94:TYR:CZ    | 2:B:98:LEU:HD11  | 2.49                     | 0.47              |
| 2:F:94:TYR:CZ    | 2:F:98:LEU:HD11  | 2.50                     | 0.47              |
| 4:P:110:VAL:HG21 | 4:P:199:GLN:HE22 | 1.78                     | 0.47              |
| 3:Y:104:GLY:C    | 3:Y:105:ASN:HD22 | 2.17                     | 0.47              |
| 1:K:247:PHE:CE2  | 1:K:249:ALA:HB2  | 2.49                     | 0.47              |
| 2:H:79:ASN:HD21  | 2:L:66:VAL:HG21  | 1.80                     | 0.47              |
| 3:I:12:LYS:HG3   | 3:I:18:VAL:HG22  | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:247:PHE:CE2  | 1:S:249:ALA:HB2  | 2.49                     | 0.47              |
| 2:B:24:TYR:CE1   | 2:B:153:ARG:HG2  | 2.49                     | 0.47              |
| 1:G:5:ILE:N      | 1:G:5:ILE:HD12   | 2.30                     | 0.47              |
| 1:S:5:ILE:N      | 1:S:5:ILE:HD12   | 2.29                     | 0.47              |
| 2:T:94:TYR:CZ    | 2:T:98:LEU:HD11  | 2.49                     | 0.47              |
| 3:V:12:LYS:HG3   | 3:V:18:VAL:HG22  | 1.97                     | 0.47              |
| 2:B:94:TYR:CD1   | 2:H:59:MET:HG3   | 2.49                     | 0.46              |
| 1:A:105:LEU:HA   | 1:A:108:ILE:HD11 | 1.96                     | 0.46              |
| 1:E:247:PHE:CE2  | 1:E:249:ALA:HB2  | 2.49                     | 0.46              |
| 3:Y:39:GLN:NE2   | 4:U:38:GLN:OE1   | 2.46                     | 0.46              |
| 2:T:24:TYR:CE1   | 2:T:153:ARG:HG2  | 2.51                     | 0.46              |
| 3:M:12:LYS:HG3   | 3:M:18:VAL:HG22  | 1.97                     | 0.46              |
| 1:S:274:CYS:SG   | 1:S:275:ASN:N    | 2.89                     | 0.46              |
| 2:R:19:ASP:HB2   | 2:R:36:ALA:HB3   | 1.97                     | 0.46              |
| 1:A:274:CYS:SG   | 1:A:275:ASN:N    | 2.89                     | 0.46              |
| 1:E:274:CYS:SG   | 1:E:275:ASN:N    | 2.89                     | 0.46              |
| 1:K:5:ILE:HD12   | 1:K:5:ILE:N      | 2.31                     | 0.46              |
| 2:T:18:VAL:O     | 3:V:57:THR:HG21  | 2.16                     | 0.46              |
| 3:C:50:ASN:HD21  | 4:D:96:ARG:NH1   | 2.14                     | 0.46              |
| 3:C:104:GLY:C    | 3:C:105:ASN:HD22 | 2.16                     | 0.46              |
| 3:C:30:ARG:HH12  | 3:C:72:ALA:HB1   | 1.81                     | 0.46              |
| 1:A:236:ASN:OD1  | 6:Z:1:NAG:C7     | 2.64                     | 0.45              |
| 1:E:5:ILE:N      | 1:E:5:ILE:HD12   | 2.31                     | 0.45              |
| 3:O:30:ARG:HH12  | 3:O:72:ALA:HB1   | 1.81                     | 0.45              |
| 3:I:70:ILE:HG22  | 3:I:81:MET:HA    | 1.98                     | 0.45              |
| 3:M:188:VAL:HG21 | 4:N:135:LEU:HD22 | 1.97                     | 0.45              |
| 3:V:30:ARG:HH12  | 3:V:72:ALA:HB1   | 1.81                     | 0.45              |
| 3:Y:12:LYS:HG3   | 3:Y:18:VAL:HG22  | 1.97                     | 0.45              |
| 1:G:274:CYS:SG   | 1:G:275:ASN:N    | 2.89                     | 0.45              |
| 1:K:274:CYS:SG   | 1:K:275:ASN:N    | 2.89                     | 0.45              |
| 1:Q:7:TYR:CZ     | 2:R:6:ILE:HG23   | 2.52                     | 0.45              |
| 1:Q:274:CYS:SG   | 1:Q:275:ASN:N    | 2.89                     | 0.45              |
| 3:V:102:TYR:O    | 3:V:102:TYR:CD2  | 2.70                     | 0.45              |
| 3:Y:102:TYR:CD2  | 3:Y:102:TYR:O    | 2.70                     | 0.45              |
| 2:B:19:ASP:HB2   | 2:B:36:ALA:HB3   | 1.99                     | 0.45              |
| 2:H:175:SER:O    | 2:L:168:LEU:HD11 | 2.16                     | 0.45              |
| 3:M:102:TYR:CD2  | 3:M:102:TYR:O    | 2.70                     | 0.45              |
| 1:S:169:GLN:NE2  | 4:J:205:VAL:HG22 | 2.31                     | 0.45              |
| 3:C:7:SER:O      | 3:C:114:THR:HG22 | 2.16                     | 0.45              |
| 3:M:70:ILE:HG22  | 3:M:81:MET:HA    | 1.99                     | 0.45              |
| 3:O:7:SER:O      | 3:O:114:THR:HG22 | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:V:70:ILE:HG22  | 3:V:81:MET:HA    | 1.98                     | 0.45              |
| 3:V:188:VAL:HG21 | 4:W:135:LEU:CD2  | 2.46                     | 0.45              |
| 3:I:7:SER:O      | 3:I:114:THR:HG22 | 2.17                     | 0.45              |
| 2:L:24:TYR:CE1   | 2:L:153:ARG:HG2  | 2.52                     | 0.45              |
| 2:R:24:TYR:CE1   | 2:R:153:ARG:HG2  | 2.51                     | 0.45              |
| 3:O:12:LYS:HG3   | 3:O:18:VAL:HG22  | 1.98                     | 0.45              |
| 3:Y:7:SER:O      | 3:Y:114:THR:HG22 | 2.17                     | 0.45              |
| 1:E:3:ILE:HD11   | 2:F:149:MET:HG2  | 1.99                     | 0.44              |
| 3:M:7:SER:O      | 3:M:114:THR:HG22 | 2.16                     | 0.44              |
| 1:E:226:MET:CE   | 1:E:248:ILE:HG21 | 2.48                     | 0.44              |
| 2:B:61:THR:HG22  | 2:L:90:ASP:OD1   | 2.18                     | 0.44              |
| 1:K:226:MET:CE   | 1:K:248:ILE:HG21 | 2.47                     | 0.44              |
| 1:Q:5:ILE:N      | 1:Q:5:ILE:HD12   | 2.32                     | 0.44              |
| 3:Y:70:ILE:HG22  | 3:Y:81:MET:HA    | 1.99                     | 0.44              |
| 3:I:102:TYR:O    | 3:I:102:TYR:CD2  | 2.70                     | 0.44              |
| 3:O:102:TYR:O    | 3:O:102:TYR:CD2  | 2.71                     | 0.44              |
| 1:S:226:MET:CE   | 1:S:248:ILE:HG21 | 2.47                     | 0.44              |
| 3:Y:30:ARG:HH12  | 3:Y:72:ALA:HB1   | 1.81                     | 0.44              |
| 1:Q:11:ASN:HD21  | 11:Q:401:NAG:C7  | 2.31                     | 0.44              |
| 3:V:7:SER:O      | 3:V:114:THR:HG22 | 2.17                     | 0.44              |
| 1:A:5:ILE:HD12   | 1:A:5:ILE:N      | 2.32                     | 0.44              |
| 2:T:19:ASP:HB2   | 2:T:36:ALA:HB3   | 1.98                     | 0.44              |
| 3:C:70:ILE:HG22  | 3:C:81:MET:HA    | 1.99                     | 0.44              |
| 3:I:126:PRO:HB2  | 3:I:149:VAL:HG13 | 2.00                     | 0.44              |
| 2:R:52:VAL:HG11  | 3:Y:28:ILE:HG21  | 2.00                     | 0.44              |
| 1:G:293:ASN:N    | 1:G:293:ASN:HD22 | 2.16                     | 0.43              |
| 3:O:70:ILE:HG22  | 3:O:81:MET:HA    | 2.00                     | 0.43              |
| 3:I:30:ARG:HH12  | 3:I:72:ALA:HB1   | 1.83                     | 0.43              |
| 2:H:83:LYS:HE2   | 2:L:66:VAL:HG23  | 2.01                     | 0.43              |
| 2:L:52:VAL:HG11  | 3:O:28:ILE:CG2   | 2.47                     | 0.43              |
| 1:Q:226:MET:CE   | 1:Q:248:ILE:HG21 | 2.48                     | 0.43              |
| 2:B:42:GLN:NE2   | 3:C:101:TYR:HB2  | 2.34                     | 0.43              |
| 1:A:226:MET:CE   | 1:A:248:ILE:HG21 | 2.48                     | 0.43              |
| 2:H:2:LEU:O      | 2:L:113:SER:OG   | 2.37                     | 0.43              |
| 2:H:175:SER:C    | 2:L:168:LEU:HD11 | 2.39                     | 0.43              |
| 3:I:91:THR:HG23  | 3:I:117:THR:HA   | 2.01                     | 0.43              |
| 3:I:202:ILE:HG21 | 3:V:164:GLY:O    | 2.19                     | 0.43              |
| 2:L:19:ASP:HB2   | 2:L:36:ALA:HB3   | 2.00                     | 0.43              |
| 3:V:126:PRO:HB2  | 3:V:149:VAL:HG13 | 2.01                     | 0.43              |
| 1:A:18:THR:OG1   | 1:A:19:ILE:N     | 2.52                     | 0.43              |
| 1:K:18:THR:OG1   | 1:K:19:ILE:N     | 2.52                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:307:LYS:HB2  | 2:B:89:LEU:HD11  | 2.01                     | 0.42              |
| 3:C:91:THR:HG23  | 3:C:117:THR:HA   | 2.01                     | 0.42              |
| 3:C:102:TYR:CD2  | 3:C:102:TYR:O    | 2.71                     | 0.42              |
| 1:E:293:ASN:N    | 1:E:293:ASN:HD22 | 2.17                     | 0.42              |
| 3:M:107:HIS:HB2  | 4:N:36:PHE:CE1   | 2.55                     | 0.42              |
| 4:W:110:VAL:HG21 | 4:W:199:GLN:NE2  | 2.34                     | 0.42              |
| 1:Q:293:ASN:N    | 1:Q:293:ASN:HD22 | 2.17                     | 0.42              |
| 1:S:18:THR:OG1   | 1:S:19:ILE:N     | 2.53                     | 0.42              |
| 2:H:24:TYR:CE1   | 2:H:153:ARG:HG2  | 2.53                     | 0.42              |
| 3:M:102:TYR:O    | 3:M:102:TYR:CG   | 2.72                     | 0.42              |
| 3:O:126:PRO:HB2  | 3:O:149:VAL:HG13 | 2.00                     | 0.42              |
| 1:Q:18:THR:OG1   | 1:Q:19:ILE:N     | 2.52                     | 0.42              |
| 3:V:33:ALA:O     | 3:V:98:ARG:O     | 2.38                     | 0.42              |
| 1:S:293:ASN:N    | 1:S:293:ASN:HD22 | 2.17                     | 0.42              |
| 2:T:20:GLY:HA2   | 3:V:55:PHE:CE1   | 2.54                     | 0.42              |
| 3:V:34:ILE:HD12  | 3:V:34:ILE:N     | 2.35                     | 0.42              |
| 3:Y:126:PRO:HB2  | 3:Y:149:VAL:HG13 | 2.01                     | 0.42              |
| 4:U:124:GLN:HE22 | 4:U:131:SER:CB   | 2.33                     | 0.42              |
| 1:A:30:GLN:OE1   | 3:C:28:ILE:HG22  | 2.20                     | 0.42              |
| 1:A:293:ASN:N    | 1:A:293:ASN:HD22 | 2.17                     | 0.42              |
| 3:O:17:SER:OG    | 2:R:143:LYS:NZ   | 2.30                     | 0.42              |
| 4:U:79:GLU:HB3   | 4:U:80:PRO:HD2   | 2.02                     | 0.42              |
| 1:E:18:THR:OG1   | 1:E:19:ILE:N     | 2.53                     | 0.42              |
| 3:O:153:PHE:HA   | 3:O:154:PRO:HA   | 1.91                     | 0.42              |
| 3:M:30:ARG:HH12  | 3:M:72:ALA:HB1   | 1.84                     | 0.42              |
| 3:M:126:PRO:HB2  | 3:M:149:VAL:HG13 | 2.02                     | 0.42              |
| 3:O:91:THR:HG23  | 3:O:117:THR:HA   | 2.01                     | 0.41              |
| 4:J:124:GLN:HE22 | 4:J:131:SER:CB   | 2.33                     | 0.41              |
| 4:D:124:GLN:HE22 | 4:D:131:SER:CB   | 2.33                     | 0.41              |
| 1:G:226:MET:CE   | 1:G:248:ILE:HG21 | 2.50                     | 0.41              |
| 1:K:293:ASN:HD22 | 1:K:293:ASN:N    | 2.16                     | 0.41              |
| 4:N:79:GLU:HB3   | 4:N:80:PRO:HD2   | 2.02                     | 0.41              |
| 1:S:1:ASP:OD1    | 2:T:28:ASN:HB2   | 2.19                     | 0.41              |
| 3:Y:153:PHE:HA   | 3:Y:154:PRO:HA   | 1.92                     | 0.41              |
| 4:N:124:GLN:HE22 | 4:N:131:SER:CB   | 2.33                     | 0.41              |
| 1:G:18:THR:OG1   | 1:G:19:ILE:N     | 2.52                     | 0.41              |
| 4:P:124:GLN:HE22 | 4:P:131:SER:CB   | 2.33                     | 0.41              |
| 3:Y:102:TYR:O    | 3:Y:102:TYR:CG   | 2.73                     | 0.41              |
| 1:S:316:GLY:O    | 2:T:111:HIS:CD2  | 2.74                     | 0.41              |
| 4:W:79:GLU:HB3   | 4:W:80:PRO:HD2   | 2.03                     | 0.41              |
| 4:W:124:GLN:HE22 | 4:W:131:SER:CB   | 2.33                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:THR:HG22 | 1:A:203:SER:N    | 2.35                     | 0.41              |
| 2:T:42:GLN:HE21  | 3:V:102:TYR:HD2  | 1.68                     | 0.41              |
| 3:V:91:THR:HG23  | 3:V:117:THR:HA   | 2.01                     | 0.41              |
| 3:Y:33:ALA:O     | 3:Y:98:ARG:O     | 2.38                     | 0.41              |
| 3:I:33:ALA:O     | 3:I:98:ARG:O     | 2.38                     | 0.41              |
| 3:M:33:ALA:O     | 3:M:98:ARG:O     | 2.39                     | 0.41              |
| 3:M:91:THR:HG23  | 3:M:117:THR:HA   | 2.03                     | 0.41              |
| 4:P:79:GLU:HB3   | 4:P:80:PRO:HD2   | 2.03                     | 0.41              |
| 3:V:188:VAL:HG11 | 4:W:135:LEU:HD22 | 2.02                     | 0.41              |
| 2:B:110:PHE:CE1  | 1:G:20:MET:HE1   | 2.55                     | 0.41              |
| 3:I:102:TYR:O    | 3:I:102:TYR:CG   | 2.73                     | 0.41              |
| 3:O:33:ALA:O     | 3:O:98:ARG:O     | 2.39                     | 0.41              |
| 3:V:102:TYR:O    | 3:V:102:TYR:CG   | 2.73                     | 0.41              |
| 3:Y:91:THR:HG23  | 3:Y:117:THR:HA   | 2.02                     | 0.41              |
| 4:D:8:PRO:HG2    | 4:D:11:LEU:HG    | 2.03                     | 0.41              |
| 4:D:79:GLU:HB3   | 4:D:80:PRO:HD2   | 2.03                     | 0.41              |
| 3:C:33:ALA:O     | 3:C:98:ARG:O     | 2.38                     | 0.41              |
| 3:C:126:PRO:HB2  | 3:C:149:VAL:HG13 | 2.02                     | 0.41              |
| 2:H:19:ASP:HB2   | 2:H:36:ALA:CB    | 2.51                     | 0.41              |
| 1:K:101:LEU:HD13 | 1:K:230:TRP:CE3  | 2.55                     | 0.41              |
| 1:K:202:THR:HG22 | 1:K:203:SER:N    | 2.36                     | 0.41              |
| 2:F:19:ASP:HB2   | 2:F:36:ALA:CB    | 2.51                     | 0.40              |
| 1:K:259:LYS:HE3  | 4:W:24:ARG:CG    | 2.51                     | 0.40              |
| 1:Q:32:ILE:HD11  | 1:Q:313:LEU:HD22 | 2.03                     | 0.40              |
| 1:S:101:LEU:HD13 | 1:S:230:TRP:CE3  | 2.56                     | 0.40              |
| 1:S:263:THR:HG21 | 2:T:67:GLY:H     | 1.86                     | 0.40              |
| 4:W:8:PRO:HG2    | 4:W:11:LEU:HG    | 2.04                     | 0.40              |
| 1:E:263:THR:HG22 | 1:E:299:ILE:CD1  | 2.52                     | 0.40              |
| 1:G:202:THR:HG22 | 1:G:203:SER:N    | 2.36                     | 0.40              |
| 1:G:293:ASN:HD22 | 1:G:293:ASN:H    | 1.69                     | 0.40              |
| 1:K:75:GLU:OE2   | 4:W:9:GLY:N      | 2.55                     | 0.40              |
| 1:Q:101:LEU:HD13 | 1:Q:230:TRP:CE3  | 2.57                     | 0.40              |
| 1:Q:293:ASN:HD22 | 1:Q:293:ASN:H    | 1.69                     | 0.40              |
| 1:E:202:THR:HG22 | 1:E:203:SER:N    | 2.36                     | 0.40              |
| 1:K:293:ASN:HD22 | 1:K:293:ASN:H    | 1.69                     | 0.40              |
| 2:L:52:VAL:CG1   | 3:O:28:ILE:HG21  | 2.47                     | 0.40              |
| 2:B:98:LEU:HD13  | 2:H:99:LEU:HD11  | 2.04                     | 0.40              |
| 1:S:202:THR:HG22 | 1:S:203:SER:N    | 2.36                     | 0.40              |
| 1:Q:16:VAL:CG1   | 2:R:104:ASN:ND2  | 2.84                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)   | 282 (88%)  | 33 (10%) | 4 (1%)   | 10          | 41 |
| 1   | E     | 319/330 (97%)   | 283 (89%)  | 32 (10%) | 4 (1%)   | 10          | 41 |
| 1   | G     | 319/330 (97%)   | 283 (89%)  | 32 (10%) | 4 (1%)   | 10          | 41 |
| 1   | K     | 319/330 (97%)   | 283 (89%)  | 31 (10%) | 5 (2%)   | 8           | 37 |
| 1   | Q     | 319/330 (97%)   | 283 (89%)  | 33 (10%) | 3 (1%)   | 14          | 48 |
| 1   | S     | 319/330 (97%)   | 284 (89%)  | 31 (10%) | 4 (1%)   | 10          | 41 |
| 2   | B     | 172/181 (95%)   | 159 (92%)  | 12 (7%)  | 1 (1%)   | 22          | 57 |
| 2   | F     | 173/181 (96%)   | 159 (92%)  | 13 (8%)  | 1 (1%)   | 22          | 57 |
| 2   | H     | 173/181 (96%)   | 159 (92%)  | 13 (8%)  | 1 (1%)   | 22          | 57 |
| 2   | L     | 173/181 (96%)   | 159 (92%)  | 13 (8%)  | 1 (1%)   | 22          | 57 |
| 2   | R     | 173/181 (96%)   | 159 (92%)  | 13 (8%)  | 1 (1%)   | 22          | 57 |
| 2   | T     | 173/181 (96%)   | 159 (92%)  | 13 (8%)  | 1 (1%)   | 22          | 57 |
| 3   | C     | 210/221 (95%)   | 181 (86%)  | 26 (12%) | 3 (1%)   | 9           | 39 |
| 3   | I     | 210/221 (95%)   | 182 (87%)  | 25 (12%) | 3 (1%)   | 9           | 39 |
| 3   | M     | 210/221 (95%)   | 182 (87%)  | 25 (12%) | 3 (1%)   | 9           | 39 |
| 3   | O     | 210/221 (95%)   | 182 (87%)  | 25 (12%) | 3 (1%)   | 9           | 39 |
| 3   | V     | 210/221 (95%)   | 183 (87%)  | 24 (11%) | 3 (1%)   | 9           | 39 |
| 3   | Y     | 210/221 (95%)   | 182 (87%)  | 25 (12%) | 3 (1%)   | 9           | 39 |
| 4   | D     | 208/215 (97%)   | 200 (96%)  | 7 (3%)   | 1 (0%)   | 25          | 60 |
| 4   | J     | 208/215 (97%)   | 198 (95%)  | 8 (4%)   | 2 (1%)   | 13          | 46 |
| 4   | N     | 208/215 (97%)   | 199 (96%)  | 8 (4%)   | 1 (0%)   | 25          | 60 |
| 4   | P     | 207/215 (96%)   | 198 (96%)  | 8 (4%)   | 1 (0%)   | 25          | 60 |
| 4   | U     | 208/215 (97%)   | 199 (96%)  | 8 (4%)   | 1 (0%)   | 25          | 60 |
| 4   | W     | 208/215 (97%)   | 200 (96%)  | 7 (3%)   | 1 (0%)   | 25          | 60 |
| All | All   | 5458/5682 (96%) | 4938 (90%) | 465 (8%) | 55 (1%)  | 13          | 46 |

All (55) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 65  | GLN  |
| 3   | I     | 65  | GLN  |
| 3   | M     | 65  | GLN  |
| 3   | O     | 65  | GLN  |
| 3   | V     | 65  | GLN  |
| 3   | Y     | 65  | GLN  |
| 2   | B     | 60  | ASN  |
| 3   | C     | 207 | HIS  |
| 2   | F     | 60  | ASN  |
| 2   | H     | 60  | ASN  |
| 3   | I     | 207 | HIS  |
| 2   | L     | 60  | ASN  |
| 3   | M     | 207 | HIS  |
| 3   | O     | 207 | HIS  |
| 4   | P     | 101 | GLY  |
| 2   | R     | 60  | ASN  |
| 1   | S     | 154 | ASN  |
| 2   | T     | 60  | ASN  |
| 3   | V     | 207 | HIS  |
| 3   | Y     | 207 | HIS  |
| 4   | U     | 101 | GLY  |
| 4   | J     | 101 | GLY  |
| 4   | D     | 101 | GLY  |
| 4   | W     | 101 | GLY  |
| 4   | N     | 101 | GLY  |
| 1   | A     | 154 | ASN  |
| 1   | A     | 194 | PRO  |
| 1   | E     | 154 | ASN  |
| 1   | E     | 194 | PRO  |
| 1   | G     | 154 | ASN  |
| 1   | G     | 194 | PRO  |
| 1   | K     | 154 | ASN  |
| 1   | K     | 194 | PRO  |
| 1   | Q     | 154 | ASN  |
| 1   | Q     | 194 | PRO  |
| 1   | S     | 194 | PRO  |
| 1   | A     | 134 | ALA  |
| 1   | E     | 134 | ALA  |
| 1   | G     | 134 | ALA  |
| 1   | K     | 134 | ALA  |
| 1   | Q     | 134 | ALA  |
| 1   | S     | 134 | ALA  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | O     | 154 | PRO  |
| 4   | J     | 29  | SER  |
| 1   | A     | 262 | SER  |
| 3   | C     | 154 | PRO  |
| 1   | E     | 133 | SER  |
| 1   | G     | 262 | SER  |
| 1   | K     | 133 | SER  |
| 1   | K     | 262 | SER  |
| 1   | S     | 262 | SER  |
| 3   | I     | 154 | PRO  |
| 3   | Y     | 154 | PRO  |
| 3   | V     | 154 | PRO  |
| 3   | M     | 154 | PRO  |

