



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:33 PM UTC

PDB ID : 4FQK / pdb\_00004fqk  
Title : Influenza B/Brisbane/60/2008 hemagglutinin Fab CR8059 complex  
Authors : Dreyfus, C.; Laursen, N.S.; Wilson, I.A.  
Deposited on : 2012-06-25  
Resolution : 5.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

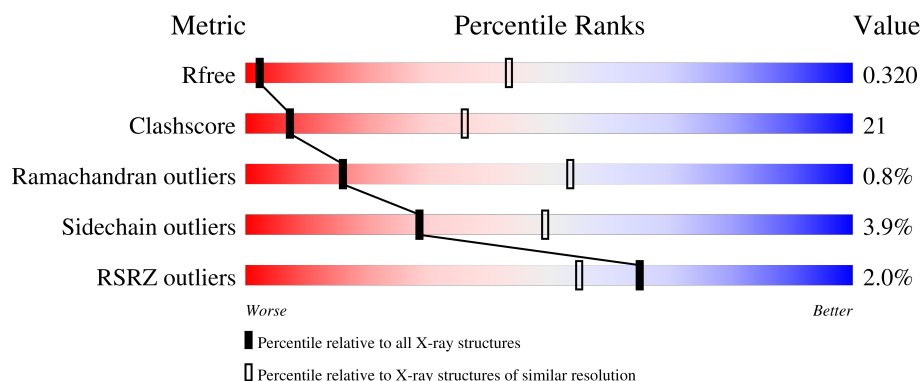
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.65 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1104 (7.32-4.00)                                      |
| Clashscore            | 190562                      | 1165 (7.32-4.00)                                      |
| Ramachandran outliers | 187476                      | 1000 (7.32-4.00)                                      |
| Sidechain outliers    | 187428                      | 1031 (7.36-3.96)                                      |
| RSRZ outliers         | 180081                      | 1097 (7.32-4.00)                                      |

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     | 347    | <div> <div>2%</div> <div> <div></div> <div>53%</div> <div>39%</div> <div>5%</div> </div> </div>               |
| 1   | C     | 347    | <div> <div>3%</div> <div> <div></div> <div>54%</div> <div>38%</div> <div>5%</div> </div> </div>               |
| 2   | B     | 179    | <div> <div>%</div> <div> <div></div> <div>55%</div> <div>20%</div> <div>•</div> <div>22%</div> </div> </div>  |
| 2   | D     | 179    | <div> <div>3%</div> <div> <div></div> <div>55%</div> <div>21%</div> <div>•</div> <div>22%</div> </div> </div> |
| 3   | E     | 234    | <div> <div>%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>•</div> <div>6%</div> </div> </div>   |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 3   | H     | 234    | <br>% 71% 23% 6%  |
| 4   | F     | 216    | <br>3% 79% 19% 2% |
| 4   | L     | 216    | <br>% 82% 15% 3%  |
| 5   | G     | 2      | <br>50% 50%       |
| 5   | I     | 2      | <br>100%          |
| 5   | J     | 2      | <br>100%          |
| 5   | N     | 2      | <br>100%          |
| 5   | O     | 2      | <br>100%          |
| 5   | P     | 2      | <br>50% 50%       |
| 6   | K     | 3      | <br>67% 33%       |
| 6   | M     | 3      | <br>33% 33% 33%   |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14080 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     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2560  | 1607 | 458 | 480 | 15 |         |         |       |
| 1   | C     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2560  | 1607 | 458 | 480 | 15 |         |         |       |

- Molecule 2 is a protein called Hemagglutinin HA2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1054  | 652 | 182 | 215 | 5 |         |         |       |
| 2   | D     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1062  | 658 | 183 | 216 | 5 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| B     | 524     | SER      | -      | linker  | UNP C0LT38 |
| B     | 525     | GLY      | -      | linker  | UNP C0LT38 |
| B     | 526     | ARG      | -      | linker  | UNP C0LT38 |
| D     | 524     | SER      | -      | linker  | UNP C0LT38 |
| D     | 525     | GLY      | -      | linker  | UNP C0LT38 |
| D     | 526     | ARG      | -      | linker  | UNP C0LT38 |

- Molecule 3 is a protein called Antibody CR8059 Heavy Chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | E     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1673  | 1061 | 278 | 327 | 7 |         |         |       |
| 3   | H     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1679  | 1064 | 279 | 328 | 8 |         |         |       |

- Molecule 4 is a protein called Antibody CR8059 Light Chain.

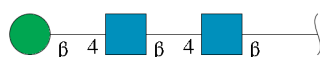
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | F     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1606  | 1006 | 269 | 327 | 4 |         |         |       |
| 4   | L     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1009 | 270 | 328 | 5 |         |         |       |

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



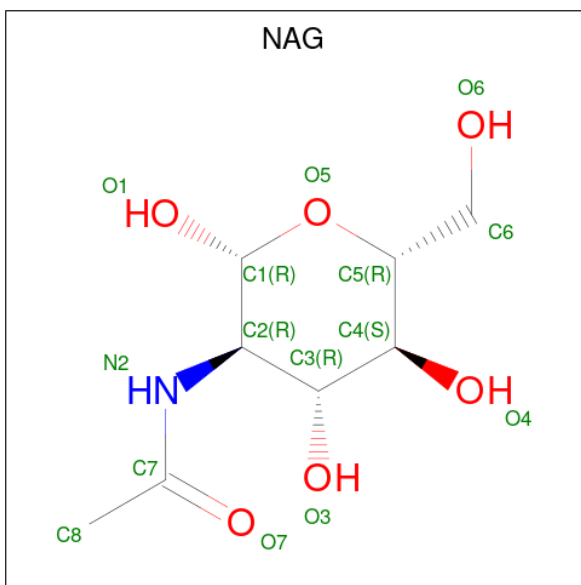
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5   | G     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 5   | I     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 5   | J     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 5   | N     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 5   | O     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 5   | P     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

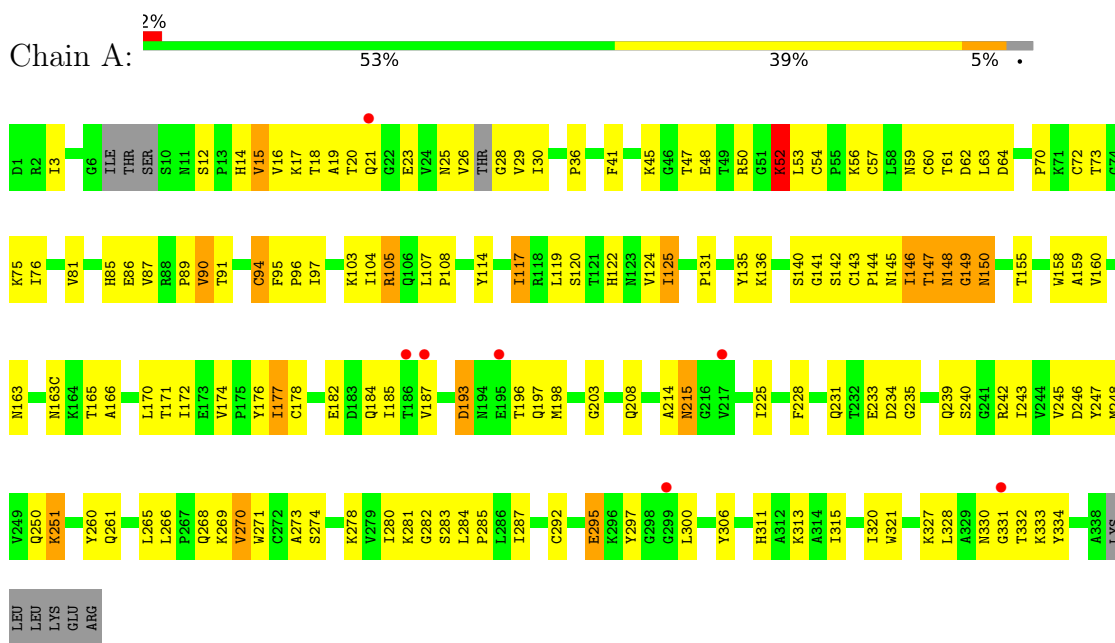


| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 7   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 7   | C     | 1        | Total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

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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



LYS  
LEU  
LEU  
LYS  
GLU  
ARG

• Molecule 2: Hemagglutinin HA2



GLY PHE PHE GLY ALA ILE ALA GLY PHE LEU GLU GLY GLY TRP GLU MET ILE ILE ALA GLY TRP H369 H373 A380 S387 A391 ILE ASN LYS I395 N398 L405 E406 V407 K408 N409 L410 Q411 R412 A416 M417 D418 H421 M422 I424 L425 E426 L427 V431 D432

R435 I439 S440 I443 E444 L448 L449 S450 N451 E452 G453 I454 E458 ASP GLU HIS TRP L463 A464 L465 S476 E479 G483 C484 F485 L496 I499 E508 F509 S510 L511 F514 ASP SER LEU ILE THR ALA ALA SER SER GLY ARG

