



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 05:30 PM BST

PDB ID : 4TZ5  
Title : Ensemble refinement of the E502A variant of sacteLam55A from *Streptomyces* sp. SirexAA-E in complex with laminarihexaose  
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.  
Deposited on : 2014-07-09  
Resolution : 1.75 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

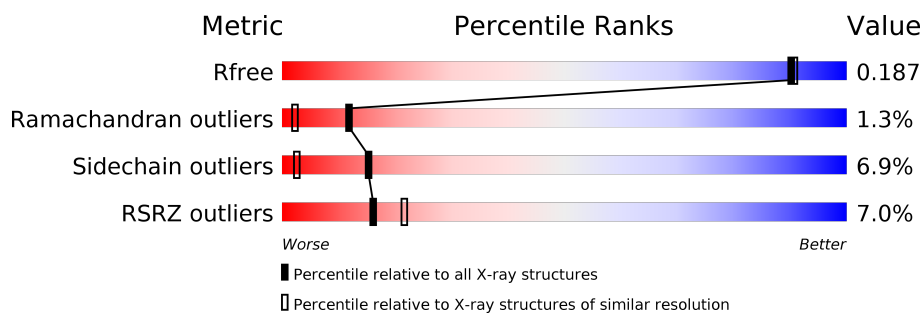
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2340 (1.76-1.76)                                      |
| Ramachandran outliers | 138981                      | 2437 (1.76-1.76)                                      |
| Sidechain outliers    | 138945                      | 2437 (1.76-1.76)                                      |
| RSRZ outliers         | 127900                      | 2298 (1.76-1.76)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 1-A   | 549    | <div> <div>7%</div> <div>91%</div> <div>9%</div> </div> |
| 1   | 1-B   | 549    | <div> <div>8%</div> <div>92%</div> <div>7%</div> </div> |
| 1   | 10-A  | 549    | <div> <div>7%</div> <div>92%</div> <div>7%</div> </div> |
| 1   | 10-B  | 549    | <div> <div>8%</div> <div>92%</div> <div>6%</div> </div> |
| 1   | 11-A  | 549    | <div> <div>7%</div> <div>94%</div> <div>5%</div> </div> |
| 1   | 11-B  | 549    | <div> <div>8%</div> <div>93%</div> <div>7%</div> </div> |
| 1   | 12-A  | 549    | <div> <div>7%</div> <div>91%</div> <div>9%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 12-B  | 549    |                  |
| 1   | 13-A  | 549    |                  |
| 1   | 13-B  | 549    |                  |
| 1   | 14-A  | 549    |                  |
| 1   | 14-B  | 549    |                  |
| 1   | 15-A  | 549    |                  |
| 1   | 15-B  | 549    |                  |
| 1   | 16-A  | 549    |                  |
| 1   | 16-B  | 549    |                  |
| 1   | 17-A  | 549    |                  |
| 1   | 17-B  | 549    |                  |
| 1   | 18-A  | 549    |                  |
| 1   | 18-B  | 549    |                  |
| 1   | 19-A  | 549    |                  |
| 1   | 19-B  | 549    |                  |
| 1   | 2-A   | 549    |                  |
| 1   | 2-B   | 549    |                  |
| 1   | 20-A  | 549    |                  |
| 1   | 20-B  | 549    |                  |
| 1   | 21-A  | 549    |                  |
| 1   | 21-B  | 549    |                  |
| 1   | 22-A  | 549    |                  |
| 1   | 22-B  | 549    |                  |
| 1   | 23-A  | 549    |                  |
| 1   | 23-B  | 549    |                  |

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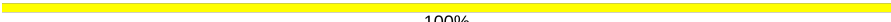
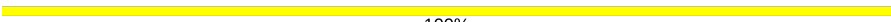
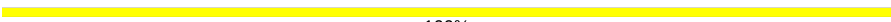
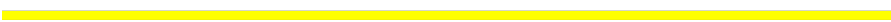











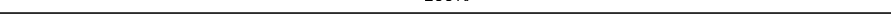
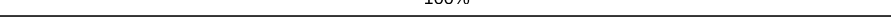
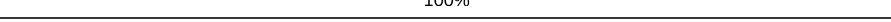
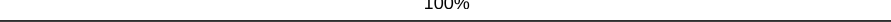
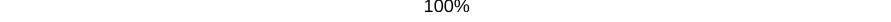
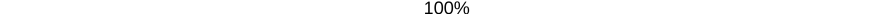
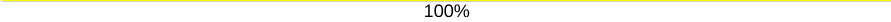
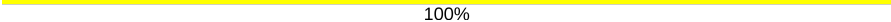
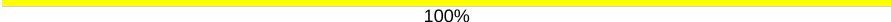
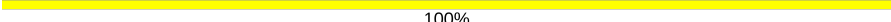
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 24-A  | 549    |                  |
| 1   | 24-B  | 549    |                  |
| 1   | 25-A  | 549    |                  |
| 1   | 25-B  | 549    |                  |
| 1   | 3-A   | 549    |                  |
| 1   | 3-B   | 549    |                  |
| 1   | 4-A   | 549    |                  |
| 1   | 4-B   | 549    |                  |
| 1   | 5-A   | 549    |                  |
| 1   | 5-B   | 549    |                  |
| 1   | 6-A   | 549    |                  |
| 1   | 6-B   | 549    |                  |
| 1   | 7-A   | 549    |                  |
| 1   | 7-B   | 549    |                  |
| 1   | 8-A   | 549    |                  |
| 1   | 8-B   | 549    |                  |
| 1   | 9-A   | 549    |                  |
| 1   | 9-B   | 549    |                  |
| 2   | 1-C   | 6      |                  |
| 2   | 1-E   | 6      |                  |
| 2   | 10-C  | 6      |                  |
| 2   | 10-E  | 6      |                  |
| 2   | 11-C  | 6      |                  |
| 2   | 11-E  | 6      |                  |
| 2   | 12-C  | 6      |                  |

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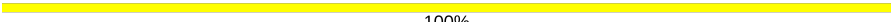
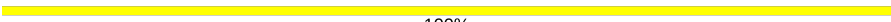
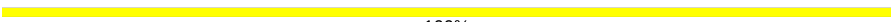
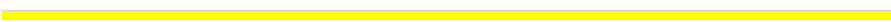











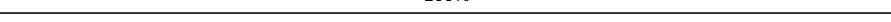
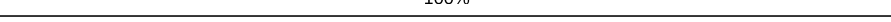
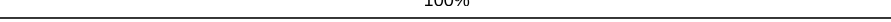
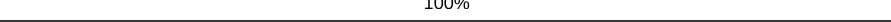
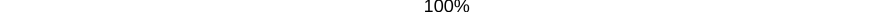
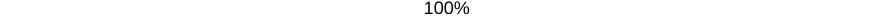
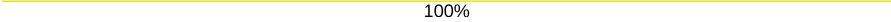
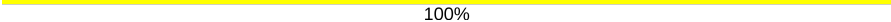
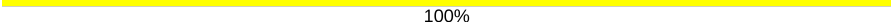
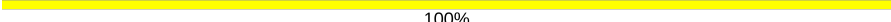


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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | 12-E  | 6      |  100%   |
| 2   | 13-C  | 6      |  100%   |
| 2   | 13-E  | 6      |  100%   |
| 2   | 14-C  | 6      |  100%   |
| 2   | 14-E  | 6      |  100%   |
| 2   | 15-C  | 6      |  100%   |
| 2   | 15-E  | 6      |  100%   |
| 2   | 16-C  | 6      |  100%   |
| 2   | 16-E  | 6      |  100%   |
| 2   | 17-C  | 6      |  100%   |
| 2   | 17-E  | 6      |  100%   |
| 2   | 18-C  | 6      |  100%   |
| 2   | 18-E  | 6      |  100% |
| 2   | 19-C  | 6      |  100% |
| 2   | 19-E  | 6      |  100% |
| 2   | 2-C   | 6      |  100% |
| 2   | 2-E   | 6      |  100% |
| 2   | 20-C  | 6      |  100% |
| 2   | 20-E  | 6      |  100% |
| 2   | 21-C  | 6      |  100% |
| 2   | 21-E  | 6      |  100% |
| 2   | 22-C  | 6      |  100% |
| 2   | 22-E  | 6      |  100% |
| 2   | 23-C  | 6      |  100% |
| 2   | 23-E  | 6      |  100% |

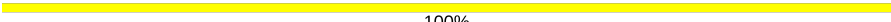
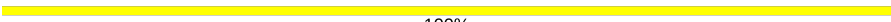
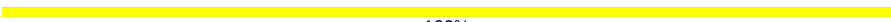
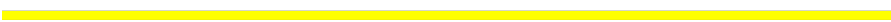











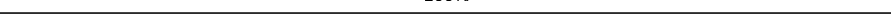
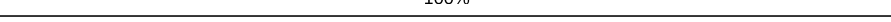
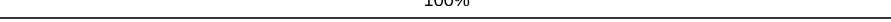
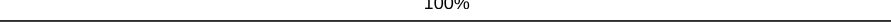
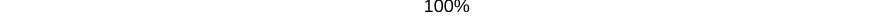
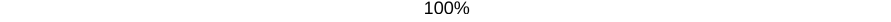
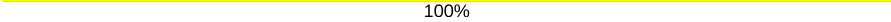
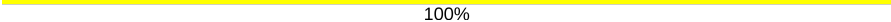
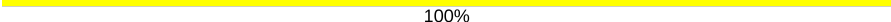
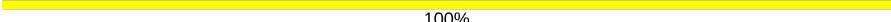
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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | 24-C  | 6      |  100%   |
| 2   | 24-E  | 6      |  100%   |
| 2   | 25-C  | 6      |  100%   |
| 2   | 25-E  | 6      |  100%   |
| 2   | 3-C   | 6      |  100%   |
| 2   | 3-E   | 6      |  100%   |
| 2   | 4-C   | 6      |  100%   |
| 2   | 4-E   | 6      |  100%   |
| 2   | 5-C   | 6      |  100%   |
| 2   | 5-E   | 6      |  100%   |
| 2   | 6-C   | 6      |  100%   |
| 2   | 6-E   | 6      |  100%   |
| 2   | 7-C   | 6      |  100% |
| 2   | 7-E   | 6      |  100% |
| 2   | 8-C   | 6      |  100% |
| 2   | 8-E   | 6      |  100% |
| 2   | 9-C   | 6      |  100% |
| 2   | 9-E   | 6      |  100% |
| 3   | 1-D   | 5      |  100% |
| 3   | 1-F   | 5      |  100% |
| 3   | 10-D  | 5      |  100% |
| 3   | 10-F  | 5      |  100% |
| 3   | 11-D  | 5      |  100% |
| 3   | 11-F  | 5      |  100% |
| 3   | 12-D  | 5      |  100% |

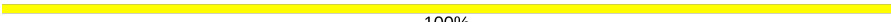
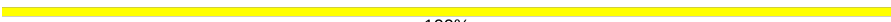
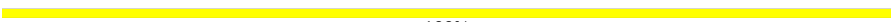
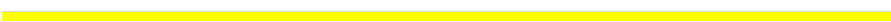








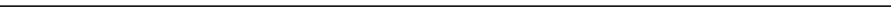


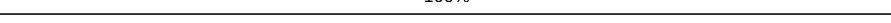
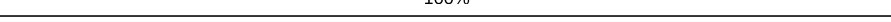
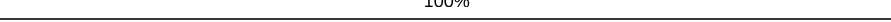
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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 3   | 12-F  | 5      |  100%   |
| 3   | 13-D  | 5      |  100%   |
| 3   | 13-F  | 5      |  100%   |
| 3   | 14-D  | 5      |  100%   |
| 3   | 14-F  | 5      |  100%   |
| 3   | 15-D  | 5      |  100%   |
| 3   | 15-F  | 5      |  100%   |
| 3   | 16-D  | 5      |  100%   |
| 3   | 16-F  | 5      |  100%   |
| 3   | 17-D  | 5      |  100%   |
| 3   | 17-F  | 5      |  100%   |
| 3   | 18-D  | 5      |  100%   |
| 3   | 18-F  | 5      |  100% |
| 3   | 19-D  | 5      |  100% |
| 3   | 19-F  | 5      |  100% |
| 3   | 2-D   | 5      |  100% |
| 3   | 2-F   | 5      |  100% |
| 3   | 20-D  | 5      |  100% |
| 3   | 20-F  | 5      |  100% |
| 3   | 21-D  | 5      |  100% |
| 3   | 21-F  | 5      |  100% |
| 3   | 22-D  | 5      |  100% |
| 3   | 22-F  | 5      |  100% |
| 3   | 23-D  | 5      |  100% |
| 3   | 23-F  | 5      |  100% |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 3   | 24-D  | 5      |  100%   |
| 3   | 24-F  | 5      |  100%   |
| 3   | 25-D  | 5      |  100%   |
| 3   | 25-F  | 5      |  100%   |
| 3   | 3-D   | 5      |  100%   |
| 3   | 3-F   | 5      |  100%   |
| 3   | 4-D   | 5      |  100%   |
| 3   | 4-F   | 5      |  100%   |
| 3   | 5-D   | 5      |  100%   |
| 3   | 5-F   | 5      |  100%   |
| 3   | 6-D   | 5      |  100%   |
| 3   | 6-F   | 5      |  100%   |
| 3   | 7-D   | 5      |  100% |
| 3   | 7-F   | 5      |  100% |
| 3   | 8-D   | 5      |  100% |
| 3   | 8-F   | 5      |  100% |
| 3   | 9-D   | 5      |  100% |
| 3   | 9-F   | 5      |  100% |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 427968 atoms, of which 195500 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 Putative secreted protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 1   | 1-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 2-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 3-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 4-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 5-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 6-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 7-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 8-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 9-A   | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 10-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 11-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 12-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 13-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 14-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 15-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 16-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 1   | 17-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 18-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 19-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 20-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 21-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 22-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 23-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 24-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 25-A  | 549      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8074  | 2629 | 3907 | 708 | 825 | 5 |         |         |       |
| 1   | 1-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 2-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 3-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 4-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 5-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 6-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 7-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 8-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 9-B   | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 10-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 11-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 12-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |

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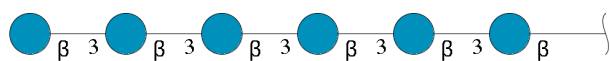
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| Mol | Chain | Residues | Atoms |      |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 1   | 13-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 14-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 15-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 16-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 17-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 18-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 19-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 20-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 21-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 22-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 23-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 24-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |
| 1   | 25-B  | 548      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 8059  | 2624 | 3901 | 707 | 822 | 5 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 502     | ALA      | GLU    | engineered mutation | UNP G2NFJ9 |
| B     | 502     | ALA      | GLU    | engineered mutation | UNP G2NFJ9 |

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms       |         |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|---------|-------|
| 2   | 1-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 2-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 3-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 4-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 5-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 6-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 7-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 8-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 9-C   | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 10-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 11-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 12-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 13-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 14-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 15-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 16-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 17-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 18-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 19-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 20-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 21-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |
| 2   | 22-C  | 6        | Total<br>67 | C<br>36 | O<br>31 | 0       | 0       | 0     |

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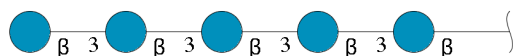
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 2   | 23-C  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 24-C  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 25-C  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 1-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 2-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 3-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 4-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 5-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 6-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 7-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 8-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 9-E   | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 10-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 11-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 12-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 13-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 14-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 15-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 16-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 17-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 18-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 2   | 19-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 20-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 21-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 22-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 23-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 24-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |
| 2   | 25-E  | 6        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 67    | 36 | 31 |         |         |       |

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 3   | 1-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 2-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 3-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 4-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 5-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 6-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 7-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 8-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 9-D   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 10-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 3   | 11-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 12-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 13-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 14-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 15-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 16-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 17-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 18-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 19-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 20-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 21-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 22-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 23-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 24-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 25-D  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 1-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 2-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 3-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 4-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 5-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 6-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 3   | 7-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 8-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 9-F   | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 10-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 11-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 12-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 13-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 14-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 15-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 16-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 17-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 18-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 19-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 20-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 21-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 22-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 23-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 24-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |
| 3   | 25-F  | 5        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 56    | 30 | 26 |         |         |       |

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | 1-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 2-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 3-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 4-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 5-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 6-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 7-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 8-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 9-A   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 10-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 11-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 12-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 13-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 14-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | 15-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 16-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 17-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 18-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 19-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 20-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 21-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 22-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 23-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 24-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 25-A  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 1-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 2-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 3-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 4-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 5-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 6-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 7-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 8-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 9-B   | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 10-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | 11-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 12-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 13-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 14-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 15-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 16-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 17-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 18-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 19-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 20-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 21-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 22-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 23-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 24-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |
| 4   | 25-B  | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | 1-A   | 355      | Total | O   | 0       | 0       |
|     |       |          | 355   | 355 |         |         |
| 5   | 2-A   | 362      | Total | O   | 0       | 0       |
|     |       |          | 362   | 362 |         |         |
| 5   | 3-A   | 360      | Total | O   | 0       | 0       |
|     |       |          | 360   | 360 |         |         |
| 5   | 4-A   | 370      | Total | O   | 0       | 0       |
|     |       |          | 370   | 370 |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | 5-A   | 364      | Total<br>364 | O<br>364 | 0       | 0       |
| 5   | 6-A   | 356      | Total<br>356 | O<br>356 | 0       | 0       |
| 5   | 7-A   | 325      | Total<br>325 | O<br>325 | 0       | 0       |
| 5   | 8-A   | 356      | Total<br>356 | O<br>356 | 0       | 0       |
| 5   | 9-A   | 327      | Total<br>327 | O<br>327 | 0       | 0       |
| 5   | 10-A  | 365      | Total<br>365 | O<br>365 | 0       | 0       |
| 5   | 11-A  | 361      | Total<br>361 | O<br>361 | 0       | 0       |
| 5   | 12-A  | 360      | Total<br>360 | O<br>360 | 0       | 0       |
| 5   | 13-A  | 335      | Total<br>335 | O<br>335 | 0       | 0       |
| 5   | 14-A  | 359      | Total<br>359 | O<br>359 | 0       | 0       |
| 5   | 15-A  | 348      | Total<br>348 | O<br>348 | 0       | 0       |
| 5   | 16-A  | 369      | Total<br>369 | O<br>369 | 0       | 0       |
| 5   | 17-A  | 351      | Total<br>351 | O<br>351 | 0       | 0       |
| 5   | 18-A  | 349      | Total<br>349 | O<br>349 | 0       | 0       |
| 5   | 19-A  | 346      | Total<br>346 | O<br>346 | 0       | 0       |
| 5   | 20-A  | 324      | Total<br>324 | O<br>324 | 0       | 0       |
| 5   | 21-A  | 347      | Total<br>347 | O<br>347 | 0       | 0       |
| 5   | 22-A  | 338      | Total<br>338 | O<br>338 | 0       | 0       |
| 5   | 23-A  | 366      | Total<br>366 | O<br>366 | 0       | 0       |
| 5   | 24-A  | 364      | Total<br>364 | O<br>364 | 0       | 0       |
| 5   | 25-A  | 359      | Total<br>359 | O<br>359 | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | 1-B   | 381      | Total<br>381 | O<br>381 | 0       | 0       |
| 5   | 2-B   | 369      | Total<br>369 | O<br>369 | 0       | 0       |
| 5   | 3-B   | 348      | Total<br>348 | O<br>348 | 0       | 0       |
| 5   | 4-B   | 377      | Total<br>377 | O<br>377 | 0       | 0       |
| 5   | 5-B   | 350      | Total<br>350 | O<br>350 | 0       | 0       |
| 5   | 6-B   | 364      | Total<br>364 | O<br>364 | 0       | 0       |
| 5   | 7-B   | 377      | Total<br>377 | O<br>377 | 0       | 0       |
| 5   | 8-B   | 372      | Total<br>372 | O<br>372 | 0       | 0       |
| 5   | 9-B   | 353      | Total<br>353 | O<br>353 | 0       | 0       |
| 5   | 10-B  | 367      | Total<br>367 | O<br>367 | 0       | 0       |
| 5   | 11-B  | 357      | Total<br>357 | O<br>357 | 0       | 0       |
| 5   | 12-B  | 379      | Total<br>379 | O<br>379 | 0       | 0       |
| 5   | 13-B  | 360      | Total<br>360 | O<br>360 | 0       | 0       |
| 5   | 14-B  | 392      | Total<br>392 | O<br>392 | 0       | 0       |
| 5   | 15-B  | 373      | Total<br>373 | O<br>373 | 0       | 0       |
| 5   | 16-B  | 361      | Total<br>361 | O<br>361 | 0       | 0       |
| 5   | 17-B  | 377      | Total<br>377 | O<br>377 | 0       | 0       |
| 5   | 18-B  | 373      | Total<br>373 | O<br>373 | 0       | 0       |
| 5   | 19-B  | 355      | Total<br>355 | O<br>355 | 0       | 0       |
| 5   | 20-B  | 372      | Total<br>372 | O<br>372 | 0       | 0       |
| 5   | 21-B  | 370      | Total<br>370 | O<br>370 | 0       | 0       |

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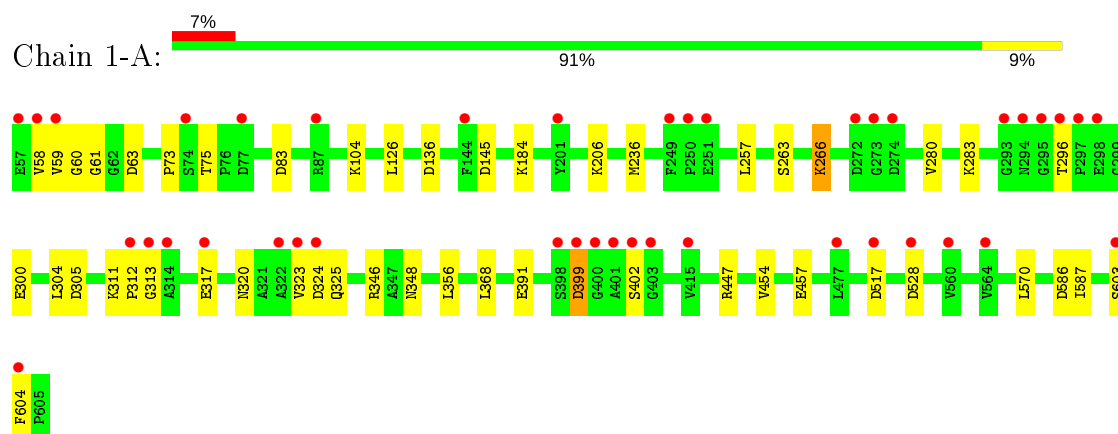
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | 22-B  | 386      | Total<br>386 | O<br>386 | 0       | 0       |
| 5   | 23-B  | 332      | Total<br>332 | O<br>332 | 0       | 0       |
| 5   | 24-B  | 360      | Total<br>360 | O<br>360 | 0       | 0       |
| 5   | 25-B  | 372      | Total<br>372 | O<br>372 | 0       | 0       |

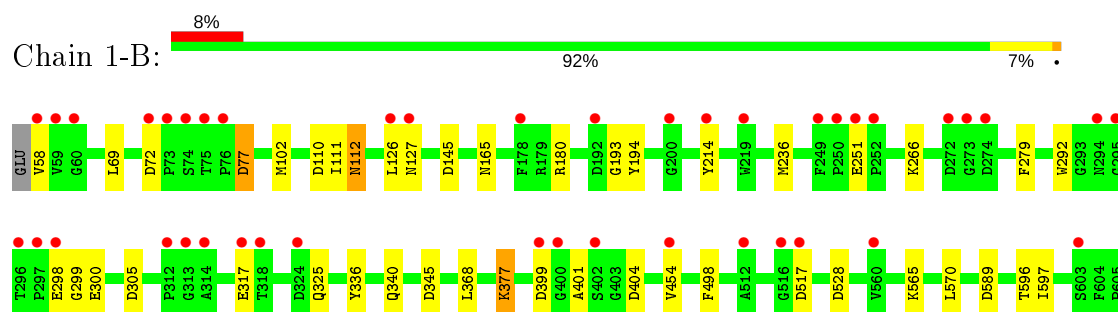
### 3 Residue-property plots [i](#)

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

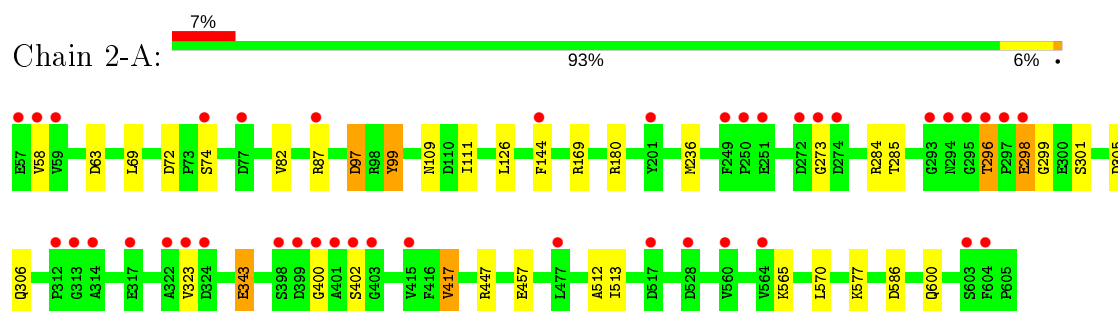
- Molecule 1: Putative secreted protein



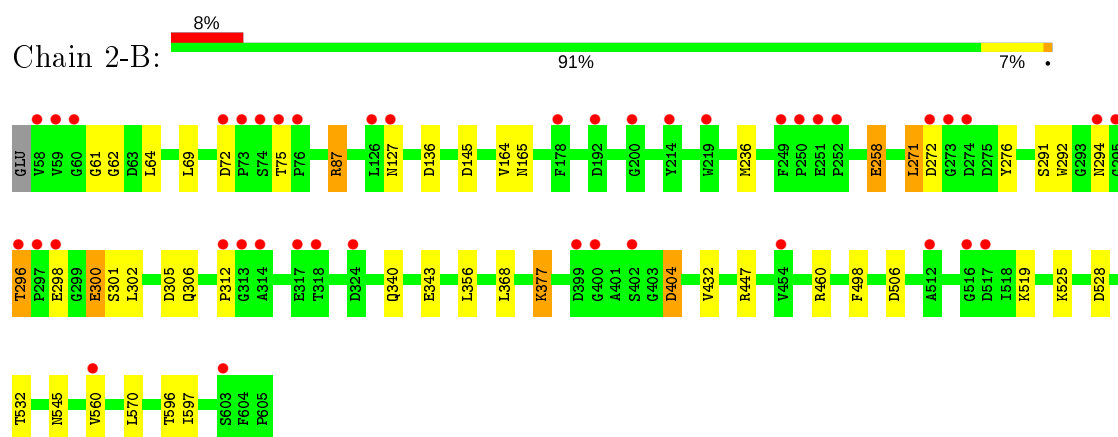
- Molecule 1: Putative secreted protein



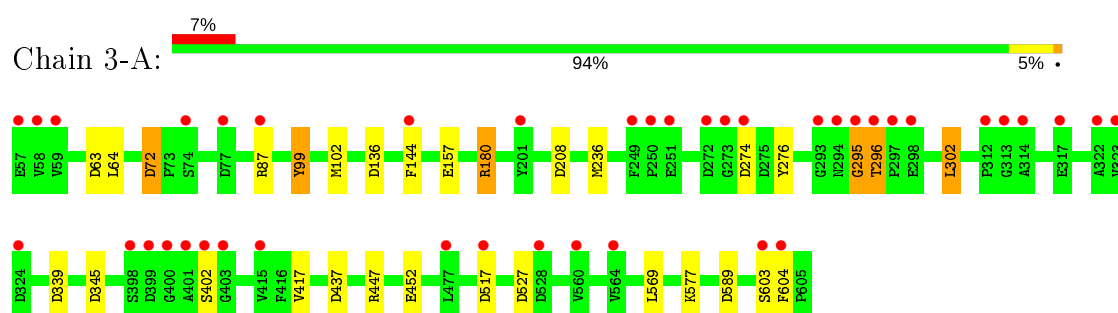
- Molecule 1: Putative secreted protein



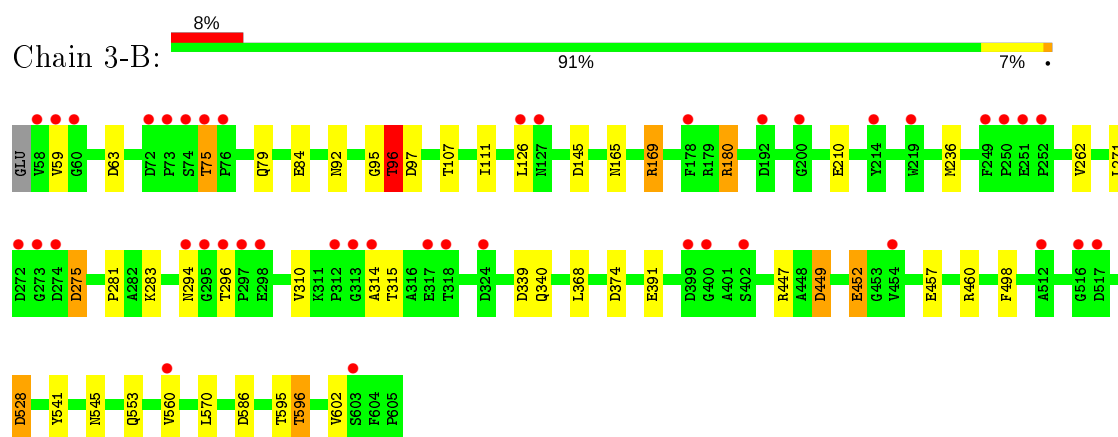
- Molecule 1: Putative secreted protein



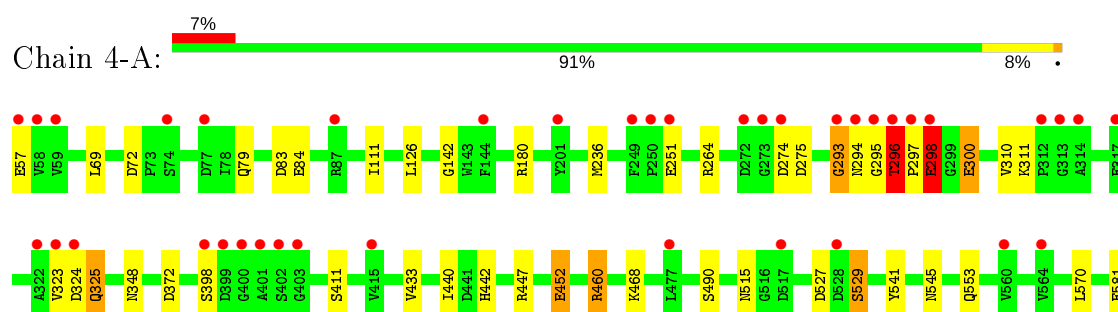
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein

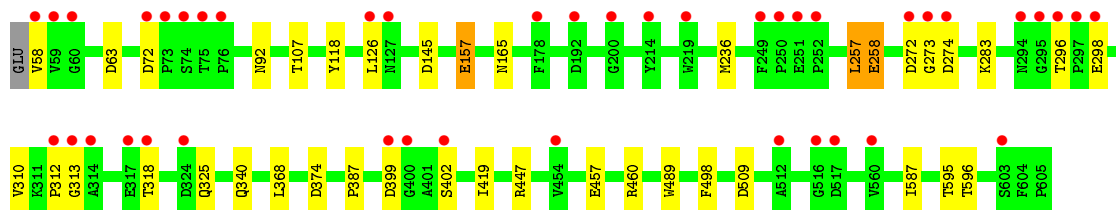


- Molecule 1: Putative secreted protein

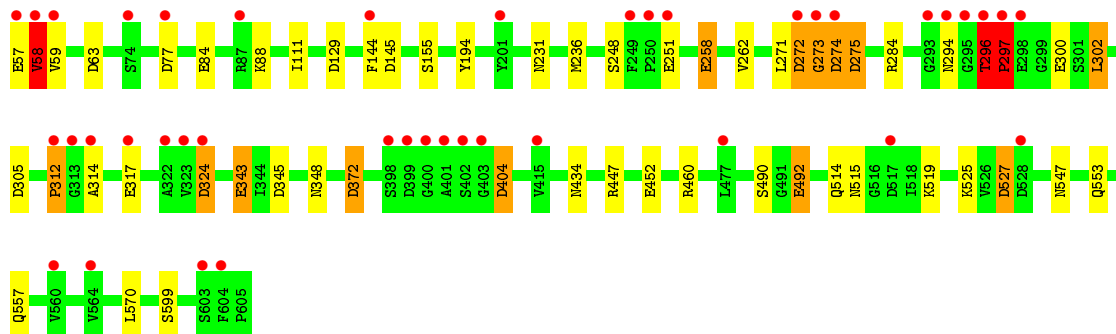
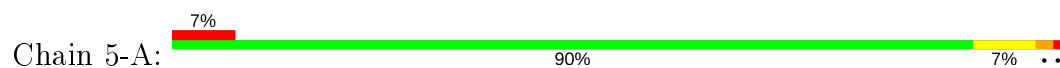




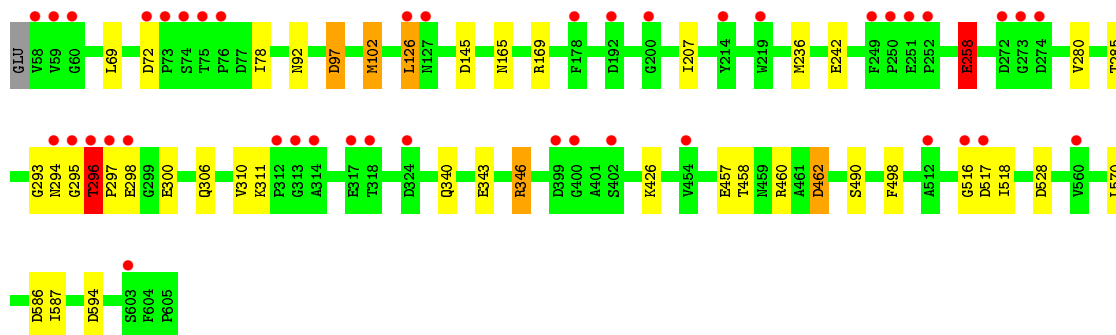
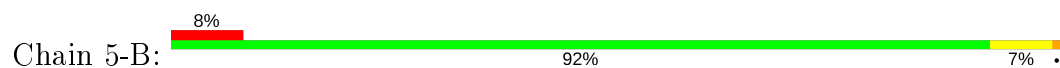
- Molecule 1: Putative secreted protein



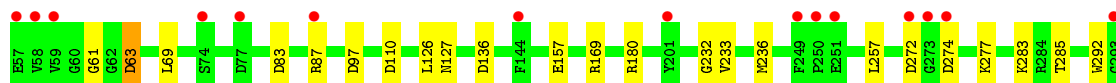
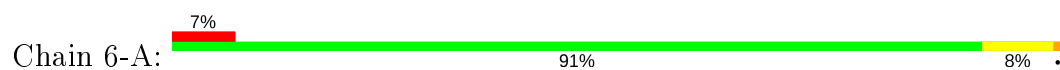
- Molecule 1: Putative secreted protein

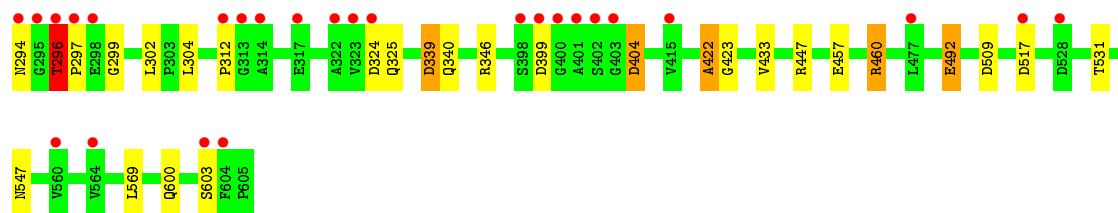


- Molecule 1: Putative secreted protein

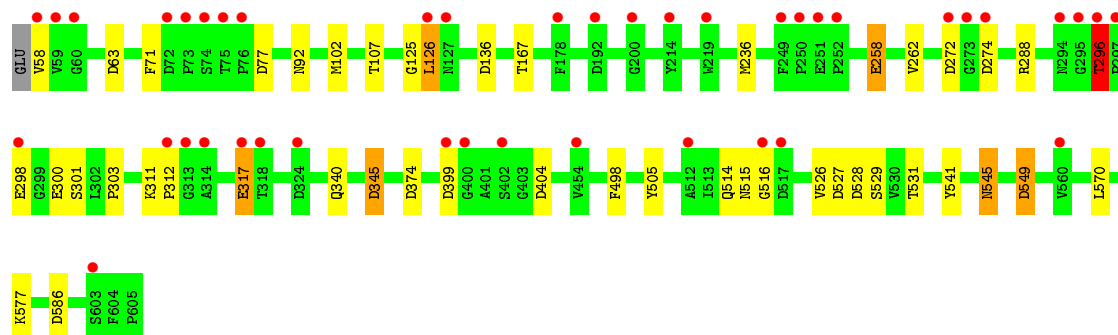


- Molecule 1: Putative secreted protein

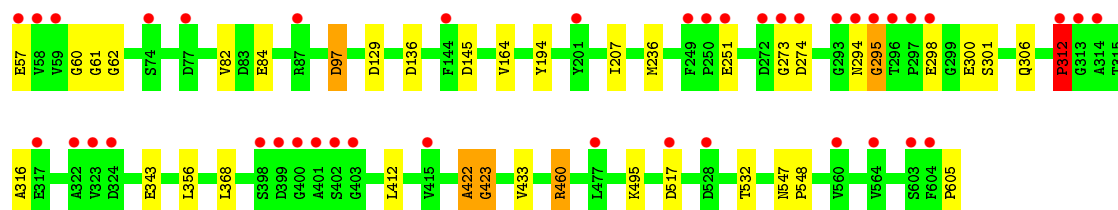




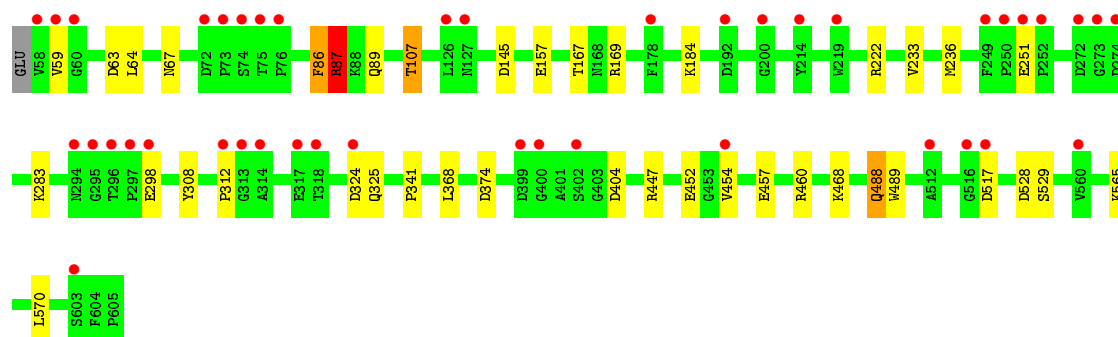
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein

