



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:43 AM UTC

PDB ID : 5O32 / pdb\_00005o32  
Title : The structure of complement complex  
Authors : Xue, X.; Wu, J.; Forneris, F.; Gros, P.  
Deposited on : 2017-05-23  
Resolution : 4.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

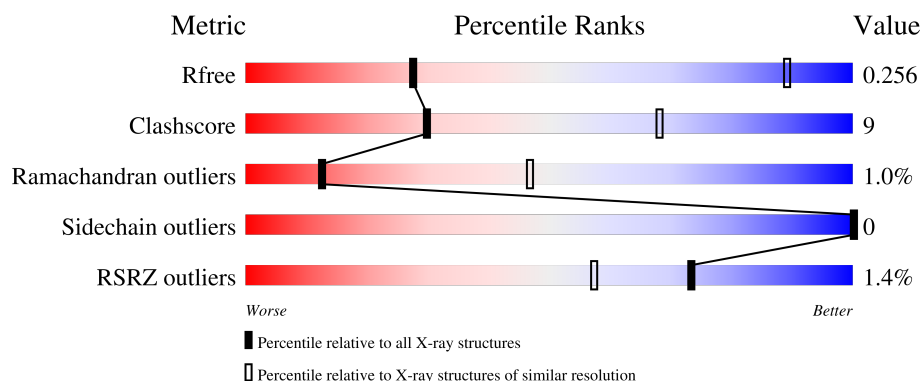
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.21 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1004 (4.52-3.88)                                      |
| Clashscore            | 190562                      | 1019 (4.50-3.90)                                      |
| Ramachandran outliers | 187476                      | 1020 (4.56-3.84)                                      |
| Sidechain outliers    | 187428                      | 1006 (4.56-3.84)                                      |
| RSRZ outliers         | 180081                      | 1001 (4.52-3.88)                                      |

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     | 645    | <div> <div>80%</div> <div>19%</div> <div>.</div> </div> |
| 1   | E     | 645    | <div> <div>82%</div> <div>17%</div> <div>.</div> </div> |
| 2   | B     | 915    | <div> <div>78%</div> <div>21%</div> <div>.</div> </div> |
| 2   | F     | 915    | <div> <div>78%</div> <div>20%</div> <div>.</div> </div> |
| 3   | C     | 383    | <div> <div>79%</div> <div>17%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                     |
|-----|-------|--------|------------------------------------------------------------------------------------------------------|
| 3   | G     | 383    | <div><div><div>%</div><div><div></div><div>81%</div><div>15%</div><div>• •</div></div></div></div>   |
| 4   | D     | 321    | <div><div><div>4%</div><div><div></div><div>73%</div><div>20%</div><div>• 6%</div></div></div></div> |
| 4   | H     | 321    | <div><div><div>2%</div><div><div></div><div>74%</div><div>18%</div><div>• 6%</div></div></div></div> |
| 5   | I     | 244    | <div><div><div>%</div><div><div></div><div>62%</div><div>34%</div><div>• •</div></div></div></div>   |
| 5   | J     | 244    | <div><div><div>3%</div><div><div></div><div>67%</div><div>30%</div><div>• •</div></div></div></div>  |
| 6   | K     | 5      | <div><div><div></div><div><div></div><div>40%</div><div>60%</div></div></div></div>                  |
| 6   | M     | 5      | <div><div><div></div><div><div></div><div>60%</div><div>40%</div></div></div></div>                  |
| 7   | L     | 2      | <div><div><div></div><div><div></div><div>100%</div></div></div></div>                               |
| 7   | N     | 2      | <div><div><div></div><div><div></div><div>50%</div><div>50%</div></div></div></div>                  |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 39091 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 Complement C3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 640      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4992  | 3179 | 846 | 952 | 15 |         |         |       |
| 1   | E     | 640      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4992  | 3179 | 846 | 952 | 15 |         |         |       |

- Molecule 2 is a protein called Complement C3.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 903      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7203  | 4565 | 1211 | 1389 | 38 |         |         |       |
| 2   | F     | 903      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7203  | 4565 | 1211 | 1389 | 38 |         |         |       |

- Molecule 3 is a protein called Complement factor H, Complement factor H.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 371      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2940  | 1836 | 510 | 565 | 29 |         |         |       |
| 3   | G     | 371      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2940  | 1836 | 510 | 565 | 29 |         |         |       |

There are 26 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| C     | 265     | LYS      | -      | linker  | UNP P08603 |
| C     | 1095    | GLY      | -      | linker  | UNP P08603 |
| C     | 1096    | GLY      | -      | linker  | UNP P08603 |
| C     | 1097    | GLY      | -      | linker  | UNP P08603 |
| C     | 1098    | GLY      | -      | linker  | UNP P08603 |
| C     | 1099    | GLY      | -      | linker  | UNP P08603 |
| C     | 1100    | GLY      | -      | linker  | UNP P08603 |
| C     | 1101    | GLY      | -      | linker  | UNP P08603 |

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| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| C     | 1102    | GLY      | -      | linker  | UNP P08603 |
| C     | 1103    | GLY      | -      | linker  | UNP P08603 |
| C     | 1104    | GLY      | -      | linker  | UNP P08603 |
| C     | 1105    | GLY      | -      | linker  | UNP P08603 |
| C     | 1106    | GLY      | -      | linker  | UNP P08603 |
| G     | 265     | LYS      | -      | linker  | UNP P08603 |
| G     | 1095    | GLY      | -      | linker  | UNP P08603 |
| G     | 1096    | GLY      | -      | linker  | UNP P08603 |
| G     | 1097    | GLY      | -      | linker  | UNP P08603 |
| G     | 1098    | GLY      | -      | linker  | UNP P08603 |
| G     | 1099    | GLY      | -      | linker  | UNP P08603 |
| G     | 1100    | GLY      | -      | linker  | UNP P08603 |
| G     | 1101    | GLY      | -      | linker  | UNP P08603 |
| G     | 1102    | GLY      | -      | linker  | UNP P08603 |
| G     | 1103    | GLY      | -      | linker  | UNP P08603 |
| G     | 1104    | GLY      | -      | linker  | UNP P08603 |
| G     | 1105    | GLY      | -      | linker  | UNP P08603 |
| G     | 1106    | GLY      | -      | linker  | UNP P08603 |

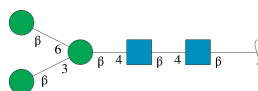
- Molecule 4 is a protein called Complement factor I.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 301      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2320  | 1422 | 407 | 456 | 35 |         |         |       |
| 4   | H     | 301      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2320  | 1422 | 407 | 456 | 35 |         |         |       |

- Molecule 5 is a protein called Complement factor I.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | I     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1911  | 1224 | 324 | 349 | 14 |         |         |       |
| 5   | J     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1911  | 1224 | 324 | 349 | 14 |         |         |       |

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



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6   | K     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 6   | M     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |

- 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   | L     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | N     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

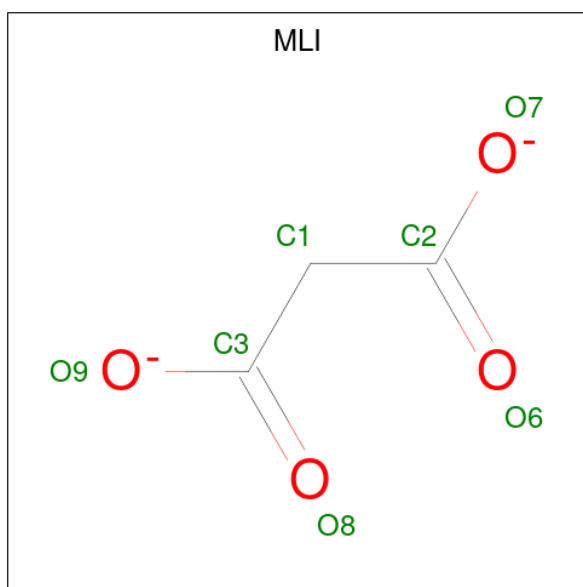
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 8   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 8   | D     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 8   | E     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 8   | H     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 9   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 9   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 10 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).

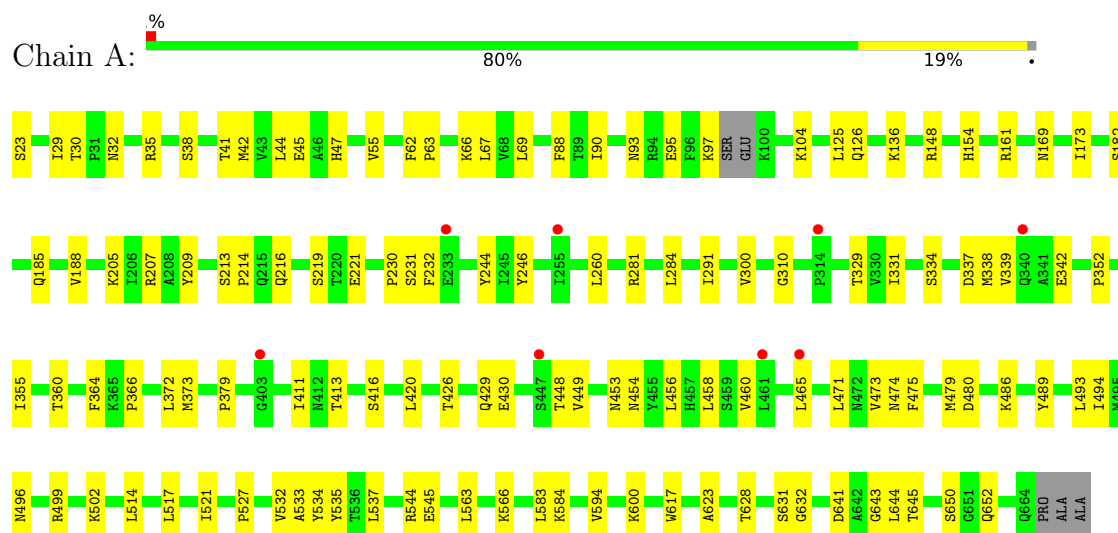


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10  | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 3 | 4 |         |         |

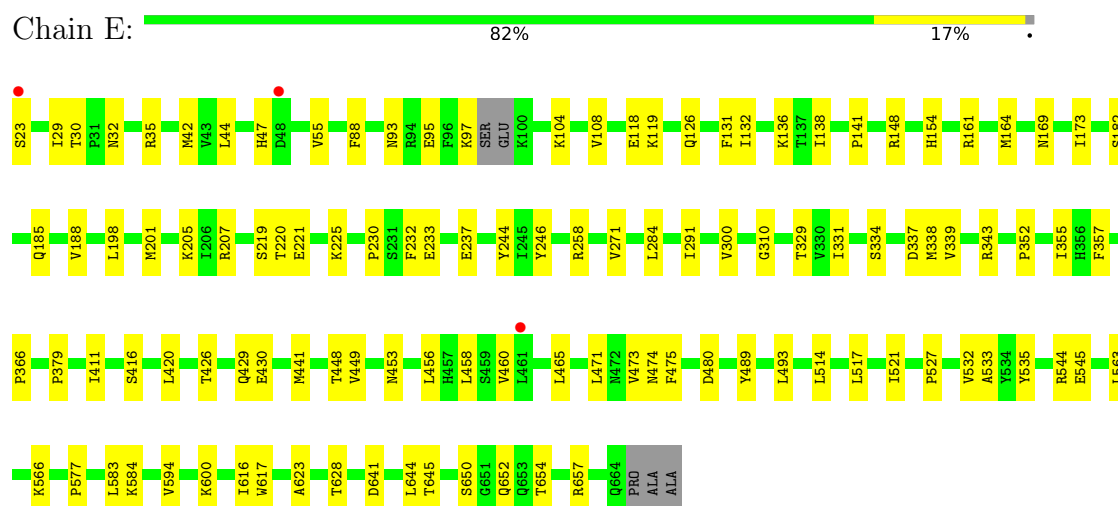
### 3 Residue-property plots

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: Complement C3

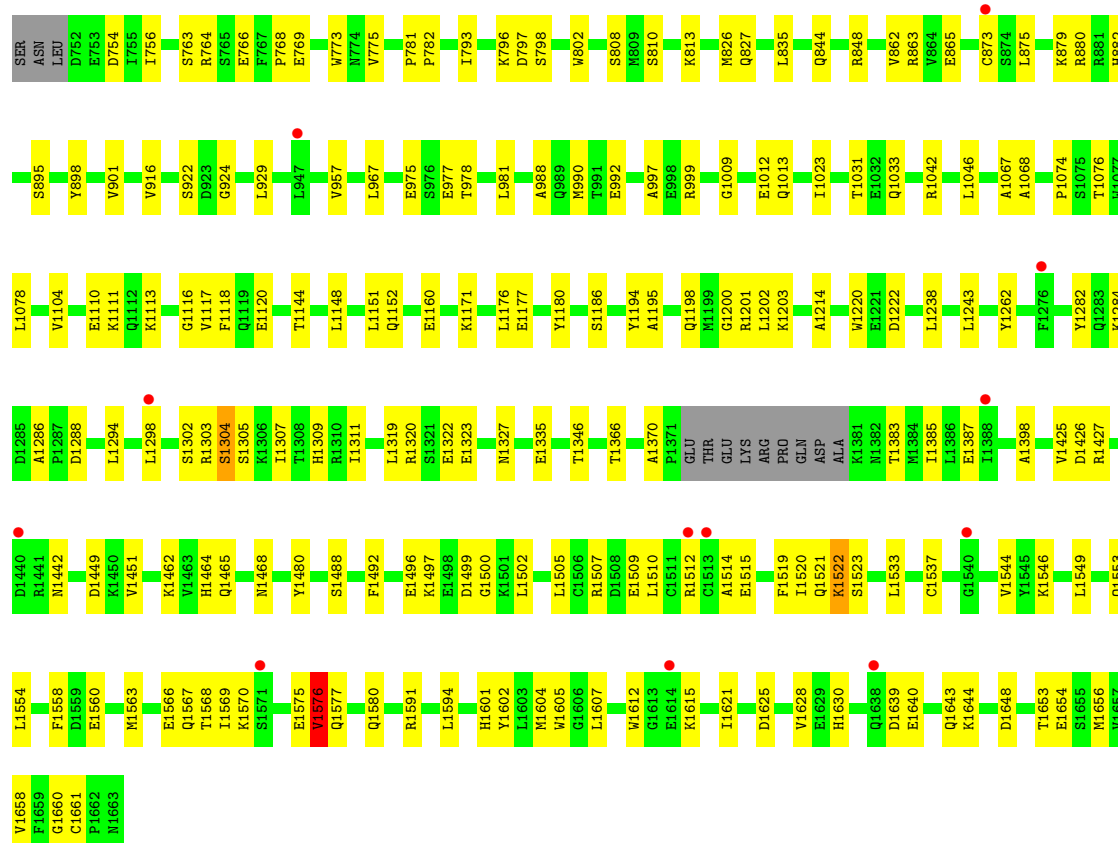


#### • Molecule 1: Complement C3

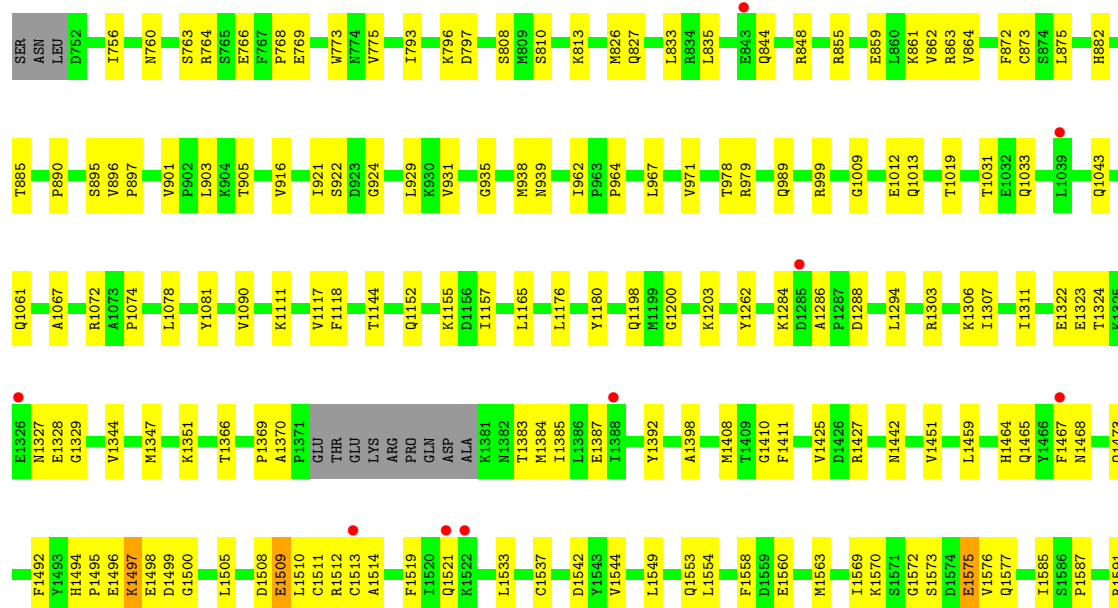
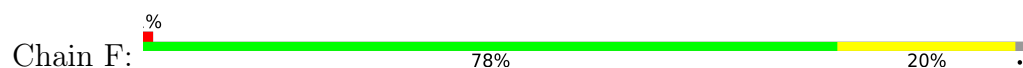


#### • Molecule 2: Complement C3



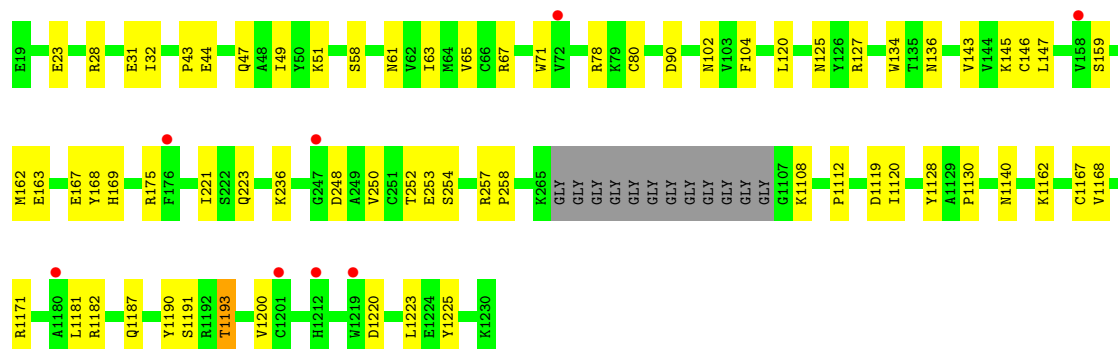
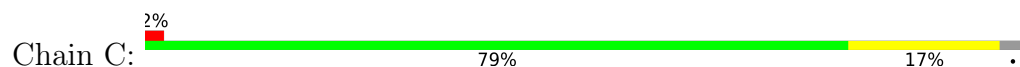