• Molecule 2: Hemagglutinin HA2



GLY PHE PHE GLY ALA ILE ALA GLY PHE LEU GLU GLY GLY TRP GLU MET ILE ILE ALA GLY TRP H369 H373 A376 A380 S387 A391 ILE ASN LYS I395 N398 L405 E406 V407 K408 N409 L410 Q411 R412 A416 M417 D418 H421 M422 I424 L425 E426

L427 V431 D432 R435 I439 S440 I443 E444 L448 L449 S450 N451 E452 G453 I454 E458 ASP GLU HIS L462 L463 L465 M472 S476 E479 G483 C484 F485 L496 I499 E508 F509 S510 L511 F514 ASP SER LEU ILE THR ALA ALA SER SER

GLY  
ARG

• Molecule 3: Antibody CR8059 Heavy Chain



Q1 V2 Q3 Q6 K12 S17 C22 S25 T30 T35 W36 A40 Q43 W50 I51 Y53 T57 K62 K71 D72 T73 M80 B82A S82B L82C D86 R94 D95 Y98 S99 G100 S100A Y100B Y100F Y100G S104 V111 SER

S113 A114 T116 K117 P123 L124 S127 SER LYS SER THR SER GLY G134 T135 G140 K143 F146 T151 V163 F166 P167 A168 V169 L170 Q171 L178 V182 T183 G190 T191 Q192 T193 H200 K201 P202 R210 V211 E212 P213 K214 S215 CYS HIS HIS HIS

HIS  
HIS  
HIS

• Molecule 3: Antibody CR8059 Heavy Chain

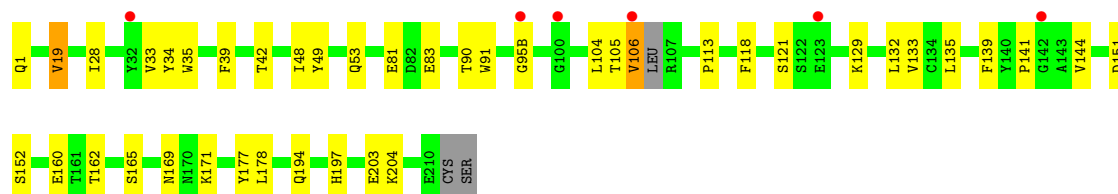
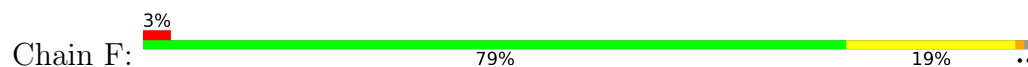


Q1 V2 Q3 Q6 K12 S17 S25 T30 T35 W36 A40 Q43 W50 I51 S52 G52A Y53 T57 K62 K71 D72 T73 M80 B82A S82B L82C D86 R94 D95 V96 Q97 Y98 S99 G100 S100A Y100B Y100F Y100G S104 V111 SER

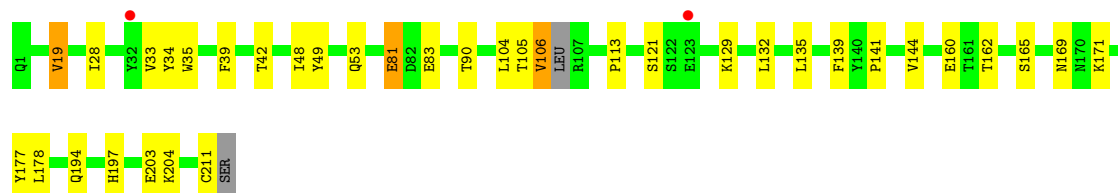
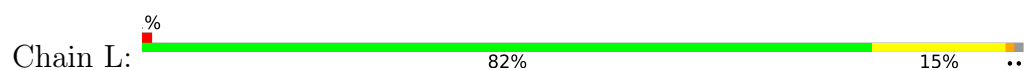
S113 A114 T116 K117 P123 S127 SER LYS SER THR SER GLY G134 T135 G139 G140 K143 F146 T151 V163 F166 P167 A168 V169 L170 Q171 S172 L178 V182 T183 T193 H200 K201 P202 T205 R210 V211 E212 P213 K214 S215 C216 HIS HIS HIS HIS



- Molecule 4: Antibody CR8059 Light Chain



- Molecule 4: Antibody CR8059 Light Chain



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



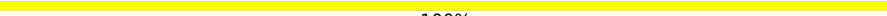
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

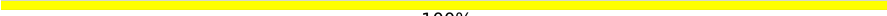


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

NAG1  
NAG2

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

Chain O:  100%

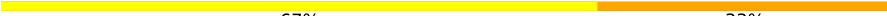
NAG1  
NAG2

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

Chain P:  50% 50%

NAG1  
NAG2

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

Chain K:  67% 33%

NAG1  
NAG2  
BMA3

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

Chain M:  33% 33% 33%

NAG1  
NAG2  
BMA3

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | H 3                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 189.20Å 189.20Å 319.31Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 48.93 – 5.65<br>48.93 – 5.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (48.93-5.65)<br>99.9 (48.93-5.65)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.66 (at 5.73Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.7.2_869)                           | Depositor        |
| R, $R_{free}$                                                           | 0.306 , 0.324<br>0.303 , 0.320                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1275 reflections (9.97%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 243.5                                                       | Xtriage          |
| Anisotropy                                                              | 0.141                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 995.2                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | 0.429 for h,-h-k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.86                                                        | EDS              |
| Total number of atoms                                                   | 14080                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 100.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 [i](#)

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

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

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     | 0.84         | 0/2618  | 1.34        | 22/3553 (0.6%)  |
| 1   | C     | 0.84         | 0/2618  | 1.34        | 23/3553 (0.6%)  |
| 2   | B     | 0.56         | 0/1063  | 1.03        | 4/1429 (0.3%)   |
| 2   | D     | 0.56         | 0/1071  | 1.03        | 4/1440 (0.3%)   |
| 3   | E     | 0.53         | 0/1714  | 0.88        | 0/2335          |
| 3   | H     | 0.53         | 0/1720  | 0.88        | 1/2343 (0.0%)   |
| 4   | F     | 0.52         | 0/1648  | 0.88        | 0/2250          |
| 4   | L     | 0.52         | 0/1654  | 0.88        | 0/2258          |
| All | All   | 0.66         | 0/14106 | 1.09        | 54/19161 (0.3%) |

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | B     | 409 | ASN  | N-CA-C | 8.63 | 122.31      | 111.69   |
| 2   | D     | 409 | ASN  | N-CA-C | 8.59 | 122.26      | 111.69   |
| 1   | C     | 90  | VAL  | N-CA-C | 7.86 | 121.25      | 108.99   |
| 1   | A     | 90  | VAL  | N-CA-C | 7.82 | 121.19      | 108.99   |
| 1   | C     | 50  | ARG  | N-CA-C | 7.74 | 120.67      | 108.67   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2560  | 0        | 2559     | 206     | 0            |
| 1   | C     | 2560  | 0        | 2559     | 197     | 0            |
| 2   | B     | 1054  | 0        | 1043     | 66      | 0            |
| 2   | D     | 1062  | 0        | 1054     | 59      | 0            |
| 3   | E     | 1673  | 0        | 1633     | 52      | 0            |
| 3   | H     | 1679  | 0        | 1638     | 53      | 0            |
| 4   | F     | 1606  | 0        | 1541     | 33      | 0            |
| 4   | L     | 1612  | 0        | 1546     | 31      | 0            |
| 5   | G     | 28    | 0        | 25       | 1       | 0            |
| 5   | I     | 28    | 0        | 25       | 0       | 0            |
| 5   | J     | 28    | 0        | 25       | 0       | 0            |
| 5   | N     | 28    | 0        | 25       | 0       | 0            |
| 5   | O     | 28    | 0        | 25       | 0       | 0            |
| 5   | P     | 28    | 0        | 25       | 5       | 0            |
| 6   | K     | 39    | 0        | 34       | 3       | 0            |
| 6   | M     | 39    | 0        | 34       | 1       | 0            |
| 7   | A     | 14    | 0        | 13       | 0       | 0            |
| 7   | C     | 14    | 0        | 13       | 0       | 0            |
| All | All   | 14080 | 0        | 13817    | 575     | 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 21.