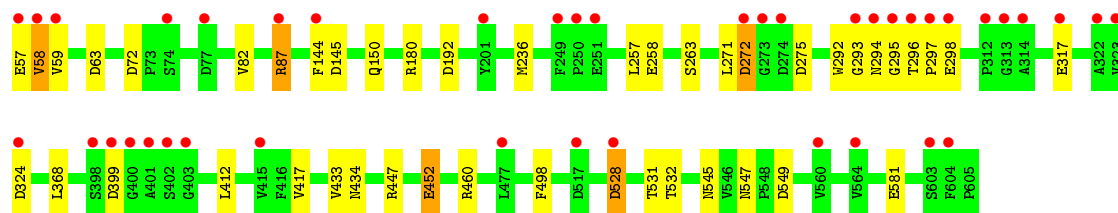


- Molecule 1: Putative secreted protein

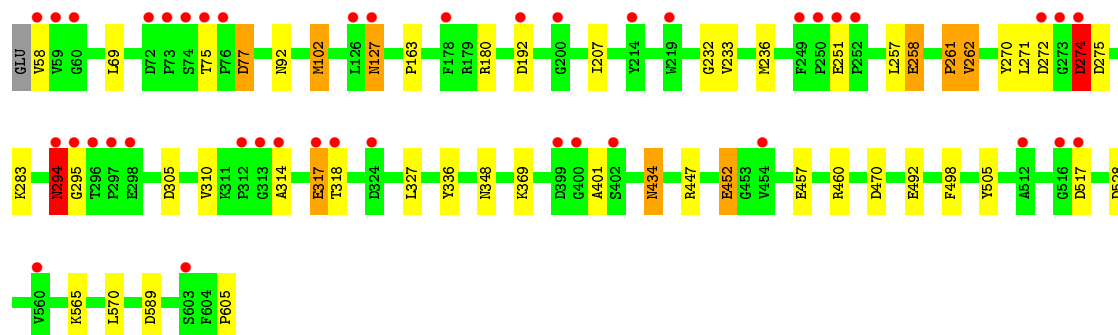


- Molecule 1: Putative secreted protein

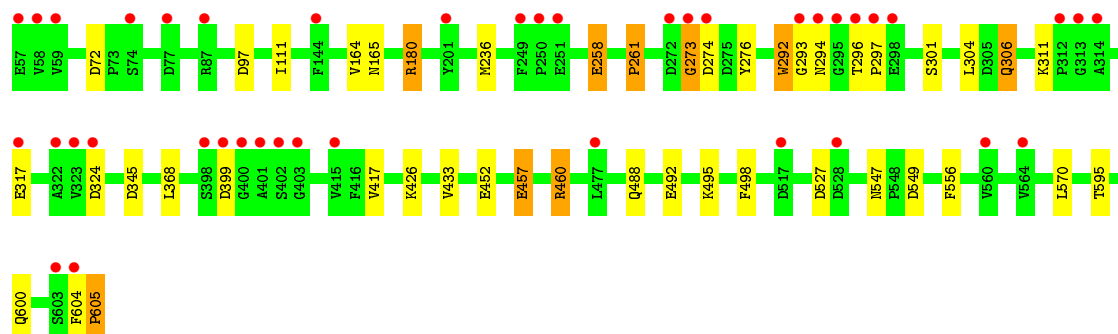




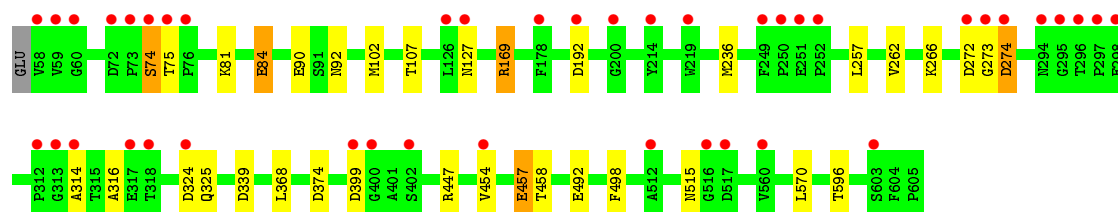
• Molecule 1: Putative secreted protein



• Molecule 1: Putative secreted protein

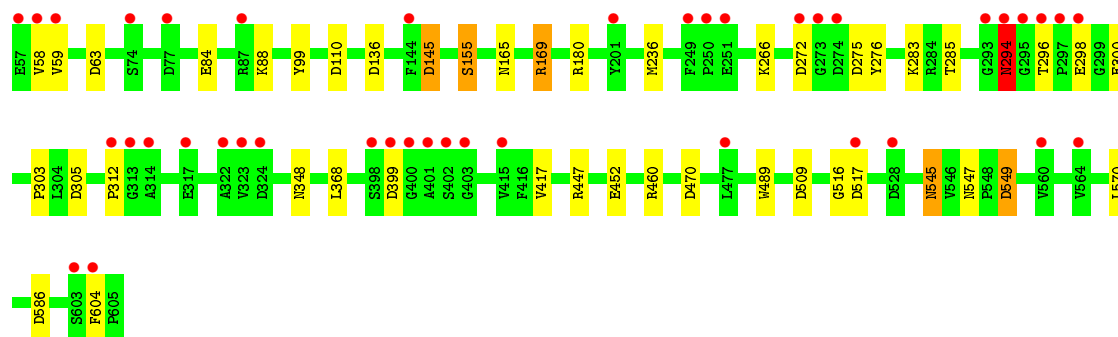


• Molecule 1: Putative secreted protein

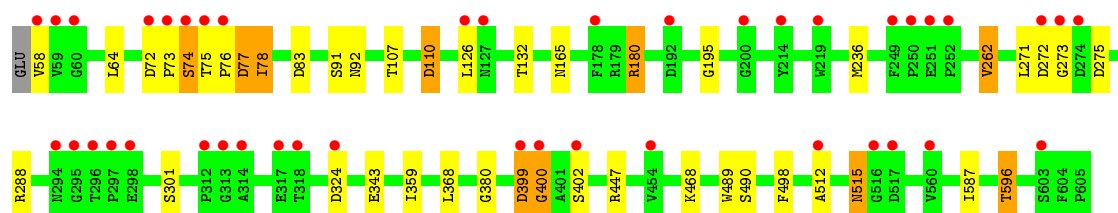


• Molecule 1: Putative secreted protein

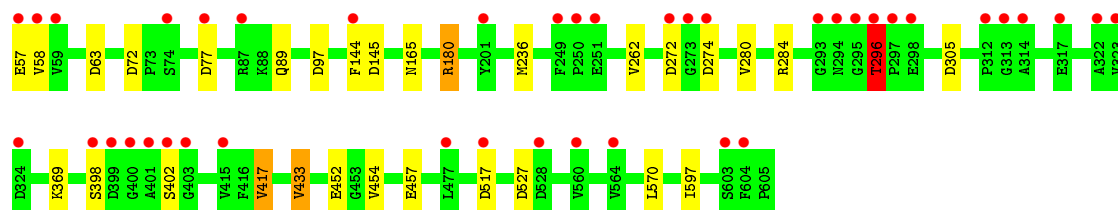




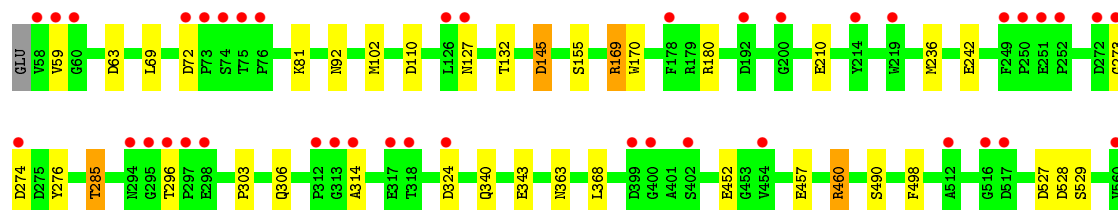
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



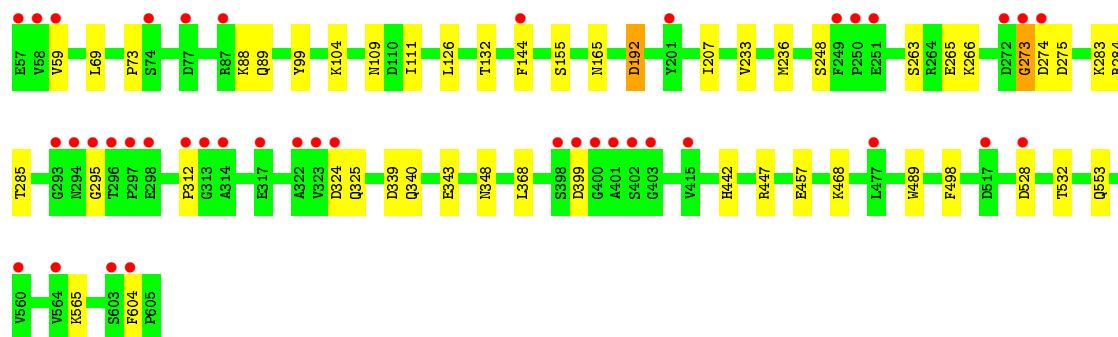
- Molecule 1: Putative secreted protein



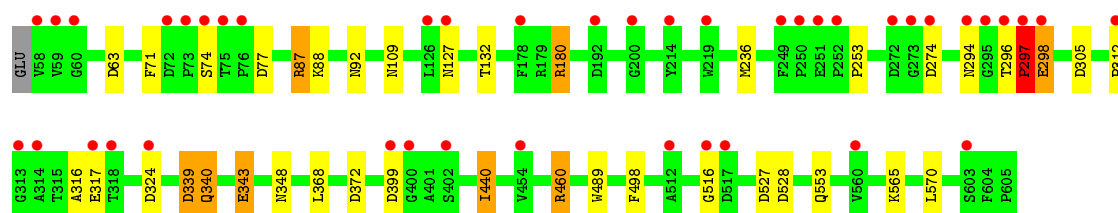
- Molecule 1: Putative secreted protein



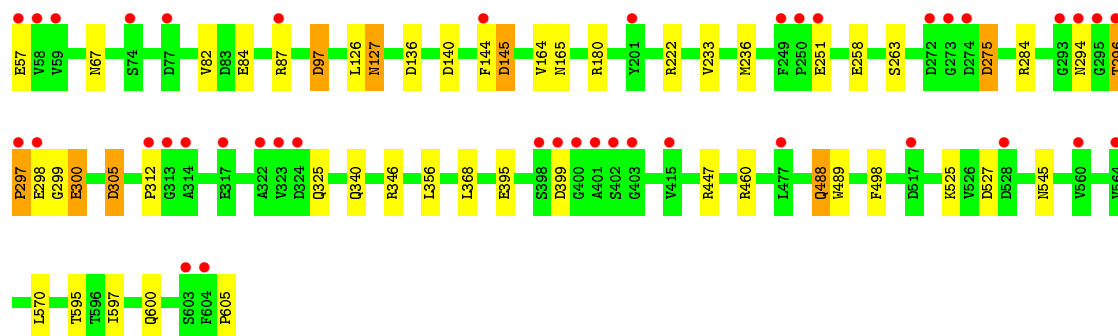




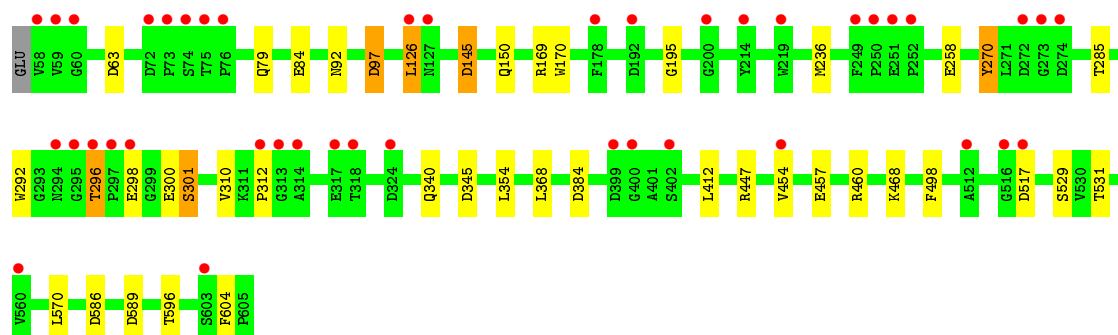
- Molecule 1: Putative secreted protein



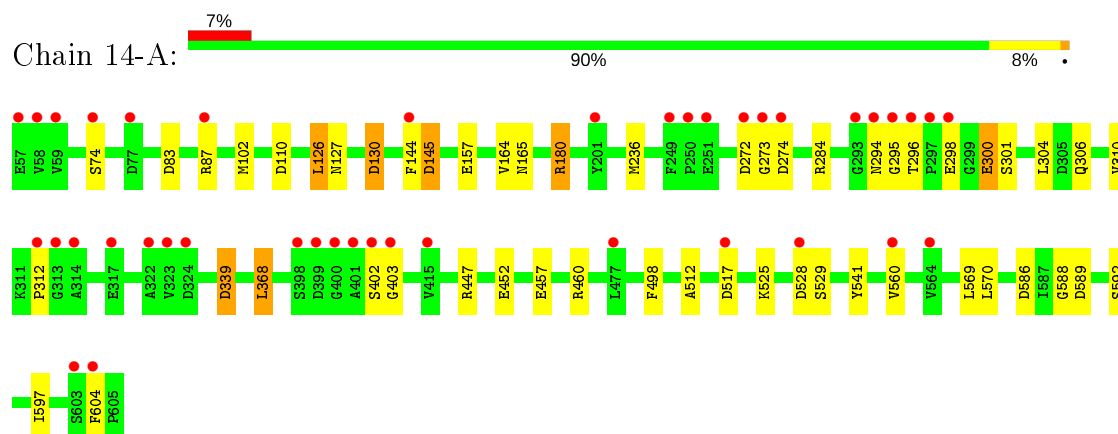
- Molecule 1: Putative secreted protein



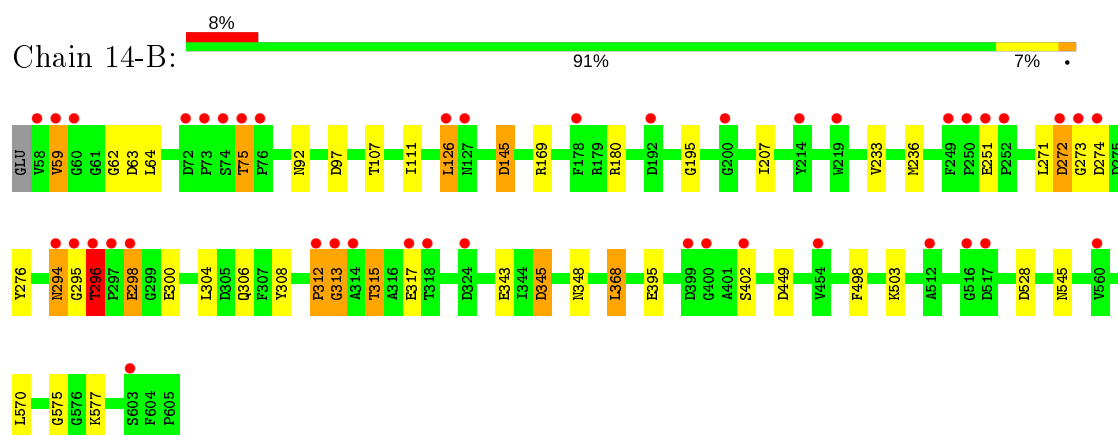
- Molecule 1: Putative secreted protein



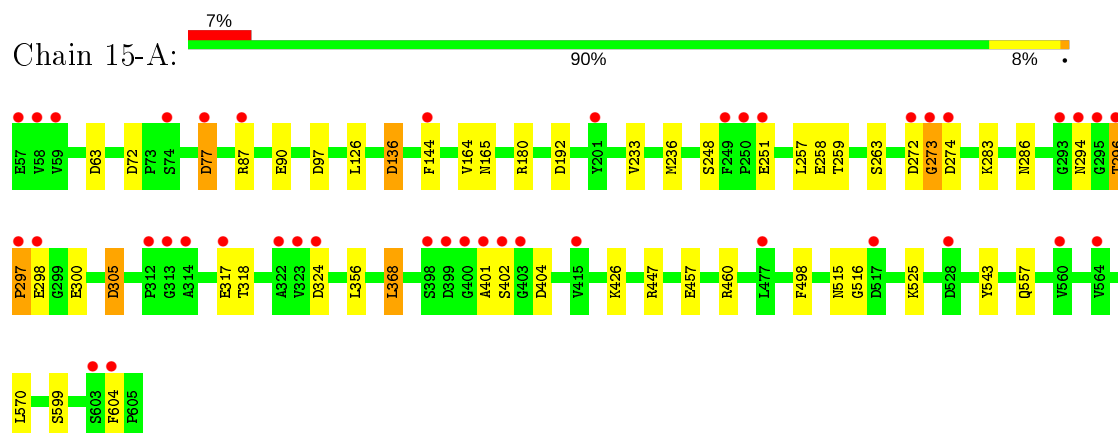
- Molecule 1: Putative secreted protein



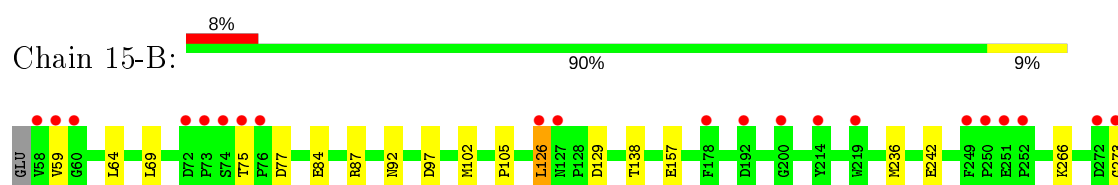
- Molecule 1: Putative secreted protein

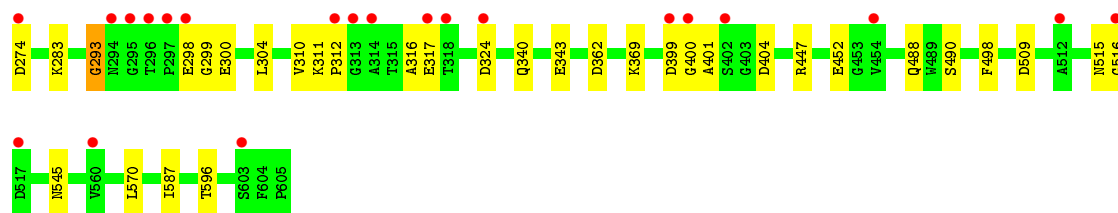


- Molecule 1: Putative secreted protein

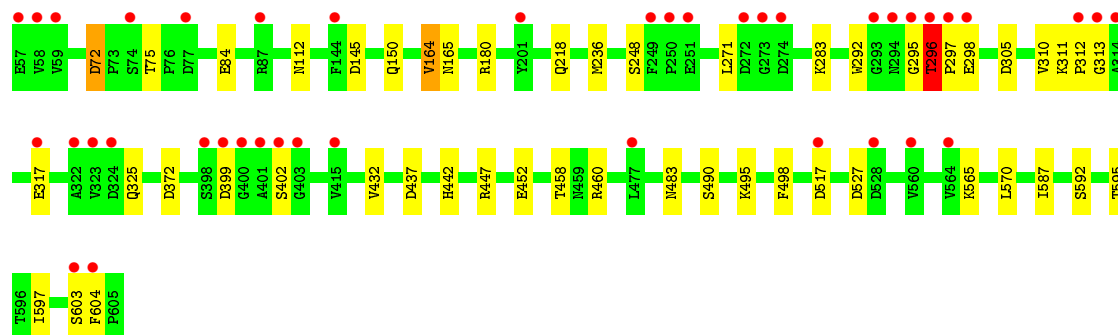


- Molecule 1: Putative secreted protein

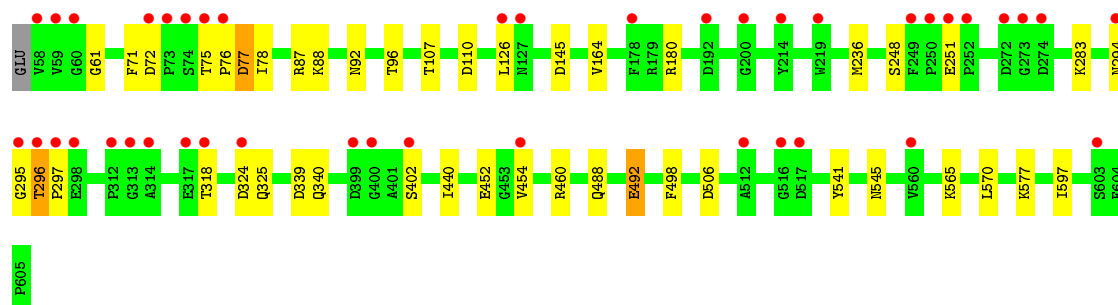




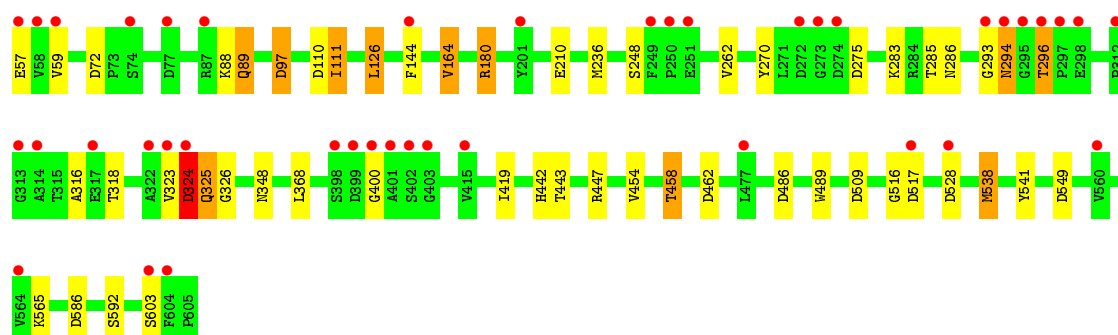
● Molecule 1: Putative secreted protein



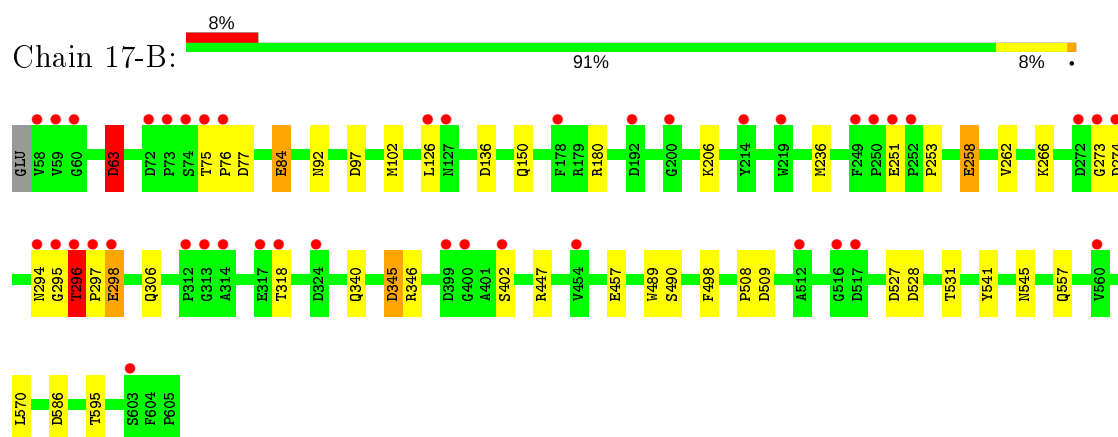
● Molecule 1: Putative secreted protein



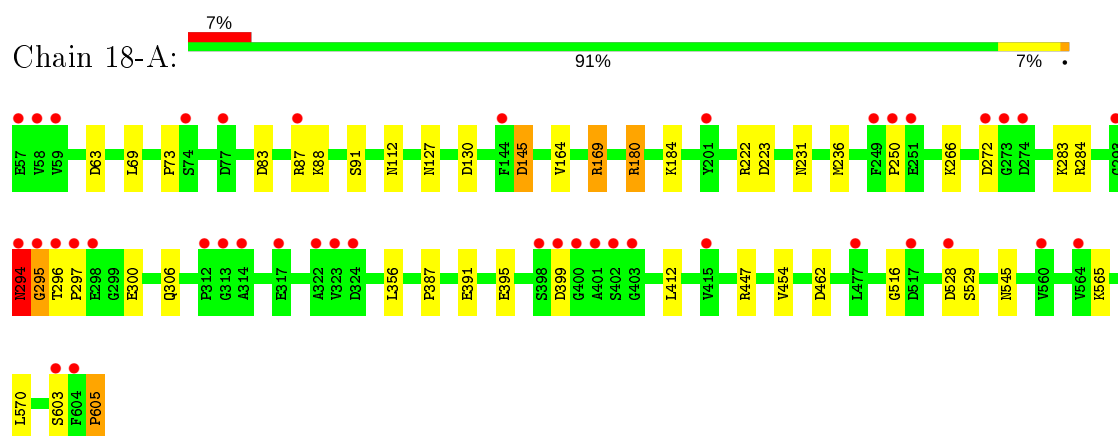
● Molecule 1: Putative secreted protein



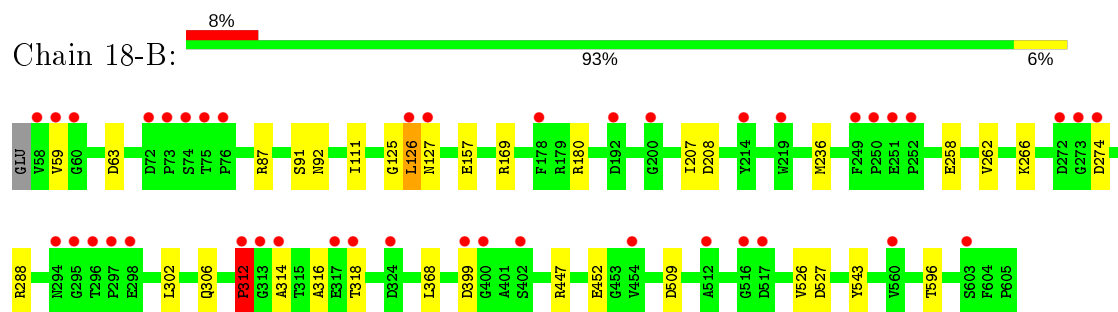
● Molecule 1: Putative secreted protein



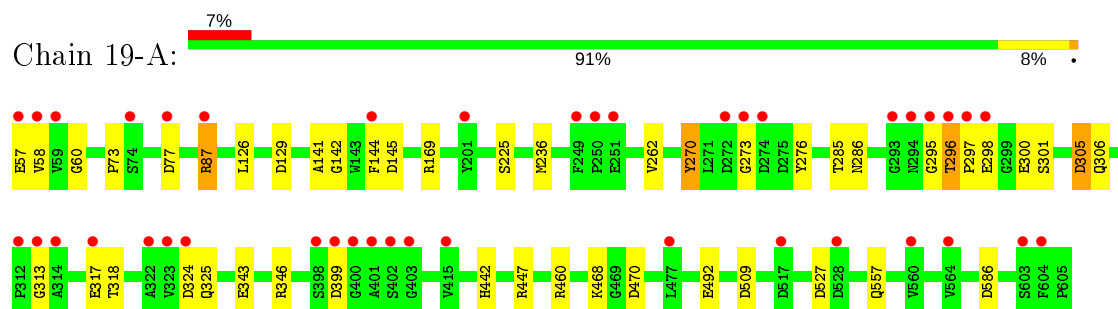
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein

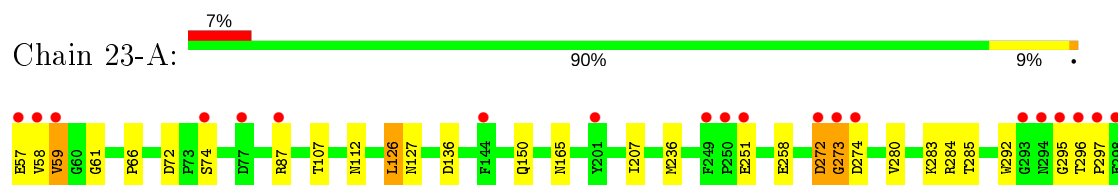
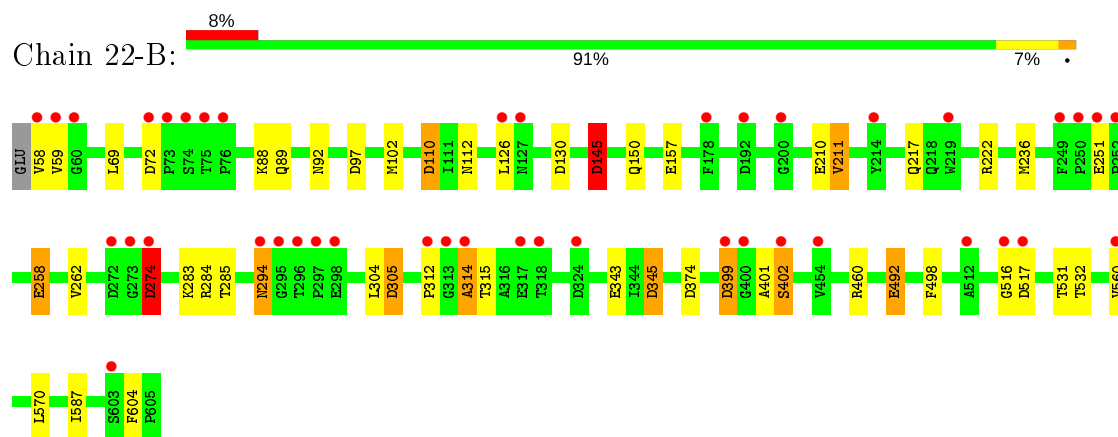
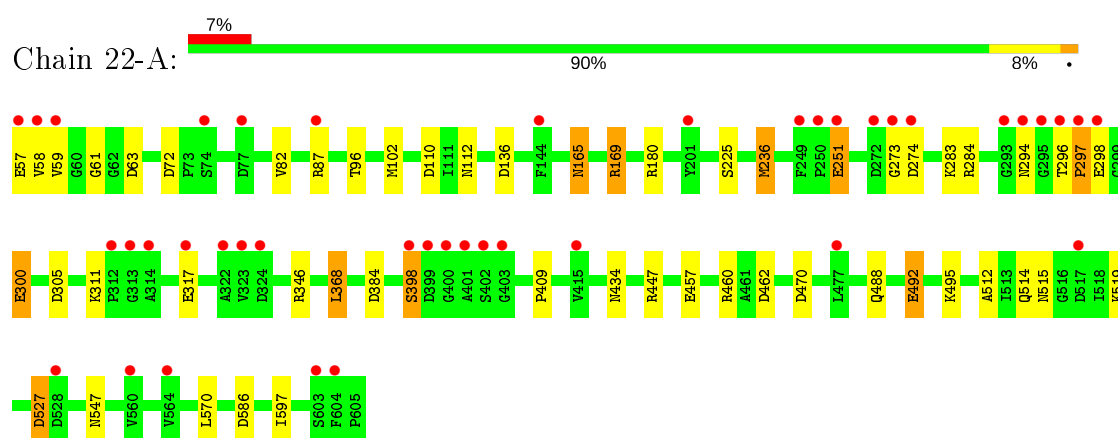
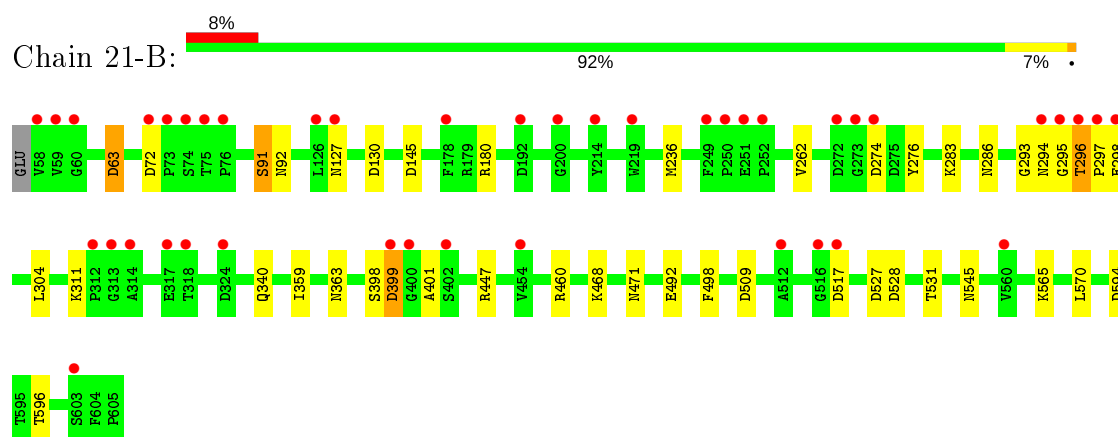


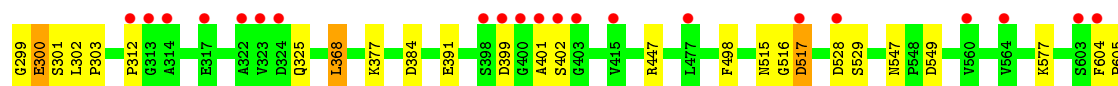
- Molecule 1: Putative secreted protein



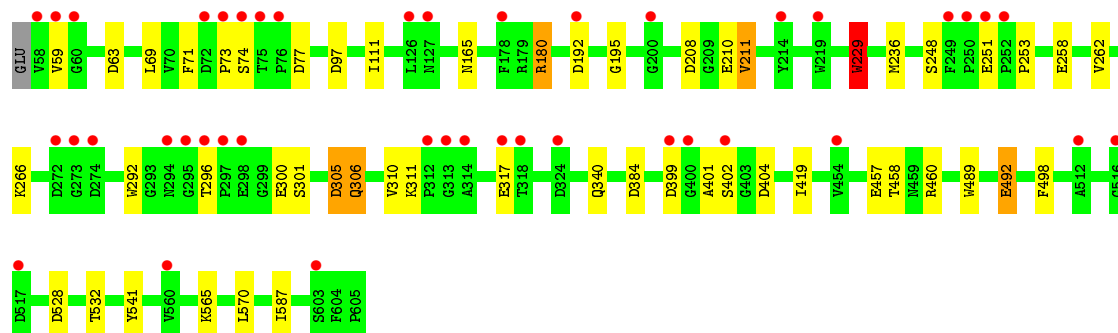
- Molecule 1: Putative secreted protein



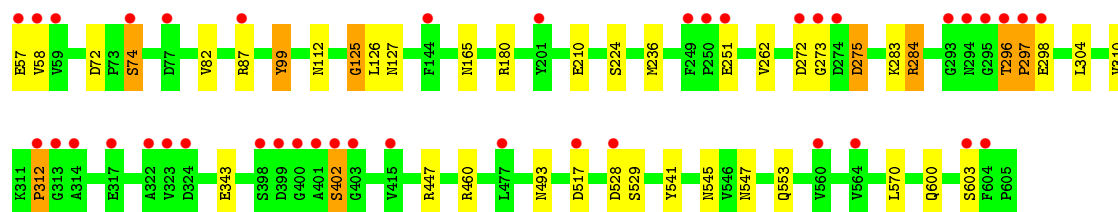




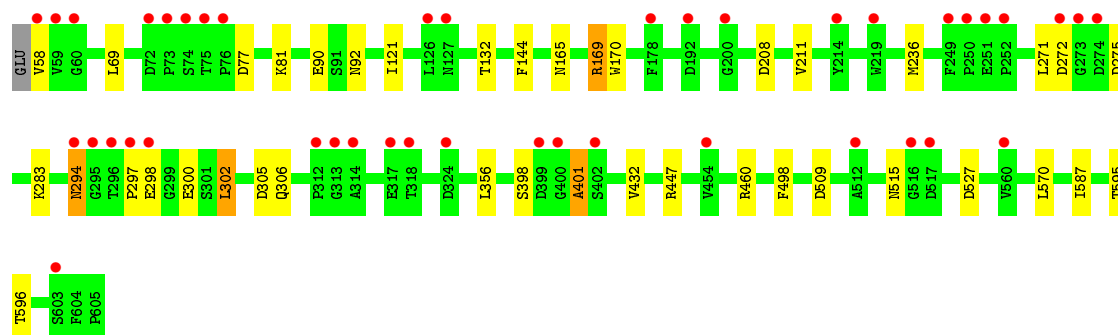
- Molecule 1: Putative secreted protein



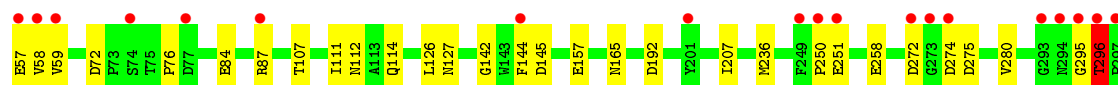
- Molecule 1: Putative secreted protein

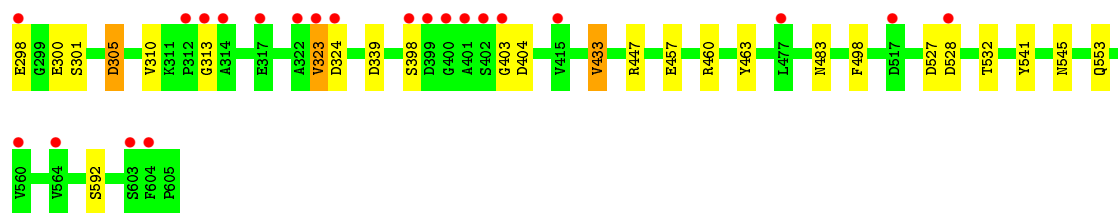


- Molecule 1: Putative secreted protein

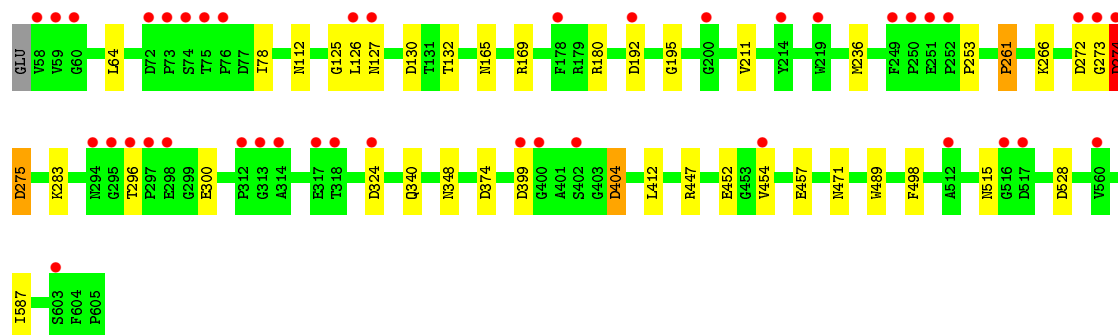


- Molecule 1: Putative secreted protein

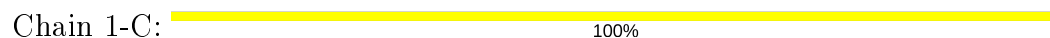




- Molecule 1: Putative secreted protein



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose





BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-E:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-C:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-E:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-E:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-C:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-C:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-E:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5  
BGC6

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 2-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 3-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



Chain 3-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 4-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 5-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 6-F:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 7-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 8-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 12-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-D:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 13-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 15-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 16-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 17-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-F:  100%


BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 21-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 22-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-D:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 25-F:  100%

