



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:49 AM UTC

PDB ID : 4HLZ / pdb\_00004hlz  
Title : Crystal Structure of Fab C179 in Complex with a H2N2 influenza virus hemagglutinin  
Authors : Dreyfus, C.; Wilson, I.A.  
Deposited on : 2012-10-17  
Resolution : 2.90 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:

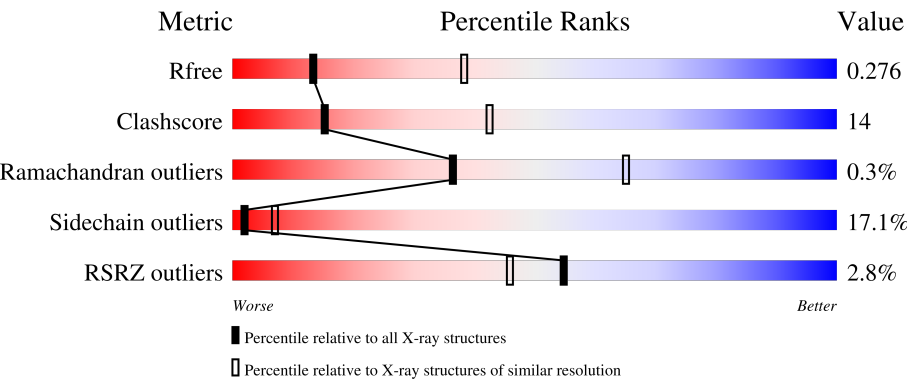
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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 <sub>free</sub>     | 180053                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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     | 327    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>63%31%5% .</div></div> |
| 1   | C     | 327    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>67%28% . .</div></div> |
| 1   | E     | 327    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>63%31%5% .</div></div> |
| 2   | B     | 174    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>70%25% . .</div></div> |
| 2   | D     | 174    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>61%31%5% .</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | F     | 174    |                  |
| 3   | G     | 229    |                  |
| 3   | I     | 229    |                  |
| 3   | K     | 229    |                  |
| 4   | H     | 214    |                  |
| 4   | J     | 214    |                  |
| 4   | L     | 214    |                  |
| 5   | M     | 3      |                  |
| 5   | P     | 3      |                  |
| 6   | N     | 4      |                  |
| 7   | O     | 2      |                  |
| 7   | Q     | 2      |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 9   | SO4  | F     | 201 | -         | -        | X       | -                |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 324      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2546  | 1600 | 441 | 490 | 15 |         |         |       |
| 1   | C     | 324      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2546  | 1600 | 441 | 490 | 15 |         |         |       |
| 1   | E     | 324      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2551  | 1605 | 441 | 490 | 15 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 9       | PRO      | -      | expression tag | UNP C7S226 |
| C     | 9       | PRO      | -      | expression tag | UNP C7S226 |
| E     | 9       | PRO      | -      | expression tag | UNP C7S226 |

- Molecule 2 is a protein called Hemagglutinin HA2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 168      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1370  | 854 | 235 | 272 | 9 |         |         |       |
| 2   | D     | 170      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1384  | 862 | 237 | 276 | 9 |         |         |       |
| 2   | F     | 172      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1404  | 876 | 240 | 279 | 9 |         |         |       |

- Molecule 3 is a protein called Fab C179 heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | G     | 223      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1696  | 1071 | 283 | 334 | 8 |         |         |       |
| 3   | I     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1675  | 1059 | 278 | 330 | 8 |         |         |       |

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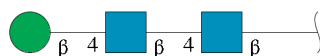
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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | K     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1532  | 970 | 253 | 302 | 7 |         |         |       |

- Molecule 4 is a protein called Fab C179 light chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | H     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1021 | 270 | 330 | 6 |         |         |       |
| 4   | J     | 212      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1025 | 272 | 332 | 6 |         |         |       |
| 4   | L     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1580  | 994  | 261 | 319 | 6 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5   | M     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |
| 5   | P     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6   | N     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 7   | O     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | Q     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 9   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 9   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 9   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 9   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 9   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 9   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 9   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

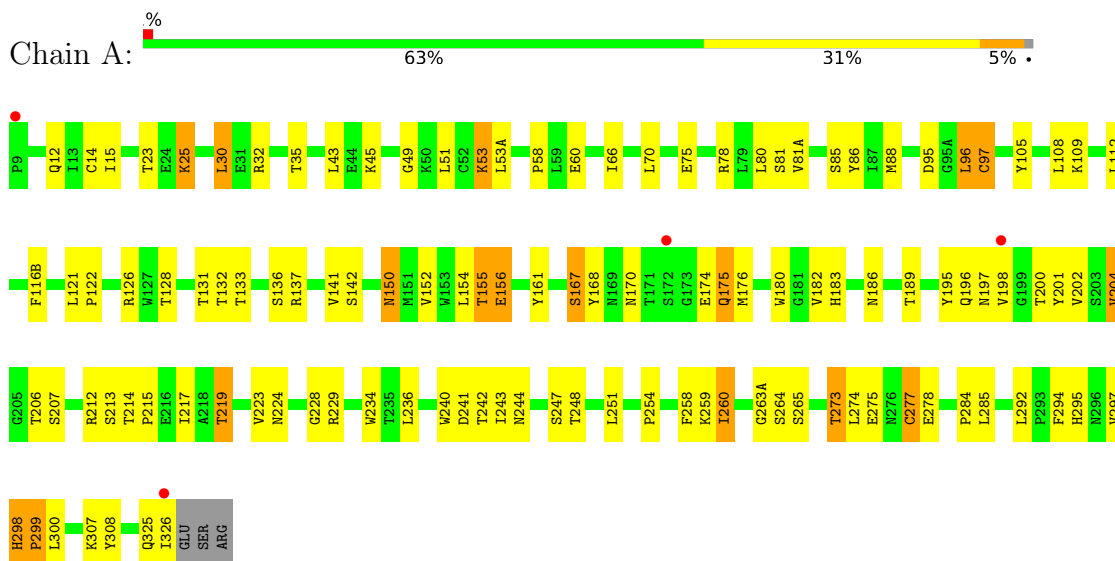


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10  | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

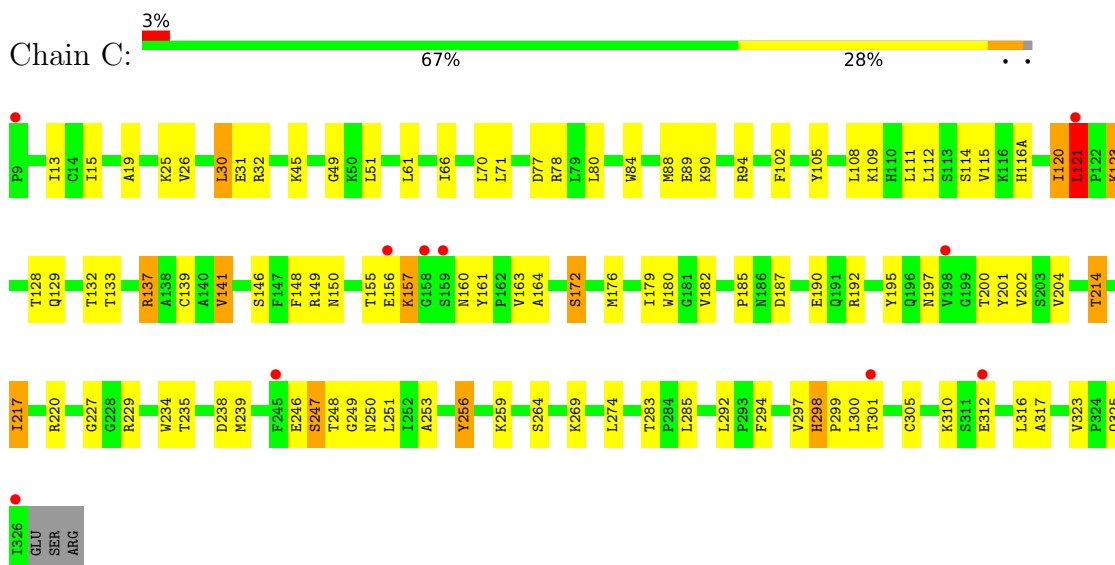
### 3 Residue-property plots

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

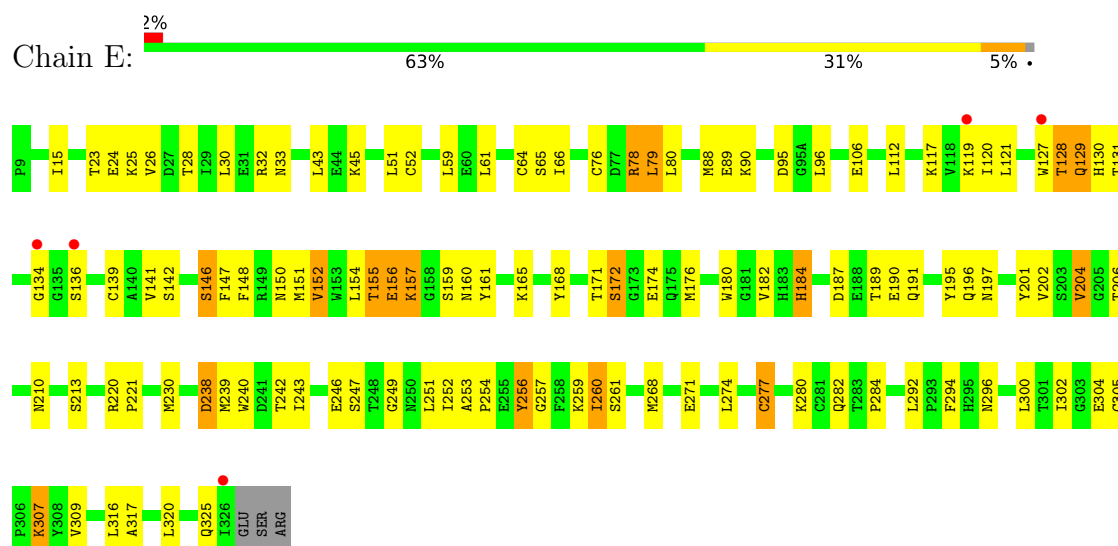
#### • Molecule 1: Hemagglutinin HA1



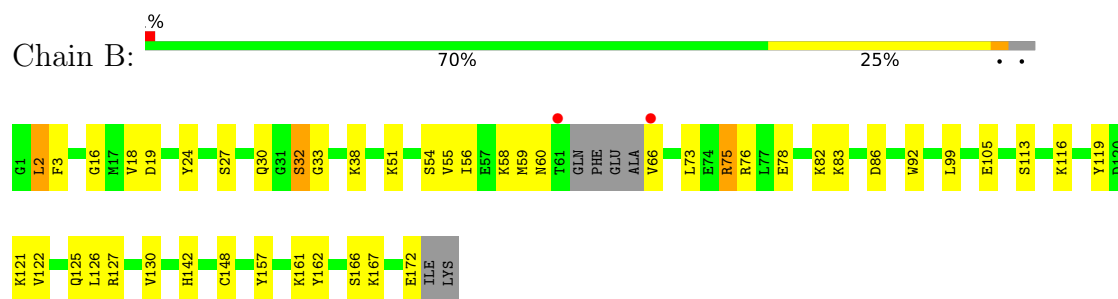
#### • Molecule 1: Hemagglutinin HA1



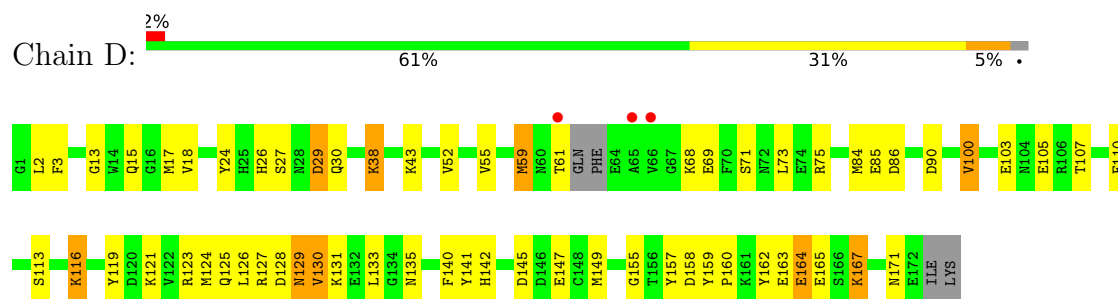
#### • Molecule 1: Hemagglutinin HA1



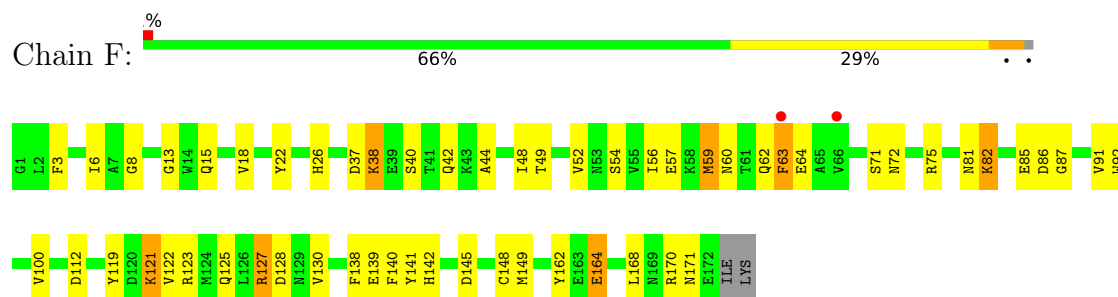
• Molecule 2: Hemagglutinin HA2



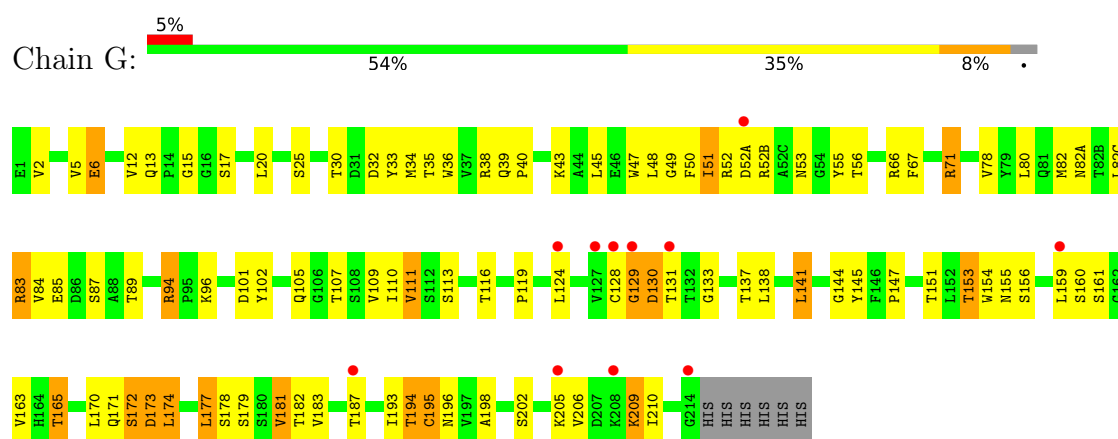
• Molecule 2: Hemagglutinin HA2



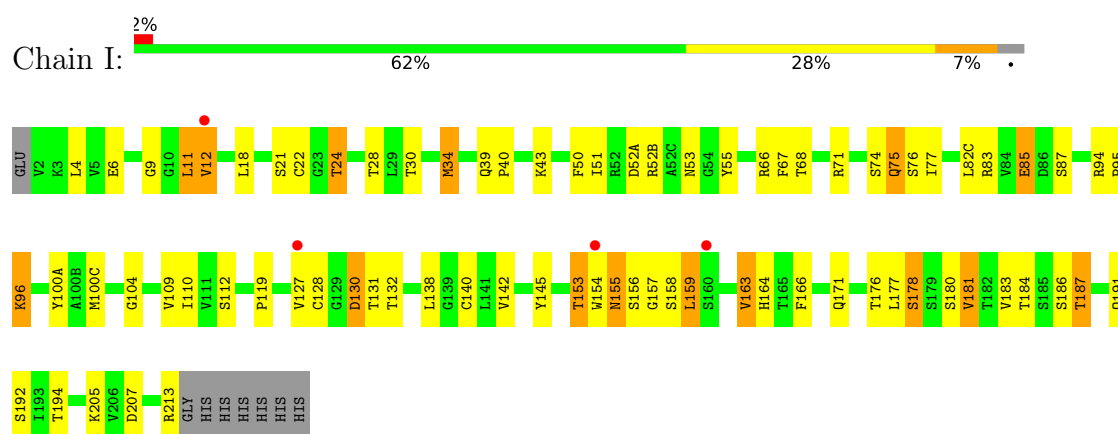
• Molecule 2: Hemagglutinin HA2



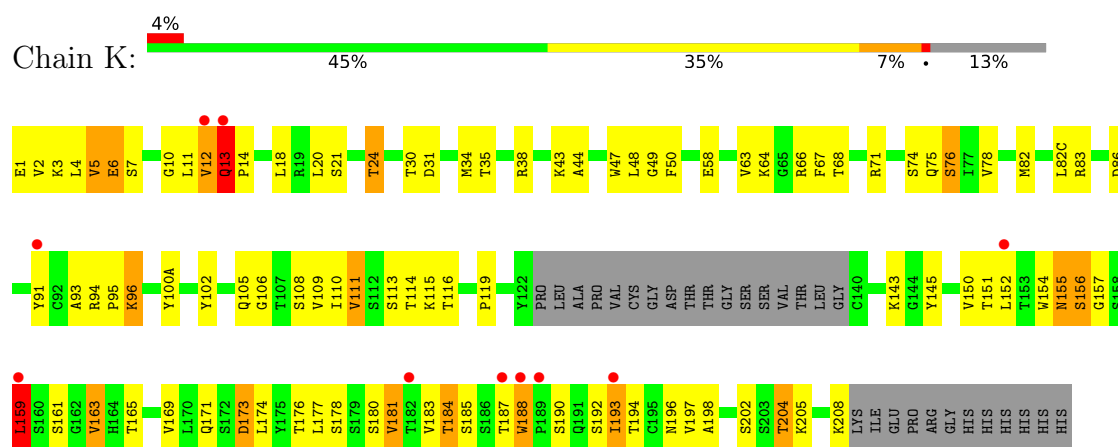
• Molecule 3: Fab C179 heavy chain



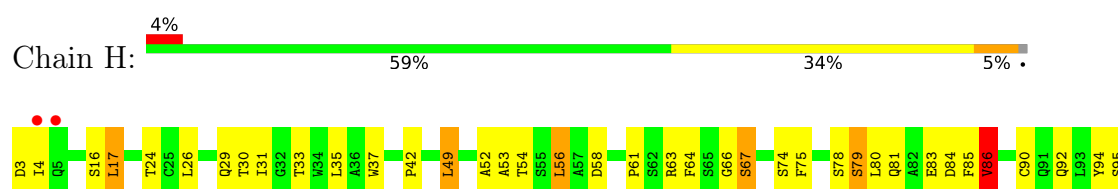
• Molecule 3: Fab C179 heavy chain

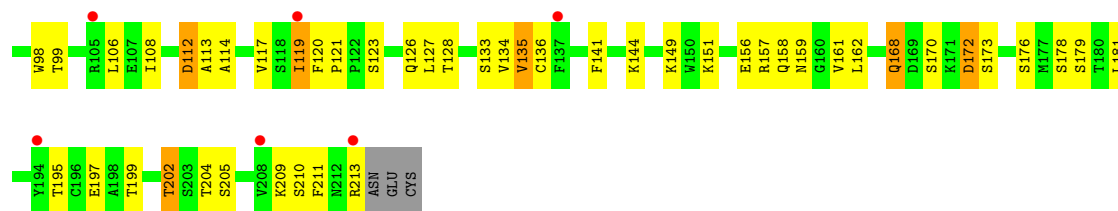


• Molecule 3: Fab C179 heavy chain

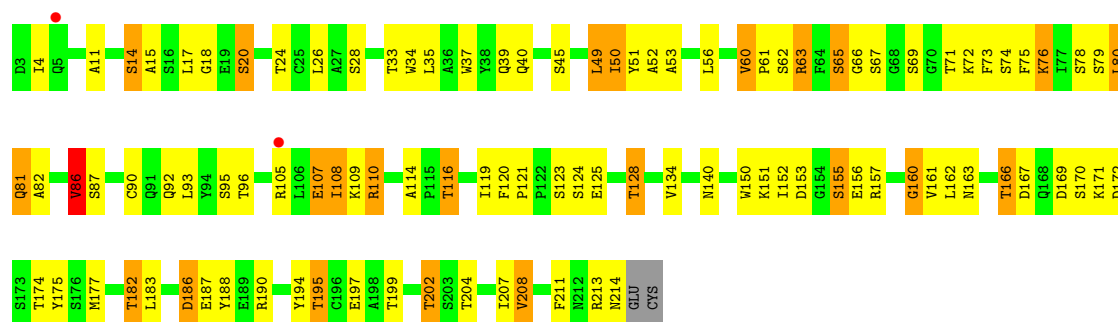


• Molecule 4: Fab C179 light chain

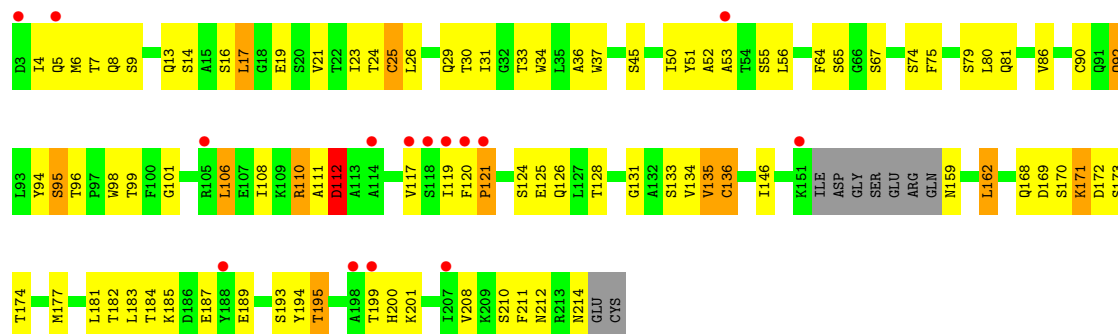




• Molecule 4: Fab C179 light chain



• Molecule 4: Fab C179 light chain



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



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



- Molecule 6:  $\alpha$ -D-mannopyranose-(1-3)- $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain N:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain O:  100%