The worst 5 of 575 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:C:214:ALA:HB2 | 1:C:248:MET:CE  | 1.62                     | 1.29              |
| 1:A:214:ALA:HB2 | 1:A:248:MET:CE  | 1.62                     | 1.27              |
| 1:A:214:ALA:HB2 | 1:A:248:MET:HE3 | 1.16                     | 1.15              |
| 1:C:214:ALA:HB2 | 1:C:248:MET:HE3 | 1.16                     | 1.14              |
| 1:A:20:THR:CG2  | 2:B:452:GLU:HG3 | 1.78                     | 1.13              |

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     | 331/347 (95%)   | 303 (92%)  | 22 (7%) | 6 (2%)   | 6           | 33  |
| 1   | C     | 331/347 (95%)   | 303 (92%)  | 22 (7%) | 6 (2%)   | 6           | 33  |
| 2   | B     | 133/179 (74%)   | 128 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 2   | D     | 134/179 (75%)   | 129 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 3   | E     | 214/234 (92%)   | 202 (94%)  | 11 (5%) | 1 (0%)   | 24          | 63  |
| 3   | H     | 215/234 (92%)   | 203 (94%)  | 11 (5%) | 1 (0%)   | 24          | 63  |
| 4   | F     | 209/216 (97%)   | 202 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 4   | L     | 210/216 (97%)   | 203 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| All | All   | 1777/1952 (91%) | 1673 (94%) | 90 (5%) | 14 (1%)  | 16          | 53  |

5 of 14 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 177 | ILE  |
| 1   | A     | 251 | LYS  |
| 1   | C     | 177 | ILE  |
| 1   | C     | 251 | LYS  |
| 1   | A     | 148 | ASN  |

### 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     | 284/294 (97%) | 271 (95%) | 13 (5%)  | 24          | 45 |
| 1   | C     | 284/294 (97%) | 272 (96%) | 12 (4%)  | 26          | 48 |
| 2   | B     | 116/143 (81%) | 112 (97%) | 4 (3%)   | 32          | 54 |
| 2   | D     | 117/143 (82%) | 113 (97%) | 4 (3%)   | 32          | 54 |
| 3   | E     | 185/198 (93%) | 176 (95%) | 9 (5%)   | 22          | 43 |
| 3   | H     | 186/198 (94%) | 177 (95%) | 9 (5%)   | 23          | 44 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 4   | F     | 180/183 (98%)   | 175 (97%)  | 5 (3%)   | 38 59       |
| 4   | L     | 181/183 (99%)   | 177 (98%)  | 4 (2%)   | 45 64       |
| All | All   | 1533/1636 (94%) | 1473 (96%) | 60 (4%)  | 28 49       |

5 of 60 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 295 | GLU  |
| 3   | H     | 183 | THR  |
| 3   | E     | 94  | ARG  |
| 3   | H     | 178 | LEU  |
| 4   | L     | 129 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 398 | ASN  |
| 3   | E     | 39  | GLN  |
| 2   | D     | 422 | ASN  |
| 3   | E     | 171 | GLN  |
| 2   | B     | 398 | 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 ⓘ

18 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  | G     | 1   | 1,5  | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.96 | 1 (5%)      |
| 5   | NAG  | G     | 2   | 5    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.88 | 1 (5%)      |
| 5   | NAG  | I     | 1   | 1,5  | 14,14,15     | 0.39 | 0           | 17,19,21    | 1.82 | 3 (17%)     |
| 5   | NAG  | I     | 2   | 5    | 14,14,15     | 0.43 | 0           | 17,19,21    | 1.29 | 3 (17%)     |
| 5   | NAG  | J     | 1   | 1,5  | 14,14,15     | 0.54 | 0           | 17,19,21    | 0.97 | 1 (5%)      |
| 5   | NAG  | J     | 2   | 5    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.88 | 1 (5%)      |
| 6   | NAG  | K     | 1   | 6,1  | 14,14,15     | 0.50 | 0           | 17,19,21    | 2.28 | 3 (17%)     |
| 6   | NAG  | K     | 2   | 6    | 14,14,15     | 0.50 | 0           | 17,19,21    | 1.35 | 3 (17%)     |
| 6   | BMA  | K     | 3   | 6    | 11,11,12     | 0.66 | 0           | 15,15,17    | 1.43 | 3 (20%)     |
| 6   | NAG  | M     | 1   | 6,1  | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.95 | 1 (5%)      |
| 6   | NAG  | M     | 2   | 6    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.88 | 1 (5%)      |
| 6   | BMA  | M     | 3   | 6    | 11,11,12     | 0.57 | 0           | 15,15,17    | 0.75 | 0           |
| 5   | NAG  | N     | 1   | 1,5  | 14,14,15     | 0.39 | 0           | 17,19,21    | 1.82 | 3 (17%)     |
| 5   | NAG  | N     | 2   | 5    | 14,14,15     | 0.42 | 0           | 17,19,21    | 1.29 | 3 (17%)     |
| 5   | NAG  | O     | 1   | 1,5  | 14,14,15     | 0.52 | 0           | 17,19,21    | 0.96 | 1 (5%)      |
| 5   | NAG  | O     | 2   | 5    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.87 | 1 (5%)      |
| 5   | NAG  | P     | 1   | 1,5  | 14,14,15     | 0.51 | 0           | 17,19,21    | 2.28 | 3 (17%)     |
| 5   | NAG  | P     | 2   | 5    | 14,14,15     | 0.49 | 0           | 17,19,21    | 1.34 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | NAG  | G     | 1   | 1,5  | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | G     | 2   | 5    | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | I     | 1   | 1,5  | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | I     | 2   | 5    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | J     | 1   | 1,5  | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | J     | 2   | 5    | -       | 3/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 1   | 6,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | BMA  | K     | 3   | 6    | -       | 2/2/19/22 | 0/1/1/1 |

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

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | P     | 1   | NAG  | O5-C1-C2 | -7.54 | 99.63       | 111.29   |
| 6   | K     | 1   | NAG  | O5-C1-C2 | -7.53 | 99.64       | 111.29   |
| 5   | I     | 1   | NAG  | C1-O5-C5 | 6.01  | 120.24      | 112.19   |
| 5   | N     | 1   | NAG  | C1-O5-C5 | 5.99  | 120.21      | 112.19   |
| 5   | J     | 1   | NAG  | C1-O5-C5 | 3.23  | 116.52      | 112.19   |

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | I     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | N     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | I     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | N     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | N     | 1   | NAG  | O5-C5-C6-O6 |

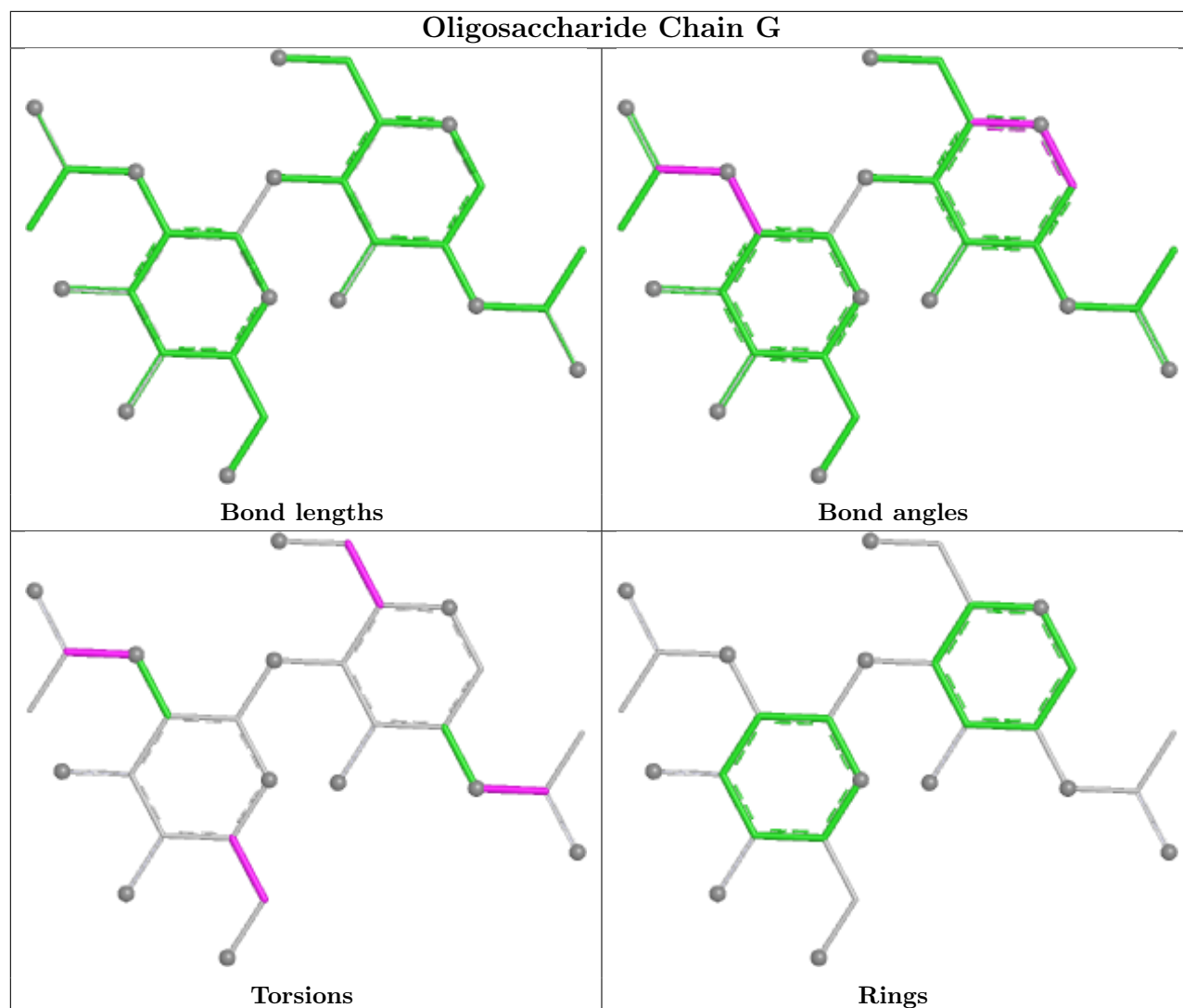
There are no ring outliers.