BGC1  
BGC2  
BGC3  
BGC4  
BGC5

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 54.10Å 100.96Å 104.18Å<br>90.00° 91.10° 90.00°              | Depositor        |
| Resolution (Å)  | 30.30 – 1.75<br>30.30 – 1.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (30.30-1.75)<br>93.6 (30.30-1.75)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.37 (at 1.75Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.ensemble_refinement: 1.9_1692)               | Depositor        |
| R, $R_{free}$   | 0.122 , 0.163<br>0.148 , 0.187                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5640 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 14.7  | Xtriage          |
| Anisotropy  | 0.140   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 229.2  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction   | 0.000 for -h,l,k<br>0.000 for -h,-l,-k<br>0.026 for h,-k,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.97  | EDS              |
| Total number of atoms   | 427968  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 13.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to  $7.0959e-05$ . The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | 1-A   | 0.86         | 3/4280 (0.1%)  | 0.95        | 14/5848 (0.2%) |
| 1   | 1-B   | 0.87         | 7/4271 (0.2%)  | 0.92        | 6/5836 (0.1%)  |
| 1   | 2-A   | 0.88         | 7/4280 (0.2%)  | 0.96        | 13/5848 (0.2%) |
| 1   | 2-B   | 0.87         | 6/4271 (0.1%)  | 0.95        | 12/5836 (0.2%) |
| 1   | 3-A   | 0.86         | 3/4280 (0.1%)  | 0.93        | 11/5848 (0.2%) |
| 1   | 3-B   | 0.89         | 9/4271 (0.2%)  | 0.97        | 12/5836 (0.2%) |
| 1   | 4-A   | 0.84         | 4/4280 (0.1%)  | 0.96        | 12/5848 (0.2%) |
| 1   | 4-B   | 0.86         | 4/4271 (0.1%)  | 0.91        | 5/5836 (0.1%)  |
| 1   | 5-A   | 0.95         | 12/4280 (0.3%) | 1.03        | 26/5848 (0.4%) |
| 1   | 5-B   | 0.87         | 5/4271 (0.1%)  | 0.97        | 16/5836 (0.3%) |
| 1   | 6-A   | 0.89         | 8/4280 (0.2%)  | 1.00        | 14/5848 (0.2%) |
| 1   | 6-B   | 0.89         | 8/4271 (0.2%)  | 0.97        | 13/5836 (0.2%) |
| 1   | 7-A   | 0.87         | 7/4280 (0.2%)  | 0.97        | 11/5848 (0.2%) |
| 1   | 7-B   | 0.83         | 4/4271 (0.1%)  | 0.92        | 6/5836 (0.1%)  |
| 1   | 8-A   | 0.88         | 8/4280 (0.2%)  | 0.98        | 11/5848 (0.2%) |
| 1   | 8-B   | 0.89         | 11/4271 (0.3%) | 0.98        | 15/5836 (0.3%) |
| 1   | 9-A   | 0.90         | 7/4280 (0.2%)  | 0.95        | 10/5848 (0.2%) |
| 1   | 9-B   | 0.86         | 6/4271 (0.1%)  | 0.90        | 8/5836 (0.1%)  |
| 1   | 10-A  | 0.91         | 9/4280 (0.2%)  | 0.99        | 14/5848 (0.2%) |
| 1   | 10-B  | 0.88         | 4/4271 (0.1%)  | 1.01        | 14/5836 (0.2%) |
| 1   | 11-A  | 0.84         | 4/4280 (0.1%)  | 0.94        | 7/5848 (0.1%)  |
| 1   | 11-B  | 0.83         | 3/4271 (0.1%)  | 0.93        | 9/5836 (0.2%)  |
| 1   | 12-A  | 0.89         | 7/4280 (0.2%)  | 0.93        | 8/5848 (0.1%)  |
| 1   | 12-B  | 0.88         | 9/4271 (0.2%)  | 0.98        | 13/5836 (0.2%) |
| 1   | 13-A  | 0.89         | 7/4280 (0.2%)  | 0.97        | 13/5848 (0.2%) |
| 1   | 13-B  | 0.84         | 3/4271 (0.1%)  | 0.96        | 17/5836 (0.3%) |
| 1   | 14-A  | 0.88         | 7/4280 (0.2%)  | 1.00        | 17/5848 (0.3%) |
| 1   | 14-B  | 0.88         | 5/4271 (0.1%)  | 0.96        | 8/5836 (0.1%)  |
| 1   | 15-A  | 0.88         | 9/4280 (0.2%)  | 0.94        | 13/5848 (0.2%) |
| 1   | 15-B  | 0.87         | 7/4271 (0.2%)  | 0.98        | 14/5836 (0.2%) |
| 1   | 16-A  | 0.87         | 5/4280 (0.1%)  | 0.95        | 12/5848 (0.2%) |
| 1   | 16-B  | 0.85         | 2/4271 (0.0%)  | 0.94        | 11/5836 (0.2%) |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 1   | 17-A  | 0.86         | 2/4280 (0.0%)     | 0.98        | 14/5848 (0.2%)    |
| 1   | 17-B  | 0.87         | 6/4271 (0.1%)     | 0.95        | 10/5836 (0.2%)    |
| 1   | 18-A  | 0.91         | 6/4280 (0.1%)     | 0.98        | 16/5848 (0.3%)    |
| 1   | 18-B  | 0.87         | 5/4271 (0.1%)     | 0.95        | 11/5836 (0.2%)    |
| 1   | 19-A  | 0.86         | 5/4280 (0.1%)     | 0.96        | 17/5848 (0.3%)    |
| 1   | 19-B  | 0.83         | 7/4271 (0.2%)     | 0.93        | 11/5836 (0.2%)    |
| 1   | 20-A  | 0.88         | 4/4280 (0.1%)     | 0.95        | 11/5848 (0.2%)    |
| 1   | 20-B  | 0.84         | 6/4271 (0.1%)     | 0.98        | 16/5836 (0.3%)    |
| 1   | 21-A  | 0.85         | 5/4280 (0.1%)     | 0.94        | 12/5848 (0.2%)    |
| 1   | 21-B  | 0.81         | 4/4271 (0.1%)     | 0.91        | 8/5836 (0.1%)     |
| 1   | 22-A  | 0.89         | 8/4280 (0.2%)     | 1.02        | 21/5848 (0.4%)    |
| 1   | 22-B  | 0.87         | 6/4271 (0.1%)     | 0.95        | 13/5836 (0.2%)    |
| 1   | 23-A  | 0.89         | 4/4280 (0.1%)     | 0.98        | 15/5848 (0.3%)    |
| 1   | 23-B  | 0.88         | 8/4271 (0.2%)     | 0.98        | 8/5836 (0.1%)     |
| 1   | 24-A  | 0.85         | 2/4280 (0.0%)     | 0.95        | 12/5848 (0.2%)    |
| 1   | 24-B  | 0.85         | 5/4271 (0.1%)     | 0.95        | 8/5836 (0.1%)     |
| 1   | 25-A  | 0.86         | 3/4280 (0.1%)     | 0.99        | 14/5848 (0.2%)    |
| 1   | 25-B  | 0.85         | 4/4271 (0.1%)     | 0.95        | 8/5836 (0.1%)     |
| All | All   | 0.87         | 290/213775 (0.1%) | 0.96        | 610/292100 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 1   | 1-A   | 0                   | 1                   |
| 1   | 1-B   | 0                   | 4                   |
| 1   | 2-A   | 0                   | 3                   |
| 1   | 2-B   | 0                   | 2                   |
| 1   | 3-A   | 0                   | 1                   |
| 1   | 3-B   | 0                   | 2                   |
| 1   | 4-A   | 0                   | 2                   |
| 1   | 4-B   | 0                   | 1                   |
| 1   | 5-A   | 0                   | 2                   |
| 1   | 5-B   | 0                   | 1                   |
| 1   | 6-A   | 0                   | 5                   |
| 1   | 6-B   | 0                   | 1                   |
| 1   | 7-A   | 0                   | 3                   |
| 1   | 7-B   | 0                   | 1                   |
| 1   | 8-A   | 0                   | 3                   |
| 1   | 8-B   | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 9-A   | 0                   | 3                   |
| 1   | 9-B   | 0                   | 1                   |
| 1   | 10-A  | 0                   | 1                   |
| 1   | 10-B  | 0                   | 4                   |
| 1   | 11-A  | 0                   | 1                   |
| 1   | 12-A  | 0                   | 2                   |
| 1   | 12-B  | 0                   | 2                   |
| 1   | 13-A  | 0                   | 4                   |
| 1   | 13-B  | 0                   | 1                   |
| 1   | 14-A  | 0                   | 1                   |
| 1   | 14-B  | 0                   | 5                   |
| 1   | 15-A  | 0                   | 1                   |
| 1   | 15-B  | 0                   | 2                   |
| 1   | 16-A  | 0                   | 2                   |
| 1   | 16-B  | 0                   | 2                   |
| 1   | 17-A  | 0                   | 4                   |
| 1   | 17-B  | 1                   | 1                   |
| 1   | 18-A  | 0                   | 1                   |
| 1   | 18-B  | 0                   | 2                   |
| 1   | 19-A  | 0                   | 1                   |
| 1   | 19-B  | 0                   | 3                   |
| 1   | 20-A  | 0                   | 1                   |
| 1   | 20-B  | 0                   | 2                   |
| 1   | 21-A  | 0                   | 1                   |
| 1   | 21-B  | 0                   | 3                   |
| 1   | 22-A  | 0                   | 4                   |
| 1   | 22-B  | 0                   | 1                   |
| 1   | 23-A  | 0                   | 3                   |
| 1   | 23-B  | 0                   | 3                   |
| 1   | 24-A  | 0                   | 2                   |
| 1   | 24-B  | 0                   | 2                   |
| 1   | 25-A  | 0                   | 4                   |
| 1   | 25-B  | 0                   | 2                   |
| All | All   | 1                   | 105                 |

The worst 5 of 290 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | 2-A   | 457 | GLU  | CB-CG  | 10.83  | 1.72        | 1.52     |
| 1   | 24-B  | 211 | VAL  | CB-CG2 | -10.77 | 1.30        | 1.52     |
| 1   | 20-A  | 170 | TRP  | CB-CG  | -10.53 | 1.31        | 1.50     |
| 1   | 10-A  | 417 | VAL  | CB-CG2 | -10.53 | 1.30        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | 3-B   | 452 | GLU  | CB-CG | 9.69 | 1.70        | 1.52     |

The worst 5 of 610 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | 14-A  | 460 | ARG  | NE-CZ-NH2 | 14.57  | 127.59      | 120.30   |
| 1   | 10-B  | 180 | ARG  | NE-CZ-NH1 | 13.36  | 126.98      | 120.30   |
| 1   | 24-B  | 460 | ARG  | NE-CZ-NH2 | -13.32 | 113.64      | 120.30   |
| 1   | 17-A  | 538 | MET  | CG-SD-CE  | -12.78 | 79.76       | 100.20   |
| 1   | 5-B   | 97  | ASP  | CB-CG-OD1 | -12.62 | 106.94      | 118.30   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | 17-B  | 345 | ASP  | CA   |

5 of 105 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 1-A   | 73  | PRO  | Peptide |
| 1   | 1-B   | 193 | GLY  | Peptide |
| 1   | 1-B   | 292 | TRP  | Peptide |
| 1   | 1-B   | 299 | GLY  | Peptide |
| 1   | 1-B   | 401 | ALA  | 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   | 1-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 1-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 2-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 2-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 3-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 3-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 4-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 4-B   | 4158  | 3901     | 3913     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 5-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 5-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 6-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 6-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 7-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 7-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 8-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 8-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 9-A   | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 9-B   | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 10-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 10-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 11-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 11-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 12-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 12-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 13-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 13-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 14-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 14-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 15-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 15-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 16-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 16-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 17-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 17-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 18-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 18-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 19-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 19-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 20-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 20-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 21-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 21-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 22-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 22-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 23-A  | 4167  | 3907     | 3918     | 0       | 0            |
| 1   | 23-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 24-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 24-B  | 4158  | 3901     | 3913     | 0       | 0            |
| 1   | 25-A  | 4167  | 3907     | 3919     | 0       | 0            |
| 1   | 25-B  | 4158  | 3901     | 3913     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 1-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 1-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 2-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 2-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 3-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 3-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 4-C   | 67    | 0        | 55       | 0       | 0            |
| 2   | 4-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 5-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 5-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 6-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 6-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 7-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 7-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 8-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 8-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 9-C   | 67    | 0        | 56       | 0       | 0            |
| 2   | 9-E   | 67    | 0        | 56       | 0       | 0            |
| 2   | 10-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 10-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 11-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 11-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 12-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 12-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 13-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 13-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 14-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 14-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 15-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 15-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 16-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 16-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 17-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 17-E  | 67    | 0        | 55       | 0       | 0            |
| 2   | 18-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 18-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 19-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 19-E  | 67    | 0        | 55       | 0       | 0            |
| 2   | 20-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 20-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 21-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 21-E  | 67    | 0        | 56       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 22-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 22-E  | 67    | 0        | 55       | 0       | 0            |
| 2   | 23-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 23-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 24-C  | 67    | 0        | 55       | 0       | 0            |
| 2   | 24-E  | 67    | 0        | 56       | 0       | 0            |
| 2   | 25-C  | 67    | 0        | 56       | 0       | 0            |
| 2   | 25-E  | 67    | 0        | 56       | 0       | 0            |
| 3   | 1-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 1-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 2-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 2-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 3-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 3-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 4-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 4-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 5-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 5-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 6-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 6-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 7-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 7-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 8-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 8-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 9-D   | 56    | 0        | 47       | 0       | 0            |
| 3   | 9-F   | 56    | 0        | 47       | 0       | 0            |
| 3   | 10-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 10-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 11-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 11-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 12-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 12-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 13-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 13-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 14-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 14-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 15-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 15-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 16-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 16-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 17-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 17-F  | 56    | 0        | 47       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 18-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 18-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 19-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 19-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 20-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 20-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 21-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 21-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 22-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 22-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 23-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 23-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 24-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 24-F  | 56    | 0        | 47       | 0       | 0            |
| 3   | 25-D  | 56    | 0        | 47       | 0       | 0            |
| 3   | 25-F  | 56    | 0        | 47       | 0       | 0            |
| 4   | 1-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 1-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 2-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 2-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 3-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 3-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 4-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 4-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 5-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 5-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 6-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 6-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 7-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 7-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 8-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 8-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 9-A   | 4     | 6        | 6        | 0       | 0            |
| 4   | 9-B   | 4     | 6        | 6        | 0       | 0            |
| 4   | 10-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 10-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 11-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 11-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 12-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 12-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 13-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 13-B  | 4     | 6        | 6        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | 14-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 14-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 15-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 15-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 16-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 16-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 17-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 17-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 18-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 18-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 19-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 19-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 20-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 20-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 21-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 21-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 22-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 22-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 23-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 23-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 24-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 24-B  | 4     | 6        | 6        | 0       | 0            |
| 4   | 25-A  | 4     | 6        | 6        | 0       | 0            |
| 4   | 25-B  | 4     | 6        | 6        | 0       | 0            |
| 5   | 1-A   | 355   | 0        | 0        | 0       | 0            |
| 5   | 1-B   | 381   | 0        | 0        | 0       | 0            |
| 5   | 2-A   | 362   | 0        | 0        | 0       | 0            |
| 5   | 2-B   | 369   | 0        | 0        | 0       | 0            |
| 5   | 3-A   | 360   | 0        | 0        | 0       | 0            |
| 5   | 3-B   | 348   | 0        | 0        | 0       | 0            |
| 5   | 4-A   | 370   | 0        | 0        | 0       | 0            |
| 5   | 4-B   | 377   | 0        | 0        | 0       | 0            |
| 5   | 5-A   | 364   | 0        | 0        | 0       | 0            |
| 5   | 5-B   | 350   | 0        | 0        | 0       | 0            |
| 5   | 6-A   | 356   | 0        | 0        | 0       | 0            |
| 5   | 6-B   | 364   | 0        | 0        | 0       | 0            |
| 5   | 7-A   | 325   | 0        | 0        | 0       | 0            |
| 5   | 7-B   | 377   | 0        | 0        | 0       | 0            |
| 5   | 8-A   | 356   | 0        | 0        | 0       | 0            |
| 5   | 8-B   | 372   | 0        | 0        | 0       | 0            |
| 5   | 9-A   | 327   | 0        | 0        | 0       | 0            |
| 5   | 9-B   | 353   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 5   | 10-A  | 365    | 0        | 0        | 0       | 0            |
| 5   | 10-B  | 367    | 0        | 0        | 0       | 0            |
| 5   | 11-A  | 361    | 0        | 0        | 0       | 0            |
| 5   | 11-B  | 357    | 0        | 0        | 0       | 0            |
| 5   | 12-A  | 360    | 0        | 0        | 0       | 0            |
| 5   | 12-B  | 379    | 0        | 0        | 0       | 0            |
| 5   | 13-A  | 335    | 0        | 0        | 0       | 0            |
| 5   | 13-B  | 360    | 0        | 0        | 0       | 0            |
| 5   | 14-A  | 359    | 0        | 0        | 0       | 0            |
| 5   | 14-B  | 392    | 0        | 0        | 0       | 0            |
| 5   | 15-A  | 348    | 0        | 0        | 0       | 0            |
| 5   | 15-B  | 373    | 0        | 0        | 0       | 0            |
| 5   | 16-A  | 369    | 0        | 0        | 0       | 0            |
| 5   | 16-B  | 361    | 0        | 0        | 0       | 0            |
| 5   | 17-A  | 351    | 0        | 0        | 0       | 0            |
| 5   | 17-B  | 377    | 0        | 0        | 0       | 0            |
| 5   | 18-A  | 349    | 0        | 0        | 0       | 0            |
| 5   | 18-B  | 373    | 0        | 0        | 0       | 0            |
| 5   | 19-A  | 346    | 0        | 0        | 0       | 0            |
| 5   | 19-B  | 355    | 0        | 0        | 0       | 0            |
| 5   | 20-A  | 324    | 0        | 0        | 0       | 0            |
| 5   | 20-B  | 372    | 0        | 0        | 0       | 0            |
| 5   | 21-A  | 347    | 0        | 0        | 0       | 0            |
| 5   | 21-B  | 370    | 0        | 0        | 0       | 0            |
| 5   | 22-A  | 338    | 0        | 0        | 0       | 0            |
| 5   | 22-B  | 386    | 0        | 0        | 0       | 0            |
| 5   | 23-A  | 366    | 0        | 0        | 0       | 0            |
| 5   | 23-B  | 332    | 0        | 0        | 0       | 0            |
| 5   | 24-A  | 364    | 0        | 0        | 0       | 0            |
| 5   | 24-B  | 360    | 0        | 0        | 0       | 0            |
| 5   | 25-A  | 359    | 0        | 0        | 0       | 0            |
| 5   | 25-B  | 372    | 0        | 0        | 0       | 0            |
| All | All   | 232468 | 195500   | 201244   | 0       | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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   | 1-A   | 547/549 (100%) | 500 (91%) | 38 (7%) | 9 (2%)   | 9           | 1   |
| 1   | 1-B   | 546/549 (100%) | 515 (94%) | 28 (5%) | 3 (0%)   | 29          | 12  |
| 1   | 2-A   | 547/549 (100%) | 509 (93%) | 35 (6%) | 3 (0%)   | 29          | 12  |
| 1   | 2-B   | 546/549 (100%) | 510 (93%) | 31 (6%) | 5 (1%)   | 17          | 5   |
| 1   | 3-A   | 547/549 (100%) | 511 (93%) | 34 (6%) | 2 (0%)   | 34          | 17  |
| 1   | 3-B   | 546/549 (100%) | 506 (93%) | 34 (6%) | 6 (1%)   | 14          | 3   |
| 1   | 4-A   | 547/549 (100%) | 505 (92%) | 32 (6%) | 10 (2%)  | 8           | 1   |
| 1   | 4-B   | 546/549 (100%) | 509 (93%) | 36 (7%) | 1 (0%)   | 47          | 29  |
| 1   | 5-A   | 547/549 (100%) | 510 (93%) | 29 (5%) | 8 (2%)   | 10          | 2   |
| 1   | 5-B   | 546/549 (100%) | 509 (93%) | 29 (5%) | 8 (2%)   | 10          | 2   |
| 1   | 6-A   | 547/549 (100%) | 505 (92%) | 36 (7%) | 6 (1%)   | 14          | 3   |
| 1   | 6-B   | 546/549 (100%) | 513 (94%) | 27 (5%) | 6 (1%)   | 14          | 3   |
| 1   | 7-A   | 547/549 (100%) | 511 (93%) | 30 (6%) | 6 (1%)   | 14          | 3   |
| 1   | 7-B   | 546/549 (100%) | 511 (94%) | 29 (5%) | 6 (1%)   | 14          | 3   |
| 1   | 8-A   | 547/549 (100%) | 511 (93%) | 29 (5%) | 7 (1%)   | 12          | 2   |
| 1   | 8-B   | 546/549 (100%) | 510 (93%) | 28 (5%) | 8 (2%)   | 10          | 2   |
| 1   | 9-A   | 547/549 (100%) | 507 (93%) | 32 (6%) | 8 (2%)   | 10          | 2   |
| 1   | 9-B   | 546/549 (100%) | 511 (94%) | 32 (6%) | 3 (0%)   | 29          | 12  |
| 1   | 10-A  | 547/549 (100%) | 507 (93%) | 34 (6%) | 6 (1%)   | 14          | 3   |
| 1   | 10-B  | 546/549 (100%) | 504 (92%) | 31 (6%) | 11 (2%)  | 7           | 1   |
| 1   | 11-A  | 547/549 (100%) | 514 (94%) | 33 (6%) | 0        | 100         | 100 |
| 1   | 11-B  | 546/549 (100%) | 507 (93%) | 35 (6%) | 4 (1%)   | 22          | 8   |
| 1   | 12-A  | 547/549 (100%) | 509 (93%) | 30 (6%) | 8 (2%)   | 10          | 2   |
| 1   | 12-B  | 546/549 (100%) | 507 (93%) | 31 (6%) | 8 (2%)   | 10          | 2   |
| 1   | 13-A  | 547/549 (100%) | 510 (93%) | 30 (6%) | 7 (1%)   | 12          | 2   |

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| Mol | Chain | Analysed           | Favoured    | Allowed   | Outliers | Percentiles |    |
|-----|-------|--------------------|-------------|-----------|----------|-------------|----|
| 1   | 13-B  | 546/549 (100%)     | 506 (93%)   | 34 (6%)   | 6 (1%)   | 14          | 3  |
| 1   | 14-A  | 547/549 (100%)     | 509 (93%)   | 28 (5%)   | 10 (2%)  | 8           | 1  |
| 1   | 14-B  | 546/549 (100%)     | 504 (92%)   | 29 (5%)   | 13 (2%)  | 6           | 1  |
| 1   | 15-A  | 547/549 (100%)     | 510 (93%)   | 28 (5%)   | 9 (2%)   | 9           | 1  |
| 1   | 15-B  | 546/549 (100%)     | 506 (93%)   | 33 (6%)   | 7 (1%)   | 12          | 2  |
| 1   | 16-A  | 547/549 (100%)     | 514 (94%)   | 27 (5%)   | 6 (1%)   | 14          | 3  |
| 1   | 16-B  | 546/549 (100%)     | 511 (94%)   | 28 (5%)   | 7 (1%)   | 12          | 2  |
| 1   | 17-A  | 547/549 (100%)     | 505 (92%)   | 29 (5%)   | 13 (2%)  | 6           | 1  |
| 1   | 17-B  | 546/549 (100%)     | 509 (93%)   | 28 (5%)   | 9 (2%)   | 9           | 1  |
| 1   | 18-A  | 547/549 (100%)     | 507 (93%)   | 34 (6%)   | 6 (1%)   | 14          | 3  |
| 1   | 18-B  | 546/549 (100%)     | 509 (93%)   | 33 (6%)   | 4 (1%)   | 22          | 8  |
| 1   | 19-A  | 547/549 (100%)     | 505 (92%)   | 34 (6%)   | 8 (2%)   | 10          | 2  |
| 1   | 19-B  | 546/549 (100%)     | 506 (93%)   | 32 (6%)   | 8 (2%)   | 10          | 2  |
| 1   | 20-A  | 547/549 (100%)     | 515 (94%)   | 26 (5%)   | 6 (1%)   | 14          | 3  |
| 1   | 20-B  | 546/549 (100%)     | 506 (93%)   | 33 (6%)   | 7 (1%)   | 12          | 2  |
| 1   | 21-A  | 547/549 (100%)     | 508 (93%)   | 30 (6%)   | 9 (2%)   | 9           | 1  |
| 1   | 21-B  | 546/549 (100%)     | 514 (94%)   | 26 (5%)   | 6 (1%)   | 14          | 3  |
| 1   | 22-A  | 547/549 (100%)     | 510 (93%)   | 34 (6%)   | 3 (0%)   | 29          | 12 |
| 1   | 22-B  | 546/549 (100%)     | 501 (92%)   | 33 (6%)   | 12 (2%)  | 6           | 1  |
| 1   | 23-A  | 547/549 (100%)     | 496 (91%)   | 37 (7%)   | 14 (3%)  | 5           | 0  |
| 1   | 23-B  | 546/549 (100%)     | 510 (93%)   | 29 (5%)   | 7 (1%)   | 12          | 2  |
| 1   | 24-A  | 547/549 (100%)     | 504 (92%)   | 34 (6%)   | 9 (2%)   | 9           | 1  |
| 1   | 24-B  | 546/549 (100%)     | 514 (94%)   | 27 (5%)   | 5 (1%)   | 17          | 5  |
| 1   | 25-A  | 547/549 (100%)     | 501 (92%)   | 36 (7%)   | 10 (2%)  | 8           | 1  |
| 1   | 25-B  | 546/549 (100%)     | 508 (93%)   | 32 (6%)   | 6 (1%)   | 14          | 3  |
| All | All   | 27325/27450 (100%) | 25409 (93%) | 1567 (6%) | 349 (1%) | 12          | 2  |

5 of 349 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 58  | VAL  |
| 1   | 1-A   | 59  | VAL  |
| 1   | 1-A   | 61  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 63  | ASP  |
| 1   | 1-A   | 75  | THR  |

### 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   | 1-A   | 436/436 (100%) | 407 (93%) | 29 (7%)  | 16          | 3 |
| 1   | 1-B   | 435/436 (100%) | 404 (93%) | 31 (7%)  | 14          | 2 |
| 1   | 2-A   | 436/436 (100%) | 409 (94%) | 27 (6%)  | 18          | 4 |
| 1   | 2-B   | 435/436 (100%) | 401 (92%) | 34 (8%)  | 12          | 2 |
| 1   | 3-A   | 436/436 (100%) | 413 (95%) | 23 (5%)  | 22          | 5 |
| 1   | 3-B   | 435/436 (100%) | 401 (92%) | 34 (8%)  | 12          | 2 |
| 1   | 4-A   | 436/436 (100%) | 401 (92%) | 35 (8%)  | 12          | 1 |
| 1   | 4-B   | 435/436 (100%) | 402 (92%) | 33 (8%)  | 13          | 2 |
| 1   | 5-A   | 436/436 (100%) | 397 (91%) | 39 (9%)  | 9           | 1 |
| 1   | 5-B   | 435/436 (100%) | 405 (93%) | 30 (7%)  | 15          | 2 |
| 1   | 6-A   | 436/436 (100%) | 402 (92%) | 34 (8%)  | 12          | 2 |
| 1   | 6-B   | 435/436 (100%) | 405 (93%) | 30 (7%)  | 15          | 2 |
| 1   | 7-A   | 436/436 (100%) | 411 (94%) | 25 (6%)  | 20          | 5 |
| 1   | 7-B   | 435/436 (100%) | 407 (94%) | 28 (6%)  | 17          | 3 |
| 1   | 8-A   | 436/436 (100%) | 411 (94%) | 25 (6%)  | 20          | 5 |
| 1   | 8-B   | 435/436 (100%) | 400 (92%) | 35 (8%)  | 12          | 1 |
| 1   | 9-A   | 436/436 (100%) | 405 (93%) | 31 (7%)  | 14          | 2 |
| 1   | 9-B   | 435/436 (100%) | 412 (95%) | 23 (5%)  | 22          | 5 |
| 1   | 10-A  | 436/436 (100%) | 407 (93%) | 29 (7%)  | 16          | 3 |
| 1   | 10-B  | 435/436 (100%) | 409 (94%) | 26 (6%)  | 19          | 4 |
| 1   | 11-A  | 436/436 (100%) | 411 (94%) | 25 (6%)  | 20          | 5 |
| 1   | 11-B  | 435/436 (100%) | 406 (93%) | 29 (7%)  | 16          | 3 |

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| Mol | Chain | Analysed           | Rotameric   | Outliers  | Percentiles |   |
|-----|-------|--------------------|-------------|-----------|-------------|---|
| 1   | 12-A  | 436/436 (100%)     | 405 (93%)   | 31 (7%)   | 14          | 2 |
| 1   | 12-B  | 435/436 (100%)     | 411 (94%)   | 24 (6%)   | 21          | 5 |
| 1   | 13-A  | 436/436 (100%)     | 403 (92%)   | 33 (8%)   | 13          | 2 |
| 1   | 13-B  | 435/436 (100%)     | 410 (94%)   | 25 (6%)   | 20          | 5 |
| 1   | 14-A  | 436/436 (100%)     | 404 (93%)   | 32 (7%)   | 14          | 2 |
| 1   | 14-B  | 435/436 (100%)     | 403 (93%)   | 32 (7%)   | 13          | 2 |
| 1   | 15-A  | 436/436 (100%)     | 403 (92%)   | 33 (8%)   | 13          | 2 |
| 1   | 15-B  | 435/436 (100%)     | 406 (93%)   | 29 (7%)   | 16          | 3 |
| 1   | 16-A  | 436/436 (100%)     | 404 (93%)   | 32 (7%)   | 14          | 2 |
| 1   | 16-B  | 435/436 (100%)     | 405 (93%)   | 30 (7%)   | 15          | 2 |
| 1   | 17-A  | 436/436 (100%)     | 400 (92%)   | 36 (8%)   | 11          | 1 |
| 1   | 17-B  | 435/436 (100%)     | 403 (93%)   | 32 (7%)   | 13          | 2 |
| 1   | 18-A  | 436/436 (100%)     | 405 (93%)   | 31 (7%)   | 14          | 2 |
| 1   | 18-B  | 435/436 (100%)     | 415 (95%)   | 20 (5%)   | 27          | 8 |
| 1   | 19-A  | 436/436 (100%)     | 412 (94%)   | 24 (6%)   | 21          | 5 |
| 1   | 19-B  | 435/436 (100%)     | 409 (94%)   | 26 (6%)   | 19          | 4 |
| 1   | 20-A  | 436/436 (100%)     | 411 (94%)   | 25 (6%)   | 20          | 5 |
| 1   | 20-B  | 435/436 (100%)     | 401 (92%)   | 34 (8%)   | 12          | 2 |
| 1   | 21-A  | 436/436 (100%)     | 406 (93%)   | 30 (7%)   | 15          | 2 |
| 1   | 21-B  | 435/436 (100%)     | 407 (94%)   | 28 (6%)   | 17          | 3 |
| 1   | 22-A  | 436/436 (100%)     | 400 (92%)   | 36 (8%)   | 11          | 1 |
| 1   | 22-B  | 435/436 (100%)     | 400 (92%)   | 35 (8%)   | 12          | 1 |
| 1   | 23-A  | 436/436 (100%)     | 402 (92%)   | 34 (8%)   | 12          | 2 |
| 1   | 23-B  | 435/436 (100%)     | 398 (92%)   | 37 (8%)   | 10          | 1 |
| 1   | 24-A  | 436/436 (100%)     | 406 (93%)   | 30 (7%)   | 15          | 2 |
| 1   | 24-B  | 435/436 (100%)     | 407 (94%)   | 28 (6%)   | 17          | 3 |
| 1   | 25-A  | 436/436 (100%)     | 402 (92%)   | 34 (8%)   | 12          | 2 |
| 1   | 25-B  | 435/436 (100%)     | 406 (93%)   | 29 (7%)   | 16          | 3 |
| All | All   | 21775/21800 (100%) | 20270 (93%) | 1505 (7%) | 15          | 2 |

5 of 1505 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 12-A  | 468 | LYS  |
| 1   | 15-A  | 251 | GLU  |
| 1   | 24-A  | 210 | GLU  |
| 1   | 12-B  | 340 | GLN  |
| 1   | 13-B  | 531 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 451 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 13-A  | 325 | GLN  |
| 1   | 16-A  | 109 | ASN  |
| 1   | 24-A  | 515 | ASN  |
| 1   | 13-B  | 114 | GLN  |
| 1   | 14-B  | 306 | GLN  |

### 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 ⓘ

550 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  | 1-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)     | 17,17,17    | 1.36 | 2 (11%)     |
| 2   | BGC  | 1-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)     | 15,15,17    | 1.43 | 2 (13%)     |
| 2   | BGC  | 1-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)     | 15,15,17    | 1.32 | 1 (6%)      |
| 2   | BGC  | 1-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)      | 15,15,17    | 1.69 | 3 (20%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 1-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 1-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 1-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 1-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 1-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 1-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 1-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 1-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 1-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 1-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 1-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 1-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 1-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 1-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 1-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 1-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 1-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 1-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 10-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 10-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 10-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 10-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 10-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 10-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 10-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 10-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 10-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 10-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 10-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 10-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 10-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 10-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 10-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 10-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 10-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 10-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 10-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 10-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 10-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 10-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 11-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 11-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 11-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 11-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 11-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 11-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 11-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 11-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 11-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 11-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 11-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 11-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 11-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 11-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 11-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 11-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 11-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 11-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 11-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 11-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 11-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 11-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 12-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 12-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 12-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 12-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 12-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 12-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 12-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 12-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 12-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 12-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 12-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 12-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 12-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 12-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 12-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 12-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 12-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 12-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 12-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 12-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 12-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 12-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 13-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 13-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 13-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 13-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 13-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 13-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 13-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 13-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 13-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 13-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 13-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 13-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 13-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 13-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 13-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 13-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 13-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 13-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 13-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 13-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 13-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 13-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 14-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 14-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 14-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 14-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 14-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 14-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 14-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 14-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 14-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 14-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 14-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 14-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 14-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 14-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 14-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 14-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 14-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 14-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 14-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 14-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 14-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 14-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 15-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 15-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 15-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 15-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 15-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 15-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 15-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 15-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 15-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 15-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 15-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 15-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 15-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 15-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 15-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 15-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 15-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 15-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 15-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 15-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 15-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 15-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 16-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 16-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 16-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 16-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 16-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 16-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 16-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 16-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 16-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 16-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 16-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 16-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 16-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 16-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 16-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 16-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 16-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 16-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 16-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 16-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 16-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 16-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 17-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 17-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 17-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 17-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 17-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 17-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 17-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 17-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 17-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 17-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 17-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 17-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 17-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 17-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 17-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 17-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 17-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 17-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 17-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 17-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 17-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 17-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 18-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 18-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 18-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 18-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 18-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 18-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 18-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 18-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 18-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 18-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 18-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 18-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 18-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 18-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 18-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 18-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 18-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 18-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 18-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 18-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 18-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 18-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 19-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 19-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 19-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 19-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 19-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 19-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 19-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 19-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 19-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 19-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 19-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 19-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 19-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 19-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 19-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 19-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 19-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 19-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 19-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 19-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 19-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 19-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 2-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 2-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 2-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 2-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 2-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 2-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 2-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 2-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 2-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 2-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 2-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 2-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 2-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 2-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 2-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 2-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 2-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 2-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 2-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 2-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 2-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 2-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 20-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 20-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 20-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 20-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 20-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 20-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 20-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 20-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 20-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 20-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 20-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 20-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 20-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 20-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 20-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 20-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 20-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 20-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 20-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 20-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 20-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 20-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 21-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 21-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 21-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 21-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 21-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 21-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 21-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 21-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 21-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 21-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 21-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 21-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 21-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 21-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 21-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 21-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 21-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 21-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 21-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 21-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 21-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 21-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 22-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 22-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 22-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 22-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 22-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 22-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 22-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 22-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 22-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 22-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 22-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 22-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 22-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 22-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 22-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 22-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 22-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 22-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 22-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 22-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 22-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 22-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 23-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 23-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 23-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 23-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 23-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 23-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 23-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 23-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 23-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 23-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 23-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 23-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 23-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 23-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 23-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 23-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 23-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 23-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 23-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 23-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 23-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 23-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 24-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 24-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 24-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 24-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 24-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 24-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 24-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 24-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 24-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 24-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 24-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 24-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 24-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 24-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 24-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 24-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 24-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 24-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 24-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 24-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 24-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 24-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 25-C  | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 25-C  | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 25-C  | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 25-C  | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 25-C  | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 25-C  | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 25-D  | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 25-D  | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 25-D  | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 25-D  | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 25-D  | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 25-E  | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 25-E  | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 25-E  | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 25-E  | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 25-E  | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 25-E  | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 25-F  | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 25-F  | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 25-F  | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 25-F  | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 25-F  | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 3-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 3-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 3-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 3-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 3-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 3-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 3-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 3-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 3-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 3-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 3-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 3-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 3-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 3-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 3-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 3-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 3-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 3-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 3-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 3-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 3-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 3-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 4-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 4-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 4-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 4-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 4-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 4-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 4-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 4-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 4-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 4-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 4-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 4-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 4-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 4-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 4-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 4-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 4-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 4-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 4-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 4-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 4-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 4-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 5-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 5-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 5-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 5-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 5-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 5-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 5-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 5-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 5-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 5-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 5-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 5-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 5-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 5-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 5-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 5-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 5-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 5-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 5-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 5-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 5-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 5-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 6-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 6-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 6-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 6-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 6-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 6-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 6-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 6-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 6-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 6-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 6-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 6-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 6-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 6-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 6-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 6-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 6-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 6-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 6-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 6-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 6-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 6-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 7-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 7-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 7-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 7-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 7-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 7-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 7-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 7-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 7-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 7-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BGC  | 7-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 7-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 7-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 7-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 7-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 7-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 7-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 7-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 7-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 7-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 7-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 7-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 8-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |
| 2   | BGC  | 8-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 8-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 8-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 8-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 8-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 8-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 8-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 8-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 8-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 8-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 8-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 8-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 8-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 8-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 8-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 8-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 8-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 8-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 8-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 8-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 8-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 0        |
| 2   | BGC  | 9-C   | 1   | 2    | 12,12,12     | 1.59 | 3 (25%)  | 17,17,17    | 1.36 | 2 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | BGC  | 9-C   | 2   | 2    | 11,11,12     | 1.41 | 3 (27%)  | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 9-C   | 3   | 2    | 11,11,12     | 1.51 | 3 (27%)  | 15,15,17    | 1.32 | 1 (6%)   |
| 2   | BGC  | 9-C   | 4   | 2    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.69 | 3 (20%)  |
| 2   | BGC  | 9-C   | 5   | 2    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 2   | BGC  | 9-C   | 6   | 2    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.37 | 3 (20%)  |
| 3   | BGC  | 9-D   | 1   | 3    | 12,12,12     | 1.29 | 1 (8%)   | 17,17,17    | 1.08 | 0        |
| 3   | BGC  | 9-D   | 2   | 3    | 11,11,12     | 1.46 | 1 (9%)   | 15,15,17    | 1.55 | 1 (6%)   |
| 3   | BGC  | 9-D   | 3   | 3    | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.53 | 3 (20%)  |
| 3   | BGC  | 9-D   | 4   | 3    | 11,11,12     | 1.34 | 2 (18%)  | 15,15,17    | 1.23 | 1 (6%)   |
| 3   | BGC  | 9-D   | 5   | 3    | 11,11,12     | 1.56 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 2   | BGC  | 9-E   | 1   | 2    | 12,12,12     | 1.57 | 3 (25%)  | 17,17,17    | 1.08 | 0        |
| 2   | BGC  | 9-E   | 2   | 2    | 11,11,12     | 1.49 | 3 (27%)  | 15,15,17    | 1.29 | 2 (13%)  |
| 2   | BGC  | 9-E   | 3   | 2    | 11,11,12     | 1.38 | 1 (9%)   | 15,15,17    | 1.36 | 2 (13%)  |
| 2   | BGC  | 9-E   | 4   | 2    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 2   | BGC  | 9-E   | 5   | 2    | 11,11,12     | 1.29 | 2 (18%)  | 15,15,17    | 2.09 | 2 (13%)  |
| 2   | BGC  | 9-E   | 6   | 2    | 11,11,12     | 1.42 | 3 (27%)  | 15,15,17    | 1.07 | 1 (6%)   |
| 3   | BGC  | 9-F   | 1   | 3    | 12,12,12     | 1.32 | 2 (16%)  | 17,17,17    | 1.00 | 1 (5%)   |
| 3   | BGC  | 9-F   | 2   | 3    | 11,11,12     | 1.57 | 1 (9%)   | 15,15,17    | 1.68 | 3 (20%)  |
| 3   | BGC  | 9-F   | 3   | 3    | 11,11,12     | 1.33 | 1 (9%)   | 15,15,17    | 2.83 | 3 (20%)  |
| 3   | BGC  | 9-F   | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | BGC  | 9-F   | 5   | 3    | 11,11,12     | 1.75 | 1 (9%)   | 15,15,17    | 0.86 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 1-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 1-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 1-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BGC  | 1-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 1-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 1-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 1-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 1-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 10-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 10-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 10-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 10-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 10-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 10-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 11-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 11-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 11-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 11-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 11-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 11-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 11-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 12-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 12-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 12-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 12-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 12-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 12-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 13-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 13-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 13-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 13-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 13-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 13-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 13-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 14-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 14-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 14-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 14-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 14-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BGC  | 14-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 14-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 15-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 15-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 15-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 15-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 15-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 15-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 16-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 16-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 16-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 16-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 16-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 16-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 16-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 17-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 17-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 17-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 17-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 17-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 17-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 18-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 18-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 18-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 18-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 18-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 18-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 19-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 19-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 19-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 19-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 19-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 19-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 2-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 2-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BGC  | 2-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 2-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 2-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 2-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 2-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 20-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 20-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 20-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 20-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 20-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 20-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 21-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 21-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 21-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 21-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 21-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 21-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 21-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 22-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 22-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 22-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 22-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 22-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 22-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 23-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 23-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 23-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 23-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 23-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 23-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 23-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 24-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 24-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 24-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 24-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BGC  | 24-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 24-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-C  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 25-C  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-C  | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-C  | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-C  | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-C  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-D  | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 25-D  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-D  | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-D  | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-D  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-E  | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 25-E  | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-E  | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-E  | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-E  | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 25-E  | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-F  | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 25-F  | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-F  | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-F  | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 25-F  | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 3-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 3-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 3-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 3-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 3-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 3-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 3-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 4-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 4-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 4-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 4-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 4-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 4-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 5-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 5-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BGC  | 5-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 5-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 5-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 5-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 5-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 6-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 6-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 6-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 6-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 6-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 6-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 7-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BGC  | 7-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 7-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 7-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 7-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 7-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 7-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 8-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 8-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 8-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 8-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 8-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 8-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-C   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 9-C   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | BGC  | 9-C   | 3   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-C   | 4   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-C   | 5   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-C   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-D   | 1   | 3    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 9-D   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-D   | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-D   | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-D   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-E   | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | BGC  | 9-E   | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-E   | 3   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-E   | 4   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-E   | 5   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | BGC  | 9-E   | 6   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-F   | 1   | 3    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | BGC  | 9-F   | 2   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-F   | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-F   | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | BGC  | 9-F   | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |

The worst 5 of 975 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | 16-F  | 5   | BGC  | C2-C3 | -4.68 | 1.45        | 1.52     |
| 3   | 11-F  | 5   | BGC  | C2-C3 | -4.68 | 1.45        | 1.52     |
| 3   | 7-F   | 5   | BGC  | C2-C3 | -4.68 | 1.45        | 1.52     |
| 3   | 21-F  | 5   | BGC  | C2-C3 | -4.68 | 1.45        | 1.52     |
| 3   | 3-F   | 5   | BGC  | C2-C3 | -4.68 | 1.45        | 1.52     |

The worst 5 of 900 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | 22-F  | 3   | BGC  | C1-O5-C5 | 9.37 | 124.88      | 112.19   |
| 3   | 3-F   | 3   | BGC  | C1-O5-C5 | 9.37 | 124.88      | 112.19   |
| 3   | 20-F  | 3   | BGC  | C1-O5-C5 | 9.37 | 124.88      | 112.19   |
| 3   | 18-F  | 3   | BGC  | C1-O5-C5 | 9.37 | 124.88      | 112.19   |
| 3   | 16-F  | 3   | BGC  | C1-O5-C5 | 9.37 | 124.88      | 112.19   |

There are no chirality outliers.