MAG1  
MAG2

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

Chain Q:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 136.58Å 150.78Å 217.78Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 39.55 – 2.90<br>39.55 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (39.55-2.90)<br>98.6 (39.55-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.19 (at 2.90Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.7.2_869)                           | Depositor        |
| R, $R_{free}$                                                           | 0.228 , 0.284<br>0.226 , 0.276                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5001 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 86.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.063                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 80.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 21839                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 101.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, EDO, SO4, NAG

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.57         | 2/2612 (0.1%)  | 1.02        | 7/3545 (0.2%)   |
| 1   | C     | 0.60         | 1/2612 (0.0%)  | 0.97        | 11/3545 (0.3%)  |
| 1   | E     | 0.57         | 0/2620         | 1.03        | 7/3556 (0.2%)   |
| 2   | B     | 0.69         | 0/1399         | 1.01        | 6/1876 (0.3%)   |
| 2   | D     | 0.66         | 0/1413         | 1.01        | 5/1895 (0.3%)   |
| 2   | F     | 0.65         | 0/1435         | 1.01        | 6/1926 (0.3%)   |
| 3   | G     | 0.59         | 0/1742         | 0.98        | 2/2378 (0.1%)   |
| 3   | I     | 0.59         | 0/1718         | 1.01        | 3/2347 (0.1%)   |
| 3   | K     | 0.60         | 1/1571 (0.1%)  | 1.00        | 5/2143 (0.2%)   |
| 4   | H     | 0.55         | 0/1666         | 0.96        | 4/2264 (0.2%)   |
| 4   | J     | 0.51         | 0/1674         | 0.99        | 7/2275 (0.3%)   |
| 4   | L     | 0.54         | 0/1618         | 0.98        | 7/2199 (0.3%)   |
| All | All   | 0.59         | 4/22080 (0.0%) | 1.00        | 70/29949 (0.2%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | C     | 298 | HIS  | C-N   | 8.96 | 1.41        | 1.33     |
| 3   | K     | 13  | GLN  | C-N   | 6.39 | 1.41        | 1.33     |
| 1   | A     | 298 | HIS  | C-N   | 5.77 | 1.41        | 1.34     |
| 1   | A     | 299 | PRO  | N-CD  | 5.42 | 1.55        | 1.47     |

All (70) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | I     | 9   | GLY  | N-CA-C | -10.40 | 88.53       | 113.18   |
| 1   | A     | 297 | VAL  | N-CA-C | 7.28   | 117.41      | 110.42   |
| 4   | L     | 121 | PRO  | CA-C-N | 7.16   | 126.92      | 119.76   |
| 4   | L     | 121 | PRO  | C-N-CA | 7.16   | 126.92      | 119.76   |
| 1   | E     | 292 | LEU  | CA-C-N | 7.05   | 127.20      | 119.87   |

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| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1   | E     | 292    | LEU  | C-N-CA | 7.05  | 127.20      | 119.87   |
| 2   | B     | 16     | GLY  | CA-C-N | -7.02 | 113.72      | 122.84   |
| 2   | B     | 16     | GLY  | C-N-CA | -7.02 | 113.72      | 122.84   |
| 2   | B     | 33     | GLY  | N-CA-C | 6.74  | 120.47      | 110.42   |
| 1   | E     | 129    | GLN  | N-CA-C | 6.74  | 118.29      | 111.07   |
| 1   | A     | 263(A) | GLY  | N-CA-C | 6.64  | 119.93      | 111.09   |
| 2   | D     | 2      | LEU  | N-CA-C | 6.63  | 118.50      | 111.28   |
| 4   | J     | 160    | GLY  | N-CA-C | -6.56 | 106.68      | 115.21   |
| 4   | H     | 135    | VAL  | N-CA-C | 6.48  | 117.21      | 107.75   |
| 2   | D     | 15     | GLN  | N-CA-C | -6.44 | 104.31      | 111.71   |
| 2   | B     | 2      | LEU  | N-CA-C | 6.42  | 118.81      | 111.11   |
| 1   | A     | 292    | LEU  | CA-C-N | 6.42  | 126.17      | 119.05   |
| 1   | A     | 292    | LEU  | C-N-CA | 6.42  | 126.17      | 119.05   |
| 1   | C     | 298    | HIS  | CA-C-N | -6.37 | 113.33      | 121.04   |
| 1   | C     | 298    | HIS  | C-N-CA | -6.37 | 113.33      | 121.04   |
| 1   | E     | 172    | SER  | N-CA-C | 6.33  | 120.10      | 112.38   |
| 4   | J     | 110    | ARG  | N-CA-C | 6.31  | 116.60      | 108.34   |
| 4   | J     | 45     | SER  | CA-C-N | -6.29 | 114.25      | 120.98   |
| 4   | J     | 45     | SER  | C-N-CA | -6.29 | 114.25      | 120.98   |
| 2   | B     | 75     | ARG  | N-CA-C | 6.27  | 117.78      | 111.07   |
| 3   | K     | 13     | GLN  | CA-C-N | -6.21 | 114.37      | 120.52   |
| 3   | K     | 13     | GLN  | C-N-CA | -6.21 | 114.37      | 120.52   |
| 4   | L     | 5      | GLN  | N-CA-C | 6.20  | 119.05      | 109.07   |
| 4   | L     | 112    | ASP  | N-CA-C | 6.09  | 118.15      | 110.24   |
| 2   | F     | 49     | THR  | N-CA-C | -6.08 | 104.57      | 111.14   |
| 2   | B     | 56     | ILE  | N-CA-C | 6.01  | 116.19      | 110.42   |
| 3   | G     | 133    | GLY  | N-CA-C | 5.93  | 122.40      | 112.85   |
| 1   | C     | 172    | SER  | N-CA-C | 5.90  | 118.50      | 111.71   |
| 2   | F     | 56     | ILE  | N-CA-C | 5.81  | 116.27      | 110.23   |
| 2   | D     | 171    | ASN  | N-CA-C | 5.79  | 117.26      | 111.07   |
| 4   | J     | 82     | ALA  | CA-C-N | 5.74  | 127.97      | 120.28   |
| 4   | J     | 82     | ALA  | C-N-CA | 5.74  | 127.97      | 120.28   |
| 2   | F     | 171    | ASN  | N-CA-C | 5.71  | 117.59      | 111.36   |
| 1   | C     | 297    | VAL  | N-CA-C | 5.60  | 115.79      | 110.42   |
| 2   | D     | 100    | VAL  | N-CA-C | 5.57  | 115.76      | 110.42   |
| 3   | I     | 30     | THR  | N-CA-C | 5.53  | 117.67      | 108.99   |
| 4   | H     | 94     | TYR  | N-CA-C | 5.48  | 116.94      | 111.07   |
| 1   | C     | 292    | LEU  | CA-C-N | 5.47  | 125.09      | 119.56   |
| 1   | C     | 292    | LEU  | C-N-CA | 5.47  | 125.09      | 119.56   |
| 2   | F     | 63     | PHE  | N-CA-C | 5.42  | 117.54      | 109.25   |
| 2   | D     | 75     | ARG  | N-CA-C | 5.40  | 117.86      | 111.33   |
| 4   | L     | 135    | VAL  | N-CA-C | 5.40  | 115.86      | 107.28   |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 4   | L     | 101    | GLY  | N-CA-C  | -5.38 | 105.19      | 112.14   |
| 1   | C     | 298    | HIS  | N-CA-C  | 5.34  | 113.03      | 108.22   |
| 3   | G     | 15     | GLY  | N-CA-C  | -5.34 | 108.73      | 115.08   |
| 3   | I     | 96     | LYS  | N-CA-C  | -5.31 | 105.41      | 111.14   |
| 4   | L     | 193    | SER  | N-CA-C  | 5.31  | 117.06      | 108.41   |
| 1   | A     | 136    | SER  | N-CA-C  | 5.25  | 116.97      | 109.14   |
| 2   | F     | 127[A] | ARG  | CB-CA-C | -5.25 | 110.50      | 116.54   |
| 2   | F     | 127[B] | ARG  | CB-CA-C | -5.25 | 110.50      | 116.54   |
| 3   | K     | 11     | LEU  | CB-CA-C | -5.25 | 110.54      | 116.63   |
| 4   | J     | 116    | THR  | N-CA-C  | -5.23 | 102.54      | 110.28   |
| 1   | C     | 121    | LEU  | CA-C-N  | 5.21  | 125.12      | 119.76   |
| 1   | C     | 121    | LEU  | C-N-CA  | 5.21  | 125.12      | 119.76   |
| 1   | A     | 298    | HIS  | CA-C-N  | -5.20 | 113.18      | 118.85   |
| 1   | A     | 298    | HIS  | C-N-CA  | -5.20 | 113.18      | 118.85   |
| 1   | E     | 184    | HIS  | CA-C-N  | 5.18  | 125.08      | 119.85   |
| 1   | E     | 184    | HIS  | C-N-CA  | 5.18  | 125.08      | 119.85   |
| 1   | E     | 134    | GLY  | N-CA-C  | 5.11  | 117.34      | 111.36   |
| 1   | C     | 214    | THR  | CA-C-N  | 5.10  | 125.39      | 119.93   |
| 1   | C     | 214    | THR  | C-N-CA  | 5.10  | 125.39      | 119.93   |
| 3   | K     | 155    | ASN  | N-CA-C  | 5.02  | 116.78      | 110.91   |
| 4   | H     | 114    | ALA  | CA-C-N  | 5.01  | 126.10      | 119.84   |
| 4   | H     | 114    | ALA  | C-N-CA  | 5.01  | 126.10      | 119.84   |
| 3   | K     | 159    | LEU  | N-CA-C  | 5.00  | 116.85      | 107.99   |

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     | 2546  | 0        | 2499     | 64      | 0            |
| 1   | C     | 2546  | 0        | 2500     | 61      | 0            |
| 1   | E     | 2551  | 0        | 2510     | 72      | 0            |
| 2   | B     | 1370  | 0        | 1282     | 23      | 0            |
| 2   | D     | 1384  | 0        | 1294     | 38      | 0            |
| 2   | F     | 1404  | 0        | 1311     | 46      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | G     | 1696  | 0        | 1661     | 55      | 0            |
| 3   | I     | 1675  | 0        | 1636     | 58      | 0            |
| 3   | K     | 1532  | 0        | 1486     | 65      | 0            |
| 4   | H     | 1627  | 0        | 1561     | 41      | 0            |
| 4   | J     | 1635  | 0        | 1567     | 62      | 0            |
| 4   | L     | 1580  | 0        | 1516     | 48      | 0            |
| 5   | M     | 39    | 0        | 34       | 0       | 0            |
| 5   | P     | 39    | 0        | 34       | 0       | 0            |
| 6   | N     | 50    | 0        | 43       | 0       | 0            |
| 7   | O     | 28    | 0        | 25       | 0       | 0            |
| 7   | Q     | 28    | 0        | 25       | 0       | 0            |
| 8   | A     | 28    | 0        | 26       | 0       | 0            |
| 8   | B     | 14    | 0        | 13       | 0       | 0            |
| 8   | E     | 14    | 0        | 13       | 0       | 0            |
| 8   | F     | 14    | 0        | 13       | 0       | 0            |
| 9   | B     | 5     | 0        | 0        | 0       | 0            |
| 9   | D     | 5     | 0        | 0        | 1       | 0            |
| 9   | E     | 5     | 0        | 0        | 0       | 0            |
| 9   | F     | 5     | 0        | 0        | 3       | 0            |
| 9   | H     | 5     | 0        | 0        | 0       | 0            |
| 9   | J     | 5     | 0        | 0        | 1       | 0            |
| 9   | L     | 5     | 0        | 0        | 1       | 0            |
| 10  | J     | 4     | 0        | 6        | 1       | 0            |
| All | All   | 21839 | 0        | 21055    | 582     | 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 14.