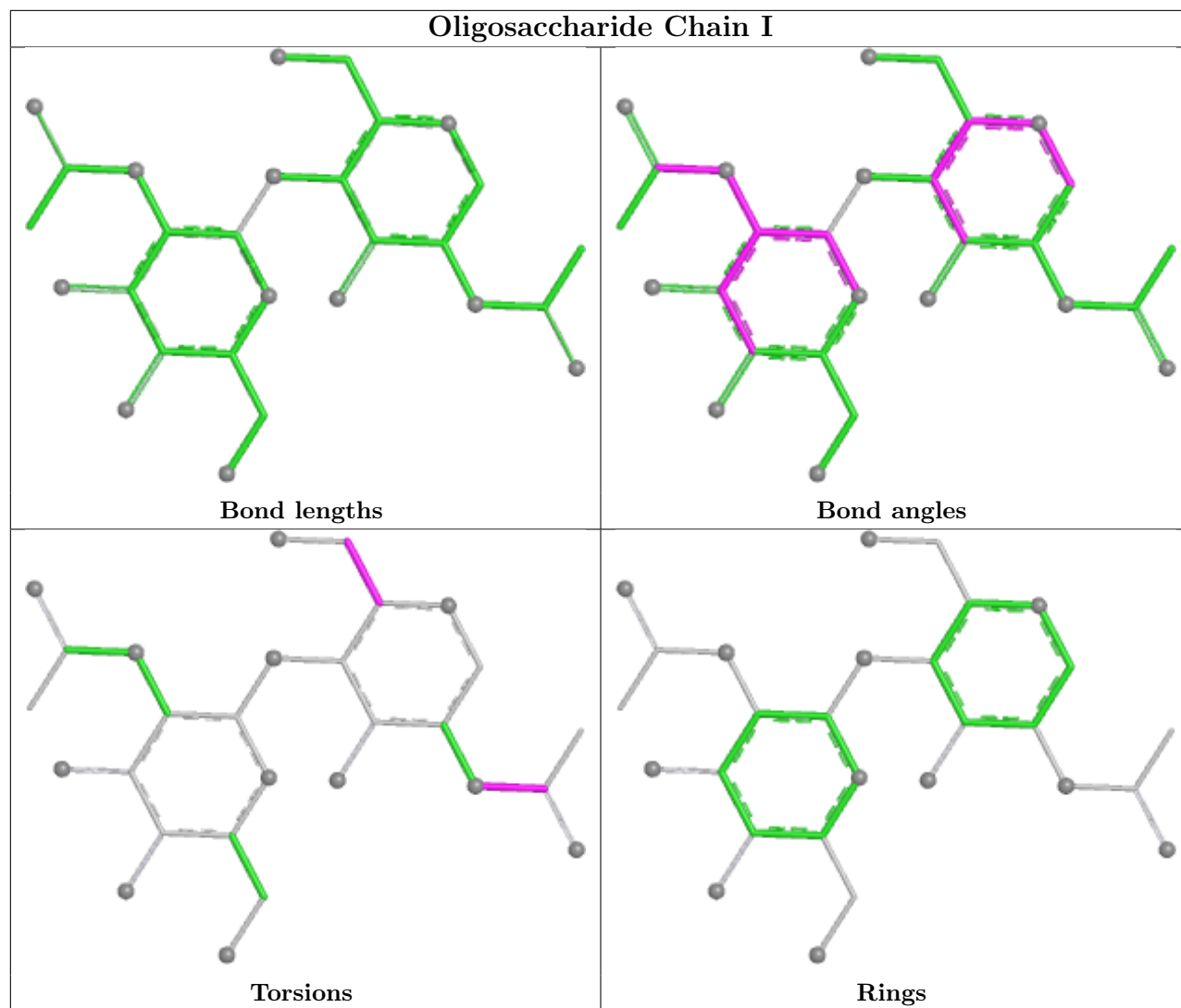
4 monomers are involved in 10 short contacts:

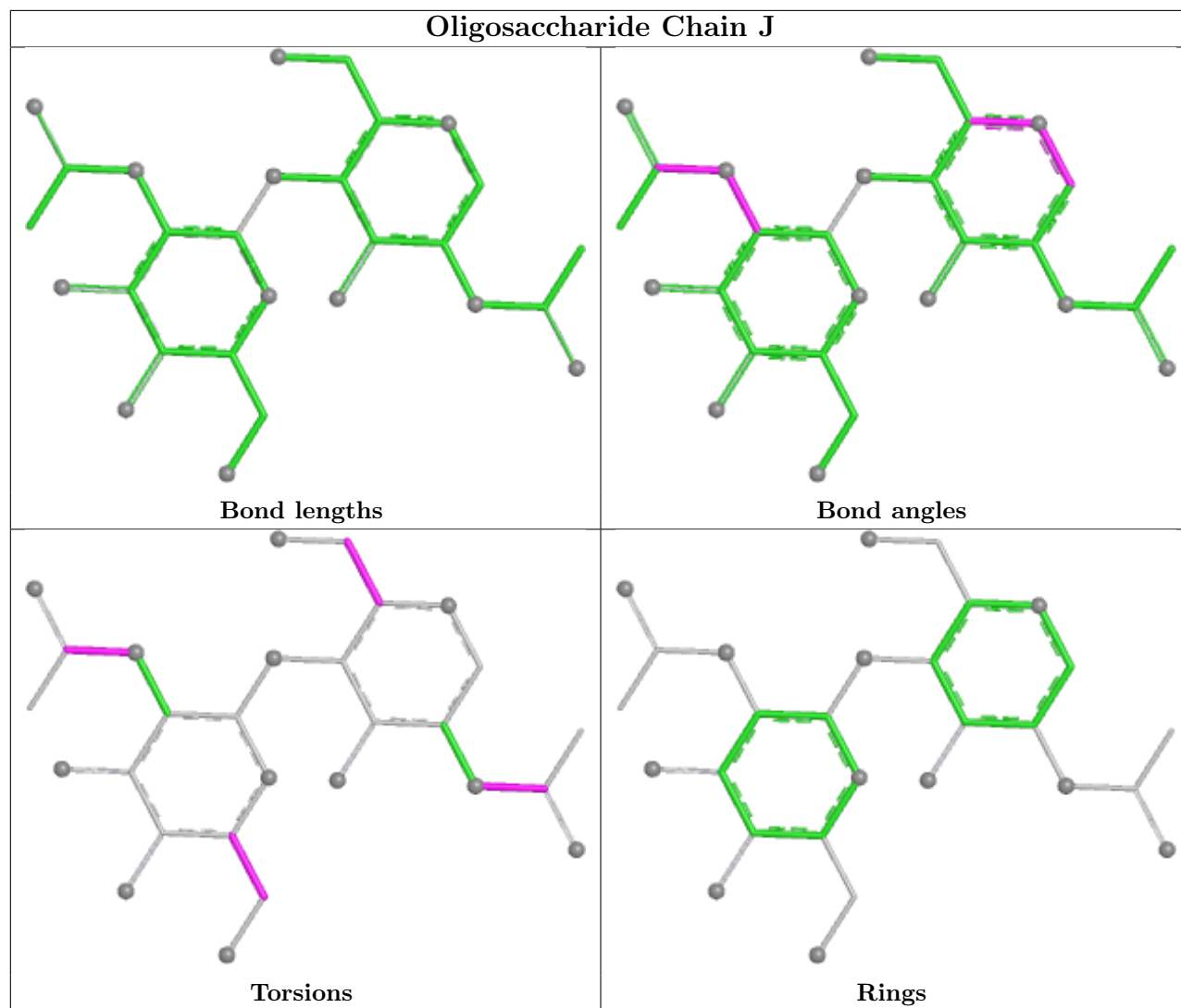
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | K     | 1   | NAG  | 3       | 0            |
| 6   | M     | 1   | NAG  | 1       | 0            |
| 5   | G     | 1   | NAG  | 1       | 0            |
| 5   | P     | 1   | NAG  | 5       | 0            |