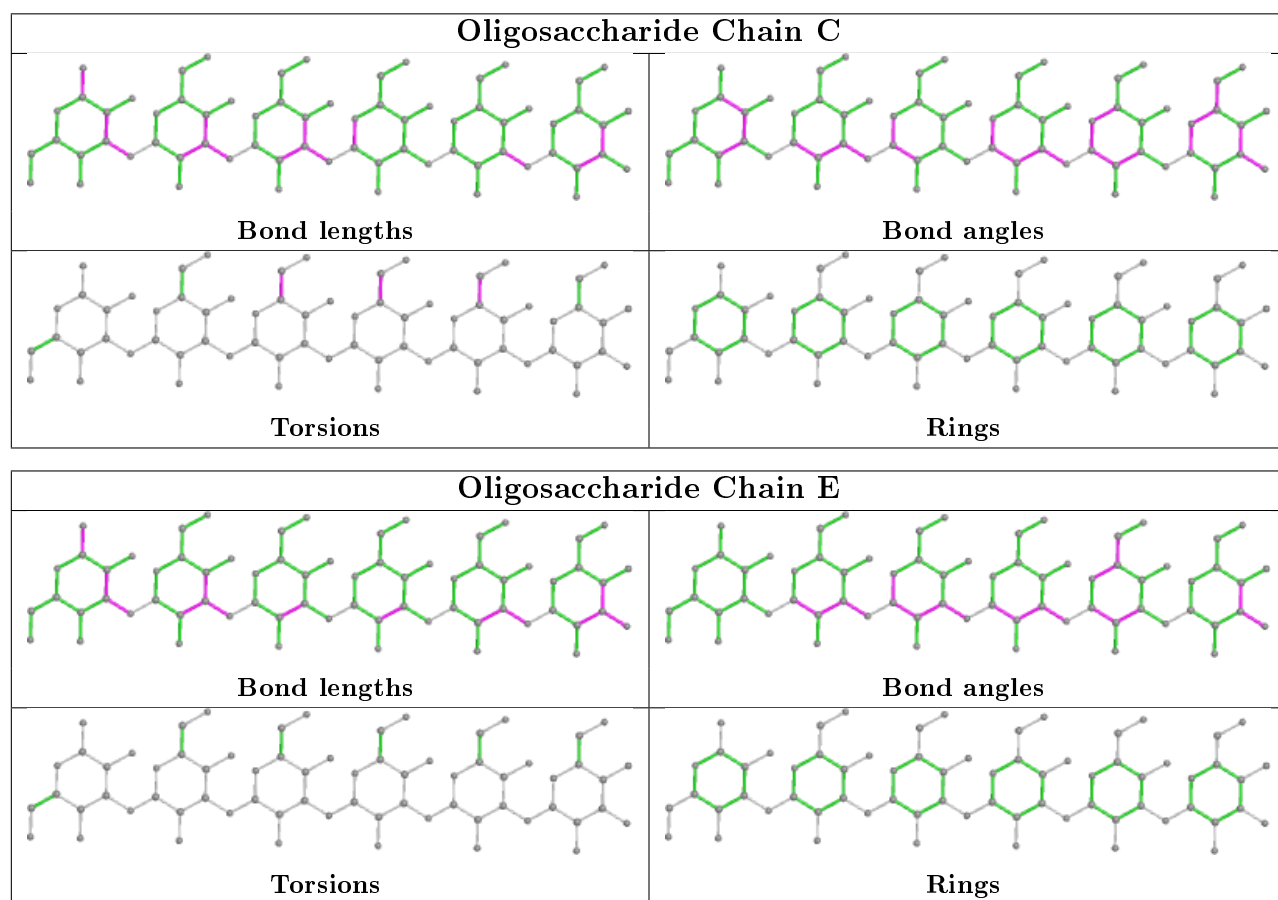
5 of 275 torsion outliers are listed below:

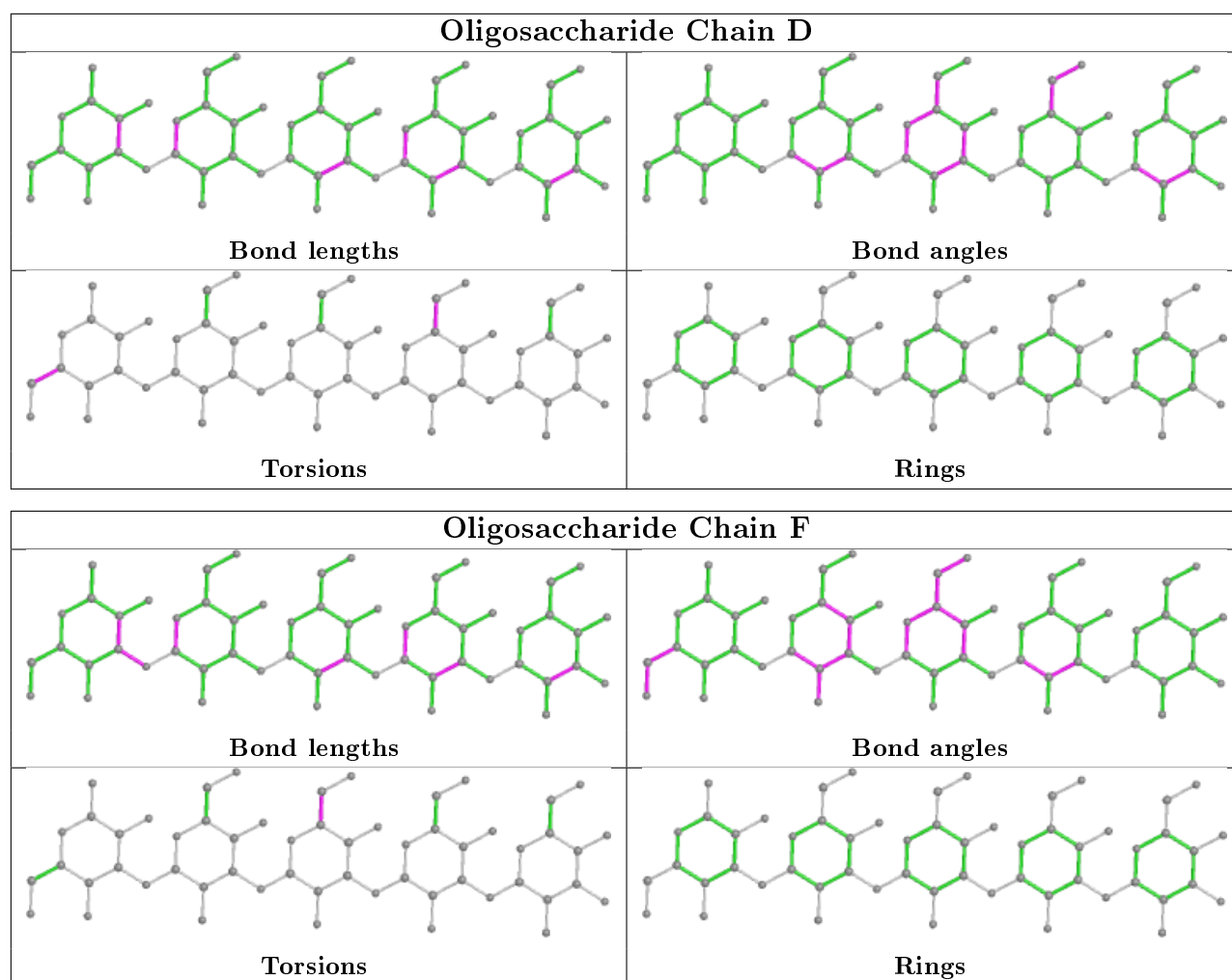
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | 4-D   | 1   | BGC  | O5-C5-C6-O6 |
| 3   | 10-D  | 1   | BGC  | O5-C5-C6-O6 |
| 3   | 5-D   | 1   | BGC  | O5-C5-C6-O6 |
| 3   | 7-D   | 1   | BGC  | O5-C5-C6-O6 |
| 3   | 14-D  | 1   | BGC  | O5-C5-C6-O6 |

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.





## 5.6 Ligand geometry [i](#)

50 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 | $\# Z  > 2$ |
| 4   | EDO  | 5-A   | 701 | -    | 3,3,3        | 0.53 | 0           | 2,2,2       | 0.20 | 0           |
| 4   | EDO  | 17-A  | 701 | -    | 3,3,3        | 0.53 | 0           | 2,2,2       | 0.20 | 0           |
| 4   | EDO  | 21-B  | 701 | -    | 3,3,3        | 0.62 | 0           | 2,2,2       | 0.74 | 0           |
| 4   | EDO  | 23-A  | 701 | -    | 3,3,3        | 0.53 | 0           | 2,2,2       | 0.20 | 0           |
| 4   | EDO  | 13-B  | 701 | -    | 3,3,3        | 0.62 | 0           | 2,2,2       | 0.74 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | EDO  | 19-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 22-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 10-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 1-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 6-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 23-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 14-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 15-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 9-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 10-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 11-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 1-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 20-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 5-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 12-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 8-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 13-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 18-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 22-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 12-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 2-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 14-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 16-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 3-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 17-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 7-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 2-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 25-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 4-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 16-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 21-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 24-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 3-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 18-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 7-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 19-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 25-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 24-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 6-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 4-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 15-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 8-A   | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | 20-B  | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | EDO  | 9-B   | 701 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.74 | 0        |
| 4   | EDO  | 11-A  | 701 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.20 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4   | EDO  | 5-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 17-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 21-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 23-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 13-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 19-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 22-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 10-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 1-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 6-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 23-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 14-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 15-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 9-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 10-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 11-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 1-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 20-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 5-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 12-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 8-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 13-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 18-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 22-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 12-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 2-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 14-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 16-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 3-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 17-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 7-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 2-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 25-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 4-B   | 701 | -    | -       | 1/1/1/1  | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 4   | EDO  | 16-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 21-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 24-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 3-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 18-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 7-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 19-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 25-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 24-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 6-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 4-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 15-A  | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 8-A   | 701 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | 20-B  | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 9-B   | 701 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | 11-A  | 701 | -    | -       | 0/1/1/1  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | 21-B  | 701 | EDO  | O1-C1-C2-O2 |
| 4   | 13-B  | 701 | EDO  | O1-C1-C2-O2 |
| 4   | 22-B  | 701 | EDO  | O1-C1-C2-O2 |
| 4   | 23-B  | 701 | EDO  | O1-C1-C2-O2 |
| 4   | 15-B  | 701 | EDO  | O1-C1-C2-O2 |

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

### 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   | 1-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 1-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 2-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 2-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 3-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 3-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 4-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 4-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 5-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 5-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 6-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 6-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 7-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 7-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 8-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 8-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 9-A   | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 9-B   | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 10-A  | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 10-B  | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 11-A  | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 11-B  | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |
| 1   | 12-A  | 549/549 (100%) | 0.24   | 41 (7%) | 14 19 | 13, 14, 15, 16        | 549 (100%) |
| 1   | 12-B  | 548/549 (99%)  | 0.17   | 42 (7%) | 13 18 | 13, 14, 15, 16        | 548 (100%) |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9        |
|-----|-------|-------------------|--------|-----------------|-----------------------|--------------|
| 1   | 13-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 13-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 14-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 14-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 15-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 15-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 16-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 16-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 17-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 17-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 18-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 18-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 19-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 19-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 20-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 20-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 21-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 21-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 22-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 22-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 23-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 23-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 24-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 24-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| 1   | 25-A  | 549/549 (100%)    | 0.24   | 41 (7%) 14 19   | 13, 14, 15, 16        | 549 (100%)   |
| 1   | 25-B  | 548/549 (99%)     | 0.17   | 42 (7%) 13 18   | 13, 14, 15, 16        | 548 (100%)   |
| All | All   | 27425/27450 (99%) | 0.21   | 2075 (7%) 16 18 | 13, 14, 15, 16        | 27425 (100%) |

The worst 5 of 2075 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 57  | GLU  | 10.3 |
| 1   | 2-A   | 57  | GLU  | 10.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 3-A   | 57  | GLU  | 10.3 |
| 1   | 4-A   | 57  | GLU  | 10.3 |
| 1   | 5-A   | 57  | GLU  | 10.3 |

## 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | BGC  | 4-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 10-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 5-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 7-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 14-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 18-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 24-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 15-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 11-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 19-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 13-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 3-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 6-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 17-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 1-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 8-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 23-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 25-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 22-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 12-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 20-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 2-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 21-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 9-D   | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |
| 3   | BGC  | 16-D  | 1   | 12/12 | 0.83 | 0.29 | 35,43,47,53                | 12    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BGC  | 22-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 24-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 14-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 2-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 17-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 9-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 18-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 8-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 16-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 4-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 20-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 7-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 23-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 21-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 1-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 10-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 5-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 6-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 25-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 13-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 19-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 3-F   | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 15-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 11-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 12-F  | 1   | 12/12 | 0.90 | 0.29 | 27,35,46,66                 | 12    |
| 3   | BGC  | 25-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 18-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 6-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 5-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 15-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 22-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 1-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 23-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 19-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 9-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 13-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 24-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 16-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 3-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 2-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 8-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 11-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BGC  | 4-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 21-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 14-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 10-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 17-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 12-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 7-D   | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 20-D  | 4   | 11/12 | 0.92 | 0.20 | 18,20,25,28                 | 11    |
| 3   | BGC  | 23-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 19-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 9-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 6-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 21-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 4-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 20-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 10-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 16-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 13-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 21-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 11-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 5-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 23-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 18-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 2-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 24-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 7-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 10-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 10-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 3-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 14-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 16-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 25-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 7-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 19-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 13-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 25-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 22-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 6-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 25-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 1-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 21-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 12-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 8-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 1-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 2-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 21-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 20-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 10-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 8-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 3-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 13-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 5-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 3-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 25-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 9-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 15-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 12-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 9-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 17-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 13-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 14-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 15-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 15-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 24-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 7-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 6-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 9-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 1-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 20-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 4-D   | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 11-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 19-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 5-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 5-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 20-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 8-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 2-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 22-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 23-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 17-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 18-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 23-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 8-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 24-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 2-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 22-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 24-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 12-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 4-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 12-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 2   | BGC  | 6-E   | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 3   | BGC  | 14-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 18-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 11-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 15-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 16-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 11-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 17-F  | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 17-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 2   | BGC  | 3-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 18-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 14-E  | 1   | 12/12 | 0.93 | 0.23 | 17,20,30,39                 | 12    |
| 2   | BGC  | 19-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 4-C   | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 2   | BGC  | 22-C  | 1   | 12/12 | 0.93 | 0.18 | 20,24,32,37                 | 12    |
| 3   | BGC  | 16-D  | 2   | 11/12 | 0.93 | 0.22 | 21,28,33,36                 | 11    |
| 3   | BGC  | 1-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 7-F   | 3   | 11/12 | 0.93 | 0.17 | 19,23,30,35                 | 11    |
| 3   | BGC  | 3-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 14-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 5-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 17-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 16-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 7-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 9-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 15-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 16-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 20-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 14-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 25-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 22-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 17-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 9-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 1-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 3-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 21-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BGC  | 24-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 2-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 6-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 10-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 4-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 25-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 8-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 1-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 11-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 23-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 18-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 8-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 15-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 2-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 6-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 18-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 11-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 10-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 12-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 20-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 12-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 19-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 24-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 19-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 23-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 4-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 21-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 22-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 13-D  | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 5-F   | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 3   | BGC  | 7-D   | 3   | 11/12 | 0.95 | 0.19 | 21,25,31,42                 | 11    |
| 3   | BGC  | 13-F  | 2   | 11/12 | 0.95 | 0.27 | 24,27,30,33                 | 11    |
| 2   | BGC  | 21-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 15-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 9-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 10-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 7-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 3-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 8-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 15-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 14-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 3   | BGC  | 12-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BGC  | 8-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 14-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 19-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 24-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 18-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 2-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 12-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 11-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 3-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 3   | BGC  | 6-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 3   | BGC  | 7-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 25-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 8-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 10-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 24-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 19-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 1-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 24-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 22-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 12-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 24-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 21-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 10-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 8-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 6-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 6-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 19-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 19-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 23-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 1-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 4-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 23-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 16-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 25-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 22-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 5-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 13-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 4-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 21-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 16-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 18-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 6-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BGC  | 1-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 20-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 4-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 21-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 3   | BGC  | 5-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 14-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 24-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 11-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 25-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 15-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 3-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 21-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 20-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 15-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 8-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 18-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 21-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 10-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 24-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 2-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 14-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 2-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 8-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 19-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 12-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 4-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 12-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 4-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 5-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 9-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 2-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 20-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 16-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 10-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 17-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 9-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 14-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 11-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 22-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 11-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 3   | BGC  | 15-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 3   | BGC  | 5-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 3-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 9-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 20-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 11-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 13-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 17-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 1-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 2-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 7-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 2-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 19-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 6-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 18-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 7-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 3   | BGC  | 11-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 5-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 9-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 22-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 11-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 25-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 14-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 17-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 24-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 15-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 3-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 19-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 6-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 14-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 25-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 7-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 10-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 3   | BGC  | 22-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 7-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 23-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 23-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 13-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 13-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 13-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 11-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 9-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 17-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 2-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BGC  | 4-F   | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 3   | BGC  | 20-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 3   | BGC  | 22-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 23-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 23-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 16-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 20-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 25-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 16-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 22-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 21-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 14-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 12-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 18-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 19-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 3-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 13-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 18-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 3-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 18-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 17-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 1-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 24-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 20-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 8-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 17-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 3   | BGC  | 10-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 16-E  | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 3   | BGC  | 13-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 4-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 20-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 4-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 10-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 6-C   | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 3   | BGC  | 6-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 23-F  | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 12-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 5-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 7-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 12-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 22-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 17-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 5-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 8-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 16-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 25-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 15-F  | 4   | 11/12 | 0.96 | 0.21 | 15,19,22,29                 | 11    |
| 2   | BGC  | 3-C   | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 3   | BGC  | 2-D   | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 15-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 7-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 3   | BGC  | 18-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 16-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 9-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 21-C  | 3   | 11/12 | 0.96 | 0.12 | 12,13,18,26                 | 11    |
| 2   | BGC  | 13-E  | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 23-C  | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 3   | BGC  | 25-D  | 5   | 11/12 | 0.96 | 0.15 | 16,19,23,27                 | 11    |
| 2   | BGC  | 5-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 2   | BGC  | 9-E   | 3   | 11/12 | 0.96 | 0.11 | 11,14,19,23                 | 11    |
| 2   | BGC  | 17-C  | 5   | 11/12 | 0.96 | 0.07 | 10,12,18,22                 | 11    |
| 2   | BGC  | 1-C   | 2   | 11/12 | 0.96 | 0.13 | 13,17,24,24                 | 11    |
| 2   | BGC  | 1-E   | 5   | 11/12 | 0.96 | 0.08 | 11,13,18,20                 | 11    |
| 3   | BGC  | 1-F   | 5   | 11/12 | 0.96 | 0.10 | 15,17,22,25                 | 11    |
| 2   | BGC  | 6-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 16-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 13-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 21-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 24-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 2-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 23-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 9-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 24-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 19-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 14-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 17-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 11-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 6-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 16-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 11-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 15-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 1-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 18-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 11-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 25-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 5-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 10-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 4-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 9-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 25-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 8-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 14-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 4-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 15-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 19-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 3-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 13-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 18-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 10-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 2-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 8-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 20-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 1-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 2-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 15-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 10-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 2-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 12-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 25-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 4-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 17-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 12-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 12-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 13-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 20-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 16-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 25-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 21-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 22-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 5-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 13-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 1-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 8-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 24-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 22-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 7-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 18-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 20-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 18-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 4-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 15-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 14-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 23-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 23-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 7-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 21-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 9-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 3-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 17-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 9-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 5-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 17-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 8-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 21-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 1-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 24-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 16-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 3-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 12-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 6-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 19-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 20-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 19-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 23-C  | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 22-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 6-C   | 4   | 11/12 | 0.97 | 0.10 | 11,12,16,17                 | 11    |
| 2   | BGC  | 10-E  | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 7-E   | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 14-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 3-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 7-E   | 4   | 11/12 | 0.97 | 0.07 | 11,12,17,18                 | 11    |
| 2   | BGC  | 11-E  | 6   | 11/12 | 0.97 | 0.08 | 10,12,13,14                 | 11    |
| 2   | BGC  | 5-E   | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 22-E  | 2   | 11/12 | 0.97 | 0.08 | 15,17,23,23                 | 11    |
| 2   | BGC  | 19-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 11-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 15-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 2-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |

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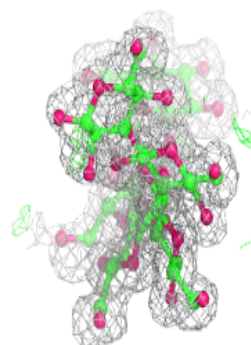
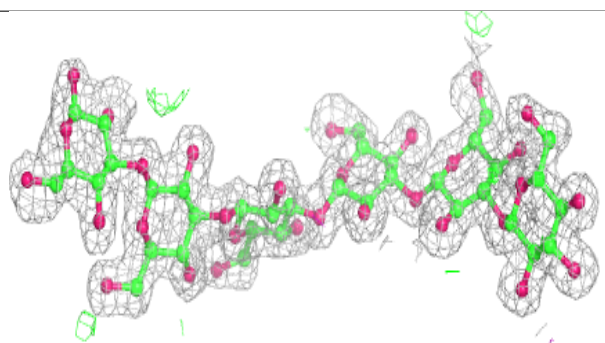
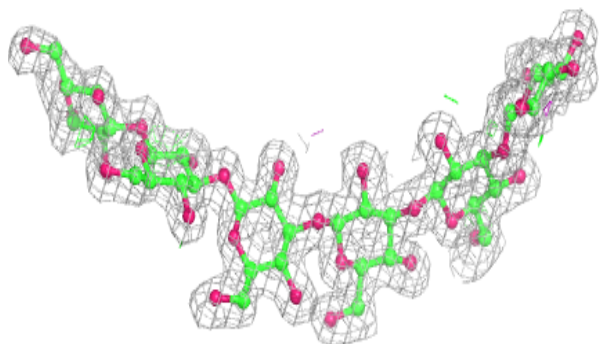
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BGC  | 16-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 21-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 22-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 10-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 18-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 4-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 7-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 9-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 17-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 25-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 13-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 14-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 8-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 20-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 24-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 3-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 23-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 1-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 6-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 5-C   | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |
| 2   | BGC  | 12-C  | 6   | 11/12 | 0.98 | 0.07 | 9,12,14,14                  | 11    |

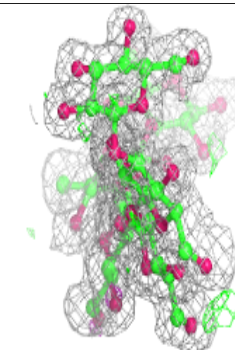
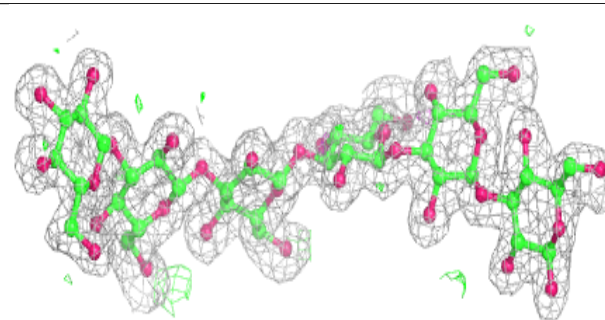
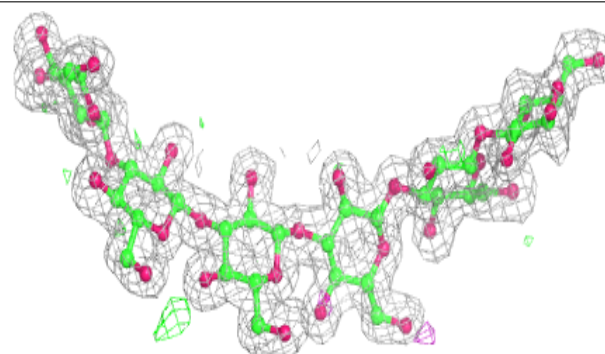
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

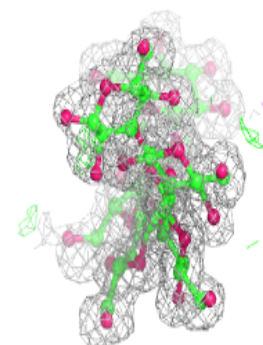
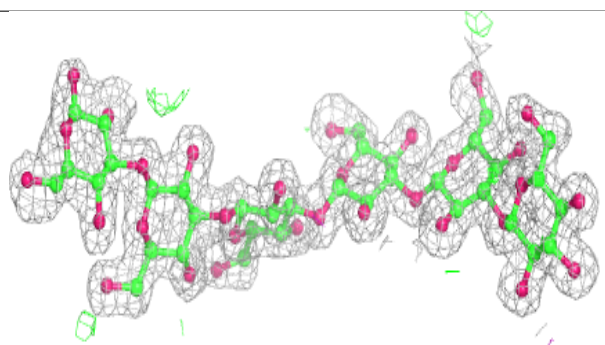
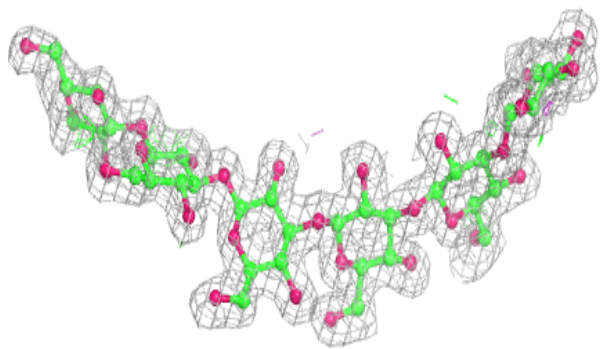
**Electron density around Chain E:**

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

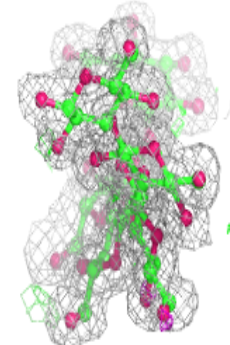
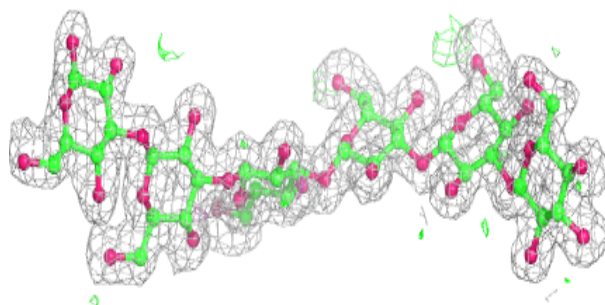
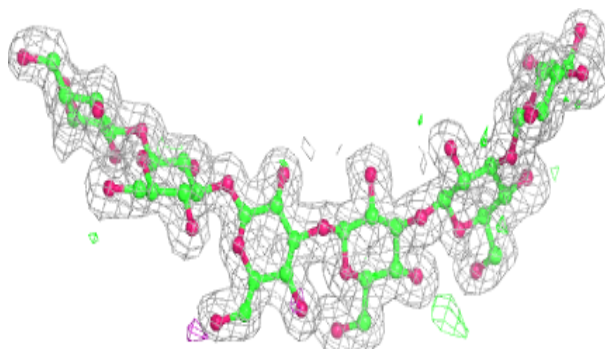


**Electron density around Chain C:**

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

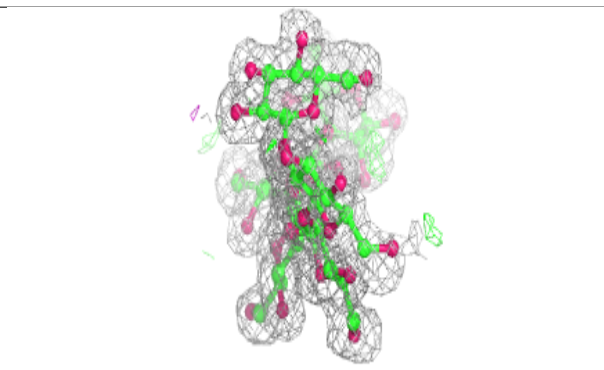
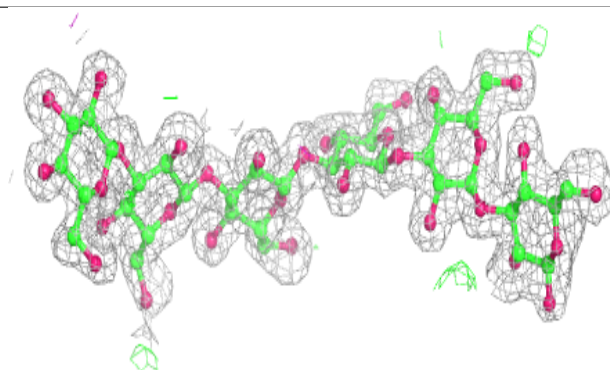
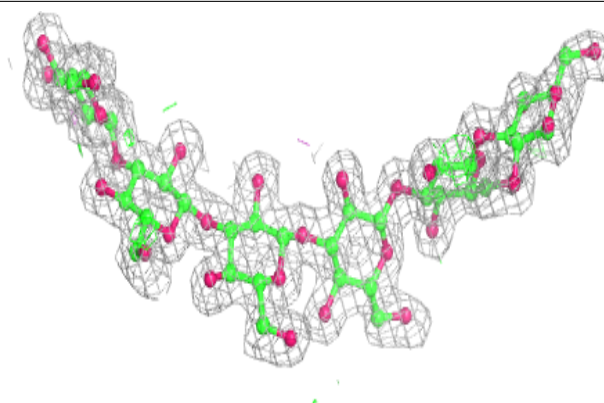
**Electron density around Chain E:**

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

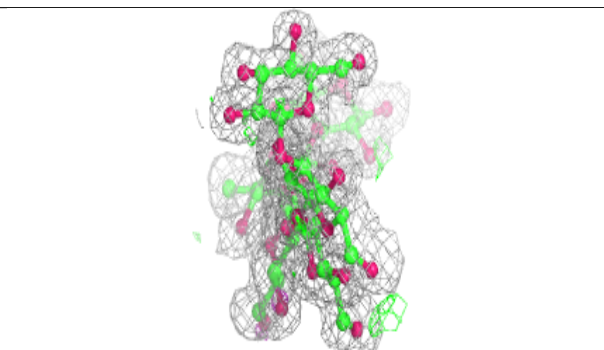
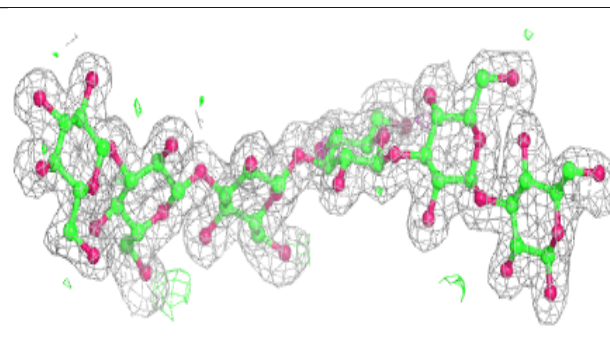
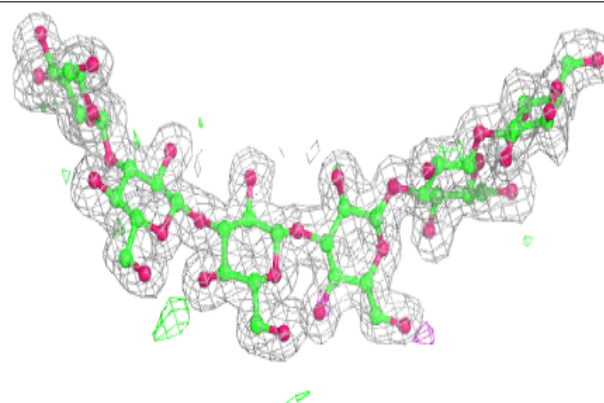


**Electron density around Chain C:**

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

**Electron density around Chain E:**

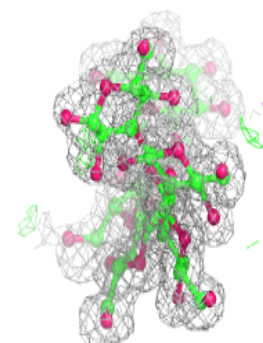
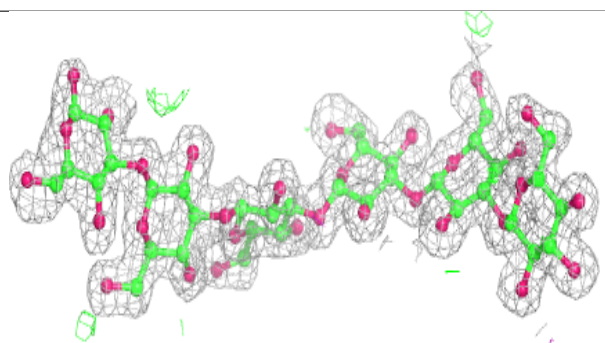
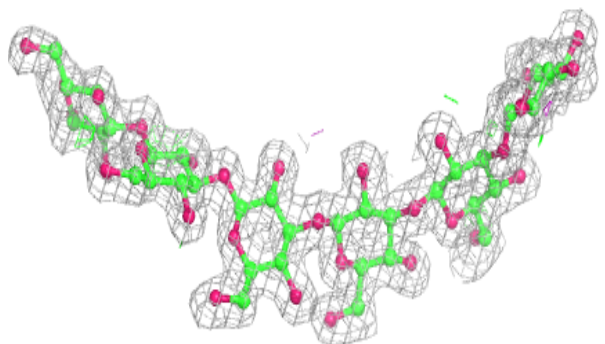
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



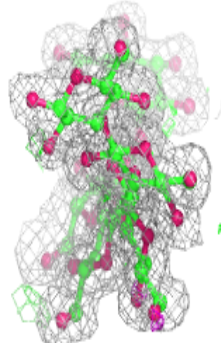
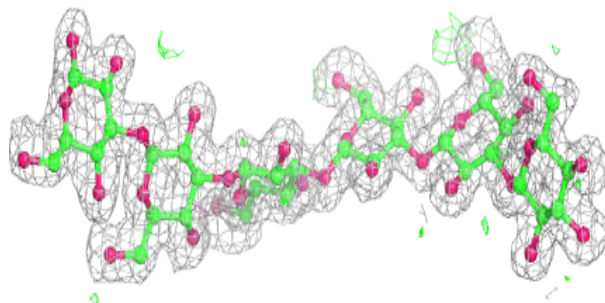
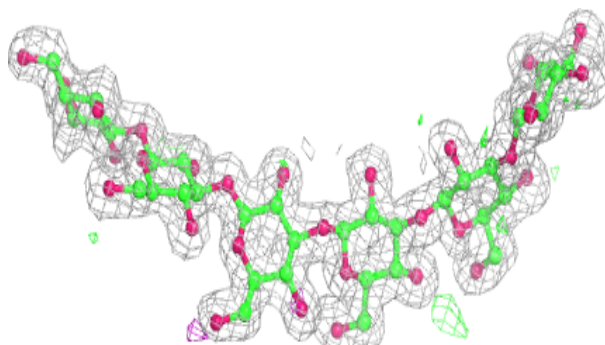


**Electron density around Chain C:**

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

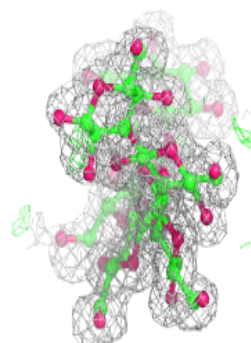
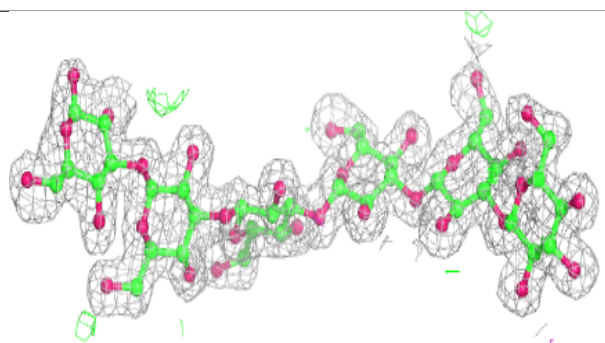
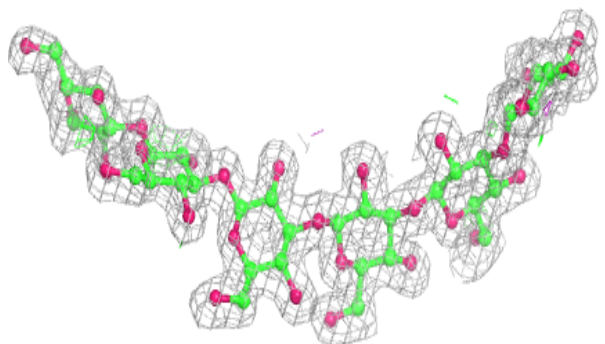
**Electron density around Chain E:**

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

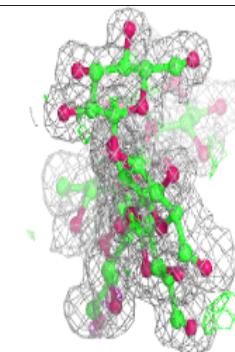
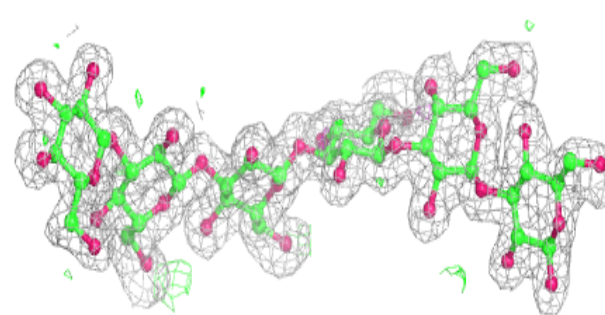
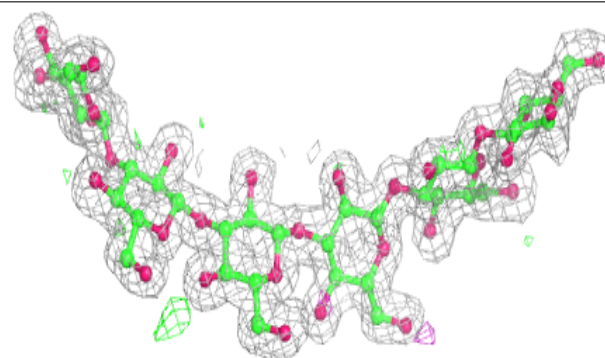


