



# Full wwPDB X-ray Structure Validation Report i

Aug 7, 2020 – 09:02 AM BST

PDB ID : 3BIW  
Title : Crystal structure of the Neuroligin-1/Neurexin-1beta synaptic adhesion complex  
Authors : Arac, D.; Boucard, A.A.; Ozkan, E.; Strop, P.; Newell, E.; Sudhof, T.C.; Brunger, A.T.  
Deposited on : 2007-12-01  
Resolution : 3.50 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 i symbol.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.1.3  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

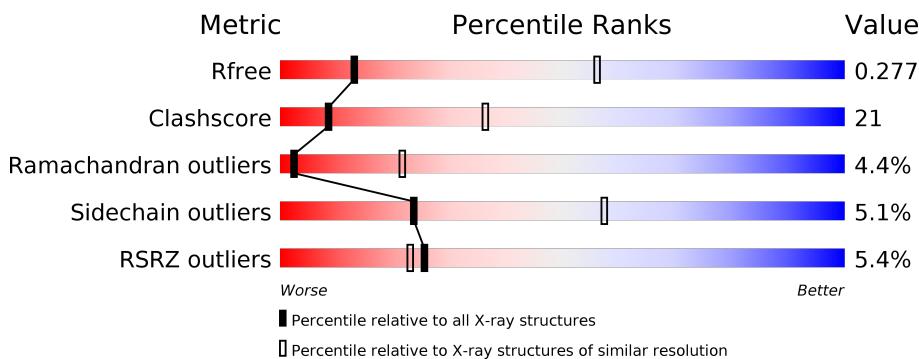
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



| Metric                | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| $R_{free}$            | 130704                   | 1659 (3.60-3.40)                                   |
| Clashscore            | 141614                   | 1036 (3.58-3.42)                                   |
| Ramachandran outliers | 138981                   | 1005 (3.58-3.42)                                   |
| Sidechain outliers    | 138945                   | 1006 (3.58-3.42)                                   |
| RSRZ outliers         | 127900                   | 1559 (3.60-3.40)                                   |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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.



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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NAG  | I     | 1   | -         | -        | X       | -                |
| 3   | NAG  | J     | 1   | -         | -        | X       | -                |
| 3   | NAG  | K     | 1   | -         | -        | X       | -                |
| 4   | NAG  | C     | 702 | -         | -        | -       | X                |
| 4   | NAG  | C     | 703 | -         | -        | -       | X                |
| 4   | NAG  | D     | 701 | -         | -        | -       | X                |
| 4   | NAG  | D     | 702 | -         | -        | -       | X                |
| 4   | NAG  | D     | 703 | -         | -        | -       | X                |

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 22438 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 Neuroligin-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 533      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4186  | 2690 | 697 | 783 | 16 |         |         |       |
| 1   | B     | 533      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4186  | 2690 | 697 | 783 | 16 |         |         |       |
| 1   | C     | 533      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4186  | 2690 | 697 | 783 | 16 |         |         |       |
| 1   | D     | 533      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4186  | 2690 | 697 | 783 | 16 |         |         |       |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 43      | ALA      | -      | expression tag | UNP Q62765 |
| A     | 44      | ASP      | -      | expression tag | UNP Q62765 |
| A     | 45      | PRO      | -      | expression tag | UNP Q62765 |
| A     | 639     | HIS      | -      | expression tag | UNP Q62765 |
| A     | 640     | HIS      | -      | expression tag | UNP Q62765 |
| A     | 641     | HIS      | -      | expression tag | UNP Q62765 |
| A     | 642     | HIS      | -      | expression tag | UNP Q62765 |
| A     | 643     | HIS      | -      | expression tag | UNP Q62765 |
| A     | 644     | HIS      | -      | expression tag | UNP Q62765 |
| B     | 43      | ALA      | -      | expression tag | UNP Q62765 |
| B     | 44      | ASP      | -      | expression tag | UNP Q62765 |
| B     | 45      | PRO      | -      | expression tag | UNP Q62765 |
| B     | 639     | HIS      | -      | expression tag | UNP Q62765 |
| B     | 640     | HIS      | -      | expression tag | UNP Q62765 |
| B     | 641     | HIS      | -      | expression tag | UNP Q62765 |
| B     | 642     | HIS      | -      | expression tag | UNP Q62765 |
| B     | 643     | HIS      | -      | expression tag | UNP Q62765 |
| B     | 644     | HIS      | -      | expression tag | UNP Q62765 |
| C     | 43      | ALA      | -      | expression tag | UNP Q62765 |
| C     | 44      | ASP      | -      | expression tag | UNP Q62765 |
| C     | 45      | PRO      | -      | expression tag | UNP Q62765 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 639     | HIS      | -      | expression tag | UNP Q62765 |
| C     | 640     | HIS      | -      | expression tag | UNP Q62765 |
| C     | 641     | HIS      | -      | expression tag | UNP Q62765 |
| C     | 642     | HIS      | -      | expression tag | UNP Q62765 |
| C     | 643     | HIS      | -      | expression tag | UNP Q62765 |
| C     | 644     | HIS      | -      | expression tag | UNP Q62765 |
| D     | 43      | ALA      | -      | expression tag | UNP Q62765 |
| D     | 44      | ASP      | -      | expression tag | UNP Q62765 |
| D     | 45      | PRO      | -      | expression tag | UNP Q62765 |
| D     | 639     | HIS      | -      | expression tag | UNP Q62765 |
| D     | 640     | HIS      | -      | expression tag | UNP Q62765 |
| D     | 641     | HIS      | -      | expression tag | UNP Q62765 |
| D     | 642     | HIS      | -      | expression tag | UNP Q62765 |
| D     | 643     | HIS      | -      | expression tag | UNP Q62765 |
| D     | 644     | HIS      | -      | expression tag | UNP Q62765 |

- Molecule 2 is a protein called Neurexin-1-beta.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | E     | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1359  | 857 | 243 | 258 | 1 |         |         |       |
| 2   | F     | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1359  | 857 | 243 | 258 | 1 |         |         |       |
| 2   | G     | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1359  | 857 | 243 | 258 | 1 |         |         |       |
| 2   | H     | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1359  | 857 | 243 | 258 | 1 |         |         |       |

There are 80 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 33      | GLY      | -      | expression tag | UNP Q63373 |
| E     | 34      | SER      | -      | expression tag | UNP Q63373 |
| E     | 35      | PRO      | -      | expression tag | UNP Q63373 |
| E     | 36      | GLY      | -      | expression tag | UNP Q63373 |
| E     | 37      | ILE      | -      | expression tag | UNP Q63373 |
| E     | 38      | SER      | -      | expression tag | UNP Q63373 |
| E     | 39      | GLY      | -      | expression tag | UNP Q63373 |
| E     | 40      | GLY      | -      | expression tag | UNP Q63373 |
| E     | 41      | GLY      | -      | expression tag | UNP Q63373 |
| E     | 42      | GLY      | -      | expression tag | UNP Q63373 |
| E     | 43      | GLY      | -      | expression tag | UNP Q63373 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 44      | ILE      | -      | expression tag | UNP Q63373 |
| E     | 45      | LEU      | -      | expression tag | UNP Q63373 |
| E     | 46      | GLU      | -      | expression tag | UNP Q63373 |
| E     | 300     | HIS      | -      | expression tag | UNP Q63373 |
| E     | 301     | HIS      | -      | expression tag | UNP Q63373 |
| E     | 302     | HIS      | -      | expression tag | UNP Q63373 |
| E     | 303     | HIS      | -      | expression tag | UNP Q63373 |
| E     | 304     | HIS      | -      | expression tag | UNP Q63373 |
| E     | 305     | HIS      | -      | expression tag | UNP Q63373 |
| F     | 33      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 34      | SER      | -      | expression tag | UNP Q63373 |
| F     | 35      | PRO      | -      | expression tag | UNP Q63373 |
| F     | 36      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 37      | ILE      | -      | expression tag | UNP Q63373 |
| F     | 38      | SER      | -      | expression tag | UNP Q63373 |
| F     | 39      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 40      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 41      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 42      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 43      | GLY      | -      | expression tag | UNP Q63373 |
| F     | 44      | ILE      | -      | expression tag | UNP Q63373 |
| F     | 45      | LEU      | -      | expression tag | UNP Q63373 |
| F     | 46      | GLU      | -      | expression tag | UNP Q63373 |
| F     | 300     | HIS      | -      | expression tag | UNP Q63373 |
| F     | 301     | HIS      | -      | expression tag | UNP Q63373 |
| F     | 302     | HIS      | -      | expression tag | UNP Q63373 |
| F     | 303     | HIS      | -      | expression tag | UNP Q63373 |
| F     | 304     | HIS      | -      | expression tag | UNP Q63373 |
| F     | 305     | HIS      | -      | expression tag | UNP Q63373 |
| G     | 33      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 34      | SER      | -      | expression tag | UNP Q63373 |
| G     | 35      | PRO      | -      | expression tag | UNP Q63373 |
| G     | 36      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 37      | ILE      | -      | expression tag | UNP Q63373 |
| G     | 38      | SER      | -      | expression tag | UNP Q63373 |
| G     | 39      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 40      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 41      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 42      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 43      | GLY      | -      | expression tag | UNP Q63373 |
| G     | 44      | ILE      | -      | expression tag | UNP Q63373 |
| G     | 45      | LEU      | -      | expression tag | UNP Q63373 |

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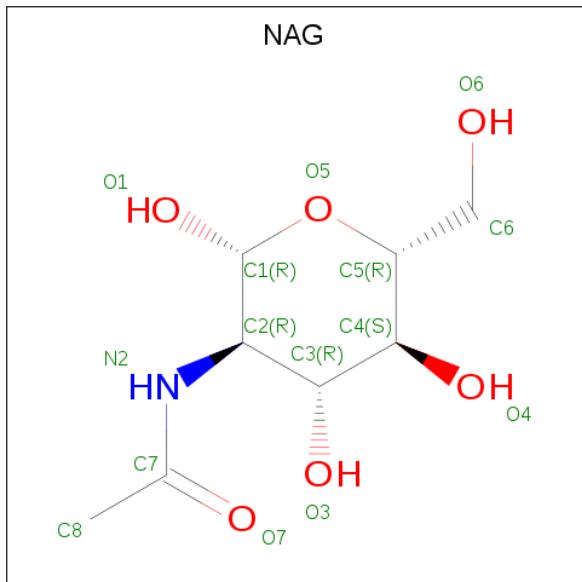
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 46      | GLU      | -      | expression tag | UNP Q63373 |
| G     | 300     | HIS      | -      | expression tag | UNP Q63373 |
| G     | 301     | HIS      | -      | expression tag | UNP Q63373 |
| G     | 302     | HIS      | -      | expression tag | UNP Q63373 |
| G     | 303     | HIS      | -      | expression tag | UNP Q63373 |
| G     | 304     | HIS      | -      | expression tag | UNP Q63373 |
| G     | 305     | HIS      | -      | expression tag | UNP Q63373 |
| H     | 33      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 34      | SER      | -      | expression tag | UNP Q63373 |
| H     | 35      | PRO      | -      | expression tag | UNP Q63373 |
| H     | 36      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 37      | ILE      | -      | expression tag | UNP Q63373 |
| H     | 38      | SER      | -      | expression tag | UNP Q63373 |
| H     | 39      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 40      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 41      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 42      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 43      | GLY      | -      | expression tag | UNP Q63373 |
| H     | 44      | ILE      | -      | expression tag | UNP Q63373 |
| H     | 45      | LEU      | -      | expression tag | UNP Q63373 |
| H     | 46      | GLU      | -      | expression tag | UNP Q63373 |
| H     | 300     | HIS      | -      | expression tag | UNP Q63373 |
| H     | 301     | HIS      | -      | expression tag | UNP Q63373 |
| H     | 302     | HIS      | -      | expression tag | UNP Q63373 |
| H     | 303     | HIS      | -      | expression tag | UNP Q63373 |
| H     | 304     | HIS      | -      | expression tag | UNP Q63373 |
| H     | 305     | HIS      | -      | expression tag | UNP Q63373 |

- Molecule 3 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 |
|-----|-------|----------|---------------------------|---------|---------|-------|
| 3   | I     | 2        | Total C N O<br>28 16 2 10 | 0       | 0       | 0     |
| 3   | J     | 2        | Total C N O<br>28 16 2 10 | 0       | 0       | 0     |
| 3   | K     | 2        | Total C N O<br>28 16 2 10 | 0       | 0       | 0     |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | G     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 5   | F     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 5   | E     | 2        | Total Ca<br>2 2 | 0       | 0       |

### 3 Residue-property plots

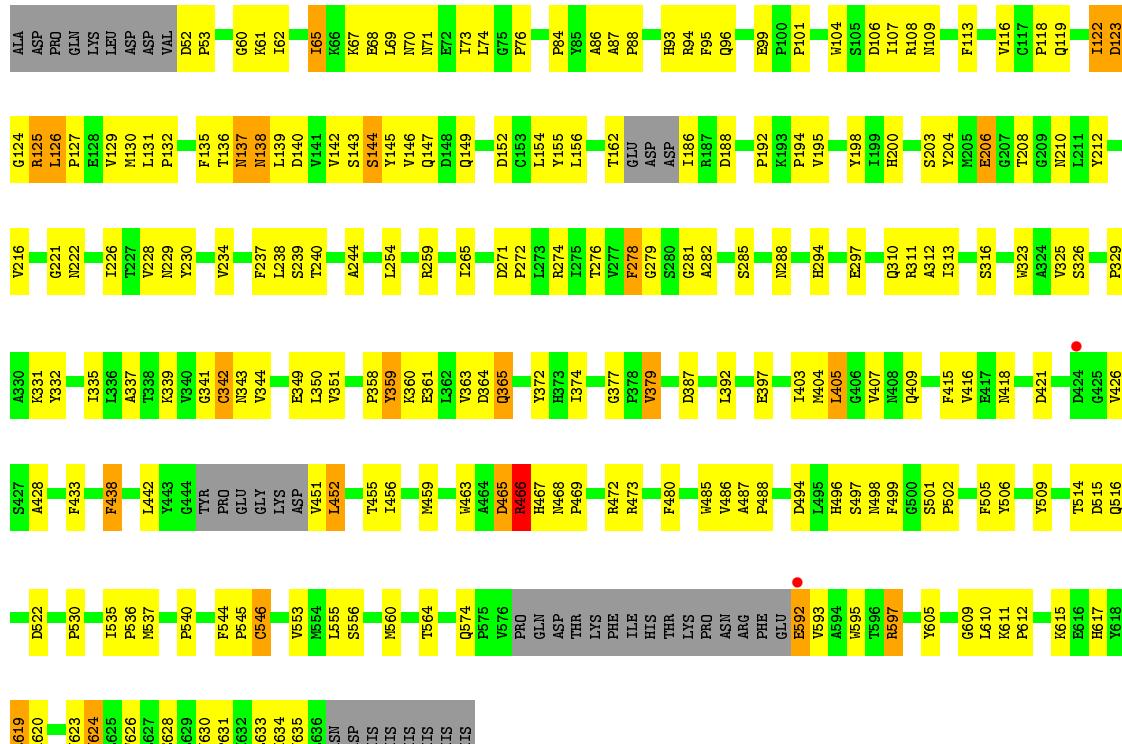
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neuroligin-1

Chain A:



