



wwPDB X-ray Structure Validation Summary Report

Aug 18, 2022 – 01:10 pm BST

PDB ID : 7PYE
Title : Structure of LPMO in complex with cellotetraose at 5.99×10^4 Gy
Authors : Tandrup, T.; Lo Leggio, L.
Deposited on : 2021-10-10
Resolution : 2.10 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

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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

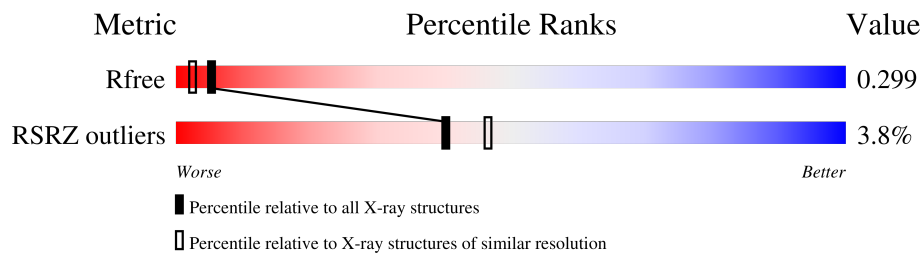
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---------------|-----------------------------|---|
| R_{free} | 130704 | 5197 (2.10-2.10) |
| RSRZ outliers | 127900 | 5083 (2.10-2.10) |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 2011 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 Auxiliary activity 9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 235 | 1821 | 1150 | 310 | 358 | 3 | 0 | 7 | 0 |

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



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| | | | Total | C | O | | | |
| 2 | B | 4 | 45 | 24 | 21 | 0 | 0 | 0 |

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| | | | Total | Cl | | |
| 5 | A | 1 | 1 | 1 | 0 | 0 |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| | | | Total | O | | |
| 6 | A | 129 | 129 | 129 | 0 | 0 |

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3 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 3 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 125.65Å 125.65Å 125.65Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 44.46 – 2.10 44.42 – 2.10 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (44.46-2.10) 100.0 (44.42-2.10) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.53 (at 2.10Å) | Xtriage |
| Refinement program | REFMAC 5.8.0267 | Depositor |
| R, R_{free} | 0.239 , 0.294 0.246 , 0.299 | Depositor DCC |
| R_{free} test set | 1050 reflections (5.15%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 41.5 | Xtriage |
| Anisotropy | 0.000 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | (Not available) , (Not available) | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 2011 | wwPDB-VP |
| Average B, all atoms (Å ²) | 45.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

1 non-standard protein/DNA/RNA residue is 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 | $\# Z > 2$ |
| 1 | HIC | A | 1 | 3,1 | 8,11,12 | 0.87 | 0 | 6,14,16 | 0.95 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | HIC | A | 1 | 3,1 | - | 0/5/6/8 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates i

4 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | BGC | B | 1 | 2 | 12,12,12 | 0.54 | 0 | 17,17,17 | 1.54 | 5 (29%) |
| 2 | BGC | B | 2 | 2 | 11,11,12 | 0.47 | 0 | 15,15,17 | 1.52 | 3 (20%) |
| 2 | BGC | B | 3 | 2 | 11,11,12 | 1.19 | 2 (18%) | 15,15,17 | 1.51 | 3 (20%) |
| 2 | BGC | B | 4 | 2 | 11,11,12 | 0.32 | 0 | 15,15,17 | 1.42 | 2 (13%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | BGC | B | 1 | 2 | - | 2/2/22/22 | 0/1/1/1 |
| 2 | BGC | B | 2 | 2 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | BGC | B | 3 | 2 | - | 2/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | BGC | B | 4 | 2 | - | 0/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | B | 3 | BGC | O5-C1 | -2.06 | 1.40 | 1.43 |
| 2 | B | 3 | BGC | C2-C3 | -2.06 | 1.49 | 1.52 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 3 | BGC | C1-C2-C3 | -3.18 | 105.75 | 109.67 |
| 2 | B | 2 | BGC | C1-C2-C3 | 3.03 | 113.39 | 109.67 |
| 2 | B | 4 | BGC | O2-C2-C3 | -2.98 | 104.16 | 110.14 |
| 2 | B | 3 | BGC | O5-C1-C2 | -2.97 | 106.18 | 110.77 |
| 2 | B | 2 | BGC | C1-O5-C5 | 2.86 | 116.07 | 112.19 |

There are no chirality outliers.