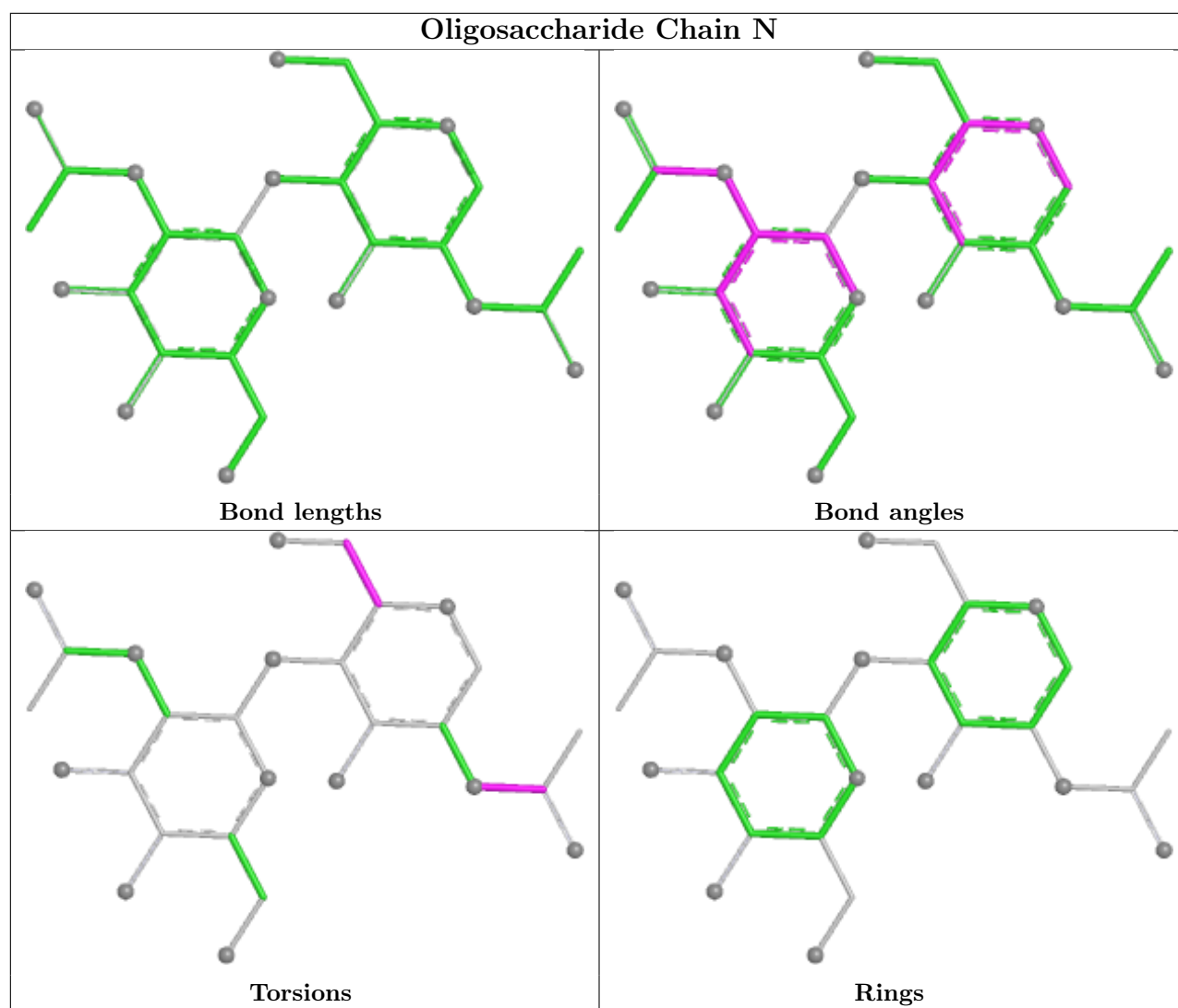
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

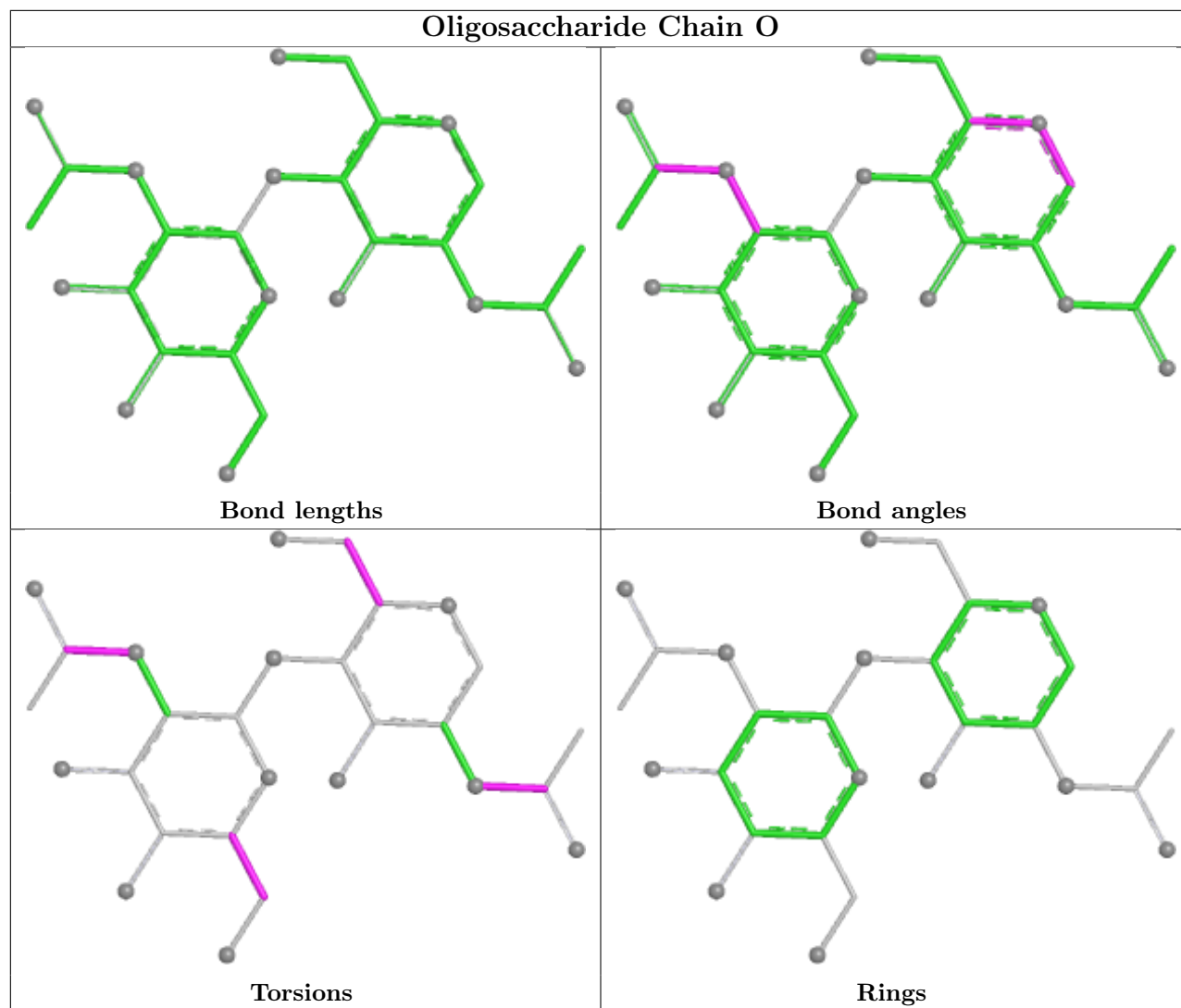
bond angles, torsion angles, and ring geometry for oligosaccharide.