**Electron density around Chain C:**

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

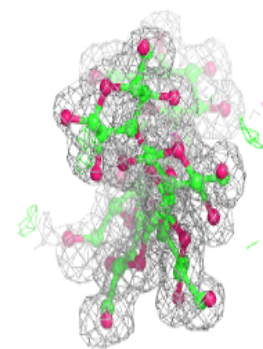
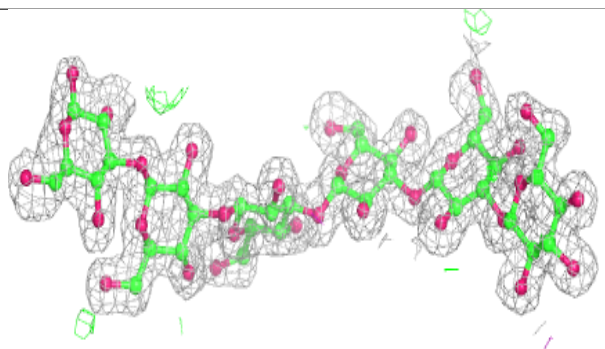
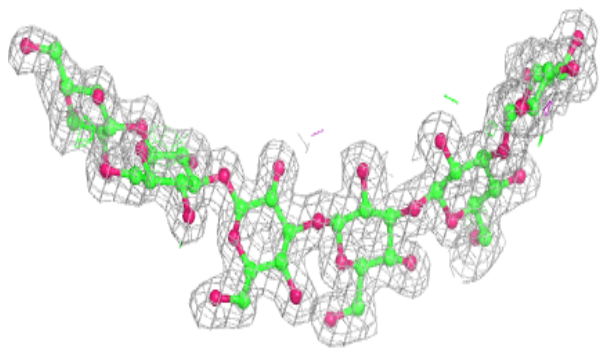
**Electron density around Chain E:**

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

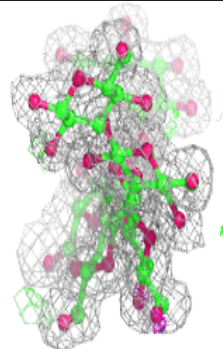
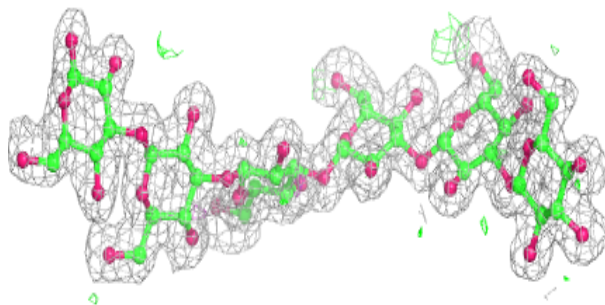
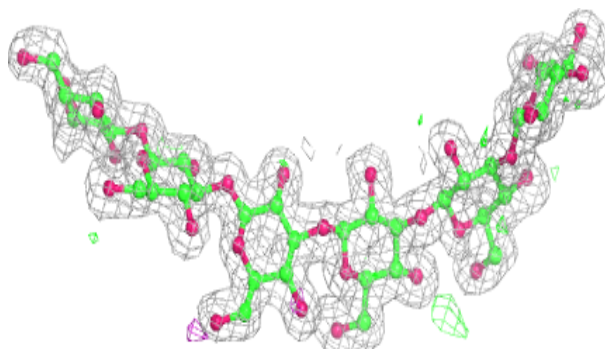


**Electron density around Chain C:**

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

**Electron density around Chain E:**

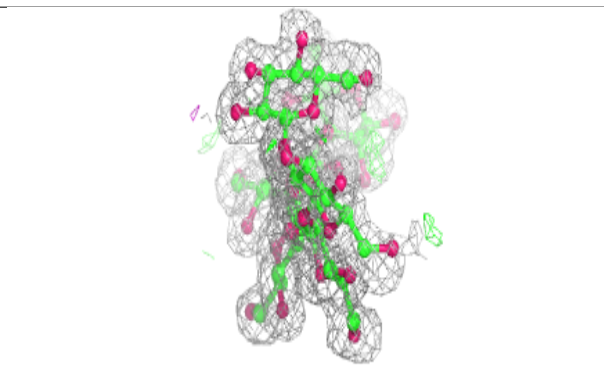
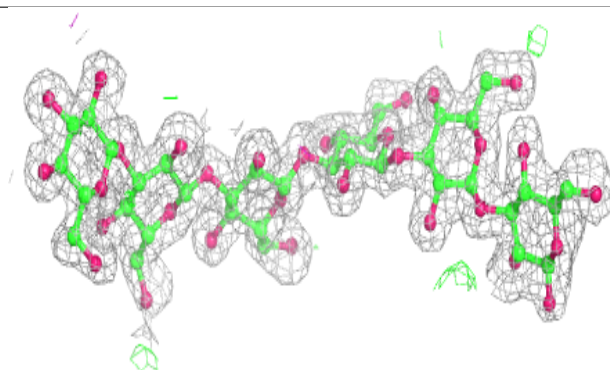
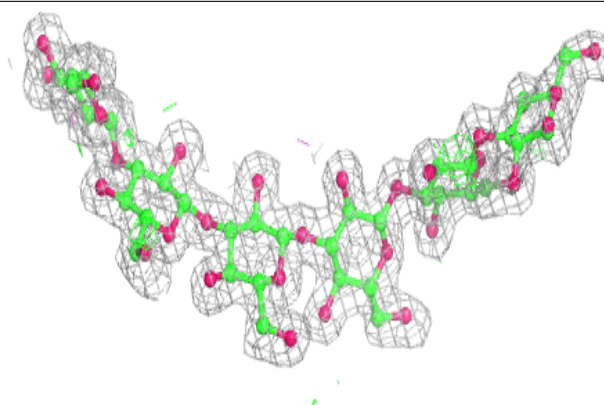
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



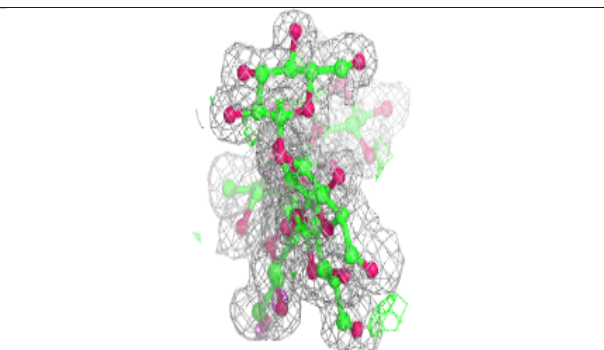
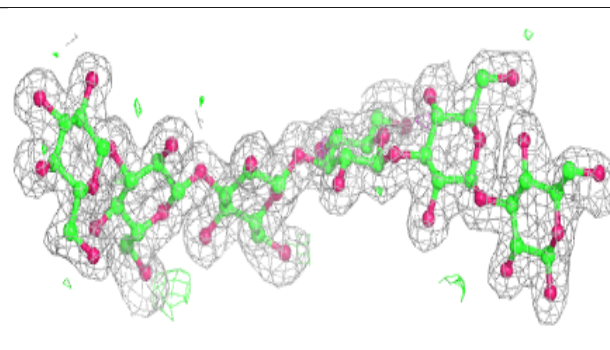
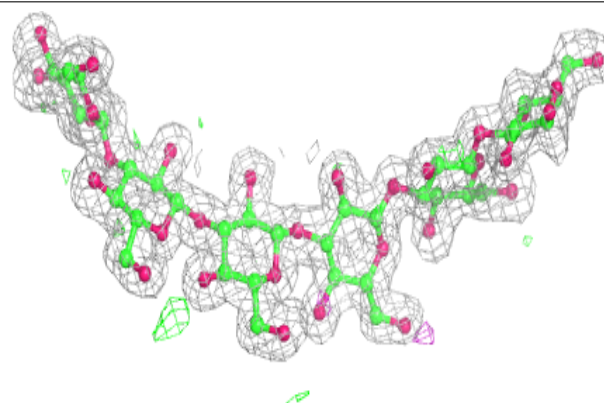


**Electron density around Chain C:**

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

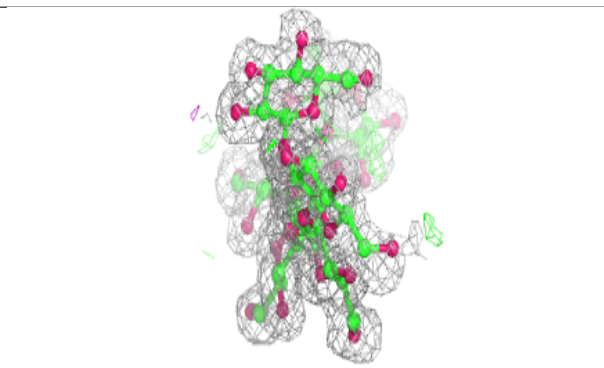
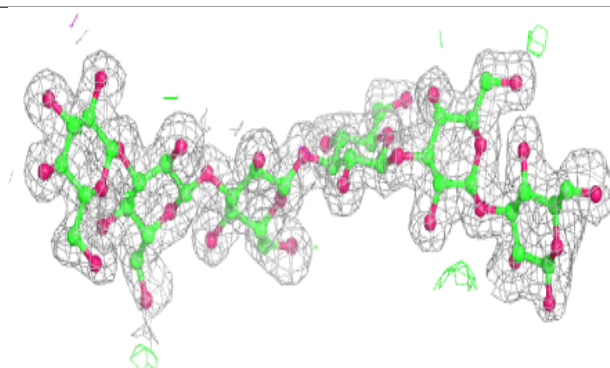
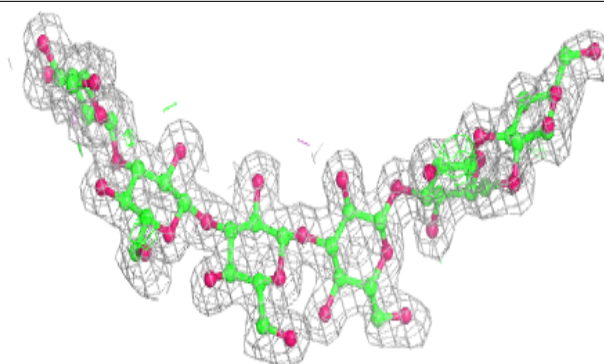
**Electron density around Chain E:**

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

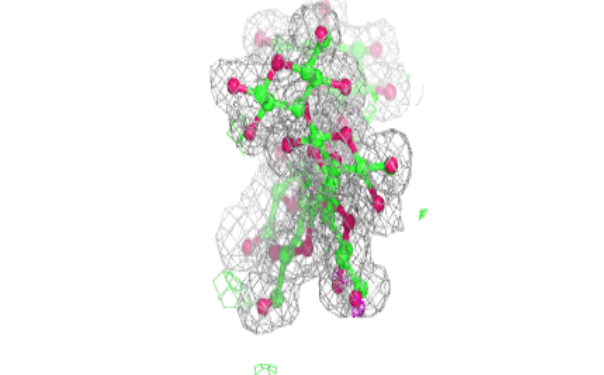
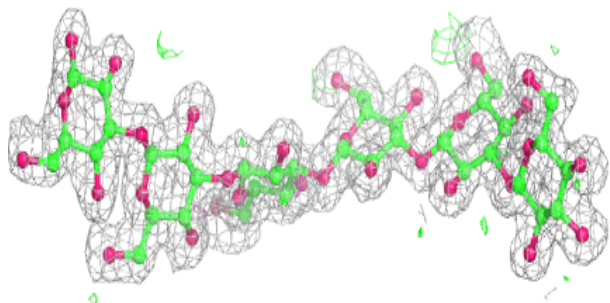
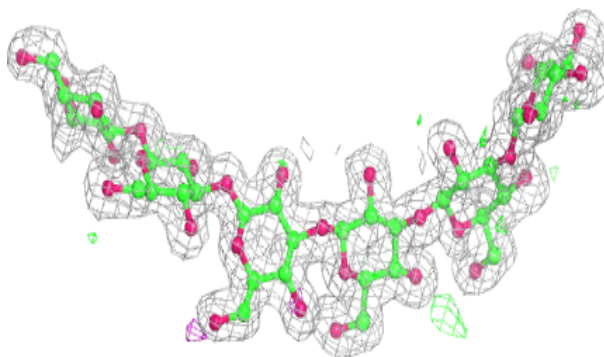


**Electron density around Chain C:**

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

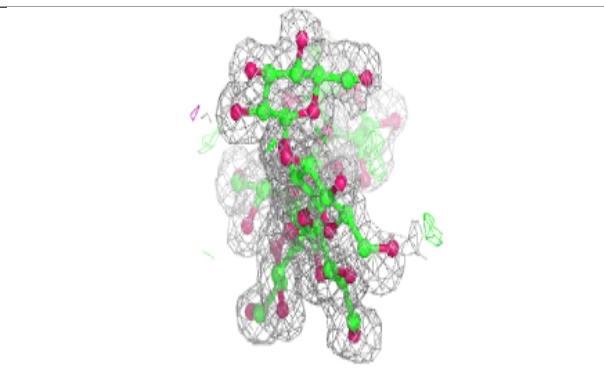
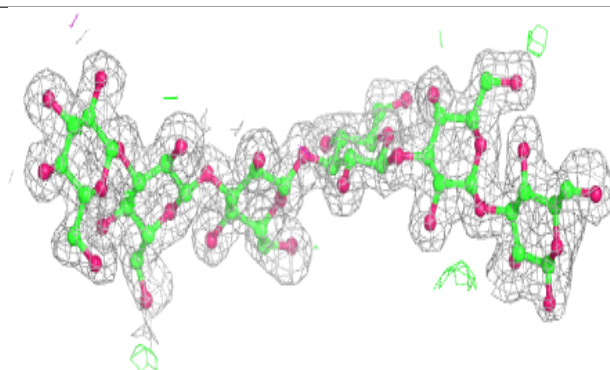
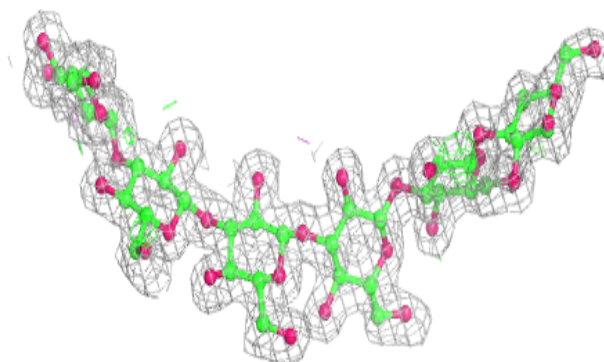
**Electron density around Chain E:**

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

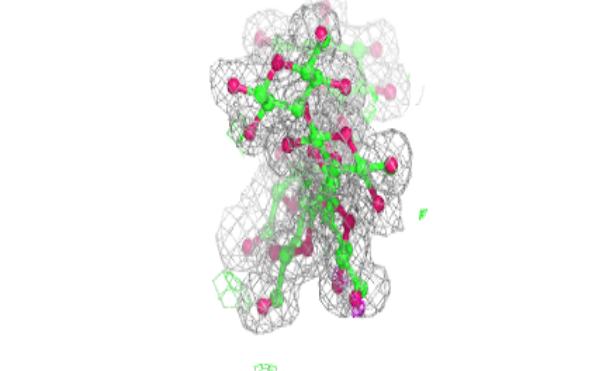
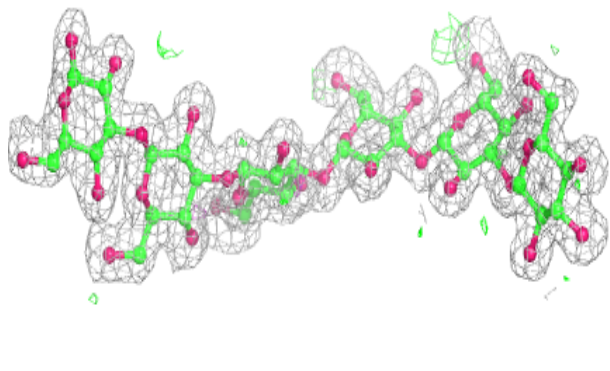
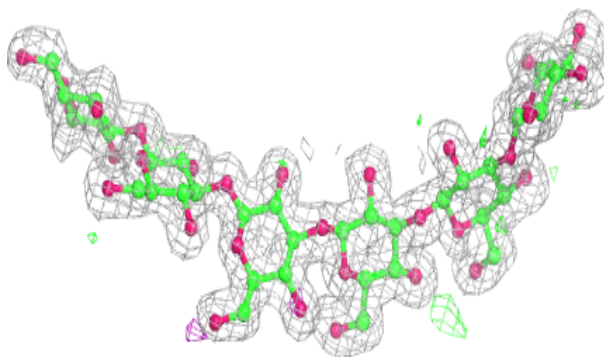


**Electron density around Chain C:**

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

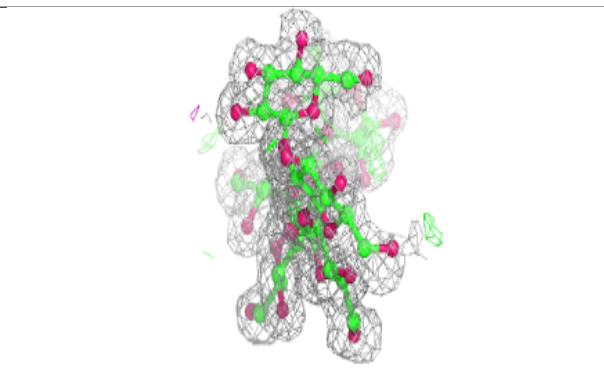
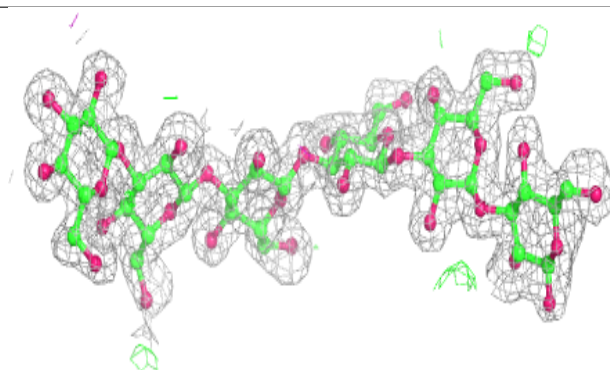
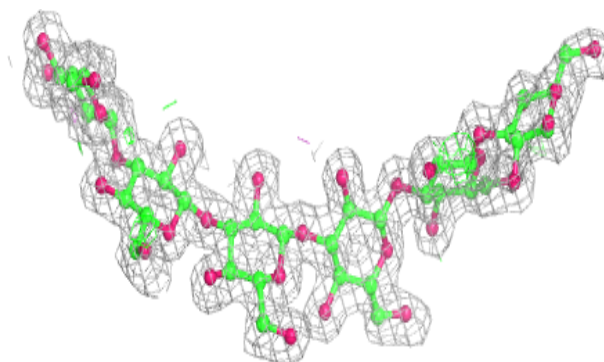
**Electron density around Chain E:**

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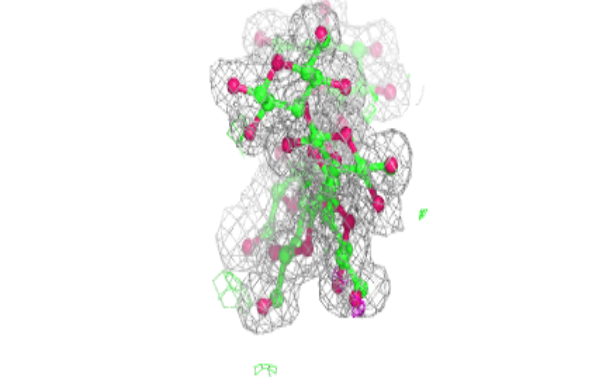
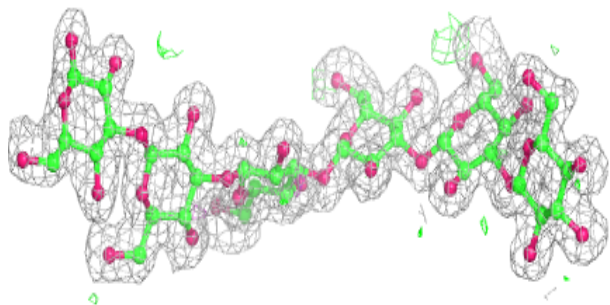
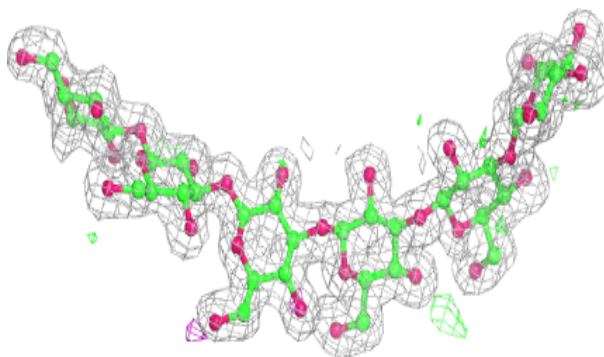


**Electron density around Chain C:**

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

**Electron density around Chain E:**

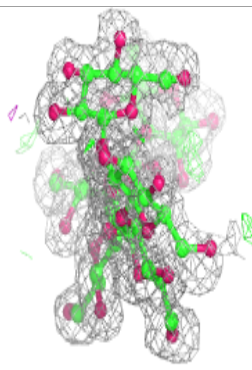
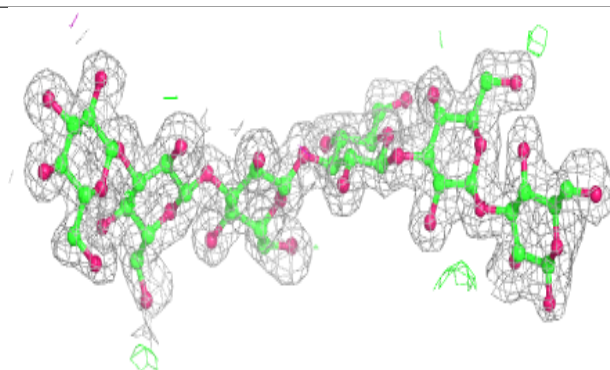
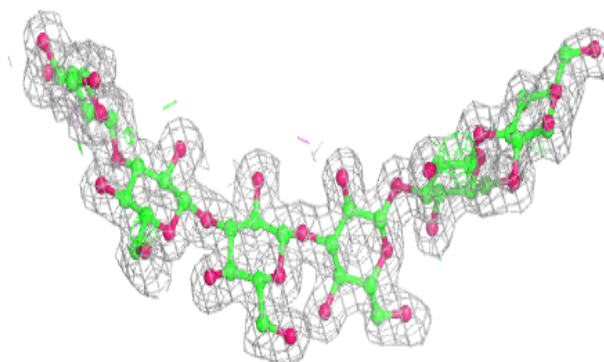
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



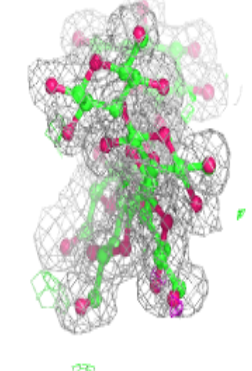
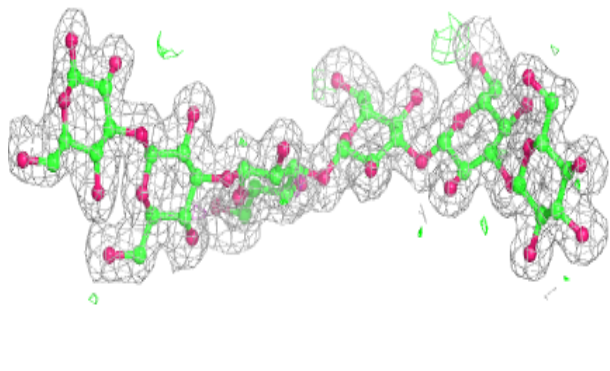
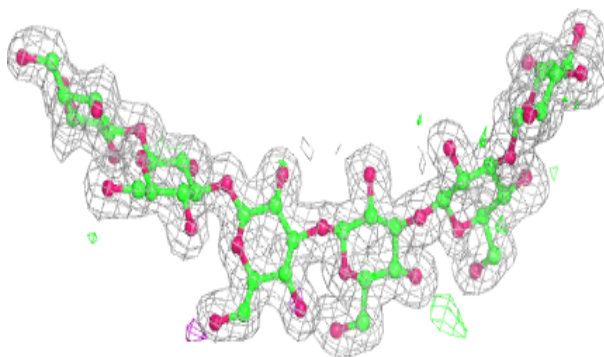


**Electron density around Chain C:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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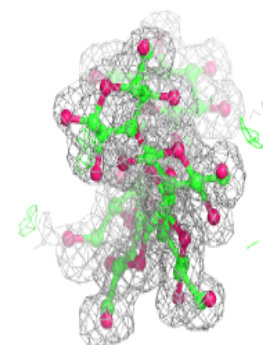
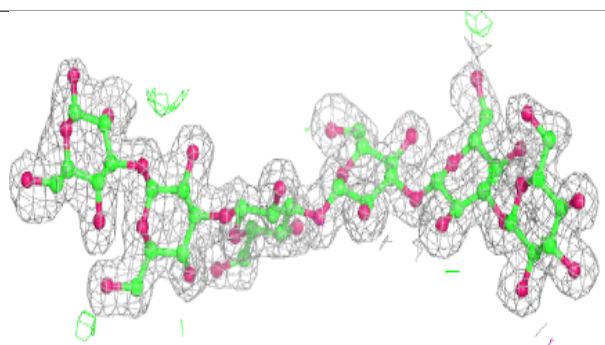
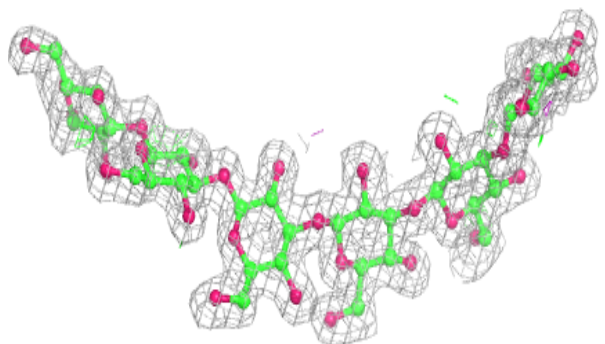
**Electron density around Chain E:**

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

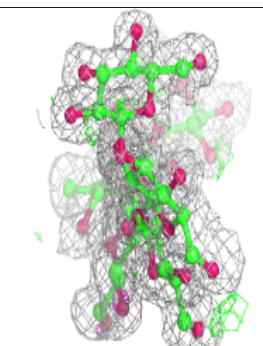
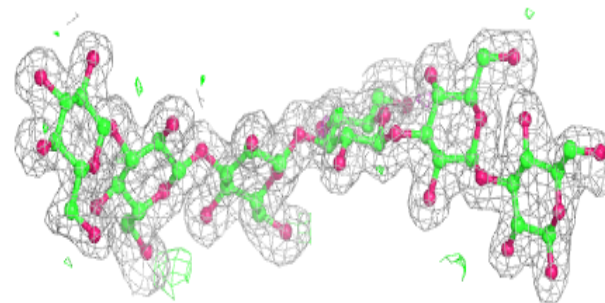
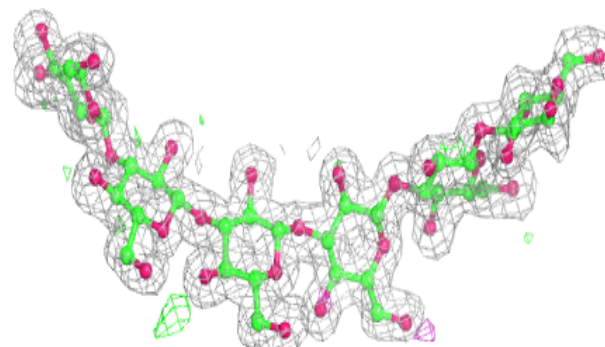


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$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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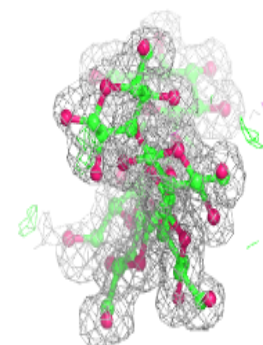
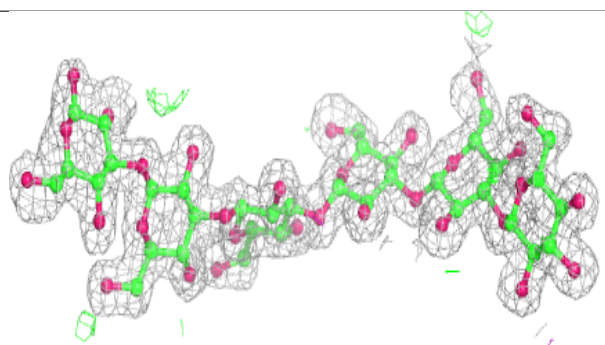
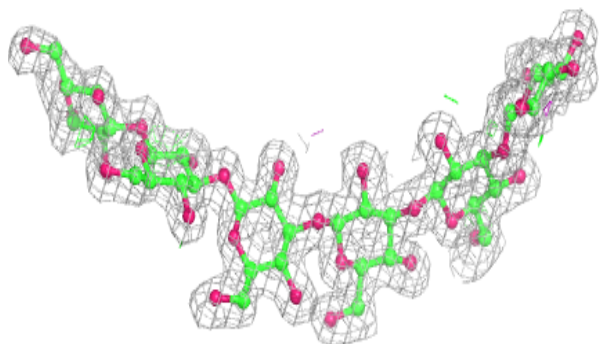
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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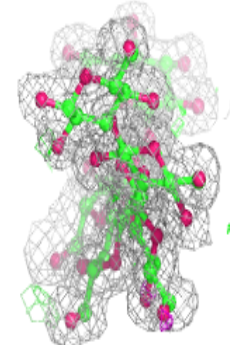
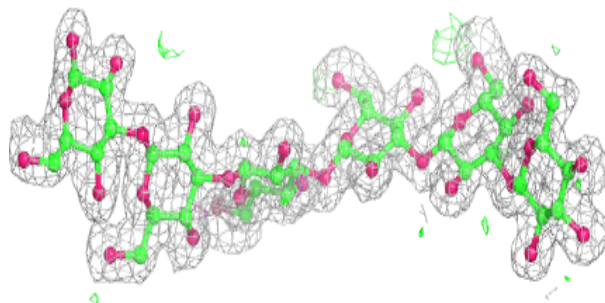
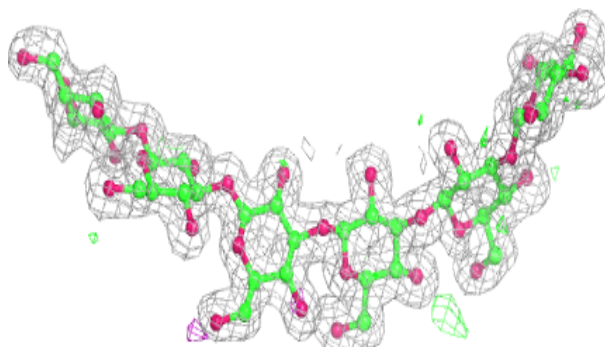


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$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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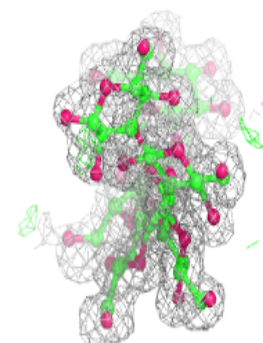
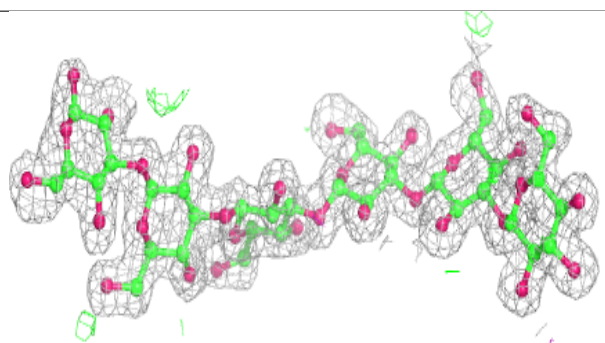
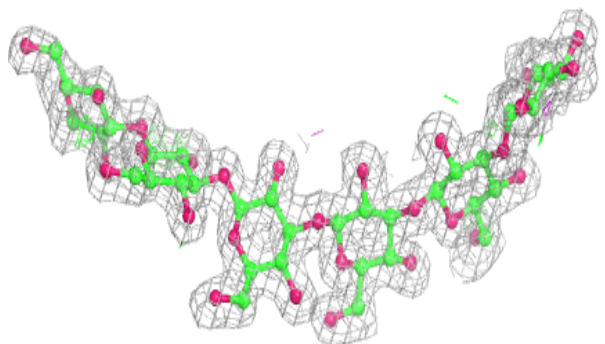
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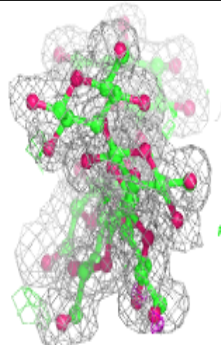
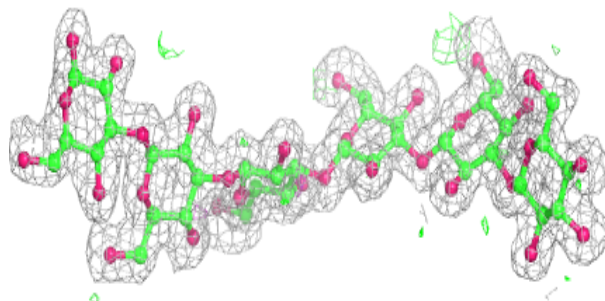
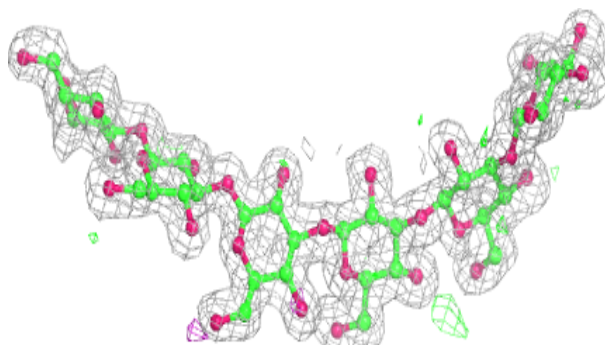


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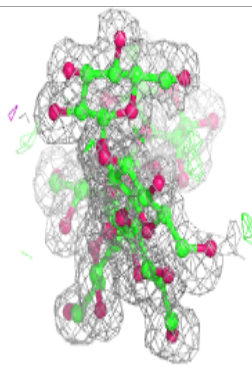
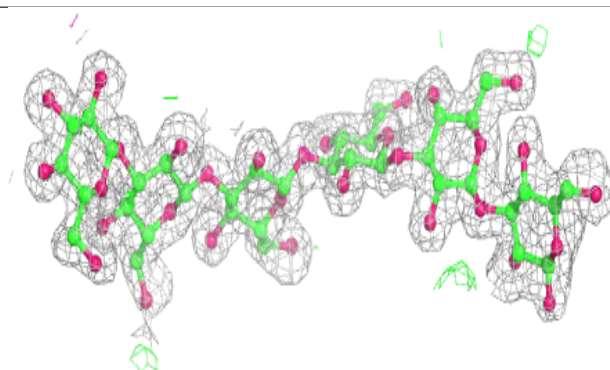
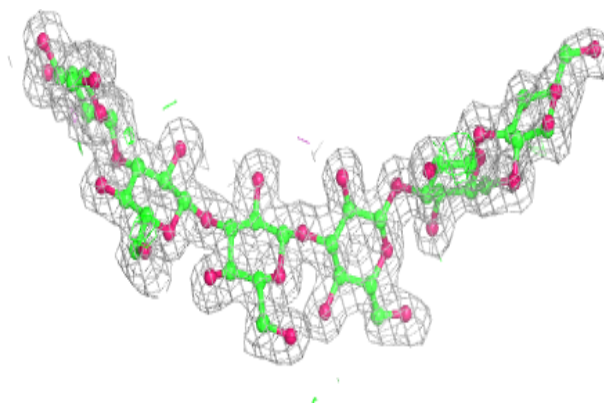
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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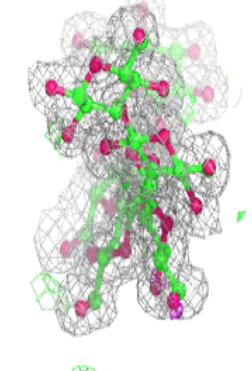
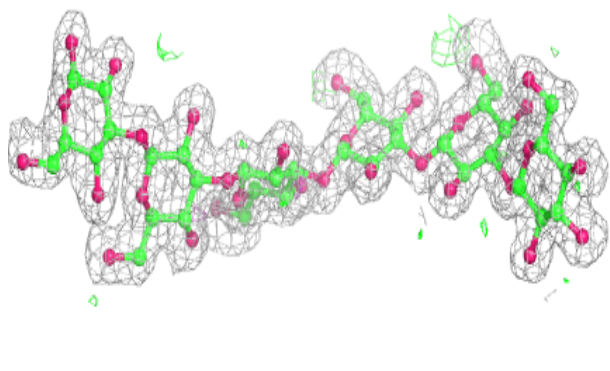
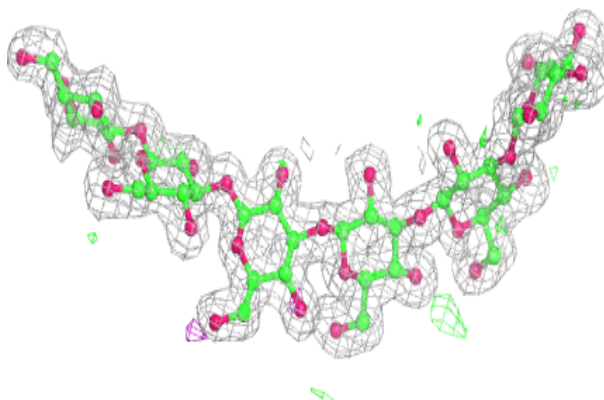


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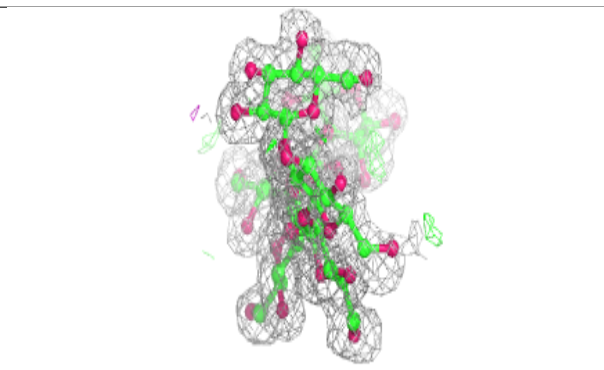
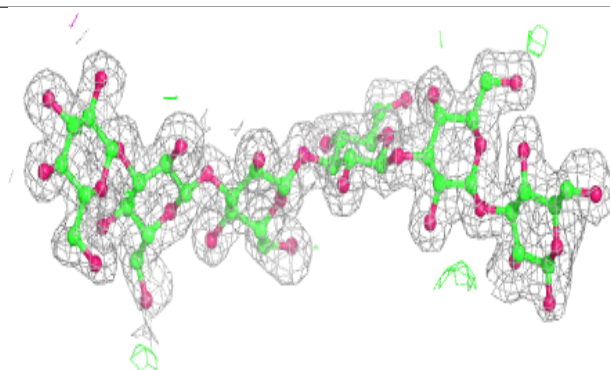
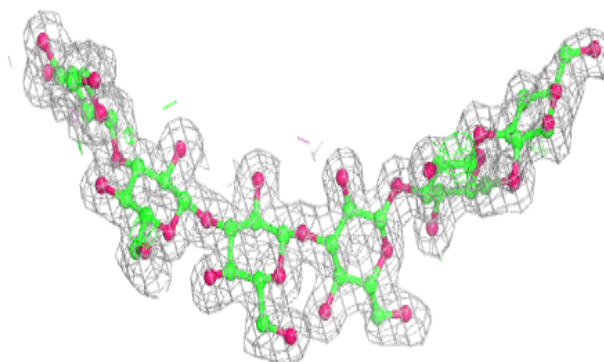
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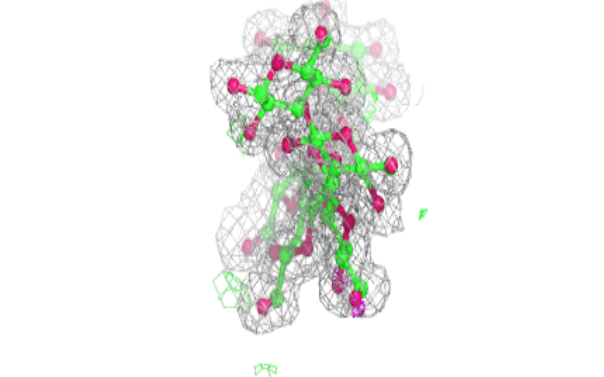
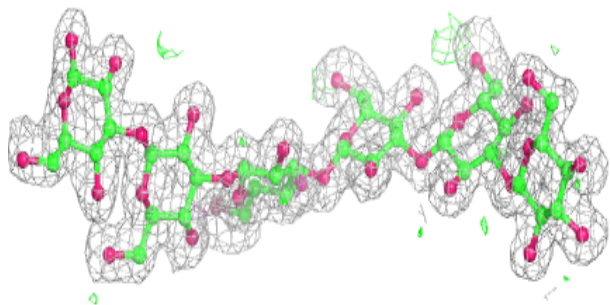
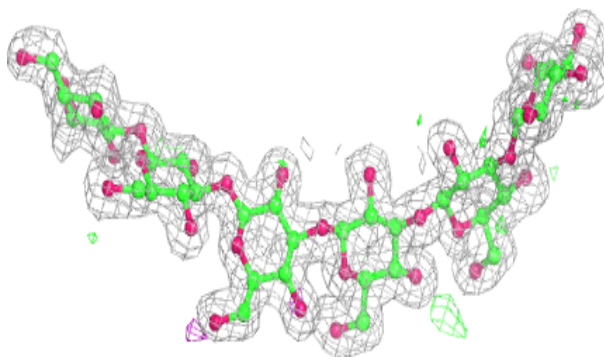