All (582) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:154:TRP:CZ3  | 3:I:163:VAL:HG21 | 1.64                     | 1.32              |
| 3:I:154:TRP:HZ3  | 3:I:163:VAL:CG2  | 1.49                     | 1.26              |
| 4:H:121:PRO:HG3  | 4:H:211:PHE:CE1  | 1.71                     | 1.24              |
| 3:I:154:TRP:CZ3  | 3:I:163:VAL:CG2  | 2.20                     | 1.23              |
| 4:H:121:PRO:HG3  | 4:H:211:PHE:CZ   | 1.88                     | 1.09              |
| 3:K:184:THR:HG22 | 3:K:185:SER:H    | 1.22                     | 1.04              |
| 1:C:298:HIS:HE1  | 1:C:300:LEU:HD12 | 1.21                     | 0.99              |
| 1:C:298:HIS:CE1  | 1:C:300:LEU:HD12 | 1.98                     | 0.99              |
| 3:G:34:MET:HG2   | 3:G:78:VAL:HG21  | 1.45                     | 0.95              |
| 3:I:159:LEU:HD12 | 3:I:159:LEU:H    | 1.36                     | 0.91              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:I:154:TRP:HZ3   | 3:I:163:VAL:HG21    | 0.74                     | 0.91              |
| 3:K:12:VAL:HG21   | 3:K:18:LEU:HD13     | 1.51                     | 0.90              |
| 3:K:6:GLU:H       | 3:K:105:GLN:HE22    | 1.20                     | 0.89              |
| 3:K:35:THR:HG22   | 3:K:50:PHE:HB3      | 1.54                     | 0.89              |
| 3:K:154:TRP:HB2   | 3:K:159:LEU:HD11    | 1.54                     | 0.89              |
| 4:H:121:PRO:CG    | 4:H:211:PHE:CE1     | 2.56                     | 0.89              |
| 3:I:130:ASP:O     | 3:I:131:THR:HG23    | 1.75                     | 0.86              |
| 3:G:163:VAL:HG22  | 3:G:181:VAL:HG23    | 1.56                     | 0.85              |
| 4:L:110:ARG:HG2   | 4:L:173:SER:HB2     | 1.59                     | 0.84              |
| 4:H:54:THR:HG22   | 4:H:66:GLY:O        | 1.77                     | 0.83              |
| 3:K:96:LYS:HB2    | 3:K:102:TYR:CE2     | 2.13                     | 0.83              |
| 3:I:163:VAL:HG23  | 3:I:181:VAL:HG13    | 1.62                     | 0.81              |
| 3:G:144:GLY:HA2   | 3:G:174:LEU:HD13    | 1.62                     | 0.81              |
| 3:G:155:ASN:O     | 3:G:156:SER:OG      | 1.98                     | 0.81              |
| 1:E:52:CYS:SG     | 1:E:277:CYS:CB      | 2.69                     | 0.80              |
| 3:I:130:ASP:O     | 3:I:131:THR:CG2     | 2.29                     | 0.80              |
| 1:C:316:LEU:HD23  | 2:D:100:VAL:HG13    | 1.64                     | 0.80              |
| 1:E:52:CYS:SG     | 1:E:277:CYS:HB2     | 2.22                     | 0.79              |
| 4:J:20:SER:HB3    | 4:J:76:LYS:HZ1      | 1.47                     | 0.79              |
| 2:F:38:LYS:HZ1    | 4:L:33:THR:HG23     | 1.49                     | 0.78              |
| 4:L:50:ILE:HG21   | 4:L:53:ALA:O        | 1.82                     | 0.78              |
| 3:K:94:ARG:HH21   | 3:K:96:LYS:HA       | 1.46                     | 0.78              |
| 4:L:195:THR:HG23  | 4:L:210:SER:HB2     | 1.65                     | 0.77              |
| 3:I:154:TRP:CZ3   | 3:I:163:VAL:HG22    | 2.18                     | 0.76              |
| 3:G:82(C):LEU:HB3 | 3:G:111:VAL:HG21    | 1.67                     | 0.75              |
| 3:G:165:THR:HG23  | 3:G:179:SER:HB2     | 1.69                     | 0.75              |
| 2:F:6:ILE:HD12    | 2:F:112:ASP:HA      | 1.68                     | 0.75              |
| 4:H:195:THR:HG23  | 4:H:210:SER:HB2     | 1.70                     | 0.74              |
| 3:G:83:ARG:O      | 3:G:111:VAL:HG11    | 1.87                     | 0.74              |
| 3:G:52(A):ASP:OD1 | 3:G:53:ASN:HB2      | 1.88                     | 0.74              |
| 3:I:159:LEU:HD12  | 3:I:159:LEU:N       | 2.02                     | 0.74              |
| 3:K:184:THR:HG22  | 3:K:185:SER:N       | 2.03                     | 0.72              |
| 3:I:191:GLN:NE2   | 3:I:192:SER:O       | 2.21                     | 0.72              |
| 1:C:141:VAL:HG12  | 1:C:146:SER:HB2     | 1.72                     | 0.72              |
| 2:D:30:GLN:OE1    | 2:D:30:GLN:N        | 2.21                     | 0.71              |
| 2:D:131:LYS:HD2   | 2:F:127[B]:ARG:HH22 | 1.54                     | 0.71              |
| 4:J:92:GLN:HE21   | 4:J:95:SER:H        | 1.36                     | 0.71              |
| 3:I:213:ARG:HH12  | 4:J:124:SER:H       | 1.37                     | 0.71              |
| 3:K:171:GLN:HB2   | 4:L:162:LEU:HD21    | 1.72                     | 0.71              |
| 1:A:70:LEU:O      | 1:A:150:ASN:ND2     | 2.24                     | 0.71              |
| 4:H:54:THR:HG22   | 4:H:67:SER:HA       | 1.74                     | 0.70              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 4:J:14:SER:HB2     | 4:J:109:LYS:HG3  | 1.72                     | 0.70              |
| 2:D:130:VAL:HG12   | 2:D:140:PHE:HA   | 1.73                     | 0.70              |
| 1:A:97:CYS:O       | 1:A:224:ASN:ND2  | 2.25                     | 0.70              |
| 4:H:172:ASP:OD1    | 4:H:172:ASP:N    | 2.24                     | 0.70              |
| 2:B:75:ARG:NH1     | 2:B:78:GLU:OE1   | 2.25                     | 0.70              |
| 1:C:150:ASN:HA     | 1:C:256:TYR:HE2  | 1.56                     | 0.70              |
| 1:A:116(B):PHE:HE1 | 1:A:260:ILE:HG22 | 1.57                     | 0.69              |
| 1:C:70:LEU:O       | 1:C:150:ASN:ND2  | 2.22                     | 0.69              |
| 1:C:301:THR:OG1    | 1:C:305:CYS:SG   | 2.51                     | 0.69              |
| 3:I:154:TRP:CH2    | 3:I:163:VAL:HG22 | 2.28                     | 0.69              |
| 3:K:1:GLU:HG2      | 3:K:2:VAL:N      | 2.06                     | 0.69              |
| 3:K:34:MET:HG2     | 3:K:78:VAL:HG21  | 1.75                     | 0.68              |
| 3:K:152:LEU:HG     | 3:K:197:VAL:HG22 | 1.73                     | 0.68              |
| 3:K:12:VAL:O       | 3:K:13:GLN:HG2   | 1.94                     | 0.67              |
| 4:H:54:THR:CG2     | 4:H:67:SER:HA    | 2.25                     | 0.67              |
| 4:L:119:ILE:HD12   | 4:L:211:PHE:HB3  | 1.76                     | 0.67              |
| 1:A:294:PHE:CZ     | 2:B:59:MET:HG2   | 2.30                     | 0.67              |
| 2:F:38:LYS:HZ1     | 4:L:33:THR:CG2   | 2.07                     | 0.67              |
| 4:H:35:LEU:HD11    | 4:H:90:CYS:HB2   | 1.77                     | 0.67              |
| 1:C:120:ILE:HD11   | 1:C:176:MET:SD   | 2.36                     | 0.66              |
| 1:E:172:SER:HB2    | 1:E:259:LYS:HD2  | 1.77                     | 0.66              |
| 3:I:12:VAL:HG21    | 3:I:18:LEU:HD22  | 1.77                     | 0.66              |
| 3:K:4:LEU:CD2      | 3:K:24:THR:HB    | 2.25                     | 0.66              |
| 4:J:188:TYR:O      | 4:J:213:ARG:NH2  | 2.28                     | 0.66              |
| 3:K:161:SER:OG     | 4:L:171:LYS:NZ   | 2.29                     | 0.66              |
| 4:L:194:TYR:HB2    | 4:L:211:PHE:HE2  | 1.61                     | 0.66              |
| 4:L:112:ASP:OD1    | 4:L:112:ASP:N    | 2.29                     | 0.65              |
| 3:I:40:PRO:HG2     | 3:I:43:LYS:HB2   | 1.79                     | 0.65              |
| 3:K:38:ARG:HG2     | 3:K:48:LEU:HD21  | 1.79                     | 0.65              |
| 4:L:110:ARG:NH1    | 4:L:111:ALA:O    | 2.30                     | 0.65              |
| 3:K:163:VAL:HG13   | 3:K:181:VAL:HG23 | 1.80                     | 0.64              |
| 1:A:307[A]:LYS:HE2 | 2:B:92:TRP:CG    | 2.33                     | 0.64              |
| 1:E:191:GLN:NE2    | 1:E:197:ASN:O    | 2.31                     | 0.64              |
| 2:D:164:GLU:HA     | 2:D:167:LYS:HG2  | 1.80                     | 0.64              |
| 1:A:206:THR:HG22   | 1:A:243:ILE:HG13 | 1.78                     | 0.64              |
| 1:E:230:MET:HE3    | 1:E:252:ILE:HG13 | 1.78                     | 0.63              |
| 1:C:180:TRP:CE2    | 1:C:204:VAL:HG21 | 2.34                     | 0.63              |
| 4:L:92:GLN:HG2     | 4:L:94:TYR:H     | 1.63                     | 0.63              |
| 1:A:299:PRO:HG2    | 1:A:300:LEU:HG   | 1.81                     | 0.63              |
| 3:K:13:GLN:O       | 3:K:111:VAL:HG23 | 1.99                     | 0.63              |
| 3:K:91:TYR:CE1     | 3:K:106:GLY:HA3  | 2.34                     | 0.63              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:25:LYS:NZ    | 1:A:35:THR:OG1     | 2.30                     | 0.62              |
| 4:H:157:ARG:NH1  | 4:H:159:ASN:O      | 2.31                     | 0.62              |
| 1:C:150:ASN:HA   | 1:C:256:TYR:CE2    | 2.34                     | 0.62              |
| 3:K:12:VAL:O     | 3:K:12:VAL:HG12    | 1.98                     | 0.62              |
| 3:I:213:ARG:NH1  | 4:J:124:SER:H      | 1.97                     | 0.62              |
| 4:J:187:GLU:HB3  | 4:J:190:ARG:HH21   | 1.64                     | 0.62              |
| 4:L:125:GLU:HA   | 4:L:128:THR:HG22   | 1.82                     | 0.62              |
| 3:G:128:CYS:C    | 3:G:130:ASP:H      | 2.08                     | 0.62              |
| 4:J:183:LEU:HB3  | 4:J:187:GLU:HG3    | 1.82                     | 0.62              |
| 4:H:80:LEU:HD13  | 4:H:85:PHE:CZ      | 2.35                     | 0.61              |
| 2:F:38:LYS:NZ    | 9:F:201:SO4:O2     | 2.34                     | 0.61              |
| 2:F:141:TYR:CE2  | 2:F:170:ARG:HD3    | 2.35                     | 0.61              |
| 1:E:325:GLN:HG2  | 2:F:13:GLY:O       | 2.01                     | 0.61              |
| 3:G:153:THR:HG23 | 3:G:196:ASN:HB2    | 1.83                     | 0.61              |
| 3:I:119:PRO:HB3  | 3:I:145:TYR:HB3    | 1.81                     | 0.61              |
| 4:L:185:LYS:O    | 4:L:189:GLU:N      | 2.33                     | 0.60              |
| 3:G:35:THR:HG22  | 3:G:50:PHE:HB3     | 1.83                     | 0.60              |
| 4:L:92:GLN:HE21  | 4:L:95:SER:H       | 1.49                     | 0.60              |
| 2:F:38:LYS:NZ    | 4:L:33:THR:HG23    | 2.16                     | 0.60              |
| 1:A:58:PRO:HD2   | 1:A:274:LEU:HD22   | 1.84                     | 0.60              |
| 1:A:105:TYR:CE2  | 1:A:109:LYS:HE3    | 2.37                     | 0.60              |
| 1:A:150:ASN:OD1  | 1:A:150:ASN:N      | 2.34                     | 0.60              |
| 1:E:316:LEU:HD13 | 2:F:52:VAL:HG12    | 1.84                     | 0.60              |
| 2:F:164:GLU:CD   | 2:F:164:GLU:H      | 2.10                     | 0.60              |
| 1:C:30:LEU:HB2   | 2:D:105:GLU:OE2    | 2.01                     | 0.60              |
| 4:J:152:ILE:HG22 | 4:J:153:ASP:HB2    | 1.83                     | 0.60              |
| 3:I:153:THR:HG22 | 3:I:154:TRP:H      | 1.66                     | 0.59              |
| 1:C:155:THR:HG22 | 1:C:156:GLU:N      | 2.17                     | 0.59              |
| 1:A:180:TRP:CE2  | 1:A:204:VAL:HG21   | 2.38                     | 0.59              |
| 1:E:238:ASP:OD2  | 1:E:238:ASP:N      | 2.36                     | 0.59              |
| 1:C:77:ASP:HA    | 1:C:80:LEU:HG      | 1.84                     | 0.59              |
| 1:E:294:PHE:HE1  | 1:E:307[A]:LYS:HZ3 | 1.49                     | 0.59              |
| 4:L:92:GLN:NE2   | 4:L:95:SER:O       | 2.35                     | 0.59              |
| 2:F:57:GLU:O     | 2:F:60:ASN:HB2     | 2.03                     | 0.59              |
| 3:K:91:TYR:CD1   | 3:K:106:GLY:CA     | 2.86                     | 0.59              |
| 3:I:130:ASP:C    | 3:I:131:THR:HG23   | 2.27                     | 0.58              |
| 4:J:37:TRP:CZ3   | 4:J:90:CYS:HB3     | 2.37                     | 0.58              |
| 1:A:196:GLN:O    | 1:A:196:GLN:HG3    | 2.02                     | 0.58              |
| 1:C:155:THR:HG22 | 1:C:156:GLU:H      | 1.67                     | 0.58              |
| 4:L:126:GLN:OE1  | 4:L:133:SER:N      | 2.22                     | 0.58              |
| 1:C:61:LEU:HD12  | 1:C:89:GLU:HG3     | 1.84                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:K:20:LEU:HD13  | 3:K:82:MET:HE2    | 1.84                     | 0.58              |
| 3:I:12:VAL:HG11  | 3:I:82(C):LEU:HG  | 1.85                     | 0.58              |
| 2:F:38:LYS:HG3   | 3:K:100(A):TYR:CZ | 2.39                     | 0.58              |
| 3:I:75:GLN:HB3   | 3:I:77:ILE:HG13   | 1.85                     | 0.58              |
| 3:K:10:GLY:O     | 3:K:12:VAL:HG23   | 2.04                     | 0.57              |
| 1:E:150:ASN:O    | 1:E:151:MET:HE2   | 2.03                     | 0.57              |
| 4:H:141:PHE:HE2  | 4:H:176:SER:HA    | 1.69                     | 0.57              |
| 3:I:155:ASN:N    | 3:I:194:THR:O     | 2.37                     | 0.57              |
| 1:C:180:TRP:HZ3  | 1:C:235:THR:HG22  | 1.68                     | 0.57              |
| 2:F:82:LYS:HD3   | 2:F:86:ASP:OD2    | 2.04                     | 0.57              |
| 3:K:76:SER:O     | 3:K:76:SER:OG     | 2.18                     | 0.57              |
| 2:F:38:LYS:NZ    | 9:F:201:SO4:O4    | 2.38                     | 0.57              |
| 1:A:277:CYS:SG   | 1:A:278:GLU:N     | 2.78                     | 0.57              |
| 3:G:172:SER:O    | 3:G:172:SER:OG    | 2.18                     | 0.57              |
| 1:E:239:MET:HE2  | 1:E:239:MET:HA    | 1.87                     | 0.57              |
| 1:E:159:SER:HA   | 1:E:196:GLN:NE2   | 2.19                     | 0.56              |
| 4:H:31:ILE:HG21  | 4:H:92:GLN:HG3    | 1.86                     | 0.56              |
| 1:C:108:LEU:HB2  | 1:C:234:TRP:CE2   | 2.39                     | 0.56              |
| 2:B:126:LEU:HD13 | 2:B:130:VAL:HG11  | 1.86                     | 0.56              |
| 2:F:130:VAL:HG12 | 2:F:140:PHE:HA    | 1.88                     | 0.56              |
| 3:K:183:VAL:HG22 | 3:K:184:THR:H     | 1.71                     | 0.56              |
| 2:D:129:ASN:ND2  | 2:D:159:TYR:HE1   | 2.04                     | 0.56              |
| 4:J:92:GLN:NE2   | 4:J:95:SER:H      | 2.03                     | 0.56              |
| 1:E:129:GLN:CD   | 1:E:129:GLN:H     | 2.14                     | 0.56              |
| 4:H:113:ALA:O    | 4:H:202:THR:HG21  | 2.04                     | 0.56              |
| 1:C:71:LEU:O     | 1:C:148:PHE:HB3   | 2.06                     | 0.56              |
| 3:K:12:VAL:O     | 3:K:12:VAL:CG1    | 2.54                     | 0.56              |
| 4:J:37:TRP:HB2   | 4:J:50:ILE:HG23   | 1.89                     | 0.55              |
| 2:D:30:GLN:HE22  | 2:D:145:ASP:HA    | 1.70                     | 0.55              |
| 3:K:184:THR:CG2  | 3:K:185:SER:H     | 2.05                     | 0.55              |
| 2:B:54:SER:HB3   | 1:E:32:ARG:NH2    | 2.21                     | 0.55              |
| 4:H:119:ILE:HG12 | 4:H:209:LYS:HB3   | 1.88                     | 0.55              |
| 3:G:84:VAL:HA    | 3:G:111:VAL:CG1   | 2.36                     | 0.55              |
| 1:E:130:HIS:HB3  | 1:E:155:THR:O     | 2.07                     | 0.55              |
| 4:J:125:GLU:OE1  | 4:J:125:GLU:N     | 2.33                     | 0.55              |
| 3:G:33:TYR:O     | 3:G:35:THR:HG23   | 2.07                     | 0.55              |
| 4:H:42:PRO:HD3   | 4:H:86:VAL:HG12   | 1.88                     | 0.55              |
| 4:J:52:ALA:O     | 4:J:53:ALA:HB3    | 2.06                     | 0.55              |
| 3:K:91:TYR:CE1   | 3:K:106:GLY:CA    | 2.90                     | 0.55              |
| 1:A:122:PRO:HD2  | 1:A:126:ARG:HH21  | 1.72                     | 0.54              |
| 1:A:66:ILE:HD12  | 1:A:112:LEU:HD12  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:105:TYR:CE2  | 1:C:109:LYS:HE3  | 2.42                     | 0.54              |
| 1:E:156:GLU:HB2  | 1:E:160:ASN:O    | 2.07                     | 0.54              |
| 1:E:316:LEU:HD23 | 2:F:100:VAL:HG13 | 1.88                     | 0.54              |
| 2:D:131:LYS:HD3  | 2:D:141:TYR:OH   | 2.07                     | 0.54              |
| 2:F:62:GLN:HB2   | 2:F:92:TRP:CE2   | 2.42                     | 0.54              |
| 3:K:91:TYR:CD1   | 3:K:106:GLY:HA2  | 2.42                     | 0.54              |
| 3:I:155:ASN:C    | 3:I:155:ASN:HD22 | 2.16                     | 0.54              |
| 4:J:163:ASN:HB3  | 4:J:177:MET:HE3  | 1.90                     | 0.54              |
| 2:F:62:GLN:NE2   | 2:F:63:PHE:O     | 2.41                     | 0.53              |
| 4:J:152:ILE:HD12 | 4:J:157:ARG:HB2  | 1.89                     | 0.53              |
| 4:L:212:ASN:OD1  | 4:L:214:ASN:ND2  | 2.40                     | 0.53              |
| 3:G:172:SER:O    | 3:G:174:LEU:HG   | 2.07                     | 0.53              |
| 4:J:33:THR:O     | 4:J:52:ALA:O     | 2.27                     | 0.53              |
| 4:H:83:GLU:OE1   | 4:H:83:GLU:N     | 2.30                     | 0.53              |
| 3:I:159:LEU:HD13 | 3:I:159:LEU:O    | 2.08                     | 0.53              |
| 4:J:15:ALA:O     | 4:J:109:LYS:N    | 2.36                     | 0.53              |
| 1:A:202:VAL:HG11 | 1:A:251:LEU:HD13 | 1.91                     | 0.53              |
| 2:F:37:ASP:OD2   | 2:F:40:SER:OG    | 2.20                     | 0.53              |
| 4:H:4:ILE:O      | 4:H:99:THR:HG21  | 2.09                     | 0.53              |
| 3:I:153:THR:HG21 | 3:I:157:GLY:HA2  | 1.91                     | 0.53              |
| 1:C:251:LEU:HD21 | 1:C:253:ALA:HB2  | 1.90                     | 0.53              |
| 1:E:156:GLU:HB3  | 1:E:161:TYR:HD1  | 1.73                     | 0.53              |
| 1:C:187:ASP:OD1  | 1:C:190:GLU:N    | 2.38                     | 0.52              |
| 1:E:152:VAL:HG23 | 1:E:253:ALA:HB3  | 1.91                     | 0.52              |
| 4:H:37:TRP:CE2   | 4:H:75:PHE:HB2   | 2.44                     | 0.52              |
| 3:I:51:ILE:HD13  | 3:I:71:ARG:HD2   | 1.90                     | 0.52              |
| 1:E:119:LYS:HB3  | 1:E:256:TYR:CD1  | 2.44                     | 0.52              |
| 4:J:35:LEU:HD13  | 4:J:73:PHE:CG    | 2.44                     | 0.52              |
| 3:K:43:LYS:HG3   | 3:K:44:ALA:H     | 1.74                     | 0.52              |
| 4:L:37:TRP:CE2   | 4:L:75:PHE:HB2   | 2.43                     | 0.52              |
| 3:K:155:ASN:CG   | 3:K:193:ILE:HG12 | 2.34                     | 0.52              |
| 3:I:4:LEU:HD22   | 3:I:24:THR:HG22  | 1.91                     | 0.52              |
| 4:J:152:ILE:O    | 4:J:155:SER:N    | 2.42                     | 0.52              |
| 1:C:32:ARG:NH2   | 2:F:54:SER:OG    | 2.41                     | 0.52              |
| 3:G:40:PRO:HG2   | 3:G:43:LYS:HB3   | 1.92                     | 0.52              |
| 3:K:173:ASP:OD2  | 3:K:173:ASP:N    | 2.41                     | 0.52              |
| 2:B:54:SER:HB3   | 1:E:32:ARG:HH22  | 1.74                     | 0.52              |
| 1:E:150:ASN:HA   | 1:E:256:TYR:HE2  | 1.75                     | 0.52              |
| 1:E:161:TYR:CE2  | 1:E:249:GLY:HA2  | 2.45                     | 0.52              |
| 4:J:49:LEU:HD12  | 4:J:60:VAL:HG11  | 1.89                     | 0.52              |
| 4:J:186:ASP:OD1  | 4:J:186:ASP:N    | 2.34                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:E:61:LEU:HD11   | 1:E:66:ILE:HD13    | 1.92                     | 0.52              |
| 1:E:280:LYS:NZ    | 1:E:304:GLU:H      | 2.08                     | 0.52              |
| 3:I:52(A):ASP:OD1 | 3:I:53:ASN:HB2     | 2.10                     | 0.52              |
| 1:C:310:LYS:NZ    | 2:D:90:ASP:OD1     | 2.36                     | 0.52              |
| 2:F:38:LYS:NZ     | 9:F:201:SO4:S      | 2.83                     | 0.52              |
| 1:C:51:LEU:HD13   | 1:C:88:MET:HE3     | 1.91                     | 0.52              |
| 2:D:38:LYS:NZ     | 9:D:201:SO4:O2     | 2.43                     | 0.52              |
| 4:H:126:GLN:OE1   | 4:H:133:SER:N      | 2.42                     | 0.51              |
| 3:K:187:THR:OG1   | 3:K:188:TRP:N      | 2.43                     | 0.51              |
| 4:L:92:GLN:NE2    | 4:L:95:SER:H       | 2.08                     | 0.51              |
| 1:C:229:ARG:NH2   | 1:E:206:THR:O      | 2.43                     | 0.51              |
| 3:G:83:ARG:C      | 3:G:111:VAL:HG11   | 2.35                     | 0.51              |
| 3:I:34:MET:HG2    | 3:I:94:ARG:HG3     | 1.91                     | 0.51              |
| 4:J:197:GLU:HG3   | 4:J:208:VAL:HB     | 1.92                     | 0.51              |
| 3:K:155:ASN:ND2   | 3:K:193:ILE:HG12   | 2.26                     | 0.51              |
| 1:A:298:HIS:CG    | 1:A:299:PRO:HD2    | 2.46                     | 0.51              |
| 1:C:298:HIS:HE1   | 1:C:300:LEU:CD1    | 2.09                     | 0.51              |
| 2:F:26:HIS:HB2    | 2:F:149:MET:HE3    | 1.92                     | 0.51              |
| 4:J:51:TYR:O      | 4:J:52:ALA:HB3     | 2.11                     | 0.51              |
| 1:A:228:GLY:O     | 1:A:229:ARG:NH1    | 2.43                     | 0.51              |
| 3:K:35:THR:HG22   | 3:K:50:PHE:CB      | 2.35                     | 0.51              |
| 3:I:140:CYS:HB2   | 3:I:154:TRP:HE1    | 1.75                     | 0.51              |
| 4:J:108:ILE:HD11  | 4:J:110:ARG:HD3    | 1.91                     | 0.51              |
| 1:A:167:SER:HB2   | 1:A:244:ASN:HD21   | 1.74                     | 0.51              |
| 1:A:244:ASN:OD1   | 1:E:221:PRO:HG3    | 2.10                     | 0.50              |
| 1:E:117:LYS:NZ    | 1:E:150:ASN:OD1    | 2.29                     | 0.50              |
| 3:I:164:HIS:NE2   | 4:J:140:ASN:OD1    | 2.34                     | 0.50              |
| 4:J:61:PRO:HB2    | 4:J:63:ARG:HD2     | 1.93                     | 0.50              |
| 1:A:174:GLU:HB2   | 1:A:259:LYS:HE3    | 1.93                     | 0.50              |
| 1:C:294:PHE:HZ    | 2:D:59:MET:HE3     | 1.76                     | 0.50              |
| 3:K:115:LYS:HD2   | 3:K:116:THR:H      | 1.77                     | 0.50              |
| 2:B:3:PHE:CE2     | 2:B:113:SER:HB2    | 2.47                     | 0.50              |
| 1:E:195:TYR:O     | 1:E:196:GLN:HB2    | 2.11                     | 0.50              |
| 4:H:63:ARG:HH21   | 4:H:84:ASP:CG      | 2.20                     | 0.50              |
| 2:B:55:VAL:HG13   | 2:B:99:LEU:HD23    | 1.94                     | 0.50              |
| 1:E:51:LEU:O      | 1:E:274:LEU:HD12   | 2.11                     | 0.50              |
| 3:I:213:ARG:HH12  | 4:J:123:SER:HA     | 1.77                     | 0.49              |
| 3:K:66:ARG:HH22   | 3:K:86:ASP:CG      | 2.20                     | 0.49              |
| 1:E:284:PRO:HD3   | 1:E:300:LEU:O      | 2.12                     | 0.49              |
| 2:F:125:GLN:O     | 2:F:127[B]:ARG:HG3 | 2.12                     | 0.49              |
| 3:K:31:ASP:HB3    | 3:K:71:ARG:NH2     | 2.26                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:D:38:LYS:HG2    | 3:I:100(A):TYR:CE2 | 2.46                     | 0.49              |
| 1:E:45:LYS:HG2    | 1:E:296:ASN:HD21   | 1.77                     | 0.49              |
| 4:J:169:ASP:OD1   | 4:J:172:ASP:HB3    | 2.13                     | 0.49              |
| 1:C:155:THR:HG22  | 1:C:156:GLU:HG2    | 1.94                     | 0.49              |
| 3:G:30:THR:HG23   | 3:G:32:ASP:H       | 1.77                     | 0.49              |
| 3:I:66:ARG:C      | 3:I:67:PHE:HD1     | 2.21                     | 0.49              |
| 1:E:106:GLU:H     | 1:E:106:GLU:CD     | 2.21                     | 0.49              |
| 1:E:294:PHE:CE1   | 1:E:307[A]:LYS:HD3 | 2.47                     | 0.49              |
| 3:G:161:SER:N     | 3:G:163:VAL:HG23   | 2.28                     | 0.49              |
| 3:I:12:VAL:CG2    | 3:I:18:LEU:HD22    | 2.42                     | 0.49              |
| 3:K:35:THR:HG21   | 4:L:98:TRP:HZ3     | 1.78                     | 0.49              |
| 1:E:64:CYS:HA     | 1:E:95:ASP:O       | 2.12                     | 0.49              |
| 1:E:128:THR:O     | 1:E:157:LYS:NZ     | 2.39                     | 0.49              |
| 1:C:13:ILE:HD11   | 2:D:24:TYR:HB3     | 1.94                     | 0.49              |
| 1:E:201:TYR:OH    | 1:E:246:GLU:OE2    | 2.31                     | 0.49              |
| 2:B:83:LYS:NZ     | 2:D:85:GLU:OE2     | 2.46                     | 0.48              |
| 3:K:1:GLU:HG2     | 3:K:2:VAL:HG23     | 1.95                     | 0.48              |
| 1:E:139:CYS:HB2   | 1:E:146:SER:O      | 2.14                     | 0.48              |
| 1:E:187:ASP:OD1   | 1:E:190:GLU:N      | 2.40                     | 0.48              |
| 2:F:38:LYS:HZ2    | 2:F:38:LYS:HB2     | 1.79                     | 0.48              |
| 3:G:52(A):ASP:OD1 | 3:G:53:ASN:N       | 2.43                     | 0.48              |
| 4:J:114:ALA:HA    | 4:J:202:THR:HG21   | 1.95                     | 0.48              |
| 1:C:220:ARG:NH1   | 1:C:227:GLY:O      | 2.45                     | 0.48              |
| 1:A:15:ILE:HD11   | 2:B:122:VAL:HG21   | 1.95                     | 0.48              |
| 1:A:183:HIS:ND1   | 1:A:195:TYR:OH     | 2.29                     | 0.48              |
| 1:C:185:PRO:HD2   | 1:C:217:ILE:HG12   | 1.95                     | 0.48              |
| 3:K:50:PHE:CD1    | 3:K:50:PHE:C       | 2.91                     | 0.48              |
| 3:I:213:ARG:HH12  | 4:J:124:SER:N      | 2.10                     | 0.48              |
| 4:L:172:ASP:OD2   | 4:L:174:THR:OG1    | 2.29                     | 0.48              |
| 1:A:51:LEU:HD13   | 1:A:88:MET:HE3     | 1.96                     | 0.47              |
| 1:A:284:PRO:HG2   | 1:A:298:HIS:CE1    | 2.49                     | 0.47              |
| 3:G:155:ASN:HD22  | 3:G:159:LEU:HD12   | 1.79                     | 0.47              |
| 3:G:177:LEU:HG    | 3:G:178:SER:H      | 1.77                     | 0.47              |
| 4:L:17:LEU:HD22   | 4:L:17:LEU:H       | 1.79                     | 0.47              |
| 3:K:1:GLU:HG2     | 3:K:2:VAL:H        | 1.76                     | 0.47              |
| 4:L:200:HIS:CD2   | 4:L:201:LYS:H      | 2.32                     | 0.47              |
| 4:J:40:GLN:O      | 4:J:86:VAL:HG13    | 2.15                     | 0.47              |
| 4:J:18:GLY:H      | 4:J:80:LEU:CB      | 2.27                     | 0.47              |
| 3:K:155:ASN:H     | 3:K:196:ASN:ND2    | 2.12                     | 0.47              |
| 4:J:124:SER:O     | 4:J:128:THR:OG1    | 2.32                     | 0.47              |
| 1:A:202:VAL:HG22  | 1:A:247:SER:OG     | 2.14                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:J:50:ILE:HD13    | 4:J:66:GLY:HA3      | 1.97                     | 0.47              |
| 1:A:96:LEU:HD12    | 1:A:96:LEU:H        | 1.80                     | 0.47              |
| 1:E:161:TYR:CZ     | 1:E:249:GLY:HA2     | 2.50                     | 0.47              |
| 2:F:164:GLU:CD     | 2:F:164:GLU:N       | 2.72                     | 0.47              |
| 3:G:32:ASP:OD1     | 3:G:52:ARG:NH2      | 2.34                     | 0.47              |
| 3:I:166:PHE:O      | 3:I:177:LEU:CD1     | 2.63                     | 0.47              |
| 4:J:151:LYS:O      | 4:J:195:THR:OG1     | 2.21                     | 0.47              |
| 3:K:83:ARG:O       | 3:K:111:VAL:HG11    | 2.15                     | 0.47              |
| 3:G:119:PRO:HB3    | 3:G:145:TYR:HB3     | 1.97                     | 0.47              |
| 1:C:161:TYR:CZ     | 1:C:249:GLY:HA2     | 2.50                     | 0.47              |
| 1:E:282:GLN:HB3    | 1:E:302[B]:ILE:HG23 | 1.97                     | 0.47              |
| 3:G:124:LEU:HD11   | 3:G:141:LEU:HB2     | 1.96                     | 0.47              |
| 4:J:150:TRP:O      | 4:J:157:ARG:N       | 2.46                     | 0.47              |
| 4:L:31:ILE:HG21    | 4:L:92:GLN:HG3      | 1.96                     | 0.47              |
| 1:A:207[B]:SER:OG  | 1:A:241:ASP:OD2     | 2.29                     | 0.46              |
| 2:D:103:GLU:OE1    | 2:D:103:GLU:HA      | 2.13                     | 0.46              |
| 2:F:127[A]:ARG:HB3 | 2:F:128:ASP:H       | 1.49                     | 0.46              |
| 1:A:170:ASN:HB3    | 1:A:240:TRP:N       | 2.31                     | 0.46              |
| 3:G:194:THR:HA     | 3:G:209:LYS:HA      | 1.97                     | 0.46              |
| 4:H:17:LEU:HD12    | 4:H:108:ILE:HD11    | 1.97                     | 0.46              |
| 2:B:82:LYS:NZ      | 2:B:86:ASP:OD2      | 2.46                     | 0.46              |
| 1:E:61:LEU:HD12    | 1:E:89:GLU:HB2      | 1.97                     | 0.46              |
| 3:G:94:ARG:O       | 3:G:101:ASP:N       | 2.48                     | 0.46              |
| 3:K:196:ASN:HB3    | 3:K:205:LYS:NZ      | 2.30                     | 0.46              |
| 1:A:53:LYS:HG3     | 1:A:277:CYS:O       | 2.16                     | 0.46              |
| 1:E:43:LEU:O       | 1:E:45:LYS:HE2      | 2.14                     | 0.46              |
| 3:K:74:SER:OG      | 3:K:75:GLN:N        | 2.47                     | 0.46              |
| 1:A:15:ILE:HG13    | 2:B:119:TYR:HA      | 1.97                     | 0.46              |
| 1:A:49:GLY:HA2     | 1:A:285:LEU:O       | 2.15                     | 0.46              |
| 4:H:108:ILE:HG22   | 4:H:168:GLN:OE1     | 2.15                     | 0.46              |
| 4:L:168:GLN:NE2    | 4:L:173:SER:O       | 2.48                     | 0.46              |
| 1:A:196:GLN:O      | 1:A:197:ASN:OD1     | 2.34                     | 0.46              |
| 2:F:3:PHE:N        | 2:F:112:ASP:OD2     | 2.49                     | 0.46              |
| 4:J:107:GLU:HG3    | 4:J:175:TYR:OH      | 2.16                     | 0.46              |
| 2:B:162:TYR:O      | 2:B:166:SER:OG      | 2.29                     | 0.46              |
| 1:C:26:VAL:HG21    | 1:C:317:ALA:HB2     | 1.97                     | 0.46              |
| 3:G:2:VAL:HG21     | 3:G:102:TYR:CE2     | 2.50                     | 0.46              |
| 3:G:116:THR:HG23   | 3:G:147:PRO:HD2     | 1.97                     | 0.46              |
| 1:A:25:LYS:CE      | 1:A:35:THR:OG1      | 2.64                     | 0.46              |
| 2:F:42:GLN:HG2     | 4:L:51:TYR:CE1      | 2.51                     | 0.46              |
| 3:G:128:CYS:C      | 3:G:130:ASP:N       | 2.73                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:H:162:LEU:O      | 4:H:179:SER:HA     | 2.16                     | 0.46              |
| 3:I:50:PHE:CD1     | 3:I:50:PHE:C       | 2.94                     | 0.46              |
| 4:L:52:ALA:O       | 4:L:53:ALA:HB3     | 2.16                     | 0.46              |
| 1:A:58:PRO:HB3     | 1:A:86:TYR:CE2     | 2.51                     | 0.46              |
| 1:A:201:TYR:HE2    | 1:A:248:THR:HG23   | 1.81                     | 0.46              |
| 1:C:30:LEU:HA      | 1:C:30:LEU:HD12    | 1.73                     | 0.46              |
| 1:C:123:LYS:NZ     | 1:C:132:THR:O      | 2.49                     | 0.46              |
| 3:G:39:GLN:HB2     | 3:G:45:LEU:HD23    | 1.98                     | 0.46              |
| 3:G:50:PHE:C       | 3:G:50:PHE:CD1     | 2.94                     | 0.46              |
| 3:I:94:ARG:HG2     | 3:I:95:PRO:HD2     | 1.96                     | 0.46              |
| 1:E:180:TRP:CE2    | 1:E:204:VAL:HG21   | 2.51                     | 0.46              |
| 4:J:34:TRP:NE1     | 9:J:301:SO4:O1     | 2.48                     | 0.46              |
| 3:K:13:GLN:C       | 3:K:111:VAL:HG23   | 2.41                     | 0.46              |
| 3:K:82:MET:HB3     | 3:K:82(C):LEU:HD21 | 1.98                     | 0.46              |
| 3:K:94:ARG:HA      | 3:K:95:PRO:HD3     | 1.81                     | 0.46              |
| 1:C:66:ILE:HB      | 1:C:105:TYR:OH     | 2.17                     | 0.45              |
| 1:E:174:GLU:C      | 1:E:239:MET:HE1    | 2.41                     | 0.45              |
| 2:F:87:GLY:O       | 2:F:91:VAL:HG23    | 2.17                     | 0.45              |
| 3:G:171:GLN:HB2    | 4:H:162:LEU:HD11   | 1.98                     | 0.45              |
| 1:E:268:MET:HE3    | 1:E:268:MET:HB2    | 1.76                     | 0.45              |
| 1:A:43:LEU:HD23    | 1:A:45:LYS:HE3     | 1.98                     | 0.45              |
| 1:C:129:GLN:O      | 1:C:157:LYS:HB3    | 2.16                     | 0.45              |
| 2:D:26:HIS:HB2     | 2:D:149:MET:HE3    | 1.99                     | 0.45              |
| 3:G:171:GLN:HG3    | 4:H:162:LEU:HD11   | 1.99                     | 0.45              |
| 4:J:20:SER:HB3     | 4:J:76:LYS:NZ      | 2.26                     | 0.45              |
| 4:J:92:GLN:NE2     | 4:J:95:SER:O       | 2.43                     | 0.45              |
| 4:L:51:TYR:O       | 4:L:52:ALA:HB3     | 2.16                     | 0.45              |
| 1:A:298:HIS:CD2    | 1:A:299:PRO:HD2    | 2.51                     | 0.45              |
| 1:E:280:LYS:HG3    | 1:E:304:GLU:HG2    | 1.98                     | 0.45              |
| 4:L:34:TRP:CD1     | 4:L:34:TRP:N       | 2.85                     | 0.45              |
| 2:B:142:HIS:CD2    | 2:B:162:TYR:HB3    | 2.52                     | 0.45              |
| 1:C:111:LEU:O      | 1:C:115:VAL:HG23   | 2.16                     | 0.45              |
| 2:F:123:ARG:HB2    | 2:F:138:PHE:CZ     | 2.52                     | 0.45              |
| 3:G:17:SER:HA      | 3:G:82(C):LEU:HD23 | 1.98                     | 0.45              |
| 4:H:61:PRO:HB2     | 4:H:64:PHE:CD2     | 2.52                     | 0.45              |
| 1:C:102:PHE:HZ     | 1:C:179:ILE:HD13   | 1.81                     | 0.45              |
| 2:D:107:THR:O      | 2:D:110:PHE:HB3    | 2.16                     | 0.45              |
| 1:E:184:HIS:HB3    | 1:E:220:ARG:NH2    | 2.32                     | 0.45              |
| 1:A:14:CYS:O       | 2:B:24:TYR:HA      | 2.16                     | 0.45              |
| 1:A:307[A]:LYS:HE2 | 2:B:92:TRP:CD2     | 2.51                     | 0.45              |
| 1:E:260:ILE:O      | 1:E:260:ILE:HG13   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:62:GLN:HB2    | 2:F:92:TRP:CZ2   | 2.52                     | 0.45              |
| 2:F:71:SER:O      | 2:F:75:ARG:NH1   | 2.49                     | 0.45              |
| 3:I:52(B):ARG:HB2 | 3:I:55:TYR:OH    | 2.17                     | 0.45              |
| 4:L:8:GLN:HE21    | 4:L:23:ILE:HG21  | 1.80                     | 0.45              |
| 1:A:58:PRO:HB3    | 1:A:86:TYR:CZ    | 2.52                     | 0.45              |
| 1:C:201:TYR:OH    | 1:C:246:GLU:OE2  | 2.32                     | 0.45              |
| 1:A:170:ASN:HB3   | 1:A:240:TRP:H    | 1.81                     | 0.45              |
| 1:C:172:SER:HB2   | 1:C:259:LYS:HD2  | 1.99                     | 0.45              |
| 1:E:247:SER:OG    | 1:E:249:GLY:O    | 2.35                     | 0.45              |
| 1:E:150:ASN:HA    | 1:E:256:TYR:CE2  | 2.52                     | 0.44              |
| 4:L:13:GLN:HG3    | 4:L:14:SER:N     | 2.33                     | 0.44              |
| 2:B:125:GLN:CD    | 2:B:157:TYR:HB3  | 2.42                     | 0.44              |
| 3:I:85:GLU:H      | 3:I:85:GLU:HG3   | 1.55                     | 0.44              |
| 4:J:187:GLU:HA    | 4:J:190:ARG:HE   | 1.82                     | 0.44              |
| 1:A:168:TYR:O     | 1:A:242:THR:HA   | 2.18                     | 0.44              |
| 1:E:247:SER:HB2   | 1:E:251:LEU:HD12 | 1.99                     | 0.44              |
| 3:K:47:TRP:CH2    | 3:K:49:GLY:HA2   | 2.53                     | 0.44              |
| 3:K:202:SER:OG    | 3:K:204:THR:OG1  | 2.28                     | 0.44              |
| 4:H:120:PHE:HB2   | 4:H:135:VAL:HB   | 1.99                     | 0.44              |
| 4:J:37:TRP:HD1    | 4:J:50:ILE:HG12  | 1.81                     | 0.44              |
| 3:K:93:ALA:HA     | 3:K:102:TYR:O    | 2.18                     | 0.44              |
| 1:E:26:VAL:HG21   | 1:E:317:ALA:HB2  | 2.00                     | 0.44              |
| 2:F:62:GLN:OE1    | 2:F:92:TRP:CD1   | 2.70                     | 0.44              |
| 3:I:39:GLN:HA     | 3:I:40:PRO:HD2   | 1.89                     | 0.44              |
| 3:K:6:GLU:HA      | 3:K:21:SER:O     | 2.18                     | 0.44              |
| 4:L:50:ILE:HG23   | 4:L:55:SER:O     | 2.18                     | 0.44              |
| 2:D:133:LEU:HB2   | 2:D:135:ASN:OD1  | 2.17                     | 0.44              |
| 1:E:171:THR:HA    | 1:E:240:TRP:HZ3  | 1.82                     | 0.44              |
| 3:G:198:ALA:HB2   | 3:G:205:LYS:HD3  | 2.00                     | 0.44              |
| 4:L:119:ILE:HG22  | 4:L:136:CYS:SG   | 2.58                     | 0.44              |
| 4:L:120:PHE:HA    | 4:L:121:PRO:HD2  | 1.87                     | 0.44              |
| 1:A:131:THR:HB    | 1:A:155:THR:HG23 | 1.99                     | 0.44              |
| 1:C:137:ARG:NE    | 1:C:137:ARG:H    | 2.15                     | 0.44              |
| 1:E:112:LEU:HD23  | 1:E:112:LEU:HA   | 1.69                     | 0.44              |
| 1:E:121:LEU:HD12  | 1:E:254:PRO:HG2  | 1.99                     | 0.44              |
| 3:G:47:TRP:CH2    | 3:G:49:GLY:HA2   | 2.53                     | 0.44              |
| 3:I:205:LYS:NZ    | 3:I:207:ASP:OD1  | 2.43                     | 0.44              |
| 2:B:76:ARG:NH1    | 2:D:69:GLU:O     | 2.48                     | 0.44              |
| 3:G:6:GLU:OE1     | 3:G:105:GLN:N    | 2.51                     | 0.44              |
| 3:G:85:GLU:CD     | 3:G:85:GLU:H     | 2.25                     | 0.44              |
| 4:H:78:SER:OG     | 4:H:79:SER:N     | 2.50                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:I:6:GLU:OE1      | 3:I:104:GLY:HA3   | 2.18                     | 0.44              |
| 3:I:52(B):ARG:HA   | 3:I:55:TYR:CE2    | 2.53                     | 0.44              |
| 4:J:63:ARG:H       | 4:J:63:ARG:HG3    | 1.34                     | 0.44              |
| 1:C:238:ASP:OD1    | 1:C:239:MET:N     | 2.50                     | 0.43              |
| 2:D:17:MET:HE3     | 2:D:17:MET:HB2    | 1.75                     | 0.43              |
| 1:E:307[A]:LYS:HE2 | 1:E:309:VAL:HG13  | 2.00                     | 0.43              |
| 3:K:5:VAL:HA       | 3:K:105:GLN:OE1   | 2.18                     | 0.43              |
| 4:L:50:ILE:CG2     | 4:L:53:ALA:O      | 2.60                     | 0.43              |
| 1:A:168:TYR:CE2    | 1:A:170:ASN:HA    | 2.53                     | 0.43              |
| 1:C:325:GLN:HG2    | 2:D:13:GLY:O      | 2.18                     | 0.43              |
| 3:G:154:TRP:CZ3    | 3:G:195:CYS:HB2   | 2.53                     | 0.43              |
| 3:K:156:SER:HB3    | 3:K:157:GLY:H     | 1.57                     | 0.43              |
| 1:A:274:LEU:HD12   | 1:A:275:GLU:H     | 1.84                     | 0.43              |
| 3:G:36:TRP:CE2     | 3:G:80:LEU:HB2    | 2.53                     | 0.43              |
| 1:A:116(B):PHE:CE1 | 1:A:260:ILE:HG22  | 2.45                     | 0.43              |
| 1:A:186:ASN:OD1    | 1:A:219:THR:HA    | 2.19                     | 0.43              |
| 1:E:184:HIS:HB3    | 1:E:220:ARG:HH22  | 1.84                     | 0.43              |
| 1:E:161:TYR:CD1    | 1:E:195:TYR:HA    | 2.54                     | 0.43              |
| 1:E:294:PHE:HE1    | 1:E:307[A]:LYS:NZ | 2.16                     | 0.43              |
| 4:J:166:THR:OG1    | 4:J:167:ASP:N     | 2.49                     | 0.43              |
| 4:J:172:ASP:OD2    | 4:J:174:THR:OG1   | 2.37                     | 0.43              |
| 1:C:164:ALA:O      | 1:C:246:GLU:HA    | 2.19                     | 0.43              |
| 1:C:195:TYR:C      | 1:C:197:ASN:H     | 2.26                     | 0.43              |
| 3:K:1:GLU:OE1      | 3:K:102:TYR:OH    | 2.22                     | 0.43              |
| 3:K:63:VAL:HB      | 3:K:67:PHE:CG     | 2.53                     | 0.43              |
| 1:C:112:LEU:HD23   | 1:C:112:LEU:HA    | 1.59                     | 0.43              |
| 3:I:11:LEU:O       | 3:I:110:ILE:O     | 2.37                     | 0.43              |
| 4:J:188:TYR:HA     | 4:J:194:TYR:OH    | 2.19                     | 0.43              |
| 3:K:151:THR:HB     | 3:K:198:ALA:HB3   | 2.01                     | 0.43              |
| 4:L:108:ILE:HG23   | 4:L:173:SER:HB3   | 2.01                     | 0.43              |
| 1:E:147:PHE:CG     | 1:E:148:PHE:N     | 2.86                     | 0.43              |
| 2:F:121:LYS:HG3    | 2:F:122:VAL:N     | 2.30                     | 0.43              |
| 2:F:142:HIS:CD2    | 2:F:162:TYR:HB3   | 2.53                     | 0.43              |
| 4:L:34:TRP:NE1     | 9:L:301:SO4:O3    | 2.36                     | 0.43              |
| 1:C:49:GLY:HA2     | 1:C:285:LEU:O     | 2.19                     | 0.43              |
| 1:C:195:TYR:CZ     | 1:C:250:ASN:HA    | 2.54                     | 0.43              |
| 1:C:298:HIS:ND1    | 1:C:299:PRO:HD2   | 2.34                     | 0.43              |
| 1:E:316:LEU:CD1    | 2:F:52:VAL:HG12   | 2.48                     | 0.43              |
| 3:I:166:PHE:HD2    | 4:J:166:THR:HG22  | 1.83                     | 0.42              |
| 4:J:37:TRP:CH2     | 4:J:90:CYS:HB3    | 2.53                     | 0.42              |
| 1:C:202:VAL:HA     | 1:C:247:SER:HB2   | 2.01                     | 0.42              |