### 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     | 289/298 (97%) | 264 (91%) | 25 (9%)  | 8           | 30 |
| 1   | E     | 289/298 (97%) | 264 (91%) | 25 (9%)  | 8           | 30 |
| 1   | G     | 289/298 (97%) | 263 (91%) | 26 (9%)  | 8           | 28 |
| 1   | K     | 289/298 (97%) | 263 (91%) | 26 (9%)  | 8           | 28 |
| 1   | Q     | 289/298 (97%) | 264 (91%) | 25 (9%)  | 8           | 30 |
| 1   | S     | 289/298 (97%) | 263 (91%) | 26 (9%)  | 8           | 28 |
| 2   | B     | 149/155 (96%) | 139 (93%) | 10 (7%)  | 13          | 38 |
| 2   | F     | 149/155 (96%) | 138 (93%) | 11 (7%)  | 11          | 34 |
| 2   | H     | 149/155 (96%) | 137 (92%) | 12 (8%)  | 9           | 32 |
| 2   | L     | 149/155 (96%) | 139 (93%) | 10 (7%)  | 13          | 38 |
| 2   | R     | 149/155 (96%) | 139 (93%) | 10 (7%)  | 13          | 38 |
| 2   | T     | 149/155 (96%) | 139 (93%) | 10 (7%)  | 13          | 38 |
| 3   | C     | 177/183 (97%) | 168 (95%) | 9 (5%)   | 20          | 45 |
| 3   | I     | 177/183 (97%) | 168 (95%) | 9 (5%)   | 20          | 45 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3   | M     | 177/183 (97%)   | 165 (93%)  | 12 (7%)  | 13          | 37 |
| 3   | O     | 177/183 (97%)   | 166 (94%)  | 11 (6%)  | 15          | 40 |
| 3   | V     | 177/183 (97%)   | 167 (94%)  | 10 (6%)  | 17          | 43 |
| 3   | Y     | 177/183 (97%)   | 167 (94%)  | 10 (6%)  | 17          | 43 |
| 4   | D     | 183/185 (99%)   | 176 (96%)  | 7 (4%)   | 28          | 52 |
| 4   | J     | 183/185 (99%)   | 177 (97%)  | 6 (3%)   | 33          | 55 |
| 4   | N     | 183/185 (99%)   | 176 (96%)  | 7 (4%)   | 28          | 52 |
| 4   | P     | 182/185 (98%)   | 176 (97%)  | 6 (3%)   | 33          | 55 |
| 4   | U     | 183/185 (99%)   | 177 (97%)  | 6 (3%)   | 33          | 55 |
| 4   | W     | 183/185 (99%)   | 177 (97%)  | 6 (3%)   | 33          | 55 |
| All | All   | 4787/4926 (97%) | 4472 (93%) | 315 (7%) | 14          | 38 |

All (315) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | THR  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 27  | THR  |
| 1   | A     | 36  | LYS  |
| 1   | A     | 41  | LEU  |
| 1   | A     | 53  | ARG  |
| 1   | A     | 55  | CYS  |
| 1   | A     | 69  | GLU  |
| 1   | A     | 173 | LEU  |
| 1   | A     | 181 | PRO  |
| 1   | A     | 192 | GLN  |
| 1   | A     | 217 | SER  |
| 1   | A     | 225 | ARG  |
| 1   | A     | 226 | MET  |
| 1   | A     | 271 | TYR  |
| 1   | A     | 274 | CYS  |
| 1   | A     | 275 | ASN  |
| 1   | A     | 277 | LYS  |
| 1   | A     | 278 | CYS  |
| 1   | A     | 280 | THR  |
| 1   | A     | 293 | ASN  |
| 1   | A     | 297 | LEU  |
| 1   | A     | 317 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 319 | ASN  |
| 1   | A     | 320 | SER  |
| 2   | B     | 28  | ASN  |
| 2   | B     | 30  | GLN  |
| 2   | B     | 42  | GLN  |
| 2   | B     | 62  | GLN  |
| 2   | B     | 112 | ASP  |
| 2   | B     | 116 | LYS  |
| 2   | B     | 117 | ASN  |
| 2   | B     | 126 | LEU  |
| 2   | B     | 127 | ARG  |
| 2   | B     | 158 | ASP  |
| 3   | C     | 28  | ILE  |
| 3   | C     | 51  | ILE  |
| 3   | C     | 52  | ILE  |
| 3   | C     | 57  | THR  |
| 3   | C     | 98  | ARG  |
| 3   | C     | 101 | TYR  |
| 3   | C     | 102 | TYR  |
| 3   | C     | 106 | SER  |
| 3   | C     | 157 | VAL  |
| 1   | E     | 18  | THR  |
| 1   | E     | 19  | ILE  |
| 1   | E     | 27  | THR  |
| 1   | E     | 36  | LYS  |
| 1   | E     | 41  | LEU  |
| 1   | E     | 53  | ARG  |
| 1   | E     | 55  | CYS  |
| 1   | E     | 69  | GLU  |
| 1   | E     | 95  | PHE  |
| 1   | E     | 173 | LEU  |
| 1   | E     | 192 | GLN  |
| 1   | E     | 217 | SER  |
| 1   | E     | 225 | ARG  |
| 1   | E     | 226 | MET  |
| 1   | E     | 271 | TYR  |
| 1   | E     | 274 | CYS  |
| 1   | E     | 275 | ASN  |
| 1   | E     | 277 | LYS  |
| 1   | E     | 278 | CYS  |
| 1   | E     | 280 | THR  |
| 1   | E     | 293 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 297 | LEU  |
| 1   | E     | 317 | LEU  |
| 1   | E     | 319 | ASN  |
| 1   | E     | 320 | SER  |
| 2   | F     | 28  | ASN  |
| 2   | F     | 30  | GLN  |
| 2   | F     | 42  | GLN  |
| 2   | F     | 60  | ASN  |
| 2   | F     | 62  | GLN  |
| 2   | F     | 112 | ASP  |
| 2   | F     | 116 | LYS  |
| 2   | F     | 117 | ASN  |
| 2   | F     | 126 | LEU  |
| 2   | F     | 127 | ARG  |
| 2   | F     | 158 | ASP  |
| 1   | G     | 18  | THR  |
| 1   | G     | 19  | ILE  |
| 1   | G     | 27  | THR  |
| 1   | G     | 36  | LYS  |
| 1   | G     | 41  | LEU  |
| 1   | G     | 53  | ARG  |
| 1   | G     | 55  | CYS  |
| 1   | G     | 69  | GLU  |
| 1   | G     | 120 | SER  |
| 1   | G     | 173 | LEU  |
| 1   | G     | 181 | PRO  |
| 1   | G     | 192 | GLN  |
| 1   | G     | 217 | SER  |
| 1   | G     | 225 | ARG  |
| 1   | G     | 226 | MET  |
| 1   | G     | 271 | TYR  |
| 1   | G     | 274 | CYS  |
| 1   | G     | 275 | ASN  |
| 1   | G     | 278 | CYS  |
| 1   | G     | 280 | THR  |
| 1   | G     | 288 | SER  |
| 1   | G     | 293 | ASN  |
| 1   | G     | 297 | LEU  |
| 1   | G     | 317 | LEU  |
| 1   | G     | 319 | ASN  |
| 1   | G     | 320 | SER  |
| 2   | H     | 28  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 30  | GLN  |
| 2   | H     | 42  | GLN  |
| 2   | H     | 62  | GLN  |
| 2   | H     | 99  | LEU  |
| 2   | H     | 112 | ASP  |
| 2   | H     | 116 | LYS  |
| 2   | H     | 117 | ASN  |
| 2   | H     | 121 | LYS  |
| 2   | H     | 126 | LEU  |
| 2   | H     | 127 | ARG  |
| 2   | H     | 158 | ASP  |
| 3   | I     | 28  | ILE  |
| 3   | I     | 51  | ILE  |
| 3   | I     | 52  | ILE  |
| 3   | I     | 57  | THR  |
| 3   | I     | 98  | ARG  |
| 3   | I     | 101 | TYR  |
| 3   | I     | 102 | TYR  |
| 3   | I     | 106 | SER  |
| 3   | I     | 157 | VAL  |
| 1   | K     | 18  | THR  |
| 1   | K     | 19  | ILE  |
| 1   | K     | 27  | THR  |
| 1   | K     | 36  | LYS  |
| 1   | K     | 40  | LYS  |
| 1   | K     | 41  | LEU  |
| 1   | K     | 53  | ARG  |
| 1   | K     | 55  | CYS  |
| 1   | K     | 69  | GLU  |
| 1   | K     | 95  | PHE  |
| 1   | K     | 173 | LEU  |
| 1   | K     | 192 | GLN  |
| 1   | K     | 217 | SER  |
| 1   | K     | 225 | ARG  |
| 1   | K     | 226 | MET  |
| 1   | K     | 271 | TYR  |
| 1   | K     | 274 | CYS  |
| 1   | K     | 275 | ASN  |
| 1   | K     | 277 | LYS  |
| 1   | K     | 278 | CYS  |
| 1   | K     | 280 | THR  |
| 1   | K     | 293 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 297 | LEU  |
| 1   | K     | 317 | LEU  |
| 1   | K     | 319 | ASN  |
| 1   | K     | 320 | SER  |
| 2   | L     | 28  | ASN  |
| 2   | L     | 42  | GLN  |
| 2   | L     | 60  | ASN  |
| 2   | L     | 62  | GLN  |
| 2   | L     | 112 | ASP  |
| 2   | L     | 116 | LYS  |
| 2   | L     | 121 | LYS  |
| 2   | L     | 126 | LEU  |
| 2   | L     | 127 | ARG  |
| 2   | L     | 158 | ASP  |
| 3   | M     | 23  | ARG  |
| 3   | M     | 28  | ILE  |
| 3   | M     | 51  | ILE  |
| 3   | M     | 52  | ILE  |
| 3   | M     | 57  | THR  |
| 3   | M     | 75  | SER  |
| 3   | M     | 98  | ARG  |
| 3   | M     | 101 | TYR  |
| 3   | M     | 102 | TYR  |
| 3   | M     | 106 | SER  |
| 3   | M     | 124 | LYS  |
| 3   | M     | 157 | VAL  |
| 3   | O     | 28  | ILE  |
| 3   | O     | 51  | ILE  |
| 3   | O     | 52  | ILE  |
| 3   | O     | 57  | THR  |
| 3   | O     | 98  | ARG  |
| 3   | O     | 101 | TYR  |
| 3   | O     | 102 | TYR  |
| 3   | O     | 106 | SER  |
| 3   | O     | 124 | LYS  |
| 3   | O     | 157 | VAL  |
| 3   | O     | 186 | SER  |
| 4   | P     | 5   | THR  |
| 4   | P     | 22  | SER  |
| 4   | P     | 29  | SER  |
| 4   | P     | 61  | ARG  |
| 4   | P     | 89  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | P     | 121 | SER  |
| 1   | Q     | 18  | THR  |
| 1   | Q     | 19  | ILE  |
| 1   | Q     | 27  | THR  |
| 1   | Q     | 36  | LYS  |
| 1   | Q     | 40  | LYS  |
| 1   | Q     | 41  | LEU  |
| 1   | Q     | 53  | ARG  |
| 1   | Q     | 55  | CYS  |
| 1   | Q     | 69  | GLU  |
| 1   | Q     | 95  | PHE  |
| 1   | Q     | 173 | LEU  |
| 1   | Q     | 192 | GLN  |
| 1   | Q     | 217 | SER  |
| 1   | Q     | 225 | ARG  |
| 1   | Q     | 226 | MET  |
| 1   | Q     | 271 | TYR  |
| 1   | Q     | 274 | CYS  |
| 1   | Q     | 275 | ASN  |
| 1   | Q     | 278 | CYS  |
| 1   | Q     | 280 | THR  |
| 1   | Q     | 293 | ASN  |
| 1   | Q     | 297 | LEU  |
| 1   | Q     | 317 | LEU  |
| 1   | Q     | 319 | ASN  |
| 1   | Q     | 320 | SER  |
| 2   | R     | 28  | ASN  |
| 2   | R     | 30  | GLN  |
| 2   | R     | 42  | GLN  |
| 2   | R     | 60  | ASN  |
| 2   | R     | 62  | GLN  |
| 2   | R     | 112 | ASP  |
| 2   | R     | 116 | LYS  |
| 2   | R     | 126 | LEU  |
| 2   | R     | 127 | ARG  |
| 2   | R     | 158 | ASP  |
| 1   | S     | 18  | THR  |
| 1   | S     | 19  | ILE  |
| 1   | S     | 27  | THR  |
| 1   | S     | 36  | LYS  |
| 1   | S     | 40  | LYS  |
| 1   | S     | 41  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 53  | ARG  |
| 1   | S     | 55  | CYS  |
| 1   | S     | 69  | GLU  |
| 1   | S     | 95  | PHE  |
| 1   | S     | 173 | LEU  |
| 1   | S     | 181 | PRO  |
| 1   | S     | 192 | GLN  |
| 1   | S     | 217 | SER  |
| 1   | S     | 225 | ARG  |
| 1   | S     | 226 | MET  |
| 1   | S     | 271 | TYR  |
| 1   | S     | 274 | CYS  |
| 1   | S     | 275 | ASN  |
| 1   | S     | 278 | CYS  |
| 1   | S     | 280 | THR  |
| 1   | S     | 293 | ASN  |
| 1   | S     | 297 | LEU  |
| 1   | S     | 317 | LEU  |
| 1   | S     | 319 | ASN  |
| 1   | S     | 320 | SER  |
| 2   | T     | 28  | ASN  |
| 2   | T     | 30  | GLN  |
| 2   | T     | 42  | GLN  |
| 2   | T     | 62  | GLN  |
| 2   | T     | 112 | ASP  |
| 2   | T     | 116 | LYS  |
| 2   | T     | 117 | ASN  |
| 2   | T     | 126 | LEU  |
| 2   | T     | 127 | ARG  |
| 2   | T     | 158 | ASP  |
| 3   | V     | 28  | ILE  |
| 3   | V     | 51  | ILE  |
| 3   | V     | 52  | ILE  |
| 3   | V     | 57  | THR  |
| 3   | V     | 98  | ARG  |
| 3   | V     | 101 | TYR  |
| 3   | V     | 102 | TYR  |
| 3   | V     | 106 | SER  |
| 3   | V     | 124 | LYS  |
| 3   | V     | 157 | VAL  |
| 3   | Y     | 28  | ILE  |
| 3   | Y     | 51  | ILE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Y     | 52  | ILE  |
| 3   | Y     | 57  | THR  |
| 3   | Y     | 98  | ARG  |
| 3   | Y     | 101 | TYR  |
| 3   | Y     | 102 | TYR  |
| 3   | Y     | 106 | SER  |
| 3   | Y     | 124 | LYS  |
| 3   | Y     | 157 | VAL  |
| 4   | U     | 5   | THR  |
| 4   | U     | 22  | SER  |
| 4   | U     | 29  | SER  |
| 4   | U     | 61  | ARG  |
| 4   | U     | 89  | GLN  |
| 4   | U     | 121 | SER  |
| 4   | J     | 5   | THR  |
| 4   | J     | 22  | SER  |
| 4   | J     | 29  | SER  |
| 4   | J     | 61  | ARG  |
| 4   | J     | 89  | GLN  |
| 4   | J     | 121 | SER  |
| 4   | D     | 5   | THR  |
| 4   | D     | 22  | SER  |
| 4   | D     | 29  | SER  |
| 4   | D     | 61  | ARG  |
| 4   | D     | 89  | GLN  |
| 4   | D     | 121 | SER  |
| 4   | D     | 168 | SER  |
| 4   | W     | 5   | THR  |
| 4   | W     | 22  | SER  |
| 4   | W     | 29  | SER  |
| 4   | W     | 61  | ARG  |
| 4   | W     | 89  | GLN  |
| 4   | W     | 121 | SER  |
| 4   | N     | 5   | THR  |
| 4   | N     | 22  | SER  |
| 4   | N     | 29  | SER  |
| 4   | N     | 61  | ARG  |
| 4   | N     | 89  | GLN  |
| 4   | N     | 121 | SER  |
| 4   | N     | 199 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | GLN  |
| 1   | A     | 138 | GLN  |
| 1   | A     | 293 | ASN  |
| 1   | A     | 319 | ASN  |
| 2   | B     | 42  | GLN  |
| 2   | B     | 79  | ASN  |
| 2   | B     | 95  | ASN  |
| 2   | B     | 117 | ASN  |
| 2   | B     | 135 | ASN  |
| 3   | C     | 39  | GLN  |
| 3   | C     | 50  | ASN  |
| 3   | C     | 178 | GLN  |
| 1   | E     | 15  | GLN  |
| 1   | E     | 109 | ASN  |
| 1   | E     | 138 | GLN  |
| 1   | E     | 192 | GLN  |
| 1   | E     | 293 | ASN  |
| 1   | E     | 319 | ASN  |
| 2   | F     | 135 | ASN  |
| 1   | G     | 15  | GLN  |
| 1   | G     | 138 | GLN  |
| 1   | G     | 293 | ASN  |
| 1   | G     | 319 | ASN  |
| 2   | H     | 79  | ASN  |
| 2   | H     | 95  | ASN  |
| 2   | H     | 117 | ASN  |
| 2   | H     | 135 | ASN  |
| 3   | I     | 39  | GLN  |
| 3   | I     | 105 | ASN  |
| 3   | I     | 178 | GLN  |
| 1   | K     | 138 | GLN  |
| 1   | K     | 293 | ASN  |
| 1   | K     | 319 | ASN  |
| 2   | L     | 30  | GLN  |
| 2   | L     | 42  | GLN  |
| 2   | L     | 95  | ASN  |
| 2   | L     | 135 | ASN  |
| 3   | M     | 39  | GLN  |
| 3   | M     | 50  | ASN  |
| 3   | M     | 178 | GLN  |
| 3   | O     | 50  | ASN  |
| 3   | O     | 107 | HIS  |
| 3   | O     | 178 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | P     | 89  | GLN  |
| 4   | P     | 124 | GLN  |
| 4   | P     | 155 | GLN  |
| 4   | P     | 199 | GLN  |
| 4   | P     | 210 | ASN  |
| 1   | Q     | 11  | ASN  |
| 1   | Q     | 15  | GLN  |
| 1   | Q     | 293 | ASN  |
| 1   | Q     | 319 | ASN  |
| 2   | R     | 42  | GLN  |
| 2   | R     | 117 | ASN  |
| 2   | R     | 135 | ASN  |
| 1   | S     | 138 | GLN  |
| 1   | S     | 293 | ASN  |
| 1   | S     | 319 | ASN  |
| 2   | T     | 42  | GLN  |
| 2   | T     | 117 | ASN  |
| 2   | T     | 135 | ASN  |
| 3   | V     | 39  | GLN  |
| 3   | V     | 105 | ASN  |
| 3   | V     | 178 | GLN  |
| 3   | Y     | 39  | GLN  |
| 3   | Y     | 50  | ASN  |
| 3   | Y     | 178 | GLN  |
| 4   | U     | 38  | GLN  |
| 4   | U     | 124 | GLN  |
| 4   | U     | 199 | GLN  |
| 4   | U     | 210 | ASN  |
| 4   | J     | 27  | GLN  |
| 4   | J     | 38  | GLN  |
| 4   | J     | 124 | GLN  |
| 4   | J     | 155 | GLN  |
| 4   | J     | 199 | GLN  |
| 4   | J     | 210 | ASN  |
| 4   | D     | 27  | GLN  |
| 4   | D     | 38  | GLN  |
| 4   | D     | 124 | GLN  |
| 4   | D     | 155 | GLN  |
| 4   | D     | 199 | GLN  |
| 4   | D     | 210 | ASN  |
| 4   | W     | 27  | GLN  |
| 4   | W     | 38  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | W     | 124 | GLN  |
| 4   | W     | 137 | ASN  |
| 4   | W     | 155 | GLN  |
| 4   | W     | 199 | GLN  |
| 4   | W     | 210 | ASN  |
| 4   | N     | 38  | GLN  |
| 4   | N     | 124 | GLN  |
| 4   | N     | 155 | GLN  |
| 4   | N     | 199 | GLN  |
| 4   | N     | 210 | ASN  |

