



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:22 AM UTC

PDB ID : 7BJ4 / pdb\_00007bj4  
Title : Inulosucrase from Halalkalicoccus jeotgali bound to kestose  
Authors : Ghauri, K.; Pijning, T.; Munawar, N.; Ali, H.; Ghauri, M.A.; Anwar, M.A.; Wallis, R.  
Deposited on : 2021-01-14  
Resolution : 2.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

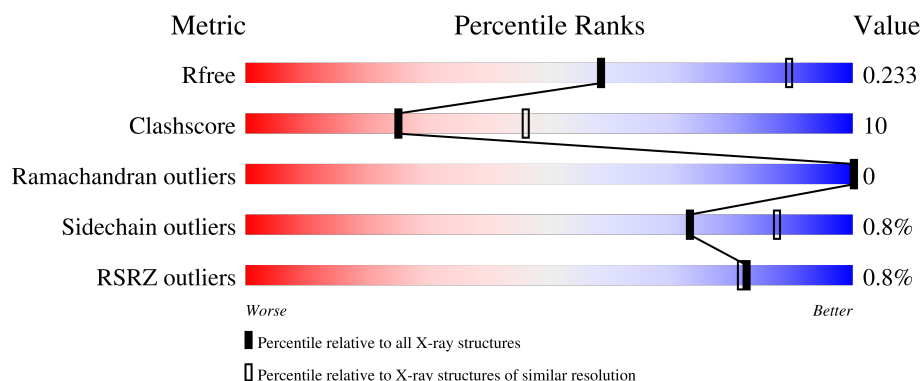
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 Å.

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



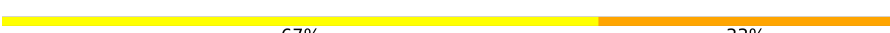
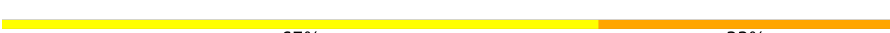
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4348 (2.74-2.70)                                      |
| Clashscore            | 190562                      | 4665 (2.74-2.70)                                      |
| Ramachandran outliers | 187476                      | 4584 (2.74-2.70)                                      |
| Sidechain outliers    | 187428                      | 4585 (2.74-2.70)                                      |
| RSRZ outliers         | 180081                      | 4348 (2.74-2.70)                                      |

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

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 428    | <div> <div>85%</div> <div>9%</div> <div>5%</div> </div>                |
| 1   | B     | 428    | <div> <div>2%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div> |
| 1   | C     | 428    | <div> <div>84%</div> <div>11%</div> <div>5%</div> </div>               |
| 1   | D     | 428    | <div> <div>82%</div> <div>13%</div> <div>5%</div> </div>               |
| 1   | E     | 428    | <div> <div>84%</div> <div>11%</div> <div>5%</div> </div>               |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | F     | 428    |    |
| 1   | G     | 428    |    |
| 1   | H     | 428    |    |
| 1   | I     | 428    |    |
| 1   | J     | 428    |    |
| 2   | K     | 3      |    |
| 2   | L     | 3      |    |
| 2   | M     | 3      |    |
| 2   | N     | 3      |    |
| 2   | O     | 3      |    |
| 2   | P     | 3      |    |
| 2   | Q     | 3      |    |
| 2   | R     | 3      |  |
| 2   | T     | 3      |  |
| 2   | U     | 3      |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | FRU  | M     | 3   | -         | -        | X       | -                |
| 2   | GLC  | Q     | 1   | -         | -        | X       | -                |
| 2   | FRU  | Q     | 3   | -         | -        | X       | -                |
| 2   | FRU  | T     | 3   | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32221 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Levansucrase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | B     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | C     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | D     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | E     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | F     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | G     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | H     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | I     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |
| 1   | J     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3180  | 2013 | 546 | 617 | 4 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 2   | K     | 3        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 34    | 18 | 16 |         |         |       |
| 2   | L     | 3        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 34    | 18 | 16 |         |         |       |

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| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-----------------------|---------|---------|-------|
| 2   | M     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | N     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | O     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | P     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | Q     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | R     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | T     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |
| 2   | U     | 3        | Total C O<br>34 18 16 | 0       | 0       | 0     |

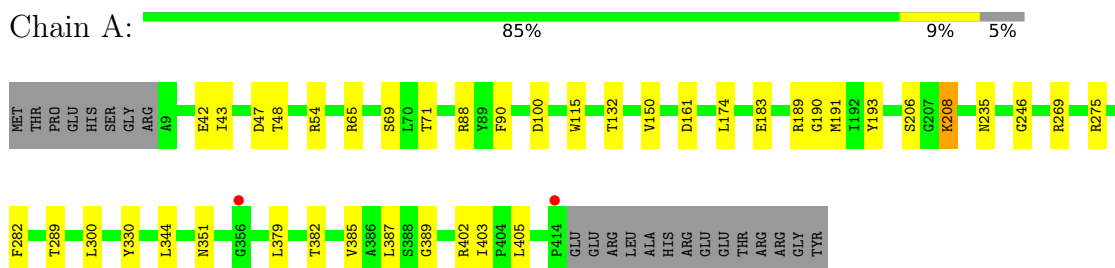
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | A     | 2        | Total O<br>2 2   | 0       | 0       |
| 3   | B     | 9        | Total O<br>9 9   | 0       | 0       |
| 3   | C     | 5        | Total O<br>5 5   | 0       | 0       |
| 3   | D     | 8        | Total O<br>8 8   | 0       | 0       |
| 3   | E     | 10       | Total O<br>10 10 | 0       | 0       |
| 3   | F     | 8        | Total O<br>8 8   | 0       | 0       |
| 3   | G     | 9        | Total O<br>9 9   | 0       | 0       |
| 3   | H     | 10       | Total O<br>10 10 | 0       | 0       |
| 3   | I     | 10       | Total O<br>10 10 | 0       | 0       |
| 3   | J     | 10       | Total O<br>10 10 | 0       | 0       |

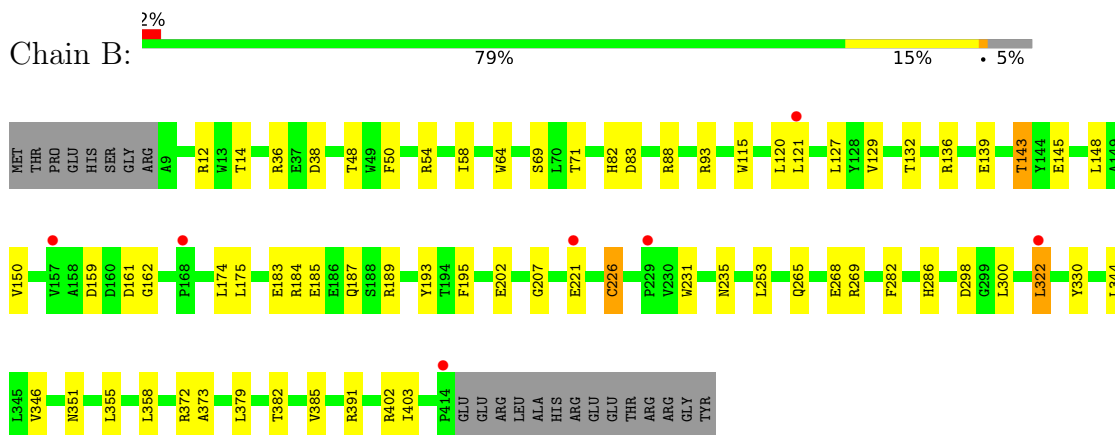
### 3 Residue-property plots [i](#)

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.

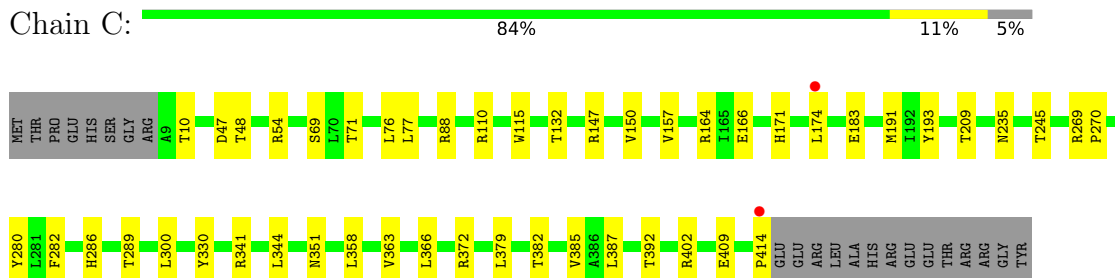
- Molecule 1: Levansucrase



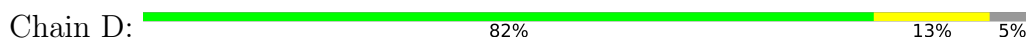
- Molecule 1: Levansucrase

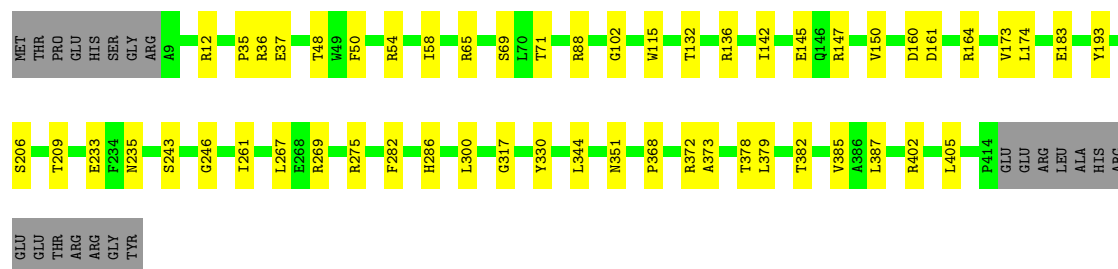


- Molecule 1: Levansucrase



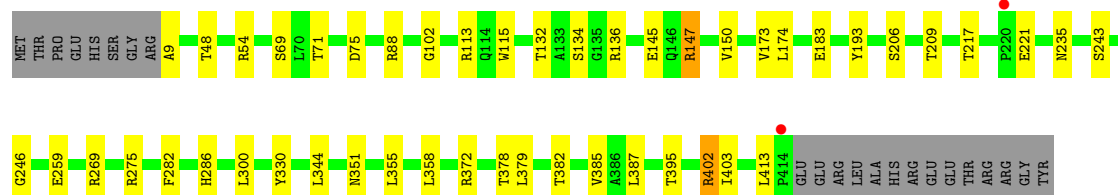
- Molecule 1: Levansucrase





• Molecule 1: Levansucrase

Chain E: 84% 11% 5%



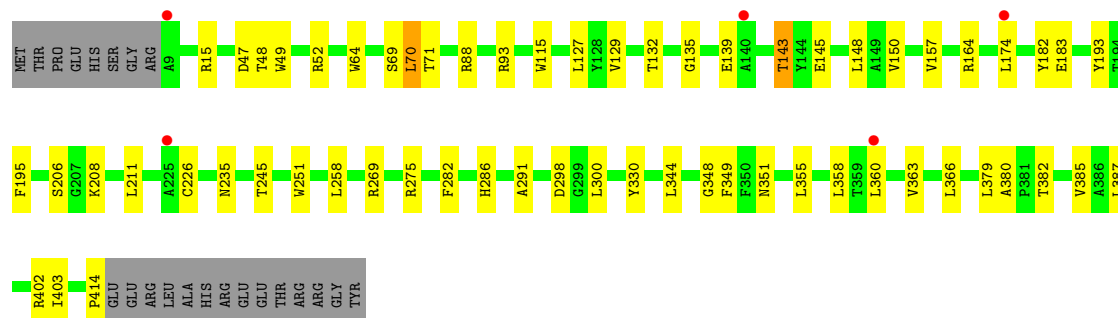
• Molecule 1: Levansucrase

Chain F: 82% 13% 5%



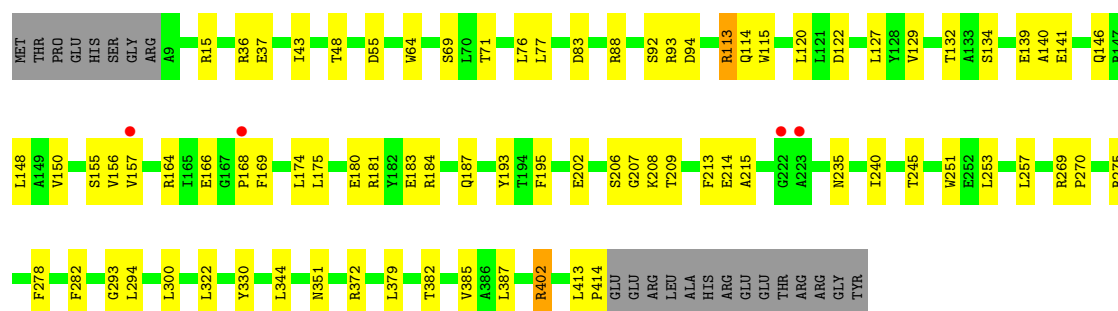
• Molecule 1: Levansucrase

Chain G: 81% 14% 5%

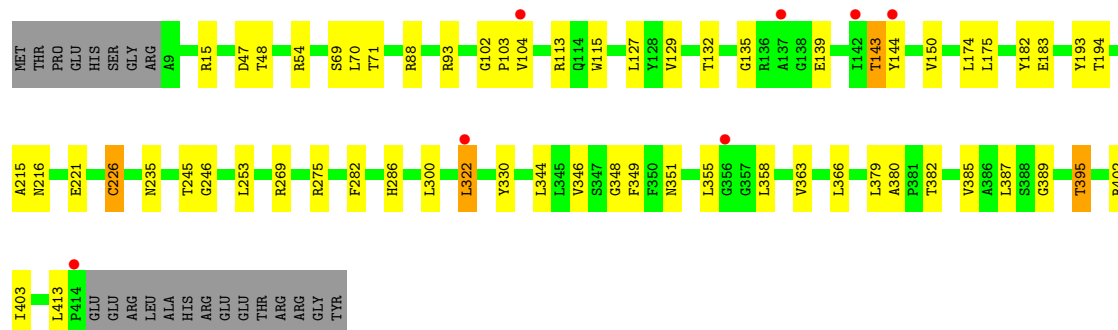
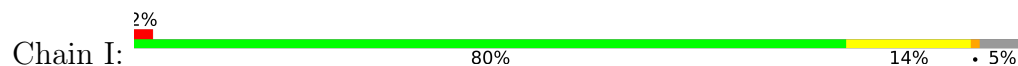


• Molecule 1: Levansucrase

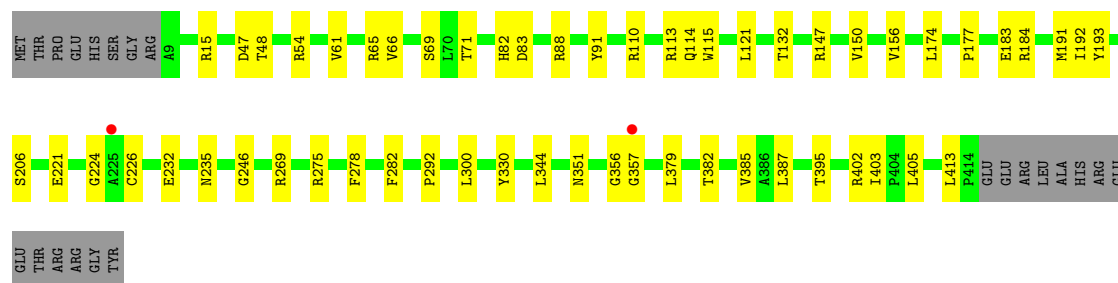
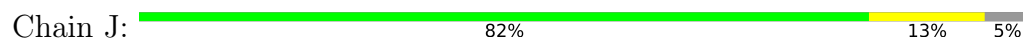
Chain H: 76% 18% 5%



• Molecule 1: Levansucrase



• Molecule 1: Levansucrase



• Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose





- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q: 100%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain R: 100%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T:  67% 33%

GLC1  
FRU2  
FRU3

- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U:  67% 33%

GLC1  
FRU2  
FRU3

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 122.30Å 142.97Å 172.87Å<br>90.00° 98.64° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 106.54 – 2.72<br>106.54 – 2.72                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 59.0 (106.54-2.72)<br>59.2 (106.54-2.72)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.66 (at 2.73Å)                                             | Xtrriage         |
| Refinement program                                                      | PHENIX 1.17.1_3660                                          | Depositor        |
| R, $R_{free}$                                                           | 0.197 , 0.225<br>0.209 , 0.233                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4758 reflections (3.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 63.8                                                        | Xtrriage         |
| Anisotropy                                                              | 0.050                                                       | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 33.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtrriage         |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 32221                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0                                                        | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.34 % 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 5.9255e-04. 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: GLC, FRU

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.97         | 0/3274      | 1.25        | 1/4466 (0.0%)   |
| 1   | B     | 0.98         | 0/3274      | 1.28        | 3/4466 (0.1%)   |
| 1   | C     | 0.97         | 0/3274      | 1.26        | 3/4466 (0.1%)   |
| 1   | D     | 0.98         | 0/3274      | 1.26        | 2/4466 (0.0%)   |
| 1   | E     | 0.96         | 0/3274      | 1.26        | 2/4466 (0.0%)   |
| 1   | F     | 0.97         | 0/3274      | 1.24        | 1/4466 (0.0%)   |
| 1   | G     | 0.98         | 0/3274      | 1.27        | 3/4466 (0.1%)   |
| 1   | H     | 0.99         | 0/3274      | 1.28        | 2/4466 (0.0%)   |
| 1   | I     | 0.97         | 0/3274      | 1.28        | 5/4466 (0.1%)   |
| 1   | J     | 0.98         | 0/3274      | 1.25        | 0/4466          |
| All | All   | 0.98         | 0/32740     | 1.26        | 22/44660 (0.0%) |

There are no bond length outliers.