55% 34% 7%

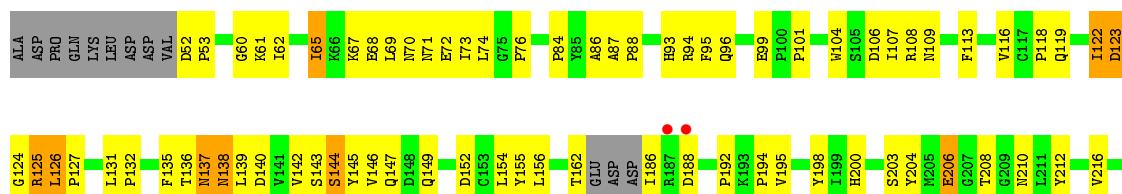


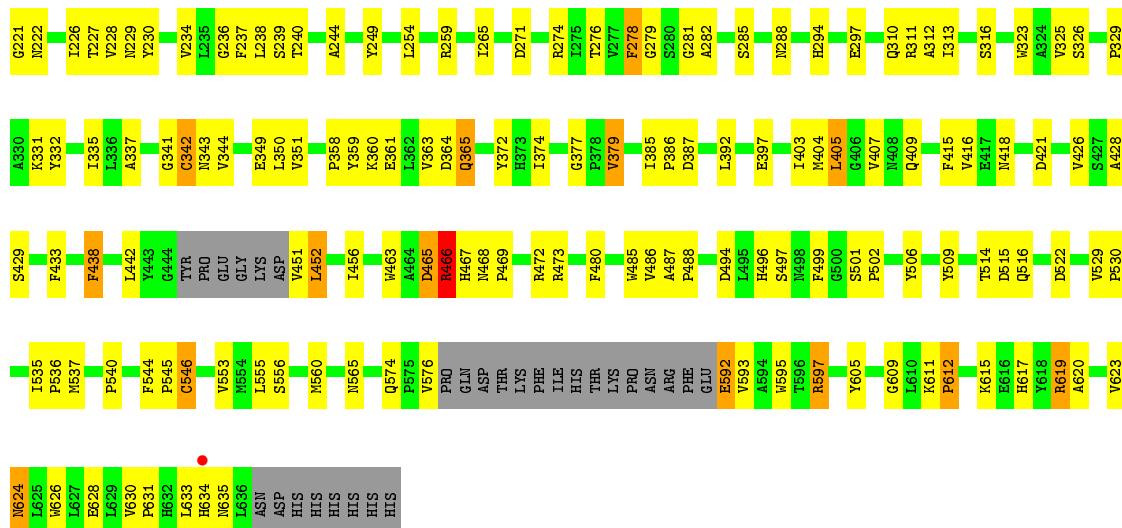
- Molecule 1: Neuroligin-1

Chain B:

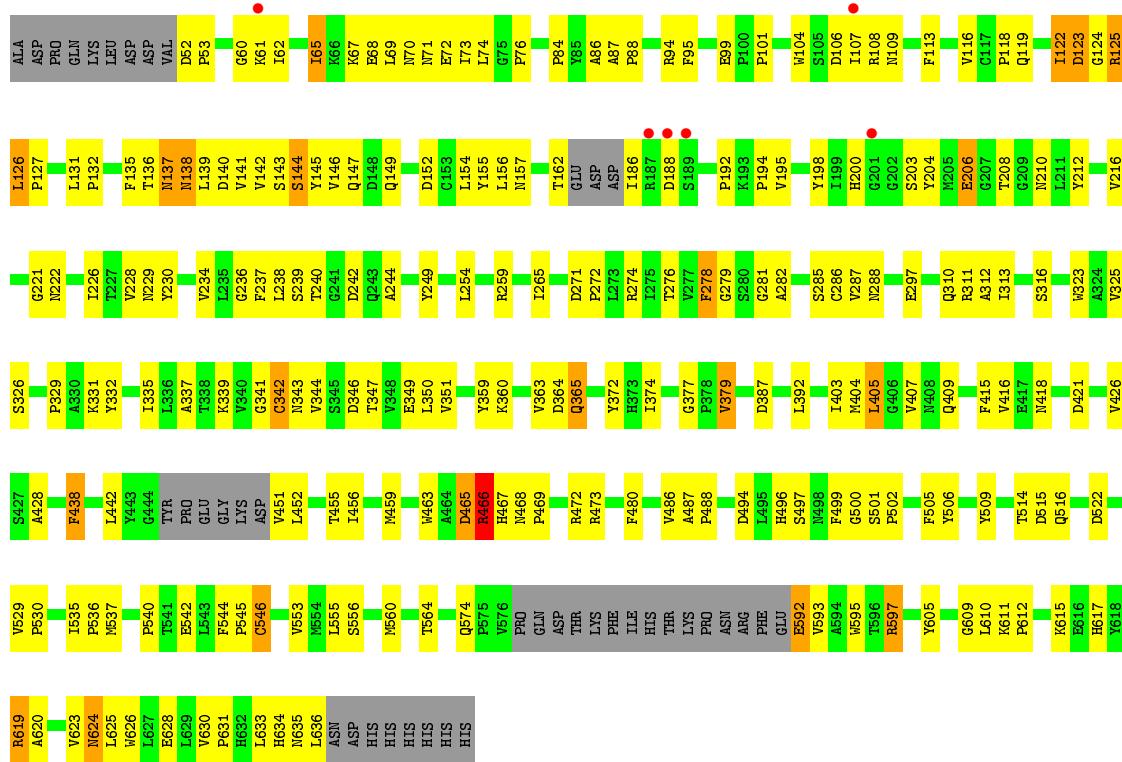


55% 34% 7%



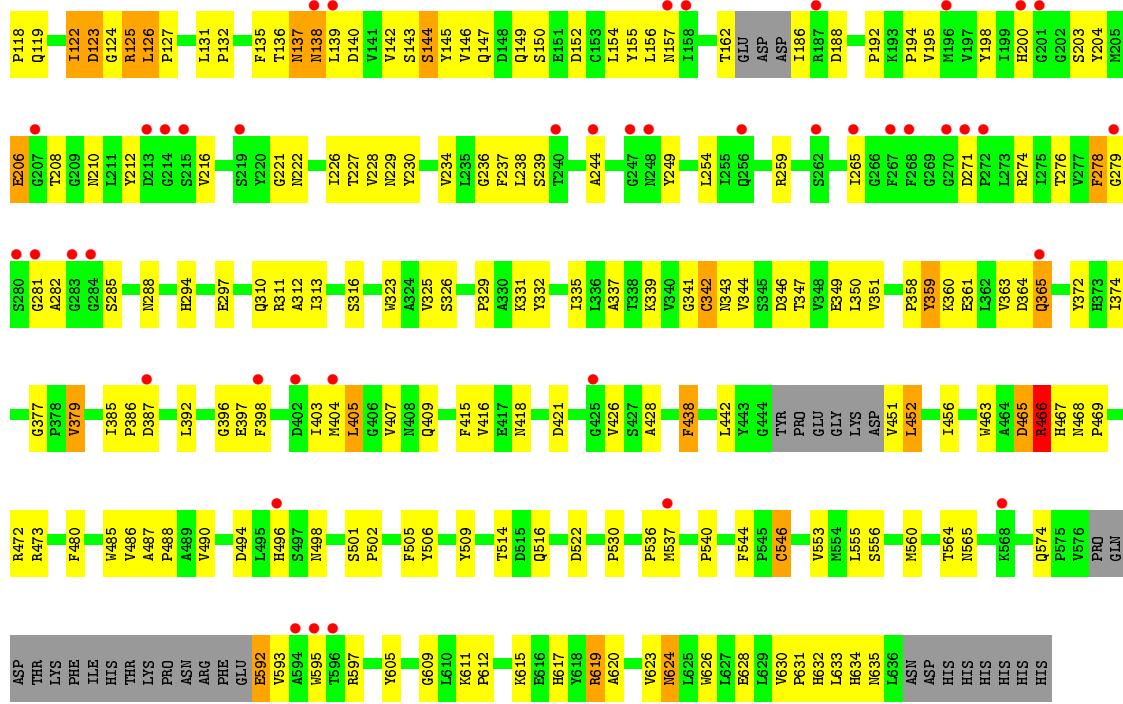


- Molecule 1: Neuroligin-1

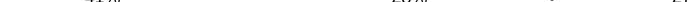


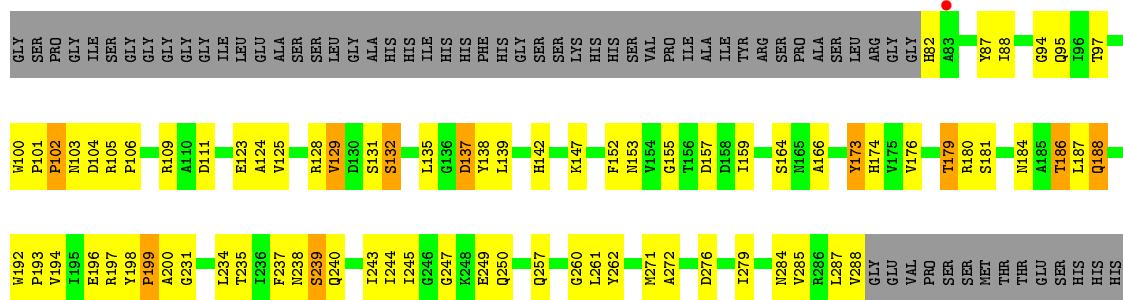
- Molecule 1: Neuroligin-1





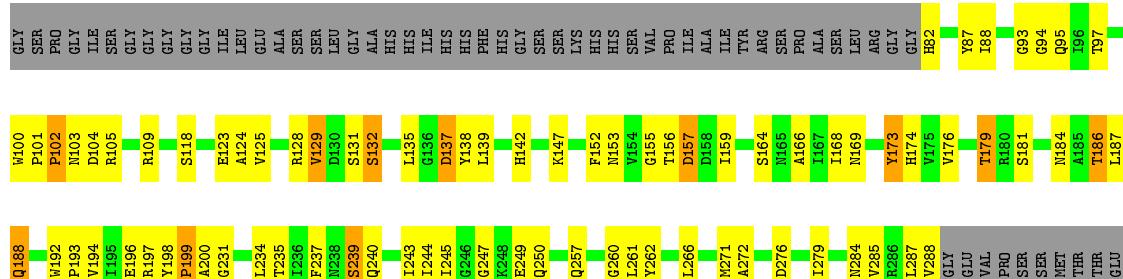
- Molecule 2: Neurexin-1-beta

Chain E:  41% 28% · 27%



- Molecule 2: Neurexin-1-beta

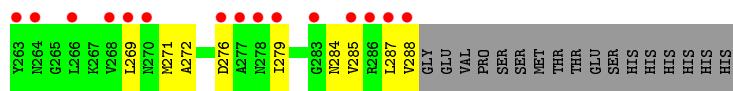
Chain F:  40%  28%  5%  27%



- Molecule 2: Neurexin-1-beta



- Molecule 2: Neurexin-1-beta



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



## 4 Data and refinement statistics (i)

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | C 1 2 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 229.83 Å    148.80 Å    123.60 Å<br>90.00°    90.38°    90.00° | Depositor        |
| Resolution (Å)  | 45.90 – 3.50<br>45.90 – 3.39                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.9 (45.90-3.50)<br>92.4 (45.90-3.39)                         | Depositor<br>EDS |
| $R_{merge}$   | 0.09   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle^1$   | 1.50 (at 3.40 Å)   | Xtriage          |
| Refinement program  | CNS 1.2  | Depositor        |
| $R$ , $R_{free}$  | 0.246 , 0.276<br>0.248 , 0.277                                 | Depositor<br>DCC |
| $R_{free}$ test set   | 2737 reflections (5.12%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 97.9   | Xtriage          |
| Anisotropy  | 0.153  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 57.0  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$    | Xtriage          |
| Estimated twinning fraction   | 0.000 for -h,-k,l  | Xtriage          |
| $F_o, F_c$ correlation  | 0.91   | EDS              |
| Total number of atoms   | 22438  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 133.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [\(i\)](#)

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

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.45         | 0/4302  | 0.65        | 1/5872 (0.0%)  |
| 1   | B     | 0.45         | 0/4302  | 0.66        | 1/5872 (0.0%)  |
| 1   | C     | 0.43         | 0/4302  | 0.65        | 0/5872         |
| 1   | D     | 0.36         | 0/4302  | 0.63        | 1/5872 (0.0%)  |
| 2   | E     | 0.44         | 0/1385  | 0.71        | 0/1877         |
| 2   | F     | 0.48         | 0/1385  | 0.71        | 0/1877         |
| 2   | G     | 0.47         | 0/1385  | 0.72        | 0/1877         |
| 2   | H     | 0.34         | 0/1385  | 0.67        | 0/1877         |
| All | All   | 0.42         | 0/22748 | 0.66        | 3/30996 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | D     | 452 | LEU  | N-CA-C | -5.23 | 96.87                  | 111.00              |
| 1   | A     | 452 | LEU  | N-CA-C | -5.09 | 97.24                  | 111.00              |
| 1   | B     | 452 | LEU  | N-CA-C | -5.07 | 97.31                  | 111.00              |

There are no chirality outliers.

There are no planarity outliers.

### 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 MolProbit. 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     | 4186  | 0        | 4046     | 176     | 0            |
| 1   | B     | 4186  | 0        | 4046     | 175     | 0            |
| 1   | C     | 4186  | 0        | 4046     | 175     | 0            |
| 1   | D     | 4186  | 0        | 4045     | 173     | 0            |
| 2   | E     | 1359  | 0        | 1345     | 54      | 1            |
| 2   | F     | 1359  | 0        | 1345     | 59      | 0            |
| 2   | G     | 1359  | 0        | 1345     | 53      | 0            |
| 2   | H     | 1359  | 0        | 1347     | 58      | 0            |
| 3   | I     | 28    | 0        | 25       | 7       | 0            |
| 3   | J     | 28    | 0        | 25       | 7       | 0            |
| 3   | K     | 28    | 0        | 25       | 7       | 0            |
| 4   | A     | 42    | 0        | 39       | 3       | 0            |
| 4   | B     | 42    | 0        | 39       | 3       | 0            |
| 4   | C     | 42    | 0        | 39       | 3       | 0            |
| 4   | D     | 42    | 0        | 39       | 2       | 0            |
| 5   | E     | 2     | 0        | 0        | 0       | 0            |
| 5   | F     | 2     | 0        | 0        | 0       | 0            |
| 5   | G     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 22438 | 0        | 21796    | 916     | 1            |

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 21.