### 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 ⓘ

56 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$ |
| 5   | NAG  | X     | 1   | 5,1  | 14,14,15     | 0.98 | 1 (7%)      | 17,19,21    | 1.43 | 3 (17%)     |
| 5   | NAG  | X     | 2   | 5    | 14,14,15     | 0.80 | 0           | 17,19,21    | 2.21 | 6 (35%)     |
| 5   | MAN  | X     | 3   | 5    | 11,11,12     | 0.84 | 0           | 15,15,17    | 1.77 | 2 (13%)     |
| 5   | MAN  | X     | 4   | 5    | 11,11,12     | 0.71 | 0           | 15,15,17    | 1.87 | 4 (26%)     |
| 6   | NAG  | Z     | 1   | 6,1  | 14,14,15     | 1.18 | 1 (7%)      | 17,19,21    | 2.71 | 7 (41%)     |
| 6   | NAG  | Z     | 2   | 6    | 14,14,15     | 0.68 | 0           | 17,19,21    | 1.10 | 1 (5%)      |
| 6   | MAN  | Z     | 3   | 6    | 11,11,12     | 0.76 | 0           | 15,15,17    | 2.02 | 3 (20%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | NAG  | a     | 1   | 7,1  | 14,14,15     | 0.81 | 0        | 17,19,21    | 0.95 | 0        |
| 7   | NAG  | a     | 2   | 7    | 14,14,15     | 0.91 | 1 (7%)   | 17,19,21    | 1.74 | 4 (23%)  |
| 7   | NAG  | b     | 1   | 7,2  | 14,14,15     | 1.13 | 1 (7%)   | 17,19,21    | 1.31 | 1 (5%)   |
| 7   | NAG  | b     | 2   | 7    | 14,14,15     | 0.85 | 1 (7%)   | 17,19,21    | 1.32 | 4 (23%)  |
| 7   | NAG  | c     | 1   | 7,1  | 14,14,15     | 0.53 | 0        | 17,19,21    | 2.05 | 3 (17%)  |
| 7   | NAG  | c     | 2   | 7    | 14,14,15     | 0.74 | 0        | 17,19,21    | 1.37 | 2 (11%)  |
| 7   | NAG  | d     | 1   | 7,1  | 14,14,15     | 1.35 | 1 (7%)   | 17,19,21    | 1.69 | 2 (11%)  |
| 7   | NAG  | d     | 2   | 7    | 14,14,15     | 0.71 | 0        | 17,19,21    | 1.30 | 2 (11%)  |
| 7   | NAG  | e     | 1   | 7,1  | 14,14,15     | 1.66 | 3 (21%)  | 17,19,21    | 1.86 | 3 (17%)  |
| 7   | NAG  | e     | 2   | 7    | 14,14,15     | 0.86 | 1 (7%)   | 17,19,21    | 1.94 | 5 (29%)  |
| 7   | NAG  | f     | 1   | 7,1  | 14,14,15     | 0.85 | 0        | 17,19,21    | 1.54 | 2 (11%)  |
| 7   | NAG  | f     | 2   | 7    | 14,14,15     | 0.46 | 0        | 17,19,21    | 1.42 | 1 (5%)   |
| 8   | NAG  | g     | 1   | 8    | 14,14,15     | 0.91 | 0        | 17,19,21    | 1.83 | 4 (23%)  |
| 8   | NAG  | g     | 2   | 8    | 14,14,15     | 0.48 | 0        | 17,19,21    | 1.97 | 5 (29%)  |
| 8   | MAN  | g     | 3   | 8    | 11,11,12     | 1.16 | 1 (9%)   | 15,15,17    | 2.22 | 5 (33%)  |
| 8   | MAN  | g     | 4   | 8    | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.33 | 2 (13%)  |
| 8   | MAN  | g     | 5   | 8    | 11,11,12     | 1.08 | 1 (9%)   | 15,15,17    | 3.53 | 3 (20%)  |
| 7   | NAG  | h     | 1   | 7,1  | 14,14,15     | 1.81 | 4 (28%)  | 17,19,21    | 1.99 | 4 (23%)  |
| 7   | NAG  | h     | 2   | 7    | 14,14,15     | 1.35 | 2 (14%)  | 17,19,21    | 1.94 | 3 (17%)  |
| 9   | NAG  | i     | 1   | 9,1  | 14,14,15     | 0.72 | 0        | 17,19,21    | 1.86 | 5 (29%)  |
| 9   | NAG  | i     | 2   | 9    | 14,14,15     | 0.64 | 0        | 17,19,21    | 1.89 | 4 (23%)  |
| 9   | MAN  | i     | 3   | 9    | 11,11,12     | 1.45 | 2 (18%)  | 15,15,17    | 2.34 | 5 (33%)  |
| 9   | MAN  | i     | 4   | 9    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.44 | 3 (20%)  |
| 9   | BMA  | i     | 5   | 9    | 11,11,12     | 2.05 | 3 (27%)  | 15,15,17    | 3.16 | 5 (33%)  |
| 10  | NAG  | j     | 1   | 10,1 | 14,14,15     | 1.74 | 4 (28%)  | 17,19,21    | 1.75 | 4 (23%)  |
| 10  | NAG  | j     | 2   | 10   | 14,14,15     | 0.65 | 0        | 17,19,21    | 1.75 | 3 (17%)  |
| 10  | MAN  | j     | 3   | 10   | 11,11,12     | 0.96 | 0        | 15,15,17    | 2.66 | 6 (40%)  |
| 10  | BMA  | j     | 4   | 10   | 11,11,12     | 1.02 | 0        | 15,15,17    | 1.47 | 2 (13%)  |
| 5   | NAG  | k     | 1   | 5,1  | 14,14,15     | 0.69 | 0        | 17,19,21    | 2.89 | 8 (47%)  |
| 5   | NAG  | k     | 2   | 5    | 14,14,15     | 0.43 | 0        | 17,19,21    | 1.35 | 4 (23%)  |
| 5   | MAN  | k     | 3   | 5    | 11,11,12     | 1.44 | 3 (27%)  | 15,15,17    | 3.08 | 9 (60%)  |
| 5   | MAN  | k     | 4   | 5    | 11,11,12     | 1.09 | 2 (18%)  | 15,15,17    | 2.97 | 5 (33%)  |
| 9   | NAG  | l     | 1   | 9,1  | 14,14,15     | 1.39 | 2 (14%)  | 17,19,21    | 2.26 | 4 (23%)  |
| 9   | NAG  | l     | 2   | 9    | 14,14,15     | 0.87 | 0        | 17,19,21    | 1.86 | 5 (29%)  |
| 9   | MAN  | l     | 3   | 9    | 11,11,12     | 1.46 | 2 (18%)  | 15,15,17    | 1.53 | 3 (20%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | MAN  | l     | 4   | 9    | 11,11,12     | 0.97 | 1 (9%)   | 15,15,17    | 1.91 | 5 (33%)  |
| 9   | BMA  | l     | 5   | 9    | 11,11,12     | 0.39 | 0        | 15,15,17    | 0.86 | 0        |
| 7   | NAG  | m     | 1   | 7,1  | 14,14,15     | 0.45 | 0        | 17,19,21    | 1.85 | 1 (5%)   |
| 7   | NAG  | m     | 2   | 7    | 14,14,15     | 0.89 | 0        | 17,19,21    | 1.84 | 5 (29%)  |
| 7   | NAG  | n     | 1   | 7,2  | 14,14,15     | 0.83 | 0        | 17,19,21    | 1.98 | 6 (35%)  |
| 7   | NAG  | n     | 2   | 7    | 14,14,15     | 0.69 | 0        | 17,19,21    | 1.50 | 1 (5%)   |
| 5   | NAG  | o     | 1   | 5,1  | 14,14,15     | 1.45 | 2 (14%)  | 17,19,21    | 1.84 | 4 (23%)  |
| 5   | NAG  | o     | 2   | 5    | 14,14,15     | 0.81 | 0        | 17,19,21    | 1.69 | 4 (23%)  |
| 5   | MAN  | o     | 3   | 5    | 11,11,12     | 0.89 | 0        | 15,15,17    | 1.43 | 3 (20%)  |
| 5   | MAN  | o     | 4   | 5    | 11,11,12     | 0.79 | 0        | 15,15,17    | 2.32 | 2 (13%)  |
| 5   | NAG  | p     | 1   | 5,1  | 14,14,15     | 0.66 | 0        | 17,19,21    | 2.22 | 1 (5%)   |
| 5   | NAG  | p     | 2   | 5    | 14,14,15     | 0.77 | 0        | 17,19,21    | 1.29 | 3 (17%)  |
| 5   | MAN  | p     | 3   | 5    | 11,11,12     | 0.70 | 0        | 15,15,17    | 0.97 | 1 (6%)   |
| 5   | MAN  | p     | 4   | 5    | 11,11,12     | 0.40 | 0        | 15,15,17    | 0.91 | 1 (6%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | NAG  | X     | 1   | 5,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | X     | 2   | 5    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | MAN  | X     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | X     | 4   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | NAG  | Z     | 1   | 6,1  | 1/1/5/7 | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | Z     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | MAN  | Z     | 3   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | a     | 1   | 7,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | a     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | b     | 1   | 7,2  | 1/1/5/7 | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | b     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | c     | 1   | 7,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | c     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | d     | 1   | 7,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | d     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | e     | 1   | 7,1  | 1/1/5/7 | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | e     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7   | NAG  | f     | 1   | 7,1  | 1/1/5/7 | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | f     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | g     | 1   | 8    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | g     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | MAN  | g     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | g     | 4   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | g     | 5   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | NAG  | h     | 1   | 7,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | h     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | i     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | i     | 2   | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | MAN  | i     | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 4   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | BMA  | i     | 5   | 9    | 1/1/4/5 | 1/2/19/22 | 0/1/1/1 |
| 10  | NAG  | j     | 1   | 10,1 | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | NAG  | j     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | MAN  | j     | 3   | 10   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | BMA  | j     | 4   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | NAG  | k     | 1   | 5,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | k     | 2   | 5    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | MAN  | k     | 3   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 5   | MAN  | k     | 4   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | NAG  | l     | 1   | 9,1  | 1/1/5/7 | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | l     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | MAN  | l     | 3   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | MAN  | l     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | BMA  | l     | 5   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | m     | 1   | 7,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | m     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | n     | 1   | 7,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | n     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | o     | 1   | 5,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | o     | 2   | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | MAN  | o     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | o     | 4   | 5    | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | NAG  | p     | 1   | 5,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | p     | 2   | 5    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | MAN  | p     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | MAN  | p     | 4   | 5    | -       | 0/2/19/22 | 0/1/1/1 |

All (39) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10  | j     | 1   | NAG  | O5-C1 | -4.72 | 1.35        | 1.43     |
| 7   | e     | 1   | NAG  | C1-C2 | 4.56  | 1.58        | 1.52     |
| 7   | h     | 1   | NAG  | O5-C1 | -4.42 | 1.36        | 1.43     |
| 9   | i     | 5   | BMA  | O5-C1 | -4.15 | 1.36        | 1.43     |
| 7   | d     | 1   | NAG  | C1-C2 | 4.05  | 1.57        | 1.52     |
| 5   | o     | 1   | NAG  | O5-C1 | -3.94 | 1.37        | 1.43     |
| 9   | i     | 5   | BMA  | C4-C5 | 3.84  | 1.61        | 1.53     |
| 9   | l     | 3   | MAN  | O2-C2 | 3.32  | 1.50        | 1.43     |
| 7   | h     | 1   | NAG  | O4-C4 | 3.24  | 1.51        | 1.43     |
| 7   | h     | 2   | NAG  | C1-C2 | 3.14  | 1.56        | 1.52     |
| 9   | l     | 1   | NAG  | C1-C2 | 3.11  | 1.56        | 1.52     |
| 9   | i     | 3   | MAN  | C2-C3 | 3.11  | 1.57        | 1.52     |
| 7   | e     | 1   | NAG  | C3-C2 | 2.99  | 1.58        | 1.52     |
| 7   | b     | 1   | NAG  | C1-C2 | 2.94  | 1.56        | 1.52     |
| 6   | Z     | 1   | NAG  | C2-N2 | -2.83 | 1.41        | 1.46     |
| 10  | j     | 1   | NAG  | C1-C2 | 2.79  | 1.56        | 1.52     |
| 7   | h     | 1   | NAG  | C4-C5 | 2.55  | 1.58        | 1.53     |
| 7   | h     | 1   | NAG  | O5-C5 | 2.53  | 1.48        | 1.43     |
| 5   | o     | 1   | NAG  | O4-C4 | 2.47  | 1.49        | 1.43     |
| 9   | i     | 3   | MAN  | C6-C5 | 2.46  | 1.60        | 1.51     |
| 7   | b     | 2   | NAG  | C1-C2 | 2.33  | 1.55        | 1.52     |
| 7   | h     | 2   | NAG  | C2-N2 | 2.31  | 1.50        | 1.46     |
| 9   | l     | 1   | NAG  | O4-C4 | 2.29  | 1.48        | 1.43     |
| 5   | k     | 4   | MAN  | C2-C3 | 2.29  | 1.56        | 1.52     |
| 9   | l     | 4   | MAN  | C2-C3 | 2.26  | 1.56        | 1.52     |
| 8   | g     | 5   | MAN  | O5-C1 | -2.25 | 1.39        | 1.43     |
| 7   | e     | 2   | NAG  | C1-C2 | 2.24  | 1.55        | 1.52     |
| 5   | k     | 3   | MAN  | C4-C5 | 2.24  | 1.57        | 1.53     |
| 5   | k     | 4   | MAN  | O5-C1 | 2.21  | 1.47        | 1.43     |
| 8   | g     | 3   | MAN  | C2-C3 | 2.21  | 1.55        | 1.52     |
| 5   | k     | 3   | MAN  | O5-C5 | 2.19  | 1.47        | 1.43     |
| 10  | j     | 1   | NAG  | O4-C4 | 2.17  | 1.48        | 1.43     |
| 9   | i     | 5   | BMA  | C4-C3 | 2.17  | 1.58        | 1.52     |
| 5   | k     | 3   | MAN  | O3-C3 | 2.11  | 1.48        | 1.43     |
| 5   | X     | 1   | NAG  | O4-C4 | 2.09  | 1.48        | 1.43     |
| 7   | a     | 2   | NAG  | C1-C2 | 2.05  | 1.55        | 1.52     |
| 9   | l     | 3   | MAN  | C1-C2 | 2.04  | 1.57        | 1.52     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 7   | e     | 1   | NAG  | C2-N2 | 2.02 | 1.49        | 1.46     |
| 10  | j     | 1   | NAG  | C4-C5 | 2.02 | 1.57        | 1.53     |

All (193) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 8   | g     | 5   | MAN  | C1-O5-C5 | -12.51 | 95.41       | 112.19   |
| 5   | k     | 4   | MAN  | C1-O5-C5 | 8.89   | 124.11      | 112.19   |
| 5   | p     | 1   | NAG  | C1-O5-C5 | 8.17   | 123.13      | 112.19   |
| 5   | o     | 4   | MAN  | C1-O5-C5 | 7.93   | 122.81      | 112.19   |
| 9   | i     | 5   | BMA  | C1-O5-C5 | -7.89  | 101.61      | 112.19   |
| 6   | Z     | 1   | NAG  | C1-C2-N2 | -7.86  | 98.05       | 110.43   |
| 5   | k     | 1   | NAG  | C1-O5-C5 | 7.01   | 121.58      | 112.19   |
| 9   | i     | 5   | BMA  | O5-C5-C4 | 6.71   | 127.16      | 110.83   |
| 7   | m     | 1   | NAG  | C1-O5-C5 | 6.43   | 120.80      | 112.19   |
| 10  | j     | 3   | MAN  | O5-C5-C6 | 6.31   | 119.95      | 107.66   |
| 7   | h     | 2   | NAG  | C2-N2-C7 | 6.23   | 131.25      | 122.90   |
| 6   | Z     | 3   | MAN  | C1-C2-C3 | 5.99   | 118.37      | 109.64   |
| 9   | l     | 1   | NAG  | C1-C2-N2 | 5.96   | 119.83      | 110.43   |
| 8   | g     | 3   | MAN  | C1-C2-C3 | 5.80   | 118.09      | 109.64   |
| 5   | k     | 3   | MAN  | O5-C5-C6 | 5.74   | 118.84      | 107.66   |
| 5   | k     | 1   | NAG  | O5-C1-C2 | 5.33   | 119.53      | 111.29   |
| 7   | d     | 1   | NAG  | C1-O5-C5 | 5.23   | 119.19      | 112.19   |
| 7   | n     | 2   | NAG  | C1-O5-C5 | 5.13   | 119.06      | 112.19   |
| 10  | j     | 3   | MAN  | C1-C2-C3 | 4.99   | 116.91      | 109.64   |
| 7   | e     | 1   | NAG  | C4-C3-C2 | 4.99   | 118.33      | 111.02   |
| 5   | X     | 2   | NAG  | C1-C2-N2 | -4.98  | 102.58      | 110.43   |
| 5   | k     | 4   | MAN  | C1-C2-C3 | 4.90   | 116.78      | 109.64   |
| 9   | i     | 3   | MAN  | C1-C2-C3 | 4.86   | 116.72      | 109.64   |
| 5   | k     | 3   | MAN  | C6-C5-C4 | -4.83  | 101.16      | 113.02   |
| 7   | m     | 2   | NAG  | C1-C2-N2 | -4.78  | 102.90      | 110.43   |
| 7   | h     | 1   | NAG  | C1-O5-C5 | 4.76   | 118.57      | 112.19   |
| 5   | X     | 3   | MAN  | O6-C6-C5 | -4.68  | 95.40       | 111.33   |
| 7   | c     | 1   | NAG  | C3-C4-C5 | 4.64   | 118.64      | 110.23   |
| 7   | c     | 1   | NAG  | C1-O5-C5 | 4.60   | 118.36      | 112.19   |
| 8   | g     | 1   | NAG  | C1-O5-C5 | 4.59   | 118.34      | 112.19   |
| 7   | f     | 2   | NAG  | C1-C2-N2 | -4.58  | 103.22      | 110.43   |
| 5   | k     | 3   | MAN  | C1-O5-C5 | 4.58   | 118.32      | 112.19   |
| 9   | l     | 1   | NAG  | C1-O5-C5 | 4.43   | 118.12      | 112.19   |
| 9   | l     | 2   | NAG  | C4-C3-C2 | 4.39   | 117.44      | 111.02   |
| 9   | l     | 4   | MAN  | C2-C3-C4 | 4.37   | 118.55      | 110.86   |
| 10  | j     | 1   | NAG  | O5-C1-C2 | -4.34  | 104.57      | 111.29   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | i     | 2   | NAG  | C4-C3-C2 | 4.31  | 117.33      | 111.02   |
| 5   | X     | 4   | MAN  | C1-O5-C5 | 4.30  | 117.95      | 112.19   |
| 5   | X     | 3   | MAN  | C1-C2-C3 | 4.28  | 115.88      | 109.64   |
| 5   | k     | 1   | NAG  | C3-C4-C5 | 4.27  | 117.97      | 110.23   |
| 10  | j     | 2   | NAG  | C1-C2-N2 | -4.24 | 103.75      | 110.43   |
| 6   | Z     | 1   | NAG  | O7-C7-C8 | 4.22  | 129.57      | 122.05   |
| 5   | o     | 2   | NAG  | C1-O5-C5 | 4.18  | 117.79      | 112.19   |
| 9   | i     | 3   | MAN  | C2-C3-C4 | 4.18  | 118.21      | 110.86   |
| 5   | k     | 3   | MAN  | O6-C6-C5 | -4.10 | 97.38       | 111.33   |
| 7   | h     | 1   | NAG  | O5-C5-C4 | 4.07  | 120.74      | 110.83   |
| 5   | k     | 3   | MAN  | C1-C2-C3 | 4.07  | 115.57      | 109.64   |
| 7   | d     | 2   | NAG  | C4-C3-C2 | 4.05  | 116.95      | 111.02   |
| 9   | i     | 3   | MAN  | C6-C5-C4 | 4.04  | 122.94      | 113.02   |
| 9   | i     | 5   | BMA  | O4-C4-C3 | -4.01 | 100.92      | 110.38   |
| 10  | j     | 1   | NAG  | C3-C4-C5 | 3.96  | 117.41      | 110.23   |
| 7   | f     | 1   | NAG  | C1-O5-C5 | 3.94  | 117.47      | 112.19   |
| 6   | Z     | 1   | NAG  | C8-C7-N2 | -3.94 | 109.58      | 116.12   |
| 8   | g     | 5   | MAN  | O5-C5-C4 | -3.93 | 101.27      | 110.83   |
| 8   | g     | 2   | NAG  | C4-C3-C2 | 3.92  | 116.76      | 111.02   |
| 7   | a     | 2   | NAG  | C1-O5-C5 | 3.89  | 117.40      | 112.19   |
| 7   | e     | 2   | NAG  | C2-N2-C7 | 3.86  | 128.08      | 122.90   |
| 7   | n     | 1   | NAG  | C2-N2-C7 | 3.81  | 128.01      | 122.90   |
| 5   | o     | 1   | NAG  | O5-C1-C2 | -3.79 | 105.43      | 111.29   |
| 9   | i     | 1   | NAG  | C2-N2-C7 | 3.78  | 127.96      | 122.90   |
| 7   | a     | 2   | NAG  | C2-N2-C7 | 3.75  | 127.93      | 122.90   |
| 5   | X     | 2   | NAG  | O4-C4-C5 | 3.68  | 118.39      | 109.32   |
| 10  | j     | 3   | MAN  | O4-C4-C5 | -3.67 | 100.28      | 109.32   |
| 7   | n     | 1   | NAG  | C4-C3-C2 | 3.67  | 116.39      | 111.02   |
| 5   | o     | 2   | NAG  | C4-C3-C2 | 3.66  | 116.38      | 111.02   |
| 5   | k     | 1   | NAG  | O4-C4-C3 | -3.65 | 101.76      | 110.38   |
| 8   | g     | 2   | NAG  | C1-C2-N2 | -3.61 | 104.74      | 110.43   |
| 10  | j     | 4   | BMA  | C6-C5-C4 | -3.57 | 104.24      | 113.02   |
| 5   | o     | 1   | NAG  | C3-C4-C5 | 3.57  | 116.70      | 110.23   |
| 9   | l     | 4   | MAN  | C1-C2-C3 | 3.57  | 114.84      | 109.64   |
| 7   | e     | 2   | NAG  | O5-C5-C6 | 3.51  | 114.49      | 107.66   |
| 9   | l     | 3   | MAN  | O2-C2-C1 | 3.48  | 117.19      | 109.22   |
| 7   | m     | 2   | NAG  | C4-C3-C2 | 3.41  | 116.02      | 111.02   |
| 5   | X     | 2   | NAG  | C2-N2-C7 | 3.38  | 127.43      | 122.90   |
| 5   | X     | 2   | NAG  | O4-C4-C3 | -3.35 | 102.47      | 110.38   |
| 9   | i     | 1   | NAG  | O5-C1-C2 | 3.35  | 116.47      | 111.29   |
| 9   | l     | 2   | NAG  | O4-C4-C5 | 3.34  | 117.55      | 109.32   |
| 9   | i     | 1   | NAG  | O5-C5-C6 | 3.33  | 114.15      | 107.66   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | i     | 2   | NAG  | C3-C4-C5 | 3.33  | 116.26      | 110.23   |
| 9   | l     | 1   | NAG  | C4-C3-C2 | 3.32  | 115.88      | 111.02   |
| 8   | g     | 1   | NAG  | C2-N2-C7 | -3.27 | 118.52      | 122.90   |
| 7   | c     | 2   | NAG  | C3-C4-C5 | 3.25  | 116.12      | 110.23   |
| 5   | X     | 1   | NAG  | C3-C4-C5 | 3.23  | 116.08      | 110.23   |
| 9   | i     | 2   | NAG  | C1-C2-N2 | -3.18 | 105.42      | 110.43   |
| 8   | g     | 2   | NAG  | O4-C4-C5 | 3.18  | 117.14      | 109.32   |
| 7   | e     | 2   | NAG  | O5-C1-C2 | 3.14  | 116.16      | 111.29   |
| 7   | h     | 2   | NAG  | O5-C5-C6 | 3.13  | 113.76      | 107.66   |
| 6   | Z     | 2   | NAG  | C4-C3-C2 | 3.12  | 115.58      | 111.02   |
| 10  | j     | 2   | NAG  | C1-O5-C5 | -3.11 | 108.02      | 112.19   |
| 6   | Z     | 3   | MAN  | C1-O5-C5 | 3.08  | 116.32      | 112.19   |
| 10  | j     | 3   | MAN  | O5-C5-C4 | -3.08 | 103.34      | 110.83   |
| 5   | o     | 1   | NAG  | C8-C7-N2 | -3.06 | 111.04      | 116.12   |
| 7   | b     | 2   | NAG  | C4-C3-C2 | 3.06  | 115.50      | 111.02   |
| 9   | i     | 4   | MAN  | C1-O5-C5 | 3.03  | 116.25      | 112.19   |
| 8   | g     | 4   | MAN  | C1-C2-C3 | 3.03  | 114.06      | 109.64   |
| 9   | i     | 5   | BMA  | O6-C6-C5 | 3.01  | 121.58      | 111.33   |
| 7   | h     | 1   | NAG  | C2-N2-C7 | 3.00  | 126.93      | 122.90   |
| 5   | k     | 3   | MAN  | C3-C4-C5 | 3.00  | 115.68      | 110.23   |
| 5   | o     | 4   | MAN  | O5-C1-C2 | 3.00  | 117.95      | 110.79   |
| 8   | g     | 3   | MAN  | C1-O5-C5 | 2.98  | 116.17      | 112.19   |
| 7   | h     | 2   | NAG  | C1-C2-N2 | 2.92  | 115.03      | 110.43   |
| 5   | o     | 3   | MAN  | C1-C2-C3 | 2.91  | 113.88      | 109.64   |
| 8   | g     | 1   | NAG  | O5-C1-C2 | -2.89 | 106.82      | 111.29   |
| 5   | p     | 2   | NAG  | C1-O5-C5 | 2.87  | 116.03      | 112.19   |
| 5   | o     | 3   | MAN  | O5-C5-C6 | 2.86  | 113.22      | 107.66   |
| 5   | k     | 1   | NAG  | O5-C5-C6 | -2.81 | 102.19      | 107.66   |
| 7   | e     | 1   | NAG  | O5-C5-C4 | -2.79 | 104.04      | 110.83   |
| 9   | l     | 2   | NAG  | C1-C2-N2 | -2.79 | 106.04      | 110.43   |
| 5   | X     | 2   | NAG  | O3-C3-C2 | 2.77  | 115.16      | 109.40   |
| 7   | b     | 1   | NAG  | C2-N2-C7 | 2.77  | 126.61      | 122.90   |
| 5   | k     | 1   | NAG  | C2-N2-C7 | 2.77  | 126.61      | 122.90   |
| 9   | l     | 3   | MAN  | O5-C5-C6 | -2.75 | 102.30      | 107.66   |
| 7   | c     | 2   | NAG  | C1-C2-N2 | -2.71 | 106.16      | 110.43   |
| 7   | b     | 2   | NAG  | C1-C2-N2 | -2.68 | 106.21      | 110.43   |
| 9   | i     | 4   | MAN  | C1-C2-C3 | 2.68  | 113.54      | 109.64   |
| 7   | e     | 2   | NAG  | O5-C5-C4 | -2.67 | 104.34      | 110.83   |
| 8   | g     | 3   | MAN  | O5-C5-C4 | -2.67 | 104.34      | 110.83   |
| 10  | j     | 2   | NAG  | C2-N2-C7 | 2.66  | 126.47      | 122.90   |
| 9   | i     | 3   | MAN  | O5-C5-C4 | -2.65 | 104.37      | 110.83   |
| 5   | o     | 1   | NAG  | C1-C2-N2 | -2.63 | 106.29      | 110.43   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | Z     | 3   | MAN  | C2-C3-C4 | 2.62  | 115.46      | 110.86   |
| 5   | k     | 1   | NAG  | O5-C5-C4 | 2.61  | 117.17      | 110.83   |
| 10  | j     | 4   | BMA  | C3-C4-C5 | 2.61  | 114.96      | 110.23   |
| 8   | g     | 3   | MAN  | C2-C3-C4 | 2.60  | 115.43      | 110.86   |
| 5   | k     | 2   | NAG  | C3-C4-C5 | 2.59  | 114.94      | 110.23   |
| 5   | X     | 1   | NAG  | C2-N2-C7 | 2.59  | 126.37      | 122.90   |
| 7   | c     | 1   | NAG  | C2-N2-C7 | 2.59  | 126.37      | 122.90   |
| 7   | n     | 1   | NAG  | C3-C4-C5 | 2.59  | 114.92      | 110.23   |
| 10  | j     | 1   | NAG  | O4-C4-C3 | -2.59 | 104.28      | 110.38   |
| 5   | p     | 4   | MAN  | C1-O5-C5 | 2.56  | 115.62      | 112.19   |
| 10  | j     | 1   | NAG  | O5-C5-C4 | 2.56  | 117.05      | 110.83   |
| 8   | g     | 2   | NAG  | O3-C3-C2 | -2.56 | 104.09      | 109.40   |
| 7   | f     | 1   | NAG  | O5-C1-C2 | 2.55  | 115.24      | 111.29   |
| 5   | p     | 3   | MAN  | C1-C2-C3 | 2.55  | 113.35      | 109.64   |
| 9   | l     | 4   | MAN  | C1-O5-C5 | 2.54  | 115.59      | 112.19   |
| 9   | i     | 2   | NAG  | O7-C7-C8 | -2.54 | 117.53      | 122.05   |
| 9   | l     | 1   | NAG  | C2-N2-C7 | 2.54  | 126.30      | 122.90   |
| 5   | o     | 2   | NAG  | C2-N2-C7 | 2.53  | 126.29      | 122.90   |
| 5   | k     | 4   | MAN  | O5-C5-C6 | 2.51  | 112.56      | 107.66   |
| 8   | g     | 4   | MAN  | C1-O5-C5 | 2.51  | 115.55      | 112.19   |
| 7   | n     | 1   | NAG  | C1-O5-C5 | 2.50  | 115.54      | 112.19   |
| 7   | a     | 2   | NAG  | C1-C2-N2 | -2.48 | 106.52      | 110.43   |
| 5   | p     | 2   | NAG  | C2-N2-C7 | 2.47  | 126.21      | 122.90   |
| 9   | i     | 1   | NAG  | C1-C2-N2 | -2.47 | 106.54      | 110.43   |
| 5   | X     | 4   | MAN  | O2-C2-C1 | -2.46 | 103.59      | 109.22   |
| 7   | m     | 2   | NAG  | C1-O5-C5 | 2.45  | 115.47      | 112.19   |
| 8   | g     | 3   | MAN  | O6-C6-C5 | 2.45  | 119.68      | 111.33   |
| 7   | n     | 1   | NAG  | O5-C1-C2 | -2.45 | 107.51      | 111.29   |
| 6   | Z     | 1   | NAG  | C2-N2-C7 | -2.43 | 119.64      | 122.90   |
| 7   | e     | 2   | NAG  | C4-C3-C2 | 2.43  | 114.58      | 111.02   |
| 7   | d     | 1   | NAG  | O4-C4-C3 | -2.42 | 104.67      | 110.38   |
| 6   | Z     | 1   | NAG  | O3-C3-C4 | 2.41  | 116.07      | 110.38   |
| 7   | n     | 1   | NAG  | O3-C3-C4 | -2.41 | 104.70      | 110.38   |
| 10  | j     | 3   | MAN  | O4-C4-C3 | 2.41  | 116.05      | 110.38   |
| 8   | g     | 1   | NAG  | O4-C4-C3 | -2.40 | 104.71      | 110.38   |
| 7   | b     | 2   | NAG  | O5-C5-C6 | 2.39  | 112.31      | 107.66   |
| 5   | k     | 1   | NAG  | C1-C2-N2 | -2.38 | 106.68      | 110.43   |
| 7   | e     | 1   | NAG  | C1-C2-N2 | 2.37  | 114.16      | 110.43   |
| 5   | X     | 4   | MAN  | O2-C2-C3 | 2.36  | 115.04      | 110.15   |
| 9   | l     | 2   | NAG  | O5-C1-C2 | -2.33 | 107.69      | 111.29   |
| 9   | i     | 5   | BMA  | C1-C2-C3 | 2.31  | 113.01      | 109.64   |
| 7   | h     | 1   | NAG  | O5-C5-C6 | -2.31 | 103.18      | 107.66   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | i     | 3   | MAN  | O2-C2-C1 | -2.30 | 103.96      | 109.22   |
| 5   | X     | 1   | NAG  | O5-C5-C4 | 2.28  | 116.37      | 110.83   |
| 8   | g     | 2   | NAG  | C2-N2-C7 | -2.25 | 119.89      | 122.90   |
| 5   | k     | 3   | MAN  | O5-C5-C4 | -2.24 | 105.37      | 110.83   |
| 5   | p     | 2   | NAG  | O4-C4-C5 | 2.23  | 114.82      | 109.32   |
| 5   | k     | 4   | MAN  | C3-C4-C5 | -2.22 | 106.21      | 110.23   |
| 5   | k     | 2   | NAG  | C1-C2-N2 | -2.22 | 106.94      | 110.43   |
| 9   | l     | 3   | MAN  | C3-C4-C5 | 2.21  | 114.24      | 110.23   |
| 5   | X     | 2   | NAG  | O3-C3-C4 | -2.20 | 105.20      | 110.38   |
| 6   | Z     | 1   | NAG  | O3-C3-C2 | -2.19 | 104.86      | 109.40   |
| 7   | m     | 2   | NAG  | O5-C5-C6 | 2.15  | 111.84      | 107.66   |
| 7   | m     | 2   | NAG  | C2-N2-C7 | 2.15  | 125.78      | 122.90   |
| 9   | l     | 4   | MAN  | O5-C5-C6 | 2.14  | 111.83      | 107.66   |
| 8   | g     | 5   | MAN  | O5-C5-C6 | 2.14  | 111.82      | 107.66   |
| 9   | l     | 2   | NAG  | O7-C7-N2 | 2.11  | 125.72      | 121.98   |
| 5   | k     | 2   | NAG  | O5-C5-C6 | 2.11  | 111.77      | 107.66   |
| 9   | i     | 4   | MAN  | O5-C5-C6 | 2.10  | 111.76      | 107.66   |
| 5   | o     | 3   | MAN  | O5-C5-C4 | -2.09 | 105.73      | 110.83   |
| 5   | k     | 2   | NAG  | O4-C4-C5 | -2.08 | 104.19      | 109.32   |
| 6   | Z     | 1   | NAG  | C1-O5-C5 | 2.08  | 114.97      | 112.19   |
| 7   | a     | 2   | NAG  | O3-C3-C2 | 2.07  | 113.69      | 109.40   |
| 7   | b     | 2   | NAG  | C3-C4-C5 | 2.06  | 113.97      | 110.23   |
| 10  | j     | 3   | MAN  | C3-C4-C5 | 2.06  | 113.97      | 110.23   |
| 5   | k     | 4   | MAN  | C6-C5-C4 | -2.06 | 107.97      | 113.02   |
| 9   | l     | 4   | MAN  | C3-C4-C5 | 2.05  | 113.96      | 110.23   |
| 5   | k     | 3   | MAN  | C2-C3-C4 | 2.05  | 114.47      | 110.86   |
| 7   | d     | 2   | NAG  | C1-C2-N2 | -2.02 | 107.25      | 110.43   |
| 5   | k     | 3   | MAN  | O3-C3-C2 | -2.02 | 105.93      | 110.05   |
| 5   | X     | 4   | MAN  | O5-C5-C4 | -2.01 | 105.94      | 110.83   |
| 9   | i     | 1   | NAG  | O4-C4-C3 | -2.01 | 105.64      | 110.38   |
| 5   | o     | 2   | NAG  | C3-C4-C5 | 2.00  | 113.86      | 110.23   |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 6   | Z     | 1   | NAG  | C1   |
| 7   | b     | 1   | NAG  | C1   |
| 7   | e     | 1   | NAG  | C1   |
| 7   | f     | 1   | NAG  | C1   |
| 9   | i     | 5   | BMA  | C5   |
| 9   | l     | 1   | NAG  | C1   |