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| Atom-1               | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|------------------|--------------------------|-------------------|
| 2:F:59:MET:HB2       | 2:F:59:MET:HE2   | 1.62                     | 0.42              |
| 3:G:52(B)[B]:ARG:HG3 | 3:G:55:TYR:CE2   | 2.54                     | 0.42              |
| 3:G:67:PHE:N         | 3:G:67:PHE:CD1   | 2.87                     | 0.42              |
| 4:H:151:LYS:HB2      | 4:H:195:THR:HB   | 2.01                     | 0.42              |
| 1:A:108:LEU:HD13     | 1:A:234:TRP:CD2  | 2.54                     | 0.42              |
| 1:A:180:TRP:NE1      | 1:A:204:VAL:HG21 | 2.33                     | 0.42              |
| 2:D:160:PRO:HA       | 2:D:163:GLU:HB2  | 2.01                     | 0.42              |
| 2:F:38:LYS:NZ        | 2:F:38:LYS:HB2   | 2.35                     | 0.42              |
| 3:G:84:VAL:HA        | 3:G:111:VAL:HG12 | 2.00                     | 0.42              |
| 3:K:13:GLN:HG3       | 3:K:14:PRO:O     | 2.19                     | 0.42              |
| 1:A:156:GLU:HB2      | 1:A:161:TYR:HB2  | 2.01                     | 0.42              |
| 2:D:84:MET:HE2       | 2:D:85:GLU:HG3   | 2.01                     | 0.42              |
| 3:G:173:ASP:OD1      | 3:G:173:ASP:N    | 2.52                     | 0.42              |
| 4:H:56:LEU:HD21      | 4:H:64:PHE:O     | 2.19                     | 0.42              |
| 3:I:130:ASP:O        | 3:I:131:THR:HG22 | 2.14                     | 0.42              |
| 4:J:26:LEU:HD13      | 4:J:72:LYS:HG2   | 2.01                     | 0.42              |
| 4:J:110:ARG:HD2      | 4:J:110:ARG:HA   | 1.81                     | 0.42              |
| 1:A:214:THR:HA       | 1:A:215:PRO:HD3  | 1.81                     | 0.42              |
| 2:B:2:LEU:HD23       | 2:D:3:PHE:HZ     | 1.84                     | 0.42              |
| 4:J:120:PHE:HA       | 4:J:121:PRO:HD3  | 1.82                     | 0.42              |
| 3:K:119:PRO:HB3      | 3:K:145:TYR:HB3  | 2.01                     | 0.42              |
| 1:A:176:MET:HA       | 1:A:258:PHE:O    | 2.20                     | 0.42              |
| 2:D:121:LYS:HB2      | 2:D:121:LYS:HE3  | 1.72                     | 0.42              |
| 3:G:129:GLY:O        | 3:G:130:ASP:HB2  | 2.19                     | 0.42              |
| 4:J:65:SER:OG        | 4:J:76:LYS:HG2   | 2.19                     | 0.42              |
| 1:A:167:SER:HB2      | 1:A:244:ASN:ND2  | 2.33                     | 0.42              |
| 1:C:120:ILE:HG22     | 1:C:121:LEU:N    | 2.33                     | 0.42              |
| 2:D:123:ARG:HH22     | 2:D:124:MET:HE3  | 1.84                     | 0.42              |
| 1:E:176:MET:HE3      | 1:E:257:GLY:C    | 2.45                     | 0.42              |
| 4:L:56:LEU:HD11      | 4:L:64:PHE:O     | 2.19                     | 0.42              |
| 1:E:247:SER:CB       | 1:E:251:LEU:HD12 | 2.50                     | 0.42              |
| 2:F:140:PHE:HB3      | 2:F:142:HIS:O    | 2.19                     | 0.42              |
| 4:H:49:LEU:HD12      | 4:H:49:LEU:HA    | 1.57                     | 0.42              |
| 4:L:19:GLU:O         | 4:L:80:LEU:HD23  | 2.18                     | 0.42              |
| 2:B:27:SER:HB3       | 2:B:32:SER:HB2   | 2.01                     | 0.42              |
| 2:D:43:LYS:HE3       | 2:D:43:LYS:HB3   | 1.90                     | 0.42              |
| 1:E:127:TRP:CZ3      | 1:E:154:LEU:HD21 | 2.55                     | 0.42              |
| 3:G:67:PHE:CE1       | 3:G:82:MET:HB3   | 2.55                     | 0.42              |
| 3:I:166:PHE:O        | 3:I:177:LEU:HD11 | 2.20                     | 0.42              |
| 2:D:116:LYS:HZ3      | 2:D:116:LYS:HG3  | 1.72                     | 0.42              |
| 2:D:142:HIS:CD2      | 2:D:162:TYR:HB3  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:90:LYS:HB3   | 1:E:271:GLU:OE1   | 2.20                     | 0.42              |
| 4:J:17:LEU:HA    | 4:J:80:LEU:HB3    | 2.01                     | 0.42              |
| 1:A:273:THR:OG1  | 1:A:274:LEU:N     | 2.52                     | 0.41              |
| 1:C:15:ILE:HG13  | 2:D:119:TYR:HA    | 2.02                     | 0.41              |
| 4:J:18:GLY:H     | 4:J:80:LEU:HB3    | 1.85                     | 0.41              |
| 1:A:175:GLN:HG2  | 1:A:236:LEU:HG    | 2.02                     | 0.41              |
| 1:A:284:PRO:HD3  | 1:A:300:LEU:O     | 2.20                     | 0.41              |
| 1:C:77:ASP:OD2   | 1:C:149:ARG:NH2   | 2.53                     | 0.41              |
| 2:D:125:GLN:HE22 | 2:D:155:GLY:C     | 2.27                     | 0.41              |
| 4:H:158:GLN:HG2  | 4:H:159:ASN:N     | 2.35                     | 0.41              |
| 1:A:105:TYR:CZ   | 1:A:109:LYS:HE3   | 2.55                     | 0.41              |
| 3:I:159:LEU:N    | 3:I:159:LEU:CD1   | 2.73                     | 0.41              |
| 4:J:78:SER:OG    | 4:J:79:SER:N      | 2.49                     | 0.41              |
| 3:K:143:LYS:HG3  | 3:K:176:THR:HG23  | 2.03                     | 0.41              |
| 1:C:90:LYS:O     | 1:C:269:LYS:NZ    | 2.43                     | 0.41              |
| 1:C:155:THR:CG2  | 1:C:156:GLU:N     | 2.83                     | 0.41              |
| 2:D:29:ASP:OD2   | 2:D:29:ASP:N      | 2.36                     | 0.41              |
| 3:I:155:ASN:O    | 3:I:155:ASN:ND2   | 2.43                     | 0.41              |
| 4:L:6:MET:HE3    | 4:L:25:CYS:SG     | 2.60                     | 0.41              |
| 1:E:320:LEU:H    | 1:E:320:LEU:HD23  | 1.85                     | 0.41              |
| 3:G:38:ARG:HD3   | 3:G:48:LEU:HD21   | 2.01                     | 0.41              |
| 4:H:52:ALA:O     | 4:H:53:ALA:HB3    | 2.20                     | 0.41              |
| 4:L:36:ALA:O     | 4:L:90:CYS:HA     | 2.21                     | 0.41              |
| 4:L:120:PHE:HB2  | 4:L:135:VAL:HB    | 2.03                     | 0.41              |
| 2:D:129:ASN:OD1  | 2:D:157:TYR:OH    | 2.38                     | 0.41              |
| 2:F:6:ILE:HD12   | 2:F:112:ASP:CA    | 2.45                     | 0.41              |
| 2:F:81:ASN:O     | 2:F:85:GLU:HG3    | 2.21                     | 0.41              |
| 4:H:33:THR:O     | 4:H:33:THR:HG23   | 2.19                     | 0.41              |
| 4:H:141:PHE:CE2  | 4:H:176:SER:HA    | 2.54                     | 0.41              |
| 3:I:184:THR:O    | 3:I:187:THR:OG1   | 2.37                     | 0.41              |
| 4:L:194:TYR:HB2  | 4:L:211:PHE:CE2   | 2.48                     | 0.41              |
| 1:C:84:TRP:CZ3   | 1:C:116(A):HIS:HA | 2.56                     | 0.41              |
| 1:E:325:GLN:OE1  | 2:F:15:GLN:HB2    | 2.21                     | 0.41              |
| 3:G:51:ILE:HD13  | 3:G:71:ARG:HG2    | 2.03                     | 0.41              |
| 3:K:155:ASN:OD1  | 3:K:193:ILE:HG12  | 2.21                     | 0.41              |
| 1:A:30:LEU:HD12  | 1:A:30:LEU:HA     | 1.73                     | 0.41              |
| 1:A:51:LEU:O     | 1:A:274:LEU:HD12  | 2.21                     | 0.41              |
| 1:A:75:GLU:HG3   | 1:A:95:ASP:OD1    | 2.21                     | 0.41              |
| 1:C:19:ALA:HB2   | 2:D:13:GLY:HA3    | 2.02                     | 0.41              |
| 1:C:123:LYS:O    | 1:C:132:THR:HG21  | 2.21                     | 0.41              |
| 1:C:155:THR:CG2  | 1:C:156:GLU:H     | 2.32                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:15:ILE:HG13    | 2:F:119:TYR:HA     | 2.02                     | 0.41              |
| 1:E:78:ARG:HG3     | 1:E:79:LEU:HD13    | 2.03                     | 0.41              |
| 2:F:44:ALA:O       | 2:F:48:ILE:HG12    | 2.21                     | 0.41              |
| 3:G:171:GLN:HB2    | 4:H:162:LEU:HD21   | 2.03                     | 0.41              |
| 3:I:52(B):ARG:HB2  | 3:I:55:TYR:CZ      | 2.56                     | 0.41              |
| 3:I:100(C):MET:HE2 | 3:I:100(C):MET:HB3 | 1.81                     | 0.41              |
| 3:I:177:LEU:HG     | 3:I:178:SER:N      | 2.36                     | 0.41              |
| 4:J:35:LEU:HB3     | 4:J:53:ALA:HB2     | 2.03                     | 0.41              |
| 4:J:80:LEU:HD12    | 4:J:81:GLN:H       | 1.85                     | 0.41              |
| 3:K:4:LEU:HD23     | 3:K:24:THR:HB      | 2.00                     | 0.41              |
| 4:J:11:ALA:H       | 10:J:302:EDO:H21   | 1.85                     | 0.41              |
| 4:J:121:PRO:HG3    | 4:J:211:PHE:CE2    | 2.56                     | 0.41              |
| 4:L:106:LEU:HD12   | 4:L:106:LEU:HA     | 1.88                     | 0.41              |
| 2:B:51:LYS:O       | 2:B:55:VAL:HG23    | 2.21                     | 0.40              |
| 2:D:38:LYS:HG2     | 3:I:100(A):TYR:CZ  | 2.56                     | 0.40              |
| 2:F:6:ILE:C        | 2:F:8:GLY:N        | 2.79                     | 0.40              |
| 3:G:52:ARG:NH2     | 3:G:53:ASN:OD1     | 2.54                     | 0.40              |
| 4:H:112:ASP:OD1    | 4:H:112:ASP:N      | 2.38                     | 0.40              |
| 1:E:168:TYR:O      | 1:E:242:THR:HA     | 2.22                     | 0.40              |
| 3:G:35:THR:HG21    | 4:H:98:TRP:HZ3     | 1.86                     | 0.40              |
| 3:G:66:ARG:HB3     | 3:G:82(A):ASN:O    | 2.21                     | 0.40              |
| 4:H:121:PRO:CG     | 4:H:211:PHE:CZ     | 2.80                     | 0.40              |
| 4:H:161:VAL:HG22   | 4:H:181:LEU:HD12   | 2.03                     | 0.40              |
| 3:I:18:LEU:HD12    | 3:I:18:LEU:HA      | 1.82                     | 0.40              |
| 3:I:155:ASN:C      | 3:I:155:ASN:ND2    | 2.79                     | 0.40              |
| 4:J:160:GLY:O      | 4:J:182:THR:OG1    | 2.36                     | 0.40              |
| 4:J:169:ASP:CG     | 4:J:172:ASP:HB3    | 2.45                     | 0.40              |
| 1:A:121:LEU:HD12   | 1:A:254:PRO:HG2    | 2.03                     | 0.40              |
| 1:A:295:HIS:O      | 1:A:308:TYR:HA     | 2.21                     | 0.40              |
| 2:B:76:ARG:HB3     | 2:D:68:LYS:HD3     | 2.03                     | 0.40              |
| 2:B:83:LYS:HE2     | 2:D:68:LYS:HZ1     | 1.86                     | 0.40              |
| 1:C:200:THR:HA     | 1:C:248:THR:OG1    | 2.21                     | 0.40              |
| 3:K:1:GLU:CG       | 3:K:2:VAL:N        | 2.73                     | 0.40              |
| 4:L:126:GLN:HG2    | 4:L:131:GLY:O      | 2.21                     | 0.40              |
| 2:F:168:LEU:HD23   | 2:F:168:LEU:HA     | 1.92                     | 0.40              |
| 4:L:37:TRP:CZ3     | 4:L:90:CYS:HB3     | 2.57                     | 0.40              |
| 1:E:129:GLN:HB2    | 1:E:130:HIS:ND1    | 2.36                     | 0.40              |
| 3:G:96:LYS:HB2     | 3:G:96:LYS:HE3     | 1.92                     | 0.40              |
| 3:G:128:CYS:O      | 3:G:130:ASP:N      | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 325/327 (99%)   | 316 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 1   | C     | 325/327 (99%)   | 315 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 1   | E     | 326/327 (100%)  | 309 (95%)  | 17 (5%)  | 0        | 100         | 100 |
| 2   | B     | 165/174 (95%)   | 157 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 2   | D     | 167/174 (96%)   | 153 (92%)  | 14 (8%)  | 0        | 100         | 100 |
| 2   | F     | 171/174 (98%)   | 162 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 3   | G     | 222/229 (97%)   | 204 (92%)  | 16 (7%)  | 2 (1%)   | 14          | 41  |
| 3   | I     | 219/229 (96%)   | 207 (94%)  | 11 (5%)  | 1 (0%)   | 24          | 54  |
| 3   | K     | 196/229 (86%)   | 177 (90%)  | 16 (8%)  | 3 (2%)   | 8           | 28  |
| 4   | H     | 209/214 (98%)   | 200 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 54  |
| 4   | J     | 210/214 (98%)   | 195 (93%)  | 14 (7%)  | 1 (0%)   | 24          | 54  |
| 4   | L     | 201/214 (94%)   | 190 (94%)  | 10 (5%)  | 1 (0%)   | 24          | 54  |
| All | All   | 2736/2832 (97%) | 2585 (94%) | 142 (5%) | 9 (0%)   | 36          | 65  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | K     | 12  | VAL  |
| 4   | L     | 86  | VAL  |
| 3   | G     | 130 | ASP  |
| 4   | J     | 86  | VAL  |
| 4   | H     | 86  | VAL  |
| 3   | K     | 184 | THR  |
| 3   | I     | 12  | VAL  |
| 3   | K     | 13  | GLN  |
| 3   | G     | 129 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 288/288 (100%)  | 243 (84%)  | 45 (16%)  | 2           | 9  |
| 1   | C     | 288/288 (100%)  | 259 (90%)  | 29 (10%)  | 7           | 24 |
| 1   | E     | 289/288 (100%)  | 249 (86%)  | 40 (14%)  | 3           | 12 |
| 2   | B     | 147/151 (97%)   | 129 (88%)  | 18 (12%)  | 5           | 16 |
| 2   | D     | 148/151 (98%)   | 124 (84%)  | 24 (16%)  | 2           | 8  |
| 2   | F     | 150/151 (99%)   | 138 (92%)  | 12 (8%)   | 11          | 34 |
| 3   | G     | 192/197 (98%)   | 150 (78%)  | 42 (22%)  | 1           | 3  |
| 3   | I     | 190/197 (96%)   | 154 (81%)  | 36 (19%)  | 1           | 5  |
| 3   | K     | 173/197 (88%)   | 137 (79%)  | 36 (21%)  | 1           | 4  |
| 4   | H     | 184/187 (98%)   | 145 (79%)  | 39 (21%)  | 1           | 4  |
| 4   | J     | 185/187 (99%)   | 137 (74%)  | 48 (26%)  | 0           | 2  |
| 4   | L     | 179/187 (96%)   | 136 (76%)  | 43 (24%)  | 1           | 2  |
| All | All   | 2413/2469 (98%) | 2001 (83%) | 412 (17%) | 2           | 7  |