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 245 | THR  | CA-C-O    | -7.43 | 113.04      | 121.81   |
| 1   | H     | 245 | THR  | CA-C-O    | -7.42 | 113.05      | 121.81   |
| 1   | C     | 245 | THR  | CA-C-O    | -7.33 | 113.16      | 121.81   |
| 1   | G     | 245 | THR  | CA-C-O    | -7.29 | 113.21      | 121.81   |
| 1   | I     | 221 | GLU  | CA-C-O    | -6.44 | 114.06      | 120.82   |
| 1   | E     | 402 | ARG  | CG-CD-NE  | 6.18  | 125.59      | 112.00   |
| 1   | A     | 208 | LYS  | CB-CG-CD  | 6.06  | 125.23      | 111.30   |
| 1   | G     | 143 | THR  | CA-CB-OG1 | -5.82 | 100.88      | 109.60   |
| 1   | H     | 402 | ARG  | CG-CD-NE  | 5.73  | 124.60      | 112.00   |
| 1   | I     | 226 | CYS  | CA-CB-SG  | -5.66 | 101.39      | 114.40   |
| 1   | C     | 372 | ARG  | CB-CG-CD  | 5.54  | 124.05      | 111.30   |
| 1   | I     | 143 | THR  | CA-CB-OG1 | -5.39 | 101.52      | 109.60   |
| 1   | B     | 38  | ASP  | CA-CB-CG  | 5.29  | 117.89      | 112.60   |
| 1   | B     | 143 | THR  | CA-CB-OG1 | -5.24 | 101.74      | 109.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 298 | ASP  | CA-CB-CG | 5.21  | 117.81      | 112.60   |
| 1   | D     | 35  | PRO  | CA-C-N   | 5.12  | 127.15      | 120.28   |
| 1   | D     | 35  | PRO  | C-N-CA   | 5.12  | 127.15      | 120.28   |
| 1   | C     | 245 | THR  | N-CA-C   | -5.12 | 103.64      | 110.55   |
| 1   | E     | 221 | GLU  | CA-C-O   | -5.07 | 115.50      | 120.82   |
| 1   | F     | 298 | ASP  | CA-CB-CG | 5.06  | 117.66      | 112.60   |
| 1   | I     | 245 | THR  | N-CA-C   | -5.03 | 103.76      | 110.55   |
| 1   | G     | 245 | THR  | N-CA-C   | -5.02 | 103.77      | 110.55   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3180  | 0        | 2977     | 31      | 0            |
| 1   | B     | 3180  | 0        | 2977     | 69      | 0            |
| 1   | C     | 3180  | 0        | 2977     | 41      | 0            |
| 1   | D     | 3180  | 0        | 2977     | 40      | 0            |
| 1   | E     | 3180  | 0        | 2977     | 42      | 0            |
| 1   | F     | 3180  | 0        | 2977     | 75      | 0            |
| 1   | G     | 3180  | 0        | 2977     | 66      | 0            |
| 1   | H     | 3180  | 0        | 2977     | 91      | 0            |
| 1   | I     | 3180  | 0        | 2977     | 72      | 0            |
| 1   | J     | 3180  | 0        | 2977     | 56      | 0            |
| 2   | K     | 34    | 0        | 31       | 4       | 0            |
| 2   | L     | 34    | 0        | 31       | 5       | 0            |
| 2   | M     | 34    | 0        | 31       | 10      | 0            |
| 2   | N     | 34    | 0        | 31       | 4       | 0            |
| 2   | O     | 34    | 0        | 31       | 6       | 0            |
| 2   | P     | 34    | 0        | 31       | 5       | 0            |
| 2   | Q     | 34    | 0        | 31       | 14      | 0            |
| 2   | R     | 34    | 0        | 31       | 4       | 0            |
| 2   | T     | 34    | 0        | 31       | 9       | 0            |
| 2   | U     | 34    | 0        | 31       | 3       | 0            |
| 3   | A     | 2     | 0        | 0        | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 9     | 0        | 0        | 20      | 0            |
| 3   | C     | 5     | 0        | 0        | 7       | 0            |
| 3   | D     | 8     | 0        | 0        | 9       | 0            |
| 3   | E     | 10    | 0        | 0        | 10      | 0            |
| 3   | F     | 8     | 0        | 0        | 39      | 0            |
| 3   | G     | 9     | 0        | 0        | 21      | 0            |
| 3   | H     | 10    | 0        | 0        | 27      | 0            |
| 3   | I     | 10    | 0        | 0        | 24      | 0            |
| 3   | J     | 10    | 0        | 0        | 25      | 0            |
| All | All   | 32221 | 0        | 30080    | 601     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (601) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:14:THR:HG23 | 3:B:503:HOH:O    | 1.17                     | 1.26              |
| 1:I:349:PHE:HA  | 3:I:501:HOH:O    | 1.31                     | 1.26              |
| 1:J:91:TYR:HA   | 3:J:501:HOH:O    | 1.35                     | 1.26              |
| 1:F:170:ALA:HB3 | 3:F:506:HOH:O    | 1.35                     | 1.24              |
| 1:H:155:SER:HA  | 3:H:503:HOH:O    | 1.27                     | 1.24              |
| 1:G:349:PHE:HA  | 3:G:503:HOH:O    | 1.34                     | 1.21              |
| 1:H:181:ARG:HA  | 3:H:506:HOH:O    | 1.38                     | 1.20              |
| 1:G:349:PHE:CA  | 3:G:503:HOH:O    | 1.88                     | 1.16              |
| 1:J:66:VAL:HA   | 3:J:501:HOH:O    | 1.47                     | 1.15              |
| 1:H:15:ARG:CZ   | 1:H:294:LEU:HD11 | 1.80                     | 1.12              |
| 1:G:52:ARG:NH1  | 3:G:501:HOH:O    | 1.83                     | 1.11              |
| 1:D:164:ARG:NH1 | 3:D:501:HOH:O    | 1.80                     | 1.11              |
| 1:B:391:ARG:NH2 | 3:B:502:HOH:O    | 1.82                     | 1.10              |
| 1:B:14:THR:N    | 3:B:503:HOH:O    | 1.87                     | 1.06              |
| 1:G:182:TYR:N   | 3:G:502:HOH:O    | 1.85                     | 1.06              |
| 1:B:187:GLN:HB2 | 3:B:507:HOH:O    | 1.55                     | 1.06              |
| 1:F:181:ARG:CD  | 3:F:503:HOH:O    | 2.03                     | 1.03              |
| 1:F:181:ARG:NE  | 3:F:503:HOH:O    | 1.89                     | 1.03              |
| 1:E:9:ALA:HB3   | 3:E:503:HOH:O    | 1.56                     | 1.03              |
| 1:H:270:PRO:HD2 | 3:H:508:HOH:O    | 1.55                     | 1.03              |
| 1:G:182:TYR:CB  | 3:G:502:HOH:O    | 2.08                     | 1.02              |
| 1:J:113:ARG:NE  | 3:J:502:HOH:O    | 1.90                     | 1.02              |
| 1:J:357:GLY:CA  | 3:J:503:HOH:O    | 2.07                     | 1.02              |
| 1:F:270:PRO:HD2 | 3:F:505:HOH:O    | 1.60                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:104:VAL:N    | 3:I:503:HOH:O    | 1.93                     | 1.02              |
| 1:H:215:ALA:HB2  | 3:H:504:HOH:O    | 1.60                     | 0.99              |
| 1:H:413:LEU:O    | 3:H:501:HOH:O    | 1.81                     | 0.98              |
| 1:H:414:PRO:O    | 3:H:501:HOH:O    | 1.82                     | 0.98              |
| 1:B:175:LEU:HD22 | 1:B:253:LEU:HD11 | 1.46                     | 0.98              |
| 1:F:270:PRO:N    | 3:F:505:HOH:O    | 1.96                     | 0.97              |
| 1:B:83:ASP:OD1   | 3:B:501:HOH:O    | 1.81                     | 0.97              |
| 3:G:505:HOH:O    | 2:Q:3:FRU:H5     | 1.65                     | 0.97              |
| 1:C:270:PRO:N    | 3:C:502:HOH:O    | 1.98                     | 0.96              |
| 1:F:181:ARG:CZ   | 3:F:503:HOH:O    | 2.12                     | 0.96              |
| 1:F:270:PRO:CD   | 3:F:505:HOH:O    | 2.09                     | 0.96              |
| 1:H:214:GLU:C    | 3:H:504:HOH:O    | 2.08                     | 0.95              |
| 1:B:162:GLY:N    | 3:B:505:HOH:O    | 1.95                     | 0.95              |
| 1:H:215:ALA:CB   | 3:H:504:HOH:O    | 2.13                     | 0.95              |
| 1:J:65:ARG:O     | 3:J:501:HOH:O    | 1.85                     | 0.94              |
| 1:D:37:GLU:OE2   | 3:D:502:HOH:O    | 1.85                     | 0.93              |
| 1:H:140:ALA:N    | 3:H:505:HOH:O    | 2.01                     | 0.93              |
| 1:J:83:ASP:HA    | 3:J:502:HOH:O    | 1.66                     | 0.93              |
| 1:J:191:MET:HB3  | 3:J:505:HOH:O    | 1.67                     | 0.93              |
| 1:G:348:GLY:O    | 3:G:503:HOH:O    | 1.87                     | 0.93              |
| 1:G:182:TYR:CG   | 3:G:502:HOH:O    | 2.22                     | 0.93              |
| 1:H:215:ALA:N    | 3:H:504:HOH:O    | 2.00                     | 0.93              |
| 1:I:348:GLY:O    | 3:I:501:HOH:O    | 1.85                     | 0.93              |
| 1:H:156:VAL:N    | 3:H:503:HOH:O    | 1.97                     | 0.93              |
| 1:F:216:ASN:N    | 3:F:504:HOH:O    | 1.89                     | 0.92              |
| 1:J:113:ARG:CD   | 3:J:502:HOH:O    | 2.14                     | 0.91              |
| 1:F:215:ALA:CA   | 3:F:504:HOH:O    | 2.19                     | 0.91              |
| 1:F:30:PRO:O     | 3:F:502:HOH:O    | 1.88                     | 0.90              |
| 1:G:298:ASP:OD2  | 3:G:504:HOH:O    | 1.87                     | 0.90              |
| 1:B:300:LEU:HB3  | 1:B:322:LEU:HG   | 1.52                     | 0.90              |
| 1:I:300:LEU:HB3  | 1:I:322:LEU:HG   | 1.53                     | 0.90              |
| 1:G:182:TYR:CD2  | 3:G:502:HOH:O    | 2.25                     | 0.90              |
| 1:B:202:GLU:OE2  | 1:B:207:GLY:O    | 1.89                     | 0.90              |
| 1:G:348:GLY:C    | 3:G:503:HOH:O    | 2.14                     | 0.89              |
| 1:A:189:ARG:C    | 3:A:501:HOH:O    | 2.17                     | 0.88              |
| 1:G:145:GLU:N    | 3:G:506:HOH:O    | 2.06                     | 0.88              |
| 1:C:270:PRO:CD   | 3:C:502:HOH:O    | 2.20                     | 0.88              |
| 1:E:136:ARG:NE   | 3:E:501:HOH:O    | 2.03                     | 0.87              |
| 1:J:357:GLY:N    | 3:J:503:HOH:O    | 2.06                     | 0.87              |
| 1:B:175:LEU:HD22 | 1:B:253:LEU:CD1  | 2.03                     | 0.87              |
| 1:C:47:ASP:OD2   | 2:M:3:FRU:H11    | 1.74                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:269:ARG:C    | 3:F:505:HOH:O    | 2.17                     | 0.86              |
| 1:H:55:ASP:O     | 3:H:502:HOH:O    | 1.91                     | 0.86              |
| 3:G:505:HOH:O    | 2:Q:3:FRU:C5     | 2.21                     | 0.85              |
| 1:B:322:LEU:HD21 | 1:B:346:VAL:HG11 | 1.57                     | 0.85              |
| 1:H:141:GLU:N    | 3:H:505:HOH:O    | 2.08                     | 0.85              |
| 1:H:114:GLN:N    | 1:H:114:GLN:OE1  | 2.09                     | 0.85              |
| 1:H:270:PRO:CD   | 3:H:508:HOH:O    | 2.17                     | 0.85              |
| 1:B:127:LEU:HD21 | 1:B:129:VAL:HG23 | 1.58                     | 0.84              |
| 1:E:145:GLU:OE1  | 3:E:501:HOH:O    | 1.94                     | 0.84              |
| 1:J:83:ASP:C     | 3:J:502:HOH:O    | 2.20                     | 0.83              |
| 1:B:64:TRP:CZ3   | 1:B:93:ARG:HG2   | 2.14                     | 0.83              |
| 1:G:414:PRO:HA   | 3:G:507:HOH:O    | 1.77                     | 0.83              |
| 1:E:136:ARG:NH2  | 3:E:501:HOH:O    | 2.12                     | 0.82              |
| 1:F:30:PRO:C     | 3:F:502:HOH:O    | 2.20                     | 0.82              |
| 1:C:270:PRO:HD2  | 3:C:502:HOH:O    | 1.77                     | 0.82              |
| 1:H:64:TRP:CZ3   | 1:H:93:ARG:HG2   | 2.14                     | 0.82              |
| 1:H:139:GLU:C    | 3:H:505:HOH:O    | 2.21                     | 0.81              |
| 1:I:115:TRP:CG   | 2:T:3:FRU:H61    | 2.15                     | 0.81              |
| 1:I:143:THR:O    | 3:I:504:HOH:O    | 1.97                     | 0.81              |
| 1:G:64:TRP:CZ3   | 1:G:93:ARG:HG2   | 2.14                     | 0.81              |
| 1:F:215:ALA:HB1  | 3:F:504:HOH:O    | 1.81                     | 0.81              |
| 1:F:152:SER:OG   | 3:F:506:HOH:O    | 1.97                     | 0.81              |
| 1:C:269:ARG:C    | 3:C:502:HOH:O    | 2.24                     | 0.81              |
| 1:H:184:ARG:HG2  | 1:H:187:GLN:OE1  | 1.81                     | 0.81              |
| 2:M:1:GLC:H2     | 2:M:2:FRU:H11    | 1.63                     | 0.80              |
| 1:E:54:ARG:HH12  | 1:E:209:THR:HG21 | 1.46                     | 0.80              |
| 1:A:190:GLY:N    | 3:A:501:HOH:O    | 2.15                     | 0.80              |
| 1:G:360:LEU:HD21 | 2:Q:1:GLC:H5     | 1.62                     | 0.80              |
| 1:I:150:VAL:HG12 | 1:I:174:LEU:HD11 | 1.64                     | 0.79              |
| 1:C:47:ASP:CG    | 2:M:3:FRU:H11    | 2.07                     | 0.79              |
| 1:B:12:ARG:O     | 3:B:503:HOH:O    | 2.01                     | 0.79              |
| 1:G:150:VAL:HG12 | 1:G:174:LEU:HD11 | 1.63                     | 0.79              |
| 1:I:113:ARG:NH2  | 3:I:504:HOH:O    | 2.03                     | 0.79              |
| 1:I:127:LEU:HD21 | 1:I:129:VAL:HG23 | 1.65                     | 0.78              |
| 1:F:170:ALA:O    | 3:F:506:HOH:O    | 2.01                     | 0.78              |
| 1:I:175:LEU:HD22 | 1:I:253:LEU:HD11 | 1.65                     | 0.78              |
| 1:C:270:PRO:O    | 3:C:502:HOH:O    | 2.00                     | 0.77              |
| 1:F:30:PRO:CD    | 3:F:502:HOH:O    | 2.29                     | 0.77              |
| 1:H:169:PHE:N    | 3:H:509:HOH:O    | 2.16                     | 0.77              |
| 1:I:349:PHE:CA   | 3:I:501:HOH:O    | 2.05                     | 0.77              |
| 1:E:9:ALA:CB     | 3:E:503:HOH:O    | 2.24                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:70:LEU:HD12  | 1:G:70:LEU:N     | 2.00                     | 0.77              |
| 1:J:83:ASP:CA    | 3:J:502:HOH:O    | 2.27                     | 0.77              |
| 1:D:164:ARG:CZ   | 3:D:501:HOH:O    | 2.18                     | 0.76              |
| 1:F:54:ARG:HH12  | 1:F:209:THR:HG21 | 1.50                     | 0.76              |
| 1:J:357:GLY:C    | 3:J:503:HOH:O    | 2.24                     | 0.76              |
| 1:B:402:ARG:NE   | 3:B:504:HOH:O    | 1.87                     | 0.76              |
| 1:E:147:ARG:NH1  | 1:E:173:VAL:HG21 | 1.99                     | 0.76              |
| 1:E:9:ALA:N      | 3:E:503:HOH:O    | 2.19                     | 0.76              |
| 1:F:269:ARG:HA   | 3:F:505:HOH:O    | 1.86                     | 0.76              |
| 1:H:92:SER:OG    | 1:H:94:ASP:O     | 2.01                     | 0.76              |
| 1:I:322:LEU:HD21 | 1:I:346:VAL:HG11 | 1.66                     | 0.76              |
| 1:D:160:ASP:CG   | 3:J:504:HOH:O    | 2.29                     | 0.75              |
| 1:J:15:ARG:NH2   | 1:J:292:PRO:O    | 2.19                     | 0.75              |
| 1:F:76:LEU:HD23  | 1:F:77:LEU:O     | 1.86                     | 0.75              |
| 1:I:175:LEU:HD22 | 1:I:253:LEU:CD1  | 2.17                     | 0.75              |
| 1:G:182:TYR:HB2  | 3:G:502:HOH:O    | 1.79                     | 0.75              |
| 1:B:184:ARG:O    | 3:B:507:HOH:O    | 2.04                     | 0.75              |
| 1:C:76:LEU:HD23  | 1:C:77:LEU:O     | 1.87                     | 0.75              |
| 1:B:402:ARG:NH2  | 3:B:504:HOH:O    | 2.17                     | 0.75              |
| 1:C:54:ARG:NH1   | 1:C:209:THR:OG1  | 2.19                     | 0.75              |
| 1:F:30:PRO:CA    | 3:F:502:HOH:O    | 2.33                     | 0.75              |
| 1:H:76:LEU:HD23  | 1:H:77:LEU:O     | 1.87                     | 0.75              |
| 1:H:240:ILE:HG21 | 1:H:257:LEU:HD11 | 1.70                     | 0.74              |
| 1:A:189:ARG:CA   | 3:A:501:HOH:O    | 2.36                     | 0.74              |
| 1:F:170:ALA:CB   | 3:F:506:HOH:O    | 2.11                     | 0.74              |
| 1:H:127:LEU:HD21 | 1:H:129:VAL:HG23 | 1.68                     | 0.74              |
| 1:H:213:PHE:HD1  | 3:H:504:HOH:O    | 1.70                     | 0.73              |
| 1:H:168:PRO:HB2  | 3:H:509:HOH:O    | 1.88                     | 0.73              |
| 1:G:49:TRP:HZ3   | 1:G:70:LEU:HD11  | 1.52                     | 0.73              |
| 1:F:210:TYR:CE1  | 3:F:501:HOH:O    | 2.41                     | 0.73              |
| 1:I:216:ASN:N    | 3:I:502:HOH:O    | 1.92                     | 0.72              |
| 1:H:15:ARG:NH1   | 1:H:294:LEU:HD11 | 2.04                     | 0.72              |
| 1:H:15:ARG:NH2   | 1:H:294:LEU:HD11 | 2.04                     | 0.72              |
| 1:J:110:ARG:NE   | 3:J:504:HOH:O    | 2.11                     | 0.72              |
| 1:F:30:PRO:HD2   | 3:F:502:HOH:O    | 1.87                     | 0.72              |
| 1:E:113:ARG:HD3  | 1:E:134:SER:OG   | 1.90                     | 0.72              |
| 1:I:395:THR:HG23 | 1:I:413:LEU:HD22 | 1.70                     | 0.71              |
| 1:H:180:GLU:O    | 3:H:506:HOH:O    | 2.06                     | 0.71              |
| 1:F:54:ARG:NH2   | 1:F:246:GLY:O    | 2.22                     | 0.71              |
| 1:D:233:GLU:O    | 3:D:503:HOH:O    | 2.07                     | 0.71              |
| 1:J:54:ARG:NH2   | 1:J:246:GLY:O    | 2.23                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:15:ARG:CZ    | 1:H:294:LEU:CD1  | 2.65                     | 0.71              |
| 1:I:54:ARG:NH2   | 1:I:246:GLY:O    | 2.22                     | 0.70              |
| 1:A:54:ARG:NH2   | 1:A:246:GLY:O    | 2.23                     | 0.70              |
| 2:L:2:FRU:H11    | 2:L:3:FRU:O1     | 1.90                     | 0.70              |
| 1:F:181:ARG:HD3  | 3:F:503:HOH:O    | 1.81                     | 0.70              |
| 1:E:54:ARG:NH2   | 1:E:246:GLY:O    | 2.23                     | 0.70              |
| 1:F:215:ALA:CB   | 3:F:504:HOH:O    | 2.35                     | 0.70              |
| 1:D:54:ARG:NH1   | 1:D:246:GLY:O    | 2.24                     | 0.70              |
| 1:H:140:ALA:C    | 3:H:505:HOH:O    | 2.33                     | 0.69              |
| 1:G:360:LEU:CD2  | 2:Q:1:GLC:H5     | 2.22                     | 0.69              |
| 1:I:103:PRO:C    | 3:I:503:HOH:O    | 2.30                     | 0.69              |
| 1:B:64:TRP:CZ2   | 1:B:93:ARG:HD3   | 2.28                     | 0.69              |
| 1:D:317:GLY:HA2  | 3:D:504:HOH:O    | 1.91                     | 0.69              |
| 1:F:30:PRO:CB    | 3:F:502:HOH:O    | 2.40                     | 0.69              |
| 1:F:170:ALA:CA   | 3:F:506:HOH:O    | 2.37                     | 0.69              |
| 1:D:54:ARG:HH11  | 1:D:209:THR:HG21 | 1.57                     | 0.69              |
| 1:J:224:GLY:O    | 1:J:232:GLU:OE2  | 2.11                     | 0.69              |
| 1:F:363:VAL:HA   | 1:F:366:LEU:CD1  | 2.23                     | 0.68              |
| 1:J:83:ASP:O     | 3:J:502:HOH:O    | 2.09                     | 0.68              |
| 1:G:47:ASP:O     | 1:G:70:LEU:HD13  | 1.92                     | 0.68              |
| 1:B:373:ALA:HA   | 1:D:36:ARG:HH21  | 1.57                     | 0.68              |
| 1:E:275:ARG:HD3  | 1:E:387:LEU:HD12 | 1.75                     | 0.68              |
| 1:G:139:GLU:OE1  | 1:G:143:THR:HG22 | 1.93                     | 0.68              |
| 1:H:15:ARG:NH2   | 1:H:294:LEU:CD1  | 2.56                     | 0.68              |
| 1:I:363:VAL:HA   | 1:I:366:LEU:CD1  | 2.24                     | 0.68              |
| 1:J:113:ARG:CG   | 3:J:502:HOH:O    | 2.41                     | 0.68              |
| 1:C:363:VAL:HA   | 1:C:366:LEU:CD1  | 2.24                     | 0.67              |
| 1:E:136:ARG:CZ   | 3:E:501:HOH:O    | 2.33                     | 0.67              |
| 1:I:322:LEU:CD2  | 1:I:346:VAL:HG11 | 2.24                     | 0.67              |
| 1:B:159:ASP:O    | 3:B:505:HOH:O    | 2.10                     | 0.67              |
| 1:B:115:TRP:HB2  | 1:B:132:THR:HB   | 1.76                     | 0.67              |
| 1:G:363:VAL:HA   | 1:G:366:LEU:CD1  | 2.24                     | 0.67              |
| 1:D:275:ARG:HD3  | 1:D:387:LEU:HD12 | 1.77                     | 0.67              |
| 1:E:217:THR:HG21 | 1:E:259:GLU:OE2  | 1.95                     | 0.67              |
| 1:G:275:ARG:HD3  | 1:G:387:LEU:HD12 | 1.75                     | 0.67              |
| 1:C:115:TRP:HB2  | 1:C:132:THR:HB   | 1.77                     | 0.67              |
| 1:J:113:ARG:HG3  | 3:J:502:HOH:O    | 1.94                     | 0.67              |
| 1:D:317:GLY:O    | 3:D:504:HOH:O    | 2.14                     | 0.66              |
| 1:I:322:LEU:C    | 1:I:322:LEU:HD12 | 2.20                     | 0.66              |
| 1:G:115:TRP:HB2  | 1:G:132:THR:HB   | 1.77                     | 0.66              |
| 2:O:1:GLC:H2     | 2:O:2:FRU:H11    | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:235:ASN:OD1  | 3:E:502:HOH:O    | 2.12                     | 0.66              |
| 1:I:115:TRP:HB2  | 1:I:132:THR:HB   | 1.78                     | 0.66              |
| 1:H:294:LEU:N    | 1:H:294:LEU:HD12 | 2.11                     | 0.66              |
| 1:I:144:TYR:CD1  | 3:I:504:HOH:O    | 2.49                     | 0.66              |
| 1:J:191:MET:CB   | 3:J:505:HOH:O    | 2.36                     | 0.66              |
| 1:E:115:TRP:HB2  | 1:E:132:THR:HB   | 1.77                     | 0.66              |
| 1:A:115:TRP:HB2  | 1:A:132:THR:HB   | 1.78                     | 0.66              |
| 1:B:322:LEU:CD2  | 1:B:346:VAL:HG11 | 2.25                     | 0.66              |
| 1:J:115:TRP:HB2  | 1:J:132:THR:HB   | 1.78                     | 0.66              |
| 1:F:215:ALA:HA   | 3:F:504:HOH:O    | 1.87                     | 0.66              |
| 1:F:175:LEU:HD22 | 1:F:253:LEU:HD11 | 1.75                     | 0.65              |
| 1:B:136:ARG:HG2  | 1:B:145:GLU:OE2  | 1.95                     | 0.65              |
| 1:F:275:ARG:HD3  | 1:F:387:LEU:HD12 | 1.77                     | 0.65              |
| 1:B:139:GLU:OE1  | 1:B:143:THR:HG22 | 1.97                     | 0.65              |
| 1:F:206:SER:OG   | 3:F:501:HOH:O    | 2.14                     | 0.65              |
| 1:H:115:TRP:HB2  | 1:H:132:THR:HB   | 1.77                     | 0.65              |
| 1:J:395:THR:HG21 | 1:J:413:LEU:HD13 | 1.78                     | 0.65              |
| 1:D:115:TRP:HB2  | 1:D:132:THR:HB   | 1.79                     | 0.65              |
| 1:F:115:TRP:HB2  | 1:F:132:THR:HB   | 1.78                     | 0.65              |
| 1:I:194:THR:O    | 3:I:502:HOH:O    | 2.15                     | 0.65              |
| 1:F:30:PRO:N     | 3:F:502:HOH:O    | 2.29                     | 0.65              |
| 1:B:322:LEU:C    | 1:B:322:LEU:HD12 | 2.22                     | 0.65              |
| 1:I:215:ALA:CA   | 3:I:502:HOH:O    | 2.45                     | 0.64              |
| 1:H:270:PRO:N    | 3:H:508:HOH:O    | 2.29                     | 0.64              |
| 1:I:322:LEU:HD12 | 1:I:322:LEU:O    | 1.97                     | 0.64              |
| 1:F:352:TYR:O    | 3:F:507:HOH:O    | 2.14                     | 0.64              |
| 2:Q:1:GLC:H2     | 2:Q:2:FRU:H11    | 1.79                     | 0.64              |
| 1:H:146:GLN:O    | 3:H:507:HOH:O    | 2.15                     | 0.64              |
| 1:B:136:ARG:CG   | 1:B:145:GLU:OE2  | 2.45                     | 0.63              |
| 1:B:148:LEU:HD13 | 1:B:195:PHE:CE2  | 2.34                     | 0.63              |
| 1:F:363:VAL:HA   | 1:F:366:LEU:HD13 | 1.80                     | 0.63              |
| 1:A:275:ARG:HD3  | 1:A:387:LEU:HD12 | 1.79                     | 0.63              |
| 1:A:189:ARG:HA   | 3:A:501:HOH:O    | 1.98                     | 0.63              |
| 1:I:139:GLU:OE1  | 1:I:143:THR:HG22 | 1.98                     | 0.63              |
| 1:H:270:PRO:O    | 3:H:508:HOH:O    | 2.15                     | 0.63              |
| 1:J:110:ARG:NH2  | 3:J:504:HOH:O    | 2.30                     | 0.63              |
| 1:D:142:ILE:HD12 | 1:D:142:ILE:O    | 1.99                     | 0.62              |
| 1:B:127:LEU:CD2  | 1:B:129:VAL:HG23 | 2.29                     | 0.62              |
| 1:G:148:LEU:HD13 | 1:G:195:PHE:CE2  | 2.35                     | 0.62              |
| 1:C:363:VAL:HA   | 1:C:366:LEU:HD13 | 1.81                     | 0.62              |
| 1:E:54:ARG:HH12  | 1:E:209:THR:CG2  | 2.12                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:148:LEU:HD13 | 1:F:195:PHE:CE2  | 2.34                     | 0.62              |
| 1:B:187:GLN:CB   | 3:B:507:HOH:O    | 2.30                     | 0.62              |
| 1:E:395:THR:HG21 | 1:E:413:LEU:HD13 | 1.81                     | 0.62              |
| 1:H:148:LEU:HD13 | 1:H:195:PHE:CE2  | 2.34                     | 0.62              |
| 1:B:322:LEU:HD12 | 1:B:322:LEU:O    | 1.99                     | 0.61              |
| 1:C:47:ASP:OD1   | 2:M:3:FRU:H11    | 2.00                     | 0.61              |
| 1:B:14:THR:CG2   | 3:B:503:HOH:O    | 1.99                     | 0.61              |
| 1:I:380:ALA:N    | 3:I:501:HOH:O    | 1.84                     | 0.61              |
| 1:H:37:GLU:HA    | 3:H:510:HOH:O    | 2.00                     | 0.61              |
| 1:G:70:LEU:N     | 1:G:70:LEU:CD1   | 2.63                     | 0.61              |
| 1:G:363:VAL:HA   | 1:G:366:LEU:HD13 | 1.82                     | 0.60              |
| 1:E:88:ARG:NH1   | 1:E:102:GLY:HA2  | 2.16                     | 0.60              |
| 1:I:88:ARG:NH1   | 1:I:102:GLY:HA2  | 2.17                     | 0.60              |
| 1:I:363:VAL:HA   | 1:I:366:LEU:HD13 | 1.81                     | 0.60              |
| 1:B:83:ASP:HA    | 3:B:501:HOH:O    | 2.01                     | 0.60              |
| 1:B:161:ASP:N    | 3:B:505:HOH:O    | 2.35                     | 0.60              |
| 1:B:127:LEU:HD21 | 1:B:129:VAL:CG2  | 2.30                     | 0.60              |
| 1:E:9:ALA:CA     | 3:E:503:HOH:O    | 2.45                     | 0.60              |
| 1:E:113:ARG:CD   | 1:E:134:SER:OG   | 2.50                     | 0.60              |
| 1:H:127:LEU:CD2  | 1:H:129:VAL:HG23 | 2.31                     | 0.60              |
| 1:I:127:LEU:CD2  | 1:I:129:VAL:HG23 | 2.30                     | 0.60              |
| 1:F:54:ARG:HH12  | 1:F:209:THR:CG2  | 2.14                     | 0.59              |
| 1:G:355:LEU:O    | 1:G:358:LEU:HD13 | 2.03                     | 0.59              |
| 1:C:157:VAL:HG23 | 1:C:164:ARG:HG2  | 1.84                     | 0.59              |
| 1:I:115:TRP:CD2  | 2:T:3:FRU:H61    | 2.36                     | 0.59              |
| 1:E:395:THR:HG22 | 1:E:413:LEU:HD22 | 1.85                     | 0.59              |
| 1:D:88:ARG:NH1   | 1:D:102:GLY:HA2  | 2.17                     | 0.59              |
| 1:I:286:HIS:CE1  | 2:T:2:FRU:O3     | 2.55                     | 0.59              |
| 1:C:115:TRP:CD1  | 2:M:3:FRU:H62    | 2.38                     | 0.58              |
| 1:C:110:ARG:HD3  | 1:C:171:HIS:HB3  | 1.84                     | 0.58              |
| 1:I:215:ALA:HB1  | 3:I:502:HOH:O    | 2.03                     | 0.58              |
| 1:H:174:LEU:O    | 1:H:175:LEU:HD13 | 2.02                     | 0.58              |
| 1:J:275:ARG:HD3  | 1:J:387:LEU:HD12 | 1.84                     | 0.58              |
| 1:H:48:THR:HG21  | 1:H:379:LEU:HD21 | 1.86                     | 0.58              |
| 1:F:175:LEU:HD22 | 1:F:253:LEU:CD1  | 2.33                     | 0.58              |
| 1:I:115:TRP:CD1  | 2:T:3:FRU:H61    | 2.39                     | 0.58              |
| 1:H:240:ILE:CG2  | 1:H:257:LEU:HD11 | 2.34                     | 0.57              |
| 1:I:344:LEU:HB3  | 1:I:385:VAL:HG23 | 1.86                     | 0.57              |
| 1:I:355:LEU:O    | 1:I:358:LEU:HD13 | 2.03                     | 0.57              |
| 1:F:115:TRP:CG   | 2:P:3:FRU:H62    | 2.39                     | 0.57              |
| 2:Q:1:GLC:H2     | 2:Q:2:FRU:C1     | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:395:THR:CG2  | 1:I:413:LEU:HD22 | 2.34                     | 0.57              |
| 1:C:48:THR:HG21  | 1:C:379:LEU:HD21 | 1.86                     | 0.57              |
| 1:D:344:LEU:HB3  | 1:D:385:VAL:HG23 | 1.87                     | 0.57              |
| 1:J:191:MET:CA   | 3:J:505:HOH:O    | 2.53                     | 0.57              |
| 1:F:48:THR:HG21  | 1:F:379:LEU:HD21 | 1.87                     | 0.57              |
| 1:E:48:THR:HG21  | 1:E:379:LEU:HD21 | 1.87                     | 0.57              |
| 1:C:115:TRP:CG   | 2:M:3:FRU:H62    | 2.39                     | 0.57              |
| 1:H:164:ARG:HD2  | 1:H:166:GLU:OE2  | 2.03                     | 0.57              |
| 1:I:48:THR:HG21  | 1:I:379:LEU:HD21 | 1.86                     | 0.57              |
| 1:I:174:LEU:N    | 1:I:174:LEU:HD12 | 2.20                     | 0.57              |
| 1:F:344:LEU:HB3  | 1:F:385:VAL:HG23 | 1.87                     | 0.57              |
| 2:M:1:GLC:H62    | 2:M:1:GLC:O3     | 2.05                     | 0.57              |
| 1:G:64:TRP:CZ2   | 1:G:93:ARG:HD3   | 2.40                     | 0.56              |
| 1:G:298:ASP:CB   | 3:G:504:HOH:O    | 2.53                     | 0.56              |
| 2:M:2:FRU:H11    | 2:M:3:FRU:O1     | 2.05                     | 0.56              |
| 2:N:2:FRU:H11    | 2:N:3:FRU:O3     | 2.05                     | 0.56              |
| 1:A:344:LEU:HB3  | 1:A:385:VAL:HG23 | 1.88                     | 0.56              |
| 2:R:2:FRU:H11    | 2:R:3:FRU:O1     | 2.04                     | 0.56              |
| 1:G:174:LEU:HD12 | 1:G:174:LEU:N    | 2.21                     | 0.56              |
| 1:G:344:LEU:HB3  | 1:G:385:VAL:HG23 | 1.86                     | 0.56              |
| 1:H:127:LEU:HD21 | 1:H:129:VAL:CG2  | 2.36                     | 0.56              |
| 1:J:177:PRO:HG2  | 1:J:184:ARG:HG2  | 1.88                     | 0.56              |
| 1:F:191:MET:HE1  | 1:F:289:THR:HG22 | 1.87                     | 0.56              |
| 1:G:135:GLY:N    | 3:G:506:HOH:O    | 2.28                     | 0.56              |
| 1:I:103:PRO:CB   | 3:I:503:HOH:O    | 2.52                     | 0.56              |
| 1:C:344:LEU:HB3  | 1:C:385:VAL:HG23 | 1.87                     | 0.56              |
| 1:H:275:ARG:HD3  | 1:H:387:LEU:HD12 | 1.86                     | 0.56              |
| 1:A:48:THR:HG21  | 1:A:379:LEU:HD21 | 1.86                     | 0.56              |
| 1:D:48:THR:HG21  | 1:D:379:LEU:HD21 | 1.87                     | 0.56              |
| 1:E:344:LEU:HB3  | 1:E:385:VAL:HG23 | 1.86                     | 0.56              |
| 2:L:1:GLC:O2     | 2:L:2:FRU:H11    | 2.06                     | 0.56              |
| 2:T:2:FRU:H11    | 2:T:3:FRU:O1     | 2.04                     | 0.56              |
| 1:J:344:LEU:HB3  | 1:J:385:VAL:HG23 | 1.87                     | 0.56              |
| 1:B:344:LEU:HB3  | 1:B:385:VAL:HG23 | 1.87                     | 0.56              |
| 1:G:49:TRP:HZ3   | 1:G:70:LEU:CD1   | 2.18                     | 0.56              |
| 1:H:344:LEU:HB3  | 1:H:385:VAL:HG23 | 1.87                     | 0.56              |
| 1:J:110:ARG:CZ   | 3:J:504:HOH:O    | 2.54                     | 0.55              |
| 1:E:355:LEU:O    | 1:E:358:LEU:HD13 | 2.06                     | 0.55              |
| 1:H:15:ARG:NH1   | 1:H:294:LEU:CD1  | 2.69                     | 0.55              |
| 1:H:157:VAL:HG13 | 1:H:164:ARG:HG2  | 1.88                     | 0.55              |
| 1:I:144:TYR:HA   | 3:I:504:HOH:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:54:ARG:NH2   | 1:B:202:GLU:OE1  | 2.40                     | 0.55              |
| 1:F:30:PRO:HB2   | 3:F:502:HOH:O    | 2.06                     | 0.55              |
| 1:H:139:GLU:HG3  | 3:H:505:HOH:O    | 2.06                     | 0.55              |
| 1:I:127:LEU:HD21 | 1:I:129:VAL:CG2  | 2.35                     | 0.55              |
| 1:F:164:ARG:HD2  | 1:F:166:GLU:OE1  | 2.06                     | 0.55              |
| 2:O:2:FRU:H11    | 2:O:3:FRU:O1     | 2.06                     | 0.55              |
| 1:A:191:MET:HE1  | 1:A:289:THR:HG22 | 1.88                     | 0.55              |
| 1:A:389:GLY:HA2  | 1:H:278:PHE:CE2  | 2.42                     | 0.55              |
| 1:J:395:THR:HG22 | 1:J:413:LEU:HD22 | 1.88                     | 0.54              |
| 1:F:210:TYR:HE1  | 3:F:501:HOH:O    | 1.87                     | 0.54              |
| 1:I:275:ARG:HD3  | 1:I:387:LEU:HD12 | 1.89                     | 0.54              |
| 1:H:174:LEU:C    | 1:H:175:LEU:HD22 | 2.33                     | 0.54              |
| 1:C:191:MET:HE1  | 1:C:289:THR:HG22 | 1.89                     | 0.54              |
| 1:I:93:ARG:NH2   | 3:I:506:HOH:O    | 2.12                     | 0.54              |
| 1:J:48:THR:HG21  | 1:J:379:LEU:HD21 | 1.89                     | 0.54              |
| 1:C:269:ARG:HG2  | 1:C:269:ARG:HH11 | 1.73                     | 0.54              |
| 1:A:269:ARG:HH11 | 1:A:269:ARG:HG2  | 1.73                     | 0.54              |
| 1:G:70:LEU:CD1   | 1:G:70:LEU:H     | 2.20                     | 0.53              |
| 1:H:257:LEU:HD12 | 1:H:257:LEU:N    | 2.21                     | 0.53              |
| 1:A:115:TRP:CD2  | 2:K:3:FRU:H61    | 2.44                     | 0.53              |
| 1:C:344:LEU:HD22 | 1:C:387:LEU:HD11 | 1.90                     | 0.53              |
| 1:G:48:THR:HG21  | 1:G:379:LEU:HD21 | 1.89                     | 0.53              |
| 1:B:48:THR:HG21  | 1:B:379:LEU:HD21 | 1.91                     | 0.53              |
| 1:I:103:PRO:CA   | 3:I:503:HOH:O    | 2.56                     | 0.53              |
| 1:F:330:TYR:HB2  | 3:F:507:HOH:O    | 2.07                     | 0.53              |
| 1:F:115:TRP:CD2  | 2:P:3:FRU:H62    | 2.43                     | 0.53              |
| 1:D:136:ARG:NH1  | 1:D:145:GLU:OE2  | 2.42                     | 0.53              |
| 1:E:286:HIS:NE2  | 2:O:1:GLC:O2     | 2.36                     | 0.53              |
| 1:H:213:PHE:CD1  | 3:H:504:HOH:O    | 2.53                     | 0.53              |
| 1:B:355:LEU:O    | 1:B:358:LEU:HD13 | 2.09                     | 0.53              |
| 1:E:269:ARG:HG2  | 1:E:269:ARG:HH11 | 1.74                     | 0.53              |
| 1:I:348:GLY:C    | 3:I:501:HOH:O    | 2.36                     | 0.53              |
| 2:Q:1:GLC:C2     | 2:Q:2:FRU:H11    | 2.38                     | 0.53              |
| 1:C:341:ARG:HH12 | 1:C:409:GLU:HG2  | 1.74                     | 0.52              |
| 1:G:115:TRP:CD2  | 2:Q:3:FRU:H62    | 2.44                     | 0.52              |
| 1:I:15:ARG:NH2   | 3:I:507:HOH:O    | 2.42                     | 0.52              |
| 1:H:64:TRP:CZ2   | 1:H:93:ARG:HD3   | 2.44                     | 0.52              |
| 1:H:240:ILE:CG2  | 1:H:257:LEU:CD1  | 2.86                     | 0.52              |
| 2:M:1:GLC:C2     | 2:M:2:FRU:H11    | 2.35                     | 0.52              |
| 1:H:269:ARG:HH11 | 1:H:269:ARG:HG2  | 1.74                     | 0.52              |
| 1:C:269:ARG:HA   | 3:C:502:HOH:O    | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:322:LEU:C    | 1:H:322:LEU:HD23 | 2.35                     | 0.52              |
| 1:J:47:ASP:OD2   | 2:U:3:FRU:H11    | 2.10                     | 0.52              |
| 1:F:269:ARG:HH11 | 1:F:269:ARG:HG2  | 1.74                     | 0.52              |
| 1:J:121:LEU:CD1  | 1:J:156:VAL:HG11 | 2.39                     | 0.52              |
| 1:D:269:ARG:HG2  | 1:D:269:ARG:HH11 | 1.75                     | 0.52              |
| 1:G:47:ASP:OD2   | 2:Q:3:FRU:H11    | 2.10                     | 0.52              |
| 1:B:402:ARG:CZ   | 3:B:504:HOH:O    | 2.31                     | 0.51              |
| 1:G:380:ALA:N    | 3:G:503:HOH:O    | 2.08                     | 0.51              |
| 1:I:269:ARG:HG2  | 1:I:269:ARG:HH11 | 1.75                     | 0.51              |
| 1:C:330:TYR:O    | 1:C:351:ASN:HB3  | 2.11                     | 0.51              |
| 3:D:506:HOH:O    | 2:N:3:FRU:H3     | 2.09                     | 0.51              |
| 1:H:206:SER:HB2  | 1:H:208:LYS:HG3  | 1.92                     | 0.51              |
| 1:I:47:ASP:OD2   | 2:T:3:FRU:H11    | 2.10                     | 0.51              |
| 1:I:389:GLY:HA2  | 1:J:278:PHE:CE2  | 2.46                     | 0.51              |
| 1:H:148:LEU:HD13 | 1:H:195:PHE:CD2  | 2.46                     | 0.51              |
| 1:H:175:LEU:HD21 | 1:H:251:TRP:HB2  | 1.92                     | 0.51              |
| 1:J:269:ARG:HG2  | 1:J:269:ARG:HH11 | 1.75                     | 0.51              |
| 1:A:42:GLU:HG3   | 1:A:43:ILE:HG12  | 1.93                     | 0.51              |
| 1:C:280:TYR:CE2  | 1:C:387:LEU:HD22 | 2.46                     | 0.51              |
| 1:D:330:TYR:O    | 1:D:351:ASN:HB3  | 2.11                     | 0.51              |
| 1:D:382:THR:HG21 | 1:D:402:ARG:O    | 2.11                     | 0.51              |
| 1:F:330:TYR:C    | 3:F:507:HOH:O    | 2.53                     | 0.51              |
| 1:F:330:TYR:CA   | 3:F:507:HOH:O    | 2.59                     | 0.51              |
| 1:B:330:TYR:O    | 1:B:351:ASN:HB3  | 2.11                     | 0.51              |
| 1:G:269:ARG:HG2  | 1:G:269:ARG:HH11 | 1.75                     | 0.51              |
| 1:G:330:TYR:O    | 1:G:351:ASN:HB3  | 2.10                     | 0.51              |
| 1:J:330:TYR:O    | 1:J:351:ASN:HB3  | 2.11                     | 0.51              |
| 1:B:36:ARG:NH2   | 1:D:373:ALA:HA   | 2.25                     | 0.50              |
| 1:C:157:VAL:CG2  | 1:C:164:ARG:HG2  | 2.41                     | 0.50              |
| 3:G:505:HOH:O    | 2:Q:3:FRU:O6     | 2.17                     | 0.50              |
| 1:A:161:ASP:OD1  | 1:C:147:ARG:NH2  | 2.45                     | 0.50              |
| 1:B:269:ARG:HG2  | 1:B:269:ARG:HH11 | 1.77                     | 0.50              |
| 1:B:83:ASP:CA    | 3:B:501:HOH:O    | 2.59                     | 0.50              |
| 1:F:382:THR:HG21 | 1:F:402:ARG:O    | 2.12                     | 0.50              |
| 1:H:36:ARG:HD2   | 1:H:36:ARG:N     | 2.26                     | 0.50              |
| 1:A:330:TYR:O    | 1:A:351:ASN:HB3  | 2.11                     | 0.50              |
| 1:C:414:PRO:C    | 3:C:503:HOH:O    | 2.54                     | 0.50              |
| 1:F:330:TYR:O    | 1:F:351:ASN:HB3  | 2.12                     | 0.50              |
| 1:I:330:TYR:O    | 1:I:351:ASN:HB3  | 2.11                     | 0.50              |
| 1:B:286:HIS:HE1  | 2:L:1:GLC:H3     | 1.75                     | 0.50              |
| 1:E:330:TYR:O    | 1:E:351:ASN:HB3  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:330:TYR:O    | 1:H:351:ASN:HB3  | 2.12                     | 0.50              |
| 1:B:148:LEU:HD13 | 1:B:195:PHE:CD2  | 2.46                     | 0.49              |
| 1:B:159:ASP:C    | 3:B:505:HOH:O    | 2.54                     | 0.49              |
| 1:E:115:TRP:CG   | 2:O:3:FRU:H62    | 2.47                     | 0.49              |
| 1:G:206:SER:HB2  | 1:G:208:LYS:HG3  | 1.92                     | 0.49              |
| 1:J:357:GLY:HA2  | 3:J:503:HOH:O    | 1.96                     | 0.49              |
| 1:B:382:THR:HG21 | 1:B:402:ARG:O    | 2.13                     | 0.49              |
| 1:C:286:HIS:NE2  | 2:M:1:GLC:O2     | 2.33                     | 0.49              |
| 1:C:282:PHE:HB3  | 1:C:300:LEU:HD11 | 1.94                     | 0.49              |
| 3:D:506:HOH:O    | 2:N:3:FRU:O4     | 2.20                     | 0.49              |
| 1:E:115:TRP:CD1  | 2:O:3:FRU:H62    | 2.47                     | 0.49              |
| 1:H:64:TRP:CD2   | 1:H:93:ARG:HD2   | 2.47                     | 0.49              |
| 1:H:115:TRP:CG   | 2:R:3:FRU:H61    | 2.48                     | 0.49              |
| 1:I:93:ARG:NH1   | 3:I:506:HOH:O    | 2.41                     | 0.49              |
| 1:E:282:PHE:HB3  | 1:E:300:LEU:HD11 | 1.95                     | 0.49              |
| 1:F:42:GLU:HG3   | 1:F:43:ILE:HG12  | 1.95                     | 0.49              |
| 1:H:83:ASP:O     | 1:H:113:ARG:HG2  | 2.12                     | 0.49              |
| 1:H:113:ARG:CD   | 1:H:134:SER:HB3  | 2.42                     | 0.49              |
| 1:J:82:HIS:HD2   | 2:U:3:FRU:H62    | 1.77                     | 0.49              |
| 1:F:148:LEU:HD13 | 1:F:195:PHE:CD2  | 2.48                     | 0.49              |
| 1:G:64:TRP:CD2   | 1:G:93:ARG:HD2   | 2.47                     | 0.49              |
| 1:G:282:PHE:HB3  | 1:G:300:LEU:HD11 | 1.95                     | 0.49              |
| 1:G:382:THR:HG21 | 1:G:402:ARG:O    | 2.13                     | 0.49              |
| 1:H:282:PHE:HB3  | 1:H:300:LEU:HD11 | 1.95                     | 0.49              |
| 1:J:382:THR:HG21 | 1:J:402:ARG:O    | 2.12                     | 0.49              |
| 1:F:330:TYR:N    | 3:F:507:HOH:O    | 2.41                     | 0.49              |
| 1:J:282:PHE:HB3  | 1:J:300:LEU:HD11 | 1.95                     | 0.49              |
| 1:D:368:PRO:HB3  | 1:D:372:ARG:HH12 | 1.78                     | 0.48              |
| 1:G:150:VAL:CG1  | 1:G:174:LEU:HD11 | 2.40                     | 0.48              |
| 1:I:215:ALA:HA   | 3:I:502:HOH:O    | 2.10                     | 0.48              |
| 1:B:50:PHE:CD2   | 1:B:58:ILE:HD11  | 2.47                     | 0.48              |
| 1:C:164:ARG:HG3  | 1:C:166:GLU:HG3  | 1.95                     | 0.48              |
| 1:F:344:LEU:HD22 | 1:F:387:LEU:HD11 | 1.95                     | 0.48              |
| 1:G:148:LEU:HD13 | 1:G:195:PHE:CD2  | 2.49                     | 0.48              |
| 1:A:382:THR:HG21 | 1:A:402:ARG:O    | 2.12                     | 0.48              |
| 1:A:282:PHE:HB3  | 1:A:300:LEU:HD11 | 1.95                     | 0.48              |
| 1:G:380:ALA:CB   | 3:G:503:HOH:O    | 2.60                     | 0.48              |
| 1:F:282:PHE:HB3  | 1:F:300:LEU:HD11 | 1.95                     | 0.48              |
| 2:P:1:GLC:O2     | 2:P:2:FRU:H11    | 2.14                     | 0.48              |
| 1:C:382:THR:HG21 | 1:C:402:ARG:O    | 2.13                     | 0.48              |
| 1:G:344:LEU:HD22 | 1:G:387:LEU:HD11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:387:LEU:HD23 | 1:C:392:THR:HG22 | 1.96                     | 0.48              |
| 1:G:157:VAL:CG2  | 1:G:164:ARG:HG2  | 2.43                     | 0.48              |
| 1:A:344:LEU:HD22 | 1:A:387:LEU:HD11 | 1.95                     | 0.48              |
| 1:D:282:PHE:HB3  | 1:D:300:LEU:HD11 | 1.95                     | 0.48              |
| 1:E:147:ARG:NH2  | 3:E:504:HOH:O    | 2.46                     | 0.48              |
| 1:J:356:GLY:C    | 3:J:503:HOH:O    | 2.47                     | 0.48              |
| 1:E:344:LEU:HD22 | 1:E:387:LEU:HD11 | 1.96                     | 0.48              |
| 1:E:382:THR:HG21 | 1:E:402:ARG:O    | 2.14                     | 0.48              |
| 1:H:155:SER:CA   | 3:H:503:HOH:O    | 2.01                     | 0.48              |
| 1:H:293:GLY:C    | 1:H:294:LEU:HD12 | 2.39                     | 0.48              |
| 1:I:382:THR:HG21 | 1:I:402:ARG:O    | 2.14                     | 0.48              |
| 1:A:47:ASP:OD2   | 2:K:3:FRU:H11    | 2.14                     | 0.47              |
| 1:B:120:LEU:HD23 | 1:B:121:LEU:C    | 2.39                     | 0.47              |
| 2:T:1:GLC:O2     | 2:T:2:FRU:H11    | 2.13                     | 0.47              |
| 1:B:282:PHE:HB3  | 1:B:300:LEU:HD11 | 1.95                     | 0.47              |
| 2:K:1:GLC:O2     | 2:K:2:FRU:H11    | 2.14                     | 0.47              |
| 1:F:209:THR:OG1  | 1:F:243:SER:HB3  | 2.15                     | 0.47              |
| 1:F:181:ARG:NH1  | 3:F:503:HOH:O    | 2.36                     | 0.47              |
| 1:I:215:ALA:CB   | 3:I:502:HOH:O    | 2.62                     | 0.47              |
| 1:B:64:TRP:CH2   | 1:B:93:ARG:HD3   | 2.50                     | 0.47              |
| 1:B:268:GLU:OE1  | 2:L:3:FRU:H12    | 2.15                     | 0.47              |
| 1:H:382:THR:HG21 | 1:H:402:ARG:O    | 2.15                     | 0.47              |
| 1:D:344:LEU:HD22 | 1:D:387:LEU:HD11 | 1.97                     | 0.47              |
| 1:I:282:PHE:HB3  | 1:I:300:LEU:HD11 | 1.95                     | 0.47              |
| 1:B:265:GLN:NE2  | 3:B:506:HOH:O    | 2.00                     | 0.47              |
| 1:G:127:LEU:CD2  | 1:G:129:VAL:HG23 | 2.45                     | 0.47              |
| 1:H:120:LEU:C    | 1:H:120:LEU:HD23 | 2.39                     | 0.47              |
| 1:I:150:VAL:CG1  | 1:I:174:LEU:HD11 | 2.40                     | 0.46              |
| 1:I:344:LEU:HD22 | 1:I:387:LEU:HD11 | 1.98                     | 0.46              |
| 1:B:372:ARG:NH2  | 1:J:221:GLU:OE1  | 2.48                     | 0.46              |
| 1:B:185:GLU:HB2  | 1:B:193:TYR:CE1  | 2.51                     | 0.46              |
| 1:F:65:ARG:NE    | 1:F:405:LEU:HD13 | 2.30                     | 0.46              |
| 1:J:65:ARG:NE    | 1:J:405:LEU:HD13 | 2.31                     | 0.46              |
| 1:B:226:CYS:SG   | 1:B:231:TRP:HB2  | 2.56                     | 0.46              |
| 1:E:209:THR:OG1  | 1:E:243:SER:HB3  | 2.16                     | 0.46              |
| 1:D:209:THR:OG1  | 1:D:243:SER:HB3  | 2.16                     | 0.46              |
| 1:J:344:LEU:HD22 | 1:J:387:LEU:HD11 | 1.98                     | 0.46              |
| 1:D:65:ARG:NE    | 1:D:405:LEU:HD13 | 2.31                     | 0.45              |
| 1:H:115:TRP:CD2  | 2:R:3:FRU:H61    | 2.51                     | 0.45              |
| 1:A:65:ARG:NE    | 1:A:405:LEU:HD13 | 2.31                     | 0.45              |
| 1:G:286:HIS:NE2  | 2:Q:1:GLC:O2     | 2.42                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:174:LEU:HB3  | 1:H:175:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:150:VAL:HB   | 1:C:174:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:136:ARG:NH1  | 1:D:145:GLU:CD   | 2.75                     | 0.45              |
| 1:H:43:ILE:CG2   | 1:H:71:THR:HB    | 2.47                     | 0.45              |
| 1:I:15:ARG:NE    | 3:I:505:HOH:O    | 2.03                     | 0.45              |
| 1:B:48:THR:HG22  | 1:B:69:SER:OG    | 2.17                     | 0.45              |
| 1:C:48:THR:HG22  | 1:C:69:SER:OG    | 2.17                     | 0.45              |
| 1:F:47:ASP:OD2   | 2:P:3:FRU:H11    | 2.17                     | 0.45              |
| 1:G:115:TRP:CE2  | 2:Q:3:FRU:H62    | 2.51                     | 0.45              |
| 1:J:48:THR:HG22  | 1:J:69:SER:OG    | 2.17                     | 0.45              |
| 1:A:90:PHE:CD1   | 1:A:100:ASP:HA   | 2.52                     | 0.45              |
| 1:H:344:LEU:HD22 | 1:H:387:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:183:GLU:OE1  | 1:D:235:ASN:ND2  | 2.50                     | 0.45              |
| 1:G:48:THR:HG22  | 1:G:69:SER:OG    | 2.17                     | 0.45              |
| 1:F:48:THR:HG22  | 1:F:69:SER:OG    | 2.17                     | 0.45              |
| 1:F:194:THR:O    | 3:F:504:HOH:O    | 2.21                     | 0.45              |
| 1:H:294:LEU:CD1  | 1:H:294:LEU:N    | 2.77                     | 0.45              |
| 1:B:120:LEU:HD23 | 1:B:121:LEU:N    | 2.33                     | 0.44              |
| 1:A:206:SER:HB2  | 1:A:208:LYS:HG2  | 1.98                     | 0.44              |
| 1:J:192:ILE:N    | 3:J:505:HOH:O    | 2.12                     | 0.44              |
| 1:C:48:THR:O     | 1:C:269:ARG:NH2  | 2.51                     | 0.44              |
| 1:H:120:LEU:HD23 | 1:H:122:ASP:N    | 2.32                     | 0.44              |
| 1:I:183:GLU:OE1  | 1:I:235:ASN:ND2  | 2.51                     | 0.44              |
| 1:J:150:VAL:HB   | 1:J:174:LEU:HD11 | 1.99                     | 0.44              |
| 1:J:91:TYR:CB    | 3:J:501:HOH:O    | 2.60                     | 0.44              |
| 1:A:183:GLU:OE1  | 1:A:235:ASN:ND2  | 2.51                     | 0.44              |
| 1:A:389:GLY:HA2  | 1:H:278:PHE:HE2  | 1.82                     | 0.44              |
| 1:B:175:LEU:CD2  | 1:B:253:LEU:CD1  | 2.88                     | 0.44              |
| 1:A:150:VAL:HB   | 1:A:174:LEU:HD11 | 1.99                     | 0.44              |
| 1:I:48:THR:HG22  | 1:I:69:SER:OG    | 2.18                     | 0.44              |
| 1:E:48:THR:HG22  | 1:E:69:SER:OG    | 2.18                     | 0.44              |
| 1:G:183:GLU:OE1  | 1:G:235:ASN:ND2  | 2.51                     | 0.44              |
| 1:D:71:THR:HG21  | 1:D:88:ARG:HD2   | 2.00                     | 0.44              |
| 1:G:174:LEU:HD23 | 1:G:251:TRP:CD1  | 2.53                     | 0.44              |
| 1:A:71:THR:HG21  | 1:A:88:ARG:HD3   | 2.00                     | 0.43              |
| 1:B:150:VAL:HB   | 1:B:174:LEU:HD11 | 2.00                     | 0.43              |
| 1:E:150:VAL:HB   | 1:E:174:LEU:HD11 | 2.00                     | 0.43              |
| 1:G:298:ASP:HB3  | 3:G:504:HOH:O    | 2.14                     | 0.43              |
| 1:I:300:LEU:HB3  | 1:I:322:LEU:CG   | 2.35                     | 0.43              |
| 1:B:82:HIS:C     | 3:B:501:HOH:O    | 2.60                     | 0.43              |
| 1:J:48:THR:O     | 1:J:269:ARG:NH2  | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:71:THR:HG21  | 1:E:88:ARG:HD2   | 2.00                     | 0.43              |
| 1:A:48:THR:O     | 1:A:269:ARG:NH2  | 2.51                     | 0.43              |
| 1:B:183:GLU:OE1  | 1:B:235:ASN:ND2  | 2.52                     | 0.43              |
| 1:H:202:GLU:OE2  | 1:H:207:GLY:O    | 2.37                     | 0.43              |
| 1:I:48:THR:O     | 1:I:269:ARG:NH2  | 2.51                     | 0.43              |
| 1:C:183:GLU:OE1  | 1:C:235:ASN:ND2  | 2.51                     | 0.43              |
| 1:D:50:PHE:CD2   | 1:D:58:ILE:HD11  | 2.52                     | 0.43              |
| 1:F:170:ALA:N    | 3:F:506:HOH:O    | 2.50                     | 0.43              |
| 1:H:48:THR:O     | 1:H:269:ARG:NH2  | 2.51                     | 0.43              |
| 1:H:183:GLU:OE1  | 1:H:235:ASN:ND2  | 2.51                     | 0.43              |
| 2:Q:2:FRU:H11    | 2:Q:3:FRU:O1     | 2.19                     | 0.43              |
| 1:E:183:GLU:OE1  | 1:E:235:ASN:ND2  | 2.51                     | 0.43              |
| 1:H:48:THR:HG22  | 1:H:69:SER:OG    | 2.18                     | 0.43              |
| 1:H:202:GLU:OE1  | 1:H:209:THR:OG1  | 2.35                     | 0.43              |
| 1:I:286:HIS:HE1  | 2:T:2:FRU:O3     | 2.00                     | 0.43              |
| 1:J:82:HIS:HD2   | 2:U:3:FRU:C6     | 2.32                     | 0.43              |
| 1:A:115:TRP:CG   | 2:K:3:FRU:H61    | 2.54                     | 0.43              |
| 1:D:317:GLY:CA   | 3:D:504:HOH:O    | 2.59                     | 0.43              |
| 1:J:183:GLU:OE1  | 1:J:235:ASN:ND2  | 2.51                     | 0.43              |
| 1:E:48:THR:O     | 1:E:269:ARG:NH2  | 2.51                     | 0.43              |
| 1:G:148:LEU:N    | 1:G:148:LEU:HD12 | 2.33                     | 0.43              |
| 1:B:148:LEU:N    | 1:B:148:LEU:HD12 | 2.34                     | 0.43              |
| 1:D:267:LEU:HD12 | 1:D:267:LEU:N    | 2.34                     | 0.43              |
| 1:H:36:ARG:HD2   | 1:H:36:ARG:H     | 1.82                     | 0.43              |
| 1:B:286:HIS:NE2  | 2:L:2:FRU:O3     | 2.49                     | 0.43              |
| 1:G:48:THR:O     | 1:G:269:ARG:NH2  | 2.51                     | 0.43              |
| 1:B:71:THR:HG21  | 1:B:88:ARG:HD3   | 2.01                     | 0.42              |
| 1:D:12:ARG:NH1   | 1:D:261:ILE:HD11 | 2.34                     | 0.42              |
| 1:F:71:THR:HG21  | 1:F:88:ARG:HD3   | 2.01                     | 0.42              |
| 1:H:257:LEU:N    | 1:H:257:LEU:CD1  | 2.81                     | 0.42              |
| 1:A:48:THR:HG22  | 1:A:69:SER:OG    | 2.18                     | 0.42              |
| 1:D:48:THR:O     | 1:D:269:ARG:NH2  | 2.51                     | 0.42              |
| 1:F:48:THR:O     | 1:F:269:ARG:NH2  | 2.52                     | 0.42              |
| 1:G:71:THR:HG21  | 1:G:88:ARG:HD3   | 2.02                     | 0.42              |
| 1:B:403:ILE:HD12 | 1:B:403:ILE:N    | 2.34                     | 0.42              |
| 1:D:150:VAL:HB   | 1:D:174:LEU:HD11 | 2.01                     | 0.42              |
| 1:F:253:LEU:HD12 | 1:F:253:LEU:N    | 2.35                     | 0.42              |
| 1:D:48:THR:HG22  | 1:D:69:SER:OG    | 2.20                     | 0.42              |
| 1:D:147:ARG:HE   | 1:D:173:VAL:HG21 | 1.84                     | 0.42              |
| 1:F:148:LEU:HD12 | 1:F:148:LEU:N    | 2.34                     | 0.42              |
| 1:G:157:VAL:HG23 | 1:G:164:ARG:HG2  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:1:GLC:H62    | 2:O:1:GLC:O3     | 2.18                     | 0.42              |
| 1:E:75:ASP:O     | 1:E:372:ARG:NE   | 2.53                     | 0.42              |
| 1:G:15:ARG:NH2   | 1:G:291:ALA:CB   | 2.82                     | 0.42              |
| 1:G:148:LEU:HD23 | 1:G:211:LEU:HD21 | 2.01                     | 0.42              |
| 1:G:135:GLY:HA2  | 1:G:143:THR:HG23 | 2.02                     | 0.42              |
| 1:H:240:ILE:HG21 | 1:H:257:LEU:CD1  | 2.43                     | 0.42              |
| 1:D:286:HIS:CE1  | 2:N:1:GLC:H3     | 2.54                     | 0.42              |
| 1:H:71:THR:HG21  | 1:H:88:ARG:HD3   | 2.02                     | 0.42              |
| 1:B:48:THR:O     | 1:B:269:ARG:NH2  | 2.52                     | 0.42              |
| 1:C:358:LEU:HD13 | 1:C:366:LEU:HD11 | 2.02                     | 0.42              |
| 1:D:136:ARG:NH1  | 1:D:145:GLU:OE1  | 2.50                     | 0.42              |
| 1:D:161:ASP:OD1  | 1:J:147:ARG:NH2  | 2.53                     | 0.42              |
| 1:H:15:ARG:NH2   | 1:H:294:LEU:HD12 | 2.35                     | 0.42              |
| 1:H:150:VAL:HB   | 1:H:174:LEU:HD11 | 2.01                     | 0.42              |
| 1:J:61:VAL:HG23  | 1:J:61:VAL:O     | 2.20                     | 0.42              |
| 1:J:224:GLY:C    | 1:J:226:CYS:H    | 2.28                     | 0.42              |
| 1:F:210:TYR:OH   | 3:F:501:HOH:O    | 1.86                     | 0.42              |
| 1:F:150:VAL:HB   | 1:F:174:LEU:HD11 | 2.02                     | 0.41              |
| 1:G:15:ARG:NH2   | 1:G:291:ALA:HB1  | 2.35                     | 0.41              |
| 1:B:189:ARG:NH2  | 1:B:221:GLU:HA   | 2.34                     | 0.41              |
| 1:C:54:ARG:HH12  | 1:C:209:THR:HG1  | 1.58                     | 0.41              |
| 1:E:403:ILE:N    | 1:E:403:ILE:HD12 | 2.35                     | 0.41              |
| 1:E:88:ARG:HH12  | 1:E:102:GLY:HA2  | 1.85                     | 0.41              |
| 1:I:395:THR:CG2  | 1:I:413:LEU:CD2  | 2.99                     | 0.41              |
| 1:B:322:LEU:C    | 1:B:322:LEU:CD1  | 2.92                     | 0.41              |
| 1:I:358:LEU:HD23 | 1:I:366:LEU:HD11 | 2.02                     | 0.41              |
| 1:J:403:ILE:N    | 1:J:403:ILE:HD12 | 2.34                     | 0.41              |
| 1:C:71:THR:HG21  | 1:C:88:ARG:HD3   | 2.02                     | 0.41              |
| 1:F:182:TYR:HD2  | 1:F:253:LEU:HD23 | 1.85                     | 0.41              |
| 1:I:71:THR:HG21  | 1:I:88:ARG:HD2   | 2.03                     | 0.41              |
| 1:I:135:GLY:HA2  | 1:I:143:THR:HG23 | 2.03                     | 0.41              |
| 1:G:403:ILE:N    | 1:G:403:ILE:HD12 | 2.36                     | 0.41              |
| 1:J:71:THR:HG21  | 1:J:88:ARG:HD3   | 2.02                     | 0.41              |
| 1:J:114:GLN:OE1  | 1:J:114:GLN:N    | 2.54                     | 0.41              |
| 1:H:175:LEU:HD12 | 1:H:253:LEU:CD1  | 2.51                     | 0.41              |
| 1:I:70:LEU:CD1   | 2:T:3:FRU:H5     | 2.50                     | 0.41              |
| 1:F:275:ARG:NH1  | 1:F:339:SER:OG   | 2.54                     | 0.40              |
| 1:I:182:TYR:HD2  | 1:I:253:LEU:HD23 | 1.87                     | 0.40              |
| 1:F:115:TRP:CD1  | 2:P:3:FRU:H62    | 2.56                     | 0.40              |
| 1:I:403:ILE:HD12 | 1:I:403:ILE:N    | 2.36                     | 0.40              |
| 2:Q:1:GLC:C2     | 2:Q:2:FRU:C1     | 2.98                     | 0.40              |