All (916) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:147:LYS:HD3  | 2:G:164:SER:HA   | 1.48                     | 0.95              |
| 2:E:147:LYS:HD3  | 2:E:164:SER:HA   | 1.47                     | 0.93              |
| 2:F:147:LYS:HD3  | 2:F:164:SER:HA   | 1.51                     | 0.92              |
| 2:H:147:LYS:HD3  | 2:H:164:SER:HA   | 1.50                     | 0.90              |
| 1:D:426:VAL:HG23 | 1:D:473:ARG:HB2  | 1.62                     | 0.80              |
| 1:A:624:ASN:HD21 | 1:D:466:ARG:NH2  | 1.80                     | 0.79              |
| 1:A:624:ASN:HD21 | 1:D:466:ARG:HH21 | 1.32                     | 0.78              |
| 1:A:466:ARG:HH21 | 1:D:624:ASN:HD21 | 1.32                     | 0.77              |
| 2:H:88:ILE:HG12  | 2:H:257:GLN:HG2  | 1.67                     | 0.77              |
| 1:D:633:LEU:C    | 1:D:635:ASN:H    | 1.88                     | 0.77              |
| 1:C:426:VAL:HG23 | 1:C:473:ARG:HB2  | 1.67                     | 0.77              |
| 2:E:88:ILE:HG12  | 2:E:257:GLN:HG2  | 1.66                     | 0.77              |
| 2:F:88:ILE:HG12  | 2:F:257:GLN:HG2  | 1.67                     | 0.77              |
| 2:G:88:ILE:HG12  | 2:G:257:GLN:HG2  | 1.67                     | 0.77              |
| 1:B:426:VAL:HG23 | 1:B:473:ARG:HB2  | 1.68                     | 0.75              |
| 2:E:173:TYR:HD1  | 2:E:174:HIS:N    | 1.85                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:173:TYR:HD1  | 2:H:174:HIS:N    | 1.85                     | 0.74              |
| 1:A:426:VAL:HG23 | 1:A:473:ARG:HB2  | 1.70                     | 0.73              |
| 2:F:173:TYR:HD1  | 2:F:174:HIS:N    | 1.87                     | 0.73              |
| 1:B:633:LEU:C    | 1:B:635:ASN:H    | 1.92                     | 0.73              |
| 2:G:173:TYR:HD1  | 2:G:174:HIS:N    | 1.86                     | 0.72              |
| 1:C:633:LEU:C    | 1:C:635:ASN:H    | 1.91                     | 0.72              |
| 1:C:360:LYS:HE3  | 1:C:364:ASP:OD2  | 1.91                     | 0.71              |
| 1:A:433:PHE:CE1  | 1:B:433:PHE:HB2  | 2.26                     | 0.71              |
| 1:A:633:LEU:C    | 1:A:635:ASN:H    | 1.92                     | 0.70              |
| 1:D:466:ARG:HH11 | 1:D:466:ARG:HG2  | 1.56                     | 0.70              |
| 1:C:514:THR:HG22 | 1:C:546:CYS:SG   | 2.31                     | 0.70              |
| 1:A:360:LYS:HE3  | 1:A:364:ASP:OD2  | 1.92                     | 0.70              |
| 1:D:415:PHE:CD2  | 1:D:480:PHE:HB2  | 2.26                     | 0.70              |
| 2:E:287:LEU:HD12 | 2:E:288:VAL:H    | 1.56                     | 0.70              |
| 1:B:466:ARG:HH11 | 1:B:466:ARG:HG2  | 1.56                     | 0.70              |
| 1:D:624:ASN:O    | 1:D:628:GLU:HB2  | 1.92                     | 0.70              |
| 1:B:360:LYS:HE3  | 1:B:364:ASP:OD2  | 1.92                     | 0.69              |
| 1:C:466:ARG:HG2  | 1:C:466:ARG:HH11 | 1.56                     | 0.69              |
| 1:D:617:HIS:HB3  | 1:D:620:ALA:HB2  | 1.75                     | 0.69              |
| 2:G:287:LEU:HD12 | 2:G:288:VAL:H    | 1.55                     | 0.69              |
| 2:F:287:LEU:HD12 | 2:F:288:VAL:H    | 1.58                     | 0.69              |
| 1:B:514:THR:HG22 | 1:B:546:CYS:SG   | 2.33                     | 0.69              |
| 1:C:123:ASP:O    | 1:C:125:ARG:N    | 2.26                     | 0.69              |
| 1:A:466:ARG:HG2  | 1:A:466:ARG:HH11 | 1.58                     | 0.69              |
| 1:B:624:ASN:O    | 1:B:628:GLU:HB2  | 1.94                     | 0.68              |
| 1:D:360:LYS:HE3  | 1:D:364:ASP:OD2  | 1.93                     | 0.68              |
| 1:B:162:THR:O    | 1:B:186:ILE:HB   | 1.93                     | 0.68              |
| 1:B:294:HIS:HA   | 2:F:109:ARG:NH2  | 2.07                     | 0.68              |
| 2:H:287:LEU:HD12 | 2:H:288:VAL:H    | 1.58                     | 0.68              |
| 1:A:162:THR:O    | 1:A:186:ILE:HB   | 1.94                     | 0.67              |
| 1:A:617:HIS:HB3  | 1:A:620:ALA:HB2  | 1.76                     | 0.67              |
| 1:B:123:ASP:O    | 1:B:125:ARG:N    | 2.27                     | 0.67              |
| 1:C:162:THR:O    | 1:C:186:ILE:HB   | 1.94                     | 0.67              |
| 1:D:123:ASP:O    | 1:D:125:ARG:N    | 2.28                     | 0.67              |
| 1:A:123:ASP:O    | 1:A:125:ARG:N    | 2.27                     | 0.67              |
| 2:G:147:LYS:HD3  | 2:G:164:SER:CA   | 2.22                     | 0.67              |
| 1:D:514:THR:HG22 | 1:D:546:CYS:SG   | 2.34                     | 0.67              |
| 1:B:415:PHE:CD2  | 1:B:480:PHE:HB2  | 2.30                     | 0.66              |
| 1:D:487:ALA:HB3  | 1:D:488:PRO:HD3  | 1.76                     | 0.66              |
| 1:C:415:PHE:CD2  | 1:C:480:PHE:HB2  | 2.30                     | 0.66              |
| 1:A:76:PRO:HG2   | 1:A:162:THR:OG1  | 1.96                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:487:ALA:HB3  | 1:C:488:PRO:HD3  | 1.75                     | 0.66              |
| 1:A:624:ASN:O    | 1:A:628:GLU:HB2  | 1.94                     | 0.66              |
| 1:B:397:GLU:OE1  | 2:F:235:THR:HB   | 1.95                     | 0.66              |
| 1:C:617:HIS:HB3  | 1:C:620:ALA:HB2  | 1.77                     | 0.66              |
| 1:D:76:PRO:HG2   | 1:D:162:THR:OG1  | 1.96                     | 0.66              |
| 2:H:147:LYS:HD3  | 2:H:164:SER:CA   | 2.24                     | 0.66              |
| 1:C:624:ASN:O    | 1:C:628:GLU:HB2  | 1.95                     | 0.65              |
| 2:E:147:LYS:HD3  | 2:E:164:SER:CA   | 2.22                     | 0.65              |
| 1:D:162:THR:O    | 1:D:186:ILE:HB   | 1.96                     | 0.65              |
| 1:C:259:ARG:HH11 | 1:C:259:ARG:HG3  | 1.60                     | 0.65              |
| 1:D:259:ARG:HH11 | 1:D:259:ARG:HG3  | 1.61                     | 0.65              |
| 1:A:514:THR:HG22 | 1:A:546:CYS:SG   | 2.36                     | 0.65              |
| 1:B:76:PRO:HG2   | 1:B:162:THR:OG1  | 1.95                     | 0.65              |
| 1:B:617:HIS:HB3  | 1:B:620:ALA:HB2  | 1.79                     | 0.65              |
| 1:A:234:VAL:HG12 | 1:A:238:LEU:HD12 | 1.79                     | 0.65              |
| 1:D:65:ILE:HD11  | 1:D:67:LYS:HE2   | 1.79                     | 0.65              |
| 1:C:76:PRO:HG2   | 1:C:162:THR:OG1  | 1.97                     | 0.65              |
| 1:D:234:VAL:HG12 | 1:D:238:LEU:HD12 | 1.78                     | 0.65              |
| 1:C:502:PRO:HA   | 1:C:597:ARG:NH1  | 2.12                     | 0.64              |
| 1:A:415:PHE:CD2  | 1:A:480:PHE:HB2  | 2.32                     | 0.64              |
| 1:B:259:ARG:HG3  | 1:B:259:ARG:HH11 | 1.63                     | 0.64              |
| 1:D:397:GLU:OE1  | 2:H:235:THR:HB   | 1.98                     | 0.64              |
| 1:A:259:ARG:HH11 | 1:A:259:ARG:HG3  | 1.62                     | 0.64              |
| 1:A:452:LEU:O    | 1:A:456:ILE:HG12 | 1.98                     | 0.63              |
| 1:D:238:LEU:HD23 | 1:D:239:SER:N    | 2.12                     | 0.63              |
| 2:F:101:PRO:HG2  | 2:F:104:ASP:HB2  | 1.80                     | 0.63              |
| 2:G:272:ALA:N    | 2:G:279:ILE:HD12 | 2.14                     | 0.63              |
| 1:D:452:LEU:O    | 1:D:456:ILE:HG12 | 1.99                     | 0.63              |
| 2:H:101:PRO:HG2  | 2:H:104:ASP:HB2  | 1.79                     | 0.63              |
| 1:C:65:ILE:HD11  | 1:C:67:LYS:HE2   | 1.79                     | 0.63              |
| 1:B:487:ALA:HB3  | 1:B:488:PRO:HD3  | 1.79                     | 0.63              |
| 1:C:452:LEU:O    | 1:C:456:ILE:HG12 | 1.98                     | 0.63              |
| 2:F:147:LYS:HD3  | 2:F:164:SER:CA   | 2.25                     | 0.63              |
| 2:H:272:ALA:N    | 2:H:279:ILE:HD12 | 2.14                     | 0.63              |
| 1:B:238:LEU:HD23 | 1:B:239:SER:N    | 2.13                     | 0.62              |
| 4:C:702:NAG:H83  | 4:C:702:NAG:O3   | 1.99                     | 0.62              |
| 1:B:624:ASN:HD21 | 1:C:466:ARG:HH21 | 1.47                     | 0.62              |
| 1:D:502:PRO:HA   | 1:D:597:ARG:NH1  | 2.14                     | 0.62              |
| 1:B:502:PRO:HA   | 1:B:597:ARG:NH1  | 2.15                     | 0.62              |
| 1:B:592:GLU:OE1  | 1:B:592:GLU:N    | 2.32                     | 0.62              |
| 1:A:65:ILE:HD11  | 1:A:67:LYS:HE2   | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:702:NAG:H83  | 4:B:702:NAG:O3   | 1.99                     | 0.62              |
| 3:I:1:NAG:C3     | 3:I:2:NAG:H2     | 2.29                     | 0.62              |
| 1:A:238:LEU:HD23 | 1:A:239:SER:N    | 2.15                     | 0.62              |
| 1:A:592:GLU:OE1  | 1:A:592:GLU:N    | 2.33                     | 0.61              |
| 1:A:487:ALA:HB3  | 1:A:488:PRO:HD3  | 1.81                     | 0.61              |
| 1:A:502:PRO:HA   | 1:A:597:ARG:NH1  | 2.15                     | 0.61              |
| 2:G:125:VAL:O    | 2:G:247:GLY:HA3  | 2.01                     | 0.61              |
| 4:A:702:NAG:O3   | 4:A:702:NAG:H83  | 2.01                     | 0.61              |
| 1:B:238:LEU:HD23 | 1:B:238:LEU:C    | 2.20                     | 0.61              |
| 1:B:337:ALA:HB2  | 1:B:350:LEU:HD21 | 1.82                     | 0.61              |
| 1:C:238:LEU:HD23 | 1:C:239:SER:N    | 2.16                     | 0.61              |
| 2:E:101:PRO:HG2  | 2:E:104:ASP:HB2  | 1.82                     | 0.61              |
| 1:B:452:LEU:O    | 1:B:456:ILE:HG12 | 2.01                     | 0.61              |
| 1:C:592:GLU:N    | 1:C:592:GLU:OE1  | 2.33                     | 0.61              |
| 3:J:1:NAG:C3     | 3:J:2:NAG:H2     | 2.30                     | 0.61              |
| 1:A:294:HIS:HA   | 2:E:109:ARG:NH2  | 2.16                     | 0.61              |
| 2:H:109:ARG:HG3  | 2:H:235:THR:CG2  | 2.31                     | 0.61              |
| 1:D:337:ALA:HB2  | 1:D:350:LEU:HD21 | 1.81                     | 0.61              |
| 1:D:244:ALA:HB1  | 1:D:351:VAL:CG2  | 2.31                     | 0.61              |
| 2:G:139:LEU:HD12 | 2:G:152:PHE:HB3  | 1.83                     | 0.61              |
| 1:D:592:GLU:N    | 1:D:592:GLU:OE1  | 2.34                     | 0.60              |
| 2:G:101:PRO:HG2  | 2:G:104:ASP:HB2  | 1.82                     | 0.60              |
| 3:K:1:NAG:C3     | 3:K:2:NAG:H2     | 2.31                     | 0.60              |
| 1:B:155:TYR:O    | 1:B:229:ASN:HB2  | 2.02                     | 0.60              |
| 1:D:116:VAL:HG21 | 1:D:146:VAL:HA   | 1.83                     | 0.60              |
| 2:F:139:LEU:HD12 | 2:F:152:PHE:HB3  | 1.84                     | 0.60              |
| 2:F:125:VAL:O    | 2:F:247:GLY:HA3  | 2.02                     | 0.60              |
| 2:F:82:HIS:HA    | 2:F:173:TYR:CE2  | 2.36                     | 0.60              |
| 2:F:272:ALA:N    | 2:F:279:ILE:HD12 | 2.16                     | 0.60              |
| 2:H:139:LEU:HD12 | 2:H:152:PHE:HB3  | 1.83                     | 0.60              |
| 1:B:234:VAL:HG12 | 1:B:238:LEU:HD12 | 1.84                     | 0.60              |
| 2:G:82:HIS:HA    | 2:G:173:TYR:CE2  | 2.37                     | 0.60              |
| 1:B:65:ILE:HD11  | 1:B:67:LYS:HE2   | 1.83                     | 0.60              |
| 1:D:238:LEU:C    | 1:D:238:LEU:HD23 | 2.22                     | 0.59              |
| 2:F:184:ASN:ND2  | 3:J:1:NAG:H61    | 2.17                     | 0.59              |
| 3:I:1:NAG:H83    | 3:I:1:NAG:H3     | 1.84                     | 0.59              |
| 1:A:276:THR:HG23 | 1:A:311:ARG:HB2  | 1.84                     | 0.59              |
| 1:A:619:ARG:O    | 1:A:623:VAL:HG23 | 2.01                     | 0.59              |
| 1:C:244:ALA:HB1  | 1:C:351:VAL:CG2  | 2.32                     | 0.59              |
| 1:B:294:HIS:HB2  | 2:F:109:ARG:CZ   | 2.32                     | 0.59              |
| 1:C:234:VAL:HG12 | 1:C:238:LEU:HD12 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:506:TYR:HB3  | 1:C:595:TRP:CZ2  | 2.37                     | 0.59              |
| 2:E:184:ASN:ND2  | 3:I:1:NAG:H61    | 2.17                     | 0.59              |
| 1:C:238:LEU:HD23 | 1:C:238:LEU:C    | 2.22                     | 0.59              |
| 1:B:619:ARG:O    | 1:B:623:VAL:HG23 | 2.03                     | 0.59              |
| 2:F:188:GLN:HG3  | 2:F:194:VAL:HG22 | 1.84                     | 0.59              |
| 2:G:188:GLN:HG3  | 2:G:194:VAL:HG22 | 1.85                     | 0.59              |
| 1:B:506:TYR:HB3  | 1:B:595:TRP:CZ2  | 2.37                     | 0.59              |
| 1:C:350:LEU:O    | 1:C:350:LEU:HD23 | 2.03                     | 0.59              |
| 2:E:82:HIS:HA    | 2:E:173:TYR:CE2  | 2.37                     | 0.59              |
| 1:B:131:LEU:HD12 | 1:B:131:LEU:N    | 2.17                     | 0.59              |