All (412) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 12    | GLN  |
| 1   | A     | 23    | THR  |
| 1   | A     | 25    | LYS  |
| 1   | A     | 30    | LEU  |
| 1   | A     | 32    | ARG  |
| 1   | A     | 53    | LYS  |
| 1   | A     | 53(A) | LEU  |
| 1   | A     | 60    | GLU  |
| 1   | A     | 78    | ARG  |
| 1   | A     | 80    | LEU  |
| 1   | A     | 81    | SER  |
| 1   | A     | 81(A) | VAL  |
| 1   | A     | 85    | SER  |
| 1   | A     | 96    | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 97  | CYS  |
| 1   | A     | 128 | THR  |
| 1   | A     | 132 | THR  |
| 1   | A     | 133 | THR  |
| 1   | A     | 137 | ARG  |
| 1   | A     | 141 | VAL  |
| 1   | A     | 142 | SER  |
| 1   | A     | 150 | ASN  |
| 1   | A     | 152 | VAL  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 155 | THR  |
| 1   | A     | 156 | GLU  |
| 1   | A     | 167 | SER  |
| 1   | A     | 175 | GLN  |
| 1   | A     | 182 | VAL  |
| 1   | A     | 189 | THR  |
| 1   | A     | 198 | VAL  |
| 1   | A     | 200 | THR  |
| 1   | A     | 204 | VAL  |
| 1   | A     | 212 | ARG  |
| 1   | A     | 213 | SER  |
| 1   | A     | 217 | ILE  |
| 1   | A     | 219 | THR  |
| 1   | A     | 223 | VAL  |
| 1   | A     | 260 | ILE  |
| 1   | A     | 264 | SER  |
| 1   | A     | 265 | SER  |
| 1   | A     | 273 | THR  |
| 1   | A     | 277 | CYS  |
| 1   | A     | 325 | GLN  |
| 1   | A     | 326 | ILE  |
| 2   | B     | 18  | VAL  |
| 2   | B     | 19  | ASP  |
| 2   | B     | 30  | GLN  |
| 2   | B     | 32  | SER  |
| 2   | B     | 38  | LYS  |
| 2   | B     | 58  | LYS  |
| 2   | B     | 60  | ASN  |
| 2   | B     | 66  | VAL  |
| 2   | B     | 73  | LEU  |
| 2   | B     | 105 | GLU  |
| 2   | B     | 116 | LYS  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | B     | 121    | LYS  |
| 2   | B     | 127[A] | ARG  |
| 2   | B     | 127[B] | ARG  |
| 2   | B     | 148    | CYS  |
| 2   | B     | 161    | LYS  |
| 2   | B     | 167    | LYS  |
| 2   | B     | 172    | GLU  |
| 1   | C     | 25     | LYS  |
| 1   | C     | 30     | LEU  |
| 1   | C     | 31     | GLU  |
| 1   | C     | 45     | LYS  |
| 1   | C     | 78     | ARG  |
| 1   | C     | 94     | ARG  |
| 1   | C     | 114    | SER  |
| 1   | C     | 120    | ILE  |
| 1   | C     | 121    | LEU  |
| 1   | C     | 123    | LYS  |
| 1   | C     | 128    | THR  |
| 1   | C     | 133    | THR  |
| 1   | C     | 137    | ARG  |
| 1   | C     | 139    | CYS  |
| 1   | C     | 141    | VAL  |
| 1   | C     | 157    | LYS  |
| 1   | C     | 160    | ASN  |
| 1   | C     | 163    | VAL  |
| 1   | C     | 182    | VAL  |
| 1   | C     | 192    | ARG  |
| 1   | C     | 214    | THR  |
| 1   | C     | 217    | ILE  |
| 1   | C     | 247    | SER  |
| 1   | C     | 256    | TYR  |
| 1   | C     | 264    | SER  |
| 1   | C     | 274    | LEU  |
| 1   | C     | 283    | THR  |
| 1   | C     | 312    | GLU  |
| 1   | C     | 323    | VAL  |
| 2   | D     | 18     | VAL  |
| 2   | D     | 27     | SER  |
| 2   | D     | 29     | ASP  |
| 2   | D     | 38     | LYS  |
| 2   | D     | 52     | VAL  |
| 2   | D     | 55     | VAL  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | D     | 59     | MET  |
| 2   | D     | 61     | THR  |
| 2   | D     | 71     | SER  |
| 2   | D     | 73     | LEU  |
| 2   | D     | 86     | ASP  |
| 2   | D     | 113    | SER  |
| 2   | D     | 116    | LYS  |
| 2   | D     | 126    | LEU  |
| 2   | D     | 127[A] | ARG  |
| 2   | D     | 127[B] | ARG  |
| 2   | D     | 128    | ASP  |
| 2   | D     | 129    | ASN  |
| 2   | D     | 130    | VAL  |
| 2   | D     | 147    | GLU  |
| 2   | D     | 158    | ASP  |
| 2   | D     | 164    | GLU  |
| 2   | D     | 165    | GLU  |
| 2   | D     | 167    | LYS  |
| 1   | E     | 23     | THR  |
| 1   | E     | 24     | GLU  |
| 1   | E     | 25     | LYS  |
| 1   | E     | 28     | THR  |
| 1   | E     | 30     | LEU  |
| 1   | E     | 33     | ASN  |
| 1   | E     | 59     | LEU  |
| 1   | E     | 65     | SER  |
| 1   | E     | 76     | CYS  |
| 1   | E     | 78     | ARG  |
| 1   | E     | 79     | LEU  |
| 1   | E     | 80     | LEU  |
| 1   | E     | 88     | MET  |
| 1   | E     | 96     | LEU  |
| 1   | E     | 120    | ILE  |
| 1   | E     | 128    | THR  |
| 1   | E     | 131    | THR  |
| 1   | E     | 136    | SER  |
| 1   | E     | 141    | VAL  |
| 1   | E     | 142    | SER  |
| 1   | E     | 146    | SER  |
| 1   | E     | 152    | VAL  |
| 1   | E     | 155    | THR  |
| 1   | E     | 156    | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | E     | 157    | LYS  |
| 1   | E     | 165    | LYS  |
| 1   | E     | 182    | VAL  |
| 1   | E     | 189    | THR  |
| 1   | E     | 202    | VAL  |
| 1   | E     | 204    | VAL  |
| 1   | E     | 210    | ASN  |
| 1   | E     | 213    | SER  |
| 1   | E     | 238    | ASP  |
| 1   | E     | 243    | ILE  |
| 1   | E     | 256    | TYR  |
| 1   | E     | 260    | ILE  |
| 1   | E     | 261    | SER  |
| 1   | E     | 277    | CYS  |
| 1   | E     | 305    | CYS  |
| 1   | E     | 307[A] | LYS  |
| 2   | F     | 18     | VAL  |
| 2   | F     | 22     | TYR  |
| 2   | F     | 38     | LYS  |
| 2   | F     | 59     | MET  |
| 2   | F     | 64     | GLU  |
| 2   | F     | 72     | ASN  |
| 2   | F     | 82     | LYS  |
| 2   | F     | 121    | LYS  |
| 2   | F     | 139    | GLU  |
| 2   | F     | 145    | ASP  |
| 2   | F     | 148    | CYS  |
| 2   | F     | 164    | GLU  |
| 3   | G     | 5      | VAL  |
| 3   | G     | 6      | GLU  |
| 3   | G     | 12     | VAL  |
| 3   | G     | 13     | GLN  |
| 3   | G     | 20     | LEU  |
| 3   | G     | 25     | SER  |
| 3   | G     | 51     | ILE  |
| 3   | G     | 56     | THR  |
| 3   | G     | 71     | ARG  |
| 3   | G     | 83     | ARG  |
| 3   | G     | 87     | SER  |
| 3   | G     | 89     | THR  |
| 3   | G     | 94     | ARG  |
| 3   | G     | 107    | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 109 | VAL  |
| 3   | G     | 110 | ILE  |
| 3   | G     | 111 | VAL  |
| 3   | G     | 113 | SER  |
| 3   | G     | 131 | THR  |
| 3   | G     | 137 | THR  |
| 3   | G     | 138 | LEU  |
| 3   | G     | 141 | LEU  |
| 3   | G     | 151 | THR  |
| 3   | G     | 153 | THR  |
| 3   | G     | 160 | SER  |
| 3   | G     | 165 | THR  |
| 3   | G     | 170 | LEU  |
| 3   | G     | 172 | SER  |
| 3   | G     | 173 | ASP  |
| 3   | G     | 174 | LEU  |
| 3   | G     | 177 | LEU  |
| 3   | G     | 181 | VAL  |
| 3   | G     | 182 | THR  |
| 3   | G     | 183 | VAL  |
| 3   | G     | 187 | THR  |
| 3   | G     | 193 | ILE  |
| 3   | G     | 194 | THR  |
| 3   | G     | 195 | CYS  |
| 3   | G     | 202 | SER  |
| 3   | G     | 206 | VAL  |
| 3   | G     | 209 | LYS  |
| 3   | G     | 210 | ILE  |
| 4   | H     | 3   | ASP  |
| 4   | H     | 16  | SER  |
| 4   | H     | 17  | LEU  |
| 4   | H     | 24  | THR  |
| 4   | H     | 26  | LEU  |
| 4   | H     | 29  | GLN  |
| 4   | H     | 30  | THR  |
| 4   | H     | 49  | LEU  |
| 4   | H     | 56  | LEU  |
| 4   | H     | 58  | ASP  |
| 4   | H     | 67  | SER  |
| 4   | H     | 74  | SER  |
| 4   | H     | 79  | SER  |
| 4   | H     | 81  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 86  | VAL  |
| 4   | H     | 95  | SER  |
| 4   | H     | 106 | LEU  |
| 4   | H     | 112 | ASP  |
| 4   | H     | 117 | VAL  |
| 4   | H     | 119 | ILE  |
| 4   | H     | 123 | SER  |
| 4   | H     | 127 | LEU  |
| 4   | H     | 128 | THR  |
| 4   | H     | 134 | VAL  |
| 4   | H     | 136 | CYS  |
| 4   | H     | 144 | LYS  |
| 4   | H     | 149 | LYS  |
| 4   | H     | 156 | GLU  |
| 4   | H     | 168 | GLN  |
| 4   | H     | 170 | SER  |
| 4   | H     | 172 | ASP  |
| 4   | H     | 173 | SER  |
| 4   | H     | 178 | SER  |
| 4   | H     | 197 | GLU  |
| 4   | H     | 199 | THR  |
| 4   | H     | 202 | THR  |
| 4   | H     | 204 | THR  |
| 4   | H     | 205 | SER  |
| 4   | H     | 213 | ARG  |
| 3   | I     | 11  | LEU  |
| 3   | I     | 21  | SER  |
| 3   | I     | 22  | CYS  |
| 3   | I     | 24  | THR  |
| 3   | I     | 28  | THR  |
| 3   | I     | 34  | MET  |
| 3   | I     | 68  | THR  |
| 3   | I     | 74  | SER  |
| 3   | I     | 75  | GLN  |
| 3   | I     | 76  | SER  |
| 3   | I     | 83  | ARG  |
| 3   | I     | 85  | GLU  |
| 3   | I     | 87  | SER  |
| 3   | I     | 96  | LYS  |
| 3   | I     | 109 | VAL  |
| 3   | I     | 112 | SER  |
| 3   | I     | 127 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 128 | CYS  |
| 3   | I     | 130 | ASP  |
| 3   | I     | 132 | THR  |
| 3   | I     | 138 | LEU  |
| 3   | I     | 142 | VAL  |
| 3   | I     | 153 | THR  |
| 3   | I     | 155 | ASN  |
| 3   | I     | 156 | SER  |
| 3   | I     | 158 | SER  |
| 3   | I     | 159 | LEU  |
| 3   | I     | 163 | VAL  |
| 3   | I     | 171 | GLN  |
| 3   | I     | 176 | THR  |
| 3   | I     | 178 | SER  |
| 3   | I     | 180 | SER  |
| 3   | I     | 181 | VAL  |
| 3   | I     | 183 | VAL  |
| 3   | I     | 186 | SER  |
| 3   | I     | 187 | THR  |
| 4   | J     | 4   | ILE  |
| 4   | J     | 14  | SER  |
| 4   | J     | 20  | SER  |
| 4   | J     | 24  | THR  |
| 4   | J     | 28  | SER  |
| 4   | J     | 39  | GLN  |
| 4   | J     | 49  | LEU  |
| 4   | J     | 50  | ILE  |
| 4   | J     | 56  | LEU  |
| 4   | J     | 60  | VAL  |
| 4   | J     | 62  | SER  |
| 4   | J     | 63  | ARG  |
| 4   | J     | 65  | SER  |
| 4   | J     | 67  | SER  |
| 4   | J     | 69  | SER  |
| 4   | J     | 71  | THR  |
| 4   | J     | 74  | SER  |
| 4   | J     | 75  | PHE  |
| 4   | J     | 76  | LYS  |
| 4   | J     | 80  | LEU  |
| 4   | J     | 81  | GLN  |
| 4   | J     | 86  | VAL  |
| 4   | J     | 87  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 93  | LEU  |
| 4   | J     | 96  | THR  |
| 4   | J     | 105 | ARG  |
| 4   | J     | 107 | GLU  |
| 4   | J     | 108 | ILE  |
| 4   | J     | 116 | THR  |
| 4   | J     | 119 | ILE  |
| 4   | J     | 128 | THR  |
| 4   | J     | 134 | VAL  |
| 4   | J     | 155 | SER  |
| 4   | J     | 156 | GLU  |
| 4   | J     | 161 | VAL  |
| 4   | J     | 162 | LEU  |
| 4   | J     | 166 | THR  |
| 4   | J     | 170 | SER  |
| 4   | J     | 171 | LYS  |
| 4   | J     | 182 | THR  |
| 4   | J     | 186 | ASP  |
| 4   | J     | 195 | THR  |
| 4   | J     | 199 | THR  |
| 4   | J     | 202 | THR  |
| 4   | J     | 204 | THR  |
| 4   | J     | 207 | ILE  |
| 4   | J     | 208 | VAL  |
| 4   | J     | 214 | ASN  |
| 3   | K     | 3   | LYS  |
| 3   | K     | 5   | VAL  |
| 3   | K     | 6   | GLU  |
| 3   | K     | 7   | SER  |
| 3   | K     | 24  | THR  |
| 3   | K     | 30  | THR  |
| 3   | K     | 58  | GLU  |
| 3   | K     | 64  | LYS  |
| 3   | K     | 68  | THR  |
| 3   | K     | 76  | SER  |
| 3   | K     | 96  | LYS  |
| 3   | K     | 108 | SER  |
| 3   | K     | 109 | VAL  |
| 3   | K     | 110 | ILE  |
| 3   | K     | 111 | VAL  |
| 3   | K     | 113 | SER  |
| 3   | K     | 114 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | K     | 150 | VAL  |
| 3   | K     | 156 | SER  |
| 3   | K     | 159 | LEU  |
| 3   | K     | 163 | VAL  |
| 3   | K     | 165 | THR  |
| 3   | K     | 169 | VAL  |
| 3   | K     | 173 | ASP  |
| 3   | K     | 174 | LEU  |
| 3   | K     | 177 | LEU  |
| 3   | K     | 178 | SER  |
| 3   | K     | 180 | SER  |
| 3   | K     | 181 | VAL  |
| 3   | K     | 188 | TRP  |
| 3   | K     | 190 | SER  |
| 3   | K     | 192 | SER  |
| 3   | K     | 193 | ILE  |
| 3   | K     | 194 | THR  |
| 3   | K     | 204 | THR  |
| 3   | K     | 208 | LYS  |
| 4   | L     | 4   | ILE  |
| 4   | L     | 7   | THR  |
| 4   | L     | 9   | SER  |
| 4   | L     | 16  | SER  |
| 4   | L     | 17  | LEU  |
| 4   | L     | 21  | VAL  |
| 4   | L     | 24  | THR  |
| 4   | L     | 25  | CYS  |
| 4   | L     | 26  | LEU  |
| 4   | L     | 29  | GLN  |
| 4   | L     | 30  | THR  |
| 4   | L     | 45  | SER  |
| 4   | L     | 65  | SER  |
| 4   | L     | 67  | SER  |
| 4   | L     | 74  | SER  |
| 4   | L     | 79  | SER  |
| 4   | L     | 81  | GLN  |
| 4   | L     | 92  | GLN  |
| 4   | L     | 95  | SER  |
| 4   | L     | 96  | THR  |
| 4   | L     | 99  | THR  |
| 4   | L     | 106 | LEU  |
| 4   | L     | 110 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L     | 112 | ASP  |
| 4   | L     | 117 | VAL  |
| 4   | L     | 124 | SER  |
| 4   | L     | 134 | VAL  |
| 4   | L     | 136 | CYS  |
| 4   | L     | 146 | ILE  |
| 4   | L     | 159 | ASN  |
| 4   | L     | 162 | LEU  |
| 4   | L     | 169 | ASP  |
| 4   | L     | 170 | SER  |
| 4   | L     | 171 | LYS  |
| 4   | L     | 177 | MET  |
| 4   | L     | 181 | LEU  |
| 4   | L     | 182 | THR  |
| 4   | L     | 183 | LEU  |
| 4   | L     | 184 | THR  |
| 4   | L     | 187 | GLU  |
| 4   | L     | 195 | THR  |
| 4   | L     | 199 | THR  |
| 4   | L     | 208 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 73  | ASN  |
| 1   | C     | 103 | ASN  |
| 1   | C     | 160 | ASN  |
| 1   | C     | 170 | ASN  |
| 2   | D     | 125 | GLN  |
| 2   | D     | 129 | ASN  |
| 2   | D     | 154 | ASN  |
| 1   | E     | 210 | ASN  |
| 1   | E     | 296 | ASN  |
| 2   | F     | 81  | ASN  |
| 2   | F     | 129 | ASN  |
| 2   | F     | 171 | ASN  |
| 3   | G     | 155 | ASN  |
| 4   | H     | 29  | GLN  |
| 4   | H     | 39  | GLN  |
| 4   | H     | 81  | GLN  |
| 3   | I     | 191 | GLN  |
| 4   | J     | 91  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 126 | GLN  |
| 3   | K     | 191 | GLN  |
| 3   | K     | 196 | ASN  |
| 4   | L     | 39  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