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| Atom-1           | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------|--------------------------|-------------------|
| 1:A:403:ILE:HD12 | 1:A:403:ILE:N | 2.35                     | 0.40              |
| 1:I:379:LEU:HA   | 3:I:501:HOH:O | 2.20                     | 0.40              |
| 2:R:1:GLC:O2     | 2:R:2:FRU:H11 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 404/428 (94%)   | 383 (95%)  | 21 (5%)  | 0        | 100         | 100 |
| 1   | B     | 404/428 (94%)   | 385 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | C     | 404/428 (94%)   | 384 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | D     | 404/428 (94%)   | 384 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | E     | 404/428 (94%)   | 383 (95%)  | 21 (5%)  | 0        | 100         | 100 |
| 1   | F     | 404/428 (94%)   | 383 (95%)  | 21 (5%)  | 0        | 100         | 100 |
| 1   | G     | 404/428 (94%)   | 385 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | H     | 404/428 (94%)   | 383 (95%)  | 21 (5%)  | 0        | 100         | 100 |
| 1   | I     | 404/428 (94%)   | 384 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | J     | 404/428 (94%)   | 380 (94%)  | 24 (6%)  | 0        | 100         | 100 |
| All | All   | 4040/4280 (94%) | 3834 (95%) | 206 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 329/348 (94%)   | 328 (100%) | 1 (0%)   | 86          | 93 |
| 1   | B     | 329/348 (94%)   | 327 (99%)  | 2 (1%)   | 78          | 90 |
| 1   | C     | 329/348 (94%)   | 327 (99%)  | 2 (1%)   | 78          | 90 |
| 1   | D     | 329/348 (94%)   | 326 (99%)  | 3 (1%)   | 70          | 86 |
| 1   | E     | 329/348 (94%)   | 325 (99%)  | 4 (1%)   | 63          | 82 |
| 1   | F     | 329/348 (94%)   | 327 (99%)  | 2 (1%)   | 78          | 90 |
| 1   | G     | 329/348 (94%)   | 325 (99%)  | 4 (1%)   | 63          | 82 |
| 1   | H     | 329/348 (94%)   | 326 (99%)  | 3 (1%)   | 70          | 86 |
| 1   | I     | 329/348 (94%)   | 325 (99%)  | 4 (1%)   | 63          | 82 |
| 1   | J     | 329/348 (94%)   | 327 (99%)  | 2 (1%)   | 78          | 90 |
| All | All   | 3290/3480 (94%) | 3263 (99%) | 27 (1%)  | 73          | 87 |