| 2:E:139:LEU:HD12 | 2:E:152:PHE:HB3  | 1.84                     | 0.59              |
| 2:H:188:GLN:HG3  | 2:H:194:VAL:HG22 | 1.85                     | 0.59              |
| 1:A:337:ALA:HB2  | 1:A:350:LEU:HD21 | 1.83                     | 0.58              |
| 1:A:506:TYR:HB3  | 1:A:595:TRP:CZ2  | 2.38                     | 0.58              |
| 1:C:342:CYS:O    | 1:C:344:VAL:N    | 2.34                     | 0.58              |
| 1:A:342:CYS:O    | 1:A:344:VAL:N    | 2.36                     | 0.58              |
| 1:A:433:PHE:HE1  | 1:B:429:SER:O    | 1.85                     | 0.58              |
| 1:C:244:ALA:HB1  | 1:C:351:VAL:HG21 | 1.84                     | 0.58              |
| 1:D:342:CYS:O    | 1:D:344:VAL:N    | 2.35                     | 0.58              |
| 1:D:633:LEU:C    | 1:D:635:ASN:N    | 2.56                     | 0.58              |
| 1:B:244:ALA:HB1  | 1:B:351:VAL:HG21 | 1.86                     | 0.58              |
| 1:B:329:PRO:HB3  | 1:B:379:VAL:HG11 | 1.85                     | 0.58              |
| 2:E:125:VAL:O    | 2:E:247:GLY:HA3  | 2.03                     | 0.58              |
| 1:B:132:PRO:HG2  | 1:B:135:PHE:HB2  | 1.86                     | 0.58              |
| 1:B:244:ALA:HB1  | 1:B:351:VAL:CG2  | 2.34                     | 0.58              |
| 1:D:466:ARG:NH1  | 1:D:466:ARG:HG2  | 2.19                     | 0.58              |
| 1:C:71:ASN:OD1   | 1:C:73:ILE:HG13  | 2.03                     | 0.58              |
| 1:D:426:VAL:O    | 1:D:472:ARG:HD2  | 2.03                     | 0.58              |
| 1:D:65:ILE:CD1   | 1:D:67:LYS:HE2   | 2.34                     | 0.58              |
| 2:F:109:ARG:HG3  | 2:F:235:THR:CG2  | 2.32                     | 0.58              |
| 1:D:294:HIS:HA   | 2:H:109:ARG:NH2  | 2.19                     | 0.58              |
| 1:A:244:ALA:HB1  | 1:A:351:VAL:CG2  | 2.34                     | 0.58              |
| 1:C:466:ARG:HG2  | 1:C:466:ARG:NH1  | 2.19                     | 0.58              |
| 1:B:198:TYR:CE1  | 1:B:279:GLY:HA2  | 2.39                     | 0.58              |
| 3:K:1:NAG:H83    | 3:K:1:NAG:H3     | 1.86                     | 0.58              |
| 1:C:337:ALA:HB2  | 1:C:350:LEU:HD21 | 1.85                     | 0.57              |
| 1:D:244:ALA:HB1  | 1:D:351:VAL:HG21 | 1.85                     | 0.57              |
| 2:E:272:ALA:N    | 2:E:279:ILE:HD12 | 2.18                     | 0.57              |
| 1:A:238:LEU:HD23 | 1:A:238:LEU:C    | 2.23                     | 0.57              |
| 1:C:155:TYR:O    | 1:C:229:ASN:HB2  | 2.03                     | 0.57              |
| 1:D:329:PRO:HB3  | 1:D:379:VAL:HG11 | 1.84                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:342:CYS:O    | 1:B:344:VAL:N    | 2.35                     | 0.57              |
| 1:B:350:LEU:HD23 | 1:B:350:LEU:O    | 2.04                     | 0.57              |
| 1:C:65:ILE:CD1   | 1:C:67:LYS:HE2   | 2.35                     | 0.57              |
| 1:D:506:TYR:HB3  | 1:D:595:TRP:CZ2  | 2.40                     | 0.57              |
| 1:A:409:GLN:OE1  | 1:A:522:ASP:HB3  | 2.05                     | 0.57              |
| 1:A:540:PRO:HG3  | 1:A:546:CYS:O    | 2.05                     | 0.57              |
| 2:E:188:GLN:HG3  | 2:E:194:VAL:HG22 | 1.84                     | 0.57              |
| 2:H:196:GLU:HB3  | 2:H:198:TYR:HE1  | 1.70                     | 0.57              |
| 3:J:1:NAG:H3     | 3:J:1:NAG:H83    | 1.86                     | 0.57              |
| 1:B:132:PRO:HG2  | 1:B:135:PHE:CB   | 2.35                     | 0.57              |
| 1:C:329:PRO:HB3  | 1:C:379:VAL:HG11 | 1.86                     | 0.57              |
| 2:H:82:HIS:HA    | 2:H:173:TYR:CE2  | 2.40                     | 0.57              |
| 1:A:329:PRO:HB3  | 1:A:379:VAL:HG11 | 1.85                     | 0.57              |
| 1:B:109:ASN:OD1  | 4:B:701:NAG:H2   | 2.05                     | 0.57              |
| 1:C:116:VAL:HG21 | 1:C:146:VAL:HA   | 1.87                     | 0.57              |
| 1:C:131:LEU:HD12 | 1:C:131:LEU:N    | 2.20                     | 0.57              |
| 1:D:203:SER:O    | 1:D:204:TYR:HB2  | 2.04                     | 0.57              |
| 1:D:619:ARG:O    | 1:D:623:VAL:HG23 | 2.04                     | 0.57              |
| 2:H:125:VAL:O    | 2:H:247:GLY:HA3  | 2.04                     | 0.57              |
| 1:A:132:PRO:HG2  | 1:A:135:PHE:HB2  | 1.86                     | 0.57              |
| 1:A:155:TYR:O    | 1:A:229:ASN:HB2  | 2.05                     | 0.57              |
| 1:A:244:ALA:HB1  | 1:A:351:VAL:HG21 | 1.86                     | 0.57              |
| 1:A:87:ALA:HB3   | 1:A:99:GLU:HB2   | 1.86                     | 0.57              |
| 2:G:184:ASN:ND2  | 3:K:1:NAG:H61    | 2.19                     | 0.57              |
| 1:D:132:PRO:HG2  | 1:D:135:PHE:HB2  | 1.87                     | 0.56              |
| 1:C:132:PRO:HG2  | 1:C:135:PHE:HB2  | 1.87                     | 0.56              |
| 1:C:87:ALA:HB3   | 1:C:99:GLU:HB2   | 1.86                     | 0.56              |
| 2:H:137:ASP:HA   | 2:H:153:ASN:O    | 2.05                     | 0.56              |
| 1:A:313:ILE:HA   | 1:A:404:MET:O    | 2.05                     | 0.56              |
| 1:A:466:ARG:NH2  | 1:D:624:ASN:HD21 | 1.99                     | 0.56              |
| 1:A:65:ILE:CD1   | 1:A:67:LYS:HE2   | 2.35                     | 0.56              |
| 1:A:109:ASN:OD1  | 4:A:701:NAG:H2   | 2.05                     | 0.56              |
| 1:B:466:ARG:NH1  | 1:B:466:ARG:HG2  | 2.19                     | 0.56              |
| 1:D:155:TYR:O    | 1:D:229:ASN:HB2  | 2.05                     | 0.56              |
| 1:A:131:LEU:HD12 | 1:A:131:LEU:N    | 2.21                     | 0.56              |
| 1:A:466:ARG:NH1  | 1:A:466:ARG:HG2  | 2.20                     | 0.56              |
| 1:A:71:ASN:OD1   | 1:A:73:ILE:HG13  | 2.05                     | 0.56              |
| 1:A:433:PHE:CD1  | 1:B:433:PHE:HB2  | 2.40                     | 0.56              |
| 1:A:624:ASN:ND2  | 1:D:466:ARG:NH2  | 2.51                     | 0.56              |
| 1:D:74:LEU:HD13  | 1:D:216:VAL:HG13 | 1.87                     | 0.56              |
| 1:A:116:VAL:HG21 | 1:A:146:VAL:HA   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:LEU:O    | 1:A:350:LEU:HD23 | 2.05                     | 0.56              |
| 1:C:540:PRO:HG3  | 1:C:546:CYS:O    | 2.06                     | 0.56              |
| 2:E:109:ARG:HG3  | 2:E:235:THR:CG2  | 2.35                     | 0.56              |
| 1:B:116:VAL:HG21 | 1:B:146:VAL:HA   | 1.88                     | 0.56              |
| 1:C:313:ILE:HA   | 1:C:404:MET:O    | 2.06                     | 0.56              |
| 1:C:109:ASN:OD1  | 4:C:701:NAG:H2   | 2.05                     | 0.56              |
| 1:D:409:GLN:OE1  | 1:D:522:ASP:HB3  | 2.06                     | 0.56              |
| 1:A:132:PRO:HG2  | 1:A:135:PHE:CB   | 2.36                     | 0.56              |
| 1:C:426:VAL:O    | 1:C:472:ARG:HD2  | 2.06                     | 0.56              |
| 1:B:624:ASN:ND2  | 1:C:466:ARG:HH21 | 2.04                     | 0.56              |
| 1:D:87:ALA:HB3   | 1:D:99:GLU:HB2   | 1.87                     | 0.56              |
| 1:A:118:PRO:HA   | 1:A:149:GLN:OE1  | 2.06                     | 0.55              |
| 1:D:350:LEU:O    | 1:D:350:LEU:HD23 | 2.07                     | 0.55              |
| 1:A:62:ILE:HG22  | 1:A:108:ARG:HB3  | 1.89                     | 0.55              |
| 1:D:74:LEU:CD1   | 1:D:216:VAL:HG13 | 2.36                     | 0.55              |
| 2:G:128:ARG:HD2  | 2:G:250:GLN:HG2  | 1.88                     | 0.55              |
| 1:B:276:THR:HG23 | 1:B:311:ARG:HB2  | 1.88                     | 0.55              |
| 1:B:71:ASN:OD1   | 1:B:73:ILE:HG13  | 2.06                     | 0.55              |
| 1:C:276:THR:HG23 | 1:C:311:ARG:HB2  | 1.88                     | 0.55              |
| 2:F:196:GLU:HB3  | 2:F:198:TYR:HE1  | 1.71                     | 0.55              |
| 2:H:173:TYR:HD1  | 2:H:174:HIS:H    | 1.55                     | 0.55              |
| 1:A:125:ARG:O    | 1:A:125:ARG:HG3  | 2.05                     | 0.55              |
| 1:C:118:PRO:HA   | 1:C:149:GLN:OE1  | 2.06                     | 0.55              |
| 2:G:196:GLU:HB3  | 2:G:198:TYR:HE1  | 1.71                     | 0.55              |
| 1:B:125:ARG:O    | 1:B:125:ARG:HG3  | 2.06                     | 0.55              |
| 1:B:540:PRO:HG3  | 1:B:546:CYS:O    | 2.06                     | 0.55              |
| 1:C:626:TRP:CE3  | 1:C:630:VAL:HG21 | 2.41                     | 0.55              |
| 1:D:118:PRO:HA   | 1:D:149:GLN:OE1  | 2.06                     | 0.55              |
| 1:D:71:ASN:OD1   | 1:D:73:ILE:HG13  | 2.06                     | 0.55              |
| 1:A:230:TYR:CD1  | 1:A:254:LEU:HD21 | 2.42                     | 0.55              |
| 1:B:372:TYR:HD2  | 1:B:442:LEU:CD2  | 2.20                     | 0.55              |
| 1:D:313:ILE:HA   | 1:D:404:MET:O    | 2.06                     | 0.55              |
| 1:D:131:LEU:HD12 | 1:D:131:LEU:N    | 2.21                     | 0.55              |
| 1:D:372:TYR:HD2  | 1:D:442:LEU:CD2  | 2.19                     | 0.55              |
| 1:D:62:ILE:HG22  | 1:D:108:ARG:HB3  | 1.88                     | 0.55              |
| 3:I:1:NAG:O3     | 3:I:2:NAG:H2     | 2.06                     | 0.55              |
| 1:A:198:TYR:CE1  | 1:A:279:GLY:HA2  | 2.42                     | 0.55              |
| 1:A:372:TYR:HD2  | 1:A:442:LEU:CD2  | 2.19                     | 0.55              |
| 1:B:203:SER:O    | 1:B:204:TYR:HB2  | 2.07                     | 0.55              |
| 1:B:65:ILE:CD1   | 1:B:67:LYS:HE2   | 2.36                     | 0.55              |
| 1:C:132:PRO:HG2  | 1:C:135:PHE:CB   | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:409:GLN:OE1  | 1:C:522:ASP:HB3  | 2.07                     | 0.54              |
| 1:D:465:ASP:OD1  | 1:D:468:ASN:HB2  | 2.06                     | 0.54              |
| 1:A:633:LEU:C    | 1:A:635:ASN:N    | 2.60                     | 0.54              |
| 1:B:515:ASP:OD2  | 4:B:703:NAG:H62  | 2.07                     | 0.54              |
| 1:C:515:ASP:OD2  | 4:C:703:NAG:H62  | 2.07                     | 0.54              |
| 1:A:466:ARG:HH21 | 1:D:624:ASN:ND2  | 2.04                     | 0.54              |
| 1:A:515:ASP:OD2  | 4:A:703:NAG:H62  | 2.08                     | 0.54              |
| 1:B:192:PRO:HB2  | 1:B:271:ASP:HB2  | 1.89                     | 0.54              |
| 1:B:465:ASP:OD1  | 1:B:468:ASN:HB2  | 2.07                     | 0.54              |
| 1:C:387:ASP:HB3  | 1:C:392:LEU:HD21 | 1.90                     | 0.54              |
| 1:D:631:PRO:O    | 1:D:635:ASN:HB2  | 2.07                     | 0.54              |
| 2:E:128:ARG:HD2  | 2:E:250:GLN:HG2  | 1.88                     | 0.54              |
| 1:A:192:PRO:HB2  | 1:A:271:ASP:HB2  | 1.90                     | 0.54              |
| 1:C:192:PRO:HB2  | 1:C:271:ASP:HB2  | 1.90                     | 0.54              |
| 1:C:372:TYR:HD2  | 1:C:442:LEU:CD2  | 2.20                     | 0.54              |
| 1:C:631:PRO:O    | 1:C:635:ASN:HB2  | 2.07                     | 0.54              |
| 1:D:259:ARG:NH1  | 1:D:259:ARG:HG3  | 2.22                     | 0.54              |
| 3:I:1:NAG:H83    | 3:I:1:NAG:C3     | 2.38                     | 0.54              |
| 1:C:125:ARG:HG3  | 1:C:125:ARG:O    | 2.06                     | 0.54              |
| 1:C:62:ILE:HG22  | 1:C:108:ARG:HB3  | 1.90                     | 0.54              |
| 2:H:173:TYR:CD1  | 2:H:174:HIS:N    | 2.72                     | 0.54              |
| 1:C:203:SER:O    | 1:C:204:TYR:HB2  | 2.07                     | 0.54              |
| 2:E:137:ASP:HA   | 2:E:153:ASN:O    | 2.08                     | 0.54              |
| 2:E:196:GLU:HB3  | 2:E:198:TYR:HE1  | 1.73                     | 0.54              |
| 2:F:179:THR:HG22 | 2:F:186:THR:HB   | 1.89                     | 0.54              |
| 1:D:398:PHE:N    | 2:H:236:ILE:HD12 | 2.23                     | 0.54              |
| 1:D:276:THR:HG23 | 1:D:311:ARG:HB2  | 1.88                     | 0.54              |
| 1:C:346:ASP:HB2  | 1:D:346:ASP:HB2  | 1.89                     | 0.54              |
| 1:D:125:ARG:O    | 1:D:125:ARG:HG3  | 2.08                     | 0.54              |
| 2:G:173:TYR:CD1  | 2:G:174:HIS:N    | 2.73                     | 0.54              |
| 1:A:426:VAL:O    | 1:A:472:ARG:HD2  | 2.08                     | 0.53              |
| 1:B:118:PRO:HA   | 1:B:149:GLN:OE1  | 2.07                     | 0.53              |
| 1:A:221:GLY:O    | 1:A:222:ASN:HB3  | 2.09                     | 0.53              |
| 1:A:259:ARG:HG3  | 1:A:259:ARG:NH1  | 2.23                     | 0.53              |
| 1:B:407:VAL:HG21 | 1:B:486:VAL:HG22 | 1.91                     | 0.53              |
| 1:D:132:PRO:HG2  | 1:D:135:PHE:CB   | 2.38                     | 0.53              |