• Molecule 2: Complement C3

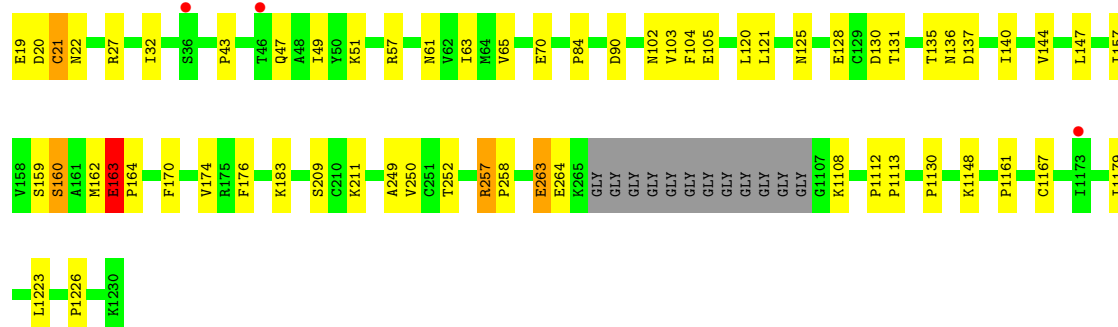
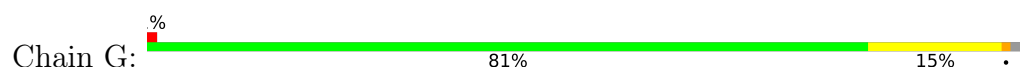




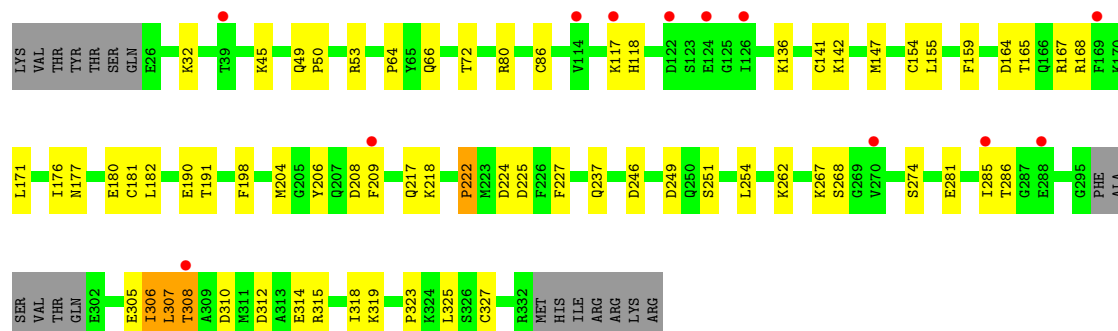
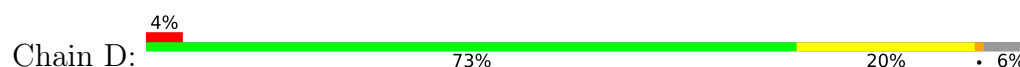
• Molecule 3: Complement factor H, Complement factor H



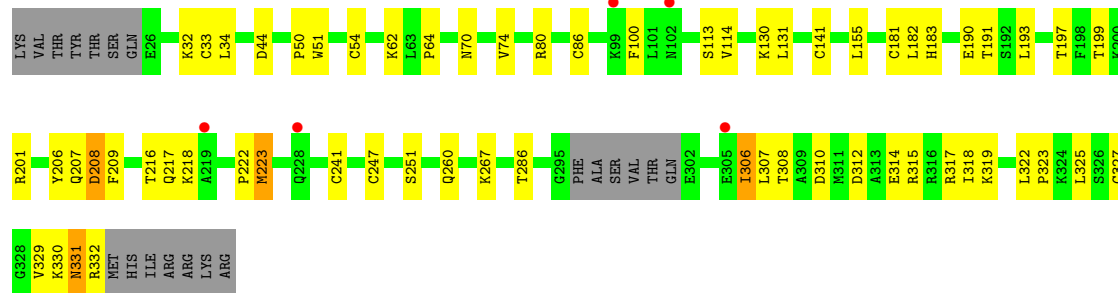
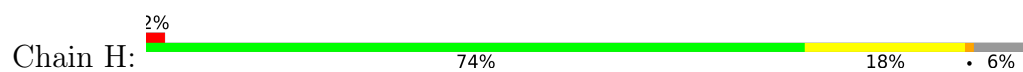
• Molecule 3: Complement factor H, Complement factor H



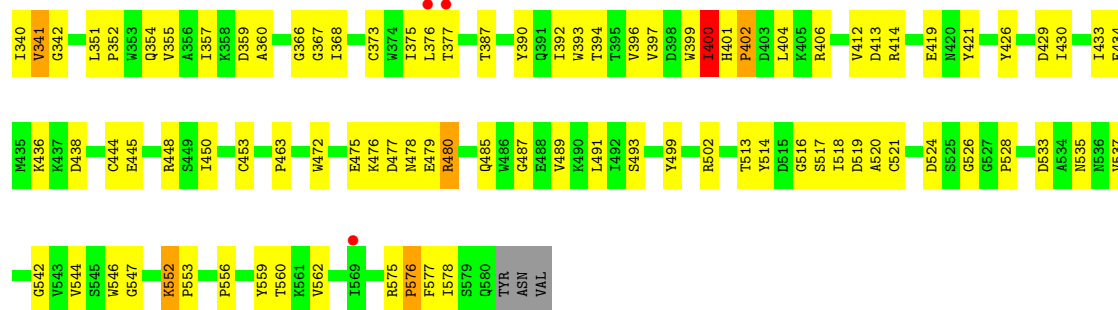
• Molecule 4: Complement factor I



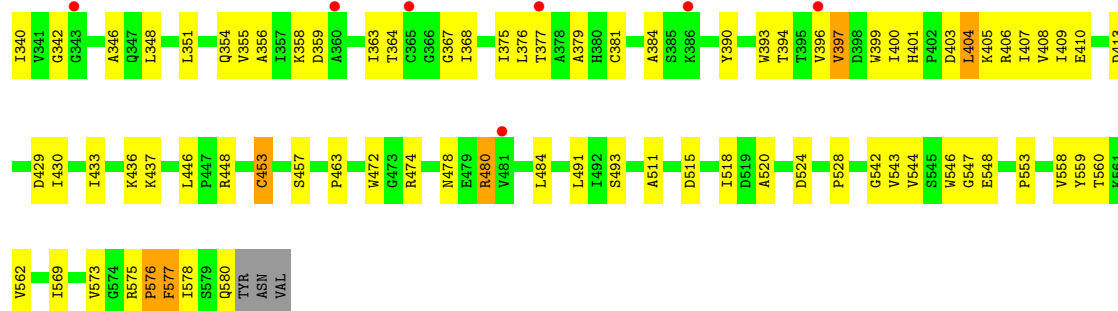
• Molecule 4: Complement factor I



• Molecule 5: Complement factor I



• Molecule 5: Complement factor I

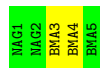


• Molecule 6: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  60% 40%



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

Chain L:  100%



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

Chain N:  50% 50%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 116.37Å 122.79Å 157.20Å<br>69.76° 76.10° 70.13°             | Depositor        |
| Resolution (Å)                                                          | 49.13 – 4.21<br>49.13 – 4.21                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.4 (49.13-4.21)<br>93.4 (49.13-4.21)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.17                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.24 (at 4.14Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.10.1_2155                                          | Depositor        |
| R, $R_{free}$                                                           | 0.229 , 0.254<br>0.231 , 0.256                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2625 reflections (5.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 83.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.010                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 73.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.82                                                        | EDS              |
| Total number of atoms                                                   | 39091                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 108.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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

### 5.1 Standard geometry

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

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     | 0.15         | 0/5092         | 0.49        | 0/6917         |
| 1   | E     | 0.17         | 0/5092         | 0.48        | 0/6917         |
| 2   | B     | 0.18         | 0/7347         | 0.61        | 3/9949 (0.0%)  |
| 2   | F     | 0.18         | 0/7347         | 0.61        | 3/9949 (0.0%)  |
| 3   | C     | 0.11         | 0/3015         | 0.35        | 0/4084         |
| 3   | G     | 0.19         | 1/3015 (0.0%)  | 0.37        | 0/4084         |
| 4   | D     | 0.11         | 0/2355         | 0.38        | 0/3163         |
| 4   | H     | 0.18         | 0/2355         | 0.39        | 0/3163         |
| 5   | I     | 0.18         | 0/1967         | 0.46        | 0/2675         |
| 5   | J     | 0.16         | 0/1967         | 0.44        | 0/2675         |
| All | All   | 0.17         | 1/39552 (0.0%) | 0.51        | 6/53576 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 2                   |
| 2   | F     | 0                   | 2                   |
| 3   | C     | 0                   | 1                   |
| 3   | G     | 0                   | 3                   |
| 4   | D     | 0                   | 1                   |
| 4   | H     | 0                   | 2                   |
| 5   | I     | 0                   | 1                   |
| All | All   | 0                   | 12                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | G     | 257 | ARG  | C-N   | 6.80 | 1.49        | 1.33     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | F     | 1497 | LYS  | N-CA-C | -6.65 | 95.92       | 107.49   |
| 2   | B     | 1660 | GLY  | CA-C-N | 6.61  | 143.73      | 121.27   |
| 2   | B     | 1660 | GLY  | C-N-CA | 6.61  | 143.73      | 121.27   |
| 2   | F     | 989  | GLN  | CA-C-N | 5.38  | 131.81      | 121.54   |
| 2   | F     | 989  | GLN  | C-N-CA | 5.38  | 131.81      | 121.54   |
| 2   | B     | 1576 | VAL  | N-CA-C | 5.11  | 116.16      | 109.21   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | B     | 1509 | GLU  | Peptide |
| 2   | B     | 1576 | VAL  | Peptide |
| 3   | C     | 1190 | TYR  | Peptide |
| 4   | D     | 222  | PRO  | Peptide |
| 2   | F     | 1509 | GLU  | Peptide |
| 2   | F     | 1575 | GLU  | Peptide |
| 3   | G     | 162  | MET  | Peptide |
| 3   | G     | 163  | GLU  | Peptide |
| 3   | G     | 263  | GLU  | Peptide |
| 4   | H     | 223  | MET  | Peptide |
| 4   | H     | 330  | LYS  | Peptide |
| 5   | I     | 400  | ILE  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4992  | 0        | 5052     | 76      | 0            |
| 1   | E     | 4992  | 0        | 5052     | 73      | 0            |
| 2   | B     | 7203  | 0        | 7119     | 137     | 0            |
| 2   | F     | 7203  | 0        | 7119     | 138     | 0            |
| 3   | C     | 2940  | 0        | 2798     | 43      | 0            |
| 3   | G     | 2940  | 0        | 2798     | 39      | 0            |
| 4   | D     | 2320  | 0        | 2223     | 45      | 0            |
| 4   | H     | 2320  | 0        | 2222     | 39      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | I     | 1911  | 0        | 1813     | 64      | 0            |
| 5   | J     | 1911  | 0        | 1811     | 60      | 0            |
| 6   | K     | 61    | 0        | 52       | 1       | 0            |
| 6   | M     | 61    | 0        | 52       | 0       | 0            |
| 7   | L     | 28    | 0        | 25       | 0       | 0            |
| 7   | N     | 28    | 0        | 25       | 1       | 0            |
| 8   | A     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | E     | 1     | 0        | 0        | 0       | 0            |
| 8   | H     | 2     | 0        | 0        | 0       | 0            |
| 9   | D     | 42    | 0        | 39       | 1       | 0            |
| 9   | H     | 42    | 0        | 39       | 0       | 0            |
| 9   | I     | 42    | 0        | 39       | 0       | 0            |
| 9   | J     | 42    | 0        | 39       | 0       | 0            |
| 10  | J     | 7     | 0        | 2        | 0       | 0            |
| All | All   | 39091 | 0        | 38319    | 659     | 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 9.