14 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | NAG  | M     | 1   | 5,1  | 14,14,15     | 0.53 | 0           | 17,19,21    | 1.01 | 1 (5%)      |
| 5   | NAG  | M     | 2   | 5    | 14,14,15     | 0.57 | 0           | 17,19,21    | 1.33 | 3 (17%)     |
| 5   | BMA  | M     | 3   | 5    | 11,11,12     | 0.67 | 0           | 15,15,17    | 0.52 | 0           |
| 6   | NAG  | N     | 1   | 1,6  | 14,14,15     | 0.50 | 0           | 17,19,21    | 1.11 | 1 (5%)      |
| 6   | NAG  | N     | 2   | 6    | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.92 | 0           |
| 6   | BMA  | N     | 3   | 6    | 11,11,12     | 0.56 | 0           | 15,15,17    | 1.14 | 2 (13%)     |
| 6   | MAN  | N     | 4   | 6    | 11,11,12     | 0.54 | 0           | 15,15,17    | 0.58 | 0           |
| 7   | NAG  | O     | 1   | 1,7  | 14,14,15     | 0.44 | 0           | 17,19,21    | 0.75 | 0           |
| 7   | NAG  | O     | 2   | 7    | 14,14,15     | 0.44 | 0           | 17,19,21    | 0.71 | 0           |
| 5   | NAG  | P     | 1   | 5,1  | 14,14,15     | 0.49 | 0           | 17,19,21    | 1.67 | 3 (17%)     |
| 5   | NAG  | P     | 2   | 5    | 14,14,15     | 0.50 | 0           | 17,19,21    | 1.25 | 2 (11%)     |
| 5   | BMA  | P     | 3   | 5    | 11,11,12     | 0.54 | 0           | 15,15,17    | 0.84 | 1 (6%)      |
| 7   | NAG  | Q     | 1   | 1,7  | 14,14,15     | 0.54 | 0           | 17,19,21    | 1.15 | 1 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | NAG  | Q     | 2   | 7    | 14,14,15     | 0.46 | 0        | 17,19,21    | 0.70 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | NAG  | M     | 1   | 5,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | M     | 2   | 5    | -       | 4/6/23/26 | 0/1/1/1 |
| 5   | BMA  | M     | 3   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | N     | 1   | 1,6  | -       | 4/6/23/26 | 0/1/1/1 |
| 6   | NAG  | N     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | N     | 3   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | MAN  | N     | 4   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | O     | 1   | 1,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | O     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | NAG  | P     | 1   | 5,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | NAG  | P     | 2   | 5    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | BMA  | P     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | NAG  | Q     | 1   | 1,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | Q     | 2   | 7    | -       | 4/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | P     | 1   | NAG  | C1-O5-C5 | 4.08  | 117.65      | 112.19   |
| 6   | N     | 1   | NAG  | C2-N2-C7 | -3.95 | 117.61      | 122.90   |
| 7   | Q     | 1   | NAG  | O5-C1-C2 | -3.21 | 106.32      | 111.29   |
| 5   | M     | 2   | NAG  | C2-N2-C7 | 3.11  | 127.06      | 122.90   |
| 5   | P     | 1   | NAG  | O5-C1-C2 | 2.75  | 115.54      | 111.29   |
| 5   | P     | 2   | NAG  | C4-C3-C2 | -2.62 | 107.18      | 111.02   |
| 5   | P     | 2   | NAG  | C1-O5-C5 | 2.42  | 115.42      | 112.19   |
| 6   | N     | 3   | BMA  | C1-O5-C5 | -2.38 | 108.99      | 112.19   |
| 5   | M     | 2   | NAG  | O7-C7-N2 | 2.33  | 126.09      | 121.98   |
| 6   | N     | 3   | BMA  | O5-C5-C6 | 2.27  | 112.07      | 107.66   |
| 5   | P     | 1   | NAG  | C2-N2-C7 | 2.23  | 125.89      | 122.90   |
| 5   | M     | 2   | NAG  | O7-C7-C8 | -2.22 | 118.09      | 122.05   |
| 5   | M     | 1   | NAG  | C4-C3-C2 | 2.01  | 113.97      | 111.02   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5   | P     | 3   | BMA  | O5-C5-C6 | 2.00 | 111.56      | 107.66   |

There are no chirality outliers.