All (62) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | X     | 2   | NAG  | C1-C2-N2-C7 |
| 7   | h     | 2   | NAG  | C1-C2-N2-C7 |
| 7   | c     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | p     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | l     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | X     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | e     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | a     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | f     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | g     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | g     | 4   | MAN  | O5-C5-C6-O6 |
| 5   | X     | 3   | MAN  | O5-C5-C6-O6 |
| 5   | X     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | X     | 4   | MAN  | C4-C5-C6-O6 |
| 7   | e     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | k     | 4   | MAN  | O5-C5-C6-O6 |
| 7   | c     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | p     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | l     | 2   | NAG  | C4-C5-C6-O6 |
| 7   | m     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | X     | 4   | MAN  | O5-C5-C6-O6 |
| 5   | p     | 3   | MAN  | O5-C5-C6-O6 |
| 7   | m     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | i     | 4   | MAN  | C4-C5-C6-O6 |
| 10  | j     | 3   | MAN  | C4-C5-C6-O6 |
| 5   | o     | 3   | MAN  | C4-C5-C6-O6 |
| 7   | f     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | p     | 3   | MAN  | C4-C5-C6-O6 |
| 7   | a     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | j     | 3   | MAN  | O5-C5-C6-O6 |
| 8   | g     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | g     | 4   | MAN  | C4-C5-C6-O6 |
| 9   | l     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | g     | 5   | MAN  | C4-C5-C6-O6 |
| 5   | o     | 3   | MAN  | O5-C5-C6-O6 |
| 7   | d     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | g     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | X     | 3   | MAN  | C4-C5-C6-O6 |
| 9   | i     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | l     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | i     | 5   | BMA  | O5-C5-C6-O6 |
| 10  | j     | 2   | NAG  | O5-C5-C6-O6 |

*Continued on next page...*

*Continued from previous page...*

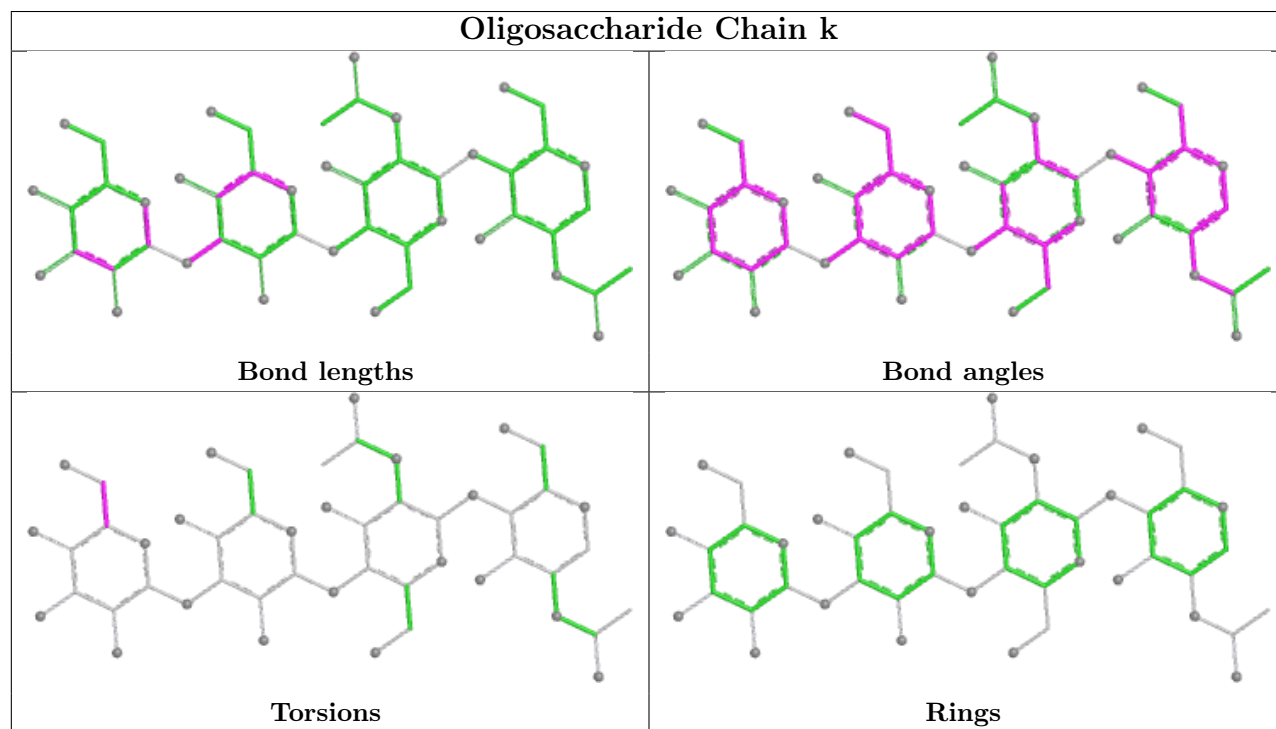
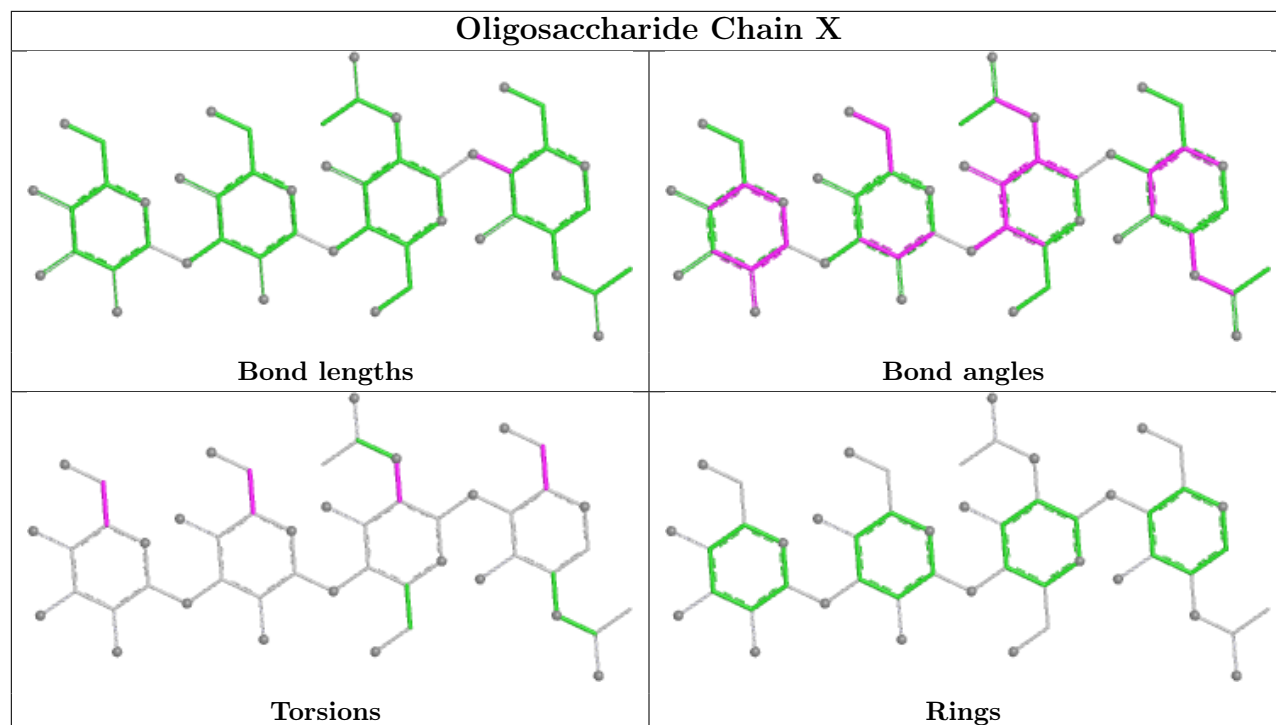
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 10  | j     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | k     | 4   | MAN  | C4-C5-C6-O6 |
| 7   | n     | 1   | NAG  | C4-C5-C6-O6 |
| 7   | h     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | o     | 4   | MAN  | O5-C5-C6-O6 |
| 10  | j     | 4   | BMA  | O5-C5-C6-O6 |
| 7   | b     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | l     | 3   | MAN  | O5-C5-C6-O6 |
| 7   | b     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | o     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | o     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | Z     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | o     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | g     | 5   | MAN  | O5-C5-C6-O6 |
| 9   | i     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | m     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | o     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | e     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | h     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | n     | 1   | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

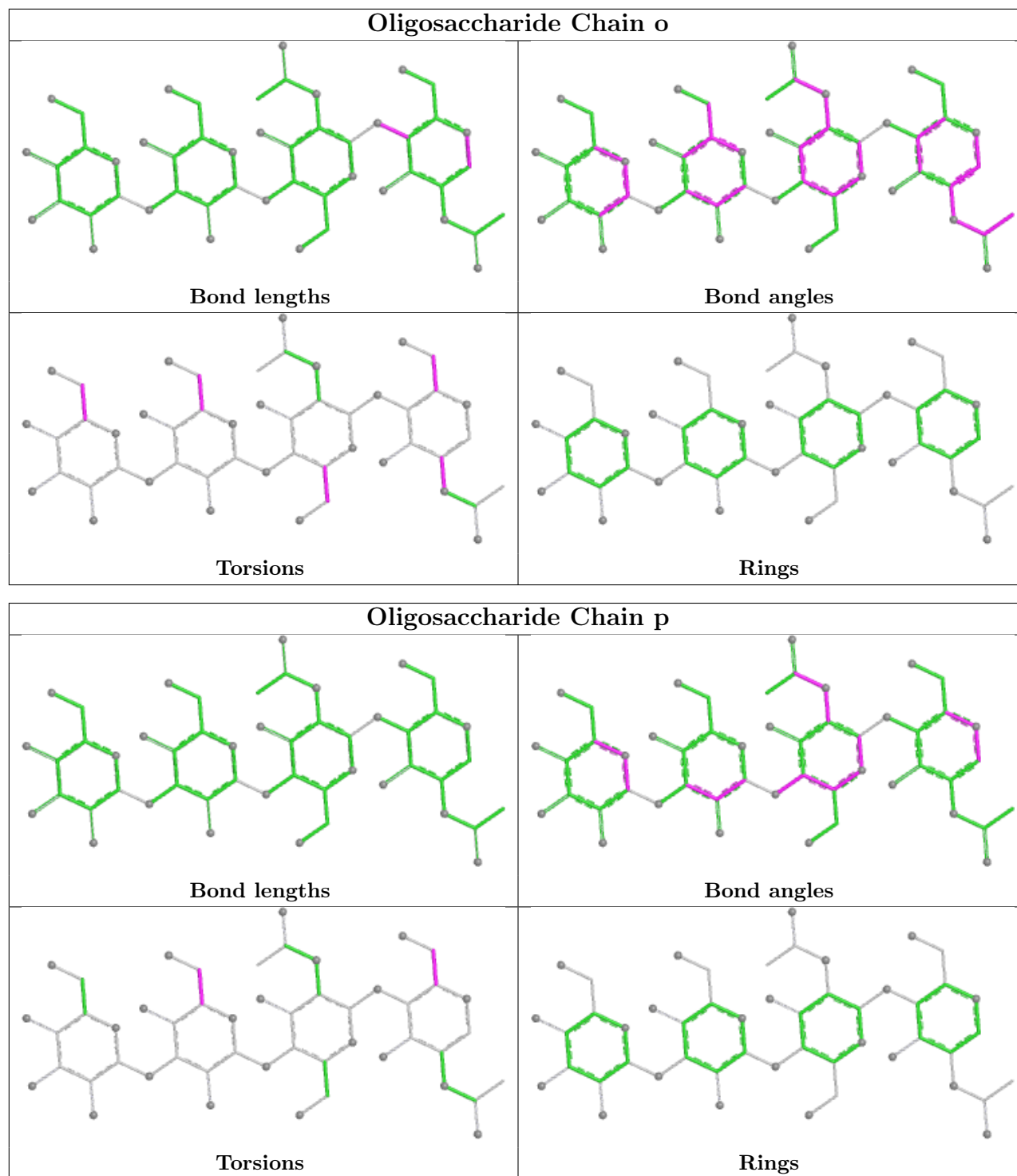
1 monomer is involved in 3 short contacts:

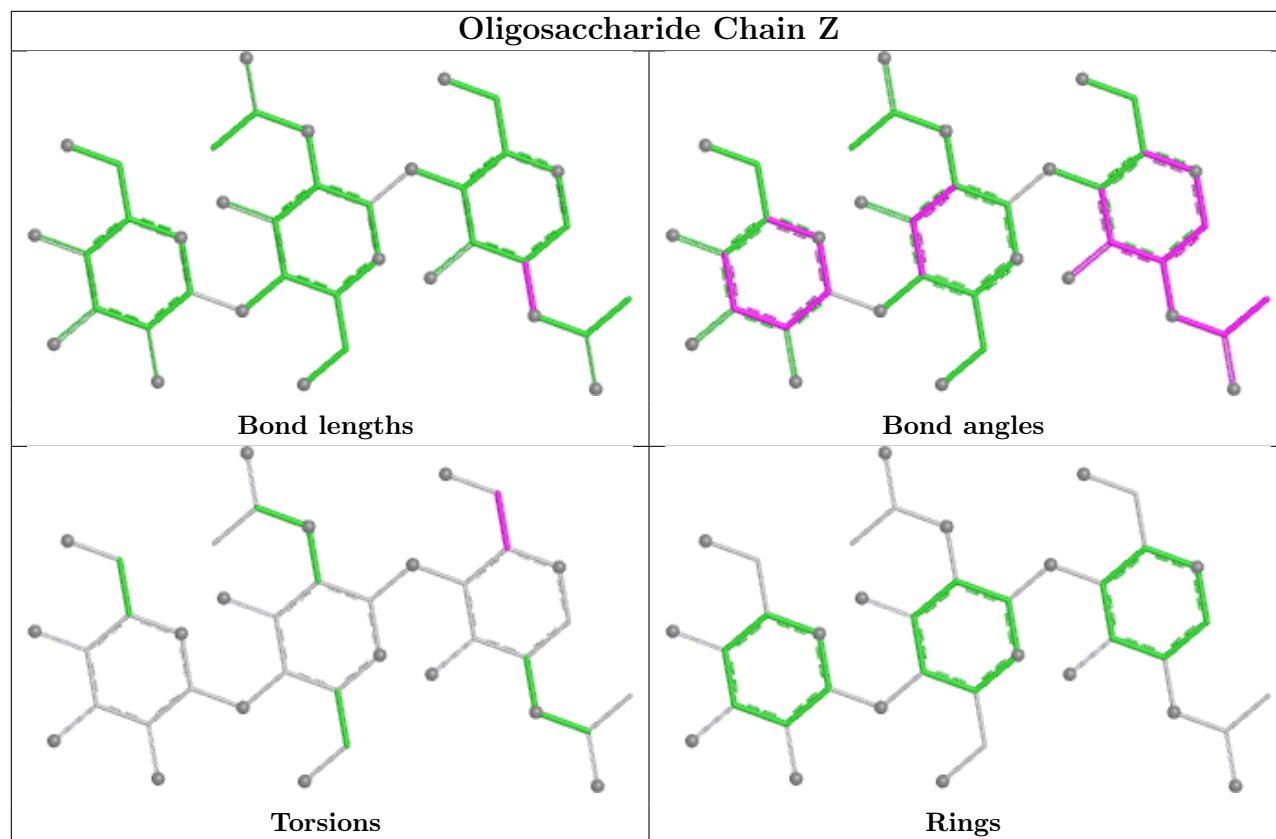
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | Z     | 1   | NAG  | 3       | 0            |