| 1:A:203:SER:O    | 1:A:204:TYR:HB2  | 2.08                     | 0.53              |
| 1:D:426:VAL:CG2  | 1:D:473:ARG:HB2  | 2.35                     | 0.53              |
| 1:B:426:VAL:O    | 1:B:472:ARG:HD2  | 2.09                     | 0.53              |
| 1:D:387:ASP:HB3  | 1:D:392:LEU:HD21 | 1.91                     | 0.53              |
| 2:F:128:ARG:HD2  | 2:F:250:GLN:HG2  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:74:LEU:HD13  | 1:C:216:VAL:HG13 | 1.90                     | 0.53              |
| 1:C:230:TYR:CD1  | 1:C:254:LEU:HD21 | 2.44                     | 0.53              |
| 1:A:387:ASP:HB3  | 1:A:392:LEU:HD21 | 1.91                     | 0.53              |
| 1:B:87:ALA:HB3   | 1:B:99:GLU:HB2   | 1.89                     | 0.53              |
| 1:B:313:ILE:HA   | 1:B:404:MET:O    | 2.08                     | 0.53              |
| 1:B:611:LYS:HD2  | 1:B:611:LYS:N    | 2.23                     | 0.53              |
| 1:B:62:ILE:HG22  | 1:B:108:ARG:HB3  | 1.91                     | 0.53              |
| 1:C:259:ARG:NH1  | 1:C:259:ARG:HG3  | 2.22                     | 0.53              |
| 1:B:259:ARG:HG3  | 1:B:259:ARG:NH1  | 2.24                     | 0.53              |
| 2:G:173:TYR:HD1  | 2:G:174:HIS:H    | 1.55                     | 0.53              |
| 1:A:631:PRO:O    | 1:A:635:ASN:HB2  | 2.09                     | 0.53              |
| 1:D:230:TYR:CD1  | 1:D:254:LEU:HD21 | 2.43                     | 0.53              |
| 2:F:109:ARG:HG3  | 2:F:235:THR:HG23 | 1.90                     | 0.53              |
| 2:G:137:ASP:HA   | 2:G:153:ASN:O    | 2.09                     | 0.53              |
| 3:J:1:NAG:O3     | 3:J:2:NAG:H2     | 2.09                     | 0.53              |
| 1:B:221:GLY:O    | 1:B:222:ASN:HB3  | 2.09                     | 0.52              |
| 1:D:200:HIS:HB2  | 1:D:212:TYR:CE2  | 2.44                     | 0.52              |
| 2:F:179:THR:HB   | 2:F:186:THR:HG22 | 1.91                     | 0.52              |
| 1:A:626:TRP:CE3  | 1:A:630:VAL:HG21 | 2.44                     | 0.52              |
| 1:A:237:PHE:HB3  | 1:A:377:GLY:O    | 2.10                     | 0.52              |
| 1:C:74:LEU:CD1   | 1:C:216:VAL:HG13 | 2.39                     | 0.52              |
| 1:A:86:ALA:HA    | 1:A:101:PRO:HD3  | 1.90                     | 0.52              |
| 1:B:294:HIS:HB2  | 2:F:109:ARG:NE   | 2.25                     | 0.52              |
| 1:B:631:PRO:O    | 1:B:635:ASN:HB2  | 2.08                     | 0.52              |
| 1:C:630:VAL:HB   | 1:C:631:PRO:HD3  | 1.92                     | 0.52              |
| 2:E:125:VAL:HG22 | 2:E:142:HIS:HB3  | 1.92                     | 0.52              |
| 1:B:409:GLN:OE1  | 1:B:522:ASP:HB3  | 2.10                     | 0.52              |
| 1:C:409:GLN:HB2  | 1:C:509:TYR:CE2  | 2.44                     | 0.52              |
| 1:C:537:MET:HG2  | 1:C:553:VAL:HG13 | 1.91                     | 0.52              |
| 2:H:128:ARG:HD2  | 2:H:250:GLN:HG2  | 1.91                     | 0.52              |
| 1:A:409:GLN:HB2  | 1:A:509:TYR:CE2  | 2.45                     | 0.52              |
| 2:F:137:ASP:HA   | 2:F:153:ASN:O    | 2.09                     | 0.52              |
| 2:H:109:ARG:HG3  | 2:H:235:THR:HG23 | 1.92                     | 0.52              |
| 1:A:574:GLN:HA   | 1:A:574:GLN:OE1  | 2.09                     | 0.52              |
| 2:F:125:VAL:HG22 | 2:F:142:HIS:HB3  | 1.92                     | 0.52              |
| 2:G:179:THR:HG22 | 2:G:186:THR:HB   | 1.92                     | 0.52              |
| 1:D:221:GLY:O    | 1:D:222:ASN:HB3  | 2.09                     | 0.52              |
| 3:J:1:NAG:H83    | 3:J:2:NAG:H2     | 1.92                     | 0.52              |
| 1:B:387:ASP:HB3  | 1:B:392:LEU:HD21 | 1.90                     | 0.52              |
| 1:C:619:ARG:O    | 1:C:623:VAL:HG23 | 2.10                     | 0.52              |
| 1:D:234:VAL:CG1  | 1:D:238:LEU:HD12 | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:109:ARG:HG3  | 2:G:235:THR:CG2  | 2.39                     | 0.52              |
| 1:A:465:ASP:OD1  | 1:A:468:ASN:HB2  | 2.11                     | 0.51              |
| 1:C:198:TYR:CE1  | 1:C:279:GLY:HA2  | 2.45                     | 0.51              |
| 1:C:221:GLY:O    | 1:C:222:ASN:HB3  | 2.10                     | 0.51              |
| 1:C:86:ALA:HA    | 1:C:101:PRO:HD3  | 1.92                     | 0.51              |
| 1:C:125:ARG:NH1  | 1:C:365:GLN:O    | 2.44                     | 0.51              |
| 1:C:465:ASP:OD1  | 1:C:468:ASN:HB2  | 2.10                     | 0.51              |
| 1:A:94:ARG:HG2   | 1:A:95:PHE:CD2   | 2.45                     | 0.51              |
| 1:A:94:ARG:O     | 1:A:95:PHE:HB2   | 2.11                     | 0.51              |
| 1:B:331:LYS:O    | 1:B:335:ILE:HG13 | 2.11                     | 0.51              |
| 1:B:626:TRP:CE3  | 1:B:630:VAL:HG21 | 2.45                     | 0.51              |
| 1:C:144:SER:HA   | 1:C:147:GLN:OE1  | 2.10                     | 0.51              |
| 3:I:1:NAG:H83    | 3:I:2:NAG:H2     | 1.92                     | 0.51              |
| 1:A:496:HIS:O    | 1:A:501:SER:HB2  | 2.11                     | 0.51              |
| 1:B:195:VAL:HG21 | 1:B:265:ILE:HG12 | 1.93                     | 0.51              |
| 1:B:94:ARG:HG2   | 1:B:95:PHE:CD2   | 2.44                     | 0.51              |
| 1:C:633:LEU:C    | 1:C:635:ASN:N    | 2.59                     | 0.51              |
| 1:D:409:GLN:HB2  | 1:D:509:TYR:CE2  | 2.45                     | 0.51              |
| 1:A:466:ARG:NH2  | 1:D:624:ASN:ND2  | 2.59                     | 0.51              |
| 1:B:409:GLN:HB2  | 1:B:509:TYR:CE2  | 2.46                     | 0.51              |
| 1:B:86:ALA:HA    | 1:B:101:PRO:HD3  | 1.93                     | 0.51              |
| 1:C:200:HIS:HB2  | 1:C:212:TYR:CE2  | 2.45                     | 0.51              |
| 1:D:540:PRO:HG3  | 1:D:546:CYS:O    | 2.10                     | 0.51              |
| 2:F:173:TYR:HD1  | 2:F:174:HIS:H    | 1.56                     | 0.51              |
| 2:H:179:THR:HB   | 2:H:186:THR:HG22 | 1.92                     | 0.51              |
| 3:J:1:NAG:H3     | 3:J:2:NAG:H2     | 1.93                     | 0.51              |
| 1:D:144:SER:HA   | 1:D:147:GLN:OE1  | 2.11                     | 0.51              |
| 1:A:195:VAL:HG21 | 1:A:265:ILE:HG12 | 1.93                     | 0.51              |
| 1:D:86:ALA:HA    | 1:D:101:PRO:HD3  | 1.92                     | 0.51              |
| 2:E:179:THR:HB   | 2:E:186:THR:HG22 | 1.93                     | 0.51              |
| 2:F:196:GLU:HB3  | 2:F:198:TYR:CE1  | 2.46                     | 0.51              |
| 3:K:1:NAG:C3     | 3:K:1:NAG:H83    | 2.41                     | 0.51              |
| 1:B:630:VAL:HB   | 1:B:631:PRO:HD3  | 1.93                     | 0.51              |
| 1:C:281:GLY:HA2  | 1:C:316:SER:O    | 2.10                     | 0.51              |
| 1:C:88:PRO:HG3   | 1:C:152:ASP:OD1  | 2.11                     | 0.51              |
| 2:G:196:GLU:HB3  | 2:G:198:TYR:CE1  | 2.46                     | 0.51              |
| 3:K:1:NAG:H3     | 3:K:2:NAG:H2     | 1.93                     | 0.51              |
| 1:C:226:ILE:HD11 | 1:C:265:ILE:HD13 | 1.92                     | 0.51              |
| 1:D:198:TYR:CE1  | 1:D:279:GLY:HA2  | 2.46                     | 0.50              |
| 1:B:119:GLN:OE1  | 1:B:206:GLU:HB2  | 2.11                     | 0.50              |
| 1:C:94:ARG:HG2   | 1:C:95:PHE:CD2   | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:179:THR:CG2  | 2:F:186:THR:HB   | 2.41                     | 0.50              |
| 2:H:196:GLU:HB3  | 2:H:198:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:200:HIS:HB2  | 1:A:212:TYR:CE2  | 2.46                     | 0.50              |
| 1:A:281:GLY:HA2  | 1:A:316:SER:O    | 2.10                     | 0.50              |
| 1:D:192:PRO:HB2  | 1:D:271:ASP:HB2  | 1.93                     | 0.50              |
| 2:H:159:ILE:HD13 | 2:H:199:PRO:HG3  | 1.94                     | 0.50              |
| 1:C:278:PHE:CB   | 1:C:313:ILE:HB   | 2.41                     | 0.50              |
| 3:K:1:NAG:O3     | 3:K:2:NAG:H2     | 2.11                     | 0.50              |
| 1:A:278:PHE:CB   | 1:A:313:ILE:HB   | 2.41                     | 0.50              |
| 1:A:88:PRO:HG3   | 1:A:152:ASP:OD1  | 2.12                     | 0.50              |
| 1:D:312:ALA:HB3  | 1:D:403:ILE:HD13 | 1.92                     | 0.50              |
| 2:E:173:TYR:CD1  | 2:E:174:HIS:N    | 2.73                     | 0.50              |
| 2:H:125:VAL:HG22 | 2:H:142:HIS:HB3  | 1.93                     | 0.50              |
| 2:E:109:ARG:HG3  | 2:E:235:THR:HG23 | 1.93                     | 0.50              |
| 1:A:234:VAL:CG1  | 1:A:238:LEU:HD12 | 2.41                     | 0.50              |
| 1:A:74:LEU:CD1   | 1:A:216:VAL:HG13 | 2.42                     | 0.50              |
| 1:C:574:GLN:OE1  | 1:C:574:GLN:HA   | 2.11                     | 0.50              |
| 2:F:173:TYR:CD1  | 2:F:174:HIS:N    | 2.74                     | 0.50              |
| 1:A:125:ARG:NH1  | 1:A:365:GLN:O    | 2.45                     | 0.50              |
| 1:A:433:PHE:CE1  | 1:B:429:SER:O    | 2.65                     | 0.50              |
| 1:B:237:PHE:HB3  | 1:B:377:GLY:O    | 2.12                     | 0.50              |
| 1:C:195:VAL:HG21 | 1:C:265:ILE:HG12 | 1.94                     | 0.50              |
| 1:B:609:GLY:O    | 1:B:612:PRO:HD3  | 2.11                     | 0.50              |
| 1:C:94:ARG:O     | 1:C:95:PHE:HB2   | 2.12                     | 0.50              |
| 1:D:195:VAL:HG21 | 1:D:265:ILE:HG12 | 1.94                     | 0.50              |
| 1:D:574:GLN:OE1  | 1:D:574:GLN:HA   | 2.12                     | 0.50              |
| 1:D:226:ILE:HD11 | 1:D:265:ILE:HD13 | 1.94                     | 0.49              |
| 1:D:278:PHE:CB   | 1:D:313:ILE:HB   | 2.42                     | 0.49              |
| 1:D:88:PRO:HG3   | 1:D:152:ASP:OD1  | 2.11                     | 0.49              |
| 2:F:249:GLU:HB3  | 2:F:250:GLN:NE2  | 2.27                     | 0.49              |
| 2:G:179:THR:CG2  | 2:G:186:THR:HB   | 2.42                     | 0.49              |
| 3:K:1:NAG:H83    | 3:K:2:NAG:H2     | 1.93                     | 0.49              |
| 1:A:278:PHE:HB2  | 1:A:313:ILE:HB   | 1.94                     | 0.49              |
| 1:A:556:SER:O    | 1:A:560:MET:HG3  | 2.12                     | 0.49              |
| 1:B:611:LYS:O    | 1:B:612:PRO:C    | 2.48                     | 0.49              |
| 1:C:208:THR:C    | 1:C:210:ASN:H    | 2.14                     | 0.49              |
| 1:C:556:SER:O    | 1:C:560:MET:HG3  | 2.13                     | 0.49              |
| 2:E:179:THR:HG22 | 2:E:186:THR:HB   | 1.94                     | 0.49              |
| 2:G:179:THR:HB   | 2:G:186:THR:HG22 | 1.94                     | 0.49              |
| 2:G:287:LEU:HD12 | 2:G:288:VAL:N    | 2.26                     | 0.49              |
| 1:A:144:SER:HA   | 1:A:147:GLN:OE1  | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:226:ILE:HD11 | 1:B:265:ILE:HD13 | 1.94                     | 0.49              |
| 1:B:281:GLY:HA2  | 1:B:316:SER:O    | 2.12                     | 0.49              |
| 1:D:137:ASN:HD22 | 1:D:516:GLN:HB3  | 1.78                     | 0.49              |
| 1:A:294:HIS:HB2  | 2:E:109:ARG:CZ   | 2.42                     | 0.49              |
| 1:B:208:THR:C    | 1:B:210:ASN:H    | 2.15                     | 0.49              |
| 1:B:230:TYR:CD1  | 1:B:254:LEU:HD21 | 2.48                     | 0.49              |
| 1:D:119:GLN:OE1  | 1:D:206:GLU:HB2  | 2.13                     | 0.49              |
| 2:G:125:VAL:HG22 | 2:G:142:HIS:HB3  | 1.93                     | 0.49              |
| 3:J:1:NAG:C3     | 3:J:1:NAG:H83    | 2.42                     | 0.49              |
| 1:A:609:GLY:O    | 1:A:612:PRO:HD3  | 2.12                     | 0.49              |
| 2:E:196:GLU:HB3  | 2:E:198:TYR:CE1  | 2.47                     | 0.49              |
| 1:A:74:LEU:HD13  | 1:A:216:VAL:HG13 | 1.93                     | 0.49              |
| 1:C:310:GLN:CD   | 1:C:310:GLN:N    | 2.66                     | 0.49              |
| 1:B:574:GLN:HA   | 1:B:574:GLN:OE1  | 2.12                     | 0.49              |
| 1:D:94:ARG:HG2   | 1:D:95:PHE:CD2   | 2.48                     | 0.49              |
| 2:F:138:TYR:CD1  | 2:F:138:TYR:C    | 2.86                     | 0.49              |
| 1:A:312:ALA:HB3  | 1:A:403:ILE:HD13 | 1.95                     | 0.49              |
| 1:A:363:VAL:O    | 1:A:363:VAL:HG12 | 2.11                     | 0.49              |
| 1:B:125:ARG:NH1  | 1:B:365:GLN:O    | 2.46                     | 0.49              |
| 1:B:137:ASN:HD22 | 1:B:516:GLN:HB3  | 1.76                     | 0.49              |
| 1:B:537:MET:HG2  | 1:B:553:VAL:HG13 | 1.94                     | 0.49              |
| 1:B:88:PRO:HG3   | 1:B:152:ASP:OD1  | 2.12                     | 0.49              |