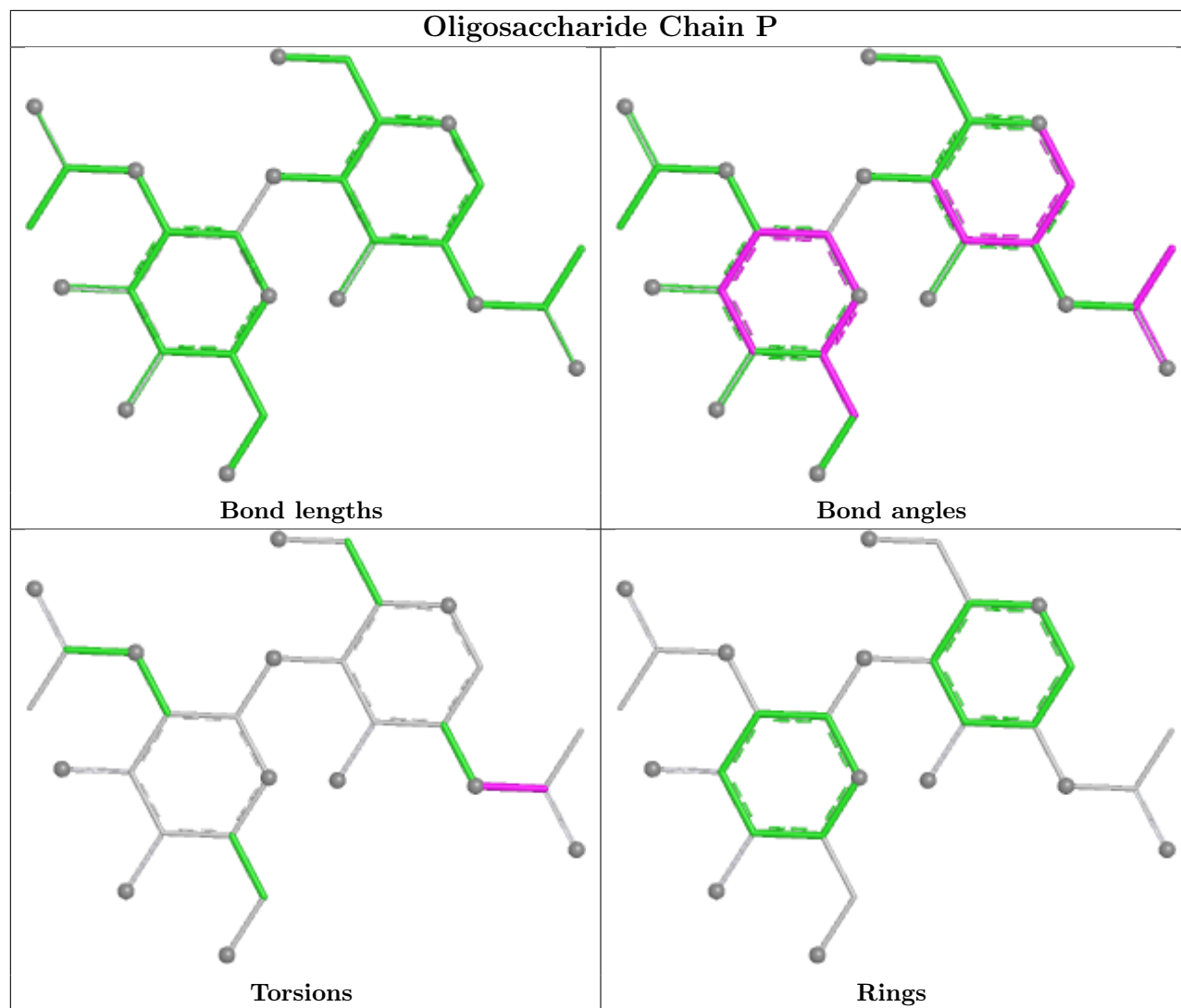


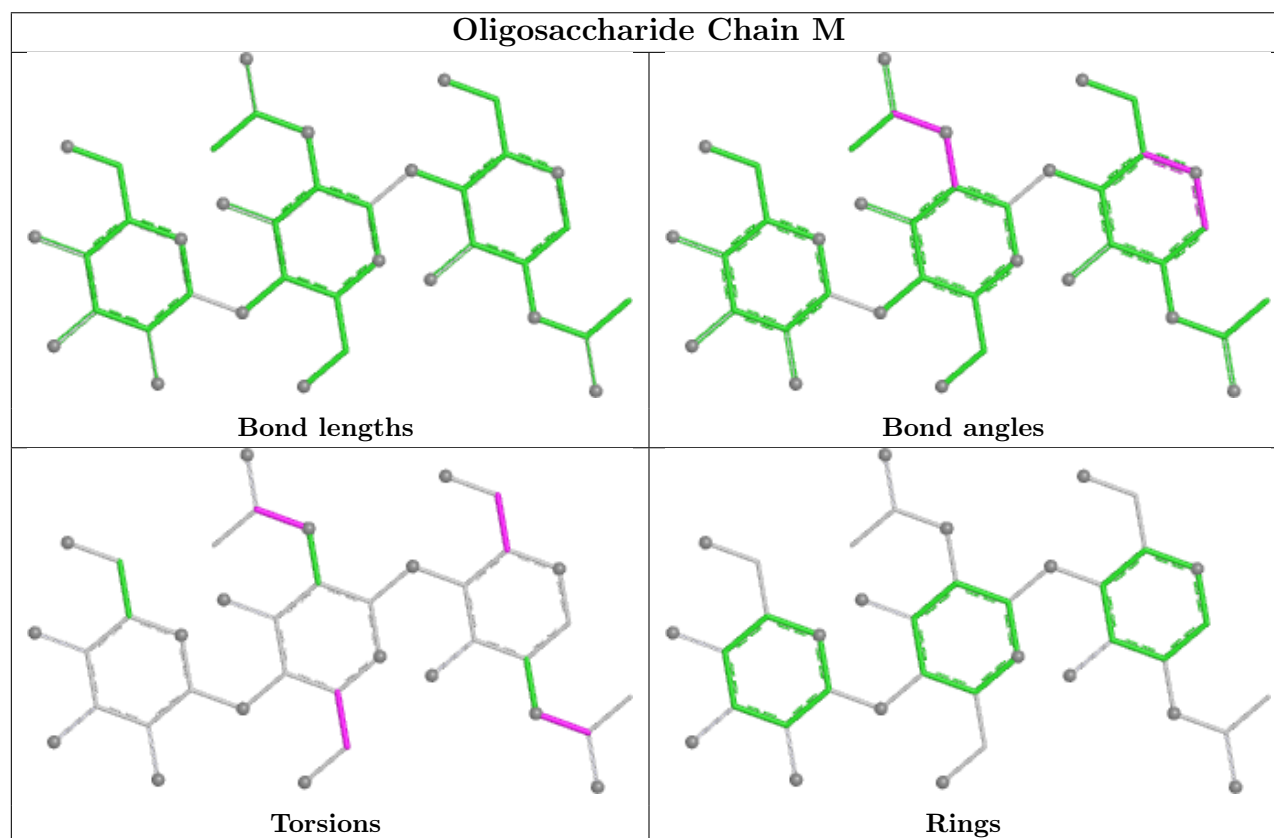
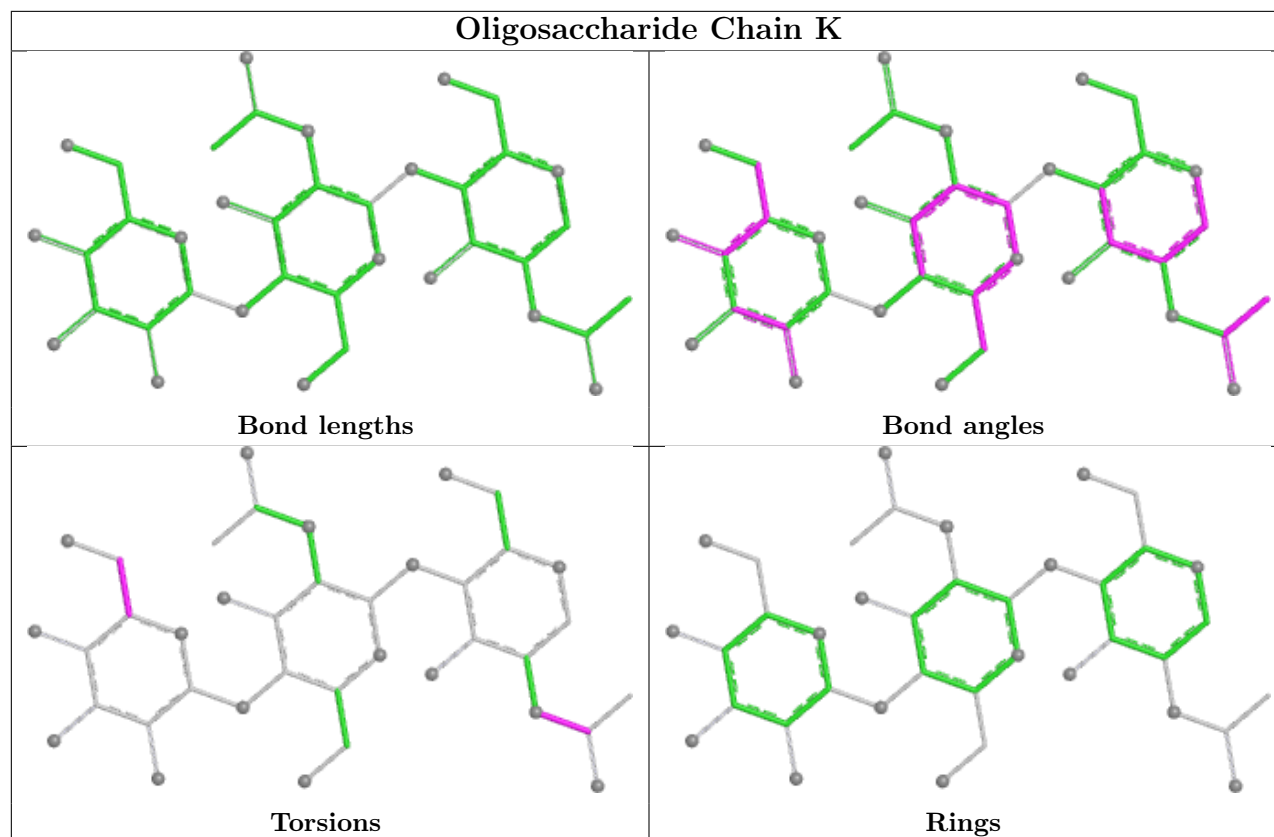