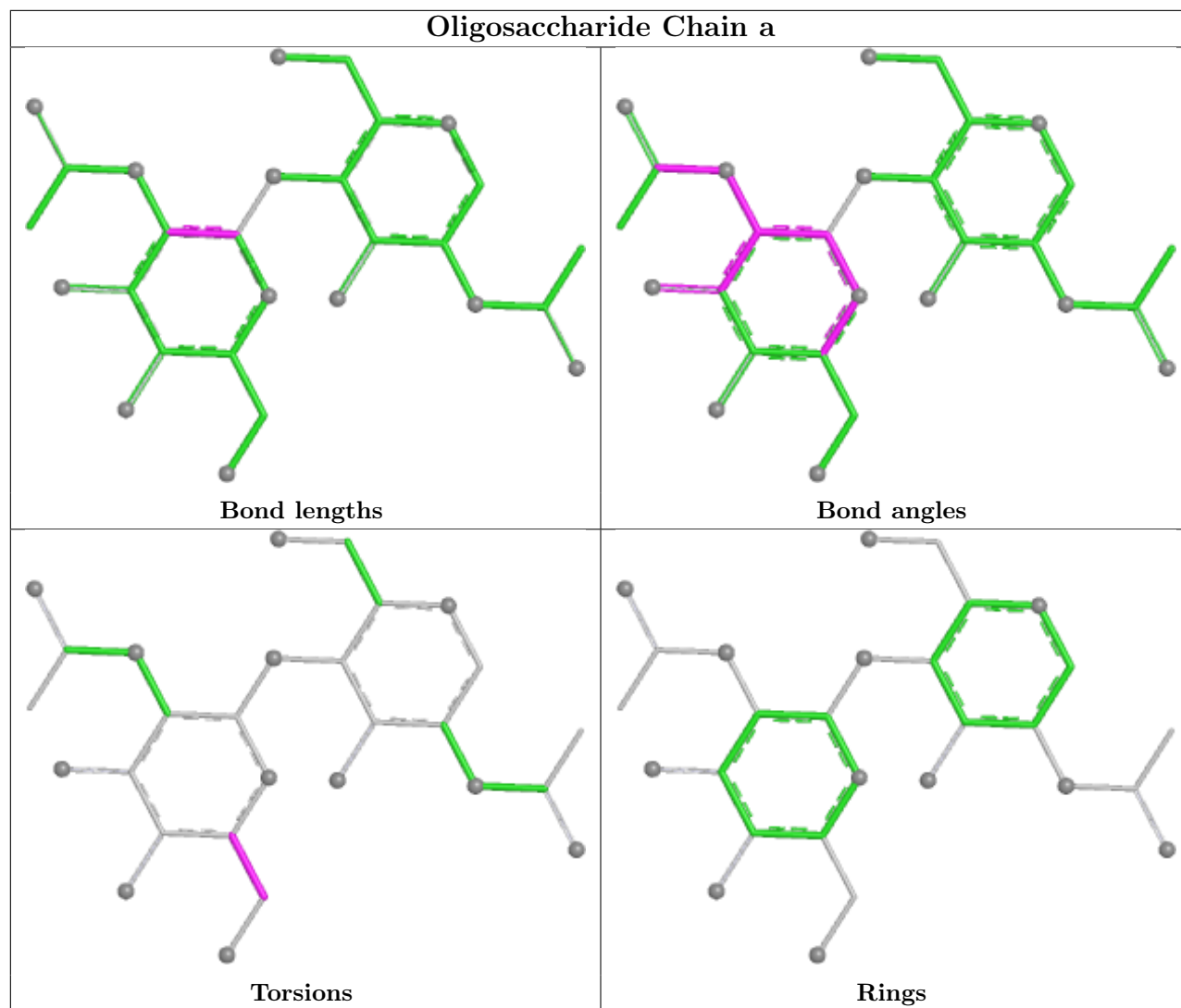
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