| 1:B:94:ARG:O     | 1:B:95:PHE:HB2   | 2.13                     | 0.49              |
| 1:A:143:SER:C    | 1:A:145:TYR:H    | 2.15                     | 0.48              |
| 1:C:609:GLY:O    | 1:C:612:PRO:HD3  | 2.13                     | 0.48              |
| 1:D:281:GLY:HA2  | 1:D:316:SER:O    | 2.13                     | 0.48              |
| 2:F:166:ALA:HB2  | 2:F:192:TRP:CE2  | 2.48                     | 0.48              |
| 1:A:208:THR:C    | 1:A:210:ASN:H    | 2.15                     | 0.48              |
| 1:A:630:VAL:HB   | 1:A:631:PRO:HD3  | 1.93                     | 0.48              |
| 1:C:237:PHE:HB3  | 1:C:377:GLY:O    | 2.13                     | 0.48              |
| 1:D:143:SER:C    | 1:D:145:TYR:H    | 2.17                     | 0.48              |
| 1:D:278:PHE:HB2  | 1:D:313:ILE:HB   | 1.95                     | 0.48              |
| 1:D:609:GLY:O    | 1:D:612:PRO:HD3  | 2.13                     | 0.48              |
| 2:F:97:THR:HG23  | 2:F:244:ILE:HG12 | 1.94                     | 0.48              |
| 1:B:278:PHE:CB   | 1:B:313:ILE:HB   | 2.42                     | 0.48              |
| 1:B:496:HIS:O    | 1:B:501:SER:HB2  | 2.13                     | 0.48              |
| 1:D:537:MET:HG2  | 1:D:553:VAL:HG13 | 1.95                     | 0.48              |
| 2:G:105:ARG:HB3  | 2:G:240:GLN:O    | 2.12                     | 0.48              |
| 1:A:537:MET:HG2  | 1:A:553:VAL:HG13 | 1.95                     | 0.48              |
| 1:B:633:LEU:C    | 1:B:635:ASN:N    | 2.60                     | 0.48              |
| 1:C:407:VAL:HG21 | 1:C:486:VAL:HG22 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:415:PHE:HB2  | 1:D:480:PHE:CD2  | 2.49                     | 0.48              |
| 2:H:179:THR:HG22 | 2:H:186:THR:HB   | 1.94                     | 0.48              |
| 2:H:105:ARG:HB3  | 2:H:240:GLN:O    | 2.14                     | 0.48              |
| 1:B:74:LEU:CD1   | 1:B:216:VAL:HG13 | 2.44                     | 0.48              |
| 1:B:325:VAL:C    | 1:B:374:ILE:HD11 | 2.34                     | 0.48              |
| 1:C:278:PHE:HB2  | 1:C:313:ILE:HB   | 1.95                     | 0.48              |
| 1:C:118:PRO:CB   | 1:C:363:VAL:HG21 | 2.44                     | 0.48              |
| 1:C:426:VAL:CG2  | 1:C:473:ARG:HB2  | 2.41                     | 0.48              |
| 1:D:331:LYS:O    | 1:D:335:ILE:HG13 | 2.14                     | 0.48              |
| 4:D:702:NAG:O3   | 4:D:702:NAG:H83  | 2.14                     | 0.48              |
| 2:G:97:THR:HG23  | 2:G:244:ILE:HG12 | 1.96                     | 0.48              |
| 2:H:166:ALA:HB2  | 2:H:192:TRP:CE2  | 2.49                     | 0.48              |
| 1:A:137:ASN:HD22 | 1:A:516:GLN:HB3  | 1.79                     | 0.48              |
| 1:B:200:HIS:HB2  | 1:B:212:TYR:CE2  | 2.48                     | 0.48              |
| 1:B:69:LEU:N     | 1:B:69:LEU:HD12  | 2.29                     | 0.48              |
| 1:D:237:PHE:HB3  | 1:D:377:GLY:O    | 2.14                     | 0.48              |
| 1:C:611:LYS:N    | 1:C:611:LYS:HD2  | 2.28                     | 0.48              |
| 1:D:496:HIS:O    | 1:D:501:SER:HB2  | 2.12                     | 0.48              |
| 2:E:173:TYR:HD1  | 2:E:174:HIS:H    | 1.55                     | 0.48              |
| 2:G:197:ARG:C    | 2:G:198:TYR:HD1  | 2.17                     | 0.48              |
| 1:D:125:ARG:NH1  | 1:D:365:GLN:O    | 2.47                     | 0.48              |
| 1:D:94:ARG:O     | 1:D:95:PHE:HB2   | 2.14                     | 0.48              |
| 1:A:310:GLN:CD   | 1:A:310:GLN:N    | 2.67                     | 0.48              |
| 1:B:144:SER:HA   | 1:B:147:GLN:OE1  | 2.13                     | 0.48              |
| 1:B:238:LEU:CD2  | 1:B:238:LEU:C    | 2.82                     | 0.48              |
| 1:C:143:SER:C    | 1:C:145:TYR:H    | 2.18                     | 0.48              |
| 1:A:142:VAL:O    | 1:A:145:TYR:HB2  | 2.14                     | 0.47              |
| 1:B:556:SER:O    | 1:B:560:MET:HG3  | 2.14                     | 0.47              |
| 2:E:271:MET:HG2  | 2:E:276:ASP:OD2  | 2.14                     | 0.47              |
| 2:G:129:VAL:HG13 | 2:G:243:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:131:LEU:HD12 | 1:B:131:LEU:H    | 1.79                     | 0.47              |
| 1:B:228:VAL:HG12 | 1:B:229:ASN:N    | 2.29                     | 0.47              |
| 1:B:405:LEU:N    | 1:B:405:LEU:HD23 | 2.28                     | 0.47              |
| 1:A:119:GLN:OE1  | 1:A:206:GLU:HB2  | 2.13                     | 0.47              |
| 1:D:142:VAL:O    | 1:D:145:TYR:HB2  | 2.14                     | 0.47              |
| 1:D:208:THR:C    | 1:D:210:ASN:H    | 2.17                     | 0.47              |
| 1:D:633:LEU:O    | 1:D:635:ASN:N    | 2.47                     | 0.47              |
| 2:F:135:LEU:CD1  | 2:F:239:SER:HB3  | 2.44                     | 0.47              |
| 2:H:135:LEU:CD1  | 2:H:239:SER:HB3  | 2.44                     | 0.47              |
| 1:B:143:SER:C    | 1:B:145:TYR:H    | 2.18                     | 0.47              |
| 1:C:363:VAL:O    | 1:C:363:VAL:HG12 | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:129:VAL:HG13 | 2:E:243:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:198:TYR:HB2  | 1:B:278:PHE:CE2  | 2.50                     | 0.47              |
| 2:E:131:SER:O    | 2:E:132:SER:C    | 2.52                     | 0.47              |
| 2:E:179:THR:CG2  | 2:E:186:THR:HB   | 2.45                     | 0.47              |
| 2:G:109:ARG:HG3  | 2:G:235:THR:HG23 | 1.95                     | 0.47              |
| 1:D:556:SER:O    | 1:D:560:MET:HG3  | 2.14                     | 0.47              |
| 1:D:630:VAL:HB   | 1:D:631:PRO:HD3  | 1.95                     | 0.47              |
| 2:G:159:ILE:HD13 | 2:G:199:PRO:HG3  | 1.97                     | 0.47              |
| 1:B:228:VAL:CG1  | 1:B:229:ASN:N    | 2.78                     | 0.47              |
| 1:C:131:LEU:HD23 | 1:C:135:PHE:CE1  | 2.50                     | 0.47              |
| 1:C:228:VAL:HG12 | 1:C:229:ASN:N    | 2.30                     | 0.47              |
| 1:D:325:VAL:C    | 1:D:374:ILE:HD11 | 2.34                     | 0.47              |
| 2:E:94:GLY:HA3   | 2:E:285:VAL:CG2  | 2.44                     | 0.47              |
| 1:A:228:VAL:HG12 | 1:A:229:ASN:N    | 2.29                     | 0.47              |
| 1:B:74:LEU:HD13  | 1:B:216:VAL:HG13 | 1.95                     | 0.47              |
| 1:C:198:TYR:HB2  | 1:C:278:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:226:ILE:HD11 | 1:A:265:ILE:HD13 | 1.97                     | 0.47              |
| 1:A:325:VAL:C    | 1:A:374:ILE:HD11 | 2.35                     | 0.47              |
| 2:F:129:VAL:HG13 | 2:F:243:ILE:HG12 | 1.97                     | 0.47              |
| 2:F:197:ARG:C    | 2:F:198:TYR:HD1  | 2.18                     | 0.47              |
| 1:C:137:ASN:HD22 | 1:C:516:GLN:HB3  | 1.80                     | 0.47              |
| 1:C:126:LEU:HD21 | 1:C:139:LEU:HD21 | 1.97                     | 0.47              |
| 1:C:194:PRO:HG3  | 1:C:274:ARG:CZ   | 2.44                     | 0.47              |
| 2:G:166:ALA:HB2  | 2:G:192:TRP:CE2  | 2.49                     | 0.47              |
| 2:G:249:GLU:HB3  | 2:G:250:GLN:NE2  | 2.30                     | 0.47              |
| 2:G:94:GLY:HA3   | 2:G:285:VAL:CG2  | 2.45                     | 0.47              |
| 2:H:129:VAL:HG13 | 2:H:243:ILE:HG12 | 1.96                     | 0.47              |
| 3:I:1:NAG:H3     | 3:I:2:NAG:H2     | 1.94                     | 0.47              |
| 1:C:119:GLN:OE1  | 1:C:206:GLU:HB2  | 2.14                     | 0.46              |
| 1:C:331:LYS:O    | 1:C:335:ILE:HG13 | 2.15                     | 0.46              |
| 1:D:486:VAL:O    | 1:D:490:VAL:HG23 | 2.15                     | 0.46              |
| 2:E:197:ARG:C    | 2:E:198:TYR:HD1  | 2.19                     | 0.46              |
| 2:F:94:GLY:HA3   | 2:F:285:VAL:CG2  | 2.45                     | 0.46              |
| 1:B:142:VAL:O    | 1:B:145:TYR:HB2  | 2.14                     | 0.46              |
| 1:B:84:PRO:HB3   | 1:B:155:TYR:CE2  | 2.51                     | 0.46              |
| 1:B:282:ALA:O    | 1:B:285:SER:HB2  | 2.14                     | 0.46              |
| 1:C:228:VAL:CG1  | 1:C:229:ASN:N    | 2.78                     | 0.46              |
| 1:D:428:ALA:HA   | 1:D:472:ARG:HD3  | 1.97                     | 0.46              |
| 2:H:271:MET:HG2  | 2:H:276:ASP:OD2  | 2.15                     | 0.46              |
| 1:D:238:LEU:CD2  | 1:D:238:LEU:C    | 2.84                     | 0.46              |
| 2:E:97:THR:HG23  | 2:E:244:ILE:HG12 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:118:PRO:CB   | 1:A:363:VAL:HG21 | 2.45                     | 0.46              |
| 1:A:52:ASP:HA    | 1:A:53:PRO:HD3   | 1.68                     | 0.46              |
| 1:B:312:ALA:HB3  | 1:B:403:ILE:HD13 | 1.97                     | 0.46              |
| 2:E:105:ARG:HB3  | 2:E:240:GLN:O    | 2.15                     | 0.46              |
| 1:A:126:LEU:HD21 | 1:A:139:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:325:VAL:C    | 1:C:374:ILE:HD11 | 2.36                     | 0.46              |
| 2:H:131:SER:O    | 2:H:132:SER:C    | 2.53                     | 0.46              |
| 1:A:228:VAL:CG1  | 1:A:229:ASN:N    | 2.79                     | 0.46              |
| 1:B:278:PHE:HB2  | 1:B:313:ILE:HB   | 1.97                     | 0.46              |
| 1:C:156:LEU:HD12 | 1:C:156:LEU:C    | 2.35                     | 0.46              |
| 1:C:415:PHE:HB2  | 1:C:480:PHE:CD2  | 2.51                     | 0.46              |
| 1:D:198:TYR:HB2  | 1:D:278:PHE:CE2  | 2.51                     | 0.46              |
| 1:D:372:TYR:CD2  | 1:D:442:LEU:CD2  | 2.98                     | 0.46              |
| 1:D:611:LYS:N    | 1:D:611:LYS:HD2  | 2.30                     | 0.46              |
| 2:G:123:GLU:O    | 2:G:124:ALA:HB2  | 2.16                     | 0.46              |
| 2:H:197:ARG:C    | 2:H:198:TYR:HD1  | 2.19                     | 0.46              |
| 2:H:94:GLY:HA3   | 2:H:285:VAL:CG2  | 2.46                     | 0.46              |
| 1:D:126:LEU:HD21 | 1:D:139:LEU:HD21 | 1.97                     | 0.46              |
| 1:D:310:GLN:CD   | 1:D:310:GLN:N    | 2.69                     | 0.46              |
| 2:F:179:THR:HB   | 2:F:186:THR:CG2  | 2.46                     | 0.46              |
| 1:B:126:LEU:HD21 | 1:B:139:LEU:HD21 | 1.98                     | 0.46              |
| 1:B:310:GLN:N    | 1:B:310:GLN:CD   | 2.69                     | 0.46              |
| 1:C:240:THR:OG1  | 1:C:244:ALA:HB3  | 2.16                     | 0.46              |
| 2:F:131:SER:O    | 2:F:132:SER:C    | 2.53                     | 0.46              |
| 2:F:271:MET:HG2  | 2:F:276:ASP:OD2  | 2.16                     | 0.46              |
| 1:A:407:VAL:HG21 | 1:A:486:VAL:HG22 | 1.98                     | 0.46              |
| 1:B:118:PRO:CB   | 1:B:363:VAL:HG21 | 2.46                     | 0.46              |
| 1:B:156:LEU:HD12 | 1:B:156:LEU:C    | 2.37                     | 0.46              |
| 2:H:179:THR:CG2  | 2:H:186:THR:HB   | 2.45                     | 0.46              |
| 1:A:131:LEU:H    | 1:A:131:LEU:HD12 | 1.80                     | 0.45              |
| 1:A:331:LYS:O    | 1:A:335:ILE:HG13 | 2.14                     | 0.45              |
| 1:B:344:VAL:HG21 | 1:B:349:GLU:HB2  | 1.98                     | 0.45              |
| 2:E:135:LEU:CD1  | 2:E:239:SER:HB3  | 2.45                     | 0.45              |
| 2:G:131:SER:O    | 2:G:132:SER:C    | 2.54                     | 0.45              |
| 1:D:203:SER:O    | 1:D:204:TYR:CB   | 2.63                     | 0.45              |
| 1:A:238:LEU:C    | 1:A:238:LEU:CD2  | 2.85                     | 0.45              |
| 1:C:84:PRO:HB3   | 1:C:155:TYR:CE2  | 2.51                     | 0.45              |
| 1:C:239:SER:HB3  | 1:C:329:PRO:HB2  | 1.99                     | 0.45              |
| 1:C:69:LEU:N     | 1:C:69:LEU:HD12  | 2.32                     | 0.45              |
| 1:D:312:ALA:HB3  | 1:D:403:ILE:CD1  | 2.46                     | 0.45              |
| 2:G:138:TYR:CD1  | 2:G:138:TYR:C    | 2.89                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:426:VAL:CG2  | 1:A:473:ARG:HB2  | 2.44                     | 0.45              |
| 1:C:238:LEU:CD2  | 1:C:238:LEU:C    | 2.84                     | 0.45              |
| 1:D:118:PRO:CB   | 1:D:363:VAL:HG21 | 2.46                     | 0.45              |
| 1:D:611:LYS:O    | 1:D:612:PRO:C    | 2.54                     | 0.45              |
| 2:E:192:TRP:HB3  | 2:E:193:PRO:HD2  | 1.98                     | 0.45              |
| 2:G:271:MET:HG2  | 2:G:276:ASP:OD2  | 2.16                     | 0.45              |
| 2:G:272:ALA:HA   | 2:G:279:ILE:HG21 | 1.99                     | 0.45              |
| 2:H:272:ALA:HA   | 2:H:279:ILE:HG21 | 1.99                     | 0.45              |