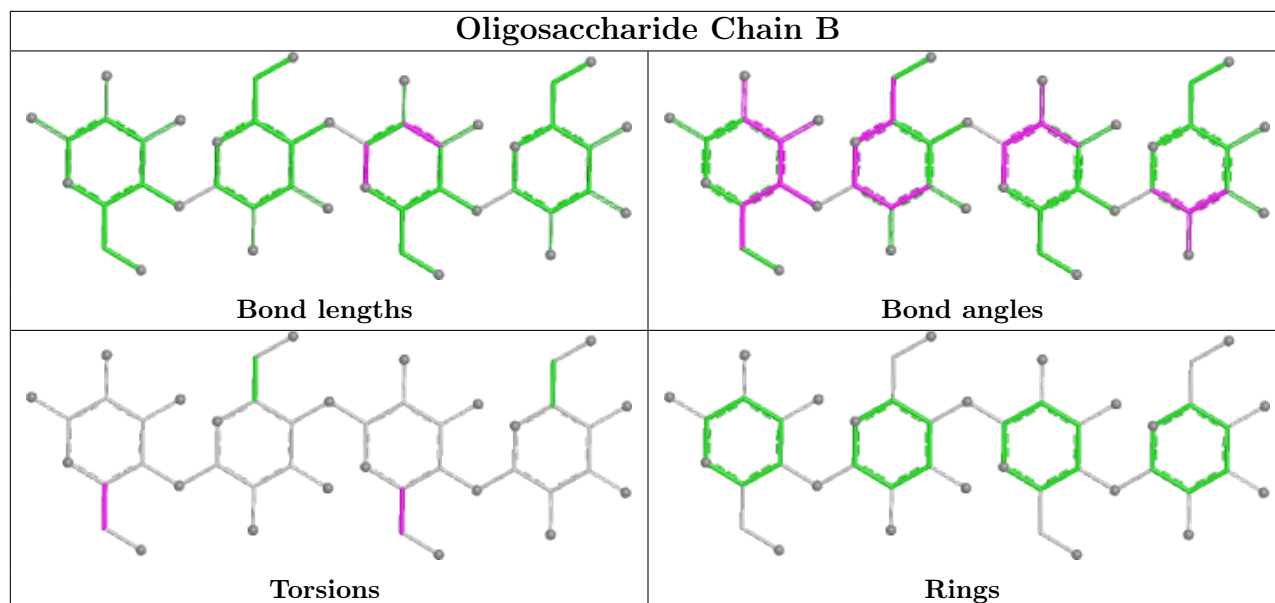
All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | B | 1 | BGC | C4-C5-C6-O6 |
| 2 | B | 1 | BGC | O5-C5-C6-O6 |
| 2 | B | 3 | BGC | O5-C5-C6-O6 |
| 2 | B | 3 | BGC | C4-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

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



4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | A | 302 | 1 | 14,14,15 | 0.48 | 0 | 17,19,21 | 1.34 | 2 (11%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | NAG | A | 302 | 1 | - | 0/6/23/26 | 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(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4 | A | 302 | NAG | C1-C2-N2 | -3.59 | 104.36 | 110.49 |
| 4 | A | 302 | NAG | O5-C5-C4 | -2.31 | 105.20 | 110.83 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

5.1 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, 95th 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 ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1 | A | 234/235 (99%) | 0.33 | 9 (3%) 40 46 | 29, 44, 61, 85 | 0 |

The worst 5 of 9 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 109 | THR | 4.0 |
| 1 | A | 111 | SER | 3.3 |
| 1 | A | 206 | PRO | 3.1 |
| 1 | A | 108 | VAL | 2.9 |
| 1 | A | 110 | ASN | 2.8 |

5.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1 | HIC | A | 1 | 11/12 | 0.89 | 0.16 | 36,40,42,42 | 0 |

5.3 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, 95th 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.