All (659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:30:THR:HG22  | 1:E:42:MET:HG2   | 1.49                     | 0.94              |
| 1:A:30:THR:HG22  | 1:A:42:MET:HG2   | 1.50                     | 0.92              |
| 2:B:1303:ARG:NH1 | 5:I:520:ALA:O    | 2.09                     | 0.86              |
| 4:D:225:ASP:HB3  | 4:D:237:GLN:HG3  | 1.59                     | 0.83              |
| 2:F:1654:GLU:OE2 | 4:H:80:ARG:NH2   | 2.12                     | 0.83              |
| 1:A:66:LYS:HB3   | 3:C:257:ARG:HD2  | 1.59                     | 0.82              |
| 2:F:939:ASN:CG   | 7:N:1:NAG:C1     | 2.53                     | 0.82              |
| 5:I:340:ILE:HD12 | 5:I:485:GLN:HB2  | 1.62                     | 0.80              |
| 2:B:764:ARG:HB3  | 2:B:797:ASP:HB3  | 1.65                     | 0.78              |
| 2:B:1383:THR:HG1 | 2:B:1464:HIS:HD1 | 1.31                     | 0.78              |
| 1:A:474:ASN:HB3  | 1:A:514:LEU:HD11 | 1.65                     | 0.77              |
| 1:E:474:ASN:HB3  | 1:E:514:LEU:HD11 | 1.66                     | 0.77              |
| 2:B:1549:LEU:HA  | 2:B:1563:MET:HG2 | 1.67                     | 0.76              |
| 5:I:399:TRP:CD1  | 5:I:400:ILE:H    | 2.02                     | 0.76              |
| 5:I:552:LYS:HB3  | 5:I:553:PRO:HD2  | 1.65                     | 0.76              |
| 1:E:650:SER:OG   | 1:E:652:GLN:OE1  | 2.04                     | 0.76              |
| 1:A:650:SER:OG   | 1:A:652:GLN:OE1  | 2.04                     | 0.76              |
| 4:H:312:ASP:OD1  | 4:H:315:ARG:NH2  | 2.20                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:J:356:ALA:HB3   | 5:J:393:TRP:HB2   | 1.69                     | 0.74              |
| 5:J:356:ALA:HB2   | 5:J:472:TRP:HZ3   | 1.51                     | 0.73              |
| 2:F:1303:ARG:NH1  | 5:J:520:ALA:O     | 2.21                     | 0.73              |
| 2:F:1505:LEU:HB3  | 2:F:1558:PHE:CE1  | 2.24                     | 0.73              |
| 1:E:161:ARG:N     | 1:E:182:SER:OG    | 2.21                     | 0.72              |
| 2:B:1563:MET:HE1  | 2:B:1604:MET:SD   | 2.30                     | 0.72              |
| 2:B:1512:ARG:NH1  | 2:B:1621:ILE:HG21 | 2.04                     | 0.72              |
| 2:F:764:ARG:HB3   | 2:F:797:ASP:HB3   | 1.72                     | 0.71              |
| 3:G:1108:LYS:HG2  | 3:G:1130:PRO:HD3  | 1.72                     | 0.71              |
| 2:B:1505:LEU:HD22 | 2:B:1514:ALA:HB2  | 1.71                     | 0.70              |
| 2:B:1658:VAL:HA   | 4:D:64:PRO:HB2    | 1.71                     | 0.70              |
| 5:J:368:ILE:HD12  | 5:J:528:PRO:HB3   | 1.71                     | 0.70              |
| 3:C:254:SER:HB2   | 3:C:257:ARG:HH12  | 1.55                     | 0.69              |
| 1:A:42:MET:HE3    | 1:A:88:PHE:CE1    | 2.28                     | 0.69              |
| 1:E:42:MET:HE3    | 1:E:88:PHE:CE1    | 2.28                     | 0.69              |
| 5:J:544:VAL:HA    | 5:J:559:TYR:HD1   | 1.57                     | 0.69              |
| 1:E:97:LYS:HB2    | 1:E:104:LYS:HE2   | 1.74                     | 0.69              |
| 5:J:463:PRO:HA    | 5:J:491:LEU:HB2   | 1.74                     | 0.68              |
| 2:F:1294:LEU:HB2  | 2:F:1311:ILE:HB   | 1.76                     | 0.68              |
| 3:G:49:ILE:HG12   | 3:G:63:ILE:HG12   | 1.76                     | 0.67              |
| 1:A:35:ARG:NH2    | 1:A:623:ALA:O     | 2.28                     | 0.67              |
| 2:B:810:SER:HB3   | 2:B:813:LYS:HB2   | 1.77                     | 0.67              |
| 5:I:463:PRO:HG3   | 5:I:493:SER:HB2   | 1.77                     | 0.67              |
| 2:F:1505:LEU:HB3  | 2:F:1558:PHE:HE1  | 1.60                     | 0.67              |
| 1:A:136:LYS:NZ    | 2:B:769:GLU:OE1   | 2.28                     | 0.67              |
| 1:A:161:ARG:H     | 1:A:182:SER:HG    | 1.41                     | 0.67              |
| 2:F:1398:ALA:HB3  | 2:F:1451:VAL:HG22 | 1.76                     | 0.67              |
| 3:G:257:ARG:HG3   | 3:G:258:PRO:HD3   | 1.77                     | 0.67              |
| 1:E:456:LEU:HB2   | 1:E:535:TYR:HE1   | 1.60                     | 0.67              |
| 2:F:1563:MET:HE1  | 2:F:1604:MET:SD   | 2.34                     | 0.66              |
| 2:F:1611:PHE:HD2  | 2:F:1618:LEU:HD21 | 1.58                     | 0.66              |
| 2:B:1575:GLU:OE2  | 5:I:575:ARG:NH2   | 2.29                     | 0.66              |
| 5:I:352:PRO:HB2   | 5:I:450:ILE:H     | 1.60                     | 0.66              |
| 2:B:1398:ALA:HB3  | 2:B:1451:VAL:HG22 | 1.78                     | 0.66              |
| 2:B:1152:GLN:OE1  | 2:B:1198:GLN:NE2  | 2.28                     | 0.66              |
| 4:H:329:VAL:HG22  | 4:H:331:ASN:H     | 1.61                     | 0.66              |
| 2:B:1607:LEU:HD11 | 2:B:1625:ASP:OD2  | 1.96                     | 0.66              |
| 2:F:862:VAL:HG22  | 2:F:916:VAL:HG12  | 1.77                     | 0.66              |
| 3:C:1108:LYS:HG2  | 3:C:1130:PRO:HD3  | 1.77                     | 0.65              |
| 5:I:445:GLU:OE2   | 4:H:332:ARG:NH1   | 2.29                     | 0.65              |
| 2:F:1427:ARG:HH21 | 2:F:1459:LEU:HB3  | 1.61                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1512:ARG:NE   | 2:F:1621:ILE:HG13 | 2.12                     | 0.64              |
| 2:B:1118:PHE:HD1  | 2:B:1144:THR:HA   | 1.61                     | 0.64              |
| 3:G:140:ILE:HG13  | 5:J:409:ILE:HD11  | 1.79                     | 0.64              |
| 2:B:875:LEU:O     | 2:B:880:ARG:NH1   | 2.30                     | 0.64              |
| 2:F:1200:GLY:O    | 2:F:1203:LYS:NZ   | 2.30                     | 0.64              |
| 2:B:756:ILE:HD12  | 2:B:922:SER:HB3   | 1.78                     | 0.64              |
| 1:A:44:LEU:HD13   | 1:A:55:VAL:HG11   | 1.79                     | 0.64              |
| 1:A:161:ARG:N     | 1:A:182:SER:OG    | 2.30                     | 0.64              |
| 2:B:1505:LEU:HD12 | 2:B:1558:PHE:HE1  | 1.63                     | 0.64              |
| 3:C:159:SER:OG    | 3:C:175:ARG:N     | 2.30                     | 0.64              |
| 5:J:346:ALA:HB3   | 5:J:484:LEU:HB3   | 1.79                     | 0.64              |
| 2:F:875:LEU:HB2   | 2:F:882:HIS:HD1   | 1.62                     | 0.63              |
| 2:B:863:ARG:NH2   | 2:B:865:GLU:OE1   | 2.31                     | 0.63              |
| 4:H:197:THR:HB    | 4:H:310:ASP:HB3   | 1.78                     | 0.63              |
| 1:A:456:LEU:HB2   | 1:A:535:TYR:HE1   | 1.63                     | 0.63              |
| 1:E:233:GLU:OE2   | 1:E:258:ARG:NH1   | 2.30                     | 0.63              |
| 1:A:232:PHE:HE1   | 1:A:337:ASP:HB3   | 1.64                     | 0.62              |
| 2:B:1654:GLU:OE2  | 4:D:80:ARG:NH1    | 2.30                     | 0.62              |
| 3:C:145:LYS:HA    | 3:C:169:HIS:HA    | 1.81                     | 0.62              |
| 2:B:1370:ALA:HB2  | 2:B:1385:ILE:HG13 | 1.81                     | 0.62              |
| 2:B:1294:LEU:HB2  | 2:B:1311:ILE:HB   | 1.80                     | 0.62              |
| 5:I:535:ASN:HB3   | 5:I:537:VAL:HG23  | 1.80                     | 0.62              |
| 5:I:375:ILE:HB    | 5:I:433:ILE:HB    | 1.81                     | 0.62              |
| 5:I:517:SER:HA    | 5:I:553:PRO:HD3   | 1.81                     | 0.62              |
| 1:E:465:LEU:HD21  | 1:E:521:ILE:HG13  | 1.81                     | 0.62              |
| 2:F:810:SER:HB3   | 2:F:813:LYS:HB2   | 1.80                     | 0.62              |
| 2:F:873:CYS:HB2   | 2:F:901:VAL:HB    | 1.82                     | 0.61              |
| 2:B:862:VAL:HG22  | 2:B:916:VAL:HG12  | 1.82                     | 0.61              |
| 2:B:1117:VAL:HG13 | 2:B:1144:THR:OG1  | 2.01                     | 0.61              |
| 2:F:1370:ALA:HB2  | 2:F:1385:ILE:HG13 | 1.81                     | 0.61              |
| 5:J:413:ASP:HB2   | 5:J:436:LYS:HB3   | 1.81                     | 0.61              |
| 4:D:325:LEU:HD13  | 5:I:577:PHE:HD2   | 1.66                     | 0.61              |
| 2:B:1303:ARG:NE   | 5:I:547:GLY:HA3   | 2.15                     | 0.61              |
| 4:H:325:LEU:HD11  | 5:J:577:PHE:HA    | 1.83                     | 0.61              |
| 5:J:348:LEU:HA    | 5:J:397:VAL:HG11  | 1.83                     | 0.61              |
| 2:B:981:LEU:HB3   | 2:B:1319:LEU:HD11 | 1.80                     | 0.60              |
| 2:B:1644:LYS:NZ   | 2:B:1648:ASP:OD2  | 2.34                     | 0.60              |
| 5:J:354:GLN:HG2   | 5:J:484:LEU:HD11  | 1.83                     | 0.60              |
| 4:H:267:LYS:HB2   | 4:H:286:THR:HG21  | 1.83                     | 0.60              |
| 1:A:230:PRO:HB3   | 1:A:339:VAL:HG22  | 1.82                     | 0.60              |
| 5:I:478:ASN:C     | 5:I:480:ARG:H     | 2.10                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:448:THR:HG21  | 1:A:453:ASN:H     | 1.67                     | 0.60              |
| 4:D:327:CYS:SG    | 5:I:453:CYS:N     | 2.74                     | 0.60              |
| 2:F:1604:MET:HE3  | 2:F:1628:VAL:HG22 | 1.83                     | 0.60              |
| 1:A:67:LEU:HD12   | 1:A:95:GLU:HG3    | 1.84                     | 0.60              |
| 2:B:1604:MET:HE3  | 2:B:1628:VAL:HG22 | 1.84                     | 0.60              |
| 1:E:44:LEU:HD13   | 1:E:55:VAL:HG11   | 1.84                     | 0.60              |
| 2:F:1117:VAL:HG13 | 2:F:1144:THR:OG1  | 2.02                     | 0.59              |
| 3:G:183:LYS:HZ2   | 3:G:209:SER:H     | 1.50                     | 0.59              |
| 2:B:1505:LEU:CD2  | 2:B:1514:ALA:HB2  | 2.31                     | 0.59              |
| 2:F:833:LEU:HG    | 2:F:835:LEU:HD13  | 1.83                     | 0.59              |
| 2:F:897:PRO:O     | 2:F:1473:GLN:NE2  | 2.30                     | 0.59              |
| 5:I:578:ILE:HD12  | 5:I:578:ILE:H     | 1.68                     | 0.59              |
| 1:E:232:PHE:HE1   | 1:E:337:ASP:HB3   | 1.67                     | 0.59              |
| 1:E:237:GLU:OE1   | 1:E:343:ARG:NH1   | 2.33                     | 0.59              |
| 5:J:375:ILE:HB    | 5:J:433:ILE:HB    | 1.85                     | 0.59              |
| 2:F:1303:ARG:HH21 | 5:J:548:GLU:H     | 1.51                     | 0.59              |
| 2:F:1549:LEU:HA   | 2:F:1563:MET:HG2  | 1.84                     | 0.59              |
| 3:G:20:ASP:O      | 3:G:22:ASN:N      | 2.36                     | 0.59              |
| 5:J:367:GLY:HA3   | 5:J:377:THR:HG22  | 1.84                     | 0.59              |
| 1:E:460:VAL:HG13  | 1:E:471:LEU:HD11  | 1.84                     | 0.59              |
| 1:E:563:LEU:HD22  | 2:F:808:SER:HB3   | 1.85                     | 0.58              |
| 3:C:47:GLN:HG2    | 3:C:65:VAL:HG22   | 1.85                     | 0.58              |
| 1:E:136:LYS:NZ    | 2:F:769:GLU:OE1   | 2.36                     | 0.58              |
| 4:D:147:MET:HE3   | 4:D:168:ARG:HH22  | 1.69                     | 0.58              |
| 3:G:19:GLU:HA     | 3:G:70:GLU:HA     | 1.85                     | 0.58              |
| 2:B:754:ASP:OD1   | 3:C:78:ARG:NH2    | 2.32                     | 0.58              |
| 2:B:873:CYS:HB3   | 2:B:901:VAL:HB    | 1.84                     | 0.58              |
| 2:F:1019:THR:HG1  | 2:F:1081:TYR:HH   | 1.47                     | 0.58              |
| 5:J:410:GLU:OE1   | 5:J:437:LYS:NZ    | 2.30                     | 0.58              |
| 1:E:118:GLU:OE2   | 2:F:1043:GLN:NE2  | 2.37                     | 0.58              |
| 2:F:756:ILE:HD12  | 2:F:922:SER:HB3   | 1.84                     | 0.58              |
| 2:F:763:SER:HA    | 2:F:924:GLY:HA3   | 1.85                     | 0.58              |
| 5:I:359:ASP:OD1   | 5:I:360:ALA:N     | 2.30                     | 0.58              |
| 5:J:342:GLY:HA3   | 5:J:518:ILE:HD12  | 1.86                     | 0.58              |
| 5:J:406:ARG:HG2   | 5:J:448:ARG:HD3   | 1.85                     | 0.58              |
| 3:G:57:ARG:HD2    | 3:G:84:PRO:HD3    | 1.85                     | 0.57              |
| 5:J:355:VAL:HG11  | 5:J:375:ILE:HD13  | 1.86                     | 0.57              |
| 2:B:1505:LEU:HD12 | 2:B:1558:PHE:CE1  | 2.38                     | 0.57              |
| 5:J:356:ALA:HB2   | 5:J:472:TRP:CZ3   | 2.37                     | 0.57              |
| 2:F:796:LYS:NZ    | 3:G:90:ASP:OD2    | 2.31                     | 0.57              |
| 1:A:281:ARG:NH1   | 1:A:342:GLU:OE2   | 2.37                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:563:LEU:HD22  | 2:B:808:SER:HB3   | 1.86                     | 0.57              |
| 1:A:583:LEU:HD22  | 2:B:793:ILE:HD13  | 1.86                     | 0.57              |
| 1:E:429:GLN:O     | 1:E:430:GLU:HG2   | 2.04                     | 0.57              |
| 2:B:796:LYS:NZ    | 3:C:90:ASP:OD2    | 2.31                     | 0.57              |
| 2:B:1200:GLY:O    | 2:B:1203:LYS:NZ   | 2.38                     | 0.57              |
| 3:G:128:GLU:N     | 3:G:135:THR:OG1   | 2.36                     | 0.56              |
| 1:A:331:ILE:HG12  | 1:A:338:MET:HG3   | 1.85                     | 0.56              |
| 1:E:334:SER:O     | 2:F:848:ARG:NH2   | 2.38                     | 0.56              |
| 1:A:460:VAL:HG13  | 1:A:471:LEU:HD11  | 1.88                     | 0.56              |
| 5:I:406:ARG:HG2   | 5:I:448:ARG:HD3   | 1.87                     | 0.56              |
| 1:E:161:ARG:N     | 1:E:182:SER:HG    | 2.01                     | 0.56              |
| 4:H:306:ILE:HG23  | 4:H:307:LEU:H     | 1.69                     | 0.56              |
| 3:C:145:LYS:HD2   | 5:I:400:ILE:HG22  | 1.88                     | 0.56              |
| 5:I:368:ILE:HD12  | 5:I:528:PRO:HB3   | 1.87                     | 0.56              |
| 5:I:413:ASP:HB2   | 5:I:436:LYS:HB2   | 1.87                     | 0.56              |
| 2:F:1510:LEU:HG   | 2:F:1612:TRP:CH2  | 2.41                     | 0.56              |
| 4:H:207:GLN:O     | 4:H:209:PHE:N     | 2.39                     | 0.56              |
| 1:A:35:ARG:HD3    | 1:A:154:HIS:CE1   | 2.41                     | 0.56              |
| 2:B:1505:LEU:HB2  | 2:B:1558:PHE:CE1  | 2.40                     | 0.56              |
| 2:B:1544:VAL:HG22 | 2:B:1605:TRP:HB2  | 1.87                     | 0.56              |
| 1:E:161:ARG:H     | 1:E:182:SER:HG    | 1.48                     | 0.56              |
| 2:F:1492:PHE:HB2  | 2:F:1500:GLY:HA3  | 1.88                     | 0.56              |
| 4:H:222:PRO:HD2   | 4:H:223:MET:HG3   | 1.88                     | 0.56              |
| 1:A:465:LEU:HD21  | 1:A:521:ILE:HG13  | 1.88                     | 0.56              |
| 1:E:291:ILE:HD13  | 1:E:300:VAL:HB    | 1.88                     | 0.56              |
| 2:B:875:LEU:HD21  | 2:B:882:HIS:CE1   | 2.41                     | 0.56              |
| 2:F:895:SER:O     | 2:F:1442:ASN:ND2  | 2.38                     | 0.56              |
| 2:B:1654:GLU:O    | 2:B:1658:VAL:HG12 | 2.05                     | 0.55              |
| 2:B:1554:LEU:HD22 | 2:B:1591:ARG:HE   | 1.72                     | 0.55              |
| 2:B:1116:GLY:HA3  | 2:B:1171:LYS:HG2  | 1.89                     | 0.55              |
| 1:A:42:MET:HE3    | 1:A:88:PHE:CZ     | 2.42                     | 0.55              |
| 4:H:70:ASN:OD1    | 4:H:317:ARG:NH2   | 2.39                     | 0.55              |
| 2:B:1512:ARG:HB3  | 2:B:1612:TRP:CH2  | 2.42                     | 0.55              |
| 3:C:49:ILE:HG12   | 3:C:63:ILE:HG12   | 1.88                     | 0.55              |
| 2:F:999:ARG:HD2   | 2:F:1262:TYR:CE2  | 2.41                     | 0.55              |
| 2:F:1611:PHE:CD2  | 2:F:1618:LEU:HD21 | 2.41                     | 0.55              |
| 4:H:216:THR:O     | 4:H:218:LYS:N     | 2.40                     | 0.55              |
| 2:F:1118:PHE:HD1  | 2:F:1144:THR:HA   | 1.70                     | 0.55              |
| 2:F:1152:GLN:OE1  | 2:F:1198:GLN:NE2  | 2.39                     | 0.55              |
| 1:A:352:PRO:O     | 1:A:379:PRO:HD3   | 2.06                     | 0.55              |
| 2:F:1544:VAL:HG22 | 2:F:1605:TRP:HB2  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:373:CYS:SG    | 5:I:444:CYS:N     | 2.80                     | 0.54              |
| 3:G:49:ILE:HG23   | 3:G:61:ASN:HB3    | 1.89                     | 0.54              |
| 3:G:160:SER:HB3   | 3:G:174:VAL:HG12  | 1.89                     | 0.54              |
| 4:D:53:ARG:NH1    | 4:D:66:GLN:OE1    | 2.40                     | 0.54              |
| 4:D:281:GLU:OE1   | 4:D:315:ARG:NH2   | 2.40                     | 0.54              |
| 5:I:367:GLY:HA3   | 5:I:377:THR:HG22  | 1.88                     | 0.54              |
| 3:C:252:THR:HG22  | 3:C:253:GLU:H     | 1.73                     | 0.54              |
| 1:E:230:PRO:HB3   | 1:E:339:VAL:HG22  | 1.90                     | 0.54              |
| 2:F:1575:GLU:HB3  | 2:F:1576:VAL:HG23 | 1.90                     | 0.54              |
| 1:A:429:GLN:O     | 1:A:430:GLU:HG2   | 2.07                     | 0.54              |
| 2:F:1654:GLU:O    | 2:F:1658:VAL:HG12 | 2.07                     | 0.54              |
| 2:B:875:LEU:HD21  | 2:B:882:HIS:HE1   | 1.72                     | 0.54              |
| 1:E:23:SER:O      | 1:E:544:ARG:NH2   | 2.40                     | 0.54              |
| 4:H:181:CYS:SG    | 4:H:182:LEU:N     | 2.79                     | 0.54              |
| 2:F:1512:ARG:CZ   | 2:F:1621:ILE:HG13 | 2.38                     | 0.54              |
| 3:G:249:ALA:HA    | 3:G:258:PRO:HB2   | 1.89                     | 0.54              |
| 4:H:183:HIS:HB2   | 4:H:199:THR:HB    | 1.90                     | 0.54              |
| 2:F:1061:GLN:NE2  | 2:F:1072:ARG:O    | 2.40                     | 0.54              |
| 2:B:1186:SER:N    | 2:B:1222:ASP:OD2  | 2.41                     | 0.54              |
| 1:A:291:ILE:HD13  | 1:A:300:VAL:HB    | 1.90                     | 0.54              |
| 2:B:1067:ALA:HB2  | 2:B:1074:PRO:HA   | 1.90                     | 0.54              |
| 5:I:387:THR:HG23  | 5:I:412:VAL:HG12  | 1.89                     | 0.54              |
| 2:F:844:GLN:HE22  | 2:F:1500:GLY:C    | 2.15                     | 0.53              |
| 1:A:473:VAL:HB    | 1:A:517:LEU:HB3   | 1.90                     | 0.53              |
| 2:B:999:ARG:HD2   | 2:B:1262:TYR:CE2  | 2.43                     | 0.53              |
| 2:F:1505:LEU:HD11 | 2:F:1587:PRO:HG3  | 1.89                     | 0.53              |
| 5:J:396:VAL:HA    | 5:J:407:ILE:HD11  | 1.88                     | 0.53              |
| 5:J:384:ALA:HB3   | 5:J:390:TYR:HE2   | 1.74                     | 0.53              |
| 3:C:1119:ASP:OD1  | 3:C:1120:ILE:N    | 2.40                     | 0.53              |
| 2:B:1568:THR:HG21 | 2:B:1576:VAL:HG11 | 1.91                     | 0.53              |
| 2:B:1576:VAL:HG12 | 2:B:1577:GLN:C    | 2.34                     | 0.53              |
| 3:G:263:GLU:HG3   | 3:G:264:GLU:HB2   | 1.91                     | 0.53              |
| 4:H:131:LEU:HD13  | 4:H:307:LEU:CD1   | 2.39                     | 0.53              |
| 4:H:327:CYS:SG    | 5:J:453:CYS:N     | 2.82                     | 0.53              |
| 1:E:594:VAL:HG12  | 2:F:775:VAL:HG22  | 1.90                     | 0.52              |
| 3:C:147:LEU:HD13  | 5:I:400:ILE:HD11  | 1.92                     | 0.52              |
| 2:F:1519:PHE:HD1  | 2:F:1521:GLN:H    | 1.56                     | 0.52              |
| 3:C:23:GLU:OE1    | 3:C:23:GLU:N      | 2.39                     | 0.52              |
| 2:F:1009:GLY:HA3  | 2:F:1013:GLN:HB2  | 1.91                     | 0.52              |
| 5:J:463:PRO:HG2   | 5:J:493:SER:HB2   | 1.92                     | 0.52              |
| 5:I:542:GLY:HA2   | 5:I:562:VAL:HG23  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1658:VAL:HA   | 4:H:64:PRO:HB2    | 1.90                     | 0.52              |
| 1:A:458:LEU:HD11  | 1:A:533:ALA:HB3   | 1.92                     | 0.52              |
| 5:I:402:PRO:HG2   | 5:I:404:LEU:HD13  | 1.90                     | 0.52              |
| 2:F:1573:SER:HB3  | 2:F:1611:PHE:CZ   | 2.44                     | 0.52              |
| 2:B:1309:HIS:HD1  | 2:B:1320:ARG:HD3  | 1.74                     | 0.52              |
| 3:G:135:THR:HG22  | 3:G:136:ASN:H     | 1.74                     | 0.52              |
| 3:G:252:THR:HG21  | 3:G:257:ARG:NE    | 2.25                     | 0.52              |
| 2:B:763:SER:HA    | 2:B:924:GLY:HA3   | 1.92                     | 0.52              |
| 1:E:331:ILE:HG12  | 1:E:338:MET:HG3   | 1.92                     | 0.52              |
| 4:D:49:GLN:N      | 4:D:49:GLN:OE1    | 2.43                     | 0.52              |
| 5:J:542:GLY:HA2   | 5:J:562:VAL:HG23  | 1.92                     | 0.52              |
| 4:D:176:ILE:HG12  | 4:D:206:TYR:CD2   | 2.45                     | 0.52              |
| 1:E:205:LYS:HG3   | 1:E:221:GLU:HG2   | 1.92                     | 0.52              |
| 3:G:21:CYS:C      | 3:G:22:ASN:HD22   | 2.17                     | 0.52              |
| 3:C:1182:ARG:HB2  | 3:C:1200:VAL:HG22 | 1.91                     | 0.51              |
| 5:I:399:TRP:C     | 5:I:401:HIS:H     | 2.18                     | 0.51              |
| 5:I:533:ASP:OD1   | 5:I:537:VAL:N     | 2.38                     | 0.51              |
| 4:H:241:CYS:O     | 4:H:260:GLN:N     | 2.25                     | 0.51              |
| 2:B:1031:THR:HB   | 2:B:1033:GLN:HE21 | 1.75                     | 0.51              |
| 3:C:162:MET:HB2   | 3:C:163:GLU:OE1   | 2.11                     | 0.51              |
| 5:I:414:ARG:HB3   | 5:I:434:GLU:HB3   | 1.92                     | 0.51              |
| 4:H:131:LEU:HD13  | 4:H:307:LEU:HD11  | 1.92                     | 0.51              |
| 1:E:448:THR:HG21  | 1:E:453:ASN:H     | 1.75                     | 0.51              |
| 2:F:760:ASN:O     | 3:G:57:ARG:NH2    | 2.44                     | 0.51              |
| 1:A:29:ILE:HG22   | 1:A:644:LEU:HD22  | 1.93                     | 0.51              |
| 3:C:127:ARG:HD3   | 3:C:134:TRP:HB3   | 1.92                     | 0.51              |
| 3:G:130:ASP:OD1   | 3:G:131:THR:N     | 2.37                     | 0.51              |
| 5:I:355:VAL:HG22  | 5:I:394:THR:HG22  | 1.93                     | 0.51              |
| 1:A:47:HIS:ND1    | 1:A:489:TYR:OH    | 2.30                     | 0.51              |
| 2:B:1148:LEU:HD23 | 2:B:1195:ALA:HB1  | 1.93                     | 0.51              |
| 3:C:146:CYS:N     | 3:C:168:TYR:O     | 2.32                     | 0.51              |
| 1:E:577:PRO:HD2   | 2:F:827:GLN:HG3   | 1.91                     | 0.51              |
| 1:E:366:PRO:HB3   | 1:E:416:SER:H     | 1.75                     | 0.51              |
| 2:F:1640:GLU:HA   | 2:F:1643:GLN:HG3  | 1.92                     | 0.51              |
| 2:B:1496:GLU:O    | 2:B:1496:GLU:HG3  | 2.11                     | 0.51              |
| 1:E:352:PRO:O     | 1:E:379:PRO:HD3   | 2.11                     | 0.51              |
| 1:A:38:SER:HB3    | 1:A:154:HIS:HD2   | 1.76                     | 0.50              |
| 2:F:872:PHE:HZ    | 2:F:929:LEU:HD11  | 1.76                     | 0.50              |
| 4:H:86:CYS:HB2    | 4:H:318:ILE:HD13  | 1.93                     | 0.50              |
| 5:J:403:ASP:C     | 5:J:405:LYS:H     | 2.19                     | 0.50              |
| 2:B:1640:GLU:HA   | 2:B:1643:GLN:HG3  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:28:ARG:HB2    | 3:C:31:GLU:HB2    | 1.93                     | 0.50              |
| 3:C:1181:LEU:H    | 3:C:1181:LEU:HD12 | 1.76                     | 0.50              |
| 2:F:903:LEU:HD22  | 2:F:1511:CYS:O    | 2.11                     | 0.50              |
| 5:J:575:ARG:N     | 5:J:576:PRO:HD2   | 2.26                     | 0.50              |
| 2:B:826:MET:HG2   | 2:B:827:GLN:N     | 2.26                     | 0.50              |
| 2:B:1568:THR:HG21 | 2:B:1576:VAL:HG21 | 1.91                     | 0.50              |
| 1:E:47:HIS:ND1    | 1:E:489:TYR:OH    | 2.27                     | 0.50              |
| 1:E:148:ARG:HG3   | 2:F:773:TRP:CZ2   | 2.46                     | 0.50              |
| 1:A:97:LYS:HB3    | 1:A:104:LYS:HE2   | 1.94                     | 0.50              |
| 4:D:164:ASP:OD2   | 4:D:167:ARG:NH1   | 2.44                     | 0.50              |
| 2:F:875:LEU:HB2   | 2:F:882:HIS:ND1   | 2.24                     | 0.50              |
| 2:B:992:GLU:HB2   | 2:B:1282:TYR:CE2  | 2.47                     | 0.50              |
| 2:B:1298:LEU:HD12 | 2:B:1307:ILE:HG21 | 1.93                     | 0.50              |
| 2:B:1507:ARG:HB3  | 2:B:1558:PHE:HE2  | 1.75                     | 0.50              |
| 4:D:50:PRO:HG3    | 4:D:319:LYS:HG3   | 1.94                     | 0.50              |
| 4:H:306:ILE:HG13  | 4:H:307:LEU:HG    | 1.93                     | 0.50              |
| 5:J:358:LYS:HA    | 5:J:363:ILE:HA    | 1.92                     | 0.50              |
| 2:B:1383:THR:HG21 | 2:B:1462:LYS:HE2  | 1.92                     | 0.50              |
| 2:F:1383:THR:OG1  | 2:F:1464:HIS:ND1  | 2.36                     | 0.50              |
| 5:I:526:GLY:N     | 5:I:544:VAL:HB    | 2.26                     | 0.49              |
| 3:G:103:VAL:O     | 3:G:105:GLU:N     | 2.46                     | 0.49              |
| 5:I:357:ILE:HG22  | 5:I:366:GLY:HA2   | 1.94                     | 0.49              |
| 1:E:35:ARG:NH2    | 1:E:623:ALA:O     | 2.44                     | 0.49              |
| 2:F:1607:LEU:HD11 | 2:F:1625:ASP:OD2  | 2.12                     | 0.49              |
| 2:F:1569:ILE:HD13 | 2:F:1653:THR:HG22 | 1.94                     | 0.49              |
| 2:B:978:THR:HA    | 2:B:1346:THR:HA   | 1.95                     | 0.49              |
| 5:I:352:PRO:HG3   | 5:I:450:ILE:HD12  | 1.95                     | 0.49              |
| 2:F:971:VAL:HG22  | 2:F:1351:LYS:HG2  | 1.94                     | 0.49              |
| 2:F:1544:VAL:HB   | 2:F:1570:LYS:HB3  | 1.94                     | 0.49              |
| 2:B:1520:ILE:C    | 2:B:1522:LYS:H    | 2.21                     | 0.49              |
| 4:D:155:LEU:HD23  | 4:D:191:THR:HA    | 1.94                     | 0.49              |
| 1:E:449:VAL:HB    | 1:E:545:GLU:HG3   | 1.95                     | 0.49              |
| 5:J:478:ASN:HB3   | 5:J:480:ARG:HG3   | 1.95                     | 0.49              |
| 1:A:411:ILE:HD11  | 1:A:420:LEU:HD21  | 1.93                     | 0.49              |
| 2:B:1546:LYS:HD3  | 2:B:1567:GLN:HG2  | 1.95                     | 0.49              |
| 1:E:198:LEU:HG    | 2:F:979:ARG:NH2   | 2.27                     | 0.49              |
| 1:A:161:ARG:N     | 1:A:182:SER:HG    | 2.07                     | 0.49              |
| 1:A:449:VAL:HB    | 1:A:545:GLU:HG3   | 1.94                     | 0.49              |
| 2:F:855:ARG:HH21  | 2:F:921:ILE:HD11  | 1.78                     | 0.49              |
| 2:F:1492:PHE:HB2  | 2:F:1500:GLY:CA   | 2.43                     | 0.49              |
| 1:A:69:LEU:HB3    | 1:A:90:ILE:HG23   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:366:PRO:HB3   | 1:A:416:SER:H     | 1.78                     | 0.49              |
| 4:D:198:PHE:O     | 4:D:307:LEU:HB3   | 2.13                     | 0.49              |
| 5:I:429:ASP:O     | 5:I:560:THR:HG21  | 2.12                     | 0.49              |
| 2:F:826:MET:HG2   | 2:F:827:GLN:H     | 1.78                     | 0.49              |
| 2:F:1505:LEU:HG   | 2:F:1514:ALA:HB2  | 1.94                     | 0.49              |
| 2:B:1426:ASP:HB3  | 2:B:1449:ASP:HB2  | 1.94                     | 0.48              |
| 5:I:340:ILE:HG23  | 5:I:524:ASP:OD2   | 2.12                     | 0.48              |
| 2:F:1284:LYS:C    | 2:F:1286:ALA:H    | 2.21                     | 0.48              |
| 4:D:142:LYS:H     | 4:D:208:ASP:HB3   | 1.77                     | 0.48              |
| 2:F:1366:THR:HG23 | 2:F:1387:GLU:HB3  | 1.95                     | 0.48              |
| 1:A:205:LYS:HG3   | 1:A:221:GLU:HG2   | 1.96                     | 0.48              |
| 3:G:1148:LYS:HA   | 3:G:1161:PRO:HG3  | 1.96                     | 0.48              |
| 3:C:250:VAL:H     | 3:C:258:PRO:HD2   | 1.78                     | 0.48              |
| 1:E:355:ILE:HD11  | 1:E:426:THR:HG23  | 1.95                     | 0.48              |
| 1:E:583:LEU:HD22  | 2:F:793:ILE:HD13  | 1.95                     | 0.48              |
| 4:H:50:PRO:HG3    | 4:H:319:LYS:HG3   | 1.96                     | 0.48              |
| 4:D:165:THR:HG21  | 4:D:246:ASP:HB3   | 1.96                     | 0.48              |
| 4:D:262:LYS:O     | 4:D:274:SER:OG    | 2.31                     | 0.48              |
| 5:I:404:LEU:H     | 5:I:404:LEU:HD22  | 1.79                     | 0.48              |
| 2:F:1306:LYS:HD2  | 5:J:474:ARG:NH2   | 2.28                     | 0.48              |
| 3:G:1167:CYS:SG   | 3:G:1223:LEU:HB2  | 2.54                     | 0.48              |
| 4:H:113:SER:HB2   | 4:H:130:LYS:HB3   | 1.95                     | 0.48              |
| 3:C:44:GLU:OE1    | 3:C:67:ARG:HA     | 2.14                     | 0.48              |
| 1:E:458:LEU:HD11  | 1:E:533:ALA:HB3   | 1.94                     | 0.48              |
| 2:B:1465:GLN:NE2  | 2:B:1468:ASN:OD1  | 2.47                     | 0.48              |
| 1:E:29:ILE:HD12   | 1:E:493:LEU:HD21  | 1.96                     | 0.48              |
| 3:G:250:VAL:HG23  | 3:G:258:PRO:HG2   | 1.96                     | 0.48              |
| 5:J:393:TRP:HE3   | 5:J:396:VAL:HG21  | 1.79                     | 0.48              |
| 4:D:72:THR:HG21   | 9:D:405:NAG:H4    | 1.96                     | 0.47              |
| 1:E:473:VAL:HB    | 1:E:517:LEU:HB3   | 1.96                     | 0.47              |
| 2:F:1425:VAL:HG11 | 2:F:1427:ARG:HH11 | 1.79                     | 0.47              |
| 2:F:1639:ASP:OD1  | 2:F:1640:GLU:N    | 2.47                     | 0.47              |
| 5:J:376:LEU:HD11  | 5:J:430:ILE:HD11  | 1.96                     | 0.47              |
| 3:C:1193:THR:HG23 | 3:C:1220:ASP:H    | 1.79                     | 0.47              |
| 5:J:359:ASP:OD2   | 5:J:364:THR:OG1   | 2.29                     | 0.47              |
| 1:A:209:TYR:CD2   | 1:A:214:PRO:HA    | 2.50                     | 0.47              |
| 2:B:1492:PHE:HB2  | 2:B:1500:GLY:HA3  | 1.97                     | 0.47              |
| 4:D:181:CYS:SG    | 4:D:182:LEU:N     | 2.87                     | 0.47              |
| 2:F:873:CYS:SG    | 2:F:903:LEU:HD21  | 2.54                     | 0.47              |
| 2:F:1012:GLU:HG2  | 2:F:1078:LEU:HD22 | 1.97                     | 0.47              |
| 2:B:1568:THR:CG2  | 2:B:1576:VAL:HG11 | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1639:ASP:OD1  | 2:B:1640:GLU:N    | 2.45                     | 0.47              |
| 4:D:154:CYS:HB3   | 4:D:159:PHE:HB2   | 1.95                     | 0.47              |
| 1:E:32:ASN:HB3    | 1:E:657:ARG:HH11  | 1.79                     | 0.47              |
| 2:B:882:HIS:CD2   | 2:B:898:TYR:HE1   | 2.32                     | 0.47              |
| 4:D:227:PHE:CE1   | 4:D:237:GLN:HG2   | 2.49                     | 0.47              |
| 4:D:267:LYS:HB2   | 4:D:286:THR:HG21  | 1.96                     | 0.47              |
| 2:F:967:LEU:HD12  | 2:F:1327:ASN:ND2  | 2.29                     | 0.47              |
| 2:F:1575:GLU:O    | 2:F:1577:GLN:HG2  | 2.14                     | 0.47              |
| 2:B:1012:GLU:HG3  | 2:B:1068:ALA:HB2  | 1.97                     | 0.47              |
| 4:D:171:LEU:HD23  | 4:D:209:PHE:CD2   | 2.49                     | 0.47              |
| 1:E:480:ASP:N     | 1:E:480:ASP:OD1   | 2.48                     | 0.47              |
| 2:F:1494:HIS:O    | 2:F:1496:GLU:N    | 2.48                     | 0.47              |
| 2:B:766:GLU:C     | 2:B:768:PRO:HD3   | 2.39                     | 0.47              |
| 2:B:1383:THR:HG1  | 2:B:1464:HIS:CE1  | 2.32                     | 0.47              |
| 2:B:1519:PHE:HD1  | 2:B:1521:GLN:H    | 1.63                     | 0.47              |
| 5:I:341:VAL:CG2   | 5:I:519:ASP:H     | 2.28                     | 0.47              |
| 2:F:935:GLY:HA3   | 2:F:971:VAL:HG21  | 1.96                     | 0.47              |
| 2:F:1307:ILE:HG21 | 2:F:1322:GLU:CD   | 2.40                     | 0.47              |
| 3:G:163:GLU:HB3   | 3:G:164:PRO:HD3   | 1.97                     | 0.47              |
| 1:A:244:TYR:CE2   | 1:A:246:TYR:HB2   | 2.49                     | 0.47              |
| 4:D:45:LYS:HB3    | 4:D:254:LEU:HD22  | 1.96                     | 0.47              |
| 2:B:1307:ILE:HG12 | 2:B:1322:GLU:CD   | 2.40                     | 0.47              |
| 5:I:341:VAL:HG23  | 5:I:342:GLY:H     | 1.78                     | 0.47              |
| 2:F:766:GLU:C     | 2:F:768:PRO:HD3   | 2.40                     | 0.47              |
| 4:H:44:ASP:HA     | 5:J:457:SER:HB2   | 1.97                     | 0.47              |
| 1:E:141:PRO:HG2   | 1:E:201:MET:HE1   | 1.96                     | 0.46              |
| 4:H:322:LEU:HB2   | 4:H:323:PRO:HD3   | 1.97                     | 0.46              |
| 1:A:480:ASP:OD1   | 1:A:480:ASP:N     | 2.48                     | 0.46              |
| 2:B:1533:LEU:O    | 2:B:1537:CYS:HB2  | 2.15                     | 0.46              |
| 4:D:325:LEU:HD21  | 5:I:577:PHE:HA    | 1.97                     | 0.46              |
| 1:A:284:LEU:HD22  | 1:A:310:GLY:HA3   | 1.97                     | 0.46              |
| 2:B:1521:GLN:C    | 2:B:1523:SER:H    | 2.23                     | 0.46              |
| 1:E:42:MET:HG3    | 1:E:88:PHE:HE1    | 1.79                     | 0.46              |
| 1:E:475:PHE:O     | 1:E:514:LEU:HA    | 2.15                     | 0.46              |
| 2:B:1302:SER:HB3  | 5:I:426:TYR:CZ    | 2.50                     | 0.46              |
| 2:F:1155:LYS:HA   | 2:F:1165:LEU:HD21 | 1.98                     | 0.46              |
| 2:F:1505:LEU:HD21 | 2:F:1587:PRO:HG3  | 1.98                     | 0.46              |
| 1:A:169:ASN:HD21  | 1:A:173:ILE:HB    | 1.79                     | 0.46              |
| 2:B:990:MET:SD    | 2:B:990:MET:N     | 2.88                     | 0.46              |
| 2:F:1303:ARG:HG3  | 5:J:546:TRP:O     | 2.16                     | 0.46              |
| 2:F:1613:GLY:O    | 2:F:1614:GLU:HB2  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:126:GLN:HG3   | 1:A:216:GLN:HG2   | 1.97                     | 0.46              |
| 1:E:32:ASN:HA     | 1:E:645:THR:HG23  | 1.98                     | 0.46              |
| 1:E:411:ILE:HD11  | 1:E:420:LEU:HD21  | 1.98                     | 0.46              |
| 2:F:1410:GLY:HA2  | 2:F:1467:PHE:HB3  | 1.98                     | 0.46              |
| 1:A:329:THR:HG21  | 1:A:338:MET:HE3   | 1.97                     | 0.46              |
| 1:A:475:PHE:O     | 1:A:514:LEU:HA    | 2.16                     | 0.46              |
| 5:I:463:PRO:HA    | 5:I:491:LEU:HB2   | 1.98                     | 0.46              |
| 1:E:532:VAL:HG11  | 1:E:644:LEU:HD12  | 1.98                     | 0.46              |
| 5:J:400:ILE:HG13  | 5:J:401:HIS:ND1   | 2.30                     | 0.46              |
| 5:J:511:ALA:HB3   | 5:J:559:TYR:HE2   | 1.81                     | 0.46              |
| 1:A:148:ARG:HG3   | 2:B:773:TRP:CZ2   | 2.50                     | 0.46              |
| 2:B:1497:LYS:HE3  | 2:B:1499:ASP:HB2  | 1.98                     | 0.46              |
| 3:C:120:LEU:HD21  | 3:C:125:ASN:HB2   | 1.97                     | 0.46              |
| 5:I:489:VAL:HG23  | 5:I:513:THR:HG23  | 1.96                     | 0.46              |
| 2:B:999:ARG:HD2   | 2:B:1262:TYR:CZ   | 2.51                     | 0.46              |
| 5:I:502:ARG:HD3   | 5:I:546:TRP:CZ3   | 2.51                     | 0.46              |
| 1:E:185:GLN:HB3   | 1:E:188:VAL:O     | 2.15                     | 0.46              |
| 2:B:875:LEU:HD23  | 2:B:875:LEU:H     | 1.81                     | 0.45              |
| 2:B:1194:TYR:CE1  | 2:B:1238:LEU:HB3  | 2.51                     | 0.45              |
| 2:B:1303:ARG:HD3  | 5:I:521:CYS:HA    | 1.96                     | 0.45              |
| 5:I:552:LYS:HB3   | 5:I:553:PRO:CD    | 2.41                     | 0.45              |
| 4:H:32:LYS:H      | 4:H:32:LYS:HD2    | 1.80                     | 0.45              |
| 1:A:125:LEU:O     | 1:A:213:SER:HB3   | 2.16                     | 0.45              |
| 2:F:1537:CYS:SG   | 2:F:1656:MET:HE1  | 2.56                     | 0.45              |
| 1:A:594:VAL:HG12  | 2:B:775:VAL:HG22  | 1.99                     | 0.45              |
| 2:F:1508:ASP:HB3  | 2:F:1509:GLU:OE1  | 2.16                     | 0.45              |
| 2:F:1542:ASP:CG   | 2:F:1608:SER:HB3  | 2.41                     | 0.45              |
| 3:G:147:LEU:HD12  | 3:G:147:LEU:H     | 1.81                     | 0.45              |
| 4:H:206:TYR:C     | 4:H:208:ASP:H     | 2.24                     | 0.45              |
| 1:A:136:LYS:HE3   | 1:A:136:LYS:HB2   | 1.83                     | 0.45              |
| 2:F:1369:PRO:HA   | 2:F:1384:MET:HG2  | 1.97                     | 0.45              |
| 3:G:144:VAL:HG23  | 3:G:170:PHE:HB2   | 1.99                     | 0.45              |
| 2:B:967:LEU:HD12  | 2:B:1327:ASN:ND2  | 2.32                     | 0.45              |
| 2:B:1012:GLU:HG2  | 2:B:1078:LEU:HD22 | 1.97                     | 0.45              |
| 5:I:340:ILE:N     | 5:I:520:ALA:HA    | 2.31                     | 0.45              |
| 5:I:514:TYR:C     | 5:I:516:GLY:H     | 2.24                     | 0.45              |
| 2:B:1160:GLU:OE2  | 3:C:223:GLN:N     | 2.36                     | 0.45              |
| 2:B:1366:THR:HG23 | 2:B:1387:GLU:HB3  | 1.97                     | 0.45              |
| 2:F:964:PRO:HB3   | 2:F:1328:GLU:HA   | 1.98                     | 0.45              |
| 2:F:1597:GLU:HB3  | 2:F:1600:LYS:HD2  | 1.99                     | 0.45              |
| 5:I:576:PRO:HB2   | 5:I:577:PHE:H     | 1.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:329:THR:HG21  | 1:E:338:MET:HE3   | 1.97                     | 0.45              |
| 2:F:1607:LEU:HG   | 2:F:1625:ASP:HB2  | 1.99                     | 0.45              |
| 2:F:1627:TRP:HE1  | 2:F:1629:GLU:HB2  | 1.81                     | 0.45              |
| 1:A:207:ARG:HD3   | 1:A:219:SER:OG    | 2.17                     | 0.45              |
| 3:C:1171:ARG:HD3  | 3:C:1187:GLN:HE22 | 1.81                     | 0.45              |
| 1:A:454:ASN:ND2   | 1:A:479:MET:HE3   | 2.32                     | 0.44              |
| 3:C:58:SER:HB3    | 3:C:80:CYS:HA     | 1.99                     | 0.44              |
| 2:F:861:LYS:HE2   | 2:F:885:THR:HG21  | 1.98                     | 0.44              |
| 2:F:962:ILE:O     | 2:F:1329:GLY:HA2  | 2.17                     | 0.44              |
| 2:F:1090:VAL:HG11 | 2:F:1157:ILE:HD13 | 1.99                     | 0.44              |
| 2:F:1307:ILE:HD13 | 2:F:1322:GLU:OE1  | 2.17                     | 0.44              |
| 2:F:1408:MET:HE3  | 2:F:1411:PHE:CD1  | 2.52                     | 0.44              |
| 3:G:211:LYS:H     | 3:G:211:LYS:HG2   | 1.52                     | 0.44              |
| 4:H:74:VAL:HB     | 4:H:100:PHE:HE1   | 1.82                     | 0.44              |
| 3:C:136:ASN:HA    | 5:I:438:ASP:CG    | 2.43                     | 0.44              |
| 5:J:396:VAL:HG22  | 5:J:407:ILE:HD11  | 1.99                     | 0.44              |
| 2:B:844:GLN:OE1   | 2:B:1502:LEU:HD12 | 2.18                     | 0.44              |
| 2:B:1499:ASP:HB3  | 2:B:1500:GLY:H    | 1.56                     | 0.44              |
| 2:F:1602:TYR:CD1  | 2:F:1630:HIS:HA   | 2.53                     | 0.44              |
| 2:B:1177:GLU:OE1  | 2:B:1201:ARG:NH2  | 2.32                     | 0.44              |
| 2:B:1569:ILE:HD13 | 2:B:1653:THR:HG22 | 1.99                     | 0.44              |
| 2:B:1570:LYS:NZ   | 2:B:1661:CYS:SG   | 2.89                     | 0.44              |
| 3:C:248:ASP:OD1   | 3:C:248:ASP:N     | 2.50                     | 0.44              |
| 1:E:136:LYS:HB2   | 1:E:136:LYS:HE3   | 1.84                     | 0.44              |
| 2:F:1465:GLN:NE2  | 2:F:1468:ASN:OD1  | 2.50                     | 0.44              |
| 5:J:404:LEU:HA    | 5:J:407:ILE:HG21  | 2.00                     | 0.44              |
| 5:J:364:THR:HG22  | 5:J:381:CYS:SG    | 2.57                     | 0.44              |
| 1:A:93:ASN:HB3    | 1:A:95:GLU:HG2    | 1.99                     | 0.44              |
| 4:D:274:SER:O     | 3:G:27:ARG:NH1    | 2.51                     | 0.44              |
| 5:I:351:LEU:HD12  | 5:I:354:GLN:HB2   | 2.00                     | 0.44              |
| 2:F:826:MET:HG2   | 2:F:827:GLN:N     | 2.32                     | 0.44              |
| 1:A:231:SER:C     | 1:A:260:LEU:HG    | 2.43                     | 0.44              |
| 5:I:478:ASN:O     | 5:I:480:ARG:N     | 2.49                     | 0.44              |
| 1:A:566:LYS:HD2   | 1:A:584:LYS:HD2   | 2.00                     | 0.44              |
| 4:D:32:LYS:H      | 4:D:32:LYS:HD2    | 1.83                     | 0.44              |
| 5:I:544:VAL:HG22  | 5:I:559:TYR:CE2   | 2.51                     | 0.44              |
| 2:F:864:VAL:HG11  | 2:F:896:VAL:HG21  | 2.00                     | 0.44              |
| 2:F:938:MET:HE2   | 2:F:938:MET:HB3   | 1.94                     | 0.44              |
| 2:F:962:ILE:HG21  | 2:F:1344:VAL:HG21 | 2.00                     | 0.44              |
| 5:J:544:VAL:HA    | 5:J:559:TYR:CD1   | 2.45                     | 0.44              |
| 1:A:62:PHE:HA     | 1:A:63:PRO:HA     | 1.75                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:185:GLN:HB3   | 1:A:188:VAL:O     | 2.18                     | 0.44              |
| 2:B:798:SER:HB2   | 2:B:802:TRP:CZ2   | 2.53                     | 0.44              |
| 2:B:1113:LYS:HG2  | 2:B:1117:VAL:O    | 2.18                     | 0.44              |
| 2:B:1480:TYR:HB3  | 2:B:1488:SER:CB   | 2.48                     | 0.44              |
| 4:D:177:ASN:C     | 4:D:177:ASN:HD22  | 2.25                     | 0.44              |
| 3:G:120:LEU:HD21  | 3:G:125:ASN:HB2   | 2.00                     | 0.44              |
| 3:G:147:LEU:HG    | 5:J:400:ILE:HD12  | 2.00                     | 0.44              |
| 5:J:543:VAL:HG23  | 5:J:560:THR:HG23  | 1.99                     | 0.44              |
| 5:J:547:GLY:HA2   | 5:J:558:VAL:HG23  | 2.00                     | 0.44              |
| 2:B:1104:VAL:HG13 | 2:B:1151:LEU:HD22 | 1.99                     | 0.43              |
| 2:B:1284:LYS:C    | 2:B:1286:ALA:H    | 2.25                     | 0.43              |
| 1:E:138:ILE:HD11  | 1:E:225:LYS:HB3   | 1.98                     | 0.43              |
| 2:F:1067:ALA:HB2  | 2:F:1074:PRO:HA   | 1.99                     | 0.43              |
| 4:H:247:CYS:SG    | 4:H:251:SER:HB2   | 2.58                     | 0.43              |
| 2:B:1042:ARG:NH1  | 2:B:1046:LEU:HD11 | 2.33                     | 0.43              |
| 4:D:147:MET:SD    | 4:D:165:THR:HG22  | 2.58                     | 0.43              |
| 1:E:93:ASN:HB3    | 1:E:95:GLU:HG2    | 2.00                     | 0.43              |
| 1:E:198:LEU:HD13  | 2:F:1347:MET:HG2  | 2.00                     | 0.43              |
| 2:F:1510:LEU:HG   | 2:F:1612:TRP:CZ2  | 2.53                     | 0.43              |
| 5:J:569:ILE:O     | 5:J:573:VAL:HG22  | 2.18                     | 0.43              |
| 3:C:1112:PRO:HD3  | 3:C:1128:TYR:CE2  | 2.53                     | 0.43              |
| 3:G:1179:ILE:HG21 | 3:G:1226:PRO:HG2  | 2.00                     | 0.43              |
| 5:J:351:LEU:HD12  | 5:J:354:GLN:HB2   | 2.00                     | 0.43              |
| 2:B:798:SER:HB2   | 2:B:802:TRP:HZ2   | 1.84                     | 0.43              |
| 2:B:1294:LEU:HD23 | 2:B:1294:LEU:HA   | 1.89                     | 0.43              |
| 2:B:1510:LEU:HG   | 2:B:1612:TRP:CZ2  | 2.53                     | 0.43              |
| 5:I:419:GLU:C     | 5:I:421:TYR:H     | 2.26                     | 0.43              |
| 1:E:244:TYR:CE2   | 1:E:246:TYR:HB2   | 2.52                     | 0.43              |
| 2:F:978:THR:HB    | 2:F:1324:THR:HG23 | 2.00                     | 0.43              |
| 4:H:131:LEU:HD11  | 4:H:182:LEU:HD11  | 2.00                     | 0.43              |
| 1:A:496:ASN:HB3   | 1:A:499:ARG:HH12  | 1.82                     | 0.43              |
| 2:B:1502:LEU:HD23 | 2:B:1515:GLU:HG2  | 2.01                     | 0.43              |
| 3:C:167:GLU:CD    | 3:C:167:GLU:H     | 2.26                     | 0.43              |
| 2:F:903:LEU:HD11  | 2:F:1513:CYS:SG   | 2.59                     | 0.43              |
| 2:F:1544:VAL:HG22 | 2:F:1605:TRP:CB   | 2.48                     | 0.43              |
| 2:F:1585:ILE:HB   | 2:F:1621:ILE:HD13 | 2.01                     | 0.43              |
| 1:A:45:GLU:OE1    | 1:A:534:TYR:OH    | 2.25                     | 0.43              |
| 4:D:310:ASP:OD1   | 4:D:312:ASP:N     | 2.52                     | 0.43              |
| 2:F:863:ARG:O     | 2:F:863:ARG:HG3   | 2.17                     | 0.43              |
| 5:J:340:ILE:HD12  | 5:J:524:ASP:OD2   | 2.19                     | 0.43              |
| 5:J:577:PHE:HB3   | 5:J:578:ILE:H     | 1.55                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:I:341:VAL:HA    | 5:I:475:GLU:HA   | 2.01                     | 0.43              |
| 1:E:357:PHE:CD2   | 1:E:441:MET:HB3  | 2.53                     | 0.43              |
| 2:F:978:THR:O     | 2:F:1323:GLU:HA  | 2.19                     | 0.43              |
| 4:H:190:GLU:N     | 4:H:190:GLU:OE2  | 2.51                     | 0.43              |
| 2:B:1009:GLY:HA3  | 2:B:1013:GLN:HB2 | 2.01                     | 0.43              |
| 2:B:1214:ALA:HB2  | 2:B:1220:TRP:CZ2 | 2.54                     | 0.43              |
| 4:H:155:LEU:HD23  | 4:H:191:THR:HA   | 2.01                     | 0.43              |
| 4:H:314:GLU:OE2   | 4:H:317:ARG:NH1  | 2.52                     | 0.43              |
| 2:B:977:GLU:OE1   | 2:B:1323:GLU:HG2 | 2.19                     | 0.43              |
| 5:I:376:LEU:HD11  | 5:I:430:ILE:HD11 | 2.00                     | 0.43              |
| 4:H:54:CYS:HB3    | 5:J:580:GLN:HG3  | 1.99                     | 0.43              |
| 5:J:515:ASP:H     | 5:J:553:PRO:HB3  | 1.84                     | 0.43              |
| 2:B:1520:ILE:HD11 | 2:B:1625:ASP:HA  | 2.01                     | 0.42              |
| 5:I:476:LYS:HB3   | 5:I:477:ASP:H    | 1.58                     | 0.42              |
| 5:I:487:GLY:HA3   | 5:I:518:ILE:HD11 | 2.00                     | 0.42              |
| 1:E:132:ILE:HB    | 1:E:220:THR:OG1  | 2.19                     | 0.42              |
| 2:F:844:GLN:HA    | 2:F:901:VAL:HG22 | 2.00                     | 0.42              |
| 2:F:859:GLU:HB3   | 2:F:890:PRO:HD3  | 2.00                     | 0.42              |
| 3:G:1112:PRO:HA   | 3:G:1113:PRO:HD3 | 1.91                     | 0.42              |
| 5:J:394:THR:HG22  | 5:J:408:VAL:O    | 2.19                     | 0.42              |
| 2:B:835:LEU:HG    | 2:B:929:LEU:HD23 | 2.02                     | 0.42              |
| 3:C:32:ILE:HG22   | 3:C:51:LYS:HB3   | 2.01                     | 0.42              |
| 3:C:1168:VAL:O    | 3:C:1225:TYR:OH  | 2.35                     | 0.42              |
| 4:D:268:SER:HB2   | 4:D:285:ILE:HD11 | 2.01                     | 0.42              |
| 1:E:29:ILE:HA     | 1:E:645:THR:O    | 2.19                     | 0.42              |
| 3:C:102:ASN:OD1   | 3:C:102:ASN:N    | 2.52                     | 0.42              |
| 1:E:566:LYS:HG3   | 1:E:584:LYS:HB3  | 2.01                     | 0.42              |
| 2:F:905:THR:HA    | 2:F:931:VAL:HB   | 2.01                     | 0.42              |
| 4:H:306:ILE:HG23  | 4:H:307:LEU:N    | 2.32                     | 0.42              |
| 2:B:895:SER:O     | 2:B:1442:ASN:ND2 | 2.43                     | 0.42              |
| 4:D:190:GLU:OE2   | 4:D:190:GLU:N    | 2.52                     | 0.42              |
| 4:D:249:ASP:OD1   | 4:D:251:SER:OG   | 2.28                     | 0.42              |
| 1:E:169:ASN:HD21  | 1:E:173:ILE:HB   | 1.85                     | 0.42              |
| 2:F:1554:LEU:HD22 | 2:F:1591:ARG:HE  | 1.83                     | 0.42              |
| 3:G:32:ILE:HG22   | 3:G:51:LYS:HB3   | 2.00                     | 0.42              |
| 2:B:1076:THR:HB   | 2:B:1120:GLU:HA  | 2.02                     | 0.42              |
| 2:B:1507:ARG:HB3  | 2:B:1558:PHE:CE2 | 2.55                     | 0.42              |
| 3:C:143:VAL:O     | 3:C:145:LYS:HE2  | 2.19                     | 0.42              |
| 4:D:305:GLU:HG2   | 4:D:306:ILE:HG23 | 2.01                     | 0.42              |
| 1:E:284:LEU:HD22  | 1:E:310:GLY:HA3  | 2.00                     | 0.42              |
| 1:E:577:PRO:HD2   | 2:F:827:GLN:CG   | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:136:LYS:HD3   | 4:D:180:GLU:OE2   | 2.19                     | 0.42              |
| 1:E:126:GLN:HB3   | 1:E:154:HIS:HE1   | 1.84                     | 0.42              |
| 2:F:1176:LEU:O    | 2:F:1180:TYR:HB2  | 2.19                     | 0.42              |
| 1:A:360:THR:HG23  | 1:A:372:LEU:HA    | 2.02                     | 0.42              |
| 1:A:628:THR:OG1   | 1:A:641:ASP:HB3   | 2.19                     | 0.42              |
| 2:B:978:THR:O     | 2:B:1323:GLU:HA   | 2.20                     | 0.42              |
| 2:B:997:ALA:HB2   | 2:B:1033:GLN:OE1  | 2.20                     | 0.42              |
| 2:B:1654:GLU:OE2  | 4:D:80:ARG:NH2    | 2.52                     | 0.42              |
| 1:A:364:PHE:CD2   | 1:A:413:THR:HG21  | 2.54                     | 0.42              |
| 1:E:527:PRO:HG3   | 1:E:617:TRP:CE3   | 2.55                     | 0.42              |
| 2:F:1392:TYR:CD1  | 2:F:1398:ALA:HB2  | 2.55                     | 0.42              |
| 5:J:358:LYS:HE2   | 5:J:393:TRP:CZ2   | 2.55                     | 0.42              |
| 2:B:1023:ILE:HD12 | 2:B:1023:ILE:HA   | 1.92                     | 0.42              |
| 3:C:1167:CYS:SG   | 3:C:1223:LEU:HB2  | 2.60                     | 0.42              |
| 4:D:217:GLN:OE1   | 4:D:217:GLN:N     | 2.47                     | 0.42              |
| 1:E:164:MET:HE3   | 1:E:164:MET:HB3   | 1.97                     | 0.42              |
| 2:F:1533:LEU:O    | 2:F:1537:CYS:HB2  | 2.20                     | 0.42              |
| 2:B:826:MET:HE2   | 2:B:826:MET:HB3   | 1.96                     | 0.42              |
| 2:B:1042:ARG:HH12 | 2:B:1046:LEU:HD11 | 1.84                     | 0.42              |
| 2:B:1425:VAL:HG11 | 2:B:1427:ARG:HH11 | 1.84                     | 0.42              |
| 3:C:49:ILE:HG23   | 3:C:61:ASN:HB3    | 2.01                     | 0.42              |
| 1:A:527:PRO:HG3   | 1:A:617:TRP:CE3   | 2.54                     | 0.41              |
| 2:B:1176:LEU:O    | 2:B:1180:TYR:HB2  | 2.20                     | 0.41              |
| 3:C:1162:LYS:HE3  | 3:C:1162:LYS:HB2  | 1.94                     | 0.41              |
| 4:D:204:MET:C     | 4:D:206:TYR:H     | 2.27                     | 0.41              |
| 2:F:1031:THR:HB   | 2:F:1033:GLN:HE21 | 1.84                     | 0.41              |
| 2:B:1118:PHE:CD1  | 2:B:1144:THR:HA   | 2.48                     | 0.41              |
| 2:B:1594:LEU:HD12 | 2:B:1594:LEU:HA   | 1.82                     | 0.41              |
| 2:B:1639:ASP:O    | 2:B:1643:GLN:HG3  | 2.19                     | 0.41              |
| 5:I:499:TYR:OH    | 5:I:556:PRO:O     | 2.34                     | 0.41              |
| 2:F:1661:CYS:HB3  | 2:F:1662:PRO:HD2  | 2.02                     | 0.41              |
| 5:J:363:ILE:HG22  | 5:J:399:TRP:CH2   | 2.55                     | 0.41              |
| 1:A:360:THR:OG1   | 1:A:373:MET:N     | 2.49                     | 0.41              |
| 1:A:494:ILE:HD12  | 1:A:502:LYS:HB3   | 2.02                     | 0.41              |
| 4:D:86:CYS:HB2    | 4:D:318:ILE:HD13  | 2.01                     | 0.41              |
| 1:E:119:LYS:NZ    | 1:E:654:THR:O     | 2.42                     | 0.41              |
| 2:F:1306:LYS:HD2  | 5:J:474:ARG:HH21  | 1.84                     | 0.41              |
| 2:F:1604:MET:HA   | 2:F:1627:TRP:O    | 2.19                     | 0.41              |
| 3:G:102:ASN:OD1   | 3:G:102:ASN:N     | 2.53                     | 0.41              |
| 3:G:159:SER:O     | 3:G:160:SER:OG    | 2.34                     | 0.41              |
| 4:H:33:CYS:SG     | 4:H:34:LEU:N      | 2.93                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:879:LYS:NZ    | 2:B:1625:ASP:OD1  | 2.35                     | 0.41              |
| 4:D:117:LYS:HB3   | 4:D:118:HIS:ND1   | 2.34                     | 0.41              |
| 4:D:314:GLU:O     | 4:D:318:ILE:HG13  | 2.21                     | 0.41              |
| 5:I:396:VAL:HG21  | 5:I:472:TRP:HE1   | 1.86                     | 0.41              |
| 3:G:121:LEU:HA    | 5:J:404:LEU:HD22  | 2.01                     | 0.41              |
| 4:H:51:TRP:C      | 4:H:62:LYS:HG2    | 2.45                     | 0.41              |
| 1:A:29:ILE:HD12   | 1:A:493:LEU:HD21  | 2.02                     | 0.41              |
| 2:B:957:VAL:HG12  | 2:B:1335:GLU:HB3  | 2.00                     | 0.41              |
| 4:D:141:CYS:N     | 4:D:181:CYS:SG    | 2.93                     | 0.41              |
| 1:E:131:PHE:CZ    | 1:E:616:ILE:HG23  | 2.55                     | 0.41              |
| 2:F:1499:ASP:OD1  | 2:F:1499:ASP:N    | 2.54                     | 0.41              |
| 2:F:1639:ASP:O    | 2:F:1643:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:23:SER:O      | 1:A:544:ARG:NH2   | 2.54                     | 0.41              |
| 1:A:32:ASN:HA     | 1:A:645:THR:HG23  | 2.02                     | 0.41              |
| 1:A:486:LYS:HD3   | 1:A:537:LEU:HB2   | 2.02                     | 0.41              |
| 3:C:253:GLU:H     | 3:C:253:GLU:HG2   | 1.58                     | 0.41              |
| 3:C:254:SER:HB2   | 3:C:257:ARG:NH1   | 2.30                     | 0.41              |
| 2:B:1304:SER:OG   | 2:B:1305:SER:N    | 2.52                     | 0.41              |
| 1:E:271:VAL:HG11  | 1:E:300:VAL:HG11  | 2.03                     | 0.41              |
| 1:A:32:ASN:ND2    | 1:A:643:GLY:HA2   | 2.36                     | 0.41              |
| 1:A:355:ILE:HD11  | 1:A:426:THR:HG23  | 2.02                     | 0.41              |
| 2:B:1110:GLU:O    | 3:C:1140:ASN:HB2  | 2.20                     | 0.41              |
| 4:D:224:ASP:O     | 4:D:225:ASP:C     | 2.64                     | 0.41              |
| 1:E:207:ARG:HD3   | 1:E:219:SER:OG    | 2.21                     | 0.41              |
| 1:A:41:THR:HG21   | 6:K:1:NAG:H82     | 2.02                     | 0.41              |
| 1:A:334:SER:O     | 2:B:848:ARG:NH2   | 2.53                     | 0.41              |
| 2:B:781:PRO:HA    | 2:B:782:PRO:HD3   | 1.95                     | 0.41              |
| 5:I:357:ILE:HD11  | 5:I:390:TYR:CD2   | 2.55                     | 0.41              |
| 5:I:544:VAL:HG22  | 5:I:559:TYR:HE2   | 1.85                     | 0.41              |
| 1:E:566:LYS:HD2   | 1:E:584:LYS:HD2   | 2.02                     | 0.41              |
| 1:E:600:LYS:HB3   | 1:E:600:LYS:HE2   | 1.86                     | 0.41              |
| 1:E:628:THR:OG1   | 1:E:641:ASP:HB3   | 2.21                     | 0.41              |
| 5:J:429:ASP:O     | 5:J:560:THR:HG21  | 2.20                     | 0.41              |
| 1:A:532:VAL:HG11  | 1:A:644:LEU:HD12  | 2.03                     | 0.41              |
| 1:A:631:SER:OG    | 1:A:632:GLY:N     | 2.54                     | 0.41              |
| 2:B:1553:GLN:HB2  | 2:B:1560:GLU:CG   | 2.51                     | 0.41              |
| 3:C:221:ILE:HD11  | 3:C:236:LYS:HB3   | 2.03                     | 0.41              |
| 2:F:1594:LEU:HD12 | 2:F:1594:LEU:HA   | 1.82                     | 0.41              |
| 2:B:1202:LEU:HD23 | 2:B:1243:LEU:HD11 | 2.03                     | 0.40              |
| 2:B:1566:GLU:OE2  | 2:B:1601:HIS:NE2  | 2.54                     | 0.40              |
| 2:B:1580:GLN:OE1  | 2:B:1580:GLN:HA   | 2.20                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:307:LEU:O     | 4:D:308:THR:C    | 2.63                     | 0.40              |
| 5:I:392:ILE:C     | 5:I:393:TRP:HD1  | 2.29                     | 0.40              |
| 2:F:1306:LYS:HB3  | 5:J:474:ARG:CZ   | 2.50                     | 0.40              |
| 1:A:600:LYS:HB3   | 1:A:600:LYS:HE2  | 1.92                     | 0.40              |
| 3:C:254:SER:HB2   | 3:C:257:ARG:HH22 | 1.86                     | 0.40              |
| 2:F:1553:GLN:HB2  | 2:F:1560:GLU:CG  | 2.51                     | 0.40              |
| 4:H:114:VAL:HG21  | 4:H:193:LEU:HD12 | 2.02                     | 0.40              |
| 2:B:1214:ALA:HB2  | 2:B:1220:TRP:CE2 | 2.56                     | 0.40              |
| 2:B:1602:TYR:CD1  | 2:B:1630:HIS:HA  | 2.56                     | 0.40              |
| 5:I:575:ARG:HD3   | 5:I:575:ARG:HA   | 1.79                     | 0.40              |
| 2:F:1294:LEU:HD23 | 2:F:1294:LEU:HA  | 1.85                     | 0.40              |
| 2:F:1542:ASP:OD1  | 2:F:1572:GLY:HA3 | 2.22                     | 0.40              |
| 2:F:1614:GLU:O    | 2:F:1615:LYS:C   | 2.64                     | 0.40              |
| 3:G:47:GLN:HG2    | 3:G:65:VAL:HG22  | 2.02                     | 0.40              |
| 2:B:1537:CYS:SG   | 2:B:1656:MET:HE1 | 2.61                     | 0.40              |
| 4:H:141:CYS:N     | 4:H:181:CYS:SG   | 2.94                     | 0.40              |
| 5:J:379:ALA:HB2   | 5:J:430:ILE:O    | 2.21                     | 0.40              |
| 5:J:446:LEU:HD13  | 5:J:448:ARG:H    | 1.87                     | 0.40              |
| 5:J:547:GLY:HA2   | 5:J:558:VAL:H    | 1.86                     | 0.40              |
| 4:D:142:LYS:HG2   | 4:D:208:ASP:HA   | 2.03                     | 0.40              |
| 1:E:108:VAL:O     | 1:E:118:GLU:HA   | 2.22                     | 0.40              |
| 2:F:826:MET:HE2   | 2:F:826:MET:HB3  | 1.82                     | 0.40              |
| 2:F:1497:LYS:HA   | 2:F:1497:LYS:HD3 | 1.79                     | 0.40              |
| 2:F:1656:MET:HE3  | 2:F:1656:MET:HA  | 2.04                     | 0.40              |
| 3:G:21:CYS:O      | 3:G:22:ASN:ND2   | 2.45                     | 0.40              |
| 3:G:157:ILE:HD11  | 3:G:176:PHE:CE2  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 636/645 (99%)   | 612 (96%)  | 24 (4%)  | 0        | 100         | 100 |
| 1   | E     | 636/645 (99%)   | 612 (96%)  | 24 (4%)  | 0        | 100         | 100 |
| 2   | B     | 899/915 (98%)   | 848 (94%)  | 44 (5%)  | 7 (1%)   | 16          | 52  |
| 2   | F     | 899/915 (98%)   | 846 (94%)  | 49 (6%)  | 4 (0%)   | 30          | 66  |
| 3   | C     | 367/383 (96%)   | 341 (93%)  | 21 (6%)  | 5 (1%)   | 9           | 39  |
| 3   | G     | 367/383 (96%)   | 339 (92%)  | 22 (6%)  | 6 (2%)   | 7           | 37  |
| 4   | D     | 297/321 (92%)   | 266 (90%)  | 25 (8%)  | 6 (2%)   | 6           | 32  |
| 4   | H     | 297/321 (92%)   | 270 (91%)  | 21 (7%)  | 6 (2%)   | 6           | 32  |
| 5   | I     | 239/244 (98%)   | 201 (84%)  | 30 (13%) | 8 (3%)   | 3           | 21  |
| 5   | J     | 239/244 (98%)   | 207 (87%)  | 26 (11%) | 6 (2%)   | 4           | 27  |
| All | All   | 4876/5016 (97%) | 4542 (93%) | 286 (6%) | 48 (1%)  | 12          | 47  |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 975  | GLU  |
| 2   | B     | 1522 | LYS  |
| 2   | B     | 1615 | LYS  |
| 3   | C     | 71   | TRP  |
| 5   | I     | 402  | PRO  |
| 2   | F     | 1498 | GLU  |
| 3   | G     | 163  | GLU  |
| 4   | H     | 208  | ASP  |
| 2   | B     | 1111 | LYS  |
| 2   | B     | 1288 | ASP  |
| 4   | D     | 218  | LYS  |
| 4   | D     | 222  | PRO  |
| 4   | D     | 306  | ILE  |
| 5   | I     | 341  | VAL  |
| 5   | I     | 479  | GLU  |
| 2   | F     | 1111 | LYS  |
| 2   | F     | 1288 | ASP  |
| 3   | G     | 21   | CYS  |
| 3   | G     | 104  | PHE  |
| 3   | G     | 137  | ASP  |
| 3   | C     | 1191 | SER  |
| 4   | D     | 308  | THR  |
| 5   | I     | 552  | LYS  |
| 5   | I     | 576  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | H     | 217  | GLN  |
| 4   | H     | 308  | THR  |
| 3   | C     | 43   | PRO  |
| 3   | C     | 104  | PHE  |
| 5   | I     | 397  | VAL  |
| 5   | I     | 400  | ILE  |
| 4   | H     | 306  | ILE  |
| 4   | H     | 331  | ASN  |
| 5   | J     | 453  | CYS  |
| 5   | J     | 577  | PHE  |
| 2   | B     | 988  | ALA  |
| 2   | B     | 1304 | SER  |
| 3   | C     | 1193 | THR  |
| 3   | G     | 160  | SER  |
| 4   | H     | 201  | ARG  |
| 5   | J     | 480  | ARG  |
| 4   | D     | 307  | LEU  |
| 5   | I     | 480  | ARG  |
| 2   | F     | 1495 | PRO  |
| 5   | J     | 404  | LEU  |
| 4   | D     | 323  | PRO  |
| 5   | J     | 397  | VAL  |
| 3   | G     | 43   | PRO  |
| 5   | J     | 576  | PRO  |