| 1:B:68:GLU:C     | 1:B:69:LEU:HD12  | 2.37                     | 0.45              |
| 1:D:228:VAL:HG12 | 1:D:229:ASN:N    | 2.31                     | 0.45              |
| 1:A:198:TYR:HB2  | 1:A:278:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:372:TYR:CD2  | 1:A:442:LEU:CD2  | 2.99                     | 0.45              |
| 1:B:239:SER:HB3  | 1:B:329:PRO:HB2  | 1.98                     | 0.45              |
| 1:B:363:VAL:HG12 | 1:B:363:VAL:O    | 2.17                     | 0.45              |
| 1:C:344:VAL:HG21 | 1:C:349:GLU:HB2  | 1.98                     | 0.45              |
| 2:G:111:ASP:OD2  | 2:G:180:ARG:NE   | 2.47                     | 0.45              |
| 1:B:240:THR:OG1  | 1:B:244:ALA:HB3  | 2.16                     | 0.45              |
| 1:A:530:PRO:HB3  | 1:A:544:PHE:CD1  | 2.52                     | 0.45              |
| 1:B:576:VAL:O    | 1:B:576:VAL:HG12 | 2.16                     | 0.45              |
| 1:C:208:THR:C    | 1:C:210:ASN:N    | 2.70                     | 0.45              |
| 1:C:387:ASP:CB   | 1:C:392:LEU:HD21 | 2.47                     | 0.45              |
| 1:D:156:LEU:HD12 | 1:D:156:LEU:C    | 2.37                     | 0.45              |
| 2:E:179:THR:HB   | 2:E:186:THR:CG2  | 2.47                     | 0.45              |
| 2:F:266:LEU:HA   | 2:F:266:LEU:HD23 | 1.81                     | 0.45              |
| 2:F:272:ALA:HA   | 2:F:279:ILE:HG21 | 1.98                     | 0.45              |
| 2:G:192:TRP:HB3  | 2:G:193:PRO:HD2  | 1.99                     | 0.45              |
| 1:C:234:VAL:CG1  | 1:C:238:LEU:HD12 | 2.46                     | 0.45              |
| 2:F:123:GLU:O    | 2:F:124:ALA:HB2  | 2.17                     | 0.45              |
| 1:C:463:TRP:C    | 1:C:465:ASP:H    | 2.20                     | 0.45              |
| 2:F:105:ARG:HB3  | 2:F:240:GLN:O    | 2.17                     | 0.45              |
| 2:H:123:GLU:O    | 2:H:124:ALA:HB2  | 2.17                     | 0.45              |
| 2:H:95:GLN:HA    | 2:H:245:ILE:O    | 2.17                     | 0.45              |
| 1:A:428:ALA:HA   | 1:A:472:ARG:HD3  | 1.99                     | 0.44              |
| 1:C:312:ALA:HB3  | 1:C:403:ILE:HD13 | 1.97                     | 0.44              |
| 1:C:500:GLY:HA3  | 2:G:239:SER:HB2  | 1.99                     | 0.44              |
| 1:C:52:ASP:HA    | 1:C:53:PRO:HD3   | 1.68                     | 0.44              |
| 1:D:69:LEU:N     | 1:D:69:LEU:HD12  | 2.32                     | 0.44              |
| 1:A:60:GLY:HA3   | 1:A:104:TRP:NE1  | 2.32                     | 0.44              |
| 1:A:69:LEU:N     | 1:A:69:LEU:HD12  | 2.32                     | 0.44              |
| 1:B:415:PHE:HB2  | 1:B:480:PHE:CD2  | 2.52                     | 0.44              |
| 1:D:194:PRO:HG3  | 1:D:274:ARG:CZ   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:467:HIS:O    | 1:D:469:PRO:HD3  | 2.17                     | 0.44              |
| 2:E:249:GLU:HB3  | 2:E:250:GLN:NE2  | 2.32                     | 0.44              |
| 1:A:416:VAL:C    | 1:A:418:ASN:N    | 2.71                     | 0.44              |
| 1:C:372:TYR:CD2  | 1:C:442:LEU:CD2  | 2.99                     | 0.44              |
| 1:D:136:THR:C    | 1:D:138:ASN:H    | 2.21                     | 0.44              |
| 1:D:282:ALA:O    | 1:D:285:SER:HB2  | 2.18                     | 0.44              |
| 1:D:331:LYS:HE3  | 1:D:332:TYR:CZ   | 2.53                     | 0.44              |
| 2:E:123:GLU:O    | 2:E:124:ALA:HB2  | 2.16                     | 0.44              |
| 2:E:138:TYR:CD1  | 2:E:138:TYR:C    | 2.91                     | 0.44              |
| 2:F:192:TRP:HB3  | 2:F:193:PRO:HD2  | 1.98                     | 0.44              |
| 2:G:272:ALA:HB2  | 2:G:279:ILE:HD13 | 1.99                     | 0.44              |
| 2:H:97:THR:HG23  | 2:H:244:ILE:HG12 | 1.99                     | 0.44              |
| 1:A:405:LEU:HD23 | 1:A:405:LEU:N    | 2.32                     | 0.44              |
| 1:A:456:ILE:HD12 | 1:A:626:TRP:CH2  | 2.53                     | 0.44              |
| 1:B:137:ASN:O    | 1:B:138:ASN:HB2  | 2.16                     | 0.44              |
| 1:C:208:THR:O    | 1:C:208:THR:HG23 | 2.17                     | 0.44              |
| 1:C:428:ALA:HA   | 1:C:472:ARG:HD3  | 2.00                     | 0.44              |
| 1:D:113:PHE:HB3  | 1:D:210:ASN:ND2  | 2.33                     | 0.44              |
| 1:D:228:VAL:CG1  | 1:D:229:ASN:N    | 2.80                     | 0.44              |
| 1:A:363:VAL:CG1  | 1:A:363:VAL:O    | 2.65                     | 0.44              |
| 1:B:136:THR:C    | 1:B:138:ASN:H    | 2.21                     | 0.44              |
| 1:B:186:ILE:HD12 | 1:B:188:ASP:OD1  | 2.18                     | 0.44              |
| 1:B:208:THR:O    | 1:B:208:THR:HG23 | 2.16                     | 0.44              |
| 2:E:95:GLN:HA    | 2:E:245:ILE:O    | 2.18                     | 0.44              |
| 2:G:135:LEU:CD1  | 2:G:239:SER:HB3  | 2.47                     | 0.44              |
| 2:H:176:VAL:CG2  | 2:H:187:LEU:HD11 | 2.48                     | 0.44              |
| 1:A:136:THR:C    | 1:A:138:ASN:H    | 2.21                     | 0.44              |
| 1:B:60:GLY:HA3   | 1:B:104:TRP:NE1  | 2.33                     | 0.44              |
| 1:C:405:LEU:HD23 | 1:C:405:LEU:N    | 2.32                     | 0.44              |
| 1:C:416:VAL:C    | 1:C:418:ASN:N    | 2.70                     | 0.44              |
| 1:D:344:VAL:HG21 | 1:D:349:GLU:HB2  | 2.00                     | 0.44              |
| 1:D:560:MET:O    | 1:D:564:THR:HG23 | 2.18                     | 0.44              |
| 2:F:176:VAL:CG2  | 2:F:187:LEU:HD11 | 2.48                     | 0.44              |
| 1:A:203:SER:O    | 1:A:204:TYR:CB   | 2.66                     | 0.44              |
| 1:B:405:LEU:CD2  | 1:B:405:LEU:N    | 2.81                     | 0.44              |
| 1:B:372:TYR:CD2  | 1:B:442:LEU:CD2  | 3.00                     | 0.44              |
| 1:C:113:PHE:HB3  | 1:C:210:ASN:ND2  | 2.32                     | 0.44              |
| 1:C:136:THR:C    | 1:C:138:ASN:H    | 2.21                     | 0.44              |
| 1:D:84:PRO:HB3   | 1:D:155:TYR:CE2  | 2.53                     | 0.44              |
| 2:E:166:ALA:HB2  | 2:E:192:TRP:CE2  | 2.53                     | 0.44              |
| 2:E:94:GLY:HA3   | 2:E:285:VAL:HG22 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:287:LEU:HD12 | 2:E:288:VAL:N    | 2.27                     | 0.44              |
| 2:G:95:GLN:HA    | 2:G:245:ILE:O    | 2.18                     | 0.44              |
| 2:H:138:TYR:CD1  | 2:H:138:TYR:C    | 2.91                     | 0.44              |
| 2:H:269:LEU:HA   | 2:H:269:LEU:HD23 | 1.87                     | 0.44              |
| 2:H:287:LEU:HD12 | 2:H:288:VAL:N    | 2.30                     | 0.44              |
| 1:A:415:PHE:HB2  | 1:A:480:PHE:CD2  | 2.53                     | 0.44              |
| 1:B:61:LYS:HB2   | 1:B:107:ILE:HG12 | 2.00                     | 0.44              |
| 1:B:416:VAL:C    | 1:B:418:ASN:N    | 2.71                     | 0.44              |
| 1:C:60:GLY:HA3   | 1:C:104:TRP:NE1  | 2.33                     | 0.44              |
| 1:C:605:TYR:CZ   | 1:C:615:LYS:HB2  | 2.53                     | 0.44              |
| 1:D:109:ASN:OD1  | 4:D:701:NAG:H2   | 2.16                     | 0.44              |
| 1:A:156:LEU:HD12 | 1:A:156:LEU:C    | 2.38                     | 0.44              |
| 1:A:611:LYS:O    | 1:A:612:PRO:C    | 2.55                     | 0.44              |
| 1:C:131:LEU:H    | 1:C:131:LEU:HD12 | 1.81                     | 0.44              |
| 1:D:236:GLY:O    | 1:D:249:TYR:HB2  | 2.17                     | 0.44              |
| 1:D:326:SER:O    | 1:D:379:VAL:HG12 | 2.17                     | 0.44              |
| 1:D:416:VAL:C    | 1:D:418:ASN:N    | 2.70                     | 0.44              |
| 2:G:179:THR:HB   | 2:G:186:THR:CG2  | 2.48                     | 0.44              |
| 2:H:105:ARG:HD3  | 2:H:241:ALA:HB2  | 2.00                     | 0.44              |
| 2:H:87:TYR:CE1   | 2:H:287:LEU:HD13 | 2.53                     | 0.44              |
| 1:A:239:SER:HB3  | 1:A:329:PRO:HB2  | 1.98                     | 0.43              |
| 1:A:282:ALA:O    | 1:A:285:SER:HB2  | 2.18                     | 0.43              |
| 1:B:203:SER:O    | 1:B:204:TYR:CB   | 2.66                     | 0.43              |
| 1:C:403:ILE:HG22 | 1:C:405:LEU:HD22 | 2.00                     | 0.43              |
| 1:D:212:TYR:O    | 1:D:227:THR:HG21 | 2.17                     | 0.43              |
| 1:D:463:TRP:C    | 1:D:465:ASP:H    | 2.21                     | 0.43              |
| 2:E:176:VAL:CG2  | 2:E:187:LEU:HD11 | 2.47                     | 0.43              |
| 2:E:159:ILE:HD13 | 2:E:199:PRO:HG3  | 2.00                     | 0.43              |
| 1:C:496:HIS:O    | 1:C:501:SER:HB2  | 2.18                     | 0.43              |
| 1:D:335:ILE:O    | 1:D:339:LYS:HG3  | 2.18                     | 0.43              |
| 1:D:385:ILE:HA   | 1:D:386:PRO:HD2  | 1.81                     | 0.43              |
| 1:D:403:ILE:HG22 | 1:D:405:LEU:HD22 | 1.99                     | 0.43              |
| 2:F:287:LEU:HD12 | 2:F:288:VAL:N    | 2.28                     | 0.43              |
| 2:H:249:GLU:HB3  | 2:H:250:GLN:NE2  | 2.33                     | 0.43              |
| 1:A:208:THR:HG23 | 1:A:208:THR:O    | 2.18                     | 0.43              |
| 1:A:68:GLU:C     | 1:A:69:LEU:HD12  | 2.39                     | 0.43              |
| 1:B:131:LEU:HD23 | 1:B:135:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:142:VAL:O    | 1:C:145:TYR:HB2  | 2.17                     | 0.43              |
| 1:C:236:GLY:O    | 1:C:249:TYR:HB2  | 2.19                     | 0.43              |
| 2:H:272:ALA:HB2  | 2:H:279:ILE:HD13 | 1.99                     | 0.43              |
| 1:A:186:ILE:HD12 | 1:A:188:ASP:OD1  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:208:THR:C    | 1:A:210:ASN:N    | 2.70                     | 0.43              |
| 1:B:387:ASP:HB3  | 1:B:392:LEU:CD2  | 2.49                     | 0.43              |
| 1:B:208:THR:C    | 1:B:210:ASN:N    | 2.72                     | 0.43              |
| 1:C:387:ASP:HB3  | 1:C:392:LEU:CD2  | 2.48                     | 0.43              |
| 1:C:530:PRO:HB3  | 1:C:544:PHE:CD1  | 2.54                     | 0.43              |
| 1:D:536:PRO:HB2  | 1:D:553:VAL:HA   | 2.00                     | 0.43              |
| 2:E:111:ASP:OD2  | 2:E:180:ARG:NE   | 2.48                     | 0.43              |
| 2:F:159:ILE:HD13 | 2:F:199:PRO:HG3  | 2.00                     | 0.43              |
| 1:B:624:ASN:ND2  | 1:C:466:ARG:NH2  | 2.66                     | 0.43              |
| 1:C:611:LYS:O    | 1:C:612:PRO:C    | 2.56                     | 0.43              |
| 1:D:122:ILE:HG13 | 1:D:123:ASP:H    | 1.83                     | 0.43              |
| 1:A:335:ILE:O    | 1:A:339:LYS:HG3  | 2.18                     | 0.43              |
| 1:A:387:ASP:HB3  | 1:A:392:LEU:CD2  | 2.49                     | 0.43              |
| 1:A:455:THR:O    | 1:A:459:MET:HG2  | 2.19                     | 0.43              |
| 1:B:326:SER:O    | 1:B:379:VAL:HG12 | 2.18                     | 0.43              |
| 1:B:529:VAL:N    | 1:B:530:PRO:HD2  | 2.34                     | 0.43              |
| 1:B:71:ASN:OD1   | 1:B:72:GLU:N     | 2.51                     | 0.43              |
| 1:C:536:PRO:HB2  | 1:C:553:VAL:HA   | 2.01                     | 0.43              |
| 1:A:122:ILE:HG13 | 1:A:123:ASP:H    | 1.84                     | 0.43              |
| 1:A:463:TRP:C    | 1:A:465:ASP:H    | 2.22                     | 0.43              |
| 1:B:194:PRO:HG3  | 1:B:274:ARG:CZ   | 2.49                     | 0.43              |
| 1:B:463:TRP:C    | 1:B:465:ASP:H    | 2.22                     | 0.43              |
| 1:C:186:ILE:HD12 | 1:C:188:ASP:OD1  | 2.19                     | 0.43              |
| 1:C:633:LEU:O    | 1:C:635:ASN:N    | 2.52                     | 0.43              |
| 1:D:186:ILE:HD12 | 1:D:188:ASP:OD1  | 2.19                     | 0.43              |
| 1:D:456:ILE:HD12 | 1:D:626:TRP:CH2  | 2.54                     | 0.43              |
| 1:A:113:PHE:HB3  | 1:A:210:ASN:ND2  | 2.33                     | 0.43              |
| 1:B:385:ILE:HA   | 1:B:386:PRO:HD2  | 1.81                     | 0.43              |
| 1:D:244:ALA:HB1  | 1:D:351:VAL:HG23 | 2.00                     | 0.43              |
| 1:D:605:TYR:CZ   | 1:D:615:LYS:HB2  | 2.53                     | 0.43              |
| 1:A:240:THR:OG1  | 1:A:244:ALA:HB3  | 2.18                     | 0.43              |
| 1:A:497:SER:C    | 1:A:499:PHE:H    | 2.22                     | 0.43              |
| 1:A:611:LYS:N    | 1:A:611:LYS:HD2  | 2.34                     | 0.43              |
| 1:B:113:PHE:HB3  | 1:B:210:ASN:ND2  | 2.33                     | 0.43              |
| 1:B:565:ASN:HB3  | 1:B:574:GLN:O    | 2.19                     | 0.43              |