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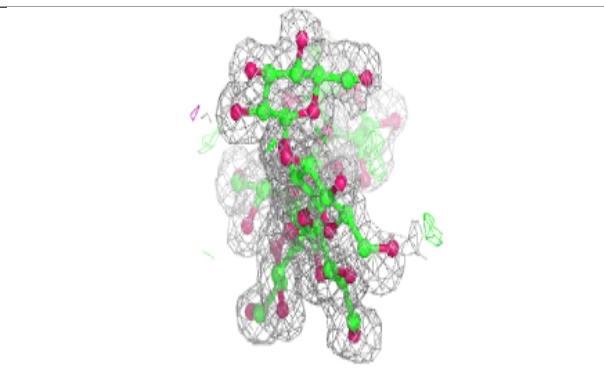
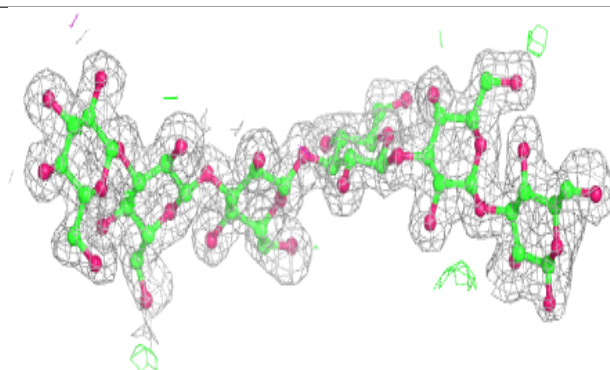
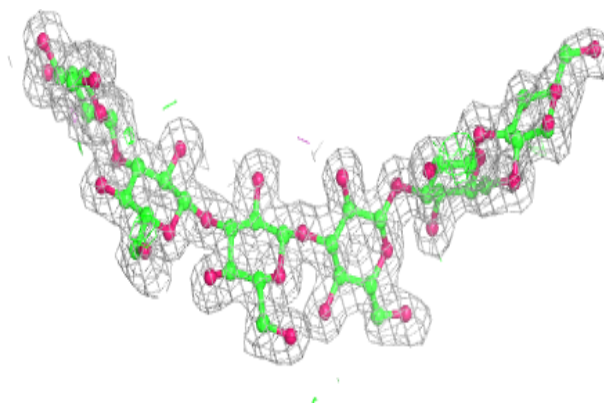
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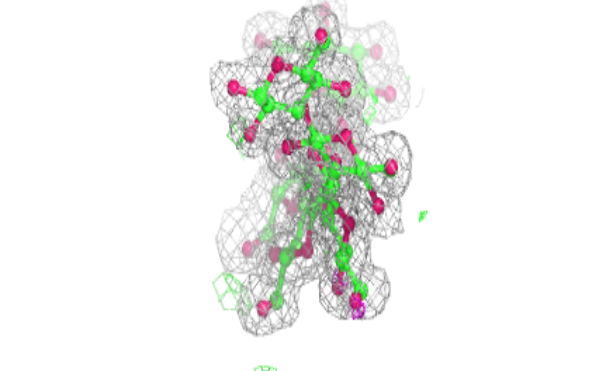
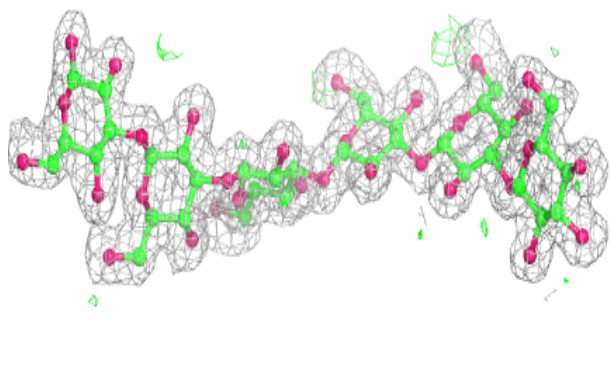
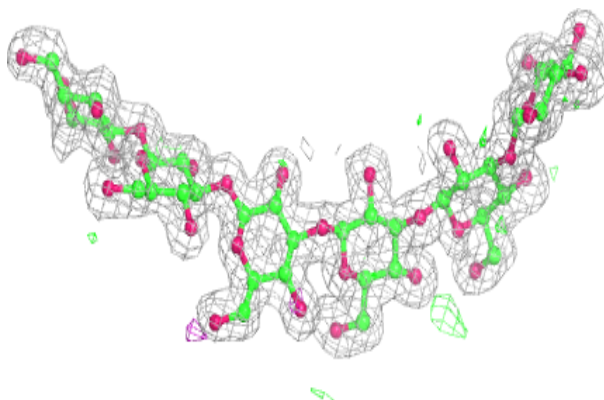


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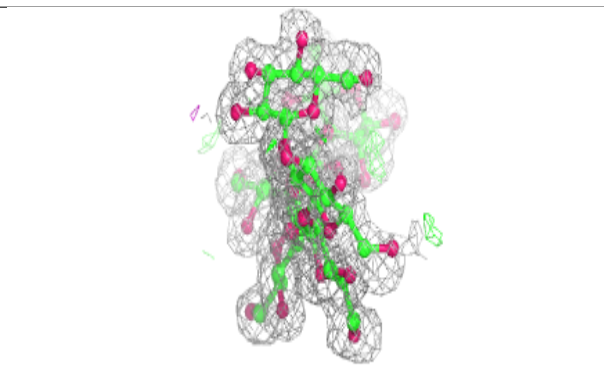
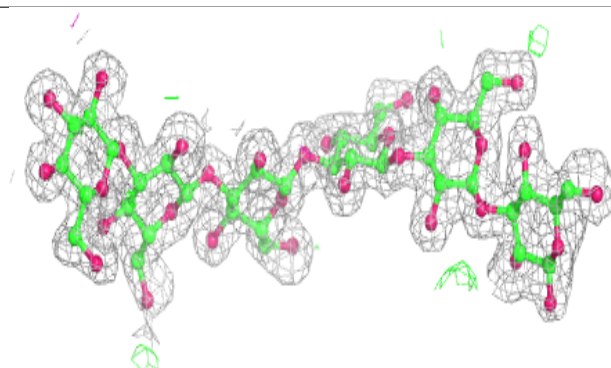
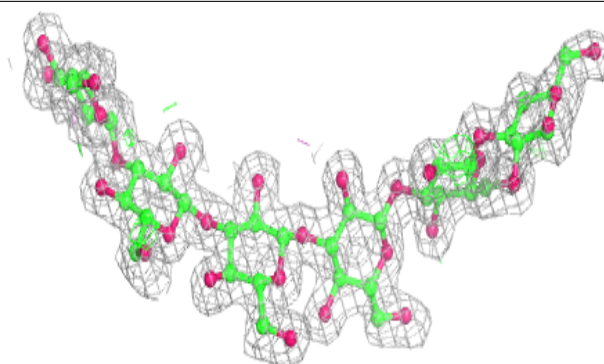
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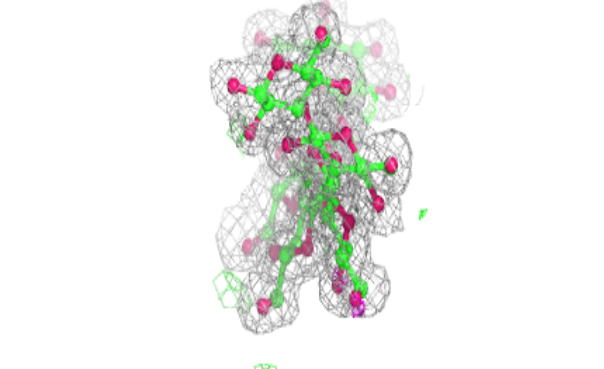
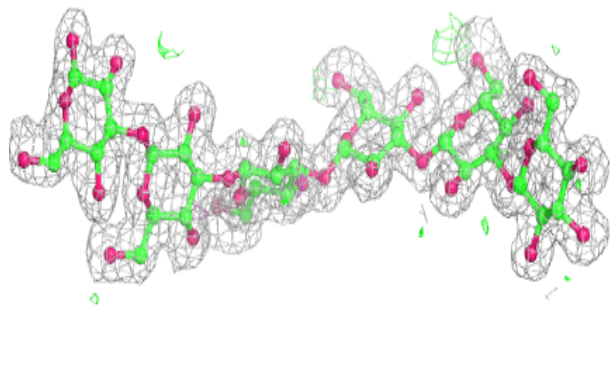
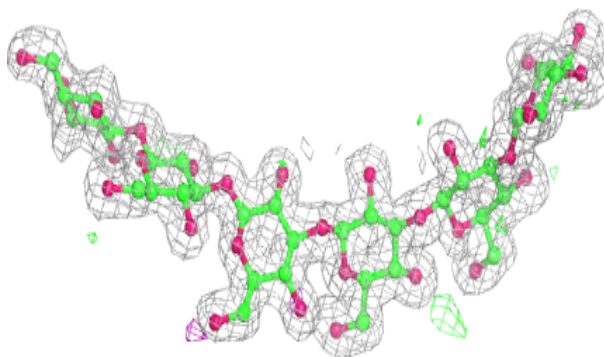


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and green (positive)

**Electron density around Chain E:**

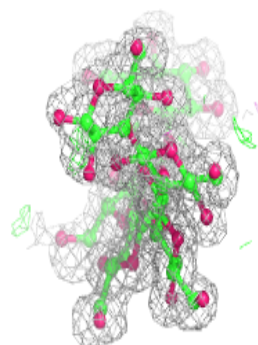
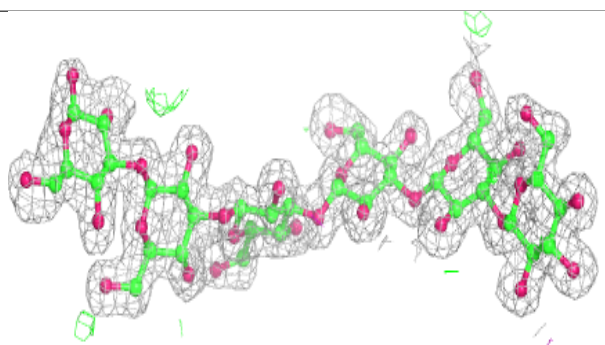
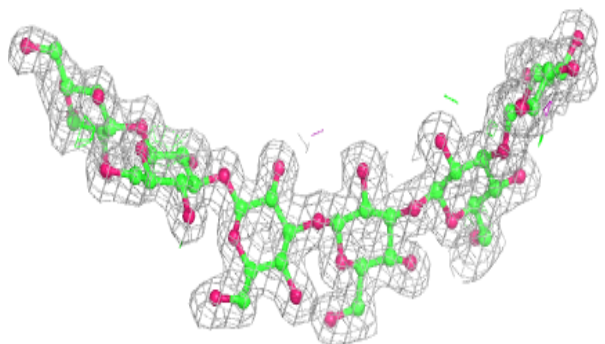
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



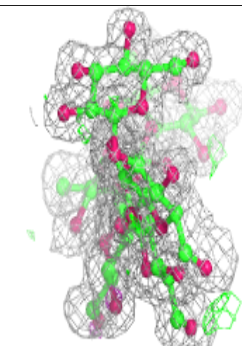
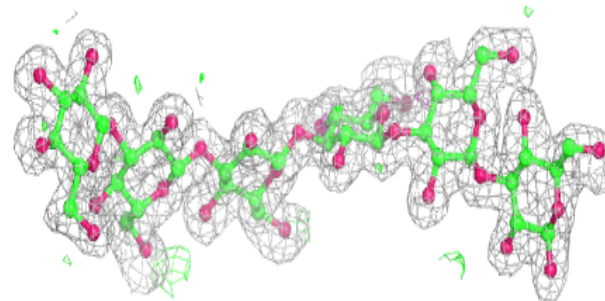
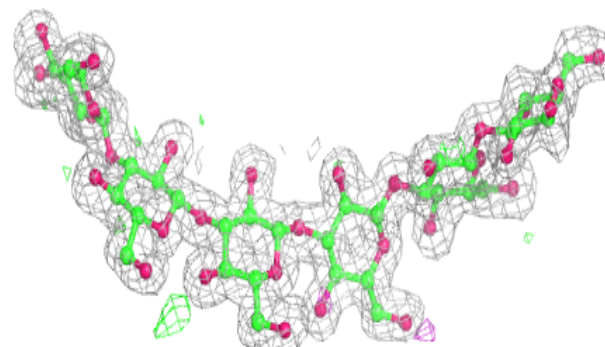


**Electron density around Chain C:**

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

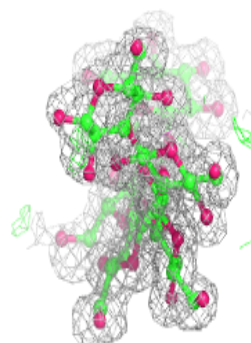
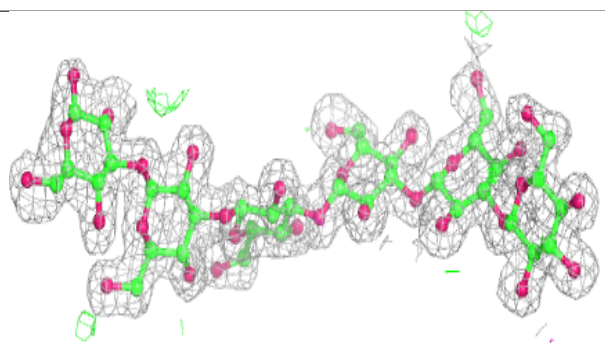
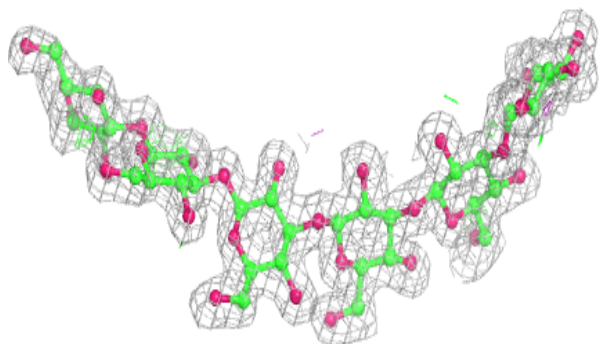
**Electron density around Chain E:**

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

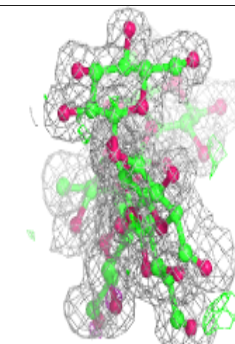
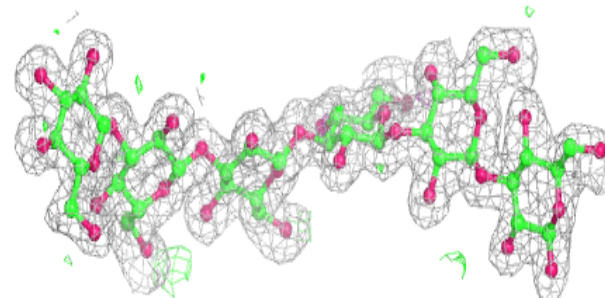
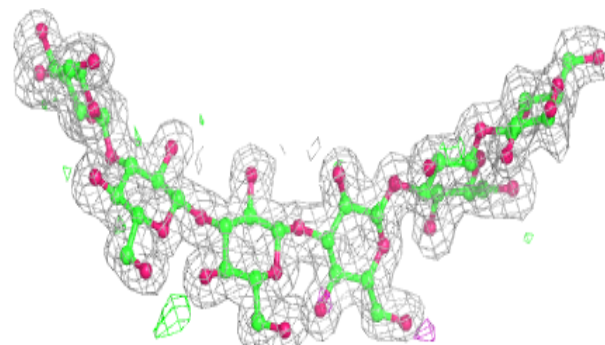


**Electron density around Chain C:**

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

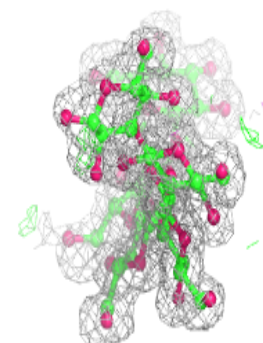
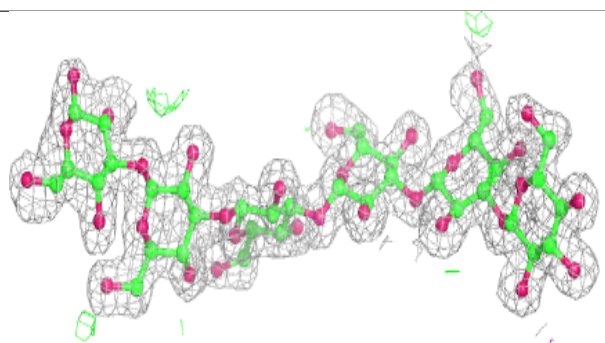
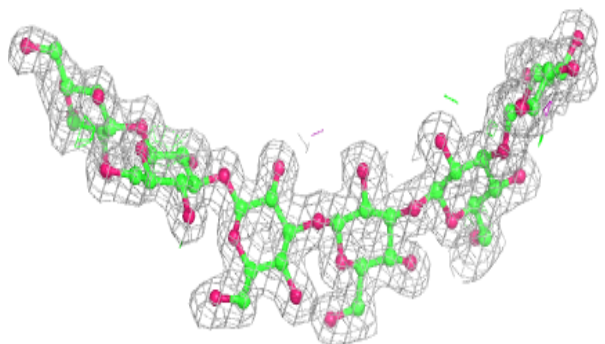
**Electron density around Chain E:**

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

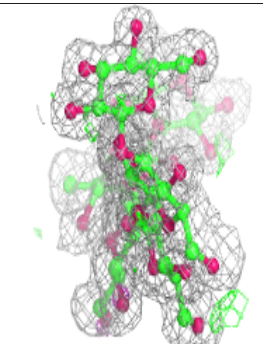
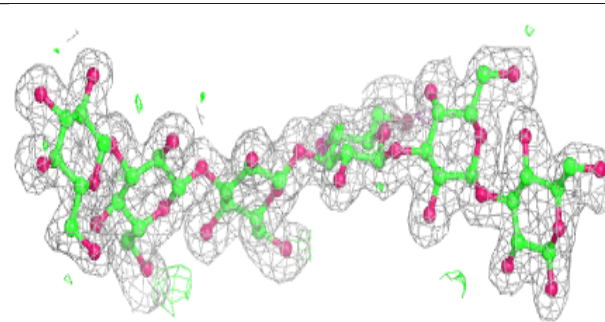
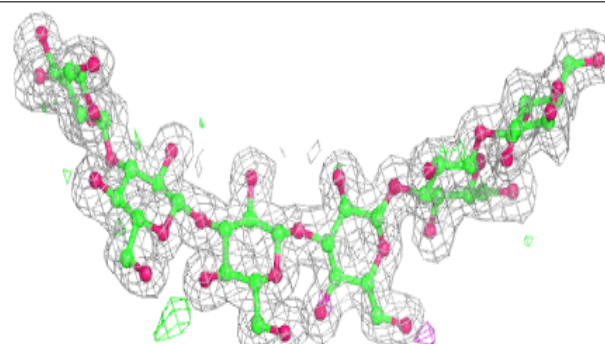


**Electron density around Chain C:**

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

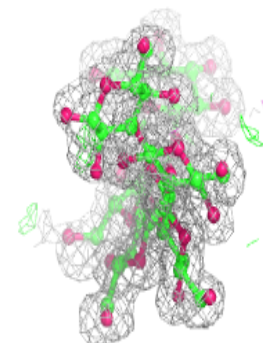
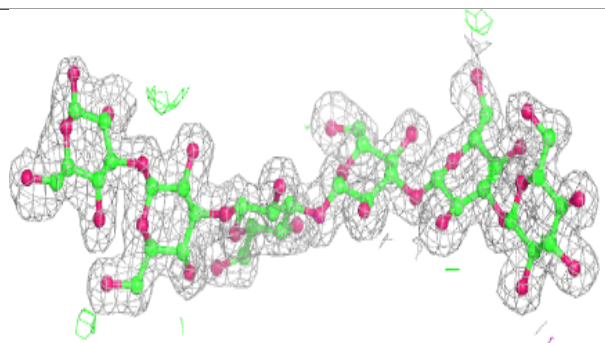
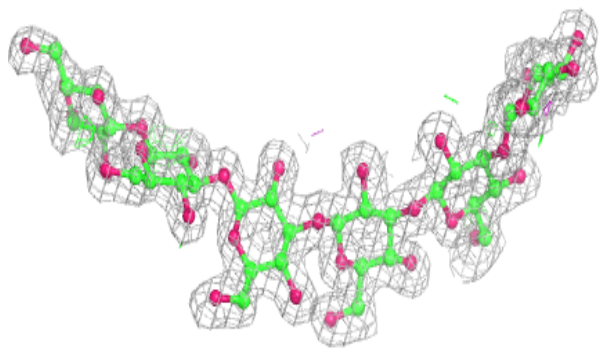
**Electron density around Chain E:**

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

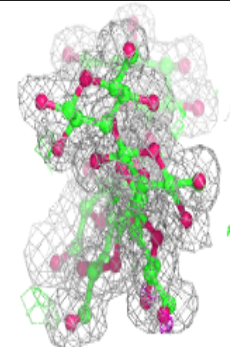
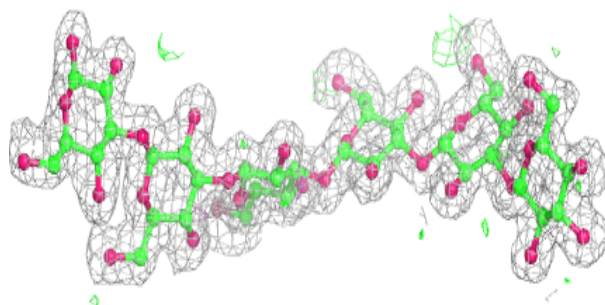
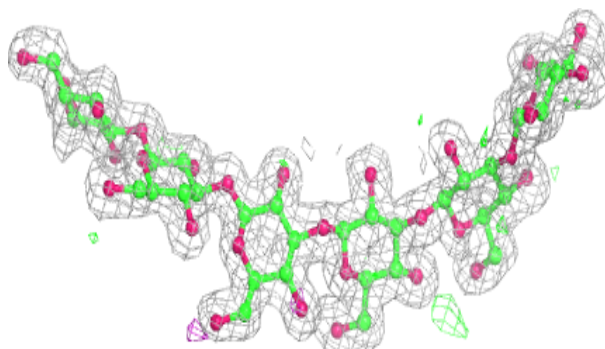


**Electron density around Chain C:**

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

**Electron density around Chain E:**

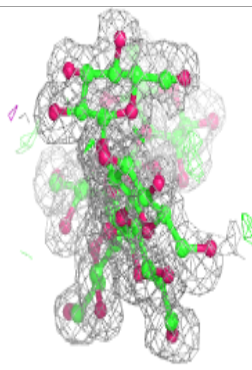
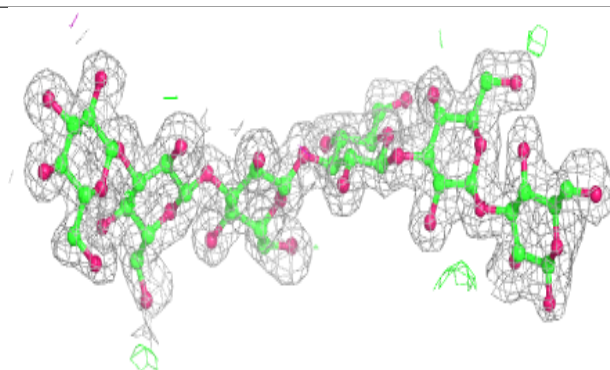
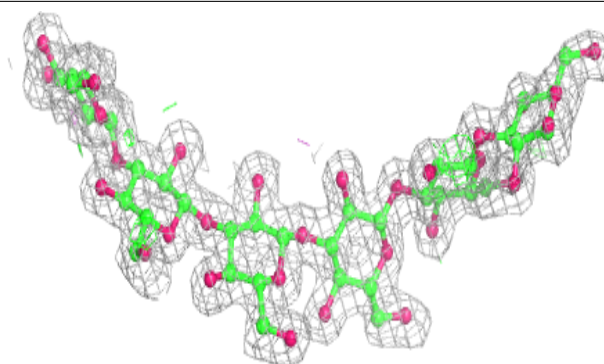
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



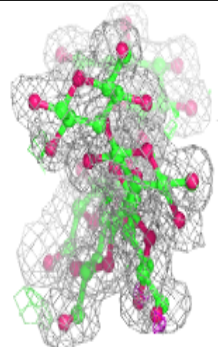
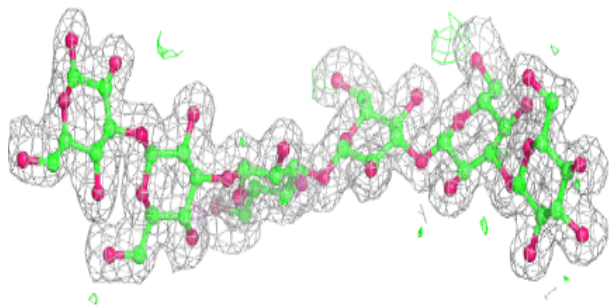
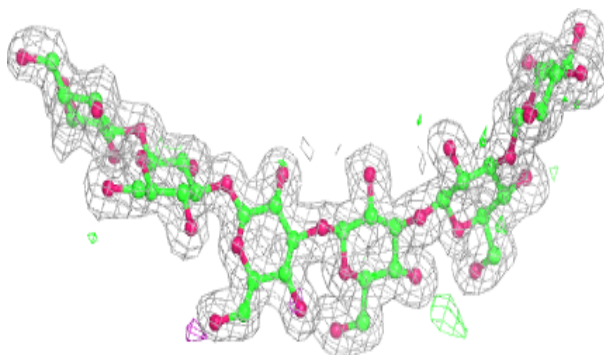


**Electron density around Chain C:**

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

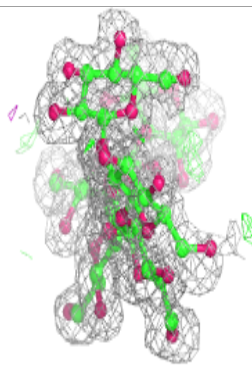
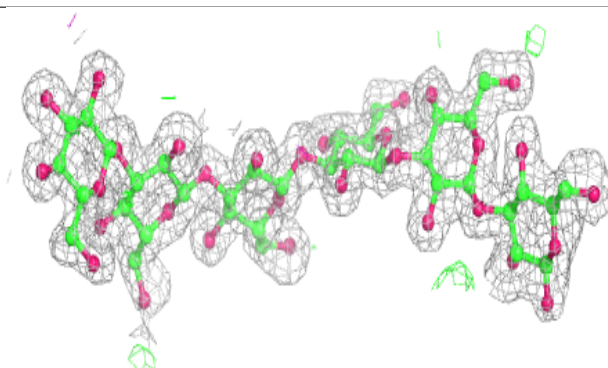
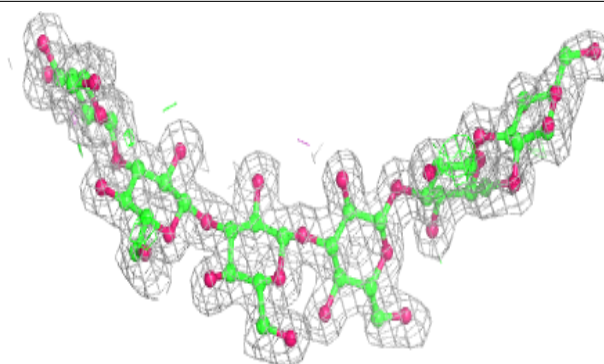
**Electron density around Chain E:**

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

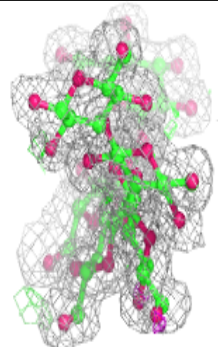
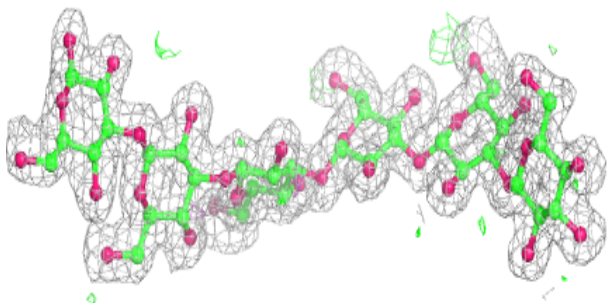
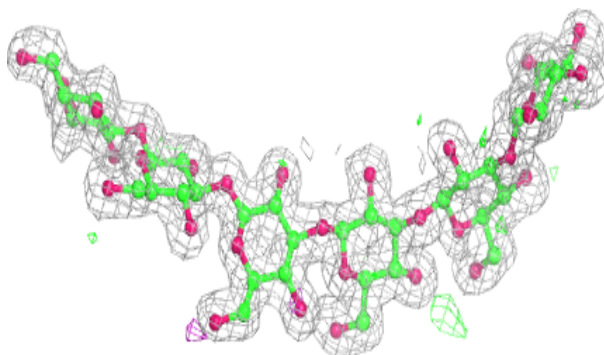


**Electron density around Chain C:**

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

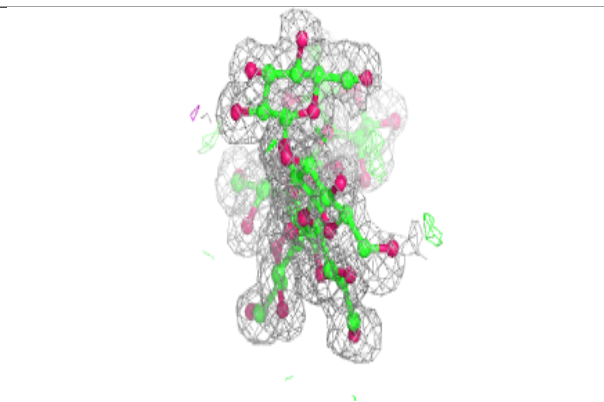
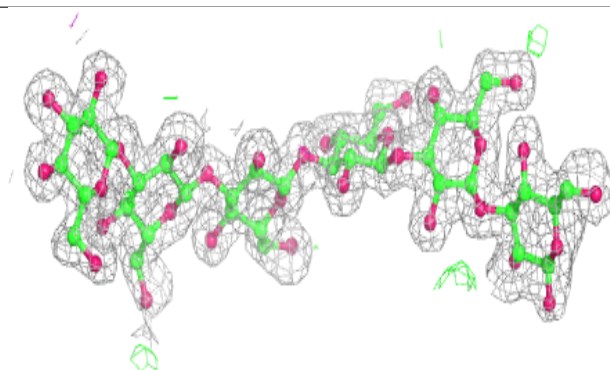
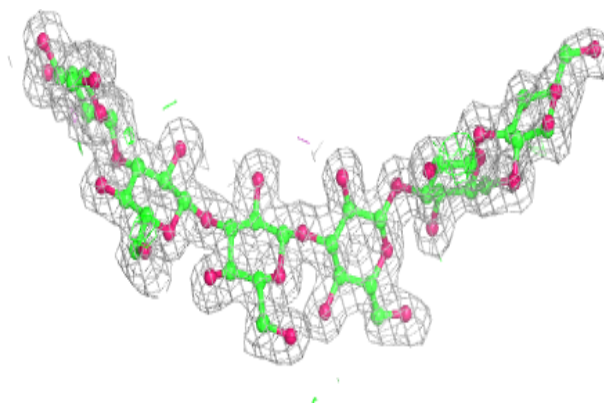
**Electron density around Chain E:**

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

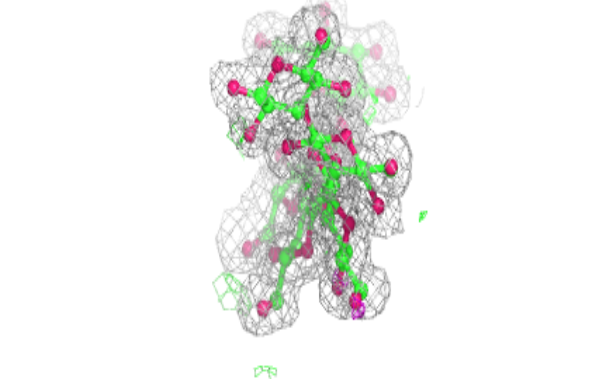
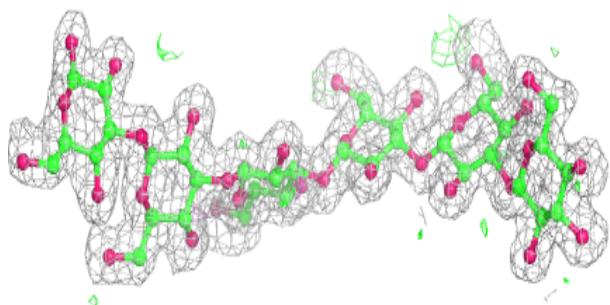
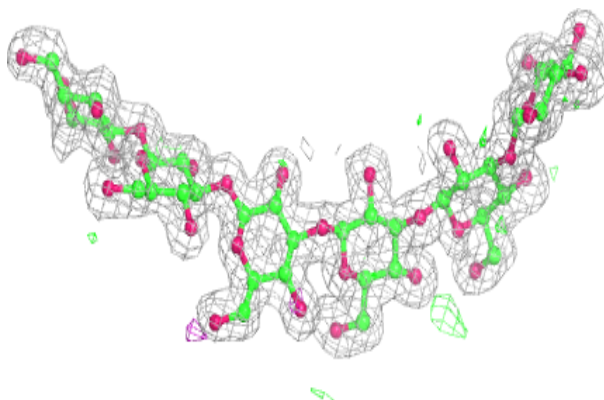


**Electron density around Chain C:**

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

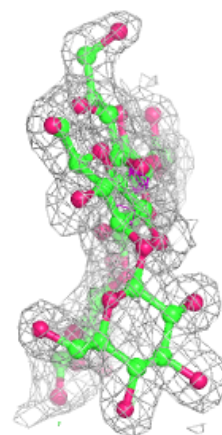
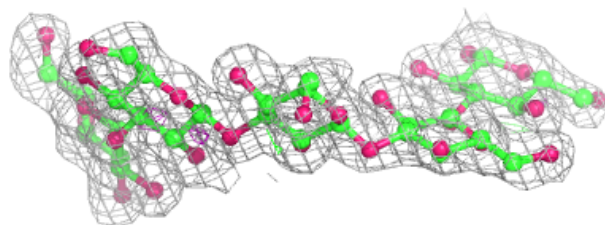
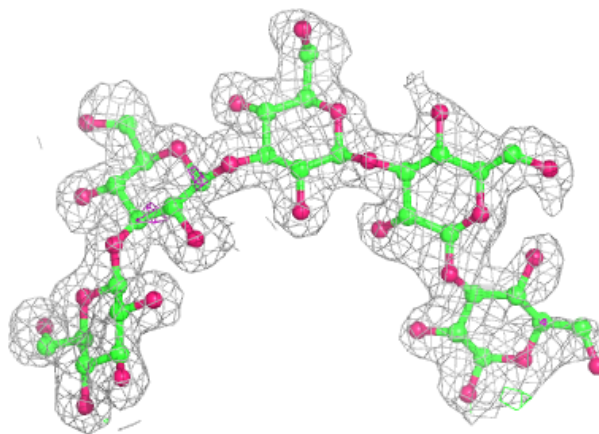
**Electron density around Chain E:**

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



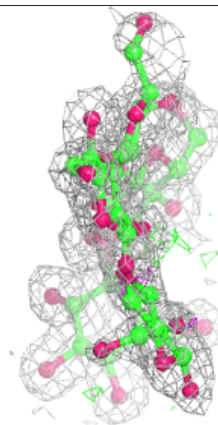
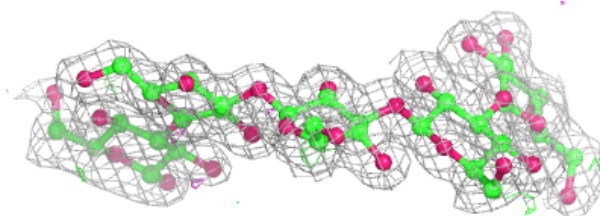
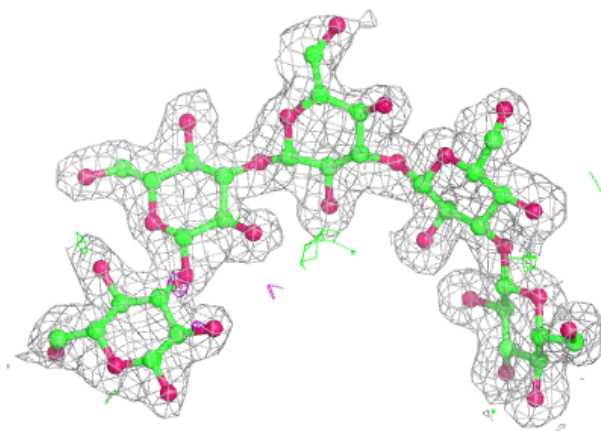
**Electron density around Chain D:**

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



**Electron density around Chain F:**

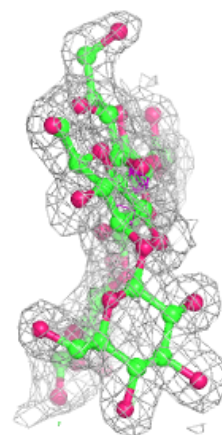
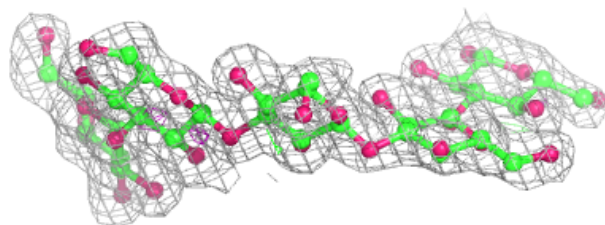
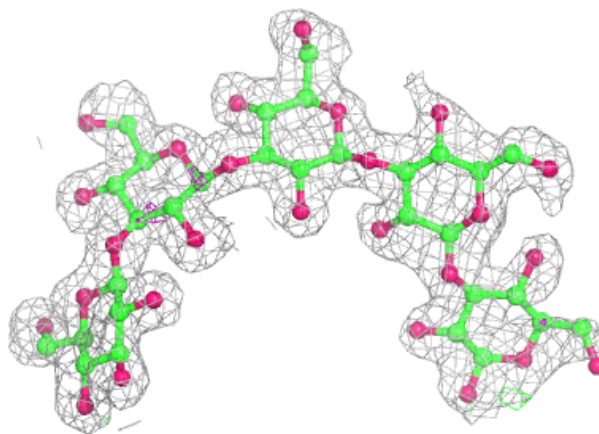
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