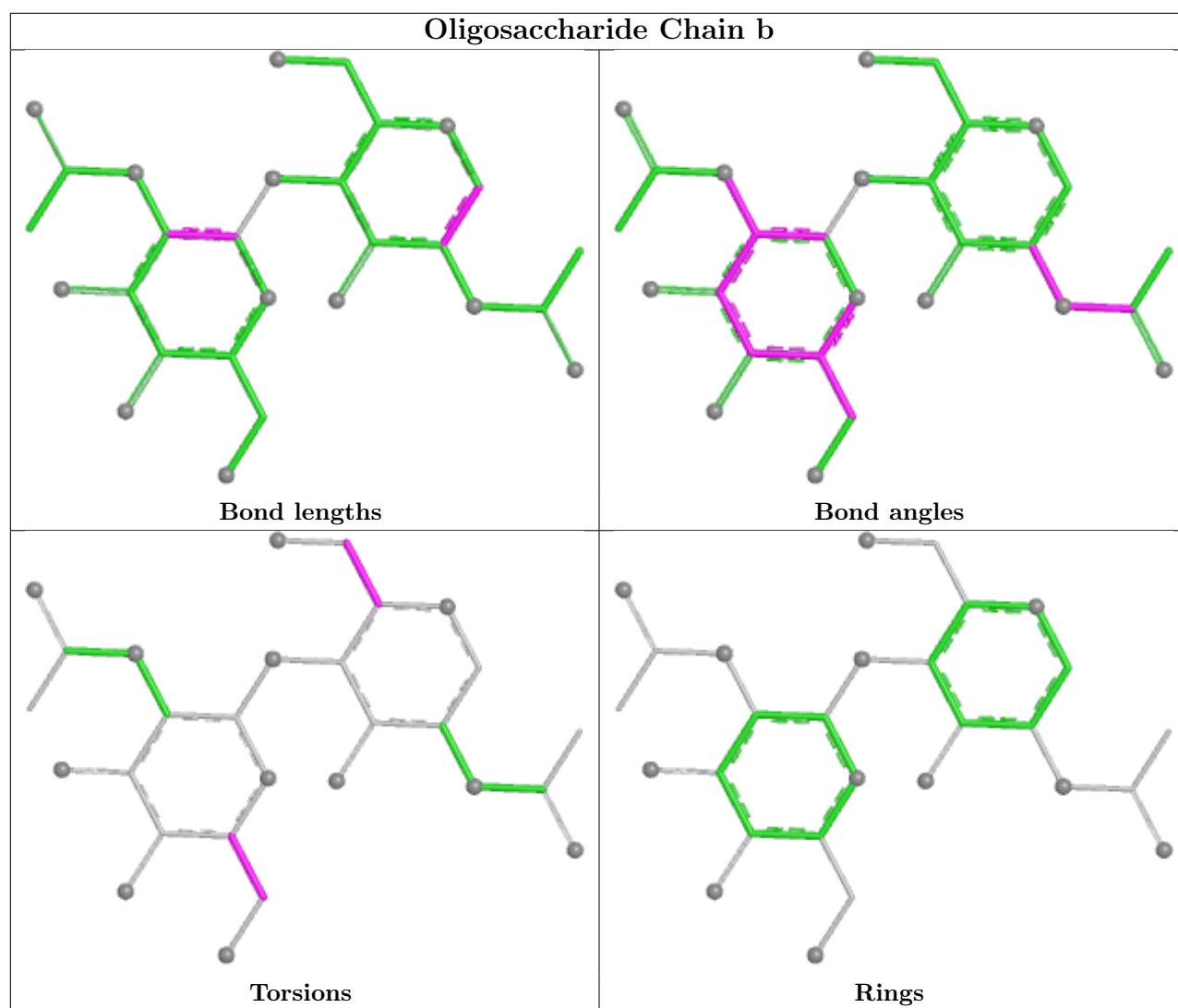


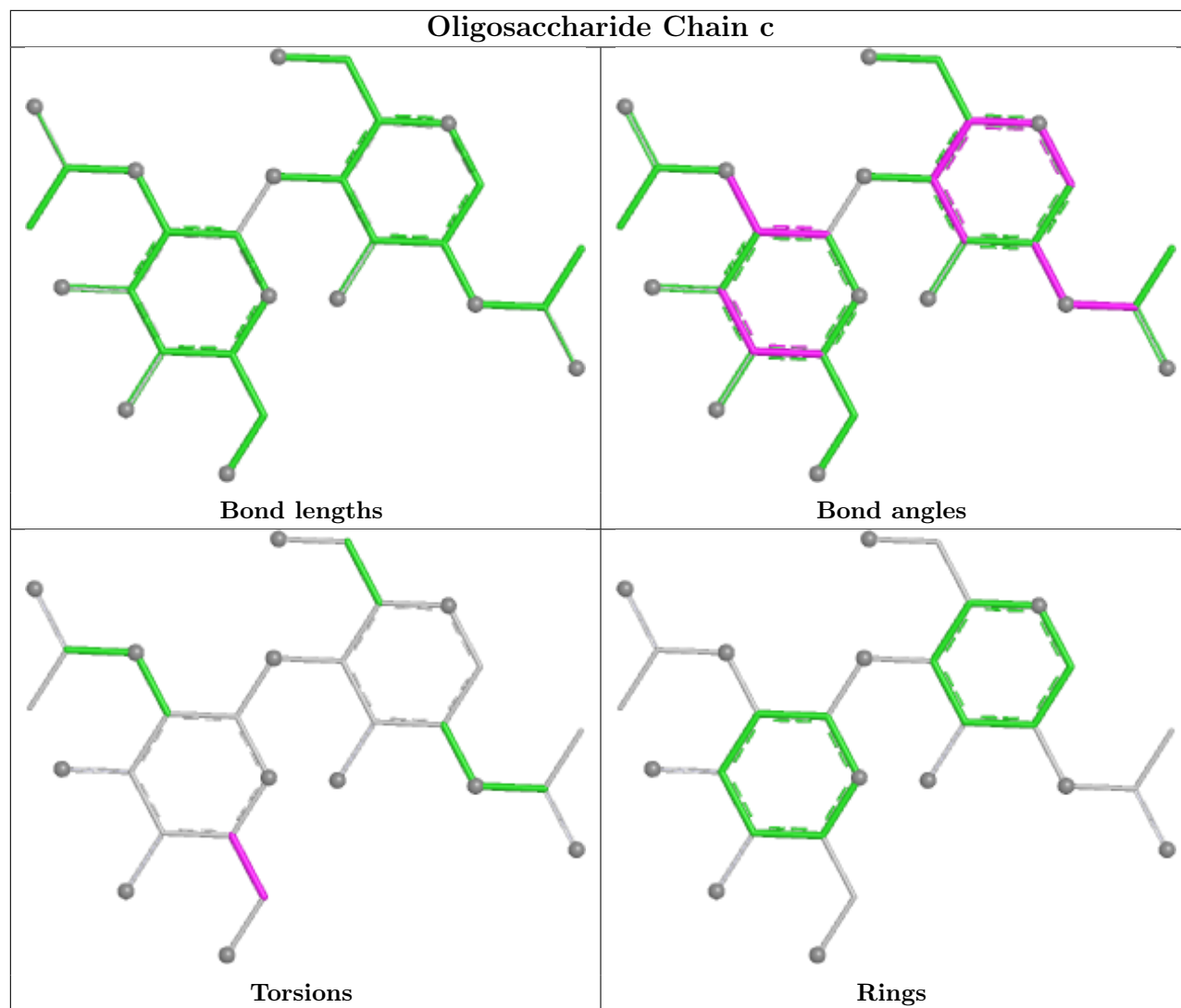


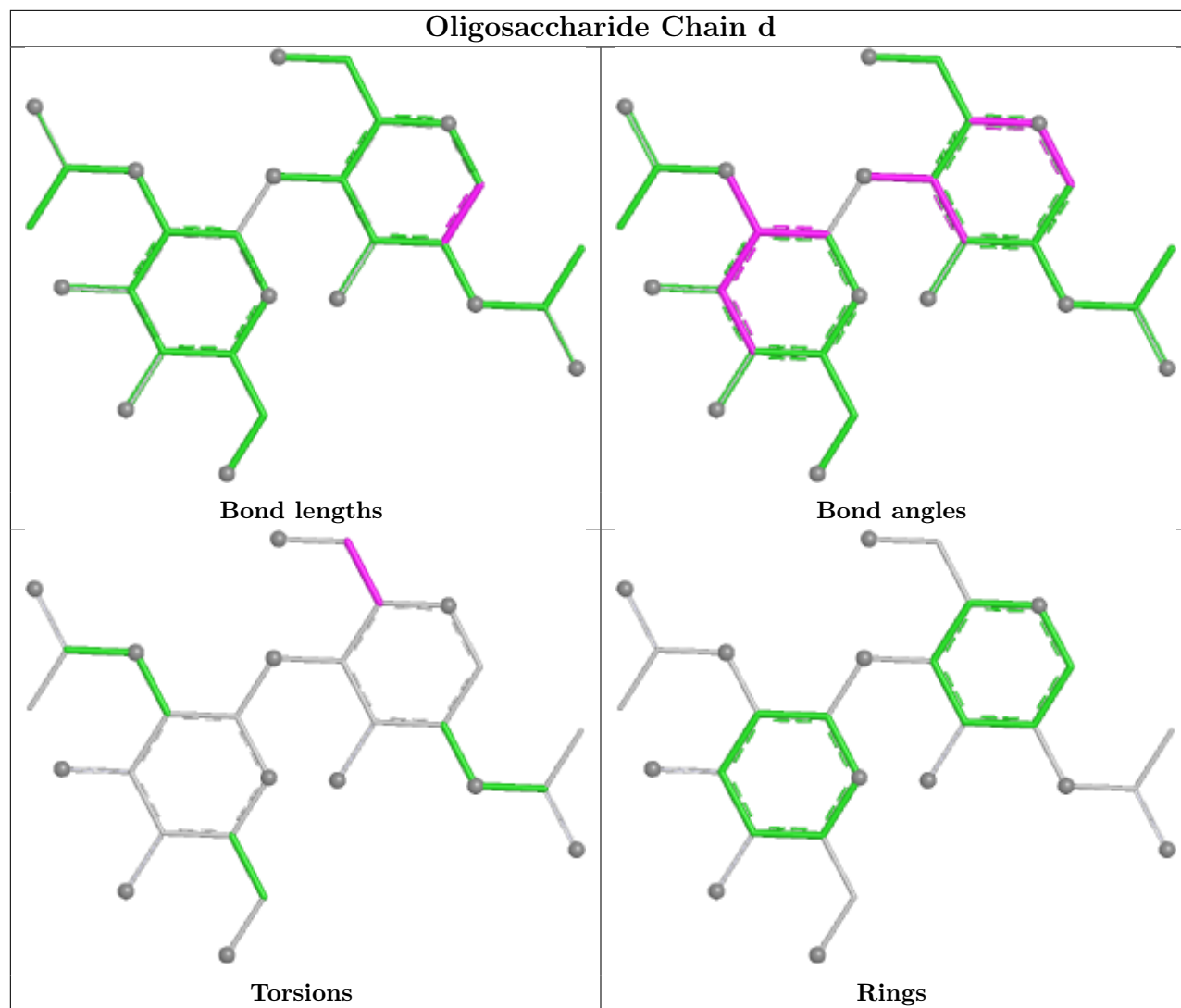


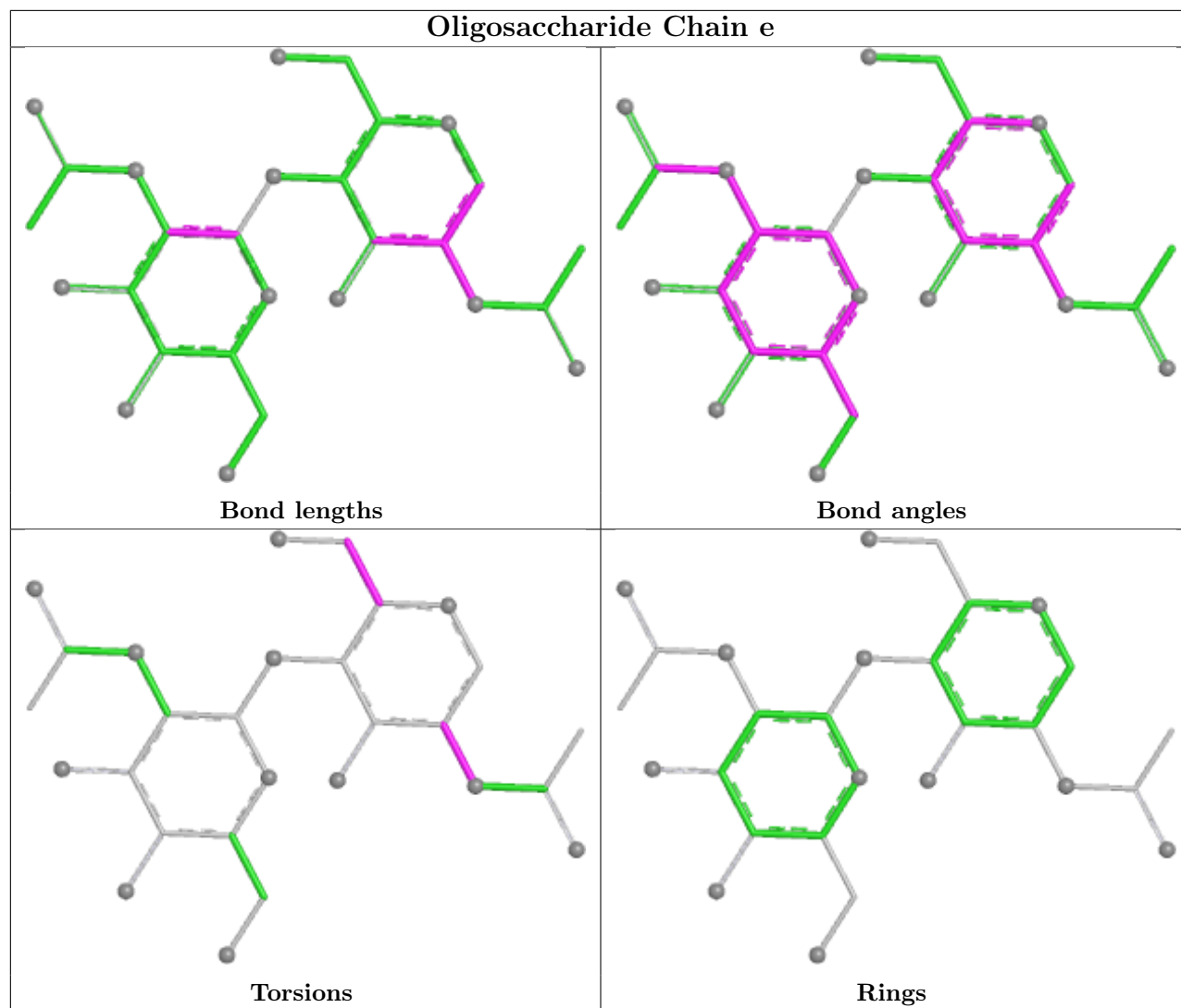


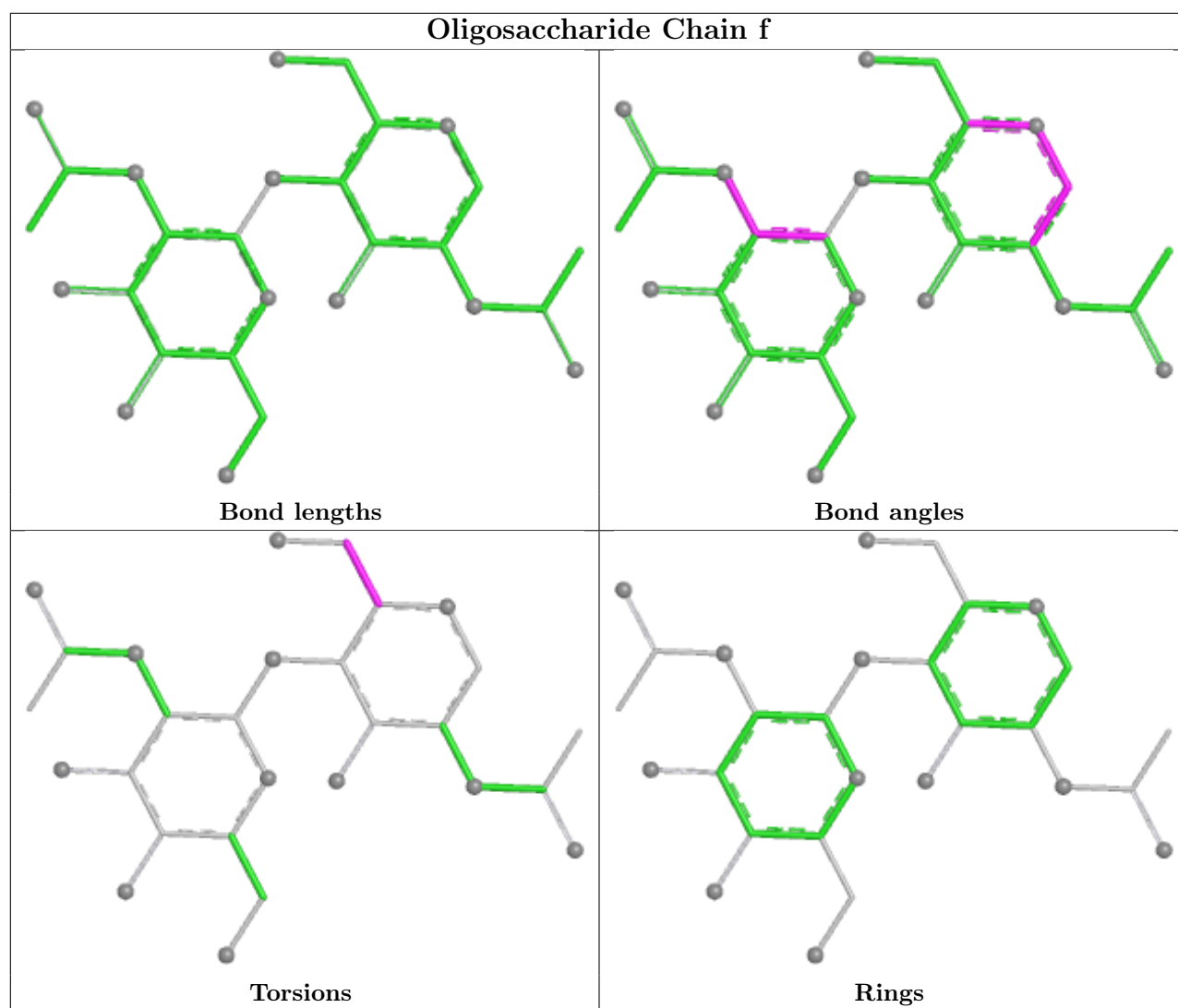




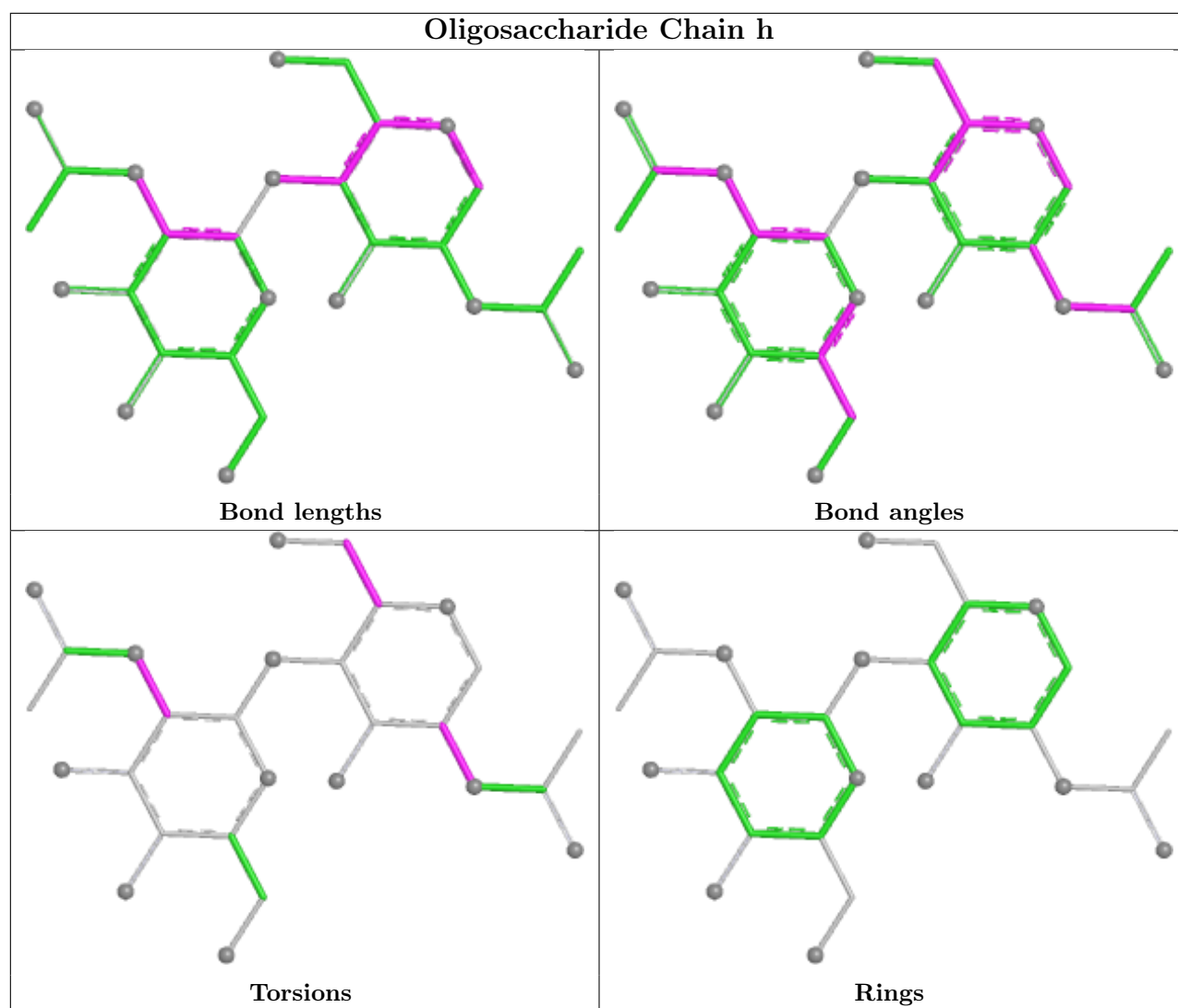


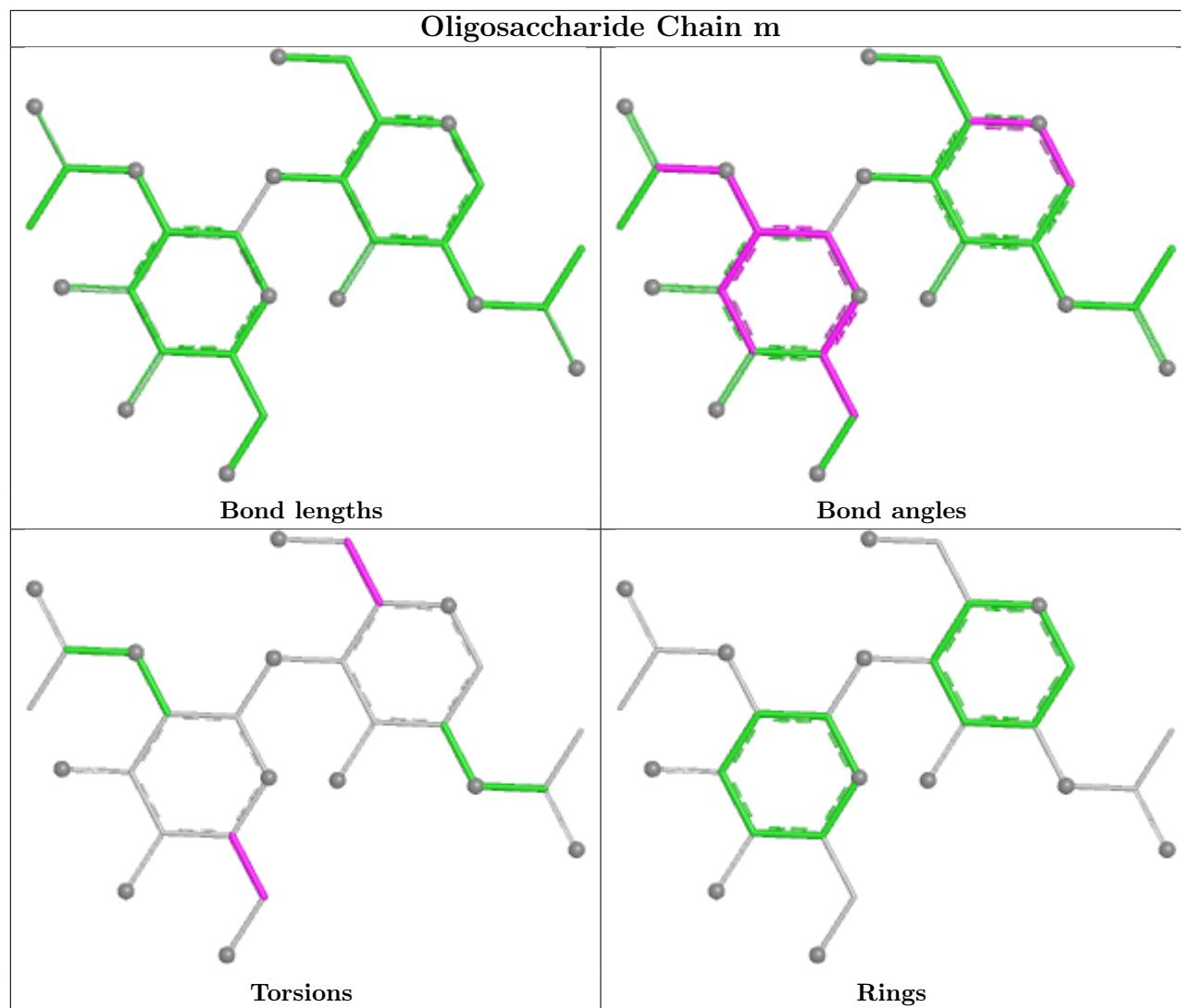


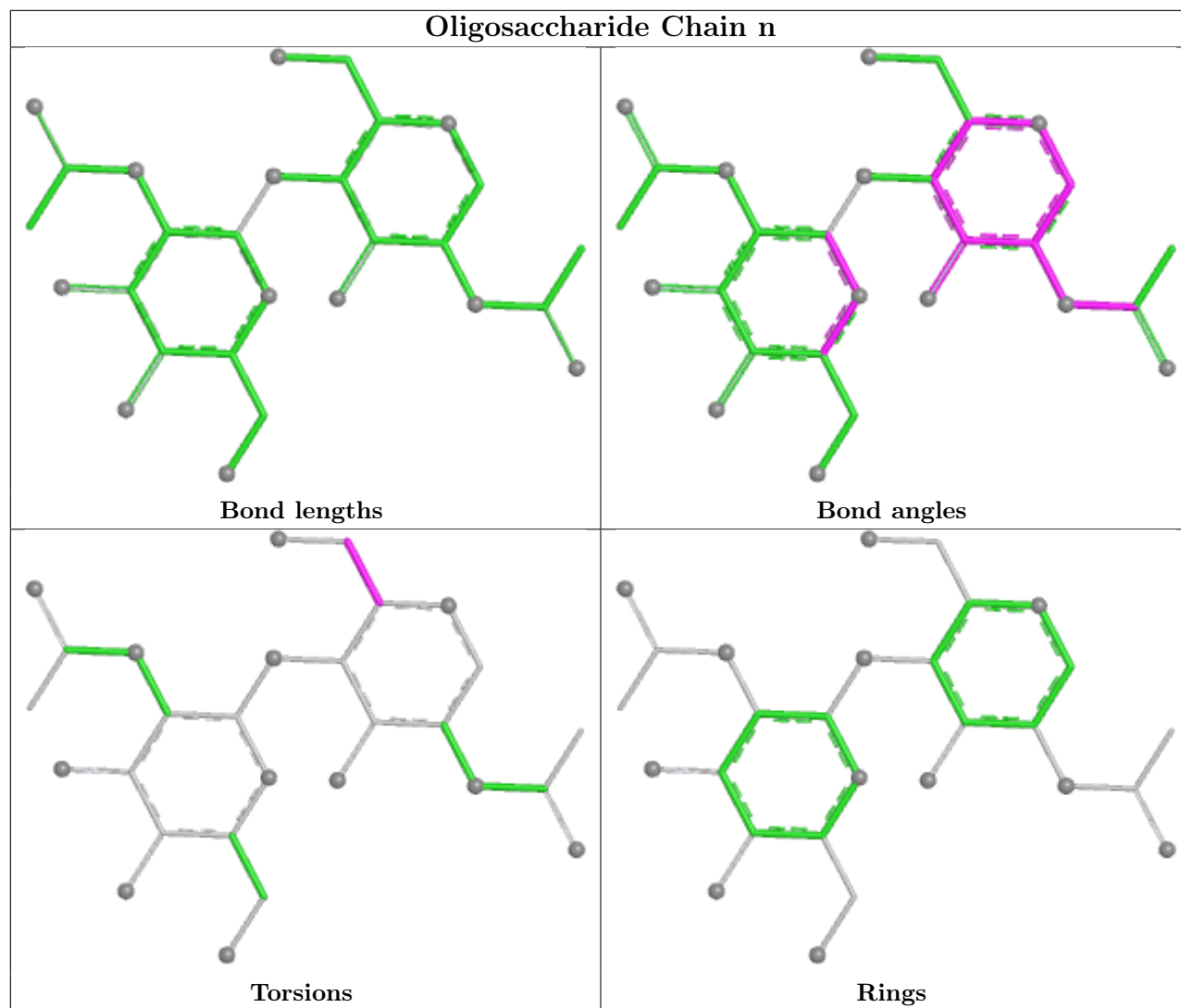


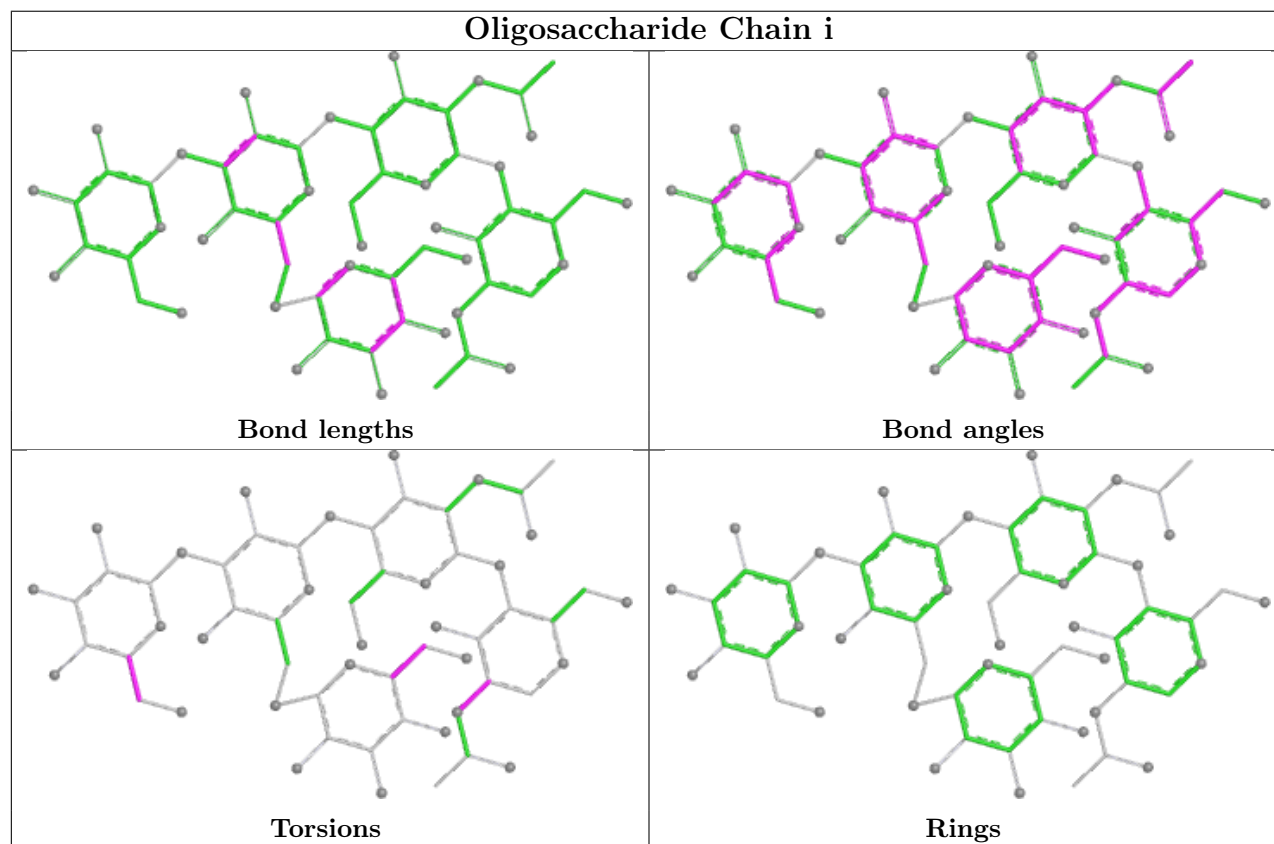
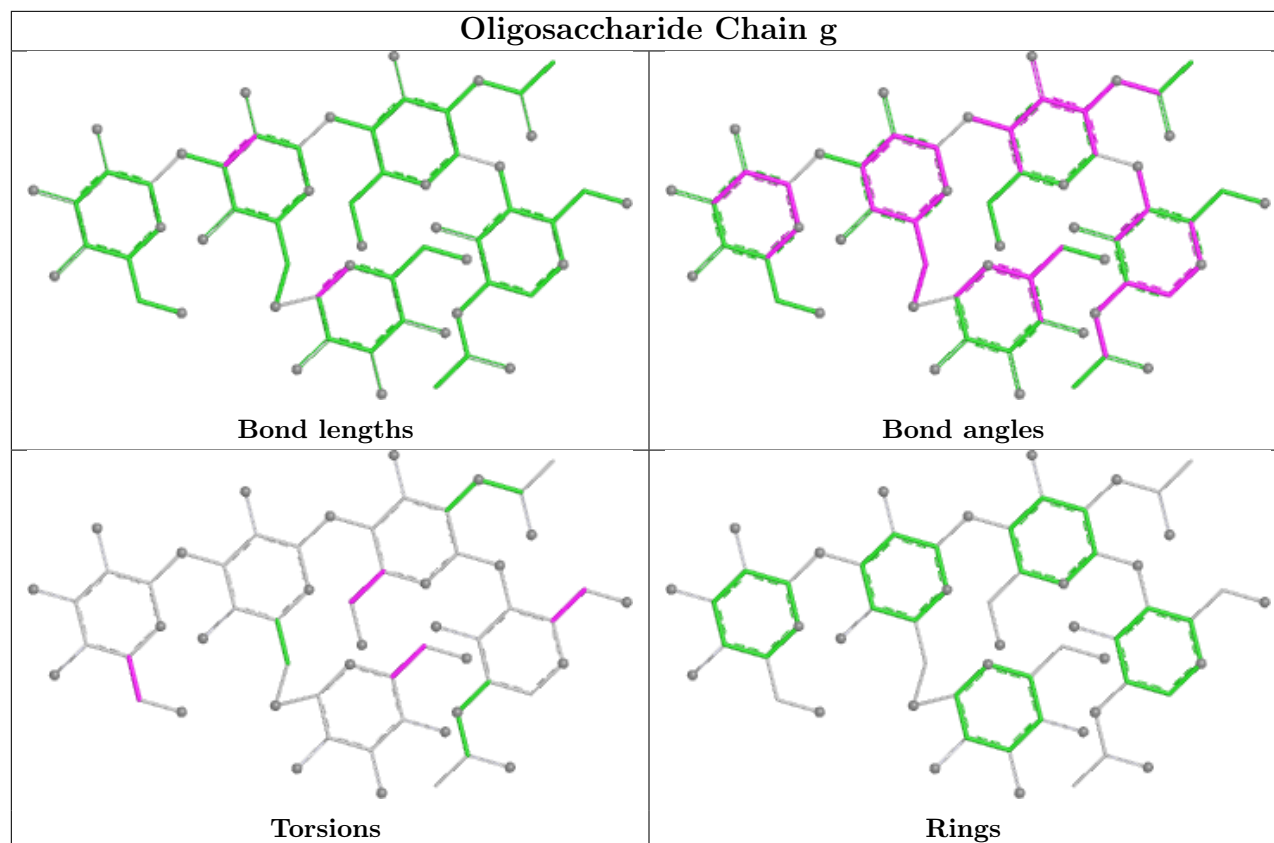


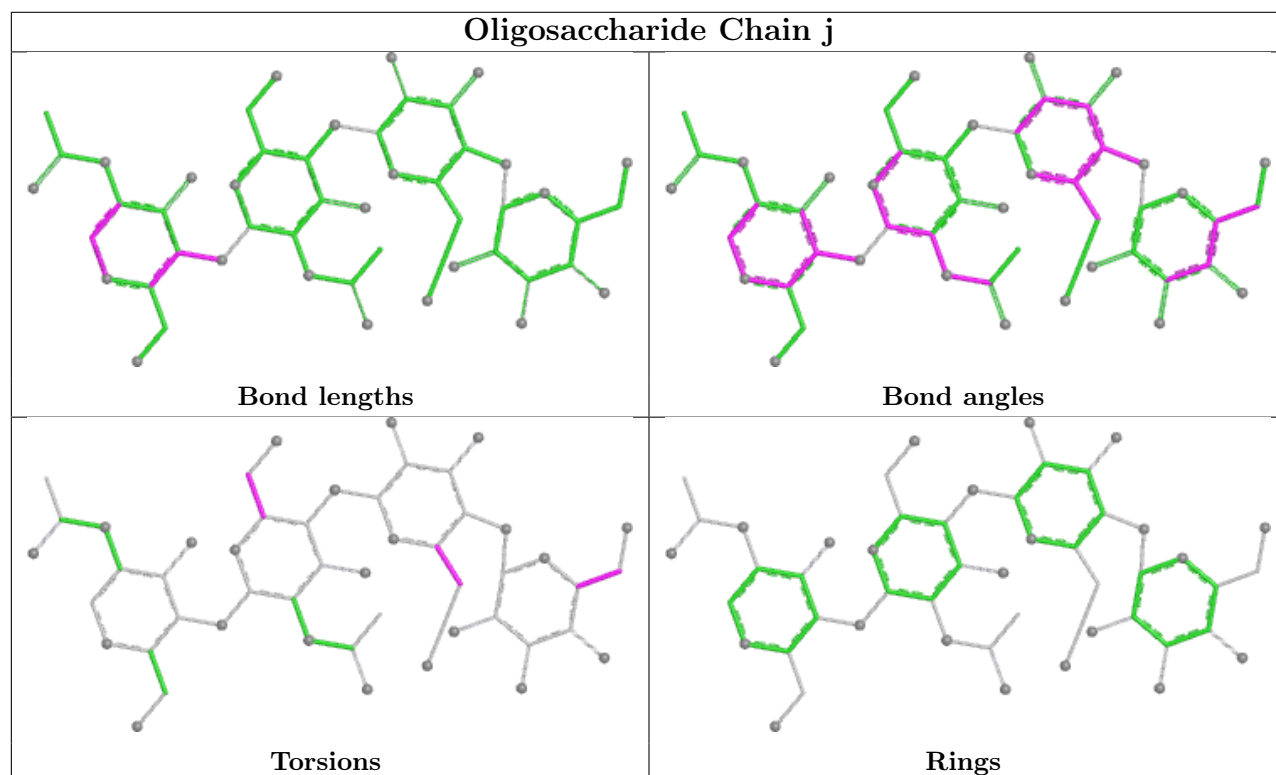
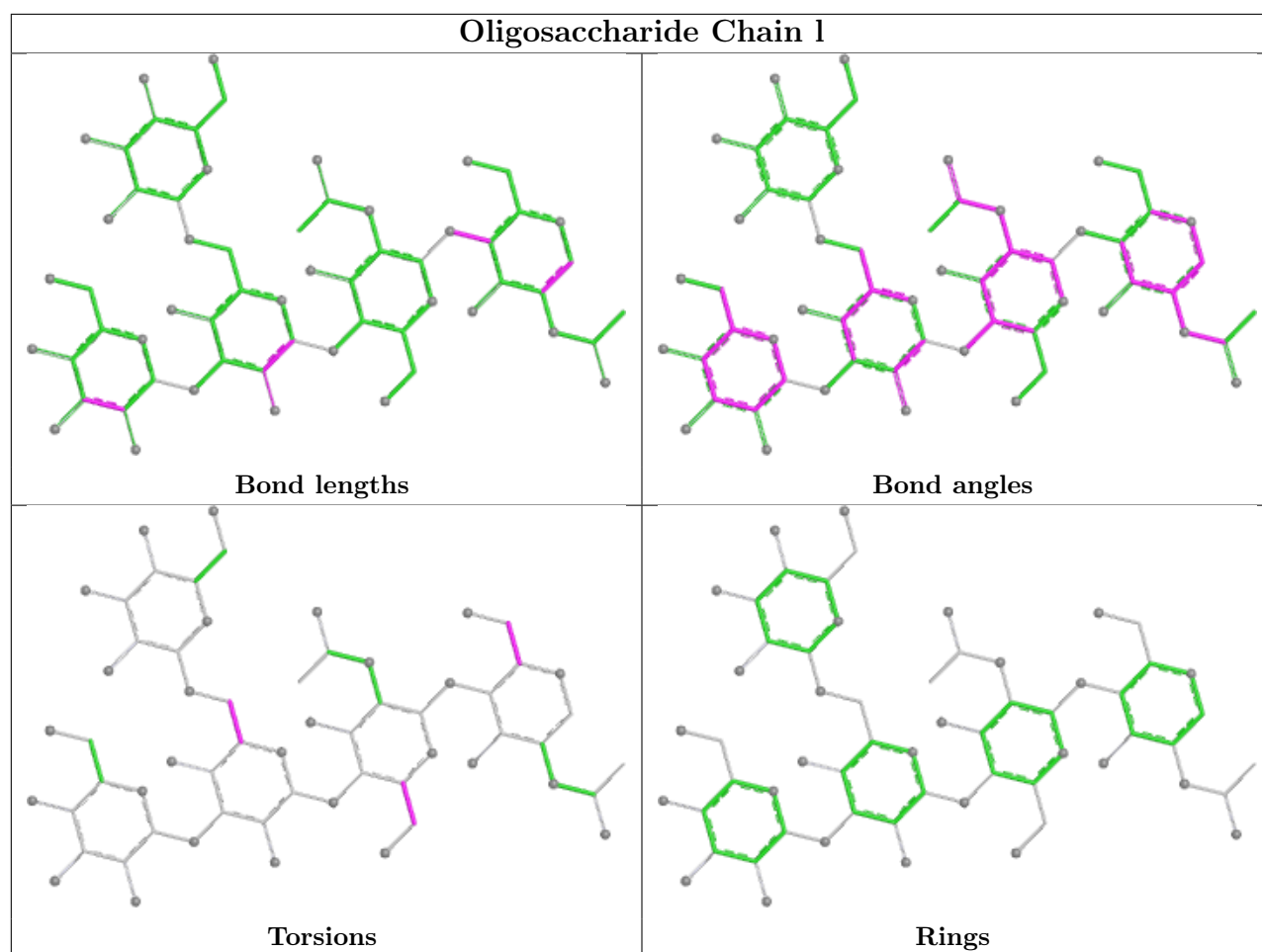