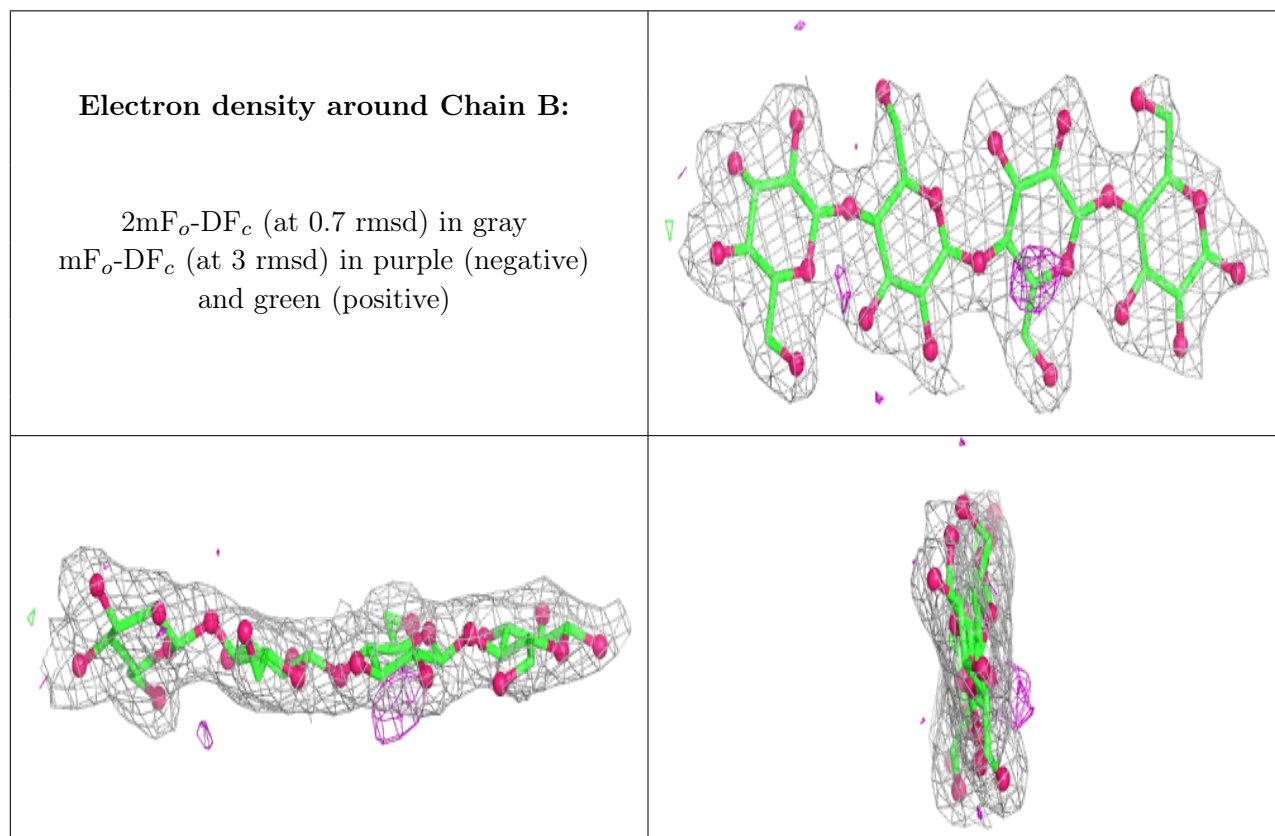
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2 | BGC | B | 2 | 11/12 | 0.87 | 0.13 | 39,47,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | BGC | B | 4 | 11/12 | 0.92 | 0.11 | 38,42,47,50 | 0 |
| 2 | BGC | B | 1 | 12/12 | 0.94 | 0.15 | 46,56,66,68 | 0 |
| 2 | BGC | B | 3 | 11/12 | 0.95 | 0.13 | 38,43,50,61 | 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.



5.4 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, 95th 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.

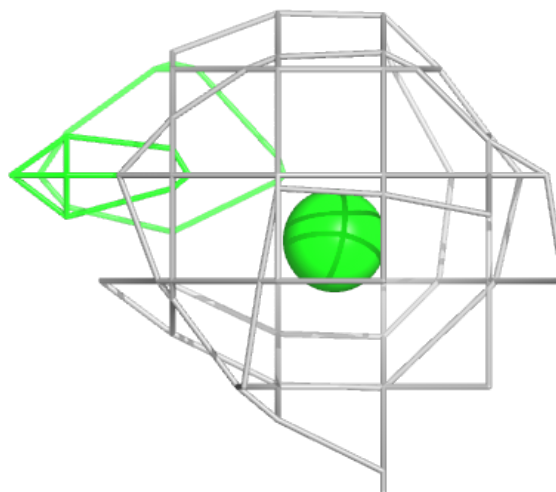
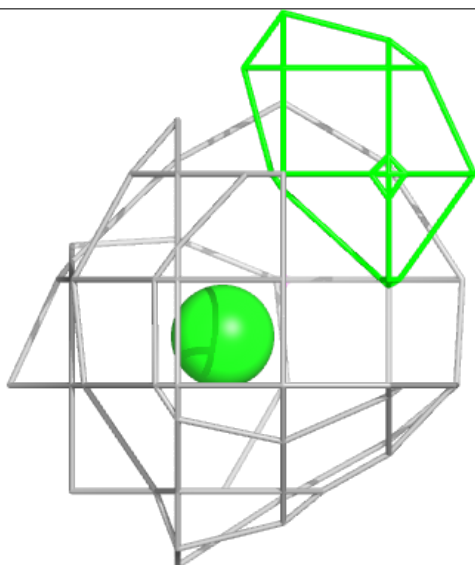
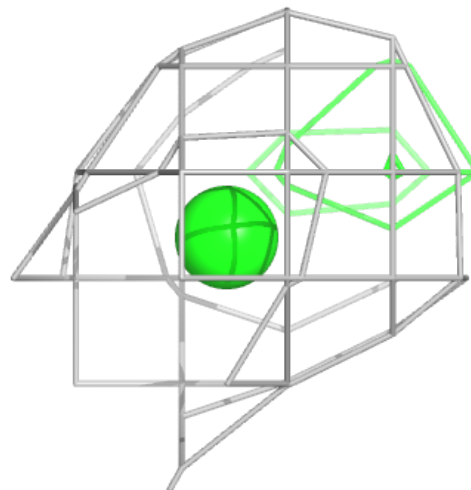
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | NAG | A | 302 | 14/15 | 0.86 | 0.21 | 46,58,67,69 | 0 |
| 5 | CL | A | 303 | 1/1 | 0.96 | 0.10 | 58,58,58,58 | 0 |
| 3 | CU | A | 301 | 1/1 | 0.99 | 0.08 | 43,43,43,43 | 0 |