## 5.6 Ligand geometry

2 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$ |
| 7   | NAG  | C     | 410 | 1    | 14,14,15     | 0.49 | 0           | 17,19,21    | 0.93 | 1 (5%)      |
| 7   | NAG  | A     | 410 | 1    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.93 | 1 (5%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7   | NAG  | C     | 410 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | A     | 410 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 7   | A     | 410 | NAG  | C1-O5-C5 | 2.49 | 115.53      | 112.19   |
| 7   | C     | 410 | NAG  | C1-O5-C5 | 2.49 | 115.52      | 112.19   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 7   | A     | 410 | NAG  | C8-C7-N2-C2 |
| 7   | C     | 410 | NAG  | C8-C7-N2-C2 |
| 7   | C     | 410 | NAG  | O7-C7-N2-C2 |
| 7   | A     | 410 | NAG  | O7-C7-N2-C2 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 337/347 (97%)   | -0.03  | 7 (2%) 63 54  | 100, 100, 100, 100    | 0     |
| 1   | C     | 337/347 (97%)   | 0.07   | 9 (2%) 56 48  | 100, 100, 100, 100    | 0     |
| 2   | B     | 139/179 (77%)   | -0.12  | 2 (1%) 73 62  | 100, 100, 100, 100    | 0     |
| 2   | D     | 140/179 (78%)   | -0.12  | 5 (3%) 46 42  | 100, 100, 100, 100    | 0     |
| 3   | E     | 220/234 (94%)   | -0.04  | 3 (1%) 73 62  | 100, 100, 100, 100    | 0     |
| 3   | H     | 221/234 (94%)   | -0.04  | 3 (1%) 73 62  | 100, 100, 100, 100    | 0     |
| 4   | F     | 213/216 (98%)   | -0.17  | 6 (2%) 55 47  | 100, 100, 100, 100    | 0     |
| 4   | L     | 214/216 (99%)   | -0.20  | 2 (0%) 81 69  | 100, 100, 100, 100    | 0     |
| All | All   | 1821/1952 (93%) | -0.06  | 37 (2%) 65 55 | 100, 100, 100, 100    | 0     |

The worst 5 of 37 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | E     | 190 | GLY  | 8.2  |
| 4   | L     | 123 | GLU  | 5.2  |
| 1   | A     | 299 | GLY  | 4.2  |
| 3   | E     | 191 | THR  | 3.8  |
| 1   | C     | 222 | VAL  | 3.6  |

### 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](#)

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,

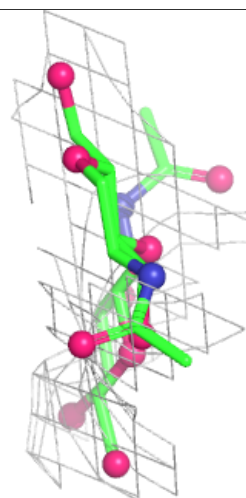
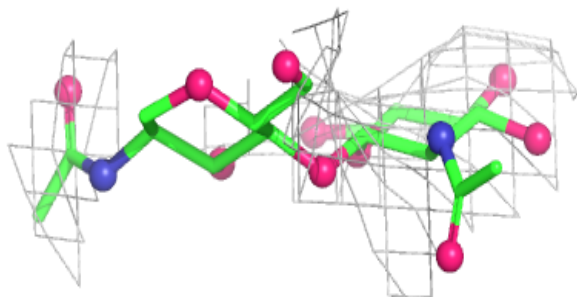
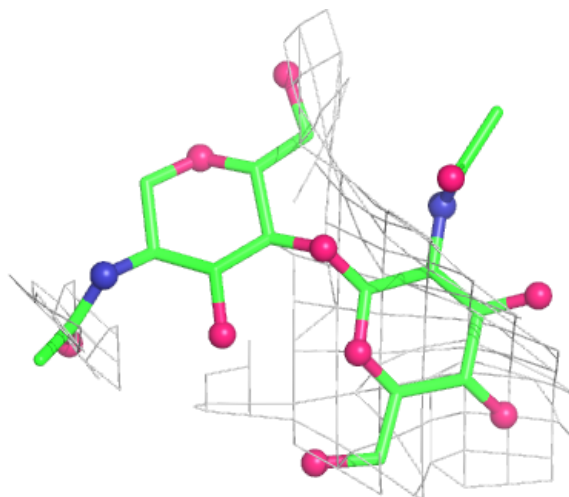
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 5   | NAG  | G     | 1   | 14/15 | -    | -    | 100,100,100,100            | 0     |
| 5   | NAG  | G     | 2   | 14/15 | -    | -    | 100,100,100,100            | 0     |
| 5   | NAG  | P     | 2   | 14/15 | 0.91 | 0.07 | 100,100,100,100            | 0     |
| 6   | NAG  | K     | 2   | 14/15 | 0.94 | 0.08 | 100,100,100,100            | 0     |
| 5   | NAG  | O     | 2   | 14/15 | 0.95 | 0.10 | 100,100,100,100            | 0     |
| 5   | NAG  | P     | 1   | 14/15 | 0.95 | 0.09 | 100,100,100,100            | 0     |
| 6   | BMA  | M     | 3   | 11/12 | 0.96 | 0.07 | 100,100,100,100            | 0     |
| 5   | NAG  | N     | 2   | 14/15 | 0.97 | 0.07 | 100,100,100,100            | 0     |
| 5   | NAG  | N     | 1   | 14/15 | 0.97 | 0.07 | 100,100,100,100            | 0     |
| 5   | NAG  | O     | 1   | 14/15 | 0.98 | 0.09 | 100,100,100,100            | 0     |
| 6   | NAG  | K     | 1   | 14/15 | 0.98 | 0.07 | 100,100,100,100            | 0     |
| 5   | NAG  | I     | 2   | 14/15 | 0.98 | 0.10 | 100,100,100,100            | 0     |
| 6   | NAG  | M     | 2   | 14/15 | 0.98 | 0.11 | 100,100,100,100            | 0     |
| 5   | NAG  | J     | 1   | 14/15 | 0.98 | 0.11 | 100,100,100,100            | 0     |
| 6   | BMA  | K     | 3   | 11/12 | -    | -    | 100,100,100,100            | 0     |
| 6   | NAG  | M     | 1   | 14/15 | 0.99 | 0.05 | 100,100,100,100            | 0     |
| 5   | NAG  | I     | 1   | 14/15 | 0.99 | 0.05 | 100,100,100,100            | 0     |
| 5   | NAG  | J     | 2   | 14/15 | 0.99 | 0.06 | 100,100,100,100            | 0     |

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

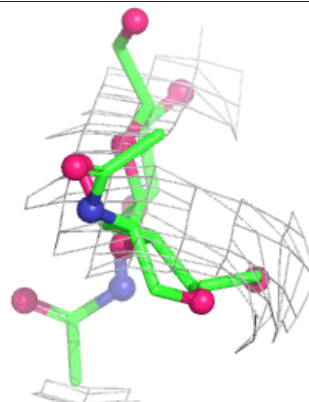
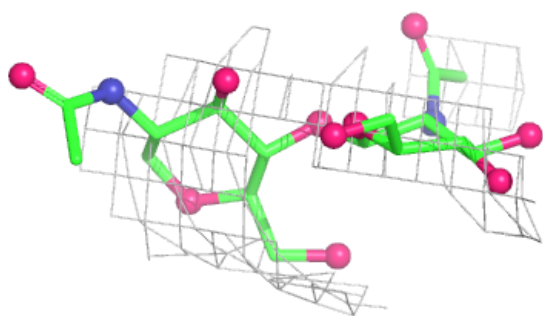
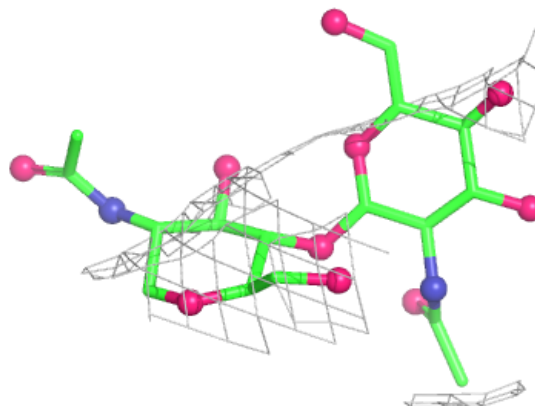
**Electron density around Chain G:**

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

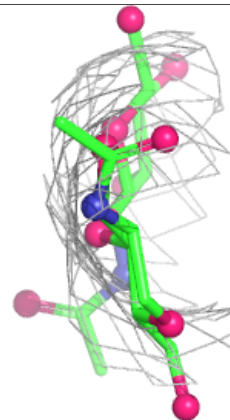
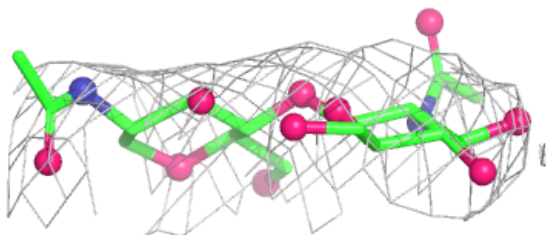
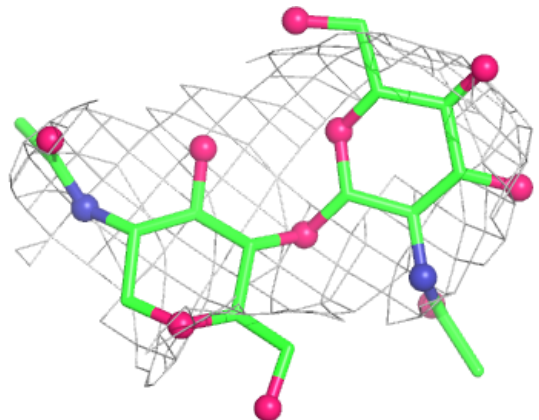