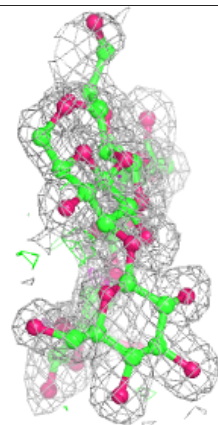
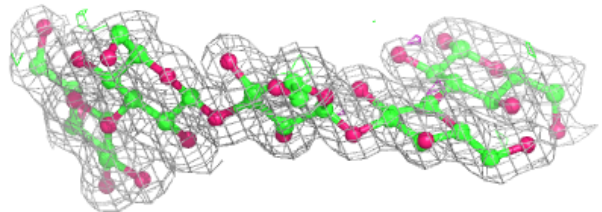
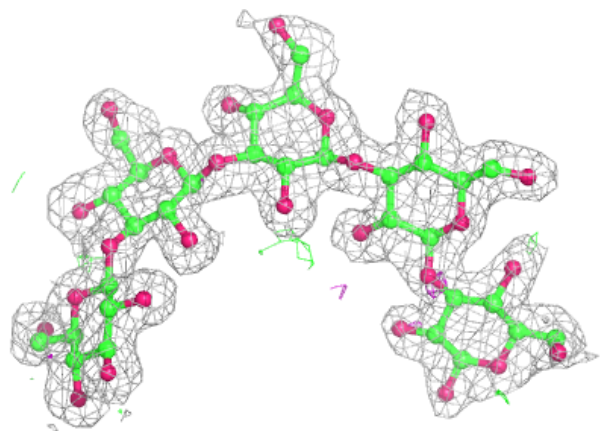
**Electron density around Chain D:**

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



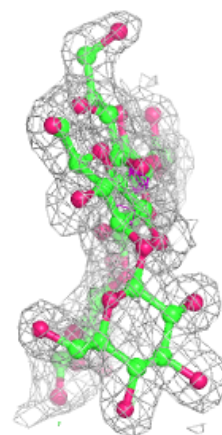
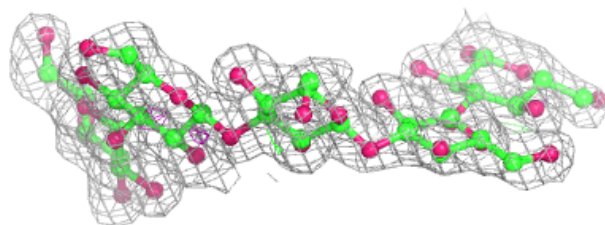
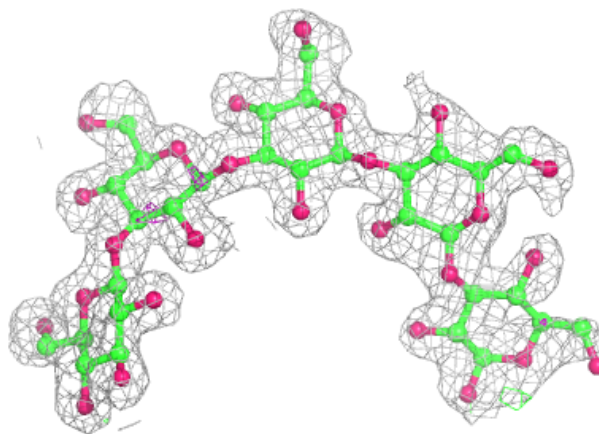
**Electron density around Chain F:**

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



**Electron density around Chain D:**

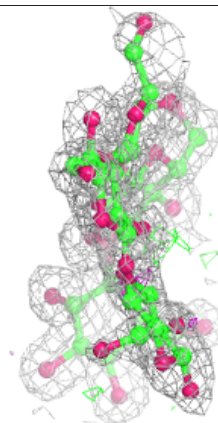
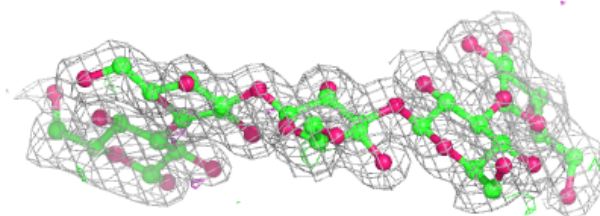
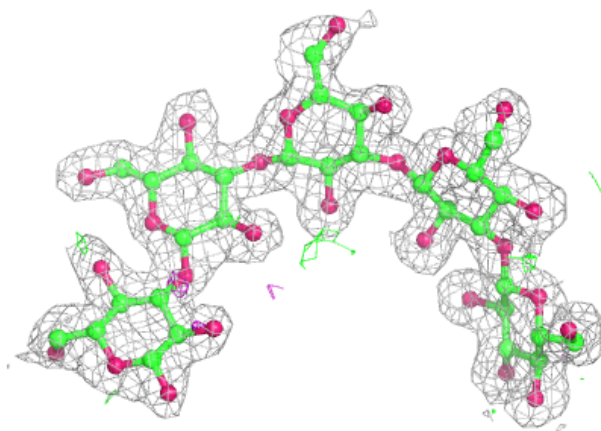
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





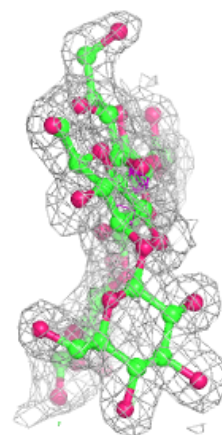
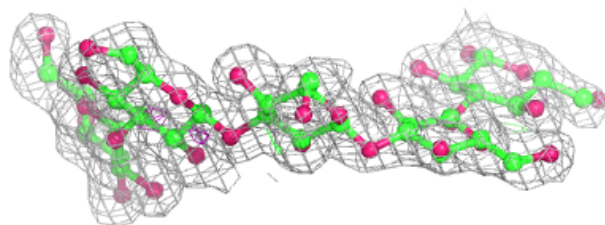
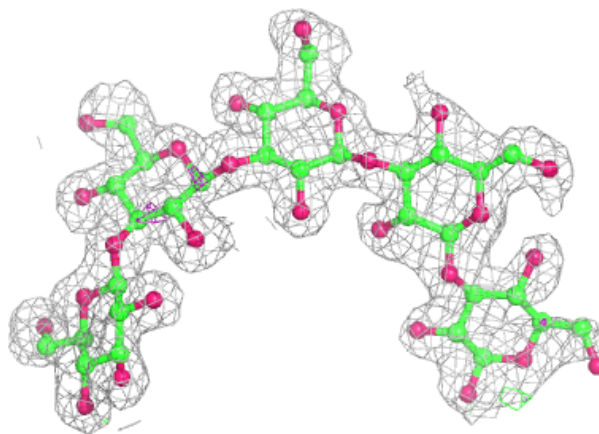
**Electron density around Chain F:**

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



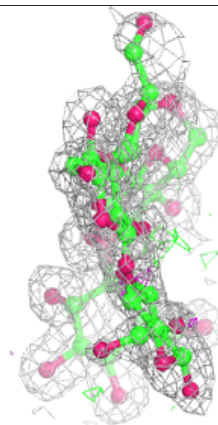
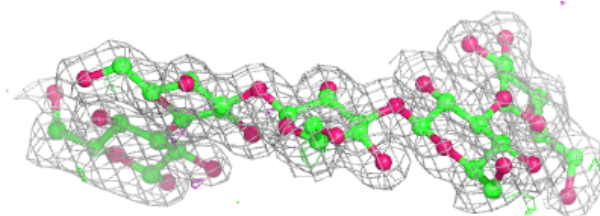
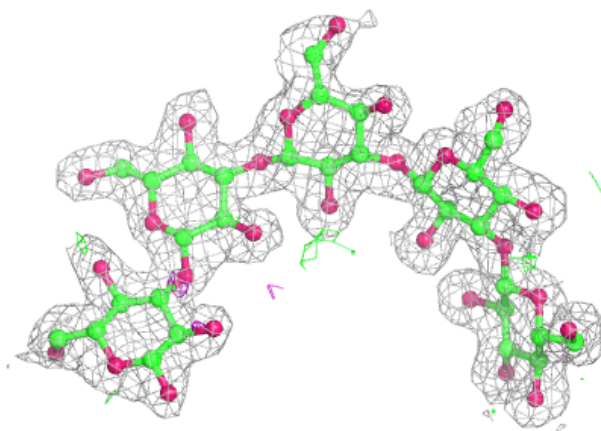
**Electron density around Chain D:**

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



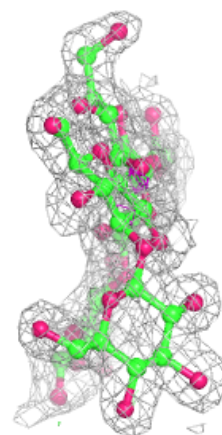
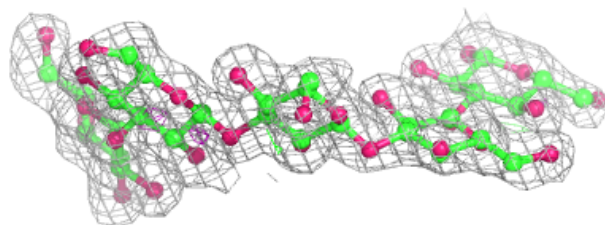
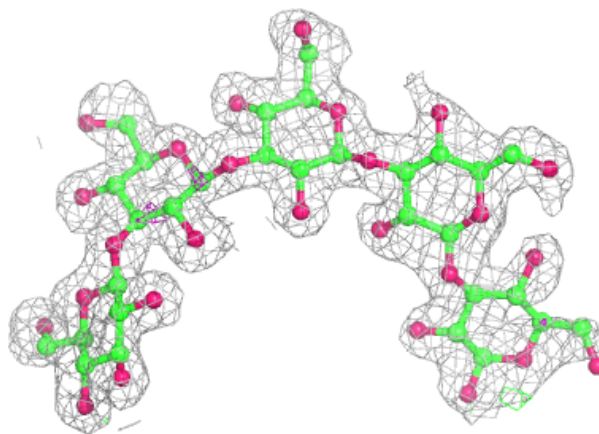
**Electron density around Chain F:**

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



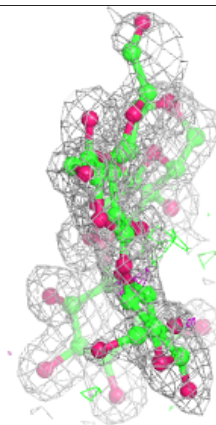
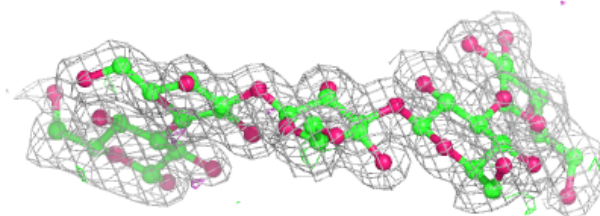
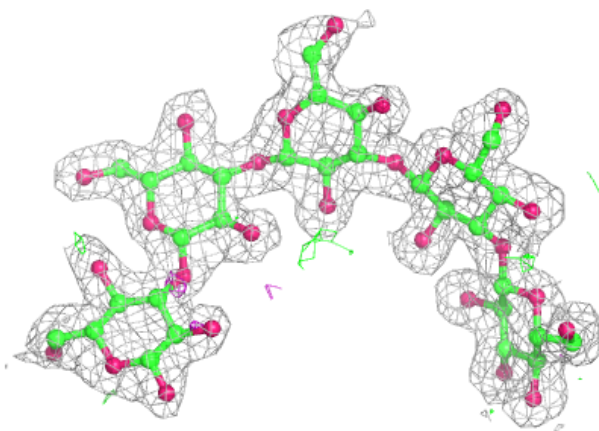
**Electron density around Chain D:**

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



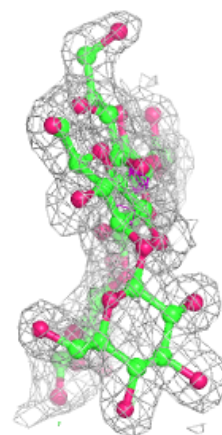
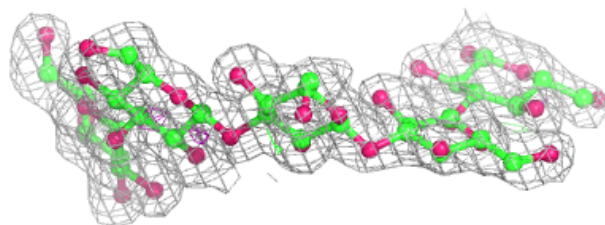
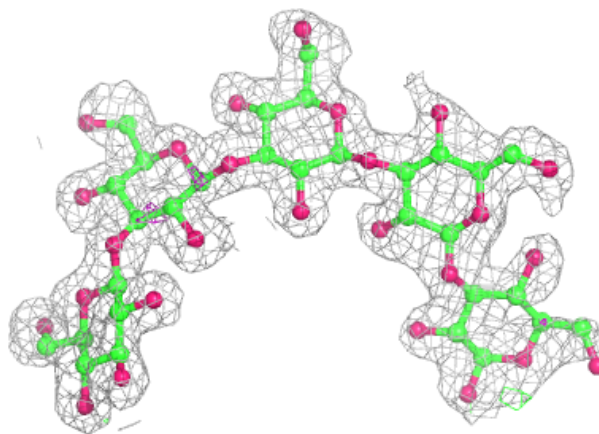
**Electron density around Chain F:**

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



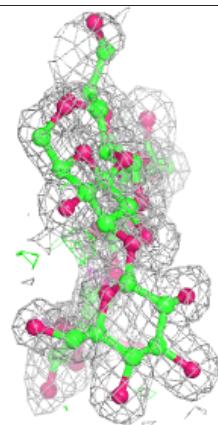
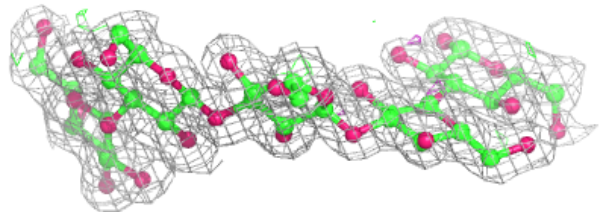
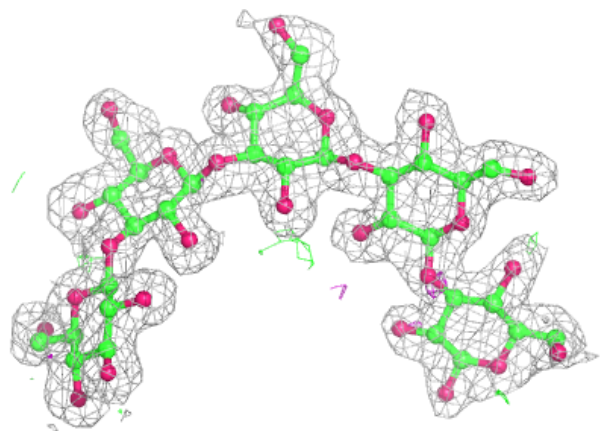
**Electron density around Chain D:**

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



**Electron density around Chain F:**

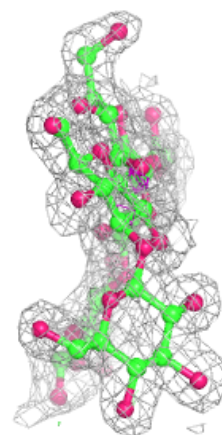
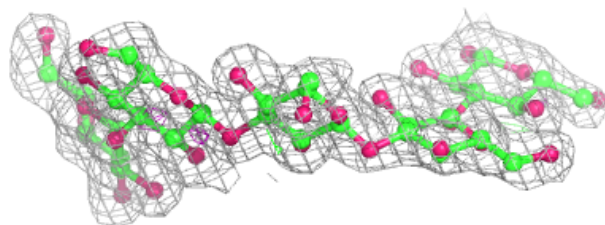
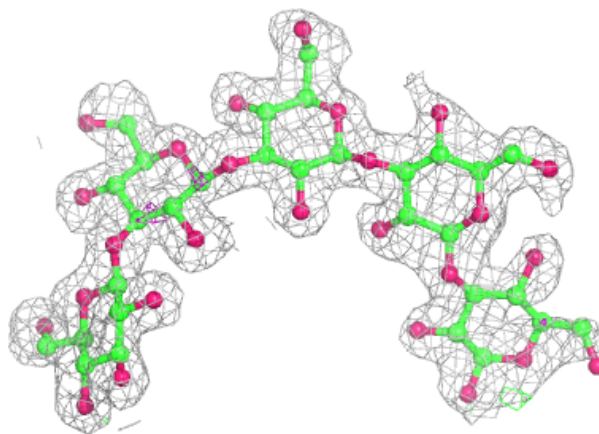
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain D:**

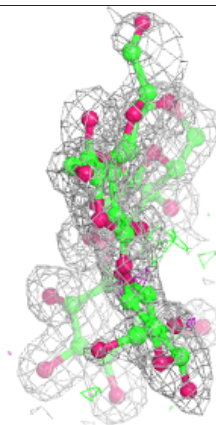
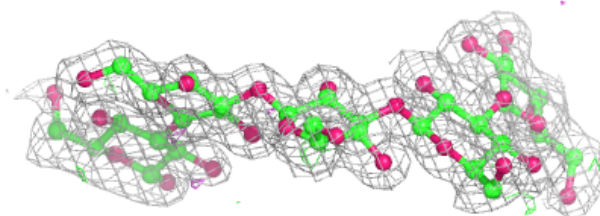
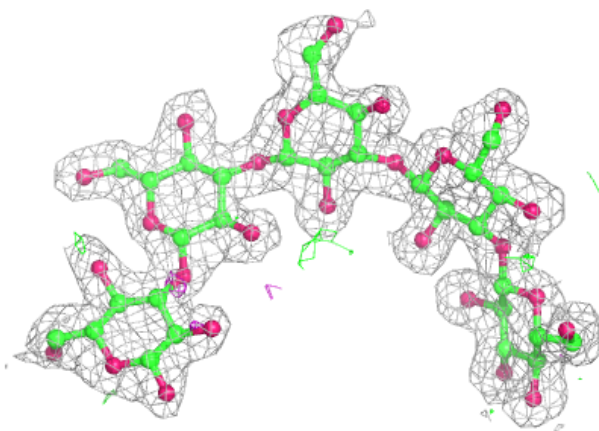
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





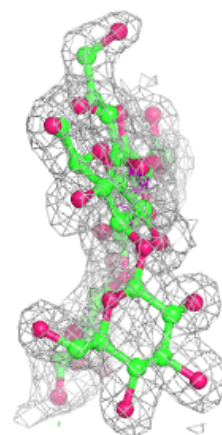
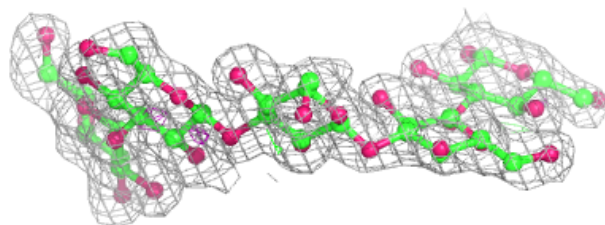
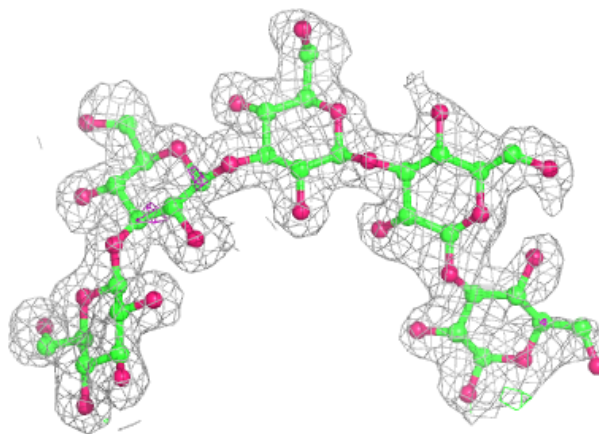
**Electron density around Chain F:**

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



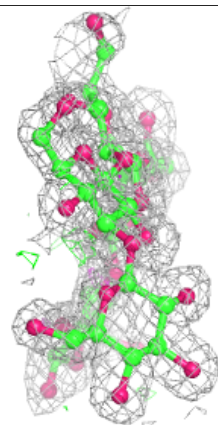
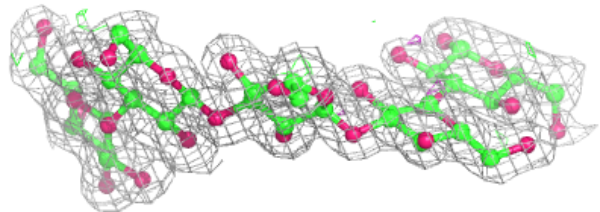
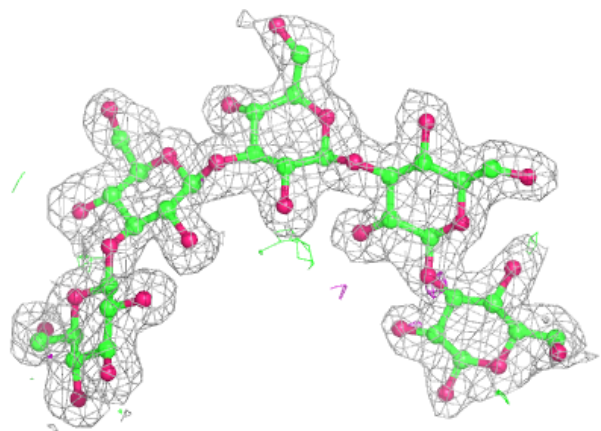
**Electron density around Chain D:**

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



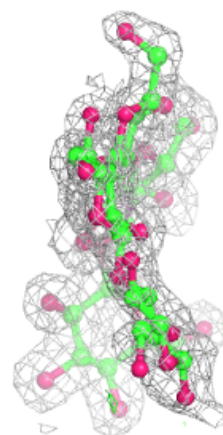
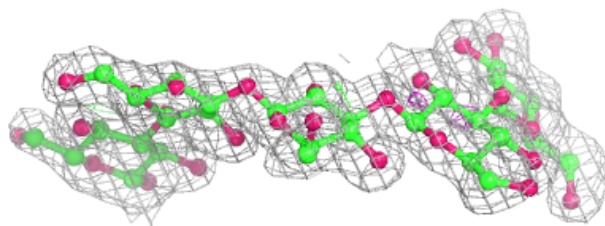
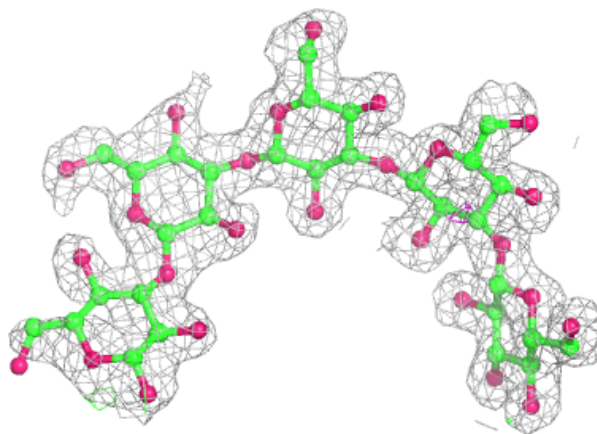
**Electron density around Chain F:**

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



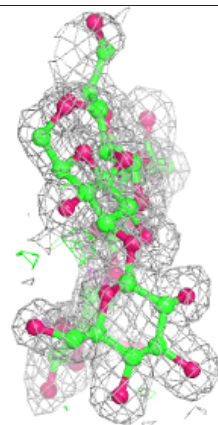
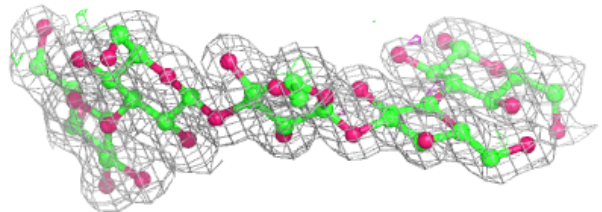
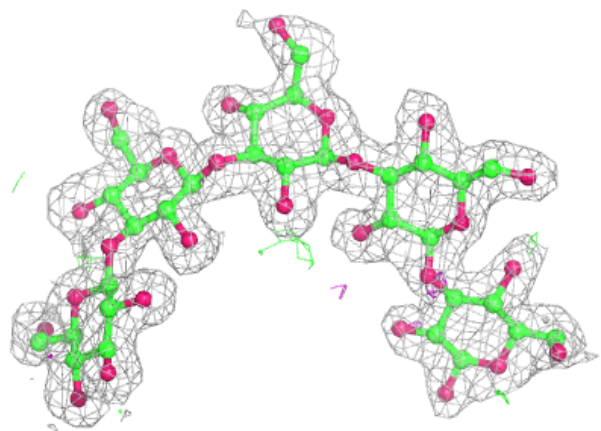
**Electron density around Chain D:**

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



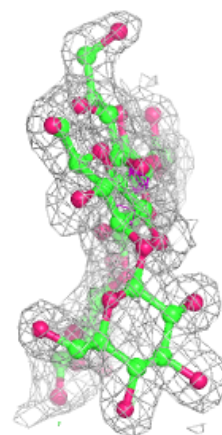
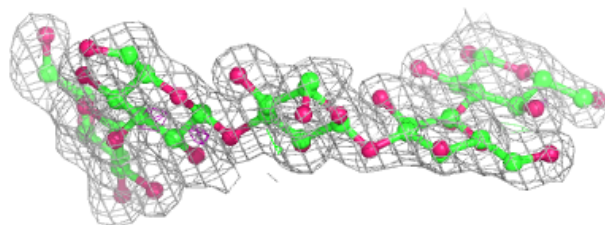
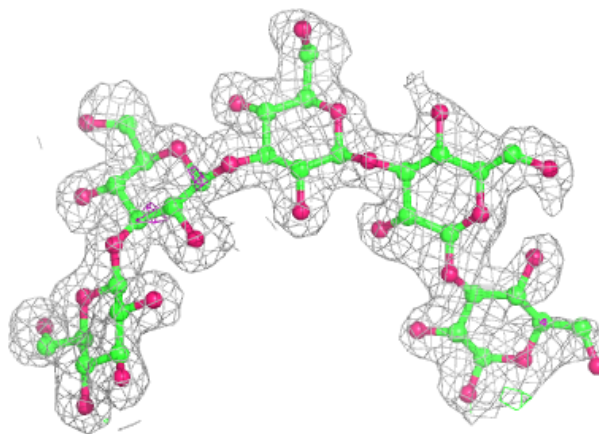
**Electron density around Chain F:**

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



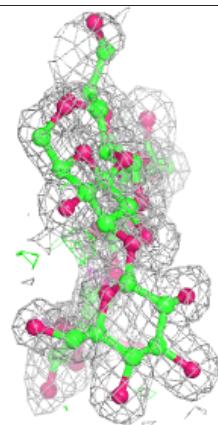
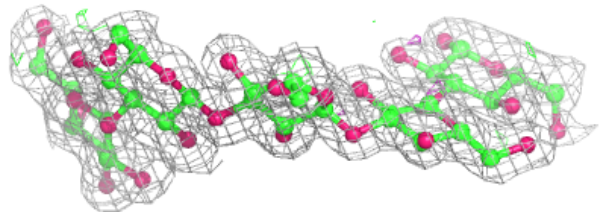
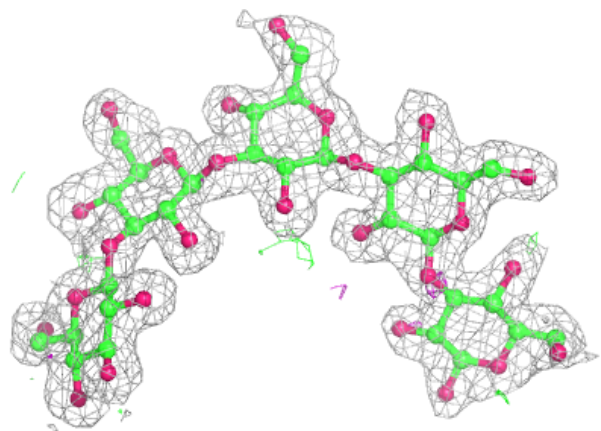
**Electron density around Chain D:**

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



**Electron density around Chain F:**

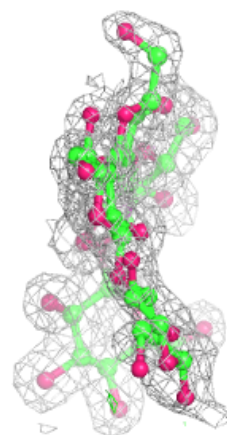
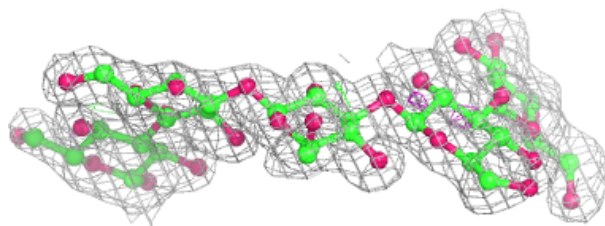
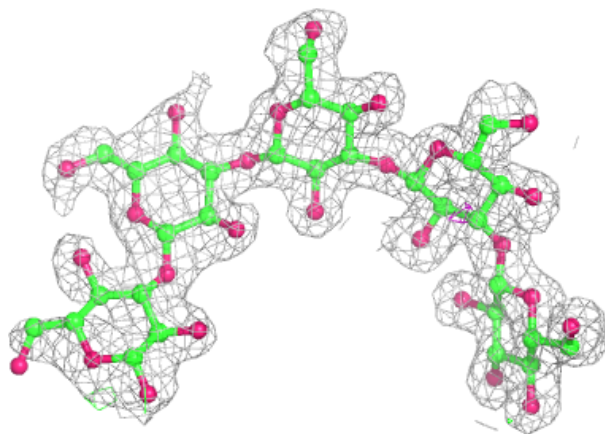
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain D:**

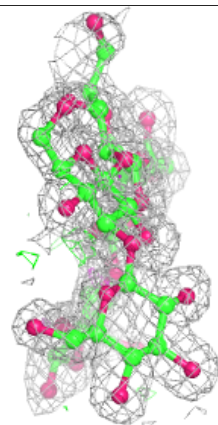
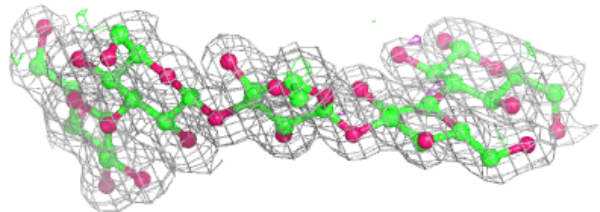
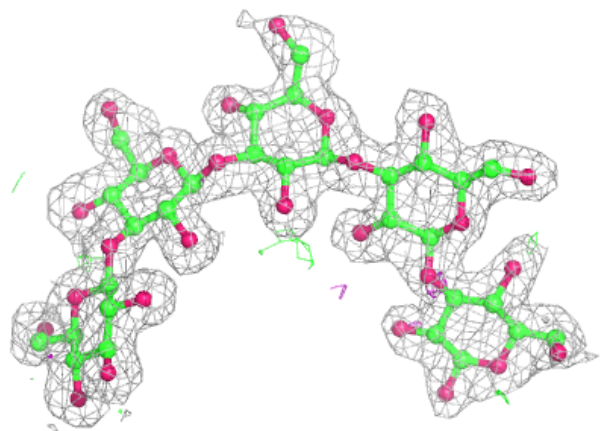
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





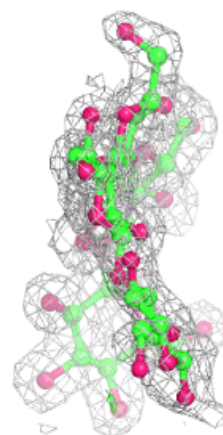
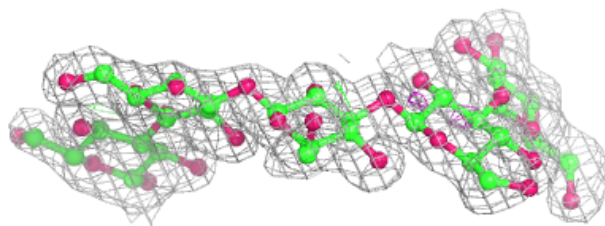
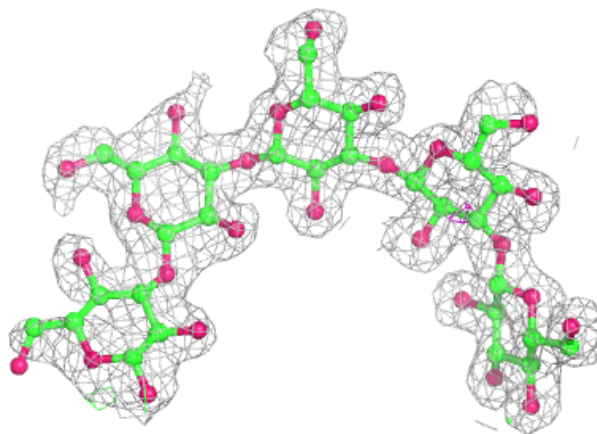
**Electron density around Chain F:**

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



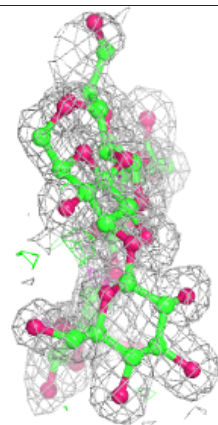
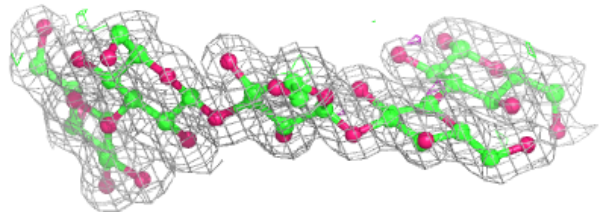
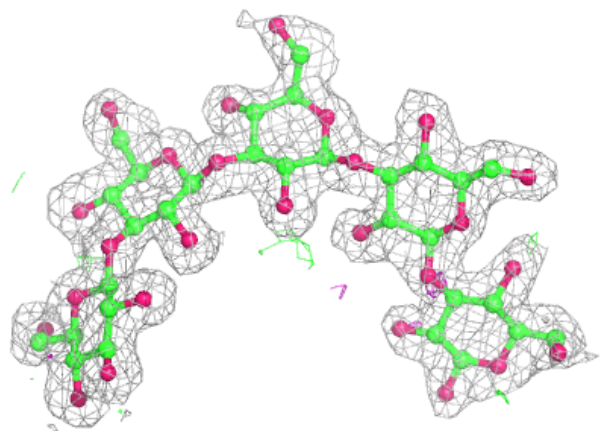
**Electron density around Chain D:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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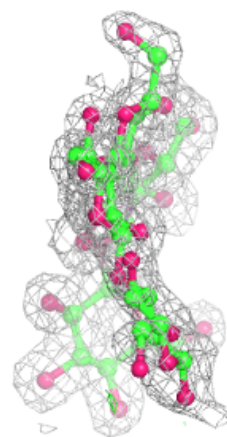
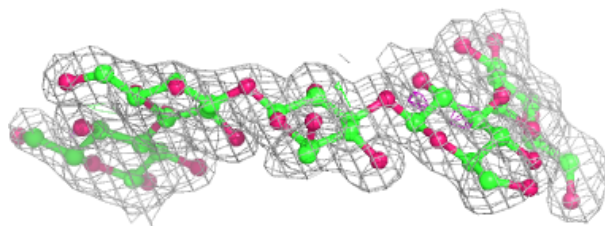
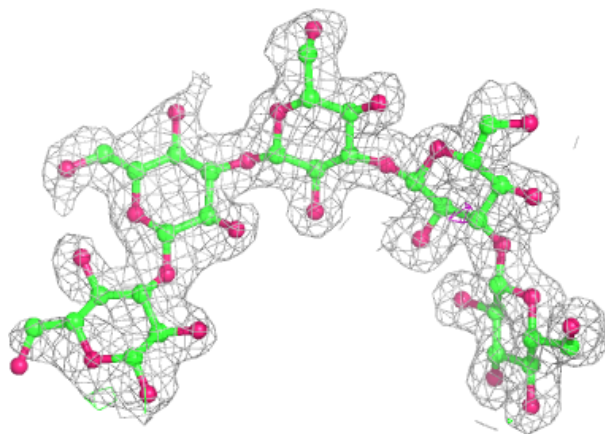
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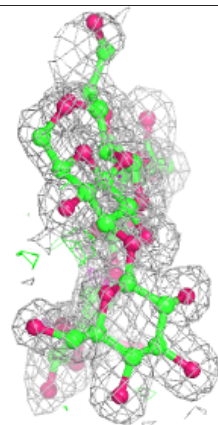
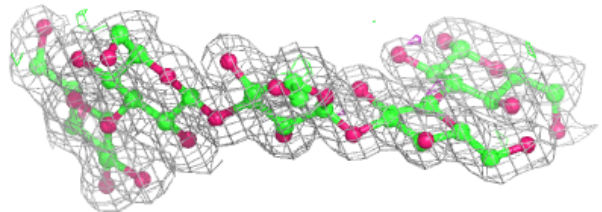
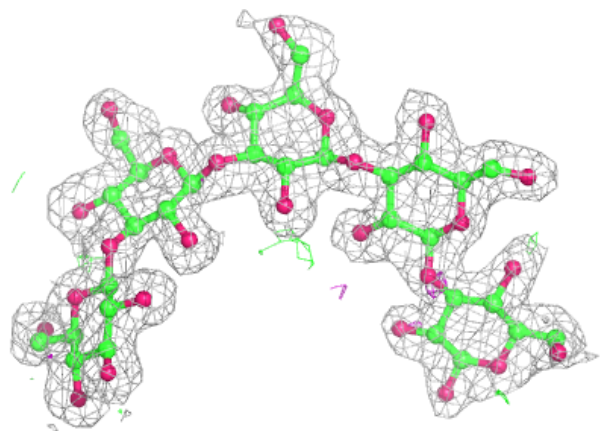
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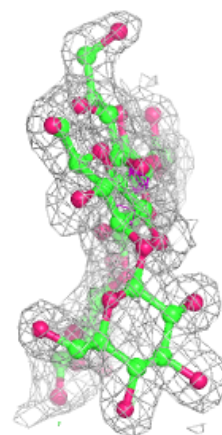
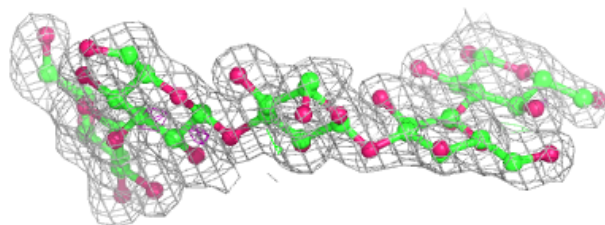
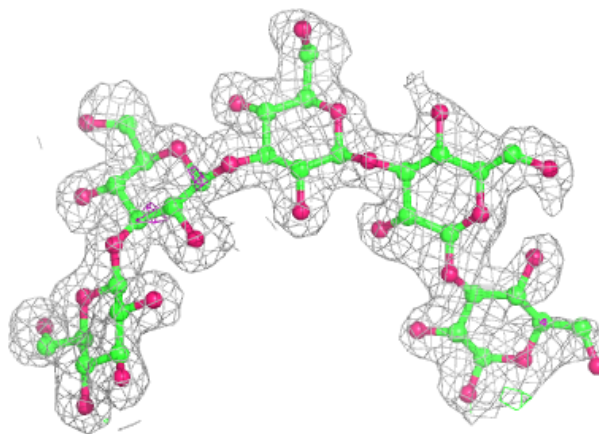
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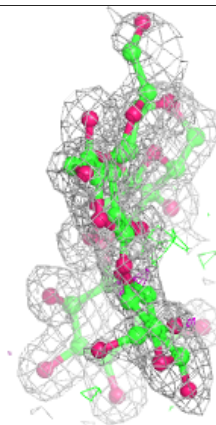
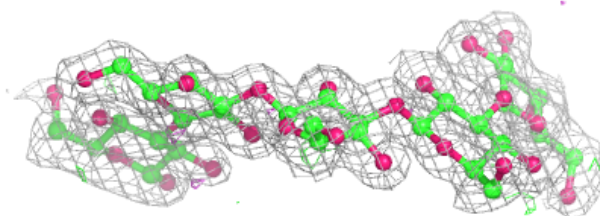
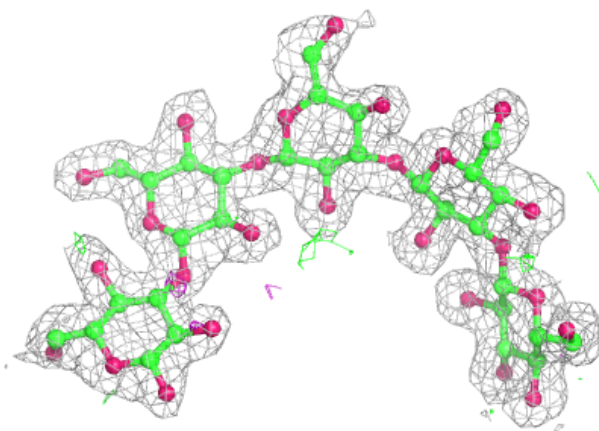
**Electron density around Chain D:**