### 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     | 564/567 (100%) | 564 (100%) | 0        | 100         | 100 |
| 1   | E     | 564/567 (100%) | 564 (100%) | 0        | 100         | 100 |
| 2   | B     | 797/810 (98%)  | 797 (100%) | 0        | 100         | 100 |
| 2   | F     | 797/810 (98%)  | 797 (100%) | 0        | 100         | 100 |
| 3   | C     | 328/328 (100%) | 328 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 3   | G     | 328/328 (100%)  | 328 (100%)  | 0        | 100         | 100 |
| 4   | D     | 264/283 (93%)   | 264 (100%)  | 0        | 100         | 100 |
| 4   | H     | 264/283 (93%)   | 264 (100%)  | 0        | 100         | 100 |
| 5   | I     | 202/207 (98%)   | 202 (100%)  | 0        | 100         | 100 |
| 5   | J     | 202/207 (98%)   | 202 (100%)  | 0        | 100         | 100 |
| All | All   | 4310/4390 (98%) | 4310 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 60   | HIS  |
| 1   | A     | 93   | ASN  |
| 1   | A     | 154  | HIS  |
| 1   | A     | 333  | HIS  |
| 1   | A     | 417  | GLN  |
| 1   | A     | 569  | GLN  |
| 1   | A     | 589  | HIS  |
| 2   | B     | 856  | GLN  |
| 2   | B     | 858  | GLN  |
| 2   | B     | 1043 | GLN  |
| 2   | B     | 1259 | GLN  |
| 2   | B     | 1293 | ASN  |
| 2   | B     | 1359 | ASN  |
| 2   | B     | 1465 | GLN  |
| 3   | C     | 172  | GLN  |
| 3   | C     | 1139 | GLN  |
| 3   | C     | 1154 | ASN  |
| 3   | C     | 1212 | HIS  |
| 5   | I     | 462  | GLN  |
| 5   | I     | 485  | GLN  |
| 1   | E     | 60   | HIS  |
| 1   | E     | 126  | GLN  |
| 1   | E     | 356  | HIS  |
| 1   | E     | 378  | ASN  |
| 2   | F     | 844  | GLN  |
| 2   | F     | 857  | ASN  |
| 2   | F     | 858  | GLN  |
| 3   | G     | 22   | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | G     | 40   | GLN  |
| 3   | G     | 75   | ASN  |
| 3   | G     | 191  | HIS  |
| 3   | G     | 1137 | GLN  |
| 3   | G     | 1178 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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 | $\# Z  > 2$ |
| 6   | NAG  | K     | 1   | 6,1  | 14,14,15     | 0.20 | 0           | 17,19,21    | 0.44 | 0           |
| 6   | NAG  | K     | 2   | 6    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.40 | 0           |
| 6   | BMA  | K     | 3   | 6    | 11,11,12     | 1.16 | 1 (9%)      | 15,15,17    | 1.26 | 2 (13%)     |
| 6   | BMA  | K     | 4   | 6    | 11,11,12     | 0.70 | 0           | 15,15,17    | 0.98 | 1 (6%)      |
| 6   | BMA  | K     | 5   | 6    | 11,11,12     | 0.59 | 0           | 15,15,17    | 0.74 | 0           |
| 7   | NAG  | L     | 1   | 7,2  | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.43 | 0           |
| 7   | NAG  | L     | 2   | 7    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.38 | 0           |
| 6   | NAG  | M     | 1   | 6,1  | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.45 | 0           |
| 6   | NAG  | M     | 2   | 6    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.40 | 0           |
| 6   | BMA  | M     | 3   | 6    | 11,11,12     | 1.15 | 1 (9%)      | 15,15,17    | 1.27 | 2 (13%)     |
| 6   | BMA  | M     | 4   | 6    | 11,11,12     | 0.66 | 0           | 15,15,17    | 0.99 | 1 (6%)      |
| 6   | BMA  | M     | 5   | 6    | 11,11,12     | 0.63 | 0           | 15,15,17    | 0.73 | 0           |
| 7   | NAG  | N     | 1   | 7,2  | 14,14,15     | 0.51 | 0           | 17,19,21    | 0.46 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | NAG  | N     | 2   | 7    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.43 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 6   | NAG  | K     | 1   | 6,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | K     | 3   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 6   | BMA  | K     | 4   | 6    | -       | 1/2/19/22 | 1/1/1/1 |
| 6   | BMA  | K     | 5   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | NAG  | L     | 1   | 7,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | L     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | M     | 1   | 6,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | M     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | BMA  | M     | 3   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 6   | BMA  | M     | 4   | 6    | -       | 1/2/19/22 | 1/1/1/1 |
| 6   | BMA  | M     | 5   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | NAG  | N     | 1   | 7,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | N     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 6   | K     | 3   | BMA  | C2-C3 | 2.60 | 1.56        | 1.52     |
| 6   | M     | 3   | BMA  | C2-C3 | 2.58 | 1.56        | 1.52     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 6   | M     | 4   | BMA  | C1-O5-C5 | 2.98 | 116.19      | 112.19   |
| 6   | K     | 4   | BMA  | C1-O5-C5 | 2.94 | 116.13      | 112.19   |
| 6   | M     | 3   | BMA  | C1-C2-C3 | 2.63 | 113.48      | 109.64   |
| 6   | K     | 3   | BMA  | C1-C2-C3 | 2.59 | 113.41      | 109.64   |
| 6   | K     | 3   | BMA  | C2-C3-C4 | 2.53 | 115.31      | 110.86   |
| 6   | M     | 3   | BMA  | C2-C3-C4 | 2.52 | 115.30      | 110.86   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | K     | 5   | BMA  | O5-C5-C6-O6 |
| 6   | M     | 5   | BMA  | O5-C5-C6-O6 |
| 7   | N     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 5   | BMA  | C4-C5-C6-O6 |
| 6   | M     | 5   | BMA  | C4-C5-C6-O6 |
| 6   | K     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | N     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 2   | NAG  | C4-C5-C6-O6 |
| 7   | N     | 1   | NAG  | C4-C5-C6-O6 |
| 7   | N     | 2   | NAG  | C4-C5-C6-O6 |
| 7   | L     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 4   | BMA  | O5-C5-C6-O6 |
| 6   | M     | 4   | BMA  | O5-C5-C6-O6 |
| 7   | L     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | M     | 3   | BMA  | C4-C5-C6-O6 |
| 6   | K     | 3   | BMA  | C4-C5-C6-O6 |