## 5.6 Ligand geometry

10 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 11  | NAG  | F     | 201 | 2    | 14,14,15     | 1.12 | 1 (7%)      | 17,19,21    | 1.60 | 3 (17%)     |
| 11  | NAG  | G     | 402 | 1    | 14,14,15     | 0.93 | 0           | 17,19,21    | 2.46 | 5 (29%)     |
| 11  | NAG  | G     | 401 | 1    | 14,14,15     | 0.84 | 0           | 17,19,21    | 1.08 | 1 (5%)      |
| 11  | NAG  | K     | 401 | 1    | 14,14,15     | 1.40 | 3 (21%)     | 17,19,21    | 2.03 | 5 (29%)     |
| 11  | NAG  | K     | 402 | 1    | 14,14,15     | 0.86 | 0           | 17,19,21    | 1.85 | 3 (17%)     |
| 11  | NAG  | Q     | 401 | -    | 14,14,15     | 0.54 | 0           | 17,19,21    | 1.81 | 4 (23%)     |
| 12  | BMA  | C     | 301 | -    | 11,11,12     | 0.56 | 0           | 15,15,17    | 1.93 | 2 (13%)     |
| 11  | NAG  | S     | 401 | 1    | 14,14,15     | 1.11 | 1 (7%)      | 17,19,21    | 1.55 | 2 (11%)     |
| 11  | NAG  | A     | 401 | 1    | 14,14,15     | 1.69 | 3 (21%)     | 17,19,21    | 2.47 | 6 (35%)     |
| 11  | NAG  | E     | 401 | 1    | 14,14,15     | 0.95 | 1 (7%)      | 17,19,21    | 1.93 | 3 (17%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 11  | NAG  | F     | 201 | 2    | 1/1/5/7 | 1/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 402 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 401 | 1    | 1/1/5/7 | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | K     | 401 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | K     | 402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | NAG  | Q     | 401 | -    | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | BMA  | C     | 301 | -    | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | NAG  | S     | 401 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | A     | 401 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | E     | 401 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 11  | A     | 401 | NAG  | C1-C2 | 4.69 | 1.58        | 1.52     |
| 11  | F     | 201 | NAG  | C1-C2 | 3.69 | 1.57        | 1.52     |
| 11  | A     | 401 | NAG  | C2-N2 | 2.95 | 1.51        | 1.46     |
| 11  | K     | 401 | NAG  | C1-C2 | 2.88 | 1.56        | 1.52     |
| 11  | K     | 401 | NAG  | C2-N2 | 2.85 | 1.51        | 1.46     |
| 11  | E     | 401 | NAG  | C1-C2 | 2.77 | 1.56        | 1.52     |
| 11  | K     | 401 | NAG  | C3-C2 | 2.42 | 1.57        | 1.52     |
| 11  | S     | 401 | NAG  | C1-C2 | 2.29 | 1.55        | 1.52     |
| 11  | A     | 401 | NAG  | C3-C2 | 2.18 | 1.57        | 1.52     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | G     | 402 | NAG  | C1-O5-C5 | 7.46  | 122.18      | 112.19   |
| 11  | K     | 401 | NAG  | C2-N2-C7 | 6.06  | 131.02      | 122.90   |
| 11  | E     | 401 | NAG  | C1-O5-C5 | 5.86  | 120.03      | 112.19   |
| 11  | A     | 401 | NAG  | C2-N2-C7 | 5.85  | 130.74      | 122.90   |
| 11  | K     | 402 | NAG  | C1-O5-C5 | 5.63  | 119.74      | 112.19   |
| 12  | C     | 301 | BMA  | C1-O5-C5 | 5.52  | 119.58      | 112.19   |
| 11  | F     | 201 | NAG  | O5-C1-C2 | 4.76  | 118.66      | 111.29   |
| 11  | Q     | 401 | NAG  | C4-C3-C2 | 4.68  | 117.88      | 111.02   |
| 11  | A     | 401 | NAG  | C1-O5-C5 | 4.63  | 118.39      | 112.19   |
| 11  | S     | 401 | NAG  | C1-C2-N2 | -3.95 | 104.21      | 110.43   |
| 12  | C     | 301 | BMA  | C1-C2-C3 | 3.83  | 115.22      | 109.64   |
| 11  | G     | 401 | NAG  | C1-O5-C5 | 3.69  | 117.13      | 112.19   |
| 11  | G     | 402 | NAG  | O5-C1-C2 | 3.65  | 116.94      | 111.29   |
| 11  | G     | 402 | NAG  | C1-C2-N2 | -3.62 | 104.72      | 110.43   |
| 11  | Q     | 401 | NAG  | C3-C4-C5 | 3.51  | 116.59      | 110.23   |
| 11  | A     | 401 | NAG  | C1-C2-N2 | 3.18  | 115.44      | 110.43   |
| 11  | A     | 401 | NAG  | O5-C1-C2 | 3.06  | 116.03      | 111.29   |
| 11  | G     | 402 | NAG  | C2-N2-C7 | 3.06  | 127.00      | 122.90   |
| 11  | A     | 401 | NAG  | C4-C3-C2 | 2.91  | 115.28      | 111.02   |
| 11  | S     | 401 | NAG  | C2-N2-C7 | 2.87  | 126.75      | 122.90   |
| 11  | K     | 401 | NAG  | C4-C3-C2 | 2.56  | 114.77      | 111.02   |
| 11  | Q     | 401 | NAG  | O5-C1-C2 | -2.52 | 107.39      | 111.29   |
| 11  | K     | 401 | NAG  | O3-C3-C2 | 2.50  | 114.60      | 109.40   |
| 11  | K     | 402 | NAG  | C1-C2-N2 | -2.44 | 106.59      | 110.43   |
| 11  | E     | 401 | NAG  | O5-C5-C4 | 2.43  | 116.73      | 110.83   |
| 11  | G     | 402 | NAG  | C3-C4-C5 | 2.36  | 114.52      | 110.23   |
| 11  | A     | 401 | NAG  | O5-C5-C4 | -2.35 | 105.12      | 110.83   |
| 11  | F     | 201 | NAG  | O5-C5-C6 | 2.31  | 112.17      | 107.66   |
| 11  | K     | 401 | NAG  | C3-C4-C5 | 2.27  | 114.35      | 110.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | K     | 401 | NAG  | O7-C7-C8 | -2.22 | 118.10      | 122.05   |
| 11  | K     | 402 | NAG  | O4-C4-C5 | 2.17  | 114.66      | 109.32   |
| 11  | E     | 401 | NAG  | O5-C5-C6 | -2.13 | 103.52      | 107.66   |
| 11  | Q     | 401 | NAG  | C1-C2-N2 | -2.11 | 107.11      | 110.43   |
| 11  | F     | 201 | NAG  | C3-C4-C5 | -2.09 | 106.44      | 110.23   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | F     | 201 | NAG  | C1   |
| 11  | G     | 401 | NAG  | C1   |

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 12  | C     | 301 | BMA  | O5-C5-C6-O6 |
| 12  | C     | 301 | BMA  | C4-C5-C6-O6 |
| 11  | G     | 401 | NAG  | O5-C5-C6-O6 |
| 11  | G     | 402 | NAG  | C4-C5-C6-O6 |
| 11  | G     | 402 | NAG  | O5-C5-C6-O6 |
| 11  | Q     | 401 | NAG  | O5-C5-C6-O6 |
| 11  | Q     | 401 | NAG  | C4-C5-C6-O6 |
| 11  | K     | 401 | NAG  | O5-C5-C6-O6 |
| 11  | S     | 401 | NAG  | O5-C5-C6-O6 |
| 11  | G     | 401 | NAG  | C4-C5-C6-O6 |
| 11  | F     | 201 | NAG  | O5-C5-C6-O6 |
| 11  | K     | 401 | NAG  | C4-C5-C6-O6 |
| 11  | A     | 401 | NAG  | C4-C5-C6-O6 |
| 11  | A     | 401 | NAG  | O5-C5-C6-O6 |
| 11  | S     | 401 | NAG  | C4-C5-C6-O6 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | Q     | 401 | NAG  | 1       | 0            |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 4   | U     | 1                |
| 4   | P     | 1                |
| 4   | J     | 1                |
| 4   | D     | 1                |
| 4   | W     | 1                |
| 4   | N     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | U     | 27:GLN    | C      | 27(A):SER | N      | 2.62         |
| 1     | P     | 27:GLN    | C      | 27(A):SER | N      | 2.61         |
| 1     | J     | 27:GLN    | C      | 27(A):SER | N      | 2.61         |
| 1     | D     | 27:GLN    | C      | 27(A):SER | N      | 2.61         |
| 1     | W     | 27:GLN    | C      | 27(A):SER | N      | 2.61         |
| 1     | N     | 27:GLN    | C      | 27(A):SER | N      | 2.61         |

## 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%) | 1.08   | 62 (19%) 4 6   | 1, 43, 128, 182       | 0     |
| 1   | E     | 321/330 (97%) | 1.11   | 45 (14%) 7 11  | 1, 56, 147, 233       | 0     |
| 1   | G     | 321/330 (97%) | 0.76   | 34 (10%) 13 14 | 1, 38, 98, 145        | 0     |
| 1   | K     | 321/330 (97%) | 0.61   | 19 (5%) 29 25  | 1, 28, 91, 189        | 0     |
| 1   | Q     | 321/330 (97%) | 0.72   | 26 (8%) 19 18  | 1, 31, 107, 145       | 0     |
| 1   | S     | 321/330 (97%) | 0.89   | 27 (8%) 18 18  | 1, 52, 111, 147       | 0     |
| 2   | B     | 174/181 (96%) | 0.46   | 5 (2%) 54 40   | 1, 13, 112, 137       | 0     |
| 2   | F     | 175/181 (96%) | 0.48   | 5 (2%) 54 40   | 1, 10, 104, 172       | 0     |
| 2   | H     | 175/181 (96%) | 0.66   | 14 (8%) 20 19  | 1, 37, 138, 210       | 0     |
| 2   | L     | 175/181 (96%) | 0.49   | 9 (5%) 34 29   | 1, 27, 138, 185       | 0     |
| 2   | R     | 175/181 (96%) | 0.67   | 7 (4%) 43 34   | 1, 20, 112, 164       | 0     |
| 2   | T     | 175/181 (96%) | 0.66   | 15 (8%) 18 17  | 1, 13, 115, 164       | 0     |
| 3   | C     | 214/221 (96%) | 0.98   | 31 (14%) 7 10  | 1, 31, 145, 197       | 0     |
| 3   | I     | 214/221 (96%) | 1.29   | 43 (20%) 3 6   | 11, 115, 242, 317     | 0     |
| 3   | M     | 214/221 (96%) | 1.55   | 64 (29%) 1 3   | 1, 64, 214, 295       | 0     |
| 3   | O     | 214/221 (96%) | 0.78   | 20 (9%) 16 16  | 1, 37, 120, 166       | 0     |
| 3   | V     | 214/221 (96%) | 1.31   | 46 (21%) 3 5   | 1, 63, 144, 180       | 0     |
| 3   | Y     | 214/221 (96%) | 1.35   | 49 (22%) 2 4   | 1, 97, 270, 367       | 0     |
| 4   | D     | 214/215 (99%) | 0.69   | 13 (6%) 28 25  | 1, 48, 131, 162       | 0     |
| 4   | J     | 214/215 (99%) | 1.39   | 41 (19%) 4 7   | 59, 137, 196, 270     | 0     |
| 4   | N     | 214/215 (99%) | 1.02   | 29 (13%) 8 11  | 1, 40, 173, 230       | 0     |
| 4   | P     | 213/215 (99%) | 0.53   | 4 (1%) 66 49   | 1, 44, 83, 111        | 0     |
| 4   | U     | 214/215 (99%) | 1.49   | 46 (21%) 3 5   | 60, 167, 283, 360     | 0     |
| 4   | W     | 214/215 (99%) | 0.80   | 27 (12%) 9 12  | 1, 42, 149, 189       | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| All | All   | 5542/5682 (97%) | 0.92   | 681 (12%) 9 12 | 1, 48, 178, 367       | 0     |