**Electron density around Chain I:**

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

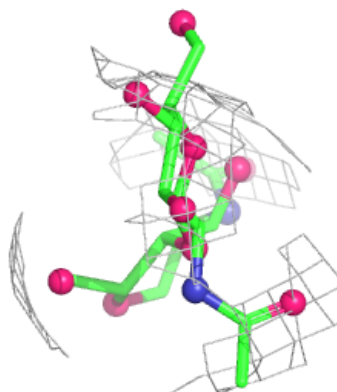
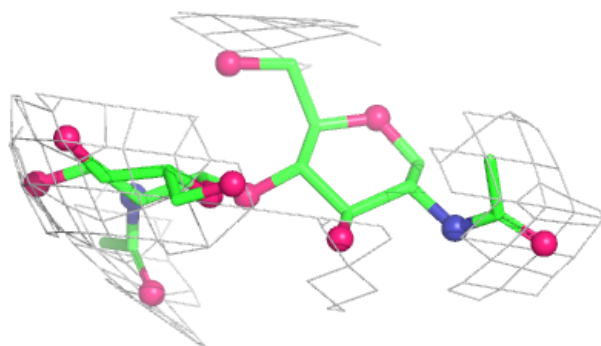
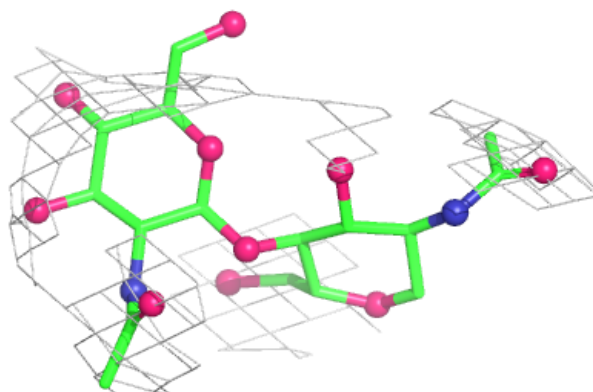
**Electron density around Chain J:**

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

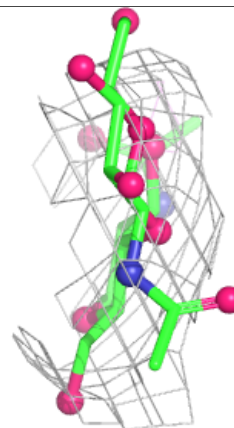
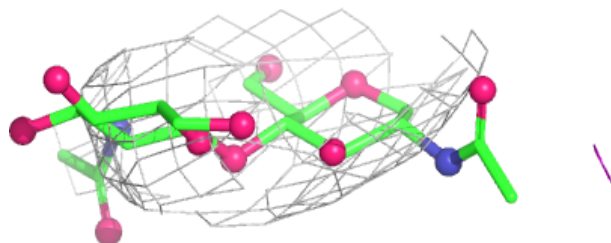
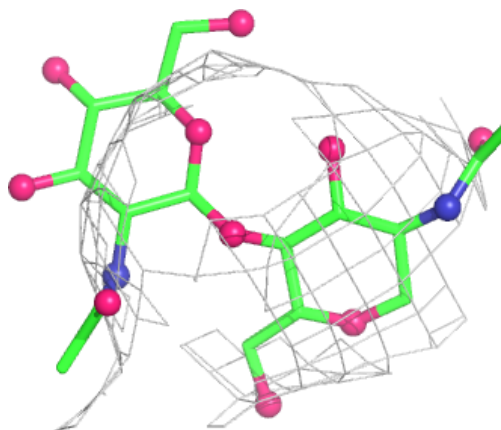


**Electron density around Chain N:**

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

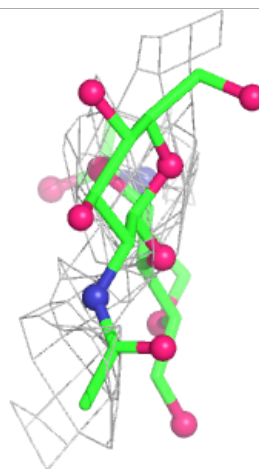
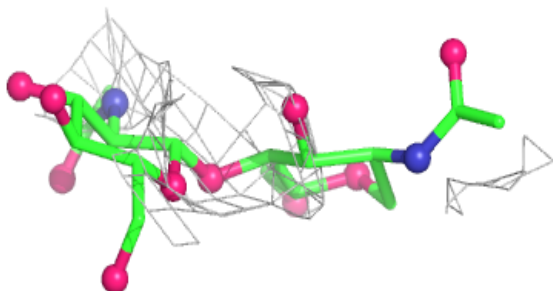
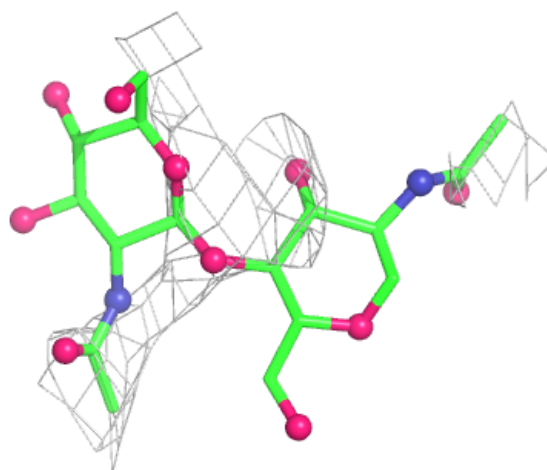
**Electron density around Chain O:**

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



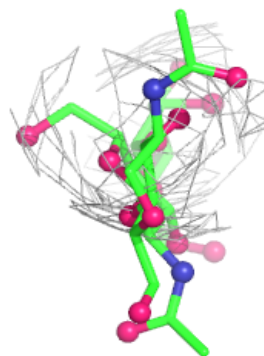
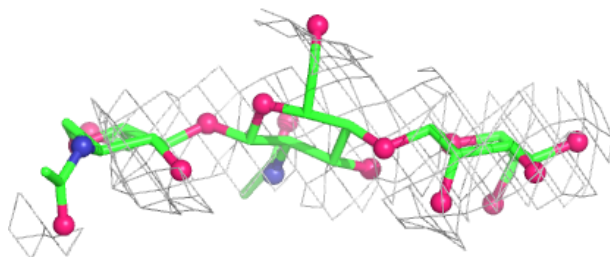
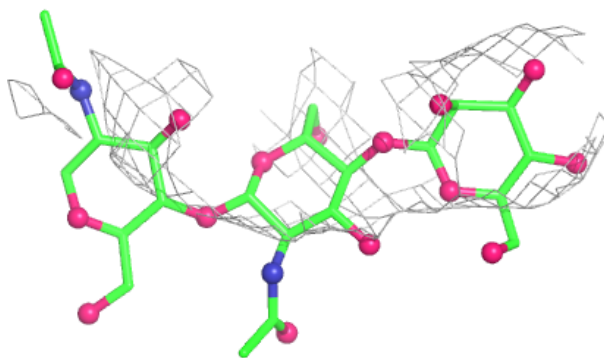
**Electron density around Chain P:**

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

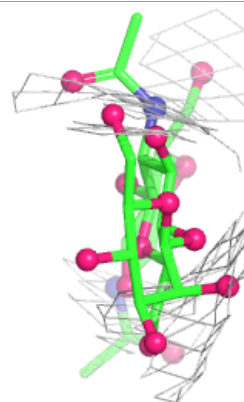
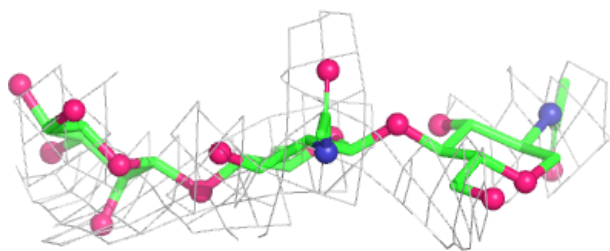
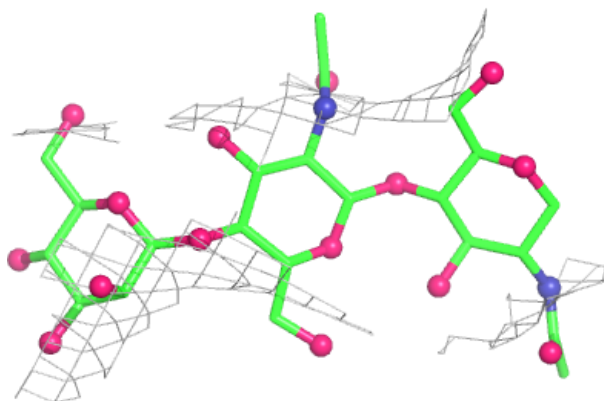


**Electron density around Chain K:**

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

**Electron density around Chain M:**

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



## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 7   | NAG  | A     | 410 | 14/15 | 0.96 | 0.11 | 100,100,100,100             | 0     |
| 7   | NAG  | C     | 410 | 14/15 | 0.98 | 0.09 | 100,100,100,100             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.