All (27) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 193 | TYR  |
| 1   | B     | 226 | CYS  |
| 1   | B     | 322 | LEU  |
| 1   | C     | 10  | THR  |
| 1   | C     | 193 | TYR  |
| 1   | D     | 193 | TYR  |
| 1   | D     | 206 | SER  |
| 1   | D     | 378 | THR  |
| 1   | E     | 147 | ARG  |
| 1   | E     | 193 | TYR  |
| 1   | E     | 206 | SER  |
| 1   | E     | 378 | THR  |
| 1   | F     | 147 | ARG  |
| 1   | F     | 193 | TYR  |
| 1   | G     | 70  | LEU  |
| 1   | G     | 193 | TYR  |
| 1   | G     | 226 | CYS  |
| 1   | G     | 258 | LEU  |
| 1   | H     | 113 | ARG  |
| 1   | H     | 193 | TYR  |
| 1   | H     | 372 | ARG  |
| 1   | I     | 193 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 226 | CYS  |
| 1   | I     | 322 | LEU  |
| 1   | I     | 395 | THR  |
| 1   | J     | 193 | TYR  |
| 1   | J     | 206 | SER  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 114 | GLN  |
| 1   | A     | 242 | HIS  |
| 1   | A     | 286 | HIS  |
| 1   | B     | 82  | HIS  |
| 1   | B     | 114 | GLN  |
| 1   | B     | 187 | GLN  |
| 1   | B     | 351 | ASN  |
| 1   | C     | 114 | GLN  |
| 1   | C     | 288 | HIS  |
| 1   | C     | 351 | ASN  |
| 1   | D     | 286 | HIS  |
| 1   | E     | 114 | GLN  |
| 1   | E     | 242 | HIS  |
| 1   | E     | 351 | ASN  |
| 1   | F     | 114 | GLN  |
| 1   | F     | 242 | HIS  |
| 1   | F     | 286 | HIS  |
| 1   | F     | 351 | ASN  |
| 1   | G     | 114 | GLN  |
| 1   | G     | 187 | GLN  |
| 1   | G     | 242 | HIS  |
| 1   | G     | 351 | ASN  |
| 1   | H     | 242 | HIS  |
| 1   | H     | 351 | ASN  |
| 1   | I     | 114 | GLN  |
| 1   | I     | 242 | HIS  |
| 1   | I     | 276 | ASN  |
| 1   | I     | 286 | HIS  |
| 1   | I     | 351 | ASN  |
| 1   | J     | 82  | HIS  |
| 1   | J     | 242 | HIS  |
| 1   | J     | 351 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