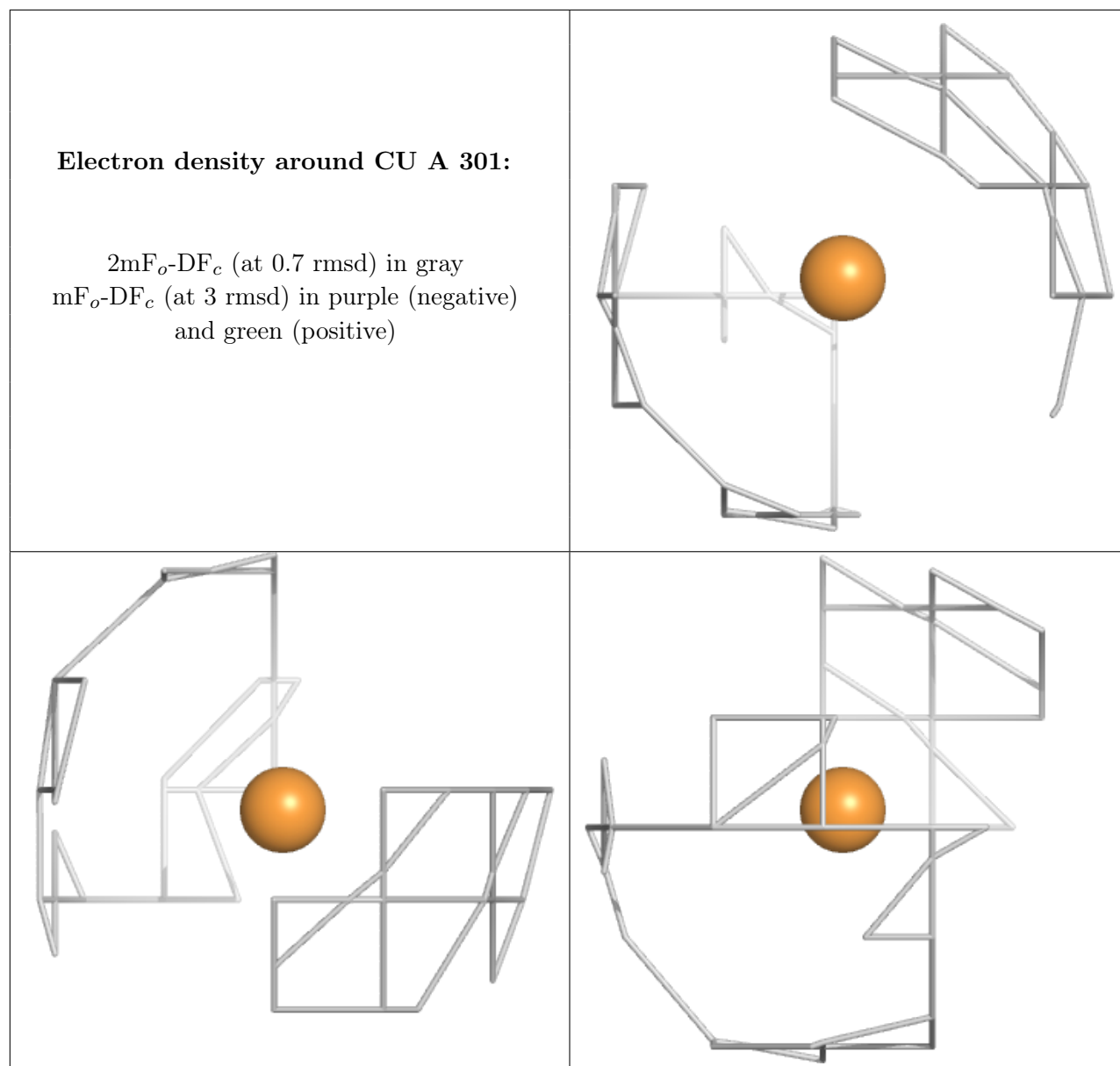
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CL A 303:

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





5.5 Other polymers [i](#)

There are no such residues in this entry.