All (681) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | O     | 130 | PRO  | 7.3  |
| 3   | V     | 145 | LEU  | 5.8  |
| 3   | M     | 148 | LEU  | 5.6  |
| 1   | A     | 151 | ILE  | 5.6  |
| 4   | N     | 146 | VAL  | 5.6  |
| 3   | M     | 186 | SER  | 5.5  |
| 1   | K     | 188 | THR  | 5.0  |
| 3   | Y     | 214 | VAL  | 5.0  |
| 3   | M     | 132 | ALA  | 4.9  |
| 4   | W     | 111 | ALA  | 4.9  |
| 3   | M     | 191 | VAL  | 4.9  |
| 1   | E     | 250 | PRO  | 4.8  |
| 1   | E     | 163 | SER  | 4.7  |
| 3   | M     | 133 | PRO  | 4.7  |
| 3   | M     | 147 | CYS  | 4.6  |
| 1   | K     | 244 | ASN  | 4.5  |
| 3   | M     | 131 | LEU  | 4.4  |
| 3   | V     | 133 | PRO  | 4.4  |
| 4   | J     | 134 | CYS  | 4.4  |
| 1   | G     | 128 | SER  | 4.3  |
| 1   | S     | 46  | GLY  | 4.3  |
| 4   | U     | 136 | LEU  | 4.3  |
| 3   | M     | 143 | ALA  | 4.3  |
| 3   | V     | 130 | PRO  | 4.3  |
| 1   | A     | 184 | ALA  | 4.2  |
| 3   | V     | 132 | ALA  | 4.2  |
| 1   | G     | 59  | GLY  | 4.1  |
| 3   | C     | 194 | SER  | 4.1  |
| 3   | M     | 144 | ALA  | 4.1  |
| 2   | L     | 141 | TYR  | 4.1  |
| 1   | A     | 131 | VAL  | 4.0  |
| 4   | J     | 85  | VAL  | 4.0  |
| 3   | M     | 205 | VAL  | 4.0  |
| 3   | Y     | 188 | VAL  | 4.0  |
| 1   | E     | 184 | ALA  | 4.0  |
| 3   | I     | 10  | GLU  | 4.0  |
| 3   | C     | 214 | VAL  | 4.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 71  | ILE  | 4.0  |
| 1   | A     | 170 | GLU  | 4.0  |
| 3   | V     | 148 | LEU  | 3.9  |
| 4   | U     | 113 | PRO  | 3.9  |
| 3   | Y     | 145 | LEU  | 3.9  |
| 1   | A     | 149 | TRP  | 3.9  |
| 3   | Y     | 205 | VAL  | 3.9  |
| 1   | E     | 124 | SER  | 3.9  |
| 1   | G     | 71  | ILE  | 3.9  |
| 3   | Y     | 157 | VAL  | 3.9  |
| 4   | U     | 175 | LEU  | 3.9  |
| 3   | Y     | 189 | VAL  | 3.8  |
| 3   | M     | 153 | PHE  | 3.8  |
| 4   | W     | 196 | VAL  | 3.8  |
| 3   | V     | 166 | LEU  | 3.8  |
| 3   | M     | 181 | GLY  | 3.7  |
| 3   | V     | 134 | SER  | 3.7  |
| 3   | M     | 183 | TYR  | 3.7  |
| 4   | J     | 113 | PRO  | 3.7  |
| 4   | N     | 134 | CYS  | 3.7  |
| 4   | N     | 135 | LEU  | 3.7  |
| 4   | J     | 86  | TYR  | 3.7  |
| 3   | I     | 135 | SER  | 3.6  |
| 1   | A     | 233 | LEU  | 3.6  |
| 3   | C     | 107 | HIS  | 3.6  |
| 3   | I     | 214 | VAL  | 3.6  |
| 3   | Y     | 133 | PRO  | 3.6  |
| 1   | E     | 241 | PHE  | 3.6  |
| 4   | U     | 119 | PRO  | 3.6  |
| 1   | G     | 93  | GLY  | 3.6  |
| 3   | Y     | 156 | PRO  | 3.6  |
| 4   | N     | 148 | TRP  | 3.6  |
| 4   | U     | 80  | PRO  | 3.5  |
| 3   | M     | 166 | LEU  | 3.5  |
| 3   | V     | 147 | CYS  | 3.5  |
| 1   | G     | 50  | LEU  | 3.5  |
| 4   | N     | 196 | VAL  | 3.5  |
| 3   | C     | 131 | LEU  | 3.5  |
| 3   | C     | 144 | ALA  | 3.5  |
| 3   | I     | 33  | ALA  | 3.5  |
| 3   | V     | 144 | ALA  | 3.5  |
| 3   | V     | 196 | LEU  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | J     | 47  | LEU  | 3.5  |
| 3   | Y     | 187 | SER  | 3.4  |
| 3   | C     | 213 | LYS  | 3.4  |
| 1   | K     | 94  | ASP  | 3.4  |
| 4   | J     | 178 | THR  | 3.4  |
| 1   | E     | 185 | ALA  | 3.4  |
| 4   | N     | 194 | CYS  | 3.4  |
| 3   | O     | 131 | LEU  | 3.4  |
| 3   | V     | 200 | THR  | 3.4  |
| 1   | K     | 72  | ASN  | 3.4  |
| 1   | K     | 132 | SER  | 3.3  |
| 3   | I     | 134 | SER  | 3.3  |
| 1   | E     | 90  | CYS  | 3.3  |
| 2   | H     | 168 | LEU  | 3.3  |
| 3   | I     | 8   | GLY  | 3.3  |
| 3   | C     | 130 | PRO  | 3.3  |
| 1   | A     | 150 | LEU  | 3.3  |
| 1   | A     | 70  | PHE  | 3.3  |
| 3   | M     | 142 | THR  | 3.3  |
| 3   | O     | 217 | LYS  | 3.3  |
| 3   | V     | 189 | VAL  | 3.3  |
| 4   | N     | 199 | GLN  | 3.3  |
| 1   | E     | 150 | LEU  | 3.3  |
| 2   | T     | 27  | SER  | 3.3  |
| 3   | C     | 186 | SER  | 3.3  |
| 1   | A     | 200 | VAL  | 3.3  |
| 3   | M     | 159 | VAL  | 3.3  |
| 3   | M     | 161 | TRP  | 3.3  |
| 4   | W     | 169 | LYS  | 3.3  |
| 1   | E     | 58  | ALA  | 3.2  |
| 3   | M     | 145 | LEU  | 3.2  |
| 4   | U     | 85  | VAL  | 3.2  |
| 3   | O     | 31  | SER  | 3.2  |
| 3   | V     | 131 | LEU  | 3.2  |
| 3   | Y     | 141 | GLY  | 3.2  |
| 1   | S     | 3   | ILE  | 3.2  |
| 3   | M     | 189 | VAL  | 3.2  |
| 3   | V     | 188 | VAL  | 3.2  |
| 1   | G     | 171 | ASP  | 3.2  |
| 4   | U     | 98  | PHE  | 3.2  |
| 4   | D     | 77  | ARG  | 3.2  |
| 2   | T     | 175 | SER  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 154 | ASN  | 3.2  |
| 3   | I     | 205 | VAL  | 3.2  |
| 3   | V     | 128 | VAL  | 3.2  |
| 3   | C     | 132 | ALA  | 3.2  |
| 3   | V     | 193 | SER  | 3.2  |
| 3   | M     | 196 | LEU  | 3.1  |
| 1   | E     | 59  | GLY  | 3.1  |
| 3   | C     | 129 | PHE  | 3.1  |
| 1   | E     | 136 | PRO  | 3.1  |
| 3   | C     | 166 | LEU  | 3.1  |
| 3   | M     | 220 | PRO  | 3.1  |
| 3   | V     | 142 | THR  | 3.1  |
| 3   | O     | 147 | CYS  | 3.1  |
| 2   | F     | 67  | GLY  | 3.1  |
| 3   | Y     | 132 | ALA  | 3.1  |
| 1   | A     | 195 | THR  | 3.1  |
| 4   | J     | 102 | THR  | 3.1  |
| 3   | C     | 202 | ILE  | 3.1  |
| 4   | U     | 29  | SER  | 3.1  |
| 3   | M     | 114 | THR  | 3.1  |
| 4   | U     | 180 | THR  | 3.1  |
| 1   | A     | 198 | ILE  | 3.1  |
| 3   | O     | 129 | PHE  | 3.1  |
| 3   | I     | 119 | SER  | 3.1  |
| 4   | N     | 12  | SER  | 3.1  |
| 1   | G     | 129 | LEU  | 3.1  |
| 1   | E     | 244 | ASN  | 3.1  |
| 3   | O     | 214 | VAL  | 3.1  |
| 1   | K     | 70  | PHE  | 3.1  |
| 3   | Y     | 196 | LEU  | 3.1  |
| 2   | L     | 27  | SER  | 3.1  |
| 1   | K     | 215 | THR  | 3.1  |
| 3   | V     | 214 | VAL  | 3.1  |
| 3   | M     | 177 | LEU  | 3.0  |
| 3   | V     | 72  | ALA  | 3.0  |
| 3   | Y     | 143 | ALA  | 3.0  |
| 2   | L     | 175 | SER  | 3.0  |
| 3   | M     | 149 | VAL  | 3.0  |
| 1   | E     | 190 | LEU  | 3.0  |
| 4   | U     | 178 | THR  | 3.0  |
| 1   | A     | 54  | ASP  | 3.0  |
| 1   | A     | 171 | ASP  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | T     | 128 | ASP  | 3.0  |
| 3   | C     | 147 | CYS  | 3.0  |
| 3   | M     | 168 | SER  | 3.0  |
| 3   | M     | 214 | VAL  | 3.0  |
| 3   | O     | 220 | PRO  | 3.0  |
| 1   | E     | 215 | THR  | 3.0  |
| 1   | S     | 167 | THR  | 3.0  |
| 4   | W     | 147 | GLN  | 3.0  |
| 1   | E     | 249 | ALA  | 3.0  |
| 3   | M     | 203 | CYS  | 3.0  |
| 4   | D     | 68  | GLY  | 3.0  |
| 4   | W     | 197 | THR  | 3.0  |
| 1   | E     | 122 | TRP  | 3.0  |
| 1   | A     | 144 | PHE  | 3.0  |
| 3   | M     | 188 | VAL  | 3.0  |
| 1   | E     | 243 | SER  | 3.0  |
| 1   | A     | 63  | GLY  | 3.0  |
| 3   | M     | 146 | GLY  | 3.0  |
| 3   | Y     | 155 | GLU  | 2.9  |
| 4   | W     | 154 | LEU  | 2.9  |
| 3   | I     | 174 | PRO  | 2.9  |
| 3   | V     | 220 | PRO  | 2.9  |
| 3   | M     | 185 | LEU  | 2.9  |
| 4   | J     | 116 | PHE  | 2.9  |
| 4   | J     | 15  | PRO  | 2.9  |
| 3   | V     | 23  | ARG  | 2.9  |
| 1   | A     | 188 | THR  | 2.9  |
| 3   | I     | 133 | PRO  | 2.9  |
| 4   | J     | 94  | SER  | 2.9  |
| 1   | E     | 253 | ALA  | 2.9  |
| 4   | J     | 51  | ALA  | 2.9  |
| 1   | K     | 71  | ILE  | 2.9  |
| 1   | Q     | 151 | ILE  | 2.9  |
| 2   | L     | 166 | ALA  | 2.9  |
| 4   | J     | 194 | CYS  | 2.9  |
| 3   | Y     | 190 | THR  | 2.9  |
| 3   | Y     | 212 | THR  | 2.9  |
| 3   | Y     | 72  | ALA  | 2.9  |
| 1   | K     | 129 | LEU  | 2.9  |
| 3   | C     | 163 | SER  | 2.9  |
| 2   | R     | 14  | TRP  | 2.9  |
| 1   | Q     | 72  | ASN  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | W     | 199 | GLN  | 2.9  |
| 3   | M     | 129 | PHE  | 2.8  |
| 3   | V     | 176 | VAL  | 2.8  |
| 4   | W     | 132 | VAL  | 2.8  |
| 1   | S     | 206 | ASN  | 2.8  |
| 4   | J     | 152 | ASN  | 2.8  |
| 1   | A     | 250 | PRO  | 2.8  |
| 1   | K     | 117 | ILE  | 2.8  |
| 4   | J     | 120 | PRO  | 2.8  |
| 4   | N     | 204 | PRO  | 2.8  |
| 3   | V     | 177 | LEU  | 2.8  |
| 3   | Y     | 66  | GLY  | 2.8  |
| 3   | M     | 128 | VAL  | 2.8  |
| 1   | E     | 261 | ASP  | 2.8  |
| 3   | I     | 184 | SER  | 2.8  |
| 3   | I     | 217 | LYS  | 2.8  |
| 3   | M     | 155 | GLU  | 2.8  |
| 4   | J     | 175 | LEU  | 2.8  |
| 2   | T     | 134 | GLY  | 2.8  |
| 3   | V     | 143 | ALA  | 2.8  |
| 1   | E     | 91  | TYR  | 2.8  |
| 3   | I     | 107 | HIS  | 2.8  |
| 1   | Q     | 188 | THR  | 2.8  |
| 4   | U     | 20  | THR  | 2.8  |
| 4   | J     | 83  | PHE  | 2.8  |
| 1   | A     | 148 | VAL  | 2.8  |
| 1   | E     | 71  | ILE  | 2.8  |
| 1   | A     | 190 | LEU  | 2.8  |
| 4   | U     | 143 | GLU  | 2.8  |
| 4   | W     | 201 | LEU  | 2.8  |
| 1   | E     | 45  | ASP  | 2.8  |
| 1   | A     | 244 | ASN  | 2.8  |
| 1   | A     | 185 | ALA  | 2.8  |
| 4   | U     | 15  | PRO  | 2.8  |
| 1   | A     | 248 | ILE  | 2.7  |
| 4   | J     | 46  | LEU  | 2.7  |
| 1   | G     | 94  | ASP  | 2.7  |
| 1   | E     | 133 | SER  | 2.7  |
| 1   | K     | 148 | VAL  | 2.7  |
| 3   | C     | 205 | VAL  | 2.7  |
| 3   | C     | 220 | PRO  | 2.7  |
| 3   | I     | 149 | VAL  | 2.7  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 150 | LEU  | 2.7  |
| 4   | W     | 116 | PHE  | 2.7  |
| 1   | Q     | 227 | GLU  | 2.7  |
| 2   | H     | 19  | ASP  | 2.7  |
| 3   | M     | 200 | THR  | 2.7  |
| 1   | S     | 132 | SER  | 2.7  |
| 3   | V     | 186 | SER  | 2.7  |
| 1   | G     | 3   | ILE  | 2.7  |
| 2   | R     | 141 | TYR  | 2.7  |
| 3   | I     | 183 | TYR  | 2.7  |
| 1   | A     | 125 | HIS  | 2.7  |
| 2   | R     | 128 | ASP  | 2.7  |
| 1   | G     | 65  | PRO  | 2.7  |
| 3   | V     | 17  | SER  | 2.7  |
| 1   | A     | 117 | ILE  | 2.7  |
| 2   | H     | 173 | ILE  | 2.7  |
| 2   | T     | 168 | LEU  | 2.7  |
| 3   | C     | 145 | LEU  | 2.7  |
| 4   | U     | 135 | LEU  | 2.7  |
| 4   | U     | 214 | CYS  | 2.7  |
| 4   | J     | 117 | ILE  | 2.7  |
| 3   | M     | 173 | PHE  | 2.7  |
| 1   | G     | 122 | TRP  | 2.7  |
| 3   | M     | 107 | HIS  | 2.7  |
| 4   | W     | 100 | GLN  | 2.7  |
| 4   | J     | 119 | PRO  | 2.7  |
| 4   | N     | 198 | HIS  | 2.7  |
| 4   | U     | 59  | PRO  | 2.7  |
| 1   | A     | 239 | ILE  | 2.7  |
| 3   | V     | 106 | SER  | 2.7  |
| 2   | H     | 148 | CYS  | 2.7  |
| 3   | M     | 123 | THR  | 2.6  |
| 3   | Y     | 200 | THR  | 2.6  |
| 4   | J     | 82  | ASP  | 2.6  |
| 1   | Q     | 155 | SER  | 2.6  |
| 3   | M     | 195 | SER  | 2.6  |
| 3   | M     | 118 | VAL  | 2.6  |
| 1   | A     | 205 | LEU  | 2.6  |
| 3   | M     | 141 | GLY  | 2.6  |
| 2   | B     | 156 | THR  | 2.6  |
| 4   | N     | 203 | SER  | 2.6  |
| 1   | S     | 244 | ASN  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 149 | TRP  | 2.6  |
| 1   | S     | 90  | CYS  | 2.6  |
| 1   | E     | 221 | GLY  | 2.6  |
| 1   | Q     | 69  | GLU  | 2.6  |
| 4   | D     | 79  | GLU  | 2.6  |
| 4   | W     | 141 | PRO  | 2.6  |
| 2   | B     | 141 | TYR  | 2.6  |
| 4   | D     | 192 | TYR  | 2.6  |
| 2   | B     | 126 | LEU  | 2.6  |
| 3   | C     | 148 | LEU  | 2.6  |
| 1   | Q     | 212 | ARG  | 2.6  |
| 1   | Q     | 143 | PHE  | 2.6  |
| 1   | E     | 231 | THR  | 2.6  |
| 2   | R     | 174 | SER  | 2.6  |
| 3   | Y     | 127 | SER  | 2.6  |
| 2   | R     | 60  | ASN  | 2.6  |
| 3   | I     | 97  | ALA  | 2.6  |
| 4   | N     | 149 | LYS  | 2.6  |
| 1   | G     | 179 | HIS  | 2.6  |
| 3   | Y     | 8   | GLY  | 2.6  |
| 1   | G     | 85  | PRO  | 2.6  |
| 4   | J     | 80  | PRO  | 2.6  |
| 1   | E     | 171 | ASP  | 2.6  |
| 2   | R     | 19  | ASP  | 2.6  |
| 1   | G     | 208 | ARG  | 2.6  |
| 1   | G     | 213 | ILE  | 2.6  |
| 3   | Y     | 179 | SER  | 2.6  |
| 1   | Q     | 211 | PRO  | 2.5  |
| 1   | A     | 164 | TYR  | 2.5  |
| 4   | W     | 140 | TYR  | 2.5  |
| 4   | J     | 135 | LEU  | 2.5  |
| 4   | U     | 117 | ILE  | 2.5  |
| 3   | M     | 106 | SER  | 2.5  |
| 3   | I     | 204 | ASN  | 2.5  |
| 3   | Y     | 162 | ASN  | 2.5  |
| 1   | A     | 130 | GLY  | 2.5  |
| 1   | E     | 200 | VAL  | 2.5  |
| 3   | Y     | 172 | THR  | 2.5  |
| 4   | U     | 205 | VAL  | 2.5  |
| 2   | H     | 121 | LYS  | 2.5  |
| 1   | A     | 213 | ILE  | 2.5  |
| 1   | G     | 144 | PHE  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | J     | 101 | GLY  | 2.5  |
| 4   | D     | 59  | PRO  | 2.5  |
| 4   | U     | 115 | VAL  | 2.5  |
| 4   | N     | 175 | LEU  | 2.5  |
| 3   | I     | 58  | ALA  | 2.5  |
| 1   | A     | 155 | SER  | 2.5  |
| 3   | C     | 135 | SER  | 2.5  |
| 1   | A     | 234 | LYS  | 2.5  |
| 3   | V     | 192 | PRO  | 2.5  |
| 3   | Y     | 192 | PRO  | 2.5  |
| 4   | D     | 161 | GLU  | 2.5  |
| 3   | I     | 11  | VAL  | 2.5  |
| 4   | N     | 200 | GLY  | 2.5  |
| 1   | A     | 132 | SER  | 2.5  |
| 3   | C     | 160 | SER  | 2.5  |
| 3   | M     | 124 | LYS  | 2.5  |
| 3   | M     | 187 | SER  | 2.5  |
| 4   | W     | 177 | SER  | 2.5  |
| 1   | G     | 92  | PRO  | 2.5  |
| 3   | M     | 130 | PRO  | 2.5  |
| 4   | U     | 81  | GLU  | 2.5  |
| 4   | U     | 38  | GLN  | 2.5  |
| 4   | U     | 55  | ALA  | 2.5  |
| 1   | S     | 247 | PHE  | 2.5  |
| 3   | V     | 197 | GLY  | 2.5  |
| 1   | Q     | 129 | LEU  | 2.5  |
| 1   | E     | 132 | SER  | 2.5  |
| 1   | E     | 141 | SER  | 2.5  |
| 3   | I     | 209 | PRO  | 2.5  |
| 3   | V     | 135 | SER  | 2.5  |
| 3   | V     | 170 | VAL  | 2.5  |
| 3   | Y     | 193 | SER  | 2.5  |
| 4   | W     | 113 | PRO  | 2.5  |
| 3   | Y     | 53  | ALA  | 2.4  |
| 1   | E     | 195 | THR  | 2.4  |
| 3   | Y     | 147 | CYS  | 2.4  |
| 3   | O     | 145 | LEU  | 2.4  |
| 4   | N     | 136 | LEU  | 2.4  |
| 4   | U     | 132 | VAL  | 2.4  |
| 1   | E     | 120 | SER  | 2.4  |
| 3   | Y     | 215 | ASP  | 2.4  |
| 4   | U     | 106 | ILE  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | I     | 155 | GLU  | 2.4  |
| 3   | M     | 91  | THR  | 2.4  |
| 1   | A     | 259 | LYS  | 2.4  |
| 3   | Y     | 221 | LYS  | 2.4  |
| 1   | G     | 145 | ARG  | 2.4  |
| 3   | I     | 148 | LEU  | 2.4  |
| 3   | O     | 135 | SER  | 2.4  |
| 4   | W     | 143 | GLU  | 2.4  |
| 1   | Q     | 192 | GLN  | 2.4  |
| 1   | S     | 182 | ASN  | 2.4  |
| 4   | N     | 112 | ALA  | 2.4  |
| 3   | V     | 71  | THR  | 2.4  |
| 3   | Y     | 148 | LEU  | 2.4  |
| 1   | G     | 135 | CYS  | 2.4  |
| 1   | A     | 176 | TRP  | 2.4  |
| 4   | U     | 110 | VAL  | 2.4  |
| 1   | K     | 179 | HIS  | 2.4  |
| 2   | T     | 132 | GLU  | 2.4  |
| 1   | S     | 88  | ASP  | 2.4  |
| 2   | H     | 128 | ASP  | 2.4  |
| 3   | C     | 150 | LYS  | 2.4  |
| 3   | M     | 163 | SER  | 2.4  |
| 3   | O     | 165 | ALA  | 2.4  |
| 3   | Y     | 144 | ALA  | 2.4  |
| 4   | J     | 177 | SER  | 2.4  |
| 3   | I     | 114 | THR  | 2.4  |
| 3   | Y     | 76  | THR  | 2.4  |
| 2   | T     | 1   | GLY  | 2.4  |
| 1   | E     | 239 | ILE  | 2.4  |
| 1   | K     | 3   | ILE  | 2.4  |
| 3   | Y     | 126 | PRO  | 2.4  |
| 4   | N     | 120 | PRO  | 2.4  |
| 4   | U     | 207 | LYS  | 2.4  |
| 1   | Q     | 187 | GLN  | 2.4  |
| 1   | S     | 163 | SER  | 2.4  |
| 2   | H     | 27  | SER  | 2.4  |
| 1   | A     | 175 | LEU  | 2.4  |
| 3   | M     | 182 | LEU  | 2.4  |
| 1   | E     | 131 | VAL  | 2.4  |
| 3   | C     | 159 | VAL  | 2.4  |
| 4   | W     | 148 | TRP  | 2.4  |
| 1   | A     | 229 | PHE  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | J     | 204 | PRO  | 2.4  |
| 3   | M     | 184 | SER  | 2.4  |
| 1   | A     | 182 | ASN  | 2.4  |
| 1   | E     | 151 | ILE  | 2.3  |
| 1   | S     | 159 | THR  | 2.3  |
| 2   | B     | 173 | ILE  | 2.3  |
| 3   | M     | 167 | THR  | 2.3  |
| 3   | C     | 217 | LYS  | 2.3  |
| 1   | K     | 192 | GLN  | 2.3  |
| 1   | Q     | 132 | SER  | 2.3  |
| 4   | J     | 114 | SER  | 2.3  |
| 1   | S     | 240 | ASN  | 2.3  |
| 3   | Y     | 159 | VAL  | 2.3  |
| 1   | Q     | 156 | THR  | 2.3  |
| 3   | V     | 198 | THR  | 2.3  |
| 3   | Y     | 197 | GLY  | 2.3  |
| 4   | U     | 97  | THR  | 2.3  |
| 4   | U     | 157 | GLY  | 2.3  |
| 1   | G     | 58  | ALA  | 2.3  |
| 1   | E     | 198 | ILE  | 2.3  |
| 1   | S     | 210 | VAL  | 2.3  |
| 4   | J     | 115 | VAL  | 2.3  |
| 4   | W     | 117 | ILE  | 2.3  |
| 3   | I     | 187 | SER  | 2.3  |
| 3   | M     | 127 | SER  | 2.3  |
| 3   | V     | 160 | SER  | 2.3  |
| 3   | Y     | 134 | SER  | 2.3  |
| 1   | A     | 59  | GLY  | 2.3  |
| 1   | E     | 105 | LEU  | 2.3  |
| 1   | E     | 129 | LEU  | 2.3  |
| 1   | S     | 105 | LEU  | 2.3  |
| 3   | V     | 24  | ALA  | 2.3  |
| 4   | W     | 119 | PRO  | 2.3  |
| 4   | N     | 179 | LEU  | 2.3  |
| 2   | T     | 144 | CYS  | 2.3  |
| 4   | P     | 214 | CYS  | 2.3  |
| 4   | U     | 88  | CYS  | 2.3  |
| 1   | A     | 160 | ILE  | 2.3  |
| 1   | Q     | 198 | ILE  | 2.3  |
| 1   | S     | 131 | VAL  | 2.3  |
| 4   | U     | 147 | GLN  | 2.3  |
| 4   | N     | 147 | GLN  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 199 | SER  | 2.3  |
| 1   | G     | 88  | ASP  | 2.3  |
| 2   | T     | 19  | ASP  | 2.3  |
| 3   | M     | 193 | SER  | 2.3  |
| 3   | Y     | 186 | SER  | 2.3  |
| 4   | J     | 176 | SER  | 2.3  |
| 4   | N     | 176 | SER  | 2.3  |
| 1   | A     | 157 | TYR  | 2.3  |
| 2   | H     | 171 | GLU  | 2.3  |
| 2   | L     | 132 | GLU  | 2.3  |
| 3   | I     | 188 | VAL  | 2.3  |
| 3   | M     | 218 | VAL  | 2.3  |
| 4   | N     | 132 | VAL  | 2.3  |
| 3   | I     | 31  | SER  | 2.3  |
| 3   | M     | 206 | ASN  | 2.3  |
| 4   | D     | 151 | ASP  | 2.3  |
| 4   | W     | 153 | ALA  | 2.3  |
| 1   | G     | 181 | PRO  | 2.3  |
| 3   | M     | 126 | PRO  | 2.3  |
| 4   | N     | 40  | PRO  | 2.3  |
| 1   | G     | 69  | GLU  | 2.3  |
| 1   | G     | 86  | VAL  | 2.3  |
| 3   | V     | 191 | VAL  | 2.3  |
| 2   | H     | 144 | CYS  | 2.3  |
| 2   | L     | 119 | TYR  | 2.3  |
| 3   | Y     | 158 | THR  | 2.3  |
| 2   | T     | 131 | LYS  | 2.2  |
| 1   | Q     | 174 | VAL  | 2.2  |
| 1   | Q     | 130 | GLY  | 2.2  |
| 3   | I     | 95  | TYR  | 2.2  |
| 3   | C     | 179 | SER  | 2.2  |
| 3   | Y     | 9   | ALA  | 2.2  |
| 4   | U     | 114 | SER  | 2.2  |
| 4   | U     | 208 | SER  | 2.2  |
| 4   | N     | 206 | THR  | 2.2  |
| 4   | W     | 145 | LYS  | 2.2  |
| 1   | A     | 65  | PRO  | 2.2  |
| 1   | E     | 194 | PRO  | 2.2  |
| 1   | G     | 143 | PHE  | 2.2  |
| 4   | N     | 139 | PHE  | 2.2  |
| 1   | A     | 173 | LEU  | 2.2  |
| 3   | Y     | 177 | LEU  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | J     | 136 | LEU  | 2.2  |
| 1   | A     | 249 | ALA  | 2.2  |
| 4   | U     | 156 | SER  | 2.2  |
| 4   | U     | 197 | THR  | 2.2  |
| 1   | G     | 68  | ASP  | 2.2  |
| 3   | M     | 154 | PRO  | 2.2  |
| 1   | Q     | 70  | PHE  | 2.2  |
| 1   | S     | 170 | GLU  | 2.2  |
| 1   | K     | 190 | LEU  | 2.2  |
| 2   | H     | 133 | LEU  | 2.2  |
| 1   | A     | 245 | GLY  | 2.2  |
| 3   | Y     | 104 | GLY  | 2.2  |
| 4   | U     | 107 | LYS  | 2.2  |
| 4   | J     | 153 | ALA  | 2.2  |
| 3   | O     | 212 | THR  | 2.2  |
| 3   | V     | 190 | THR  | 2.2  |
| 1   | A     | 147 | VAL  | 2.2  |
| 1   | E     | 199 | SER  | 2.2  |
| 1   | G     | 141 | SER  | 2.2  |
| 2   | F     | 167 | ARG  | 2.2  |
| 3   | M     | 11  | VAL  | 2.2  |
| 3   | M     | 120 | SER  | 2.2  |
| 3   | O     | 205 | VAL  | 2.2  |
| 4   | U     | 177 | SER  | 2.2  |
| 4   | J     | 62  | PHE  | 2.2  |
| 4   | N     | 116 | PHE  | 2.2  |
| 3   | C     | 196 | LEU  | 2.2  |
| 3   | I     | 145 | LEU  | 2.2  |
| 4   | N     | 101 | GLY  | 2.2  |
| 1   | Q     | 131 | VAL  | 2.2  |
| 1   | S     | 208 | ARG  | 2.2  |
| 3   | I     | 57  | THR  | 2.2  |
| 4   | J     | 132 | VAL  | 2.2  |
| 3   | Y     | 220 | PRO  | 2.2  |
| 4   | U     | 62  | PHE  | 2.2  |
| 4   | W     | 146 | VAL  | 2.2  |
| 1   | G     | 72  | ASN  | 2.2  |
| 3   | C     | 119 | SER  | 2.2  |
| 3   | I     | 120 | SER  | 2.2  |
| 3   | M     | 215 | ASP  | 2.2  |
| 4   | U     | 174 | SER  | 2.2  |
| 4   | D     | 121 | SER  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | O     | 166 | LEU  | 2.2  |
| 1   | A     | 126 | GLU  | 2.2  |
| 1   | E     | 189 | LYS  | 2.2  |
| 3   | I     | 124 | LYS  | 2.2  |
| 1   | A     | 177 | GLY  | 2.2  |
| 1   | A     | 192 | GLN  | 2.2  |
| 2   | T     | 141 | TYR  | 2.2  |
| 4   | W     | 198 | HIS  | 2.2  |
| 4   | J     | 106 | ILE  | 2.2  |
| 3   | I     | 189 | VAL  | 2.2  |
| 3   | V     | 11  | VAL  | 2.2  |
| 1   | G     | 52  | LEU  | 2.2  |
| 2   | F     | 168 | LEU  | 2.2  |
| 3   | I     | 172 | THR  | 2.2  |
| 4   | N     | 214 | CYS  | 2.2  |
| 3   | I     | 192 | PRO  | 2.2  |
| 3   | O     | 126 | PRO  | 2.2  |
| 1   | A     | 146 | ASN  | 2.2  |
| 1   | A     | 183 | ASP  | 2.2  |
| 2   | F     | 60  | ASN  | 2.2  |
| 4   | J     | 63  | SER  | 2.2  |
| 4   | W     | 122 | ASP  | 2.2  |
| 4   | P     | 143 | GLU  | 2.1  |
| 3   | I     | 169 | GLY  | 2.1  |
| 3   | M     | 169 | GLY  | 2.1  |
| 1   | A     | 222 | GLN  | 2.1  |
| 2   | R     | 30  | GLN  | 2.1  |
| 3   | V     | 171 | HIS  | 2.1  |
| 1   | E     | 247 | PHE  | 2.1  |
| 3   | C     | 128 | VAL  | 2.1  |
| 1   | G     | 175 | LEU  | 2.1  |
| 3   | I     | 130 | PRO  | 2.1  |
| 3   | O     | 142 | THR  | 2.1  |
| 4   | U     | 35  | TRP  | 2.1  |
| 4   | U     | 148 | TRP  | 2.1  |
| 3   | M     | 122 | SER  | 2.1  |
| 1   | S     | 75  | GLU  | 2.1  |
| 2   | L     | 19  | ASP  | 2.1  |
| 1   | S     | 248 | ILE  | 2.1  |
| 4   | J     | 75  | ILE  | 2.1  |
| 1   | E     | 53  | ARG  | 2.1  |
| 3   | V     | 159 | VAL  | 2.1  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 258 | LYS  | 2.1  |
| 1   | E     | 235 | PRO  | 2.1  |
| 1   | A     | 202 | THR  | 2.1  |
| 3   | I     | 190 | THR  | 2.1  |
| 4   | J     | 202 | SER  | 2.1  |
| 4   | N     | 137 | ASN  | 2.1  |
| 1   | S     | 151 | ILE  | 2.1  |
| 3   | C     | 146 | GLY  | 2.1  |
| 1   | A     | 247 | PHE  | 2.1  |
| 1   | G     | 169 | GLN  | 2.1  |
| 4   | J     | 38  | GLN  | 2.1  |
| 3   | Y     | 182 | LEU  | 2.1  |
| 4   | D     | 191 | VAL  | 2.1  |
| 4   | D     | 197 | THR  | 2.1  |
| 1   | S     | 256 | ILE  | 2.1  |
| 2   | H     | 164 | GLU  | 2.1  |
| 2   | H     | 174 | SER  | 2.1  |
| 2   | T     | 112 | ASP  | 2.1  |
| 3   | I     | 141 | GLY  | 2.1  |
| 3   | O     | 26  | GLY  | 2.1  |
| 3   | Y     | 23  | ARG  | 2.1  |
| 3   | Y     | 195 | SER  | 2.1  |
| 4   | U     | 171 | SER  | 2.1  |
| 3   | I     | 215 | ASP  | 2.1  |
| 3   | I     | 177 | LEU  | 2.1  |
| 3   | M     | 170 | VAL  | 2.1  |
| 4   | U     | 154 | LEU  | 2.1  |
| 1   | A     | 71  | ILE  | 2.1  |
| 3   | O     | 23  | ARG  | 2.1  |
| 4   | U     | 58  | ILE  | 2.1  |
| 4   | P     | 123 | GLU  | 2.1  |
| 1   | G     | 70  | PHE  | 2.1  |
| 1   | K     | 247 | PHE  | 2.1  |
| 1   | S     | 127 | ALA  | 2.1  |
| 1   | S     | 320 | SER  | 2.1  |
| 2   | B     | 174 | SER  | 2.1  |
| 2   | L     | 135 | ASN  | 2.1  |
| 3   | C     | 134 | SER  | 2.1  |
| 3   | V     | 119 | SER  | 2.1  |
| 1   | A     | 209 | LEU  | 2.1  |
| 2   | T     | 116 | LYS  | 2.1  |
| 3   | I     | 176 | VAL  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | M     | 18  | VAL  | 2.1  |
| 4   | W     | 135 | LEU  | 2.1  |
| 4   | W     | 163 | VAL  | 2.1  |
| 1   | K     | 115 | GLN  | 2.1  |
| 4   | J     | 24  | ARG  | 2.1  |
| 4   | D     | 18  | ARG  | 2.1  |
| 3   | M     | 172 | THR  | 2.1  |
| 2   | H     | 150 | GLU  | 2.1  |
| 2   | T     | 164 | GLU  | 2.1  |
| 3   | V     | 169 | GLY  | 2.1  |
| 4   | D     | 118 | PHE  | 2.1  |
| 1   | S     | 214 | ALA  | 2.1  |
| 1   | E     | 223 | SER  | 2.1  |
| 1   | K     | 182 | ASN  | 2.1  |
| 3   | C     | 149 | VAL  | 2.1  |
| 4   | D     | 134 | CYS  | 2.1  |
| 3   | V     | 127 | SER  | 2.1  |
| 4   | U     | 182 | SER  | 2.1  |
| 4   | J     | 168 | SER  | 2.1  |
| 1   | A     | 231 | THR  | 2.0  |
| 1   | S     | 202 | THR  | 2.0  |
| 2   | H     | 156 | THR  | 2.0  |
| 3   | M     | 190 | THR  | 2.0  |
| 1   | E     | 259 | LYS  | 2.0  |
| 1   | Q     | 247 | PHE  | 2.0  |
| 3   | I     | 196 | LEU  | 2.0  |
| 1   | S     | 200 | VAL  | 2.0  |
| 3   | I     | 175 | ALA  | 2.0  |
| 3   | V     | 18  | VAL  | 2.0  |
| 4   | J     | 133 | VAL  | 2.0  |
| 1   | A     | 206 | ASN  | 2.0  |
| 1   | G     | 182 | ASN  | 2.0  |
| 3   | Y     | 163 | SER  | 2.0  |
| 2   | T     | 145 | ASP  | 2.0  |
| 4   | P     | 147 | GLN  | 2.0  |
| 4   | U     | 37  | GLN  | 2.0  |
| 1   | A     | 92  | PRO  | 2.0  |
| 1   | Q     | 117 | ILE  | 2.0  |
| 1   | Q     | 194 | PRO  | 2.0  |
| 3   | V     | 209 | PRO  | 2.0  |
| 4   | N     | 141 | PRO  | 2.0  |
| 3   | O     | 221 | LYS  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | Y     | 217 | LYS  | 2.0  |
| 4   | U     | 39  | LYS  | 2.0  |
| 4   | J     | 78  | LEU  | 2.0  |
| 1   | G     | 91  | TYR  | 2.0  |
| 1   | Q     | 186 | GLU  | 2.0  |
| 3   | C     | 189 | VAL  | 2.0  |
| 3   | Y     | 56  | GLY  | 2.0  |
| 3   | V     | 10  | GLU  | 2.0  |
| 2   | L     | 174 | SER  | 2.0  |
| 1   | A     | 208 | ARG  | 2.0  |
| 1   | Q     | 94  | ASP  | 2.0  |
| 2   | F     | 112 | ASP  | 2.0  |
| 3   | O     | 215 | ASP  | 2.0  |
| 4   | W     | 139 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 11  | NAG  | F     | 201 | 14/15 | 0.51 | 0.15 | 65,85,92,97                | 0     |
| 11  | NAG  | Q     | 401 | 14/15 | 0.59 | 0.17 | 91,97,112,116              | 0     |
| 11  | NAG  | G     | 401 | 14/15 | 0.69 | 0.13 | 41,63,75,78                | 0     |
| 11  | NAG  | A     | 401 | 14/15 | 0.72 | 0.13 | 34,44,48,50                | 0     |
| 11  | NAG  | K     | 401 | 14/15 | 0.77 | 0.13 | 32,48,55,57                | 0     |
| 11  | NAG  | E     | 401 | 14/15 | 0.79 | 0.12 | 24,29,31,31                | 0     |
| 11  | NAG  | S     | 401 | 14/15 | 0.81 | 0.12 | 18,23,28,31                | 0     |
| 11  | NAG  | G     | 402 | 14/15 | 0.82 | 0.12 | 25,35,39,40                | 0     |
| 11  | NAG  | K     | 402 | 14/15 | 0.88 | 0.10 | 16,21,39,42                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 12  | BMA  | C     | 301 | 11/12 | 0.88 | 0.14 | 25,30,35,38                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.