30 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   | GLC  | K     | 1   | 2    | 11,11,12     | 0.26 | 0           | 15,15,17    | 0.53 | 0           |
| 2   | FRU  | K     | 2   | 2    | 11,12,12     | 0.54 | 0           | 10,18,18    | 0.92 | 0           |
| 2   | FRU  | K     | 3   | 2    | 11,11,12     | 0.39 | 0           | 15,15,18    | 1.17 | 1 (6%)      |
| 2   | GLC  | L     | 1   | 2    | 11,11,12     | 0.26 | 0           | 15,15,17    | 0.53 | 0           |
| 2   | FRU  | L     | 2   | 2    | 11,12,12     | 0.54 | 0           | 10,18,18    | 0.87 | 0           |
| 2   | FRU  | L     | 3   | 2    | 11,11,12     | 0.40 | 0           | 15,15,18    | 1.16 | 1 (6%)      |
| 2   | GLC  | M     | 1   | 2    | 11,11,12     | 0.25 | 0           | 15,15,17    | 0.50 | 0           |
| 2   | FRU  | M     | 2   | 2    | 11,12,12     | 0.57 | 0           | 10,18,18    | 0.87 | 0           |
| 2   | FRU  | M     | 3   | 2    | 11,11,12     | 0.39 | 0           | 15,15,18    | 1.18 | 1 (6%)      |
| 2   | GLC  | N     | 1   | 2    | 11,11,12     | 0.26 | 0           | 15,15,17    | 0.56 | 0           |
| 2   | FRU  | N     | 2   | 2    | 11,12,12     | 0.54 | 0           | 10,18,18    | 0.90 | 0           |
| 2   | FRU  | N     | 3   | 2    | 11,11,12     | 0.40 | 0           | 15,15,18    | 1.17 | 1 (6%)      |
| 2   | GLC  | O     | 1   | 2    | 11,11,12     | 0.25 | 0           | 15,15,17    | 0.51 | 0           |
| 2   | FRU  | O     | 2   | 2    | 11,12,12     | 0.58 | 0           | 10,18,18    | 0.88 | 0           |
| 2   | FRU  | O     | 3   | 2    | 11,11,12     | 0.39 | 0           | 15,15,18    | 1.17 | 1 (6%)      |
| 2   | GLC  | P     | 1   | 2    | 11,11,12     | 0.25 | 0           | 15,15,17    | 0.52 | 0           |
| 2   | FRU  | P     | 2   | 2    | 11,12,12     | 0.53 | 0           | 10,18,18    | 0.91 | 0           |
| 2   | FRU  | P     | 3   | 2    | 11,11,12     | 0.40 | 0           | 15,15,18    | 1.17 | 1 (6%)      |
| 2   | GLC  | Q     | 1   | 2    | 11,11,12     | 0.26 | 0           | 15,15,17    | 0.53 | 0           |
| 2   | FRU  | Q     | 2   | 2    | 11,12,12     | 0.58 | 0           | 10,18,18    | 0.87 | 0           |
| 2   | FRU  | Q     | 3   | 2    | 11,11,12     | 0.40 | 0           | 15,15,18    | 1.15 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | GLC  | R     | 1   | 2    | 11,11,12     | 0.26 | 0        | 15,15,17    | 0.55 | 0        |
| 2   | FRU  | R     | 2   | 2    | 11,12,12     | 0.57 | 0        | 10,18,18    | 0.91 | 0        |
| 2   | FRU  | R     | 3   | 2    | 11,11,12     | 0.40 | 0        | 15,15,18    | 1.13 | 0        |
| 2   | GLC  | T     | 1   | 2    | 11,11,12     | 0.26 | 0        | 15,15,17    | 0.53 | 0        |
| 2   | FRU  | T     | 2   | 2    | 11,12,12     | 0.54 | 0        | 10,18,18    | 0.90 | 0        |
| 2   | FRU  | T     | 3   | 2    | 11,11,12     | 0.39 | 0        | 15,15,18    | 1.14 | 1 (6%)   |
| 2   | GLC  | U     | 1   | 2    | 11,11,12     | 0.26 | 0        | 15,15,17    | 0.55 | 0        |
| 2   | FRU  | U     | 2   | 2    | 11,12,12     | 0.57 | 0        | 10,18,18    | 0.92 | 0        |
| 2   | FRU  | U     | 3   | 2    | 11,11,12     | 0.40 | 0        | 15,15,18    | 1.15 | 1 (6%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | GLC  | K     | 1   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | FRU  | K     | 2   | 2    | -       | 3/5/24/24 | 0/1/1/1 |
| 2   | FRU  | K     | 3   | 2    | -       | 3/4/20/24 | 0/1/1/1 |
| 2   | GLC  | L     | 1   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | FRU  | L     | 2   | 2    | -       | 5/5/24/24 | 0/1/1/1 |
| 2   | FRU  | L     | 3   | 2    | -       | 3/4/20/24 | 0/1/1/1 |
| 2   | GLC  | M     | 1   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | FRU  | M     | 2   | 2    | -       | 4/5/24/24 | 0/1/1/1 |
| 2   | FRU  | M     | 3   | 2    | -       | 0/4/20/24 | 0/1/1/1 |
| 2   | GLC  | N     | 1   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | FRU  | N     | 2   | 2    | -       | 5/5/24/24 | 0/1/1/1 |
| 2   | FRU  | N     | 3   | 2    | -       | 4/4/20/24 | 0/1/1/1 |
| 2   | GLC  | O     | 1   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | FRU  | O     | 2   | 2    | -       | 3/5/24/24 | 0/1/1/1 |
| 2   | FRU  | O     | 3   | 2    | -       | 0/4/20/24 | 0/1/1/1 |
| 2   | GLC  | P     | 1   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | FRU  | P     | 2   | 2    | -       | 3/5/24/24 | 0/1/1/1 |
| 2   | FRU  | P     | 3   | 2    | -       | 2/4/20/24 | 0/1/1/1 |
| 2   | GLC  | Q     | 1   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | FRU  | Q     | 2   | 2    | -       | 3/5/24/24 | 0/1/1/1 |
| 2   | FRU  | Q     | 3   | 2    | -       | 3/4/20/24 | 0/1/1/1 |
| 2   | GLC  | R     | 1   | 2    | -       | 2/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | FRU  | R     | 2   | 2    | -       | 3/5/24/24 | 0/1/1/1 |
| 2   | FRU  | R     | 3   | 2    | -       | 2/4/20/24 | 0/1/1/1 |
| 2   | GLC  | T     | 1   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | FRU  | T     | 2   | 2    | -       | 5/5/24/24 | 0/1/1/1 |
| 2   | FRU  | T     | 3   | 2    | -       | 3/4/20/24 | 0/1/1/1 |
| 2   | GLC  | U     | 1   | 2    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | FRU  | U     | 2   | 2    | -       | 4/5/24/24 | 0/1/1/1 |
| 2   | FRU  | U     | 3   | 2    | -       | 2/4/20/24 | 0/1/1/1 |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | M     | 3   | FRU  | C1-C2-C3 | -2.08 | 110.18      | 115.10   |
| 2   | K     | 3   | FRU  | C1-C2-C3 | -2.06 | 110.22      | 115.10   |
| 2   | O     | 3   | FRU  | C1-C2-C3 | -2.05 | 110.27      | 115.10   |
| 2   | N     | 3   | FRU  | C1-C2-C3 | -2.04 | 110.27      | 115.10   |
| 2   | P     | 3   | FRU  | C1-C2-C3 | -2.04 | 110.27      | 115.10   |
| 2   | L     | 3   | FRU  | C1-C2-C3 | -2.01 | 110.34      | 115.10   |
| 2   | U     | 3   | FRU  | C1-C2-C3 | -2.00 | 110.37      | 115.10   |
| 2   | T     | 3   | FRU  | C1-C2-C3 | -2.00 | 110.37      | 115.10   |

There are no chirality outliers.

All (73) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | K     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | K     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | L     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | L     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | M     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | M     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | M     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | N     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | O     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | O     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | P     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | P     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | Q     | 2   | FRU  | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | Q     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | Q     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | R     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | R     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | T     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | T     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | U     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | U     | 2   | FRU  | O1-C1-C2-O2 |
| 2   | T     | 2   | FRU  | O5-C5-C6-O6 |
| 2   | T     | 2   | FRU  | C4-C5-C6-O6 |
| 2   | N     | 2   | FRU  | O5-C5-C6-O6 |
| 2   | L     | 2   | FRU  | O5-C5-C6-O6 |
| 2   | O     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | L     | 2   | FRU  | C4-C5-C6-O6 |
| 2   | O     | 1   | GLC  | C4-C5-C6-O6 |
| 2   | P     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | N     | 2   | FRU  | C4-C5-C6-O6 |
| 2   | R     | 1   | GLC  | C4-C5-C6-O6 |
| 2   | N     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | Q     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | N     | 1   | GLC  | C4-C5-C6-O6 |
| 2   | R     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | K     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | L     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | O     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | P     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | R     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | T     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | U     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | P     | 1   | GLC  | C4-C5-C6-O6 |
| 2   | Q     | 3   | FRU  | C4-C5-C6-O6 |
| 2   | M     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | T     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | N     | 3   | FRU  | O5-C5-C6-O6 |
| 2   | T     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | K     | 3   | FRU  | O5-C5-C6-O6 |
| 2   | K     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | L     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | L     | 3   | FRU  | O5-C5-C6-O6 |
| 2   | P     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | R     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | U     | 3   | FRU  | O1-C1-C2-O5 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | N     | 2   | FRU  | O1-C1-C2-C3 |
| 2   | K     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | L     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | R     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | U     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | Q     | 1   | GLC  | C4-C5-C6-O6 |
| 2   | U     | 1   | GLC  | C4-C5-C6-O6 |
| 2   | P     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | Q     | 3   | FRU  | O5-C5-C6-O6 |
| 2   | N     | 3   | FRU  | C4-C5-C6-O6 |
| 2   | U     | 1   | GLC  | O5-C5-C6-O6 |
| 2   | N     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | T     | 3   | FRU  | O5-C5-C6-O6 |
| 2   | N     | 3   | FRU  | O1-C1-C2-C3 |
| 2   | N     | 2   | FRU  | O1-C1-C2-O5 |
| 2   | Q     | 3   | FRU  | O1-C1-C2-O5 |
| 2   | U     | 2   | FRU  | O5-C5-C6-O6 |
| 2   | M     | 2   | FRU  | O5-C5-C6-O6 |

There are no ring outliers.

28 monomers are involved in 64 short contacts:

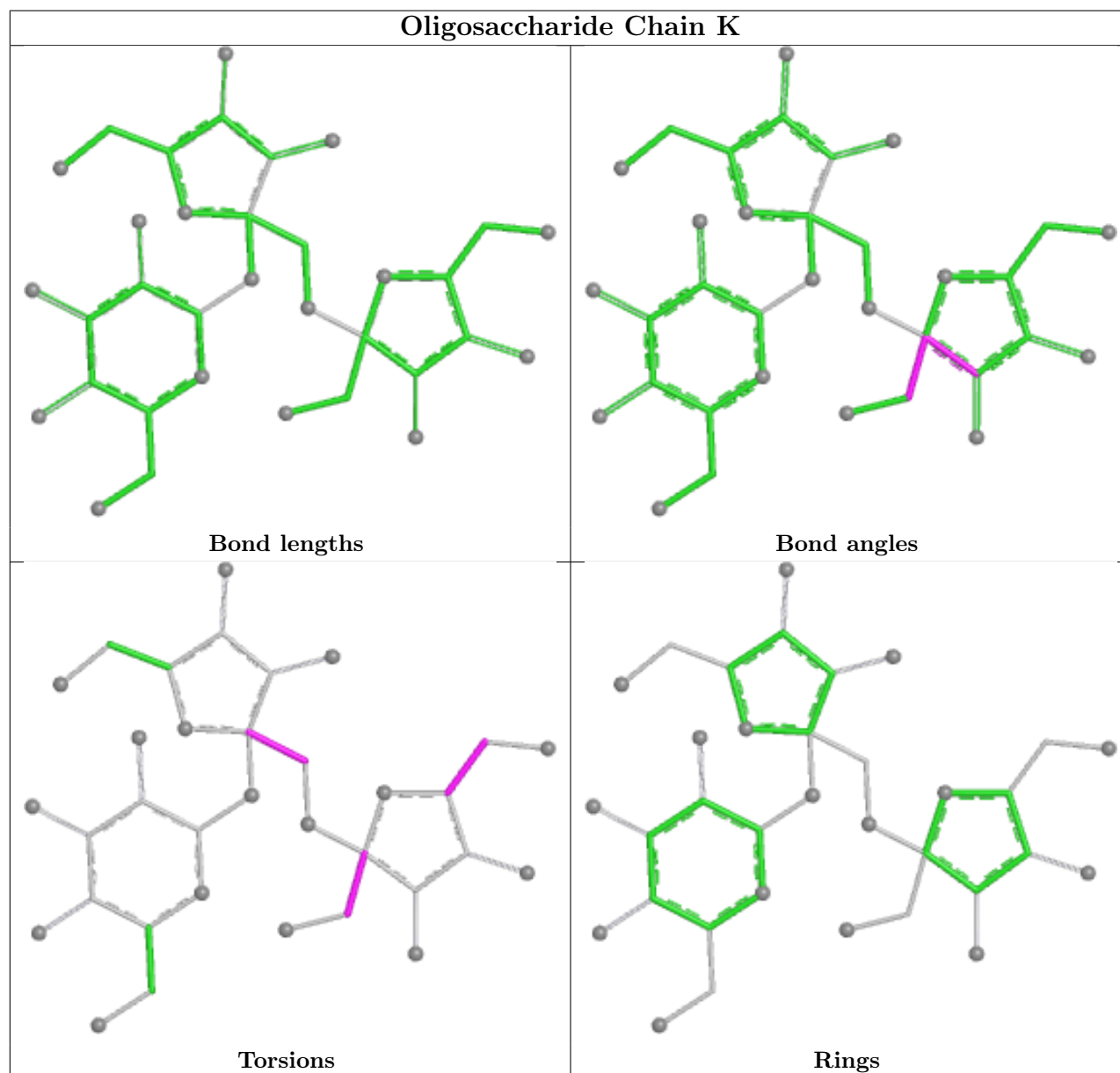
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | P     | 1   | GLC  | 1       | 0            |
| 2   | Q     | 2   | FRU  | 5       | 0            |
| 2   | L     | 1   | GLC  | 2       | 0            |
| 2   | N     | 1   | GLC  | 1       | 0            |
| 2   | P     | 3   | FRU  | 4       | 0            |
| 2   | P     | 2   | FRU  | 1       | 0            |
| 2   | O     | 2   | FRU  | 2       | 0            |
| 2   | R     | 1   | GLC  | 1       | 0            |
| 2   | M     | 3   | FRU  | 6       | 0            |
| 2   | R     | 3   | FRU  | 3       | 0            |
| 2   | M     | 2   | FRU  | 3       | 0            |
| 2   | K     | 1   | GLC  | 1       | 0            |
| 2   | L     | 2   | FRU  | 3       | 0            |
| 2   | N     | 2   | FRU  | 1       | 0            |
| 2   | O     | 1   | GLC  | 3       | 0            |
| 2   | R     | 2   | FRU  | 2       | 0            |
| 2   | Q     | 3   | FRU  | 7       | 0            |
| 2   | O     | 3   | FRU  | 3       | 0            |
| 2   | U     | 3   | FRU  | 3       | 0            |