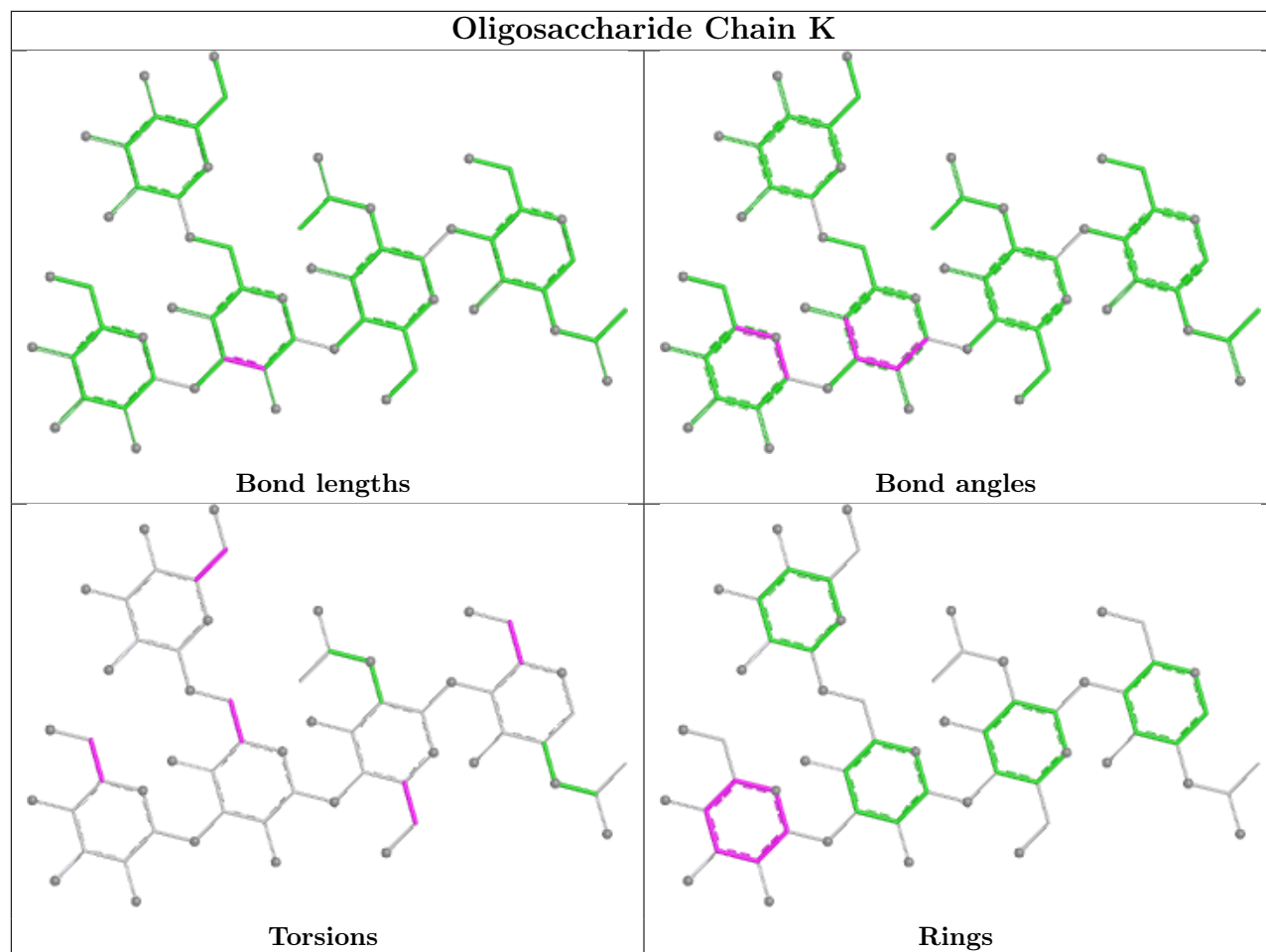
All (2) ring outliers are listed below:

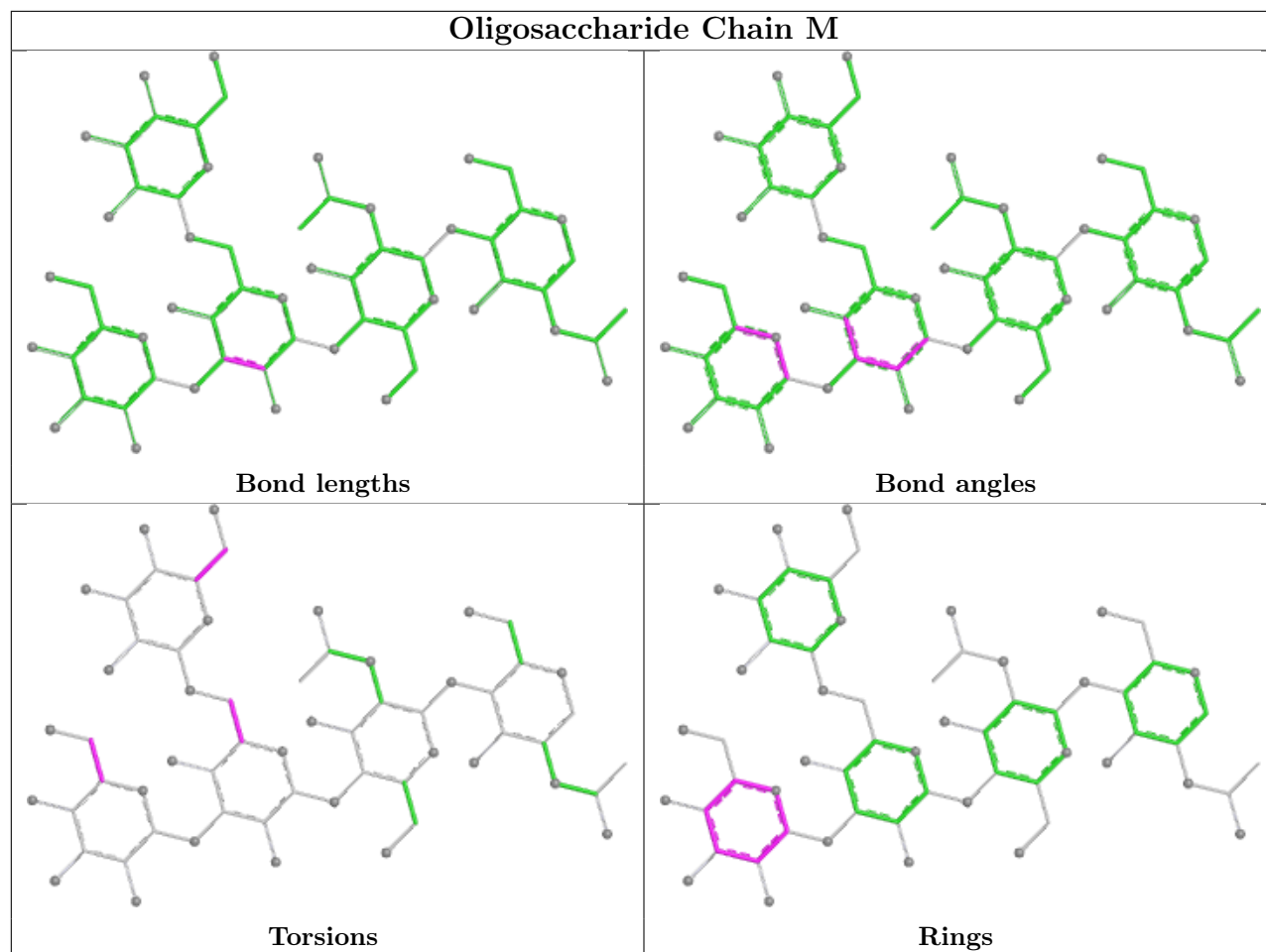
| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 6   | K     | 4   | BMA  | C1-C2-C3-C4-C5-O5 |
| 6   | M     | 4   | BMA  | C1-C2-C3-C4-C5-O5 |