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**Electron density around Chain F:**

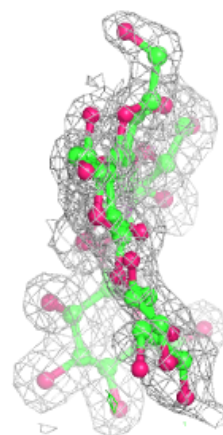
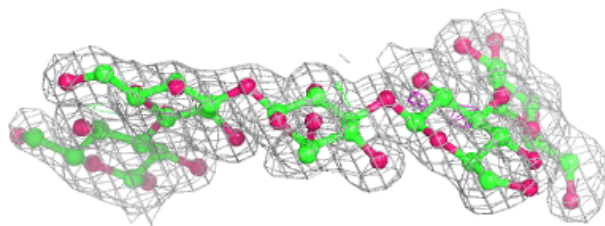
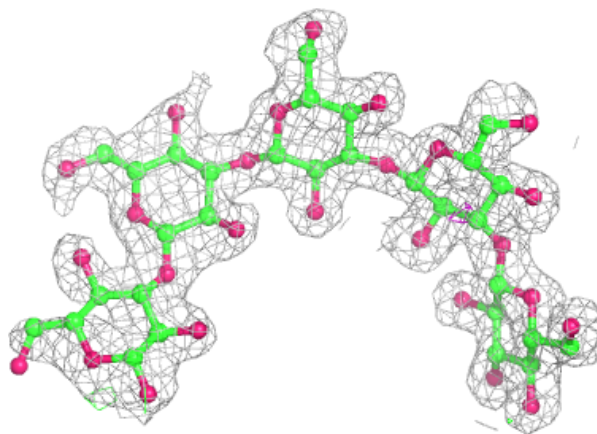
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
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**Electron density around Chain D:**

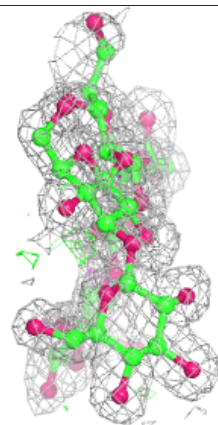
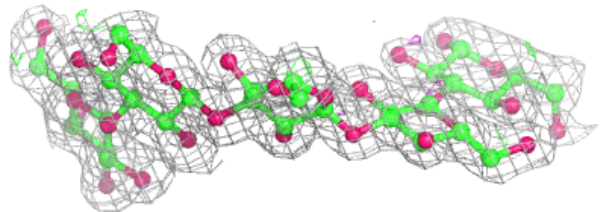
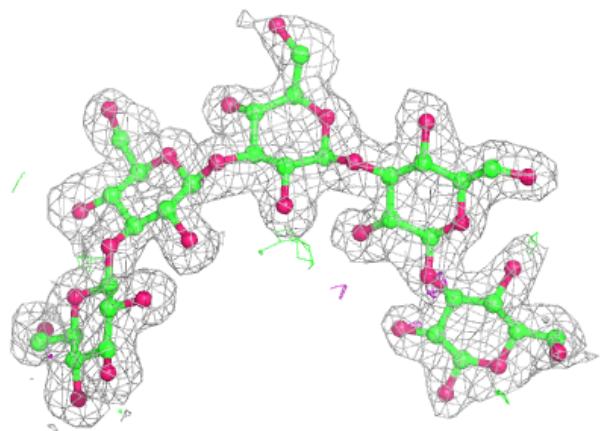
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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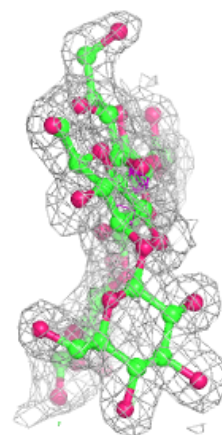
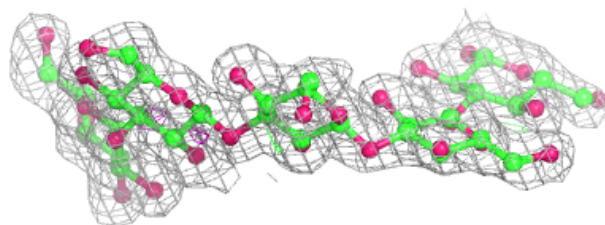
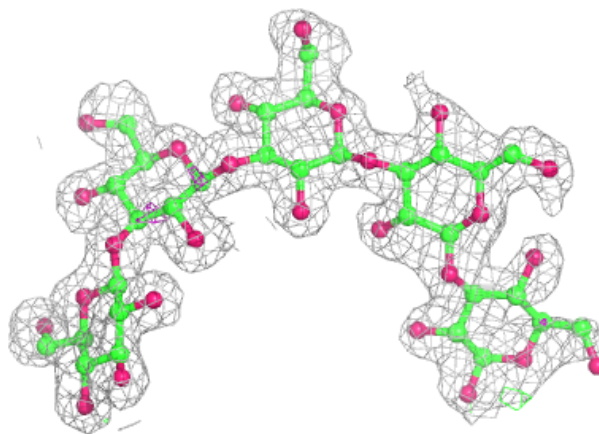
**Electron density around Chain F:**

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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
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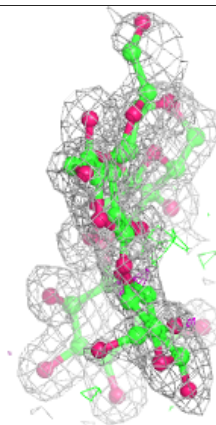
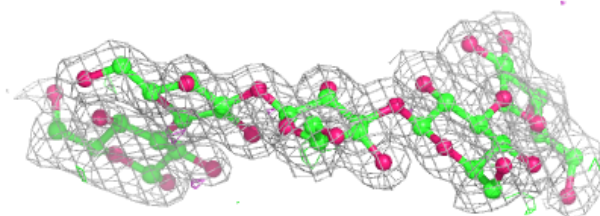
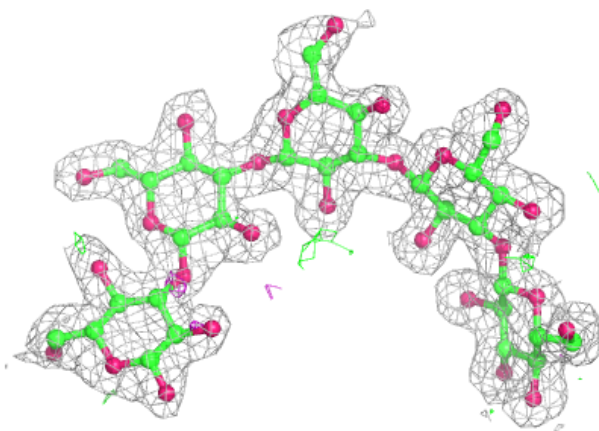
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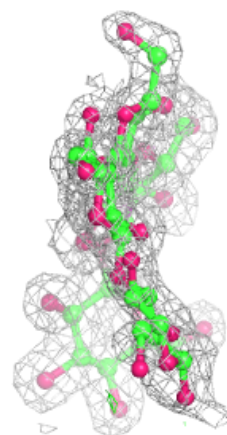
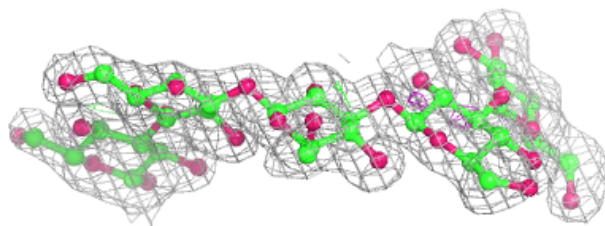
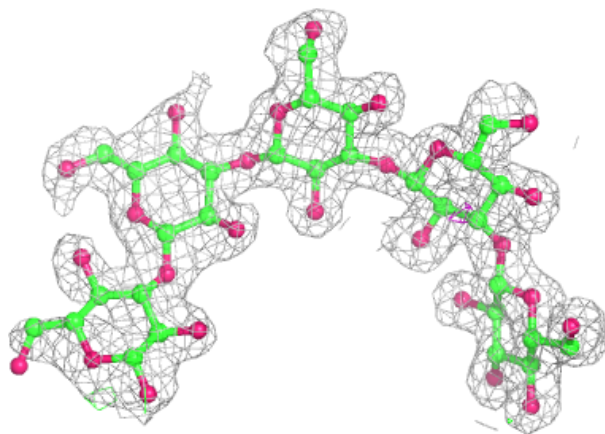
**Electron density around Chain F:**

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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
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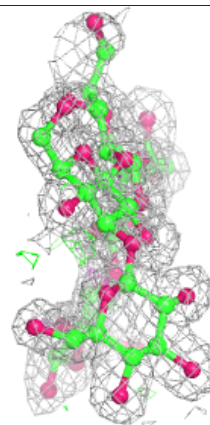
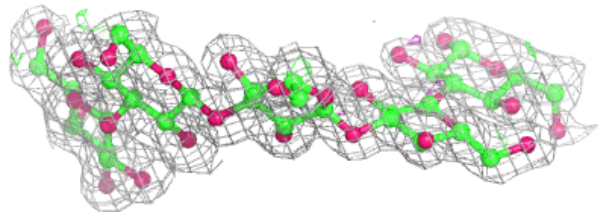
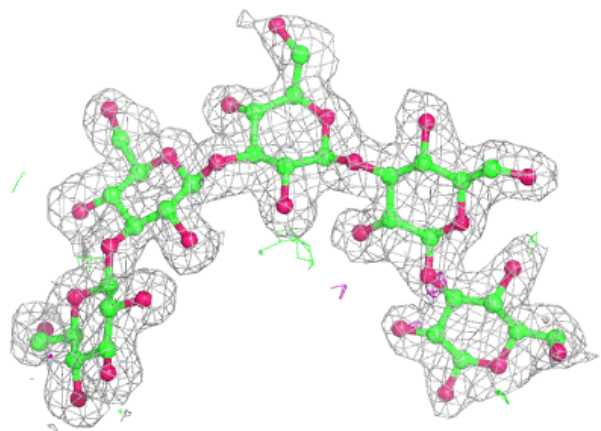
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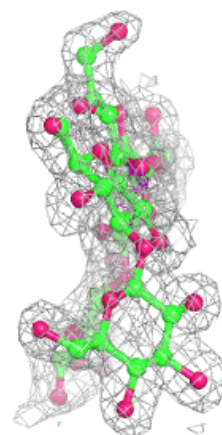
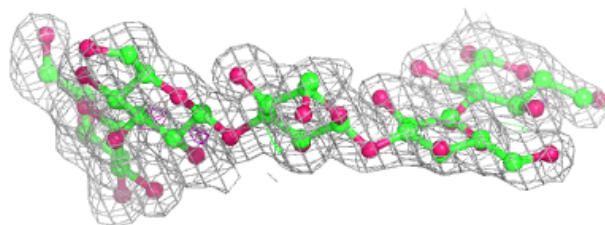
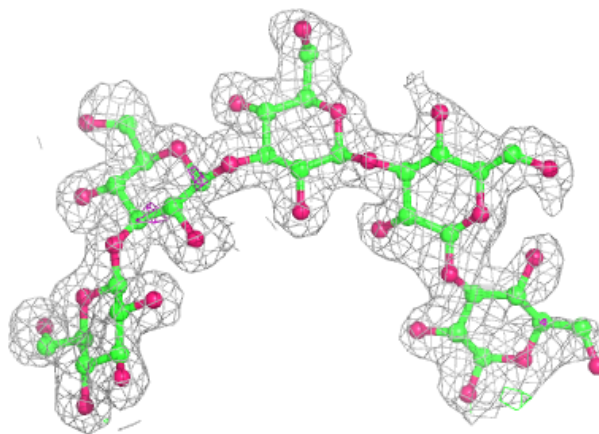
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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
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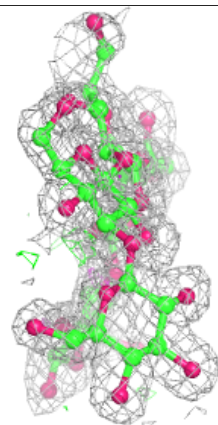
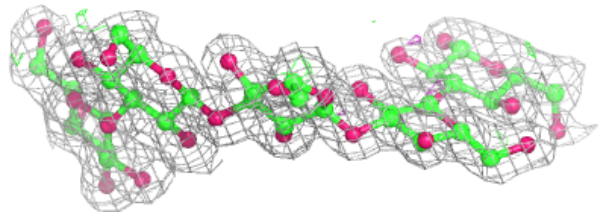
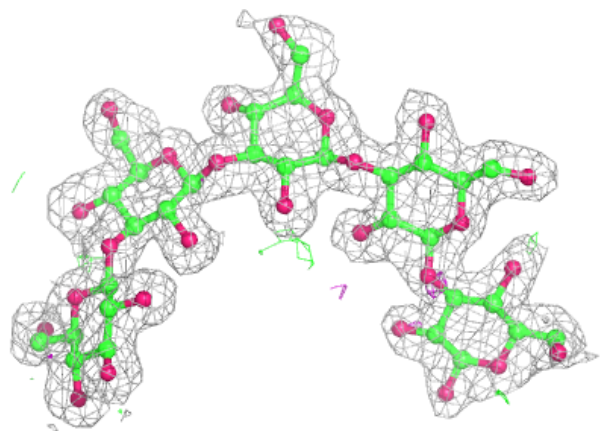
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**Electron density around Chain F:**

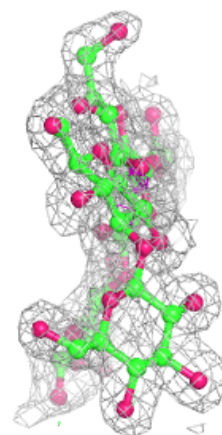
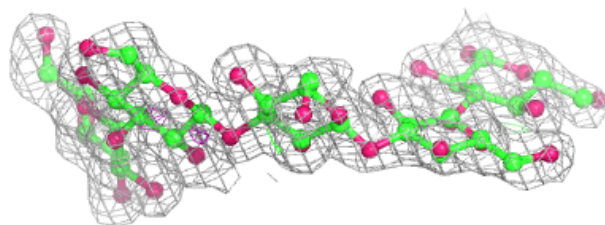
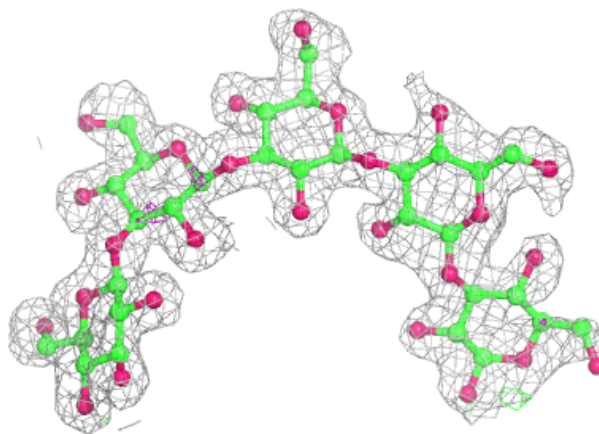
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
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**Electron density around Chain D:**

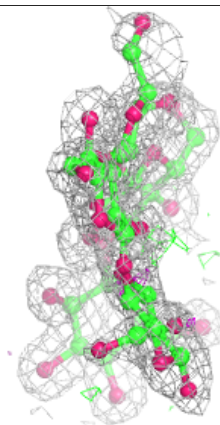
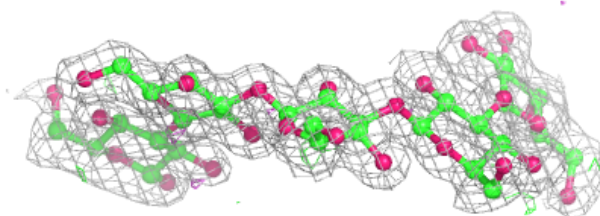
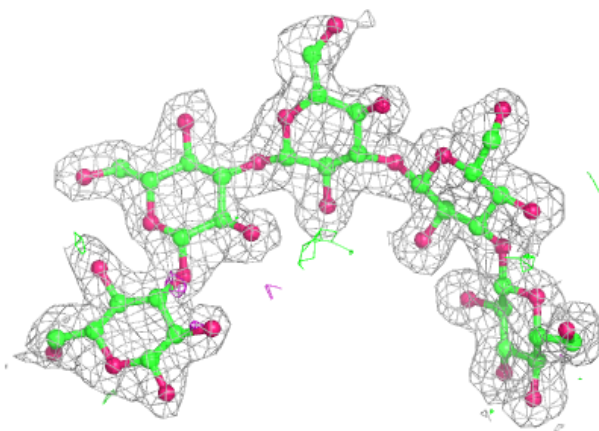
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and green (positive)





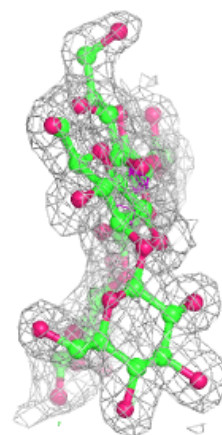
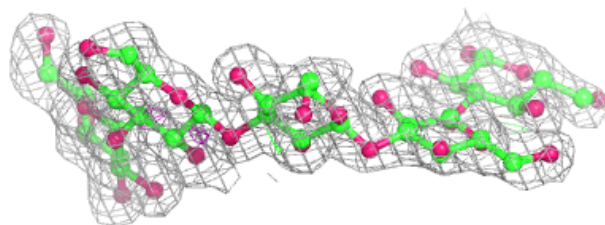
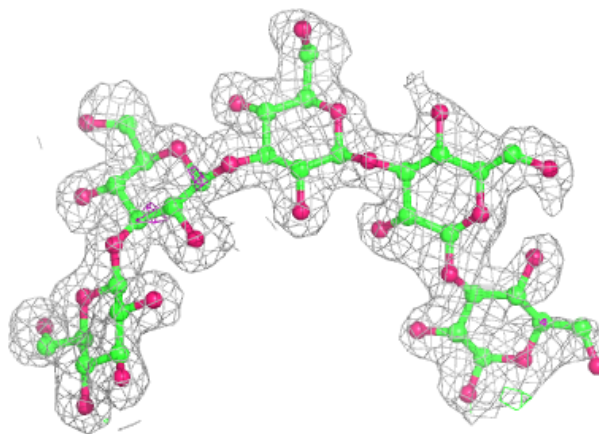
**Electron density around Chain F:**

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



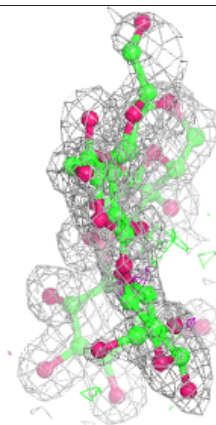
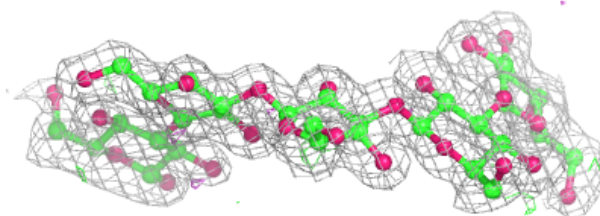
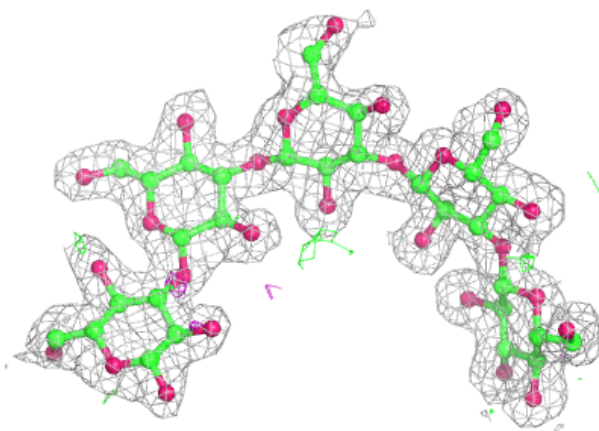
**Electron density around Chain D:**

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



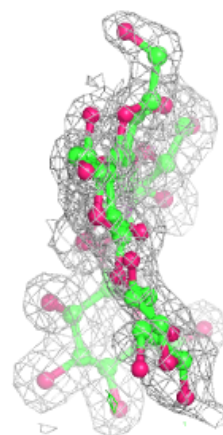
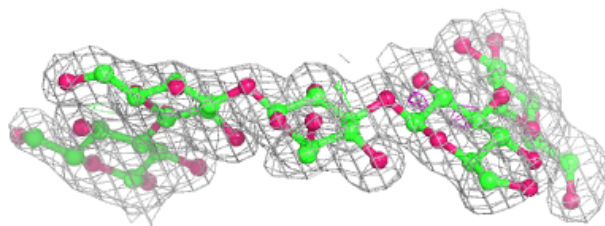
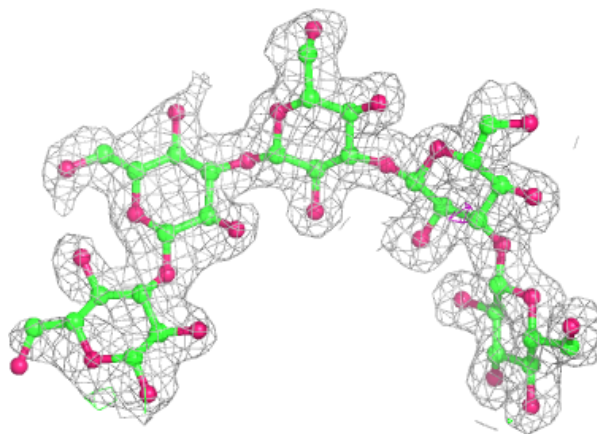
**Electron density around Chain F:**

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



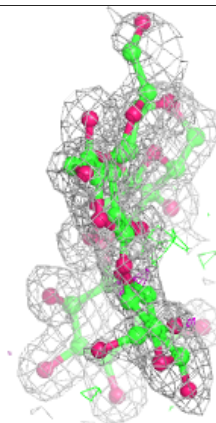
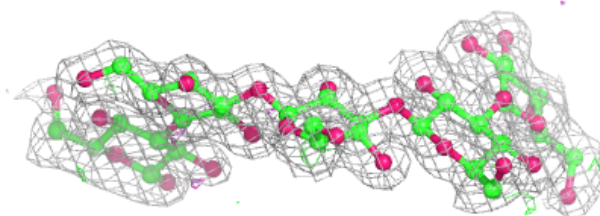
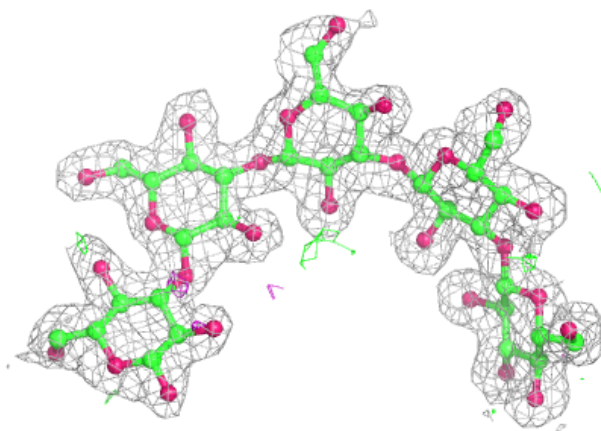
**Electron density around Chain D:**

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



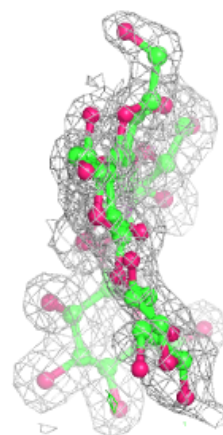
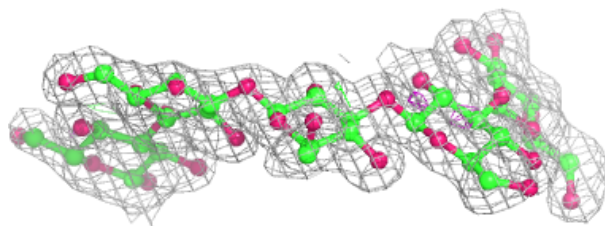
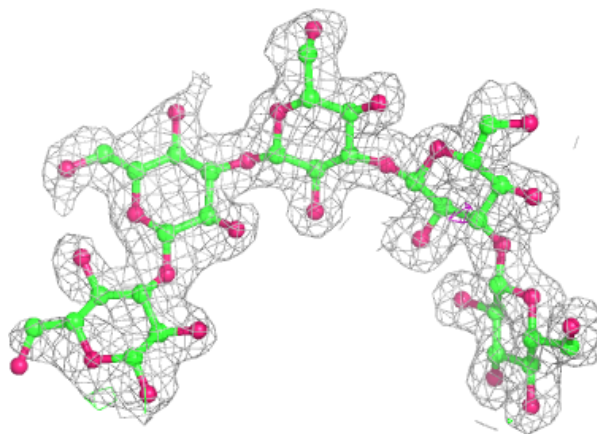
**Electron density around Chain F:**

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



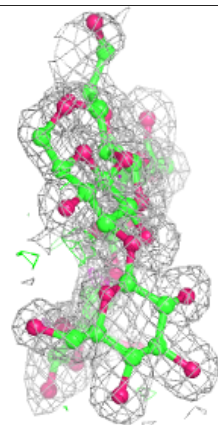
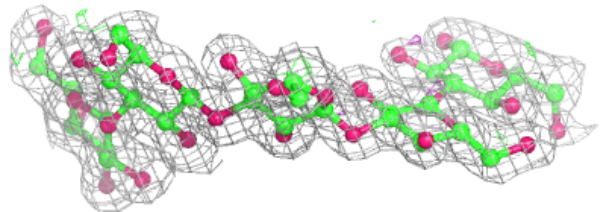
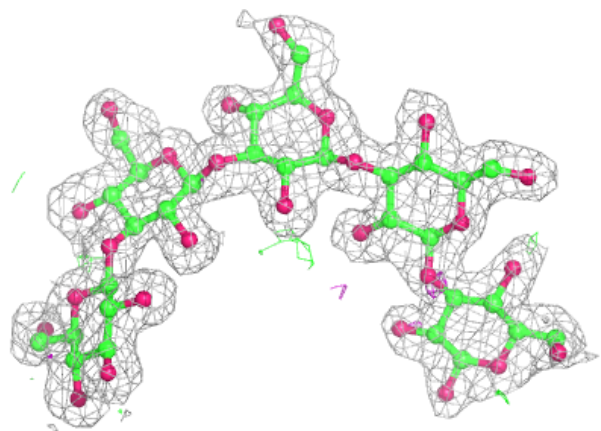
**Electron density around Chain D:**

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



**Electron density around Chain F:**

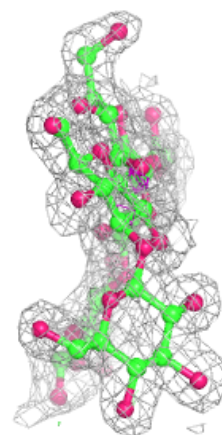
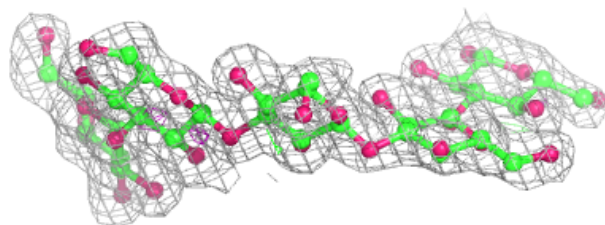
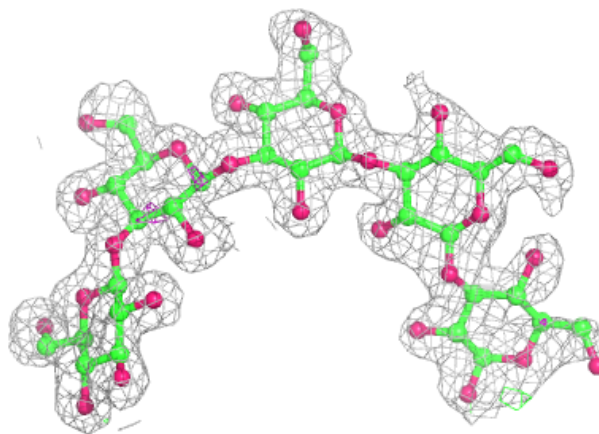
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain D:**

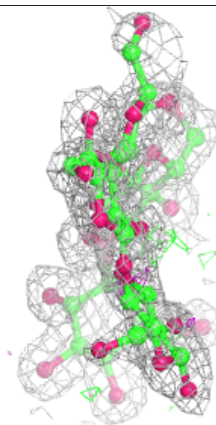
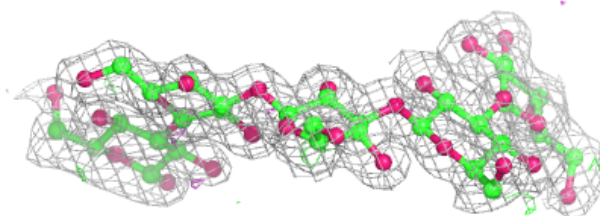
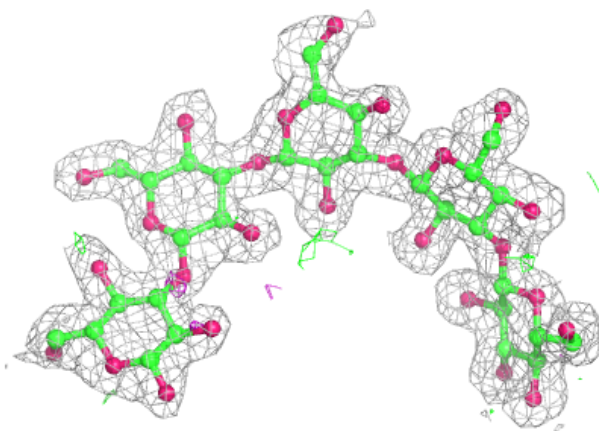
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





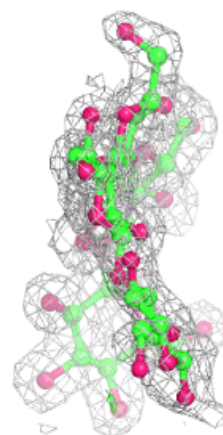
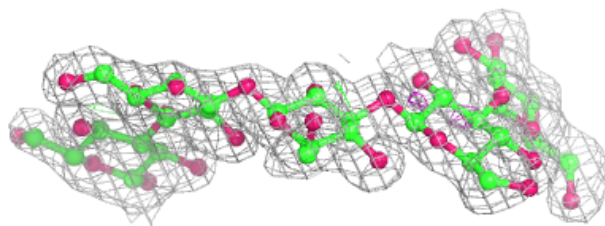
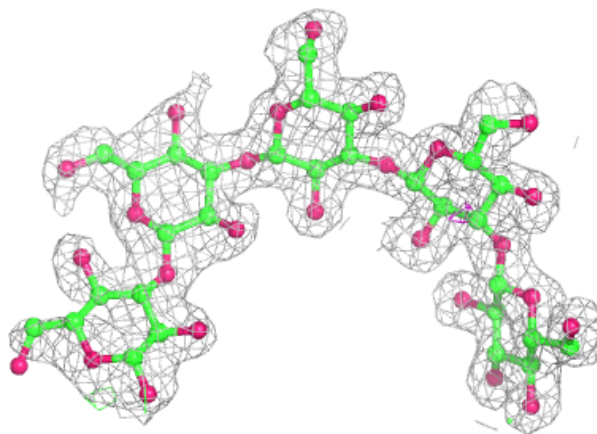
**Electron density around Chain F:**

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



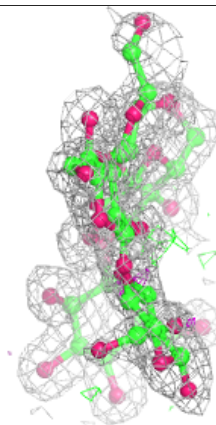
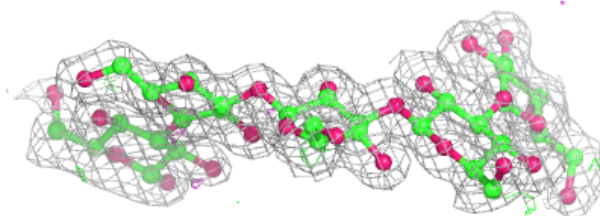
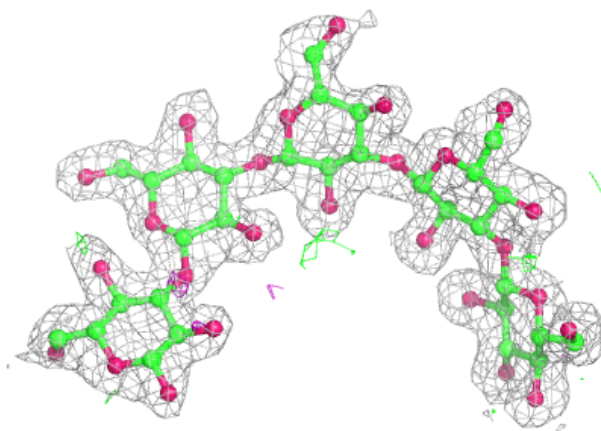
**Electron density around Chain D:**

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



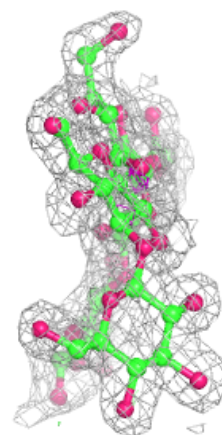
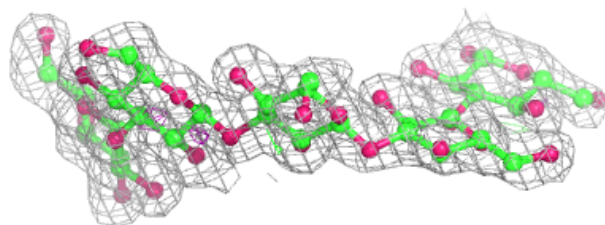
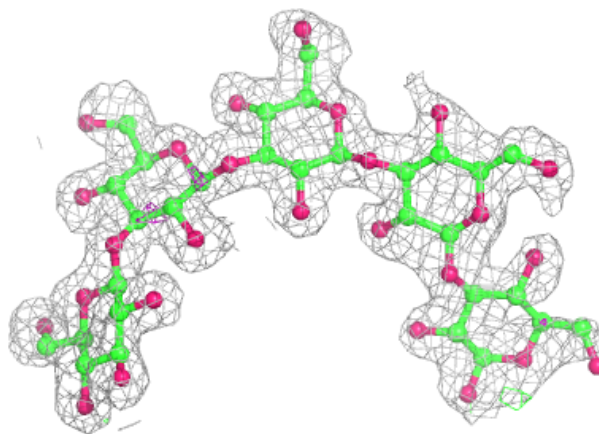
**Electron density around Chain F:**

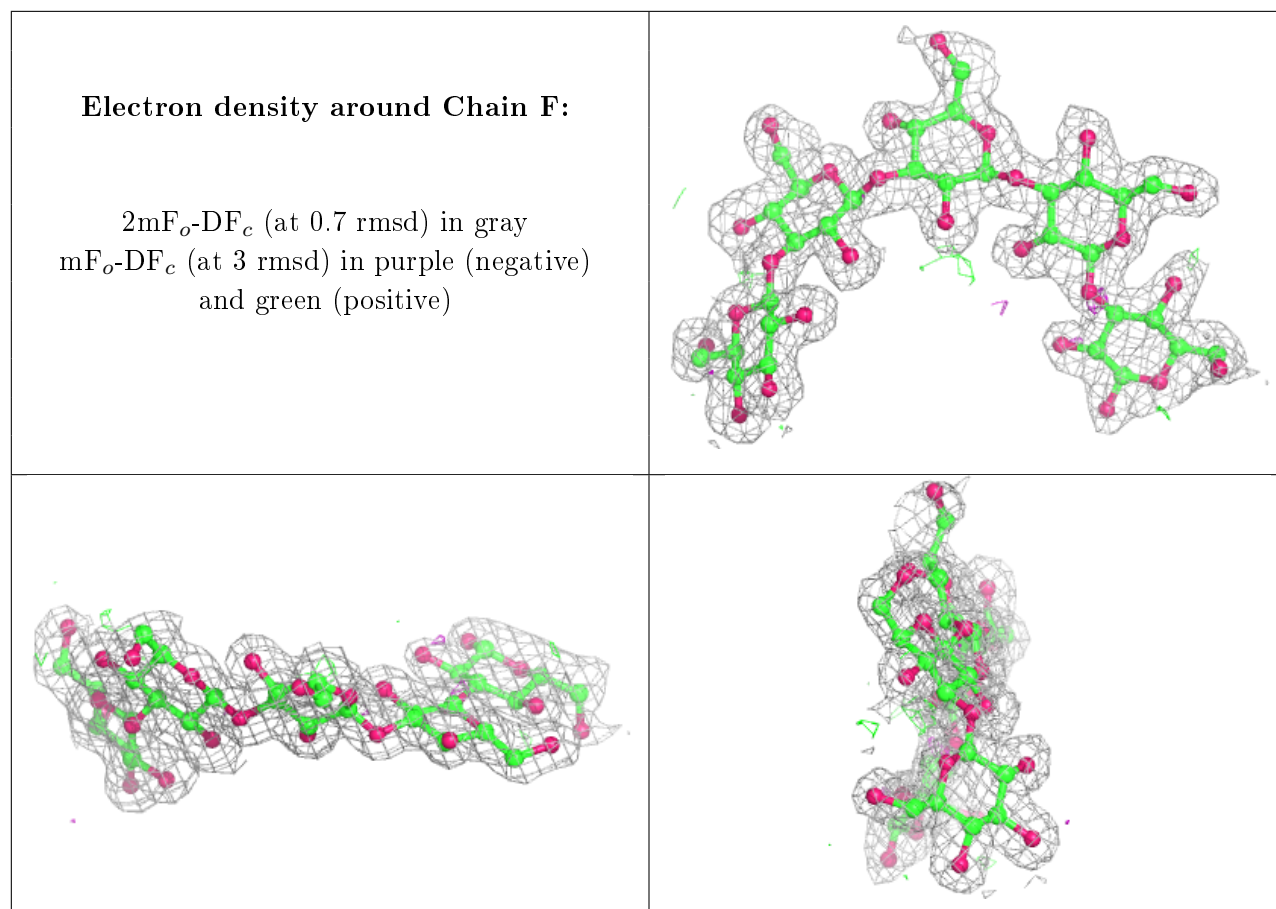
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

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





## 6.4 Ligands ⓘ

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | EDO  | 21-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 13-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 22-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 23-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 15-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 10-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 1-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 5-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 12-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 8-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 18-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 2-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |
| 4   | EDO  | 17-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                | 10    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | EDO  | 16-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 4-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 11-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 24-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 3-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 7-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 19-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 25-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 14-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 6-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 20-B  | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 9-B   | 701 | 4/4   | 0.93 | 0.11 | 13,21,21,22                 | 10    |
| 4   | EDO  | 11-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 24-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 16-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 3-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 14-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 7-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 23-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 2-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 25-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 9-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 17-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 21-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 19-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 20-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 18-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 5-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 10-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 1-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 13-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 6-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 4-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 15-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 8-A   | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 22-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |
| 4   | EDO  | 12-A  | 701 | 4/4   | 0.98 | 0.07 | 13,13,19,19                 | 10    |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.