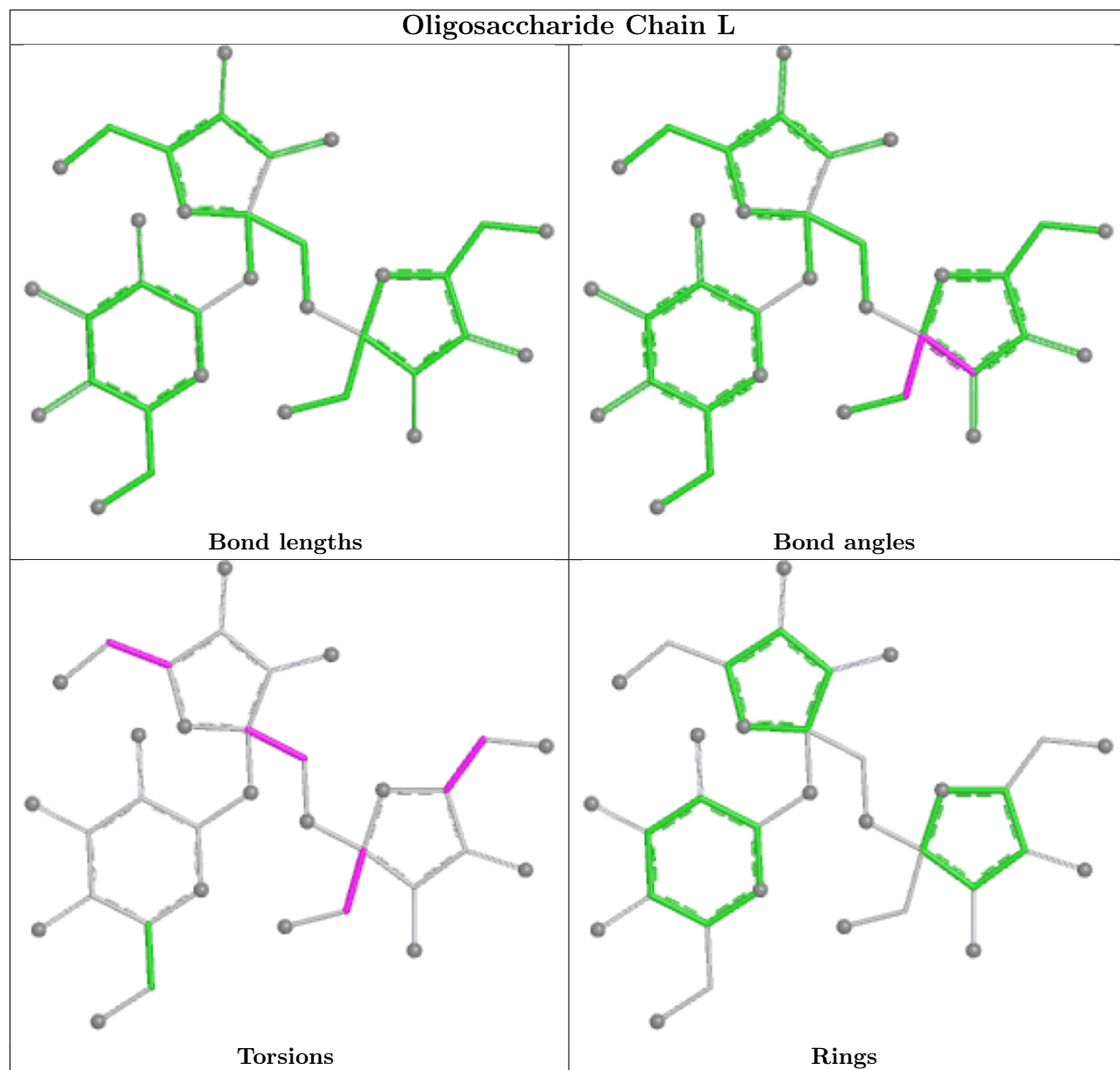
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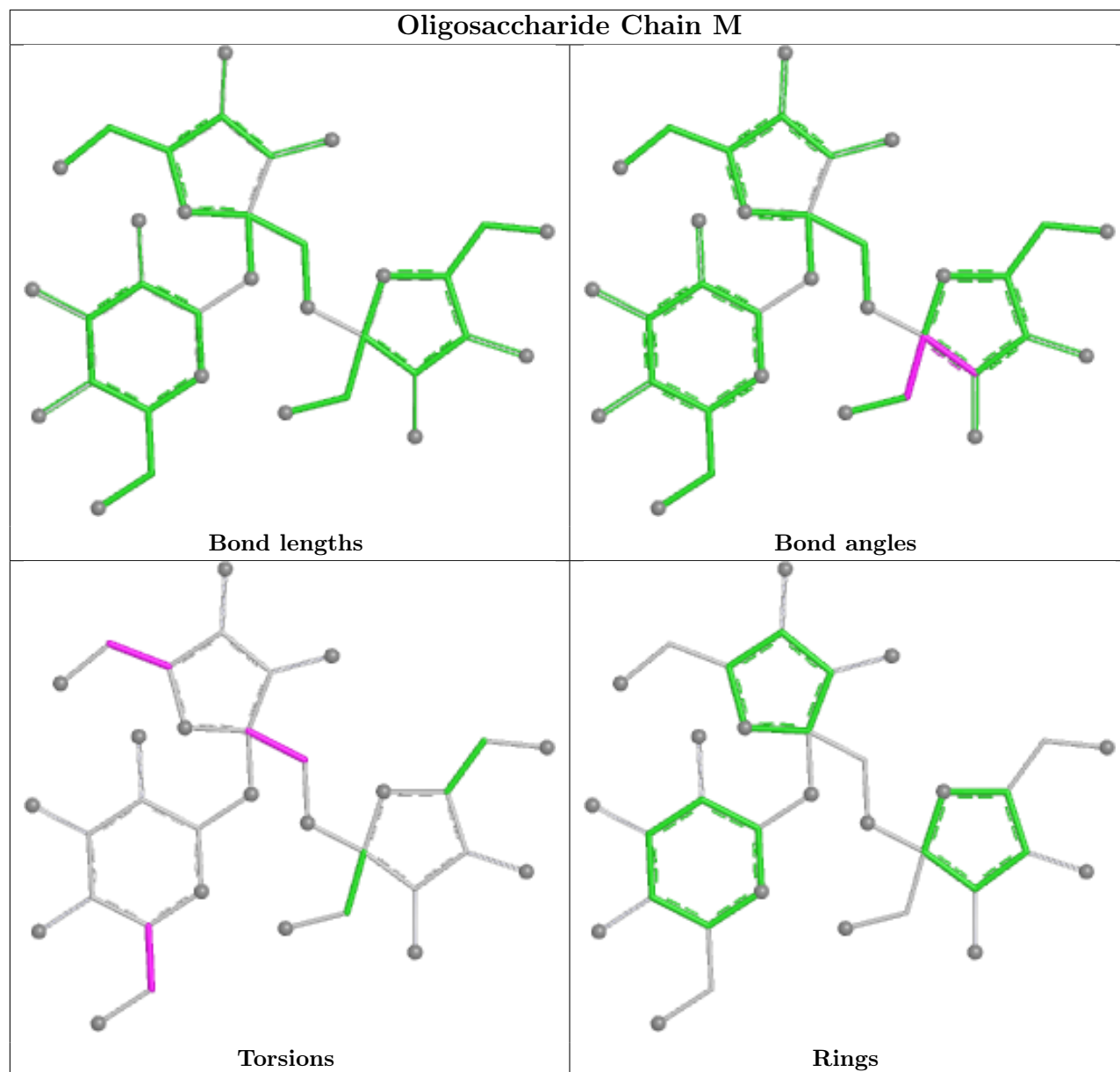
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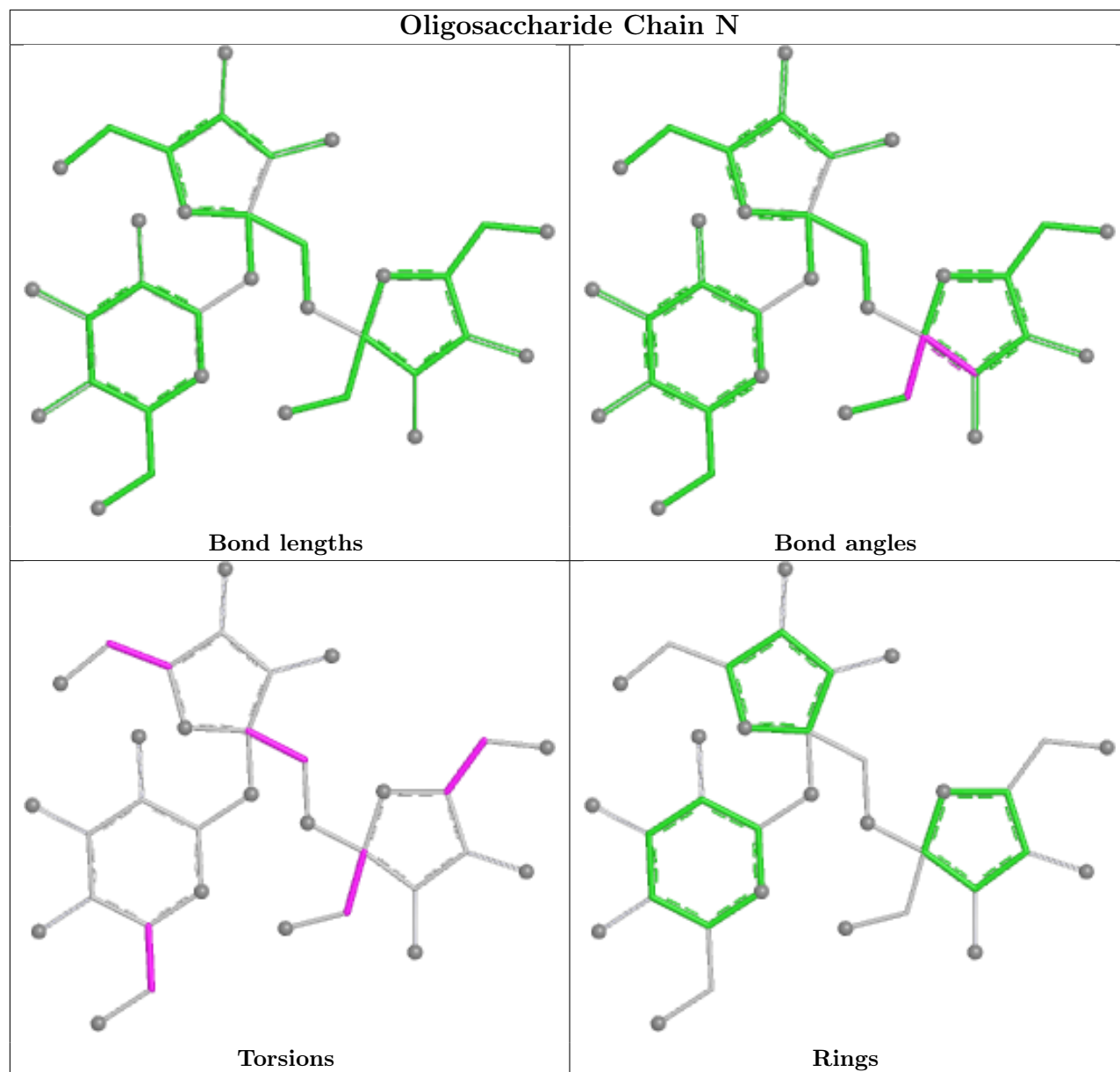
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | T     | 1   | GLC  | 1       | 0            |
| 2   | T     | 3   | FRU  | 6       | 0            |
| 2   | T     | 2   | FRU  | 4       | 0            |
| 2   | K     | 2   | FRU  | 1       | 0            |
| 2   | K     | 3   | FRU  | 3       | 0            |
| 2   | L     | 3   | FRU  | 2       | 0            |
| 2   | N     | 3   | FRU  | 3       | 0            |
| 2   | M     | 1   | GLC  | 4       | 0            |
| 2   | Q     | 1   | GLC  | 7       | 0            |

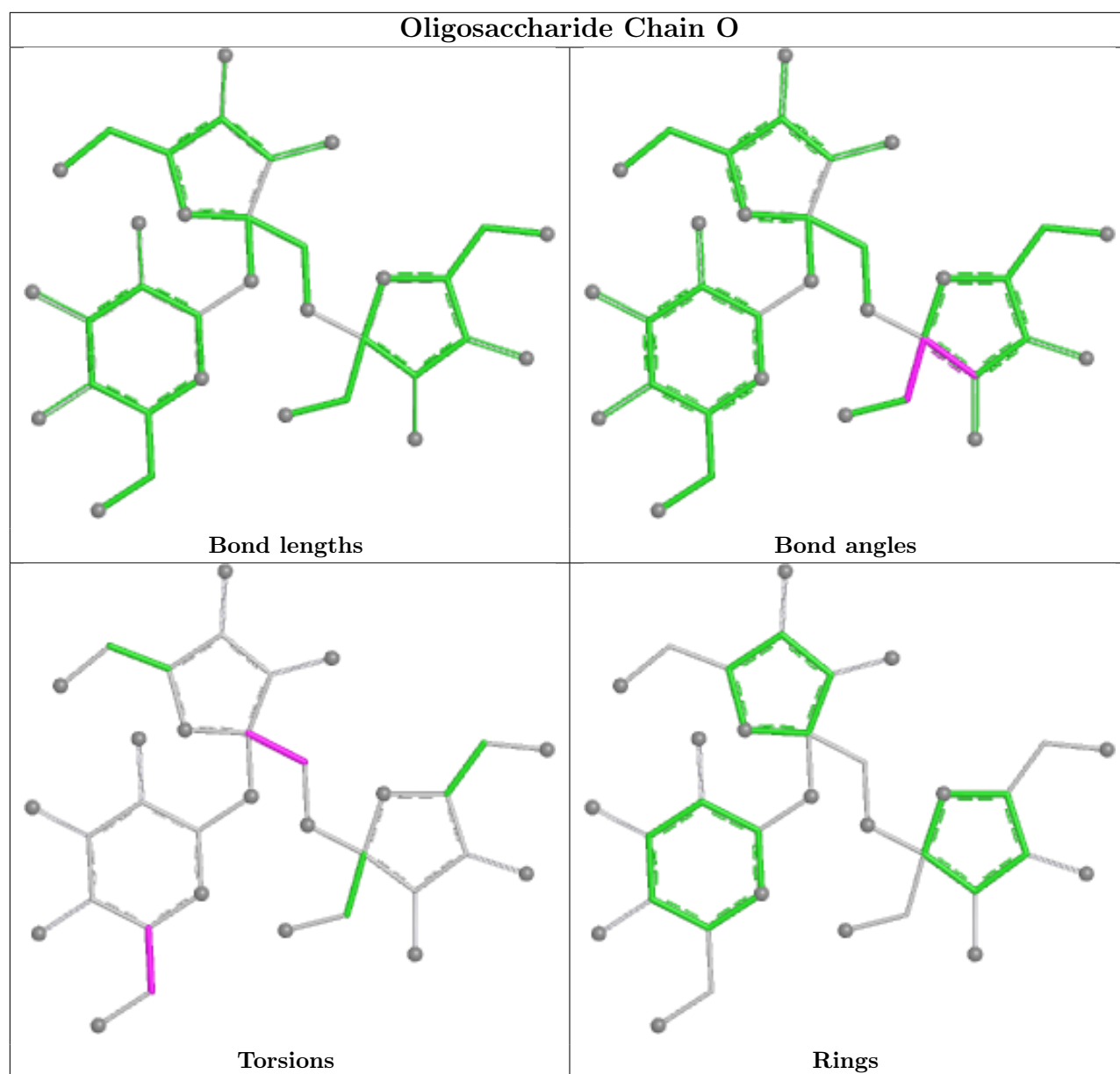
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