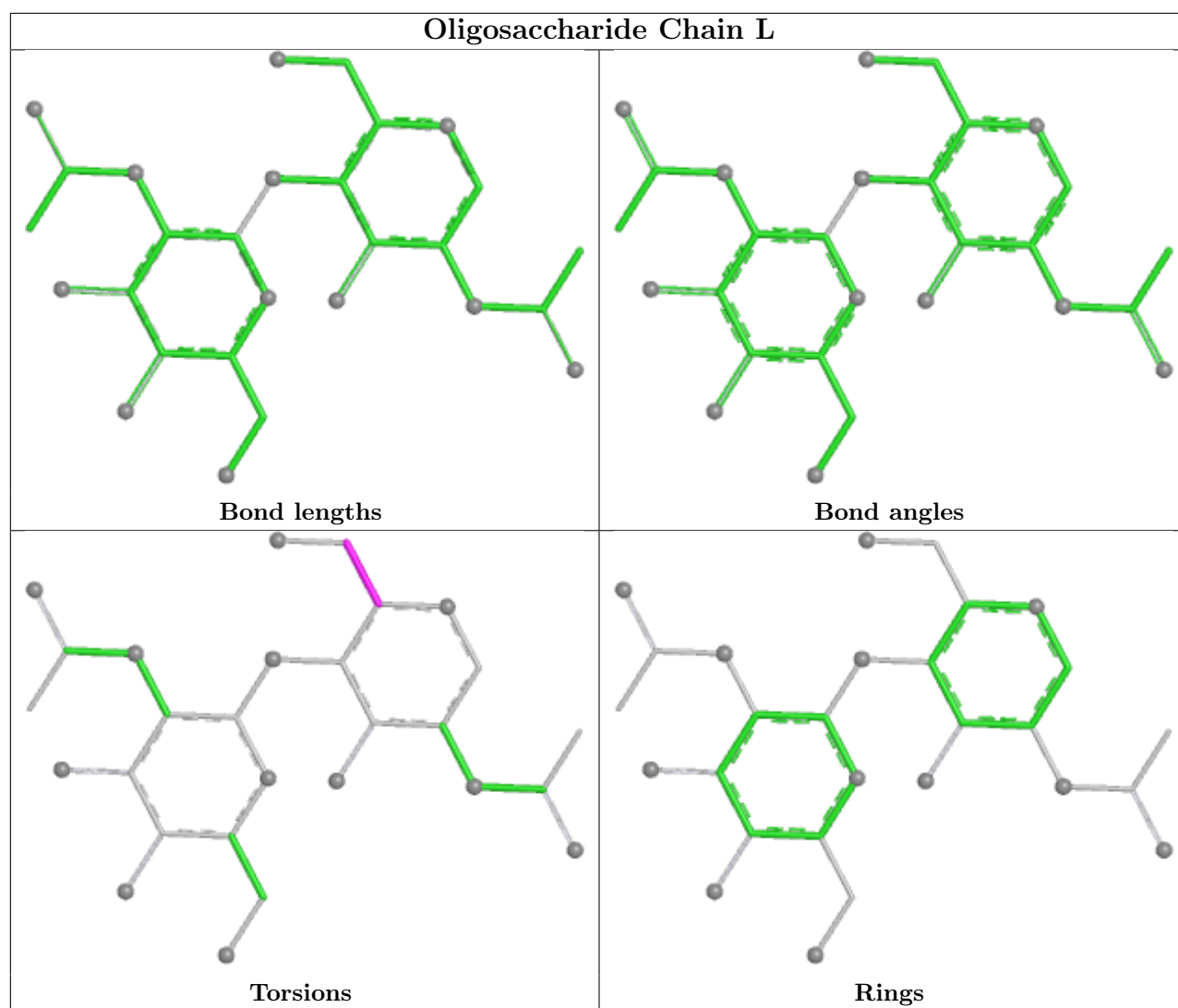
2 monomers are involved in 2 short contacts:

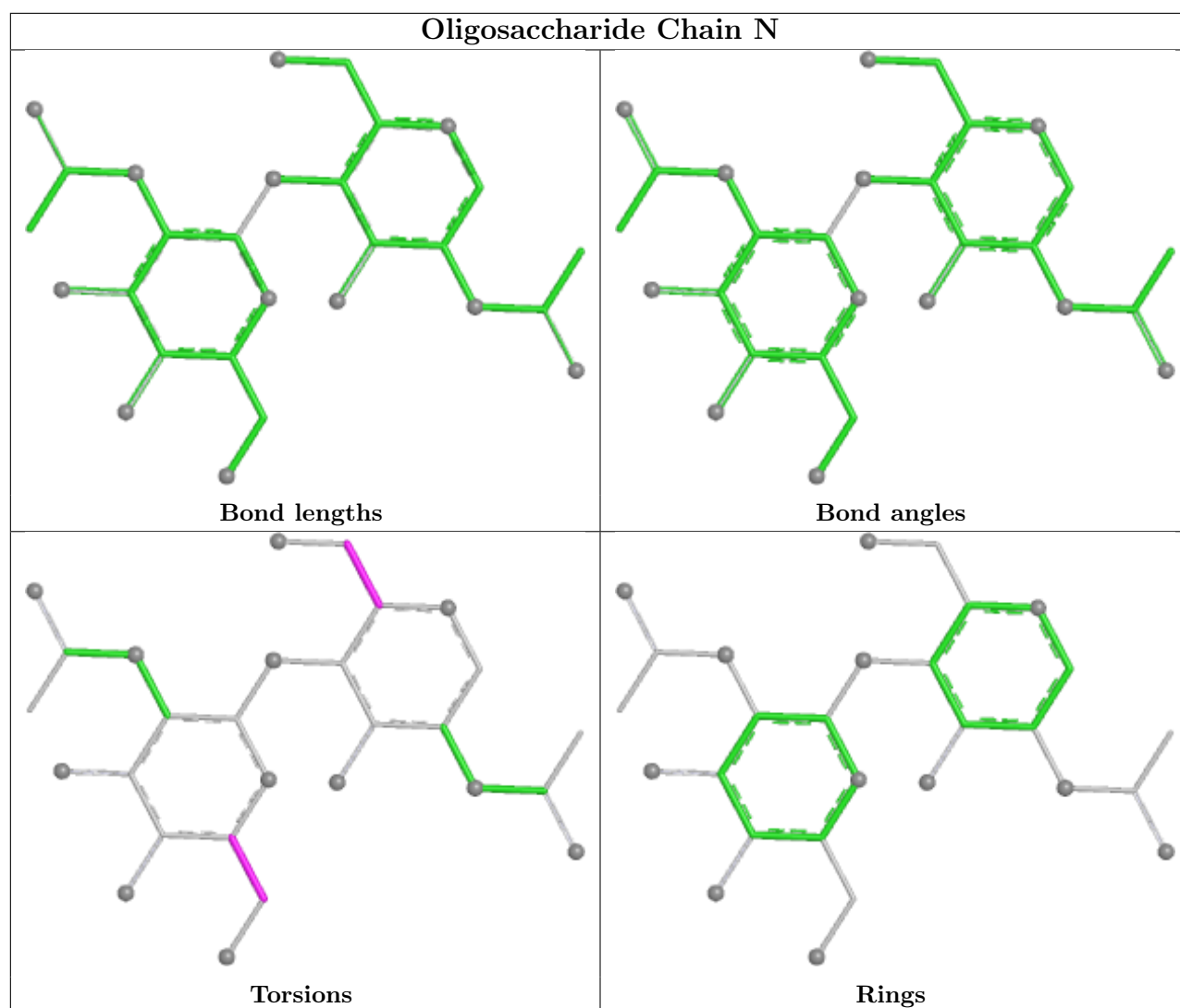
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | K     | 1   | NAG  | 1       | 0            |
| 7   | N     | 1   | NAG  | 1       | 0            |

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









## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 9   | NAG  | D     | 405 | 4    | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.42 | 0           |
| 9   | NAG  | H     | 403 | 4    | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.78 | 1 (5%)      |
| 10  | MLI  | J     | 604 | -    | 6,6,6        | 1.35 | 0           | 7,7,7       | 1.27 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | NAG  | H     | 404 | 4    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.42 | 0        |
| 9   | NAG  | I     | 602 | 5    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.44 | 0        |
| 9   | NAG  | I     | 601 | 5    | 14,14,15     | 0.46 | 0        | 17,19,21    | 0.46 | 0        |
| 9   | NAG  | D     | 404 | 4    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.45 | 0        |
| 9   | NAG  | J     | 602 | 5    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.51 | 0        |
| 9   | NAG  | D     | 403 | 4    | 14,14,15     | 0.72 | 0        | 17,19,21    | 1.21 | 1 (5%)   |
| 9   | NAG  | J     | 601 | 5    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.62 | 0        |
| 9   | NAG  | H     | 405 | 4    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.42 | 0        |
| 9   | NAG  | J     | 603 | 5    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.79 | 1 (5%)   |
| 9   | NAG  | I     | 603 | 5    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.39 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 9   | NAG  | D     | 405 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | H     | 403 | 4    | -       | 4/6/23/26 | 0/1/1/1 |
| 10  | MLI  | J     | 604 | -    | -       | 4/4/4/4   | -       |
| 9   | NAG  | H     | 404 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | I     | 602 | 5    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | I     | 601 | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | D     | 404 | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | J     | 602 | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | D     | 403 | 4    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | J     | 601 | 5    | -       | 4/6/23/26 | 0/1/1/1 |
| 9   | NAG  | H     | 405 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | J     | 603 | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | I     | 603 | 5    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 9   | D     | 403 | NAG  | C1-O5-C5 | 4.55 | 118.28      | 112.19   |
| 9   | J     | 603 | NAG  | C1-O5-C5 | 2.97 | 116.17      | 112.19   |
| 9   | H     | 403 | NAG  | C1-O5-C5 | 2.50 | 115.54      | 112.19   |

There are no chirality outliers.

All (28) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 9   | J     | 603 | NAG  | O5-C5-C6-O6 |
| 9   | J     | 603 | NAG  | C4-C5-C6-O6 |
| 9   | H     | 403 | NAG  | O5-C5-C6-O6 |
| 9   | I     | 601 | NAG  | C4-C5-C6-O6 |
| 9   | J     | 601 | NAG  | O5-C5-C6-O6 |
| 9   | J     | 602 | NAG  | O5-C5-C6-O6 |
| 9   | H     | 403 | NAG  | C4-C5-C6-O6 |
| 9   | J     | 602 | NAG  | C4-C5-C6-O6 |
| 9   | I     | 601 | NAG  | O5-C5-C6-O6 |
| 9   | I     | 603 | NAG  | C4-C5-C6-O6 |
| 9   | H     | 404 | NAG  | C8-C7-N2-C2 |
| 9   | H     | 404 | NAG  | O7-C7-N2-C2 |
| 9   | H     | 405 | NAG  | C8-C7-N2-C2 |
| 9   | H     | 405 | NAG  | O7-C7-N2-C2 |
| 9   | I     | 603 | NAG  | O5-C5-C6-O6 |
| 9   | J     | 601 | NAG  | C4-C5-C6-O6 |
| 9   | D     | 403 | NAG  | O5-C5-C6-O6 |
| 9   | D     | 405 | NAG  | C4-C5-C6-O6 |
| 10  | J     | 604 | MLI  | C3-C1-C2-O7 |
| 9   | D     | 405 | NAG  | O5-C5-C6-O6 |
| 9   | H     | 403 | NAG  | C3-C2-N2-C7 |
| 9   | J     | 601 | NAG  | C3-C2-N2-C7 |
| 10  | J     | 604 | MLI  | C2-C1-C3-O9 |
| 10  | J     | 604 | MLI  | C3-C1-C2-O6 |
| 9   | H     | 403 | NAG  | C1-C2-N2-C7 |
| 9   | J     | 601 | NAG  | C1-C2-N2-C7 |
| 10  | J     | 604 | MLI  | C2-C1-C3-O8 |
| 9   | I     | 602 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | D     | 405 | NAG  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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     | 640/645 (99%)   | 0.35   | 8 (1%) 75 59  | 40, 87, 131, 170      | 0     |
| 1   | E     | 640/645 (99%)   | 0.38   | 3 (0%) 87 75  | 41, 91, 132, 156      | 0     |
| 2   | B     | 903/915 (98%)   | 0.41   | 12 (1%) 75 59 | 48, 115, 159, 180     | 0     |
| 2   | F     | 903/915 (98%)   | 0.39   | 10 (1%) 78 62 | 47, 110, 152, 182     | 0     |
| 3   | C     | 371/383 (96%)   | 0.40   | 8 (2%) 62 48  | 65, 124, 192, 207     | 0     |
| 3   | G     | 371/383 (96%)   | 0.44   | 3 (0%) 82 68  | 60, 126, 197, 217     | 0     |
| 4   | D     | 301/321 (93%)   | 0.62   | 12 (3%) 42 35 | 96, 123, 157, 187     | 0     |
| 4   | H     | 301/321 (93%)   | 0.49   | 5 (1%) 69 54  | 77, 102, 140, 170     | 0     |
| 5   | I     | 241/244 (98%)   | 0.59   | 3 (1%) 76 61  | 71, 111, 148, 164     | 0     |
| 5   | J     | 241/244 (98%)   | 0.52   | 7 (2%) 53 41  | 64, 96, 126, 145      | 0     |
| All | All   | 4912/5016 (97%) | 0.43   | 71 (1%) 73 57 | 40, 107, 159, 217     | 0     |