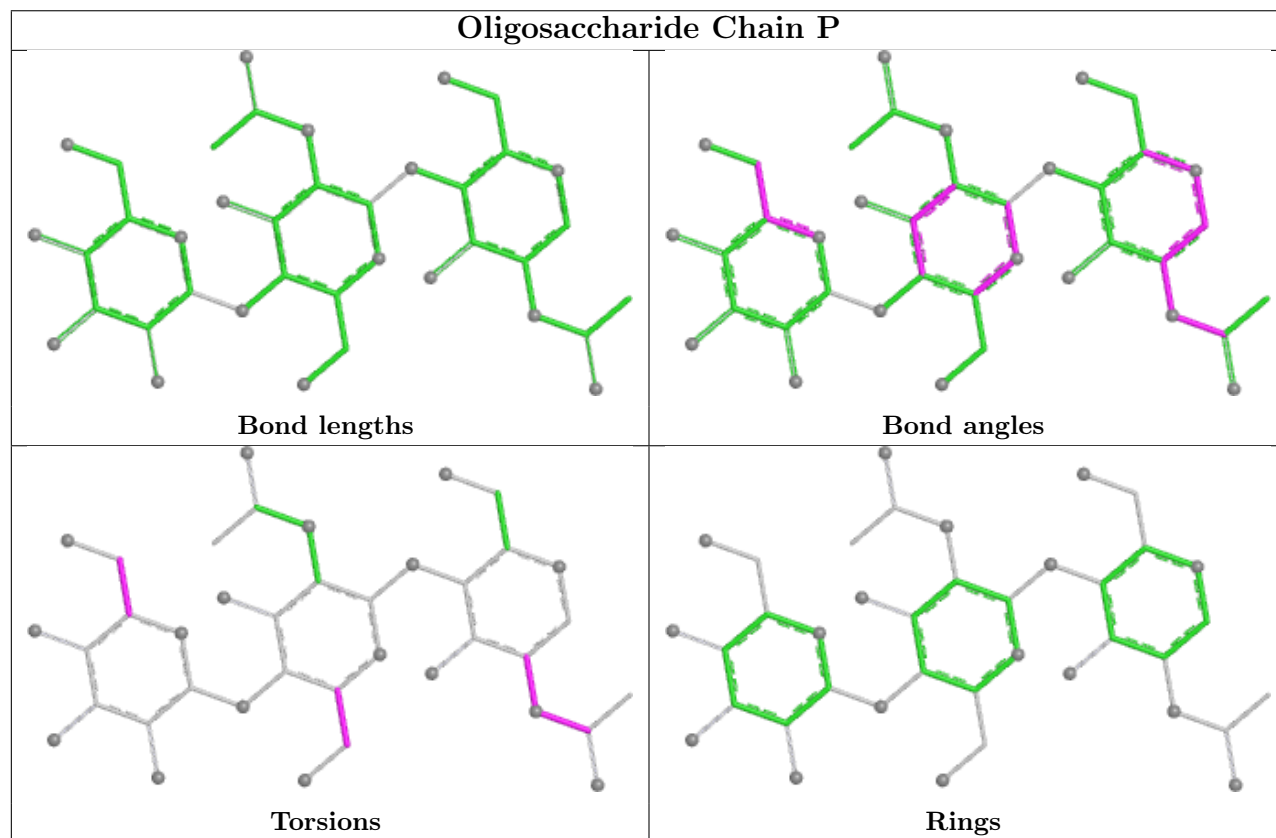
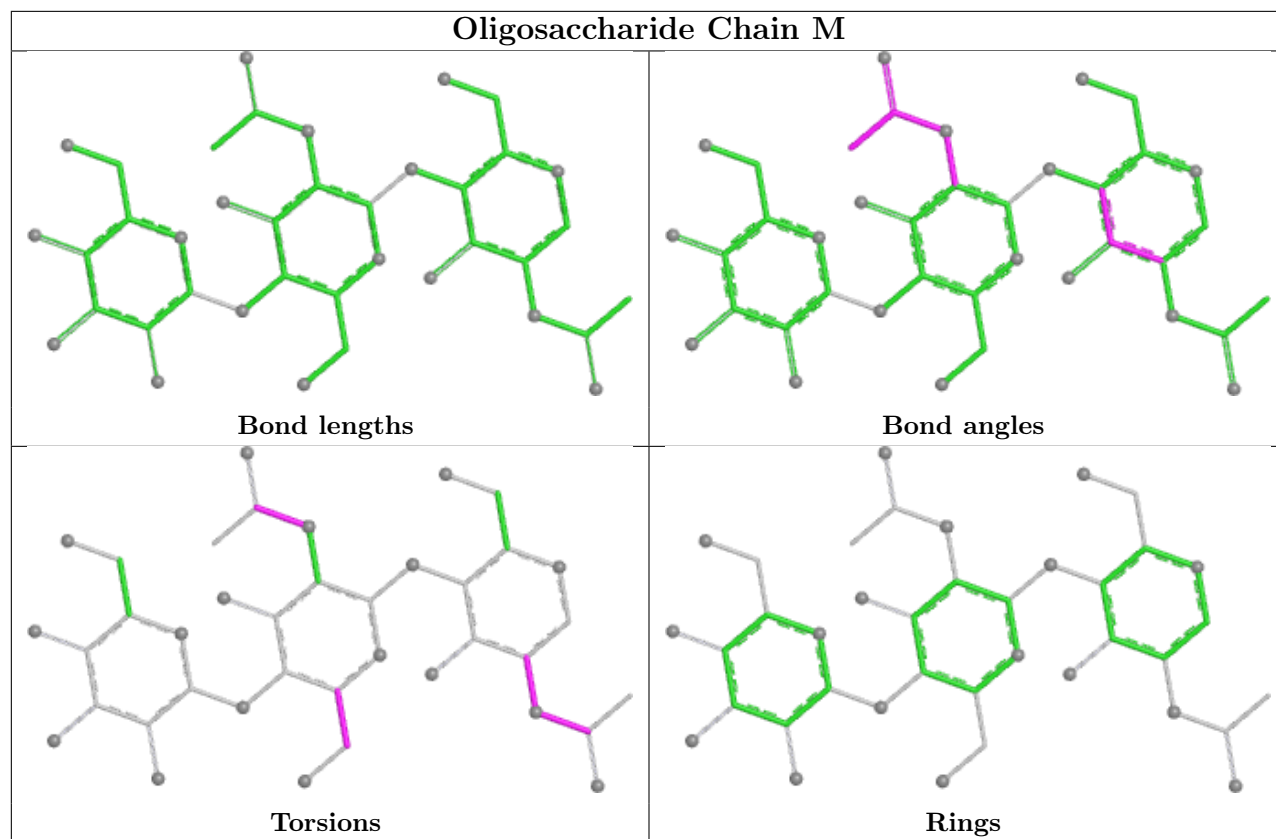
All (29) torsion outliers are listed below:

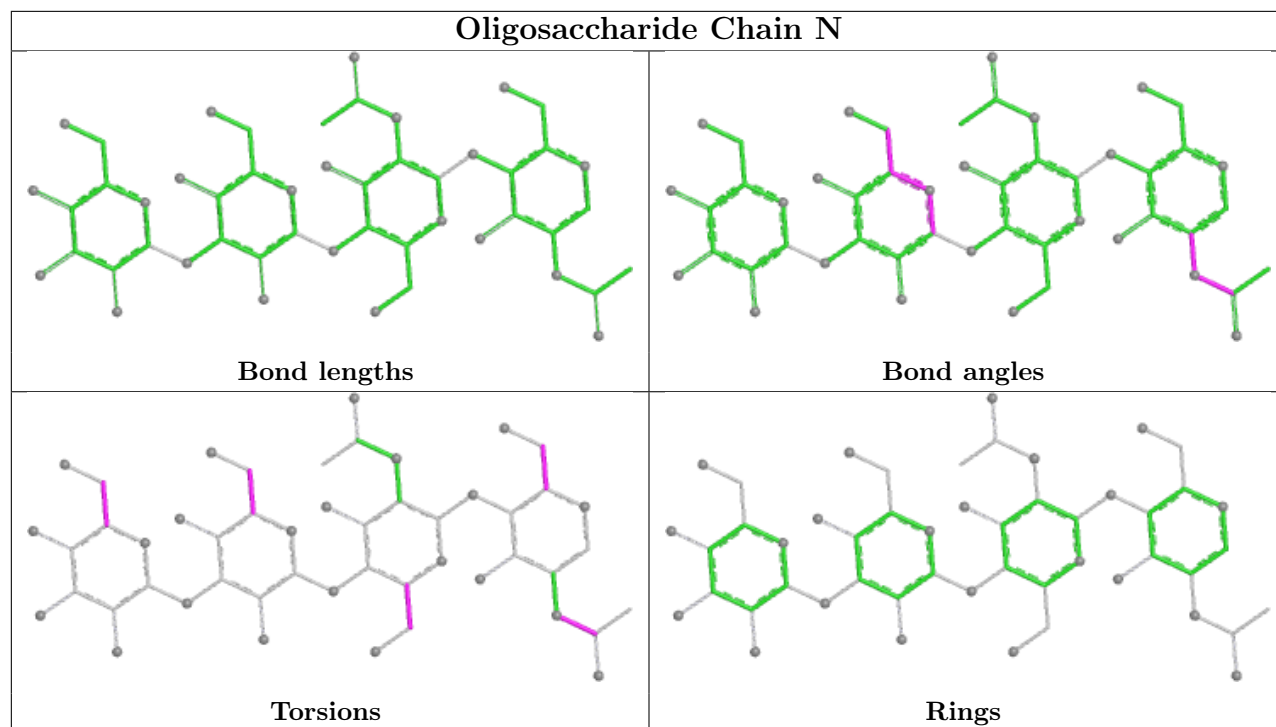
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | M     | 1   | NAG  | C3-C2-N2-C7 |
| 5   | M     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | M     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | P     | 1   | NAG  | C3-C2-N2-C7 |
| 5   | P     | 1   | NAG  | C8-C7-N2-C2 |
| 5   | P     | 1   | NAG  | O7-C7-N2-C2 |
| 7   | Q     | 2   | NAG  | C8-C7-N2-C2 |
| 7   | Q     | 2   | NAG  | O7-C7-N2-C2 |
| 7   | O     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | P     | 3   | BMA  | O5-C5-C6-O6 |
| 7   | Q     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | N     | 1   | NAG  | C8-C7-N2-C2 |
| 6   | N     | 1   | NAG  | O7-C7-N2-C2 |
| 5   | M     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | Q     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | N     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | N     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | M     | 2   | NAG  | C8-C7-N2-C2 |
| 5   | P     | 3   | BMA  | C4-C5-C6-O6 |
| 7   | O     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | N     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | M     | 2   | NAG  | O7-C7-N2-C2 |
| 6   | N     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | M     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | N     | 4   | MAN  | O5-C5-C6-O6 |
| 5   | P     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | N     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | N     | 2   | NAG  | C4-C5-C6-O6 |
| 7   | O     | 2   | NAG  | C1-C2-N2-C7 |

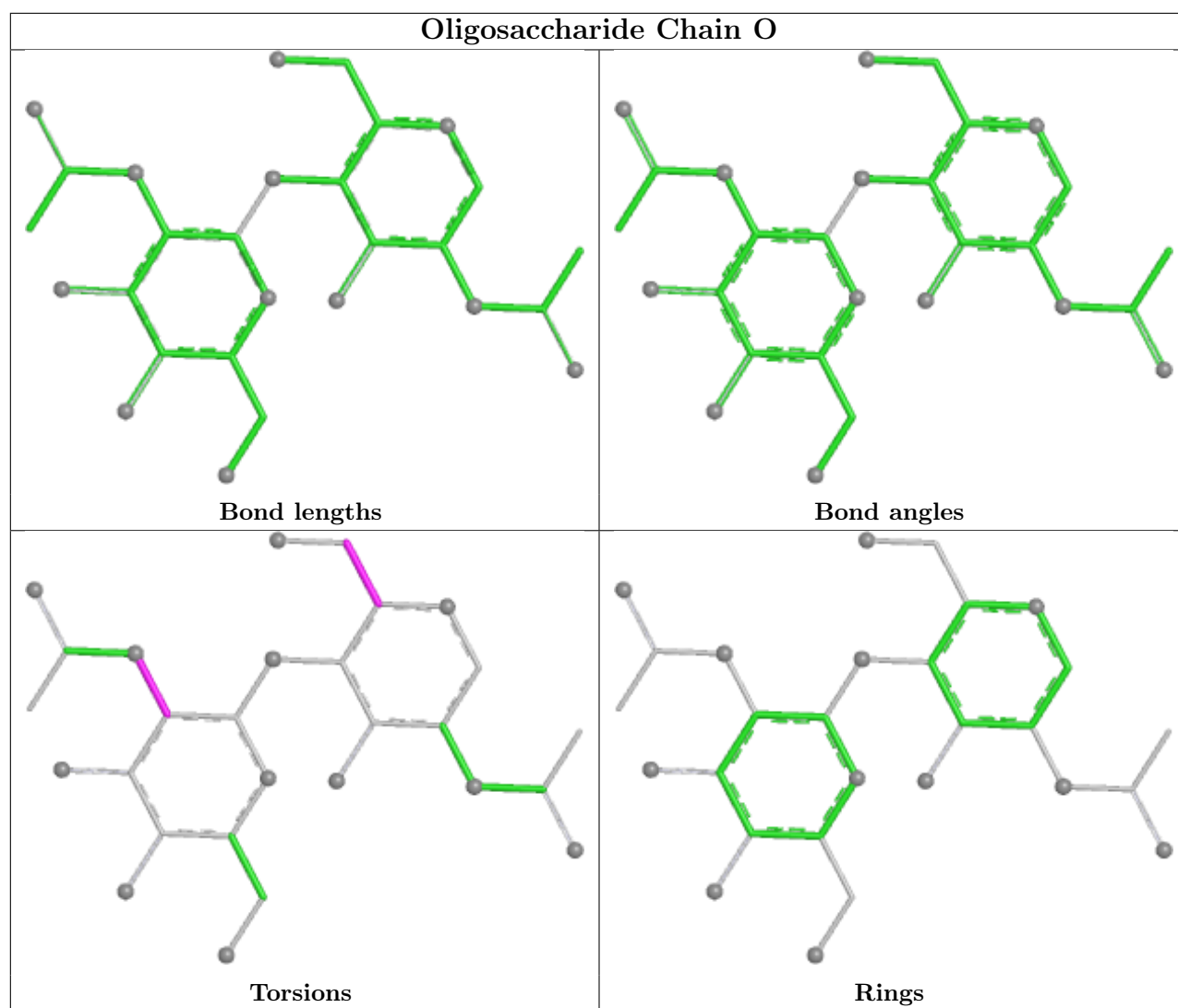
There are no ring outliers.

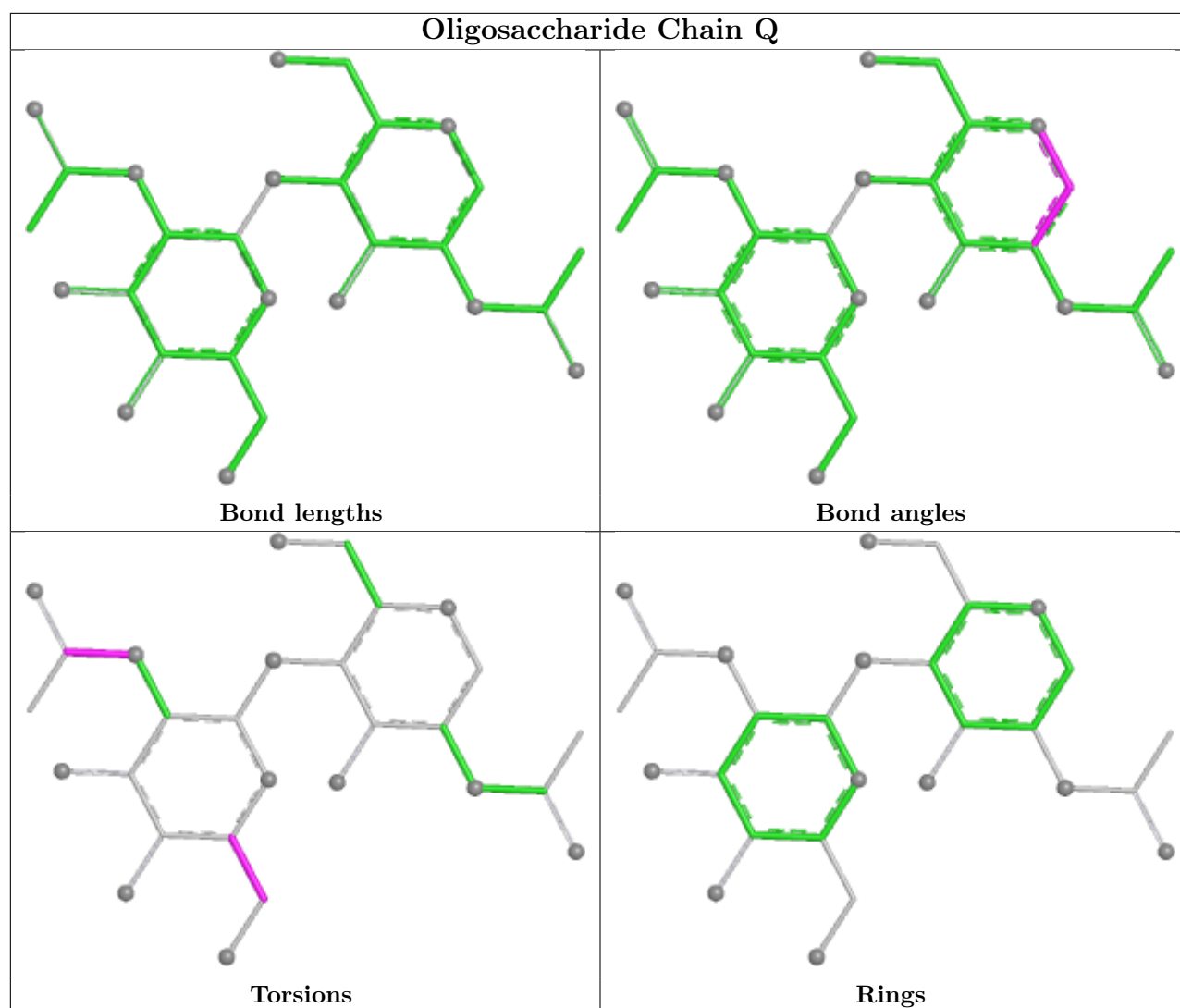
No monomer is involved in short contacts.

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









## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 8   | NAG  | E     | 401 | 1    | 14,14,15     | 0.39 | 0           | 17,19,21    | 1.39 | 3 (17%)     |
| 9   | SO4  | F     | 201 | -    | 4,4,4        | 0.28 | 0           | 6,6,6       | 0.30 | 0           |
| 8   | NAG  | B     | 202 | 2    | 14,14,15     | 0.78 | 0           | 17,19,21    | 1.32 | 2 (11%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | NAG  | A     | 405 | 1    | 14,14,15     | 0.58 | 0        | 17,19,21    | 1.05 | 1 (5%)   |
| 8   | NAG  | F     | 202 | 2    | 14,14,15     | 0.57 | 0        | 17,19,21    | 0.86 | 1 (5%)   |
| 9   | SO4  | H     | 301 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.20 | 0        |
| 9   | SO4  | J     | 301 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.16 | 0        |
| 9   | SO4  | E     | 402 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.18 | 0        |
| 9   | SO4  | B     | 201 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.24 | 0        |
| 9   | SO4  | L     | 301 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.24 | 0        |
| 10  | EDO  | J     | 302 | -    | 3,3,3        | 0.56 | 0        | 2,2,2       | 0.21 | 0        |
| 9   | SO4  | D     | 201 | -    | 4,4,4        | 0.22 | 0        | 6,6,6       | 0.20 | 0        |
| 8   | NAG  | A     | 401 | 1    | 14,14,15     | 0.50 | 0        | 17,19,21    | 1.02 | 1 (5%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | NAG  | E     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 8   | NAG  | B     | 202 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | A     | 405 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 8   | NAG  | F     | 202 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | EDO  | J     | 302 | -    | -       | 0/1/1/1   | -       |
| 8   | NAG  | A     | 401 | 1    | -       | 2/6/23/26 | 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(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | E     | 401 | NAG  | C1-O5-C5 | 3.87  | 117.37      | 112.19   |
| 8   | A     | 401 | NAG  | C1-O5-C5 | 3.62  | 117.04      | 112.19   |
| 8   | A     | 405 | NAG  | C1-O5-C5 | 3.01  | 116.22      | 112.19   |
| 8   | B     | 202 | NAG  | C2-N2-C7 | 2.85  | 126.72      | 122.90   |
| 8   | E     | 401 | NAG  | O5-C1-C2 | -2.72 | 107.09      | 111.29   |
| 8   | E     | 401 | NAG  | C2-N2-C7 | -2.58 | 119.45      | 122.90   |
| 8   | B     | 202 | NAG  | C1-O5-C5 | 2.54  | 115.58      | 112.19   |
| 8   | F     | 202 | NAG  | C2-N2-C7 | -2.41 | 119.67      | 122.90   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | E     | 401 | NAG  | C4-C5-C6-O6 |
| 8   | E     | 401 | NAG  | C8-C7-N2-C2 |
| 8   | E     | 401 | NAG  | O7-C7-N2-C2 |
| 8   | A     | 405 | NAG  | O5-C5-C6-O6 |
| 8   | F     | 202 | NAG  | C4-C5-C6-O6 |
| 8   | A     | 401 | NAG  | O5-C5-C6-O6 |
| 8   | E     | 401 | NAG  | O5-C5-C6-O6 |
| 8   | A     | 405 | NAG  | C4-C5-C6-O6 |
| 8   | F     | 202 | NAG  | O5-C5-C6-O6 |
| 8   | A     | 405 | NAG  | C8-C7-N2-C2 |
| 8   | A     | 405 | NAG  | O7-C7-N2-C2 |
| 8   | A     | 401 | NAG  | C4-C5-C6-O6 |

There are no ring outliers.