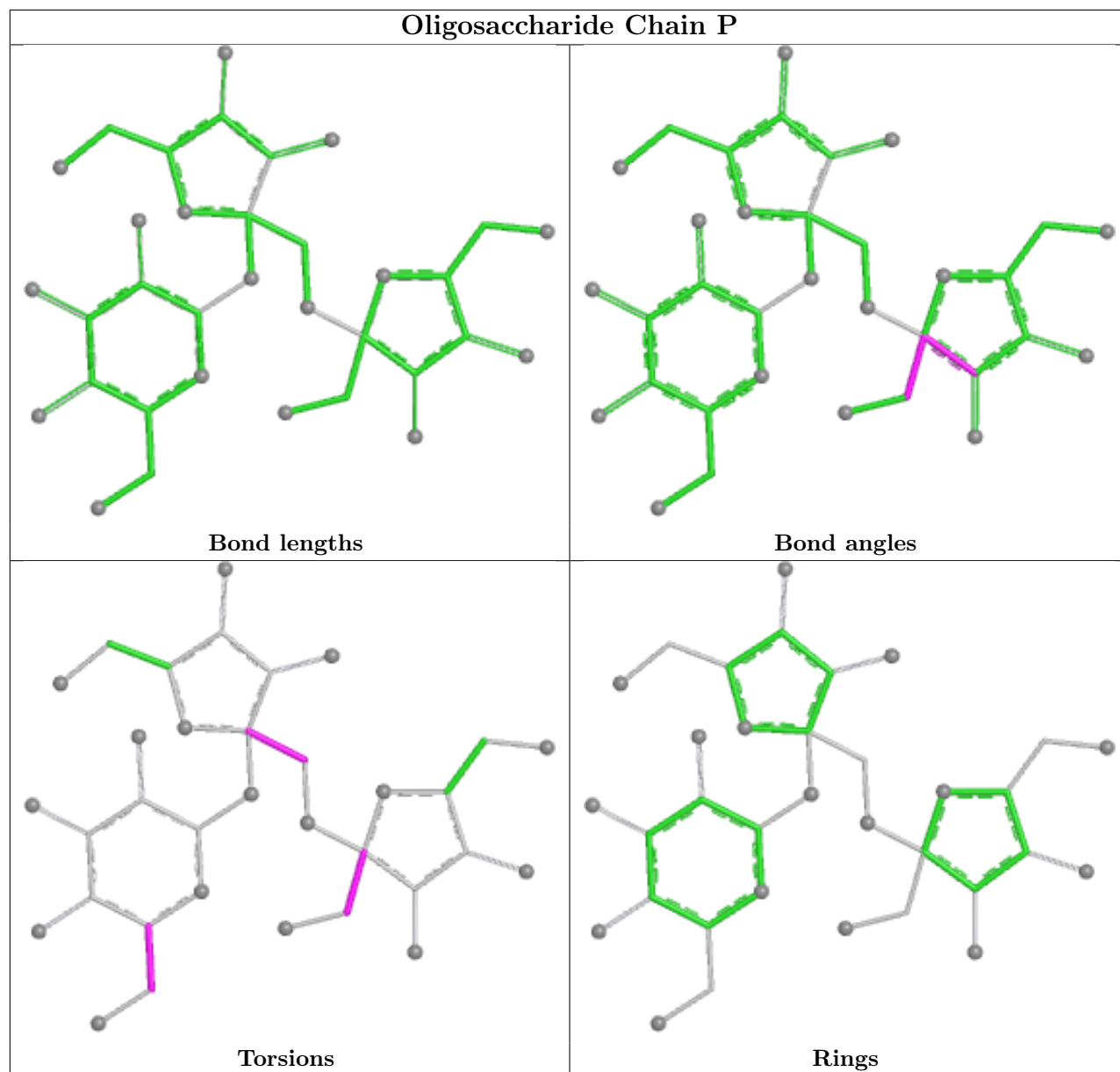


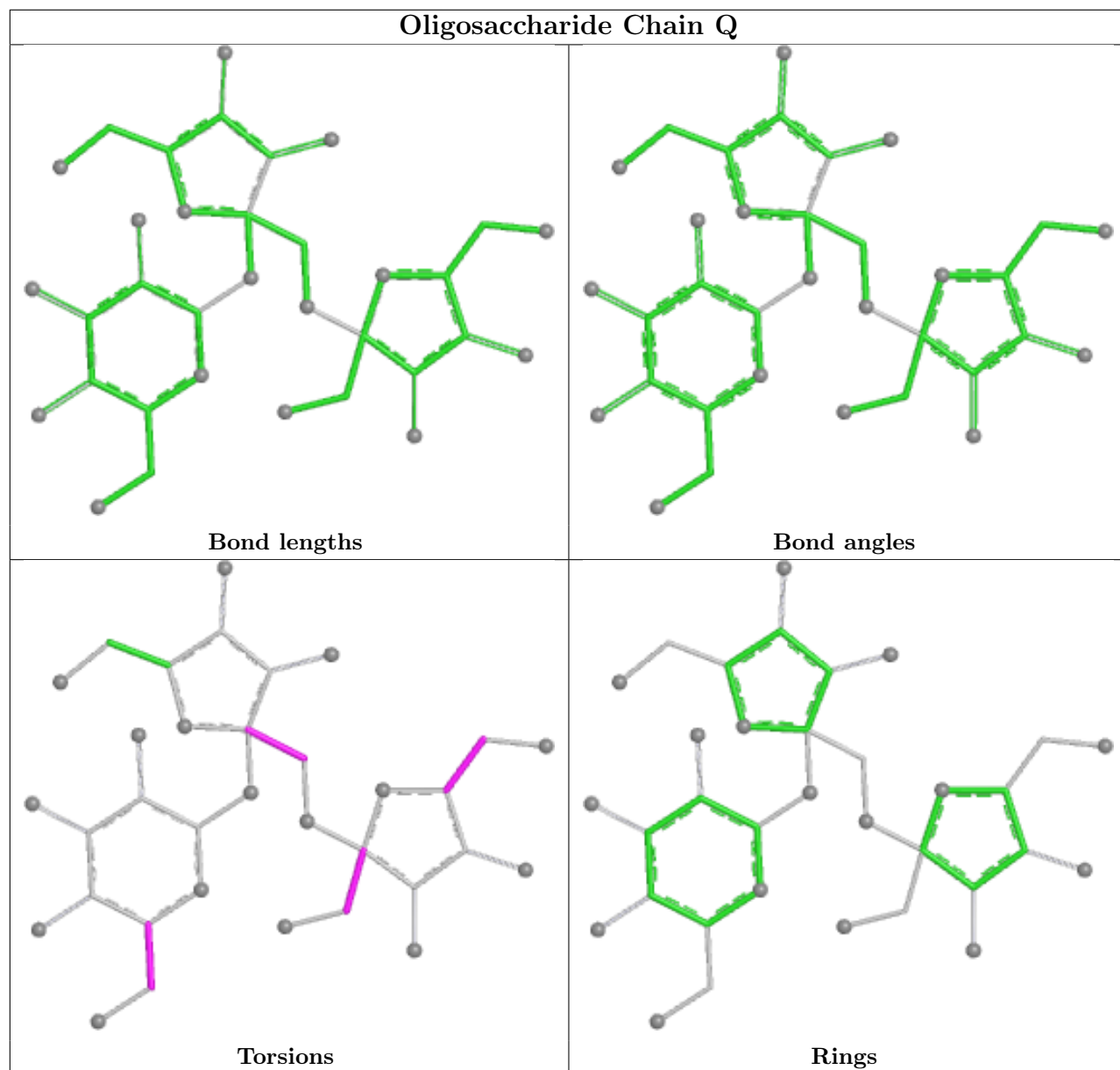


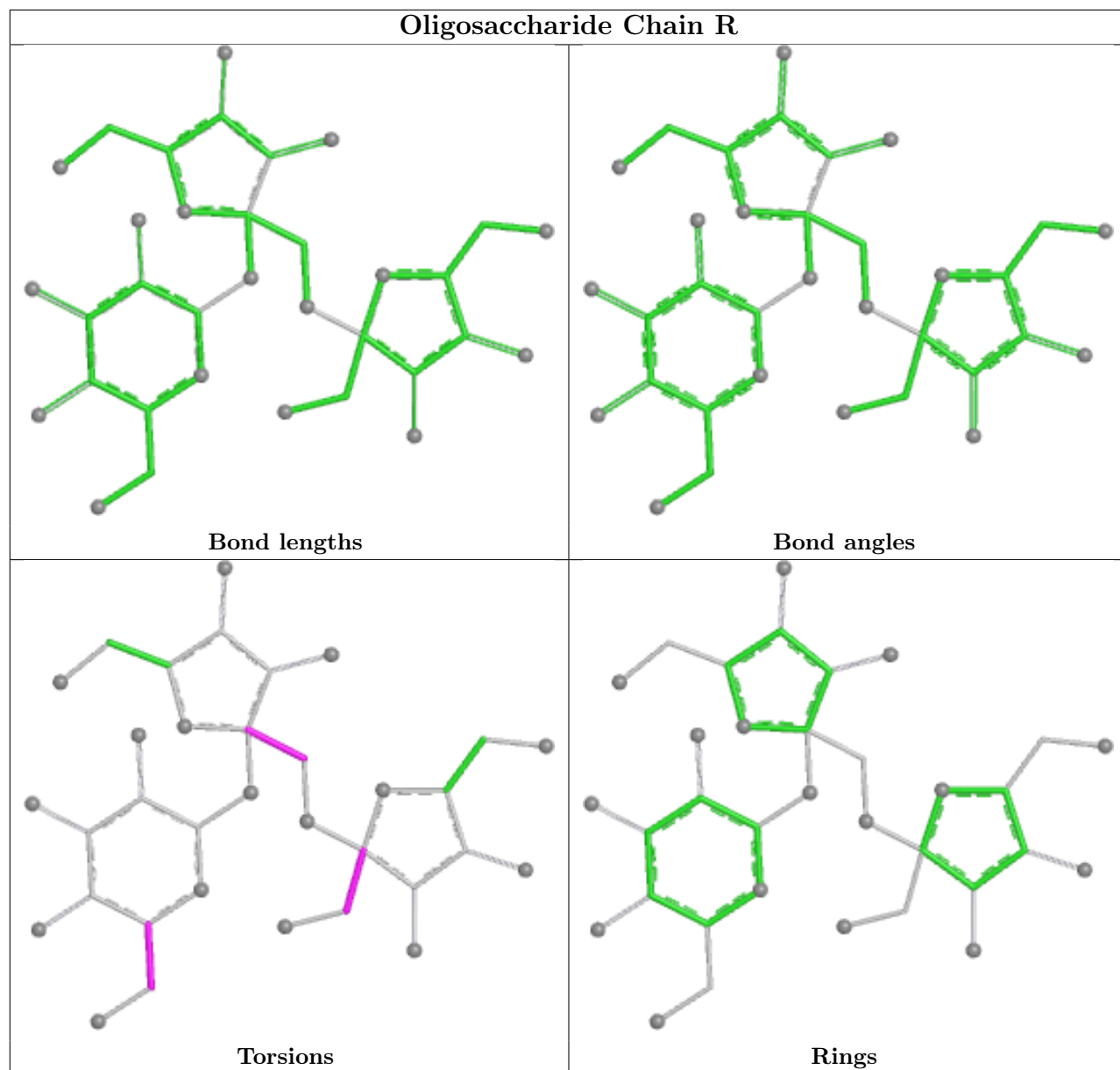


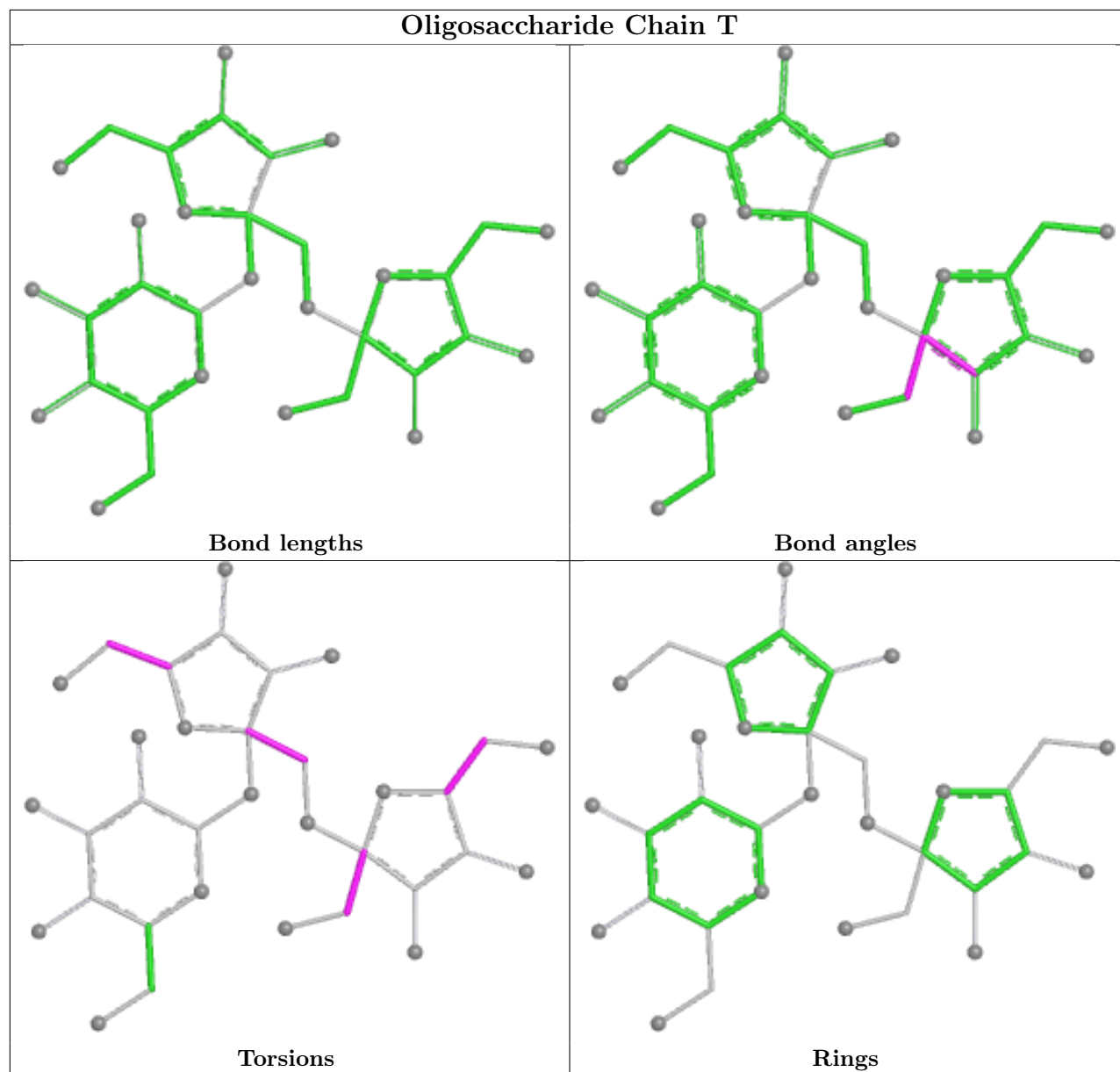


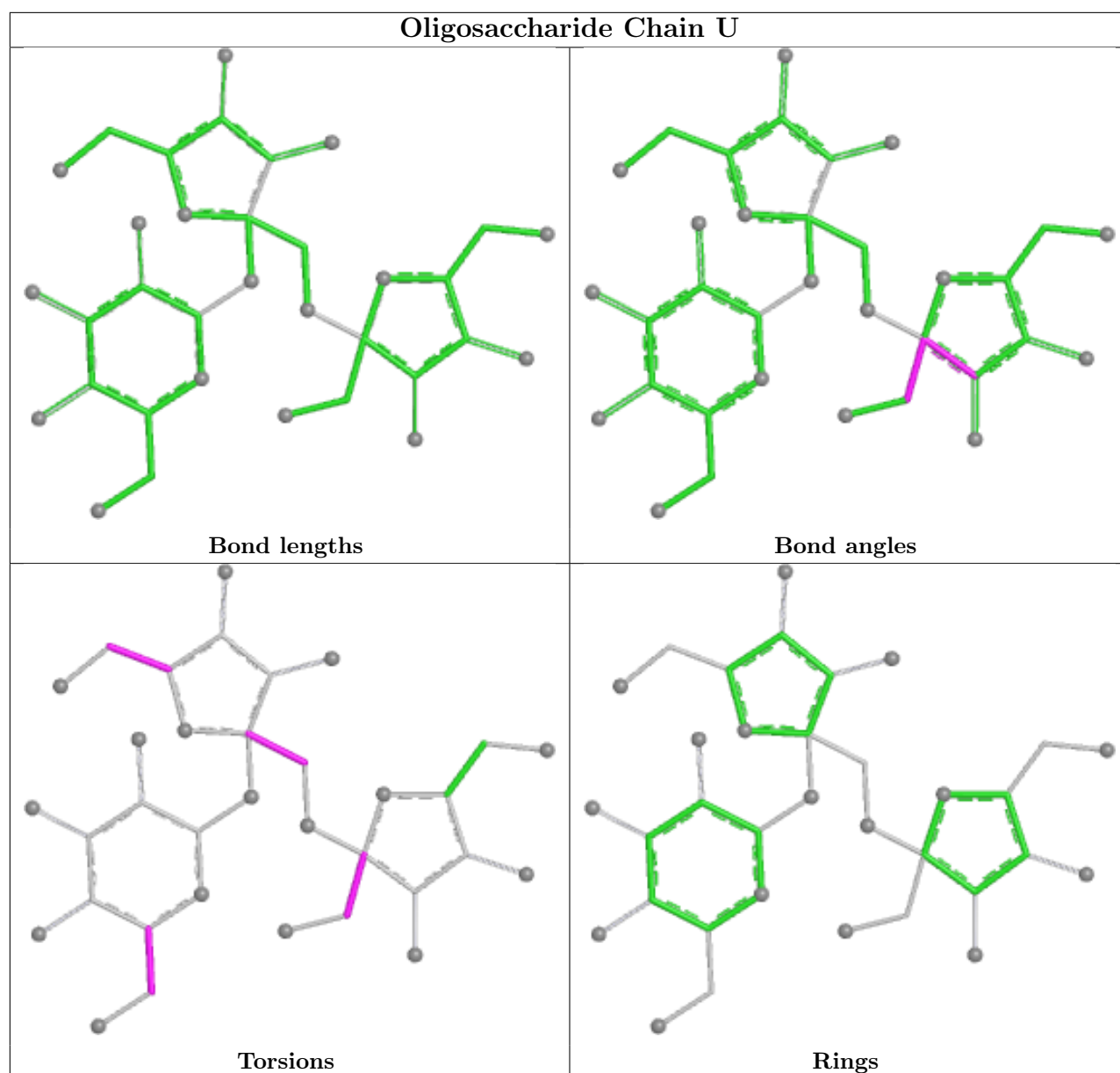












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 406/428 (94%)   | -0.34  | 2 (0%) 87 86  | 34, 51, 77, 94        | 0     |
| 1   | B     | 406/428 (94%)   | 0.14   | 7 (1%) 69 66  | 43, 77, 118, 135      | 0     |
| 1   | C     | 406/428 (94%)   | -0.31  | 2 (0%) 87 86  | 37, 56, 81, 93        | 0     |
| 1   | D     | 406/428 (94%)   | -0.41  | 0 100 100     | 28, 47, 70, 89        | 0     |
| 1   | E     | 406/428 (94%)   | -0.35  | 2 (0%) 87 86  | 28, 50, 81, 104       | 0     |
| 1   | F     | 406/428 (94%)   | -0.23  | 2 (0%) 87 86  | 37, 57, 83, 106       | 0     |
| 1   | G     | 406/428 (94%)   | -0.00  | 5 (1%) 76 75  | 43, 73, 109, 128      | 0     |
| 1   | H     | 406/428 (94%)   | 0.04   | 4 (0%) 79 78  | 37, 72, 113, 136      | 0     |
| 1   | I     | 406/428 (94%)   | 0.02   | 7 (1%) 69 66  | 44, 72, 103, 121      | 0     |
| 1   | J     | 406/428 (94%)   | -0.24  | 2 (0%) 87 86  | 37, 54, 77, 94        | 0     |
| All | All   | 4060/4280 (94%) | -0.17  | 33 (0%) 82 81 | 28, 58, 102, 136      | 0     |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 414 | PRO  | 4.1  |
| 1   | A     | 414 | PRO  | 3.7  |
| 1   | C     | 414 | PRO  | 3.1  |
| 1   | G     | 360 | LEU  | 3.1  |
| 1   | B     | 168 | PRO  | 3.0  |
| 1   | G     | 140 | ALA  | 2.9  |
| 1   | H     | 222 | GLY  | 2.9  |
| 1   | J     | 357 | GLY  | 2.7  |
| 1   | H     | 168 | PRO  | 2.7  |
| 1   | G     | 174 | LEU  | 2.6  |
| 1   | B     | 229 | PRO  | 2.6  |
| 1   | I     | 144 | TYR  | 2.5  |
| 1   | I     | 137 | ALA  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 414 | PRO  | 2.4  |
| 1   | I     | 414 | PRO  | 2.4  |
| 1   | B     | 322 | LEU  | 2.4  |
| 1   | A     | 356 | GLY  | 2.3  |
| 1   | G     | 225 | ALA  | 2.3  |
| 1   | H     | 223 | ALA  | 2.3  |
| 1   | G     | 9   | ALA  | 2.2  |
| 1   | C     | 174 | LEU  | 2.2  |
| 1   | I     | 322 | LEU  | 2.2  |
| 1   | E     | 220 | PRO  | 2.2  |
| 1   | B     | 157 | VAL  | 2.2  |
| 1   | B     | 121 | LEU  | 2.2  |
| 1   | H     | 157 | VAL  | 2.2  |
| 1   | I     | 356 | GLY  | 2.1  |
| 1   | J     | 225 | ALA  | 2.1  |
| 1   | I     | 104 | VAL  | 2.1  |
| 1   | I     | 142 | ILE  | 2.1  |
| 1   | F     | 39  | ALA  | 2.0  |
| 1   | B     | 221 | GLU  | 2.0  |
| 1   | E     | 414 | PRO  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | FRU  | R     | 2   | 12/12 | 0.59 | 0.23 | 45,49,62,63                 | 12    |
| 2   | GLC  | N     | 1   | 11/12 | 0.60 | 0.31 | 45,58,75,83                 | 11    |
| 2   | GLC  | T     | 1   | 11/12 | 0.60 | 0.29 | 45,49,63,70                 | 11    |
| 2   | GLC  | M     | 1   | 11/12 | 0.61 | 0.27 | 45,53,63,69                 | 11    |
| 2   | GLC  | O     | 1   | 11/12 | 0.63 | 0.33 | 45,45,66,70                 | 11    |
| 2   | GLC  | P     | 1   | 11/12 | 0.63 | 0.29 | 45,51,63,73                 | 11    |
| 2   | FRU  | O     | 2   | 12/12 | 0.65 | 0.22 | 45,54,66,70                 | 12    |
| 2   | GLC  | R     | 1   | 11/12 | 0.65 | 0.26 | 45,45,56,61                 | 11    |

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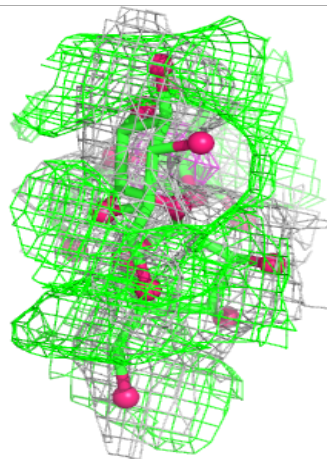
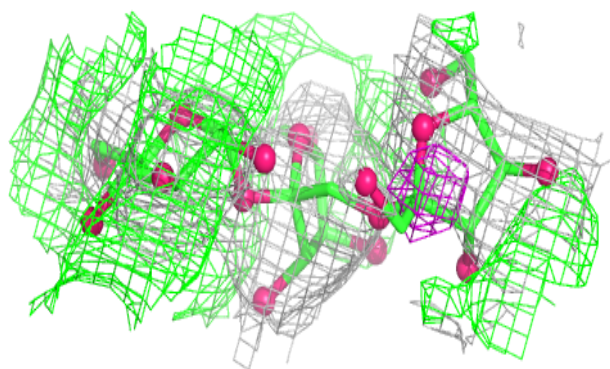
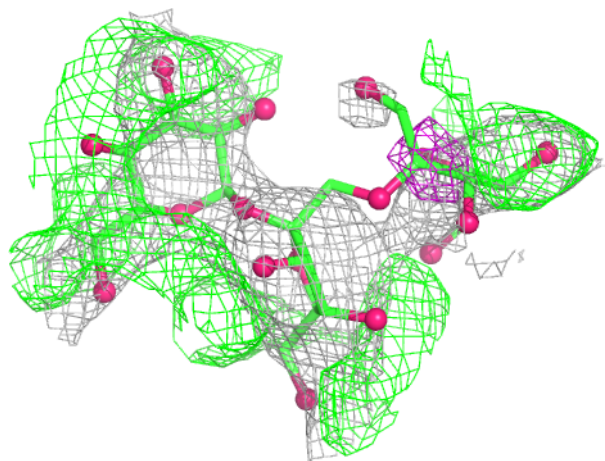
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | GLC  | K     | 1   | 11/12 | 0.68 | 0.28 | 45,46,65,78                 | 11    |
| 2   | FRU  | K     | 2   | 12/12 | 0.68 | 0.18 | 45,50,63,64                 | 12    |
| 2   | FRU  | L     | 2   | 12/12 | 0.70 | 0.17 | 45,56,62,65                 | 12    |
| 2   | FRU  | T     | 2   | 12/12 | 0.70 | 0.20 | 45,53,62,66                 | 12    |
| 2   | GLC  | L     | 1   | 11/12 | 0.73 | 0.24 | 45,47,62,63                 | 11    |
| 2   | GLC  | Q     | 1   | 11/12 | 0.73 | 0.27 | 45,52,65,66                 | 11    |
| 2   | FRU  | N     | 2   | 12/12 | 0.75 | 0.18 | 45,47,57,61                 | 12    |
| 2   | FRU  | M     | 3   | 11/12 | 0.76 | 0.25 | 45,47,57,58                 | 11    |
| 2   | FRU  | Q     | 3   | 11/12 | 0.76 | 0.30 | 45,54,69,72                 | 11    |
| 2   | FRU  | Q     | 2   | 12/12 | 0.77 | 0.23 | 47,57,67,70                 | 12    |
| 2   | FRU  | K     | 3   | 11/12 | 0.78 | 0.23 | 45,48,62,64                 | 11    |
| 2   | FRU  | M     | 2   | 12/12 | 0.82 | 0.15 | 45,50,60,61                 | 12    |
| 2   | FRU  | T     | 3   | 11/12 | 0.82 | 0.24 | 45,49,58,60                 | 11    |
| 2   | FRU  | R     | 3   | 11/12 | 0.85 | 0.19 | 45,49,54,55                 | 11    |
| 2   | FRU  | P     | 2   | 12/12 | 0.85 | 0.18 | 45,54,60,64                 | 12    |
| 2   | FRU  | P     | 3   | 11/12 | 0.86 | 0.21 | 45,50,63,73                 | 11    |
| 2   | FRU  | O     | 3   | 11/12 | 0.86 | 0.23 | 45,45,60,63                 | 11    |
| 2   | FRU  | N     | 3   | 11/12 | 0.88 | 0.19 | 45,45,52,54                 | 11    |
| 2   | FRU  | L     | 3   | 11/12 | 0.88 | 0.23 | 45,54,70,75                 | 11    |
| 2   | GLC  | U     | 1   | 11/12 | -    | -    | 45,46,66,68                 | 11    |
| 2   | FRU  | U     | 2   | 12/12 | -    | -    | 45,54,58,60                 | 12    |
| 2   | FRU  | U     | 3   | 11/12 | -    | -    | 45,51,57,60                 | 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.