All (71) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | H     | 305  | GLU  | 4.6  |
| 1   | A     | 403  | GLY  | 4.5  |
| 5   | J     | 360  | ALA  | 4.1  |
| 4   | D     | 117  | LYS  | 3.9  |
| 4   | D     | 209  | PHE  | 3.6  |
| 4   | D     | 169  | PHE  | 3.1  |
| 1   | E     | 461  | LEU  | 2.9  |
| 5   | I     | 377  | THR  | 2.9  |
| 5   | I     | 376  | LEU  | 2.9  |
| 2   | F     | 1326 | GLU  | 2.8  |
| 4   | H     | 102  | ASN  | 2.8  |
| 3   | C     | 247  | GLY  | 2.8  |
| 2   | F     | 1388 | ILE  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | F     | 843  | GLU  | 2.7  |
| 5   | J     | 365  | CYS  | 2.7  |
| 3   | C     | 72   | VAL  | 2.7  |
| 2   | B     | 1276 | PHE  | 2.6  |
| 1   | A     | 314  | PRO  | 2.6  |
| 1   | A     | 465  | LEU  | 2.5  |
| 3   | C     | 158  | VAL  | 2.5  |
| 2   | F     | 1647 | GLN  | 2.5  |
| 2   | B     | 1513 | CYS  | 2.5  |
| 2   | B     | 947  | LEU  | 2.4  |
| 4   | H     | 219  | ALA  | 2.4  |
| 2   | B     | 873  | CYS  | 2.4  |
| 3   | C     | 1201 | CYS  | 2.4  |
| 4   | D     | 122  | ASP  | 2.4  |
| 5   | J     | 343  | GLY  | 2.4  |
| 2   | F     | 1467 | PHE  | 2.4  |
| 3   | G     | 46   | THR  | 2.4  |
| 1   | E     | 48   | ASP  | 2.4  |
| 1   | A     | 461  | LEU  | 2.3  |
| 4   | D     | 126  | ILE  | 2.3  |
| 2   | B     | 1512 | ARG  | 2.3  |
| 2   | B     | 1614 | GLU  | 2.3  |
| 2   | B     | 1638 | GLN  | 2.3  |
| 2   | F     | 1521 | GLN  | 2.3  |
| 4   | D     | 124  | GLU  | 2.3  |
| 1   | A     | 233  | GLU  | 2.3  |
| 5   | J     | 386  | LYS  | 2.2  |
| 3   | C     | 176  | PHE  | 2.2  |
| 4   | D     | 285  | ILE  | 2.2  |
| 4   | D     | 288  | GLU  | 2.2  |
| 4   | D     | 114  | VAL  | 2.2  |
| 5   | J     | 396  | VAL  | 2.2  |
| 3   | G     | 36   | SER  | 2.2  |
| 4   | D     | 308  | THR  | 2.2  |
| 2   | B     | 1388 | ILE  | 2.2  |
| 1   | E     | 23   | SER  | 2.2  |
| 5   | J     | 481  | VAL  | 2.2  |
| 2   | F     | 1285 | ASP  | 2.1  |
| 1   | A     | 340  | GLN  | 2.1  |
| 2   | F     | 1513 | CYS  | 2.1  |
| 1   | A     | 255  | ILE  | 2.1  |
| 2   | B     | 1540 | GLY  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | F     | 1522 | LYS  | 2.1  |
| 1   | A     | 447  | SER  | 2.1  |
| 2   | B     | 1571 | SER  | 2.1  |
| 4   | H     | 99   | LYS  | 2.1  |
| 5   | I     | 569  | ILE  | 2.1  |
| 4   | H     | 228  | GLN  | 2.1  |
| 2   | B     | 1298 | LEU  | 2.1  |
| 5   | J     | 377  | THR  | 2.1  |
| 2   | B     | 1440 | ASP  | 2.1  |
| 2   | F     | 1039 | LEU  | 2.1  |
| 3   | C     | 1212 | HIS  | 2.1  |
| 4   | D     | 270  | VAL  | 2.0  |
| 3   | G     | 1173 | ILE  | 2.0  |
| 3   | C     | 1180 | ALA  | 2.0  |
| 3   | C     | 1219 | TRP  | 2.0  |
| 4   | D     | 39   | 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.

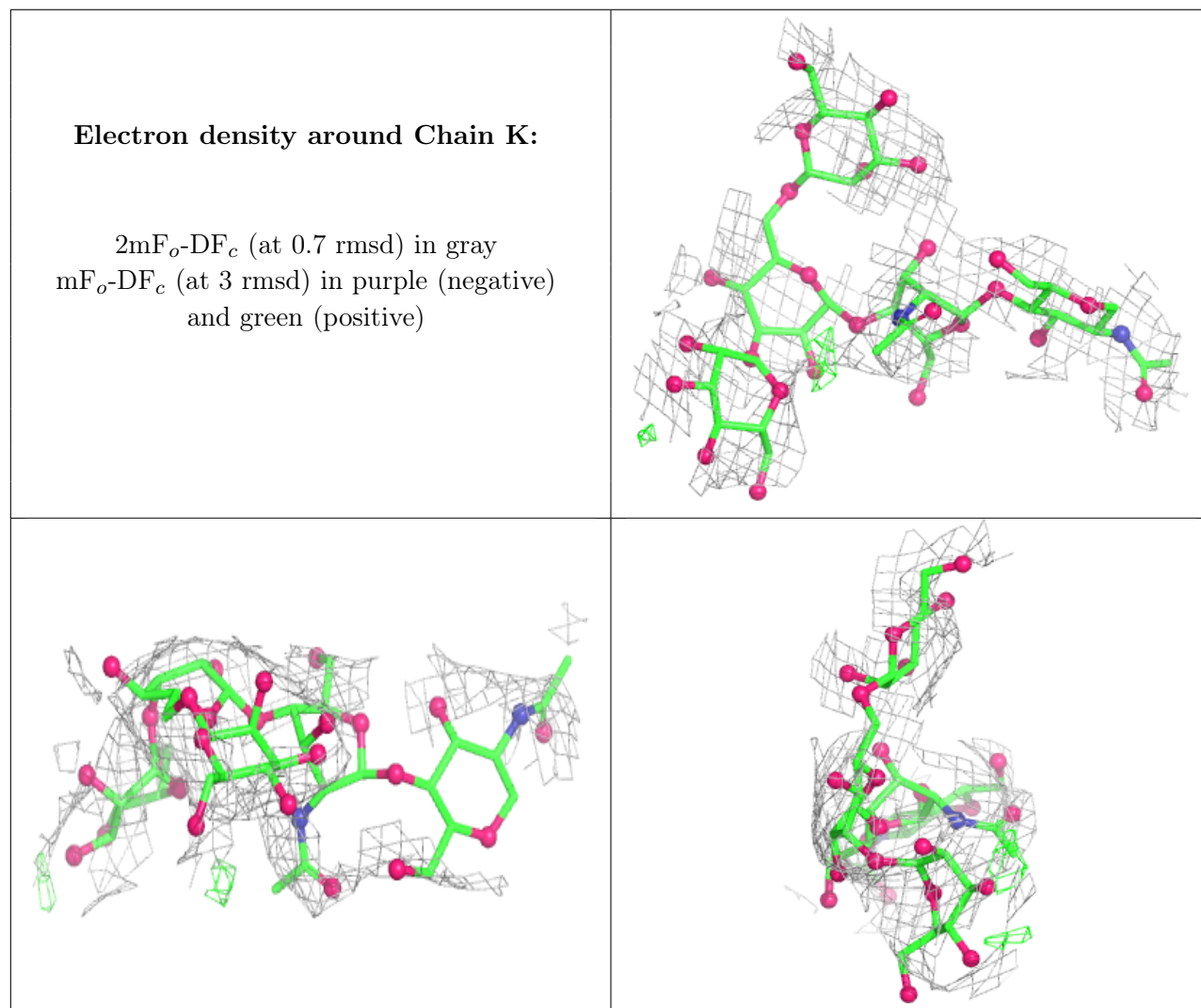
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | BMA  | K     | 4   | 11/12 | 0.24 | 0.20 | 147,152,164,167            | 0     |
| 6   | BMA  | M     | 5   | 11/12 | 0.29 | 0.17 | 175,182,188,191            | 0     |
| 6   | BMA  | M     | 4   | 11/12 | 0.35 | 0.17 | 164,170,183,188            | 0     |
| 7   | NAG  | L     | 2   | 14/15 | 0.43 | 0.18 | 158,160,163,166            | 0     |
| 6   | BMA  | K     | 5   | 11/12 | 0.49 | 0.13 | 142,150,163,167            | 0     |
| 6   | BMA  | K     | 3   | 11/12 | 0.54 | 0.14 | 141,151,155,161            | 0     |
| 7   | NAG  | N     | 2   | 14/15 | 0.57 | 0.15 | 139,145,158,162            | 0     |
| 6   | BMA  | M     | 3   | 11/12 | 0.62 | 0.14 | 160,170,176,183            | 0     |
| 6   | NAG  | K     | 2   | 14/15 | 0.71 | 0.14 | 116,124,130,132            | 0     |
| 7   | NAG  | N     | 1   | 14/15 | 0.73 | 0.15 | 133,139,145,145            | 0     |
| 7   | NAG  | L     | 1   | 14/15 | 0.73 | 0.12 | 143,146,150,152            | 0     |
| 6   | NAG  | M     | 2   | 14/15 | 0.79 | 0.12 | 136,142,152,154            | 0     |

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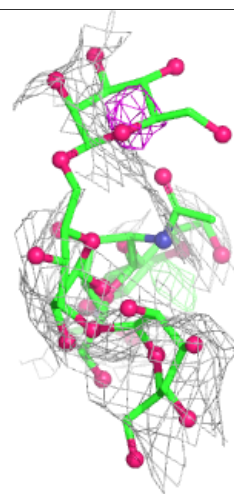
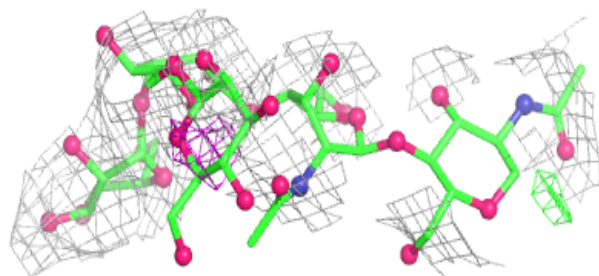
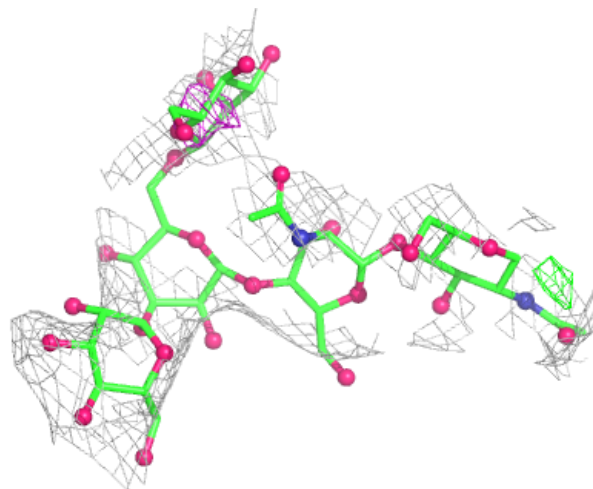
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | NAG  | K     | 1   | 14/15 | 0.85 | 0.15 | 77,90,98,102                | 0     |
| 6   | NAG  | M     | 1   | 14/15 | 0.87 | 0.15 | 86,100,111,112              | 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.



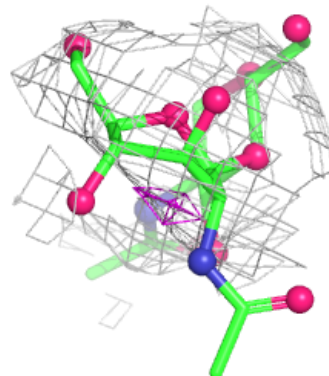
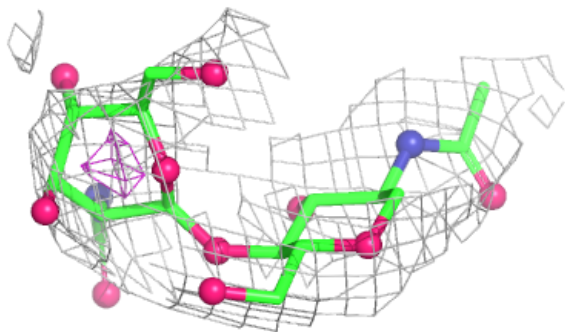
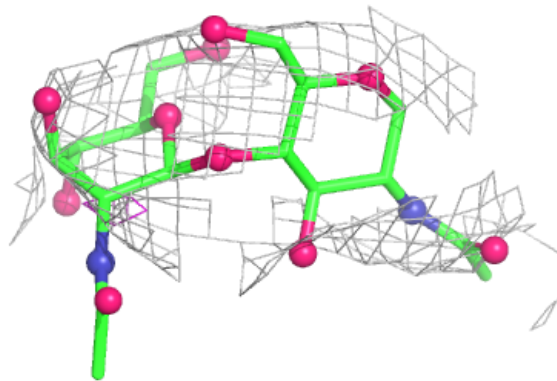
**Electron density around Chain M:**

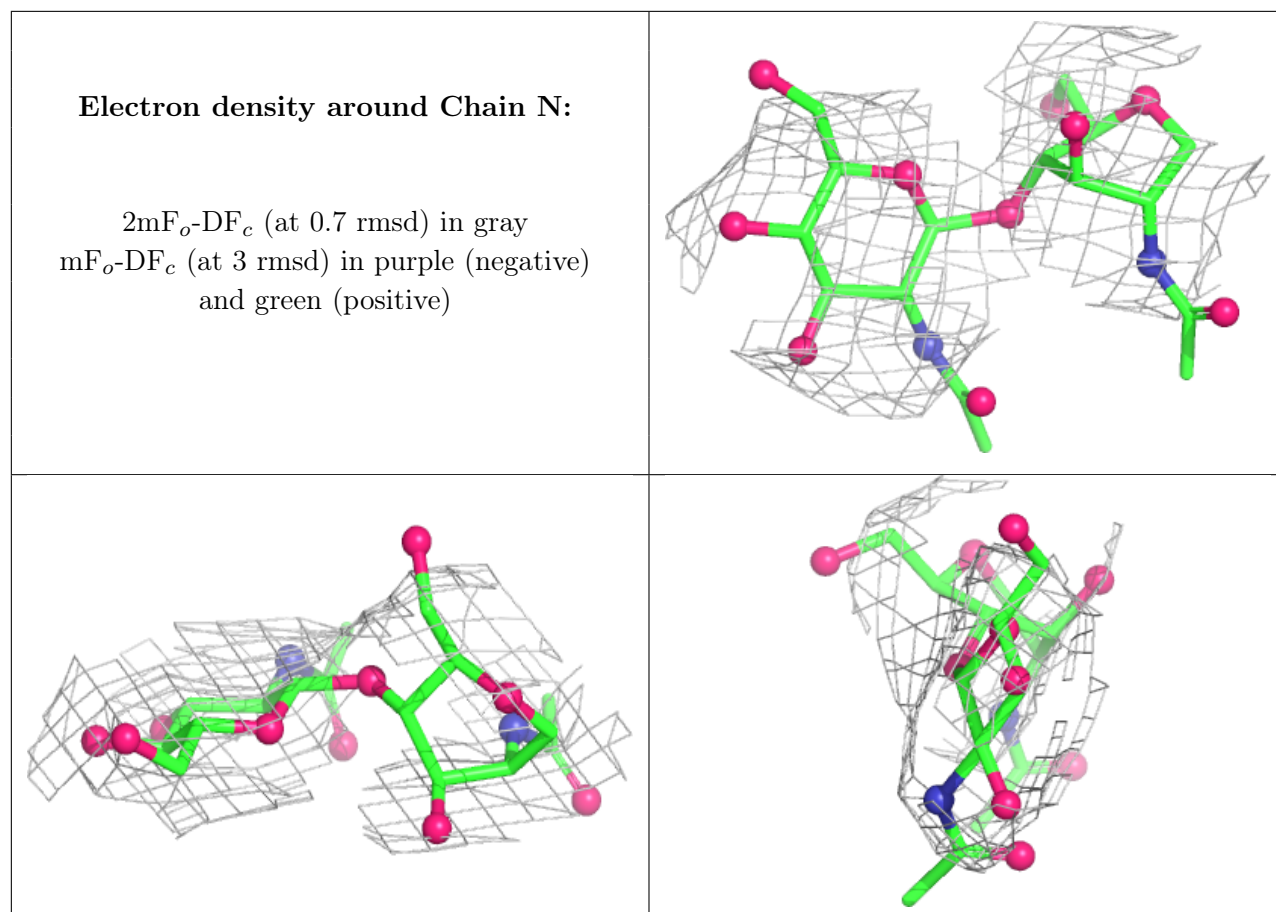
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

$2mF_o - DF_c$  (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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 9   | NAG  | I     | 601 | 14/15 | 0.46 | 0.17 | 153,155,161,162            | 0     |
| 9   | NAG  | I     | 603 | 14/15 | 0.55 | 0.16 | 171,178,187,187            | 0     |
| 9   | NAG  | J     | 602 | 14/15 | 0.55 | 0.16 | 139,143,147,149            | 0     |
| 9   | NAG  | H     | 404 | 14/15 | 0.56 | 0.21 | 129,134,140,141            | 0     |
| 9   | NAG  | I     | 602 | 14/15 | 0.58 | 0.15 | 156,158,165,170            | 0     |
| 9   | NAG  | J     | 603 | 14/15 | 0.63 | 0.18 | 144,151,157,159            | 0     |
| 9   | NAG  | H     | 405 | 14/15 | 0.65 | 0.17 | 119,129,144,149            | 0     |
| 9   | NAG  | J     | 601 | 14/15 | 0.67 | 0.13 | 122,128,137,140            | 0     |
| 9   | NAG  | H     | 403 | 14/15 | 0.68 | 0.13 | 118,125,131,134            | 0     |
| 9   | NAG  | D     | 403 | 14/15 | 0.70 | 0.14 | 128,138,147,147            | 0     |
| 9   | NAG  | D     | 405 | 14/15 | 0.72 | 0.15 | 122,133,143,148            | 0     |
| 9   | NAG  | D     | 404 | 14/15 | 0.73 | 0.14 | 159,162,167,169            | 0     |

*Continued on next page...*

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 10  | MLI  | J     | 604 | 7/7   | 0.83 | 0.09 | 91,94,99,103                | 0     |
| 8   | CA   | D     | 401 | 1/1   | 0.97 | 0.05 | 123,123,123,123             | 0     |
| 8   | CA   | E     | 701 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 8   | CA   | A     | 701 | 1/1   | 0.97 | 0.06 | 61,61,61,61                 | 0     |
| 8   | CA   | H     | 401 | 1/1   | 0.99 | 0.07 | 93,93,93,93                 | 0     |
| 8   | CA   | H     | 402 | 1/1   | 0.99 | 0.09 | 102,102,102,102             | 0     |
| 8   | CA   | D     | 402 | 1/1   | 0.99 | 0.06 | 124,124,124,124             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.