5 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | F     | 201 | SO4  | 3       | 0            |
| 9   | J     | 301 | SO4  | 1       | 0            |
| 9   | L     | 301 | SO4  | 1       | 0            |
| 10  | J     | 302 | EDO  | 1       | 0            |
| 9   | D     | 201 | SO4  | 1       | 0            |

## 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     | 324/327 (99%)   | -0.20  | 4 (1%) 76 69  | 39, 94, 147, 177      | 5 (1%)  |
| 1   | C     | 324/327 (99%)   | -0.02  | 10 (3%) 51 42 | 41, 100, 147, 169     | 5 (1%)  |
| 1   | E     | 324/327 (99%)   | -0.09  | 5 (1%) 72 64  | 40, 104, 153, 223     | 6 (1%)  |
| 2   | B     | 168/174 (96%)   | -0.42  | 2 (1%) 76 69  | 45, 66, 108, 138      | 1 (0%)  |
| 2   | D     | 170/174 (97%)   | -0.27  | 3 (1%) 67 59  | 44, 79, 145, 169      | 1 (0%)  |
| 2   | F     | 172/174 (98%)   | -0.32  | 2 (1%) 76 69  | 44, 81, 126, 176      | 1 (0%)  |
| 3   | G     | 223/229 (97%)   | 0.20   | 11 (4%) 35 27 | 30, 100, 151, 246     | 1 (0%)  |
| 3   | I     | 221/229 (96%)   | 0.02   | 4 (1%) 67 59  | 45, 95, 166, 190      | 0       |
| 3   | K     | 200/229 (87%)   | -0.01  | 10 (5%) 34 27 | 32, 89, 195, 245      | 0       |
| 4   | H     | 211/214 (98%)   | 0.05   | 8 (3%) 44 36  | 42, 108, 155, 185     | 0       |
| 4   | J     | 212/214 (99%)   | 0.09   | 2 (0%) 81 75  | 49, 122, 158, 213     | 0       |
| 4   | L     | 205/214 (95%)   | 0.26   | 15 (7%) 21 17 | 46, 120, 185, 268     | 0       |
| All | All   | 2754/2832 (97%) | -0.05  | 76 (2%) 55 46 | 30, 97, 158, 268      | 20 (0%) |

All (76) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 66  | VAL  | 5.0  |
| 3   | G     | 129 | GLY  | 4.9  |
| 4   | L     | 3   | ASP  | 4.7  |
| 4   | L     | 105 | ARG  | 4.5  |
| 3   | G     | 159 | LEU  | 4.4  |
| 4   | H     | 137 | PHE  | 4.3  |
| 4   | L     | 117 | VAL  | 4.2  |
| 3   | I     | 154 | TRP  | 4.2  |
| 2   | D     | 66  | VAL  | 4.2  |
| 4   | J     | 105 | ARG  | 4.1  |
| 4   | L     | 5   | GLN  | 4.0  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 4   | J     | 5     | GLN  | 4.0  |
| 2   | B     | 66    | VAL  | 3.9  |
| 4   | H     | 105   | ARG  | 3.8  |
| 1   | C     | 326   | ILE  | 3.8  |
| 4   | L     | 119   | ILE  | 3.8  |
| 4   | H     | 5     | GLN  | 3.7  |
| 4   | L     | 120   | PHE  | 3.7  |
| 3   | K     | 189   | PRO  | 3.6  |
| 1   | C     | 159   | SER  | 3.5  |
| 4   | L     | 53    | ALA  | 3.3  |
| 3   | K     | 12    | VAL  | 3.2  |
| 1   | C     | 245   | PHE  | 3.2  |
| 4   | H     | 208   | VAL  | 3.2  |
| 2   | D     | 61    | THR  | 3.2  |
| 1   | A     | 326   | ILE  | 3.2  |
| 1   | A     | 9     | PRO  | 3.1  |
| 3   | I     | 12    | VAL  | 3.1  |
| 1   | E     | 326   | ILE  | 3.1  |
| 3   | K     | 193   | ILE  | 3.1  |
| 4   | L     | 188   | TYR  | 3.0  |
| 4   | L     | 207   | ILE  | 3.0  |
| 1   | C     | 121   | LEU  | 3.0  |
| 3   | G     | 127   | VAL  | 2.9  |
| 3   | G     | 52(A) | ASP  | 2.8  |
| 3   | G     | 124   | LEU  | 2.7  |
| 2   | D     | 65    | ALA  | 2.7  |
| 3   | K     | 159   | LEU  | 2.7  |
| 3   | K     | 182   | THR  | 2.7  |
| 4   | H     | 119   | ILE  | 2.6  |
| 1   | C     | 156   | GLU  | 2.6  |
| 4   | H     | 4     | ILE  | 2.6  |
| 2   | F     | 63    | PHE  | 2.6  |
| 4   | L     | 118   | SER  | 2.6  |
| 4   | H     | 213   | ARG  | 2.6  |
| 3   | G     | 208   | LYS  | 2.6  |
| 1   | C     | 301   | THR  | 2.6  |
| 4   | L     | 114   | ALA  | 2.6  |
| 1   | C     | 9     | PRO  | 2.5  |
| 3   | G     | 205   | LYS  | 2.5  |
| 3   | K     | 188   | TRP  | 2.5  |
| 3   | I     | 127   | VAL  | 2.5  |
| 3   | K     | 187   | THR  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 61  | THR  | 2.4  |
| 3   | G     | 214 | GLY  | 2.3  |
| 1   | E     | 127 | TRP  | 2.3  |
| 1   | C     | 158 | GLY  | 2.3  |
| 3   | G     | 131 | THR  | 2.2  |
| 1   | A     | 172 | SER  | 2.2  |
| 3   | G     | 128 | CYS  | 2.2  |
| 4   | L     | 151 | LYS  | 2.2  |
| 1   | C     | 198 | VAL  | 2.2  |
| 3   | K     | 91  | TYR  | 2.2  |
| 4   | H     | 194 | TYR  | 2.2  |
| 3   | K     | 13  | GLN  | 2.1  |
| 3   | K     | 152 | LEU  | 2.1  |
| 1   | E     | 134 | GLY  | 2.1  |
| 1   | C     | 312 | GLU  | 2.1  |
| 1   | E     | 136 | SER  | 2.1  |
| 1   | E     | 119 | LYS  | 2.1  |
| 4   | L     | 121 | PRO  | 2.1  |
| 3   | G     | 187 | THR  | 2.1  |
| 4   | L     | 198 | ALA  | 2.1  |
| 3   | I     | 160 | SER  | 2.0  |
| 1   | A     | 198 | VAL  | 2.0  |
| 4   | L     | 199 | THR  | 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.

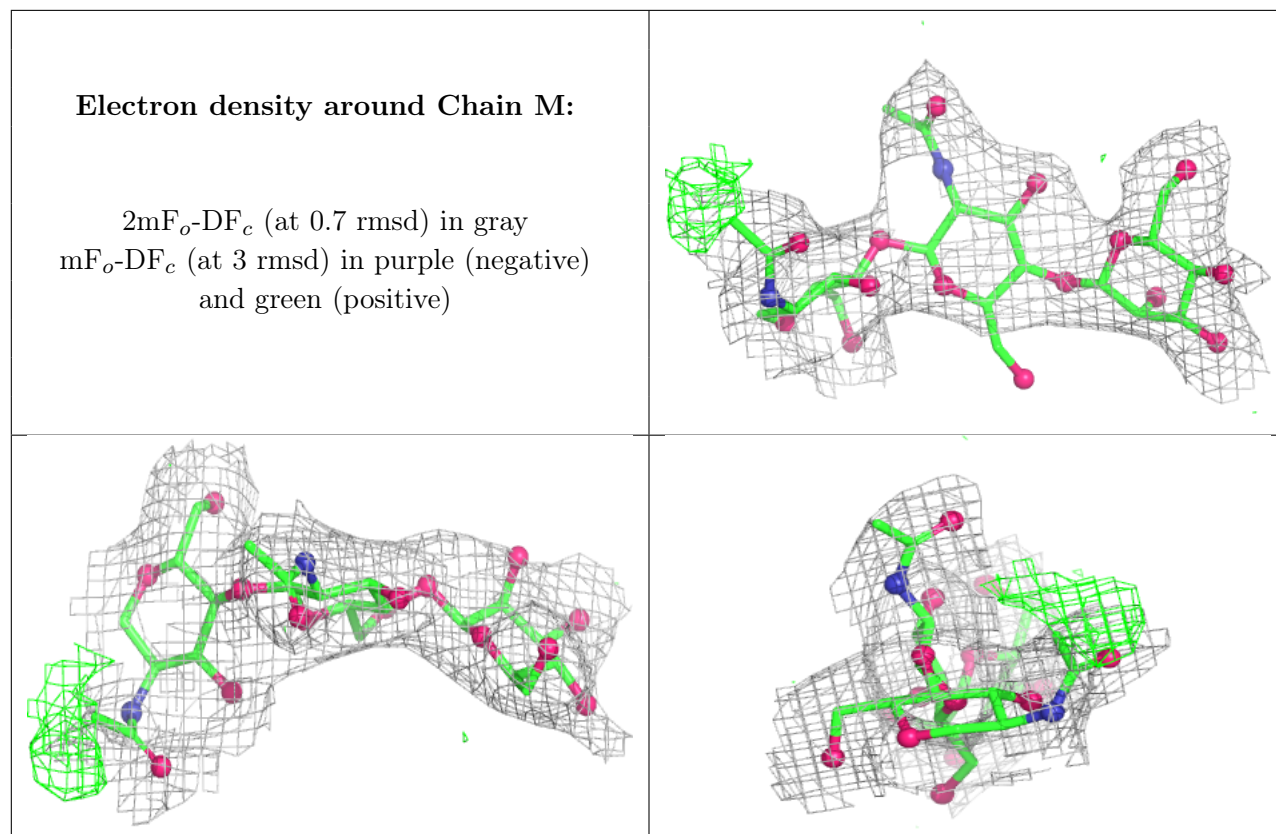
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 5   | BMA  | P     | 3   | 11/12 | 0.24 | 0.12 | 143,165,176,185            | 0     |
| 6   | MAN  | N     | 4   | 11/12 | 0.37 | 0.13 | 145,159,166,169            | 0     |
| 7   | NAG  | Q     | 2   | 14/15 | 0.50 | 0.10 | 143,165,173,175            | 0     |
| 5   | BMA  | M     | 3   | 11/12 | 0.53 | 0.11 | 105,121,129,135            | 0     |
| 5   | NAG  | M     | 1   | 14/15 | 0.60 | 0.13 | 90,122,136,143             | 0     |

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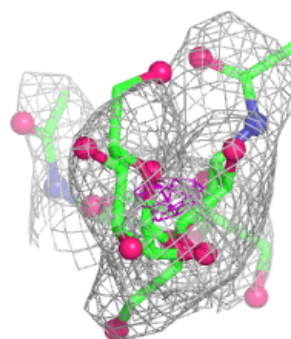
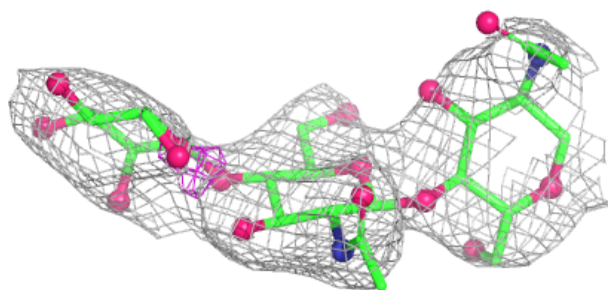
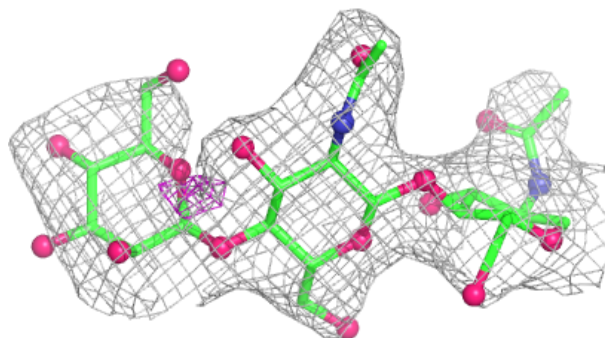
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | NAG  | N     | 1   | 14/15 | 0.61 | 0.14 | 94,109,131,134              | 0     |
| 6   | BMA  | N     | 3   | 11/12 | 0.72 | 0.08 | 103,119,135,148             | 0     |
| 7   | NAG  | O     | 2   | 14/15 | 0.74 | 0.13 | 135,182,189,192             | 0     |
| 7   | NAG  | Q     | 1   | 14/15 | 0.78 | 0.09 | 108,135,153,164             | 0     |
| 5   | NAG  | P     | 1   | 14/15 | 0.80 | 0.11 | 78,117,137,139              | 0     |
| 7   | NAG  | O     | 1   | 14/15 | 0.81 | 0.12 | 134,152,166,178             | 0     |
| 5   | NAG  | M     | 2   | 14/15 | 0.85 | 0.10 | 97,113,135,138              | 0     |
| 6   | NAG  | N     | 2   | 14/15 | 0.87 | 0.10 | 82,112,130,131              | 0     |
| 5   | NAG  | P     | 2   | 14/15 | 0.91 | 0.09 | 89,125,140,155              | 0     |

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

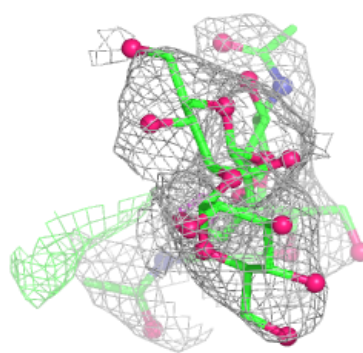
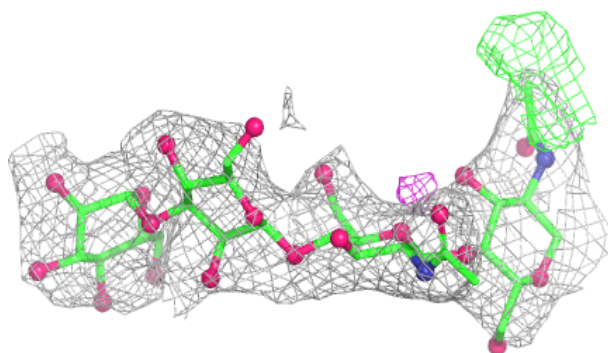
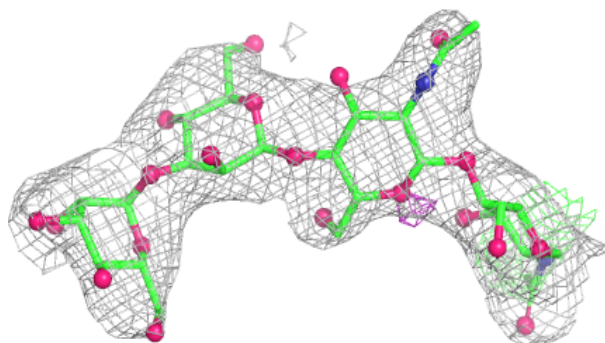


**Electron density around Chain P:**

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

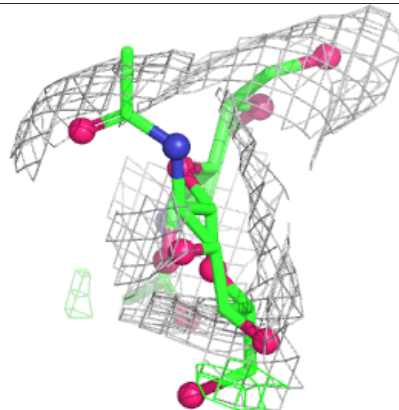
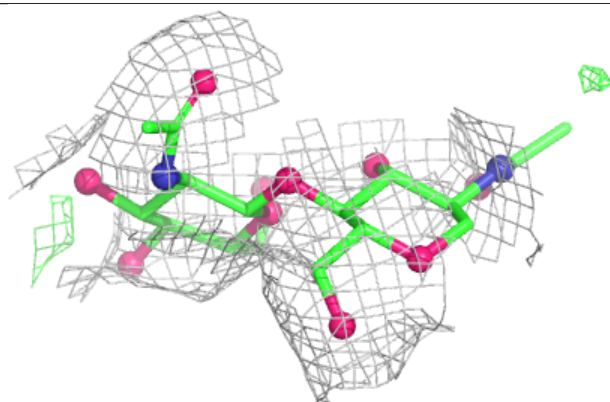
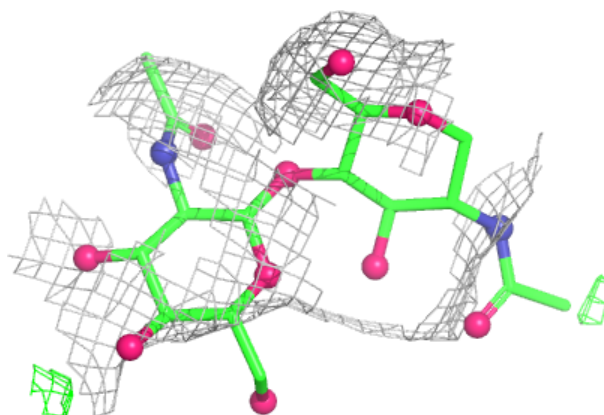
**Electron density around Chain N:**

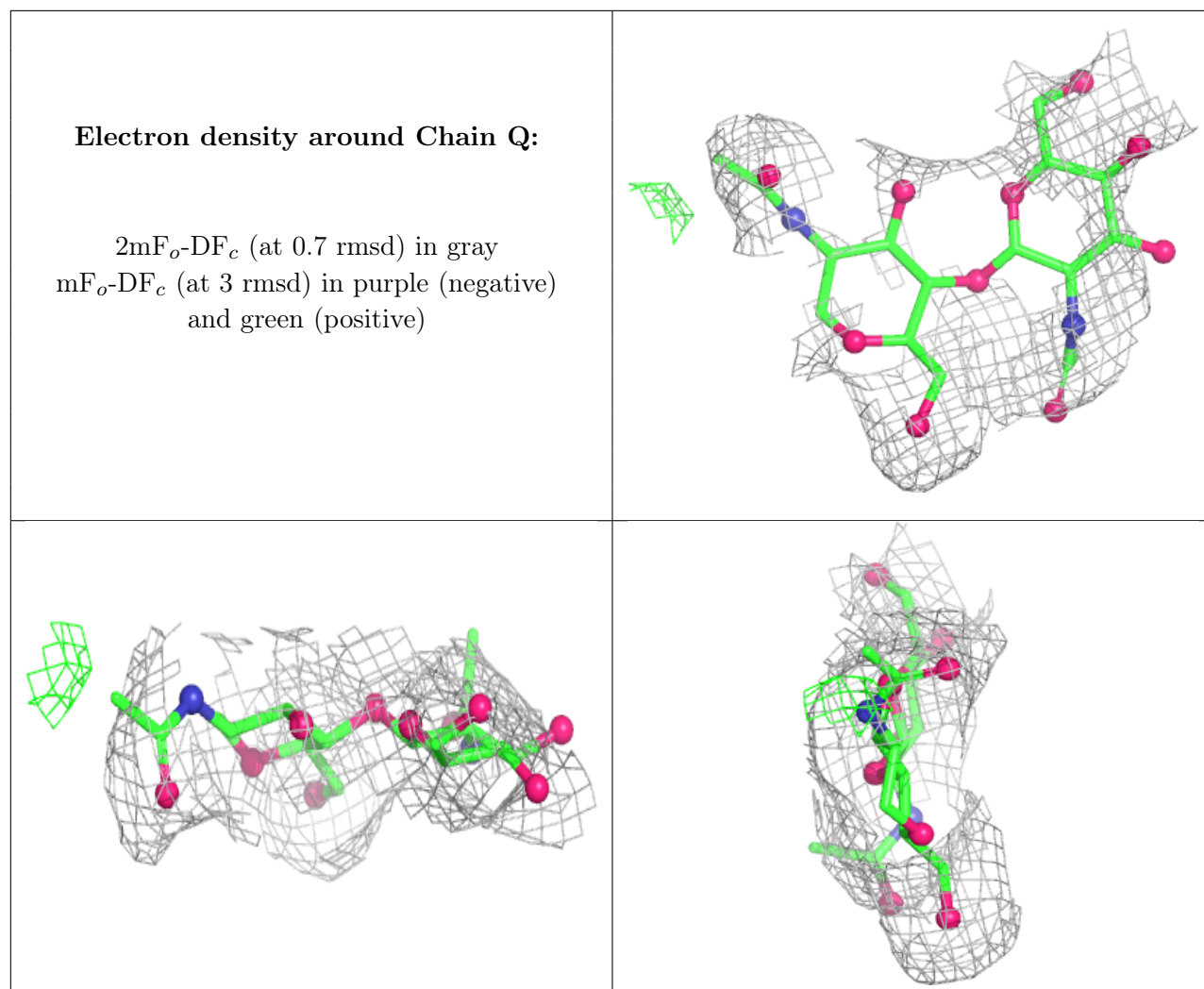
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 8   | NAG  | A     | 405 | 14/15 | 0.65 | 0.12 | 113,129,153,159            | 0     |
| 8   | NAG  | B     | 202 | 14/15 | 0.68 | 0.14 | 103,114,125,125            | 0     |
| 8   | NAG  | A     | 401 | 14/15 | 0.70 | 0.12 | 129,142,146,150            | 0     |
| 9   | SO4  | E     | 402 | 5/5   | 0.74 | 0.12 | 107,124,128,130            | 0     |
| 8   | NAG  | F     | 202 | 14/15 | 0.78 | 0.12 | 100,114,121,125            | 0     |
| 9   | SO4  | J     | 301 | 5/5   | 0.80 | 0.14 | 110,123,135,151            | 0     |
| 8   | NAG  | E     | 401 | 14/15 | 0.82 | 0.10 | 92,106,121,124             | 0     |
| 10  | EDO  | J     | 302 | 4/4   | 0.82 | 0.15 | 72,74,76,81                | 0     |
| 9   | SO4  | L     | 301 | 5/5   | 0.86 | 0.11 | 89,106,111,123             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 9   | SO4  | H     | 301 | 5/5   | 0.91 | 0.09 | 84,88,102,104               | 0     |
| 9   | SO4  | D     | 201 | 5/5   | 0.95 | 0.08 | 80,90,96,101                | 0     |
| 9   | SO4  | F     | 201 | 5/5   | 0.95 | 0.07 | 84,89,95,99                 | 0     |
| 9   | SO4  | B     | 201 | 5/5   | 0.98 | 0.04 | 54,69,74,74                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.