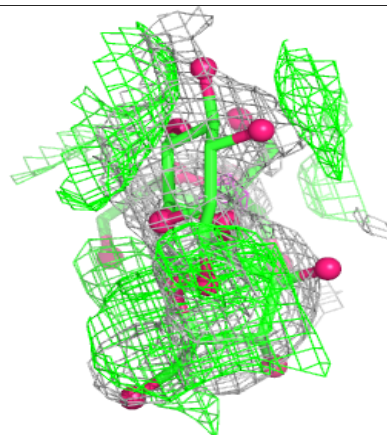
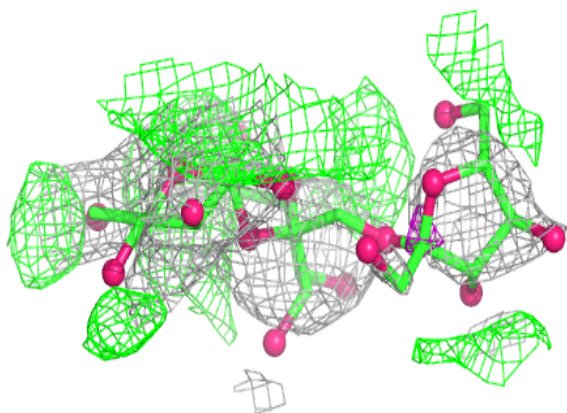
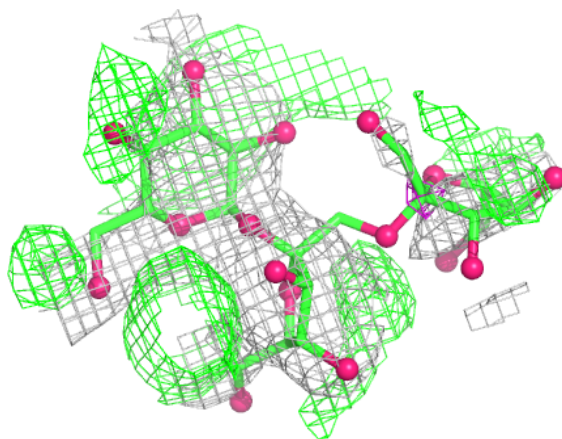
**Electron density around Chain K:**

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



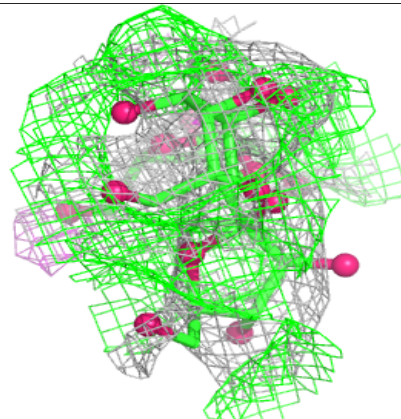
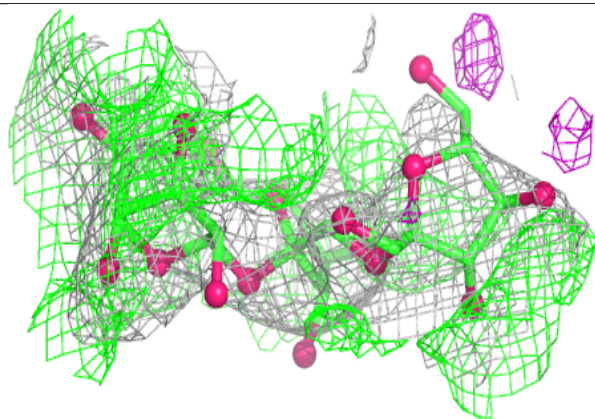
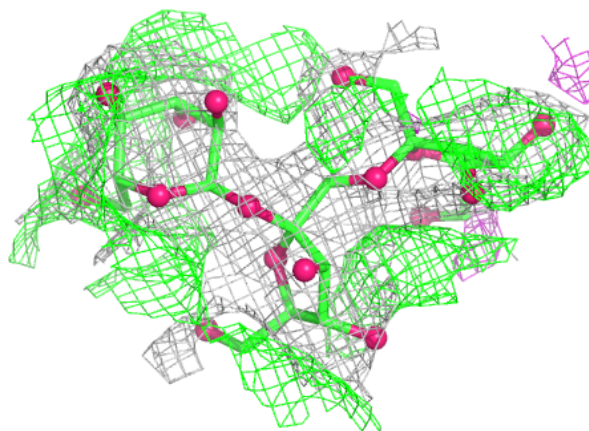
**Electron density around Chain L:**

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



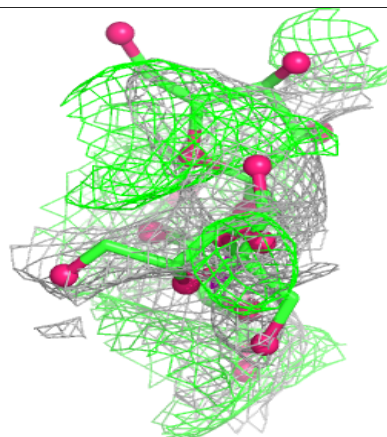
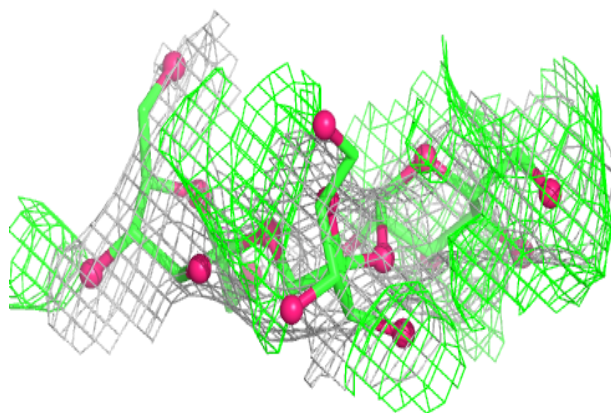
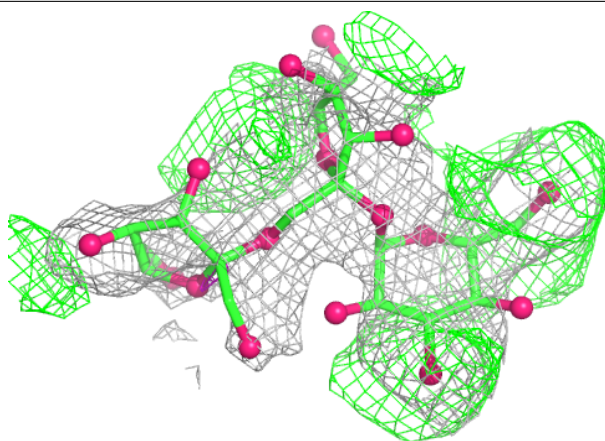
**Electron density around Chain M:**

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



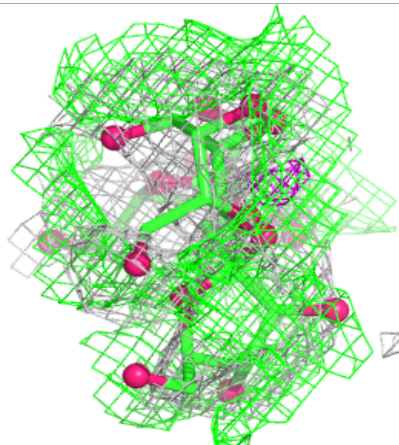
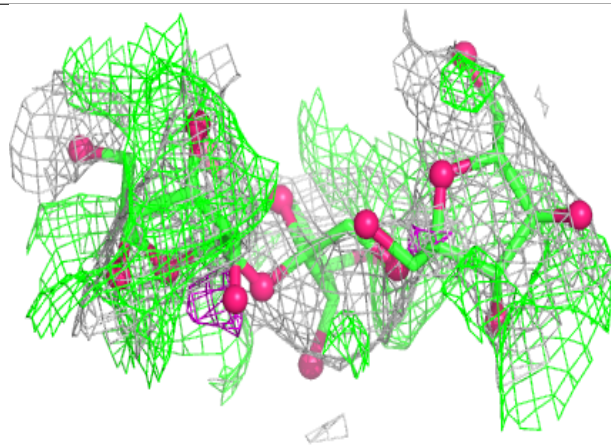
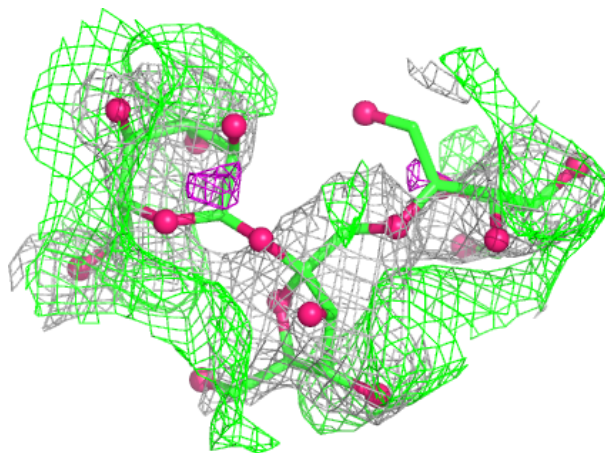
**Electron density around Chain N:**

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



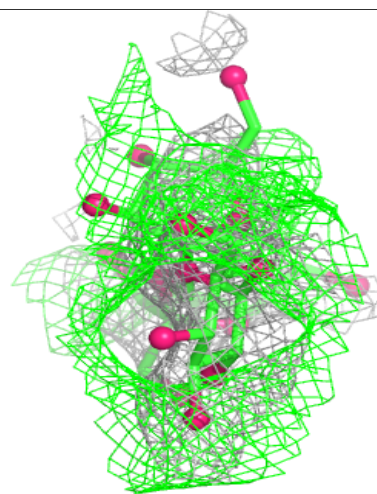
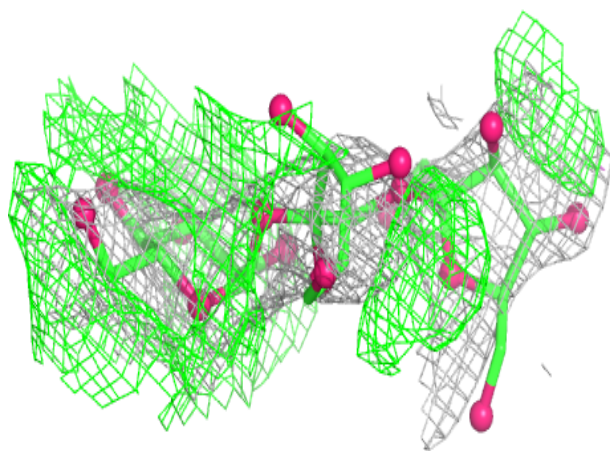
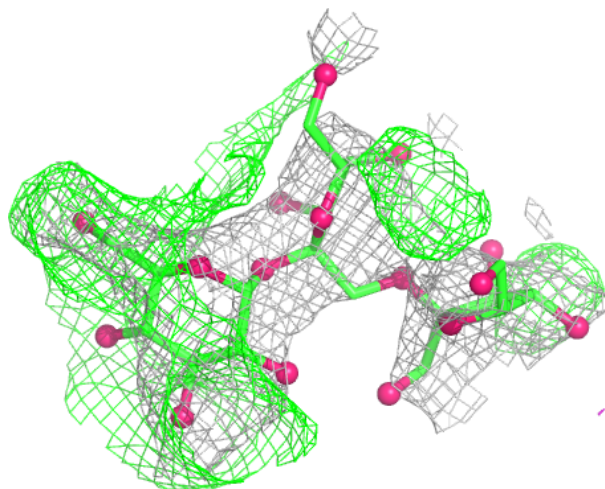
**Electron density around Chain O:**

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



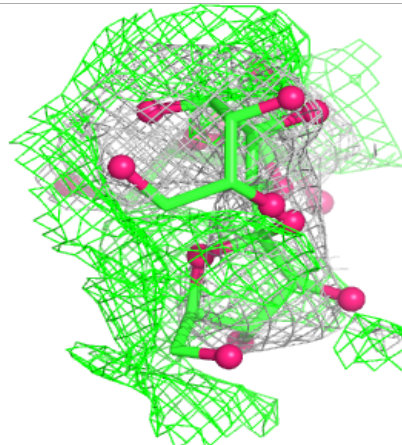
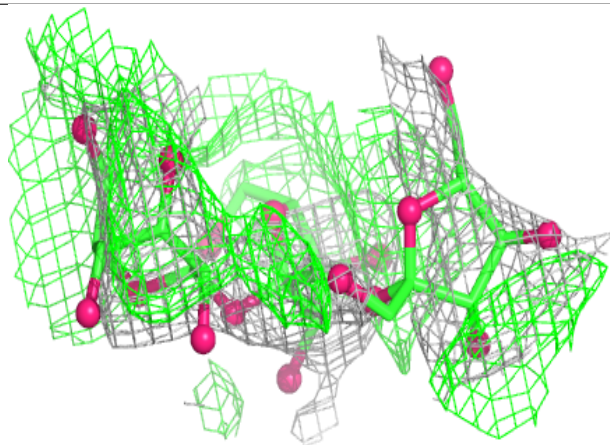
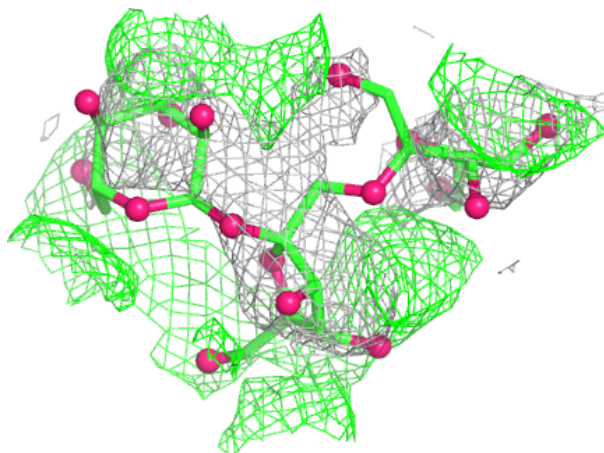
**Electron density around Chain P:**

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



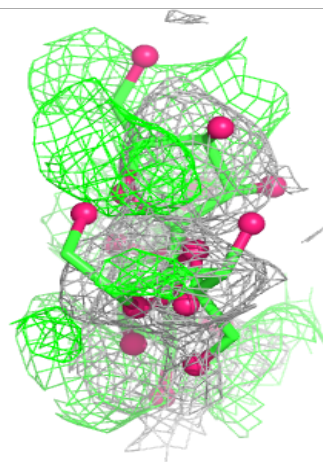
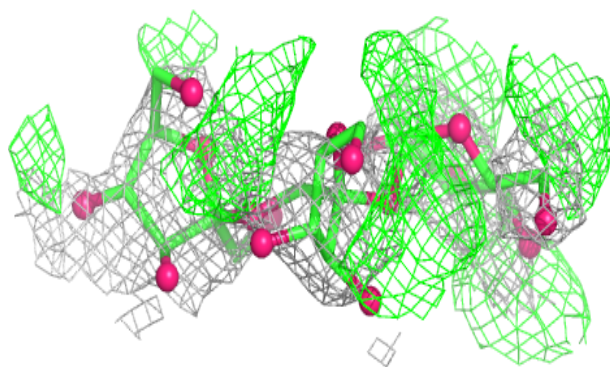
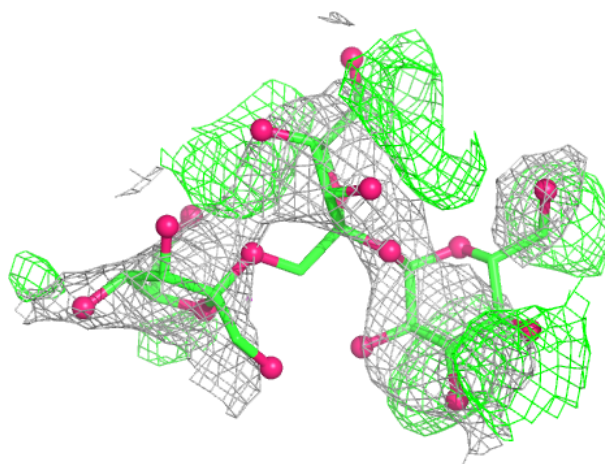
**Electron density around Chain Q:**

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



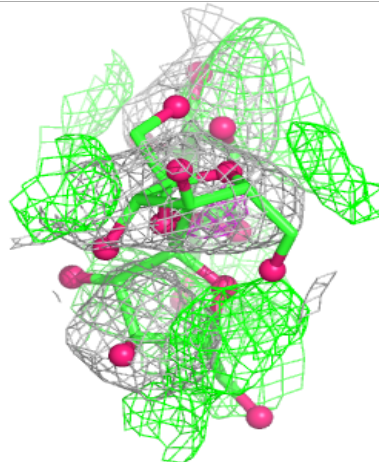
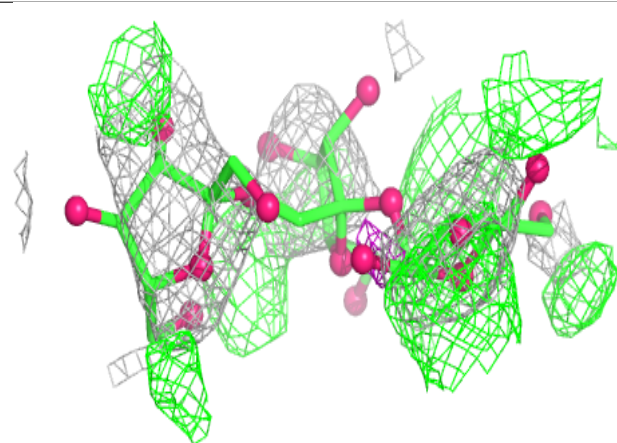
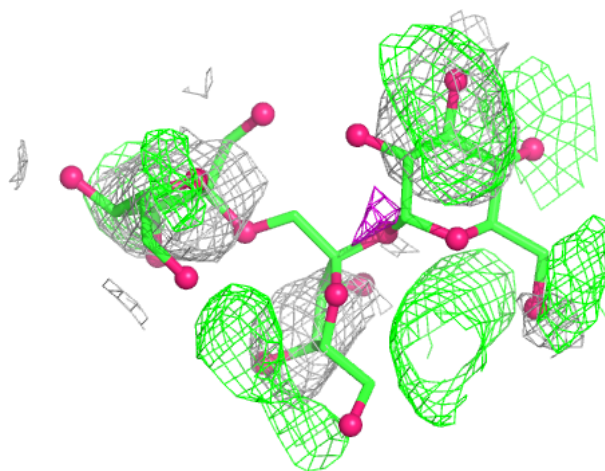
**Electron density around Chain R:**

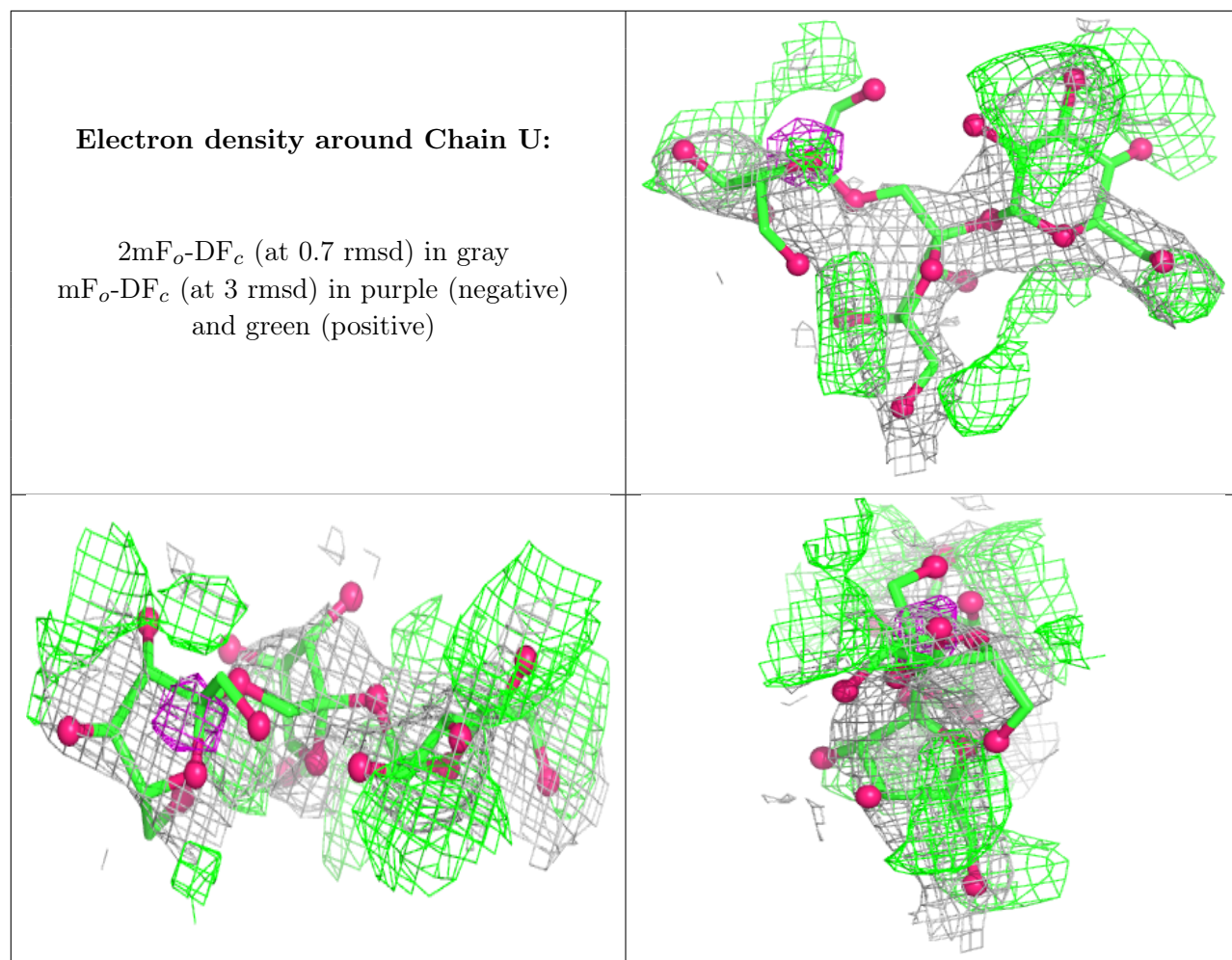
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain T:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.