| 2:E:272:ALA:HA   | 2:E:279:ILE:HG21 | 2.01                     | 0.43              |
| 1:C:282:ALA:O    | 1:C:285:SER:HB2  | 2.19                     | 0.42              |
| 1:D:407:VAL:HG21 | 1:D:486:VAL:HG22 | 2.00                     | 0.42              |
| 2:F:234:LEU:HA   | 2:F:234:LEU:HD23 | 1.91                     | 0.42              |
| 2:G:94:GLY:HA3   | 2:G:285:VAL:HG22 | 2.00                     | 0.42              |
| 2:H:192:TRP:HB3  | 2:H:193:PRO:HD2  | 1.99                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:272:ALA:CB   | 2:H:279:ILE:HG21 | 2.49                     | 0.42              |
| 1:C:68:GLU:C     | 1:C:69:LEU:HD12  | 2.39                     | 0.42              |
| 1:D:61:LYS:HB2   | 1:D:107:ILE:HG12 | 2.00                     | 0.42              |
| 2:F:155:GLY:C    | 2:F:234:LEU:HD12 | 2.40                     | 0.42              |
| 2:F:261:LEU:HD12 | 2:F:262:TYR:N    | 2.34                     | 0.42              |
| 2:G:135:LEU:H    | 2:G:135:LEU:HG   | 1.55                     | 0.42              |
| 1:A:605:TYR:CZ   | 1:A:615:LYS:HB2  | 2.54                     | 0.42              |
| 1:B:236:GLY:O    | 1:B:249:TYR:HB2  | 2.19                     | 0.42              |
| 1:B:331:LYS:HE3  | 1:B:332:TYR:CZ   | 2.54                     | 0.42              |
| 1:B:592:GLU:CD   | 1:B:592:GLU:N    | 2.71                     | 0.42              |
| 1:D:68:GLU:C     | 1:D:69:LEU:HD12  | 2.40                     | 0.42              |
| 2:E:88:ILE:HG12  | 2:E:257:GLN:CG   | 2.44                     | 0.42              |
| 2:G:269:LEU:HD23 | 2:G:269:LEU:HA   | 1.88                     | 0.42              |
| 1:A:344:VAL:HG21 | 1:A:349:GLU:HB2  | 2.01                     | 0.42              |
| 1:A:497:SER:C    | 1:A:499:PHE:N    | 2.73                     | 0.42              |
| 1:B:428:ALA:HA   | 1:B:472:ARG:HD3  | 2.00                     | 0.42              |
| 1:B:485:TRP:O    | 1:B:488:PRO:HD2  | 2.18                     | 0.42              |
| 1:B:633:LEU:O    | 1:B:635:ASN:N    | 2.52                     | 0.42              |
| 1:C:118:PRO:HB3  | 1:C:363:VAL:HG21 | 2.01                     | 0.42              |
| 1:C:469:PRO:HA   | 1:C:472:ARG:NH1  | 2.35                     | 0.42              |
| 1:D:363:VAL:O    | 1:D:363:VAL:HG12 | 2.18                     | 0.42              |
| 1:D:387:ASP:HB3  | 1:D:392:LEU:CD2  | 2.48                     | 0.42              |
| 1:D:485:TRP:O    | 1:D:488:PRO:HD2  | 2.19                     | 0.42              |
| 1:D:626:TRP:CE3  | 1:D:630:VAL:HG21 | 2.53                     | 0.42              |
| 1:A:131:LEU:HD23 | 1:A:135:PHE:CE1  | 2.54                     | 0.42              |
| 1:B:426:VAL:CG2  | 1:B:473:ARG:HB2  | 2.41                     | 0.42              |
| 1:C:326:SER:O    | 1:C:379:VAL:HG12 | 2.19                     | 0.42              |
| 1:D:131:LEU:HD12 | 1:D:131:LEU:H    | 1.82                     | 0.42              |
| 1:A:312:ALA:HB3  | 1:A:403:ILE:CD1  | 2.50                     | 0.42              |
| 1:A:610:LEU:HD23 | 1:A:610:LEU:HA   | 1.83                     | 0.42              |
| 1:C:405:LEU:O    | 1:C:505:PHE:HA   | 2.20                     | 0.42              |
| 1:D:131:LEU:HD23 | 1:D:135:PHE:CE1  | 2.55                     | 0.42              |
| 1:D:565:ASN:HB3  | 1:D:574:GLN:O    | 2.20                     | 0.42              |
| 2:E:155:GLY:C    | 2:E:234:LEU:HD12 | 2.40                     | 0.42              |
| 2:F:272:ALA:HB2  | 2:F:279:ILE:HD13 | 2.02                     | 0.42              |
| 2:H:179:THR:HB   | 2:H:186:THR:CG2  | 2.48                     | 0.42              |
| 1:B:358:PRO:HD2  | 1:B:361:GLU:OE2  | 2.19                     | 0.42              |
| 1:B:536:PRO:HB2  | 1:B:553:VAL:HA   | 2.02                     | 0.42              |
| 1:C:203:SER:O    | 1:C:204:TYR:CB   | 2.66                     | 0.42              |
| 1:C:536:PRO:O    | 1:C:553:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:294:HIS:HB2  | 2:E:109:ARG:NE   | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:94:GLY:HA3   | 2:H:285:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:118:PRO:HB3  | 1:A:363:VAL:HG21 | 2.02                     | 0.42              |
| 1:C:113:PHE:HB3  | 1:C:210:ASN:HD22 | 1.85                     | 0.42              |
| 1:C:635:ASN:C    | 1:C:636:LEU:HG   | 2.40                     | 0.42              |
| 1:D:239:SER:HB3  | 1:D:329:PRO:HB2  | 2.01                     | 0.42              |
| 2:F:94:GLY:HA3   | 2:F:285:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:560:MET:O    | 1:A:564:THR:HG23 | 2.20                     | 0.42              |
| 1:B:122:ILE:HG13 | 1:B:123:ASP:H    | 1.85                     | 0.42              |
| 1:B:132:PRO:HG2  | 1:B:135:PHE:HB3  | 2.02                     | 0.42              |
| 1:B:312:ALA:HB3  | 1:B:403:ILE:CD1  | 2.50                     | 0.42              |
| 1:B:387:ASP:CB   | 1:B:392:LEU:HD21 | 2.50                     | 0.42              |
| 1:B:540:PRO:HB3  | 1:B:545:PRO:O    | 2.20                     | 0.42              |
| 1:C:335:ILE:O    | 1:C:339:LYS:HG3  | 2.19                     | 0.42              |
| 1:C:529:VAL:N    | 1:C:530:PRO:HD2  | 2.34                     | 0.42              |
| 2:F:87:TYR:CE1   | 2:F:287:LEU:HD13 | 2.55                     | 0.42              |
| 2:G:88:ILE:HG12  | 2:G:257:GLN:CG   | 2.45                     | 0.42              |
| 1:A:326:SER:O    | 1:A:379:VAL:HG12 | 2.19                     | 0.41              |
| 1:A:633:LEU:O    | 1:A:635:ASN:N    | 2.52                     | 0.41              |
| 1:C:61:LYS:HB2   | 1:C:107:ILE:HG12 | 2.01                     | 0.41              |
| 1:C:141:VAL:HG21 | 1:C:542:GLU:O    | 2.19                     | 0.41              |
| 1:C:312:ALA:HB3  | 1:C:403:ILE:CD1  | 2.50                     | 0.41              |
| 1:C:540:PRO:HB3  | 1:C:545:PRO:O    | 2.20                     | 0.41              |
| 1:D:359:TYR:C    | 1:D:359:TYR:CD1  | 2.94                     | 0.41              |
| 2:E:87:TYR:CE1   | 2:E:287:LEU:HD13 | 2.54                     | 0.41              |
| 2:F:95:GLN:HA    | 2:F:245:ILE:O    | 2.20                     | 0.41              |
| 1:A:194:PRO:HG3  | 1:A:274:ARG:CZ   | 2.50                     | 0.41              |
| 1:A:485:TRP:O    | 1:A:488:PRO:HD2  | 2.20                     | 0.41              |
| 1:A:497:SER:O    | 1:A:499:PHE:N    | 2.53                     | 0.41              |
| 1:B:438:PHE:C    | 1:B:438:PHE:CD2  | 2.93                     | 0.41              |
| 1:D:186:ILE:HG23 | 1:D:186:ILE:O    | 2.20                     | 0.41              |
| 1:D:387:ASP:CB   | 1:D:392:LEU:HD21 | 2.49                     | 0.41              |
| 2:F:272:ALA:CB   | 2:F:279:ILE:HG21 | 2.50                     | 0.41              |
| 2:G:176:VAL:CG2  | 2:G:187:LEU:HD11 | 2.50                     | 0.41              |
| 1:A:129:VAL:HG23 | 1:A:130:MET:N    | 2.34                     | 0.41              |
| 1:C:137:ASN:O    | 1:C:138:ASN:HB2  | 2.20                     | 0.41              |
| 1:D:438:PHE:C    | 1:D:438:PHE:CD2  | 2.93                     | 0.41              |
| 1:D:405:LEU:O    | 1:D:505:PHE:HA   | 2.20                     | 0.41              |
| 1:B:212:TYR:O    | 1:B:227:THR:HG21 | 2.20                     | 0.41              |
| 1:B:234:VAL:CG1  | 1:B:238:LEU:HD12 | 2.47                     | 0.41              |
| 1:B:403:ILE:HG22 | 1:B:405:LEU:HD22 | 2.01                     | 0.41              |
| 1:B:530:PRO:HB3  | 1:B:544:PHE:CD1  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:60:GLY:HA3   | 1:D:104:TRP:NE1  | 2.35                     | 0.41              |
| 2:G:272:ALA:CB   | 2:G:279:ILE:HG21 | 2.50                     | 0.41              |
| 2:H:111:ASP:OD2  | 2:H:180:ARG:NE   | 2.51                     | 0.41              |
| 1:A:61:LYS:HB2   | 1:A:107:ILE:HG12 | 2.03                     | 0.41              |
| 1:A:271:ASP:HA   | 1:A:272:PRO:HD2  | 1.94                     | 0.41              |
| 1:B:467:HIS:O    | 1:B:469:PRO:HD3  | 2.21                     | 0.41              |
| 1:B:535:ILE:HB   | 1:B:536:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:438:PHE:C    | 1:C:438:PHE:CD2  | 2.94                     | 0.41              |
| 1:C:625:LEU:O    | 1:C:630:VAL:HG23 | 2.20                     | 0.41              |
| 1:D:157:ASN:O    | 1:D:226:ILE:HA   | 2.20                     | 0.41              |
| 1:D:208:THR:O    | 1:D:208:THR:HG23 | 2.19                     | 0.41              |
| 1:A:403:ILE:HG22 | 1:A:405:LEU:HD22 | 2.03                     | 0.41              |
| 1:B:93:HIS:O     | 1:B:96:GLN:HB2   | 2.21                     | 0.41              |
| 2:G:137:ASP:OD1  | 2:G:154:VAL:C    | 2.59                     | 0.41              |
| 1:A:93:HIS:O     | 1:A:96:GLN:HB2   | 2.21                     | 0.41              |
| 1:C:456:ILE:HD12 | 1:C:626:TRP:CH2  | 2.56                     | 0.41              |
| 1:D:536:PRO:O    | 1:D:553:VAL:HG22 | 2.20                     | 0.41              |
| 2:H:137:ASP:OD1  | 2:H:154:VAL:C    | 2.59                     | 0.41              |
| 1:B:186:ILE:O    | 1:B:186:ILE:HG23 | 2.21                     | 0.41              |
| 1:B:605:TYR:CZ   | 1:B:615:LYS:HB2  | 2.56                     | 0.41              |
| 1:C:467:HIS:O    | 1:C:469:PRO:HD3  | 2.21                     | 0.41              |
| 1:A:397:GLU:OE1  | 2:E:235:THR:HB   | 2.20                     | 0.41              |
| 1:A:84:PRO:HB3   | 1:A:155:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:405:LEU:O    | 1:A:505:PHE:HA   | 2.21                     | 0.41              |
| 1:A:540:PRO:HB3  | 1:A:545:PRO:O    | 2.20                     | 0.41              |
| 1:B:294:HIS:HA   | 2:F:109:ARG:CZ   | 2.51                     | 0.41              |
| 1:C:122:ILE:HG13 | 1:C:123:ASP:H    | 1.86                     | 0.41              |
| 1:C:497:SER:C    | 1:C:499:PHE:H    | 2.24                     | 0.41              |
| 1:C:535:ILE:HB   | 1:C:536:PRO:HD3  | 2.03                     | 0.41              |
| 1:D:498:ASN:O    | 1:D:498:ASN:CG   | 2.59                     | 0.41              |
| 1:D:530:PRO:HB3  | 1:D:544:PHE:CD1  | 2.55                     | 0.41              |
| 2:F:156:THR:HG22 | 2:F:157:ASP:N    | 2.36                     | 0.41              |
| 2:H:190:ASP:OD2  | 2:H:192:TRP:HZ3  | 2.04                     | 0.41              |
| 1:A:438:PHE:CD2  | 1:A:438:PHE:C    | 2.94                     | 0.41              |
| 1:B:113:PHE:HB3  | 1:B:210:ASN:HD22 | 1.86                     | 0.41              |
| 1:B:212:TYR:CD2  | 1:B:212:TYR:N    | 2.89                     | 0.41              |
| 1:B:52:ASP:HA    | 1:B:53:PRO:HD3   | 1.70                     | 0.41              |
| 1:D:208:THR:C    | 1:D:210:ASN:N    | 2.74                     | 0.41              |
| 1:D:358:PRO:HD2  | 1:D:361:GLU:OE2  | 2.21                     | 0.41              |
| 1:D:409:GLN:HB2  | 1:D:509:TYR:CD2  | 2.56                     | 0.41              |
| 2:G:155:GLY:C    | 2:G:234:LEU:HD12 | 2.41                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:155:GLY:HA3  | 2:H:234:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:358:PRO:HD2  | 1:A:361:GLU:OE2  | 2.21                     | 0.41              |
| 1:A:387:ASP:CB   | 1:A:392:LEU:HD21 | 2.51                     | 0.41              |
| 1:A:535:ILE:HB   | 1:A:536:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:628:GLU:C    | 1:A:631:PRO:HD2  | 2.42                     | 0.41              |
| 1:C:271:ASP:HA   | 1:C:272:PRO:HD2  | 1.95                     | 0.41              |
| 1:C:242:ASP:OD1  | 1:C:347:THR:HG21 | 2.21                     | 0.41              |
| 1:D:63:ARG:NH2   | 1:D:107:ILE:HG21 | 2.36                     | 0.41              |
| 1:A:331:LYS:HE3  | 1:A:332:TYR:CZ   | 2.57                     | 0.40              |
| 1:C:359:TYR:CD1  | 1:C:360:LYS:N    | 2.90                     | 0.40              |
| 1:C:409:GLN:HB2  | 1:C:509:TYR:CD2  | 2.56                     | 0.40              |
| 1:C:560:MET:O    | 1:C:564:THR:HG23 | 2.21                     | 0.40              |
| 1:C:610:LEU:HA   | 1:C:610:LEU:HD23 | 1.87                     | 0.40              |
| 1:D:632:HIS:O    | 1:D:635:ASN:HB3  | 2.21                     | 0.40              |
| 2:H:155:GLY:HA3  | 2:H:234:LEU:HD12 | 2.02                     | 0.40              |
| 1:B:405:LEU:HD23 | 1:B:405:LEU:H    | 1.85                     | 0.40              |
| 1:C:497:SER:C    | 1:C:499:PHE:N    | 2.74                     | 0.40              |
| 1:D:115:PRO:HB2  | 1:D:150:SER:HB3  | 2.04                     | 0.40              |
| 1:D:113:PHE:HB3  | 1:D:210:ASN:HD22 | 1.86                     | 0.40              |
| 1:D:325:VAL:HG12 | 1:D:326:SER:N    | 2.35                     | 0.40              |
| 1:C:157:ASN:O    | 1:C:226:ILE:HA   | 2.21                     | 0.40              |
| 1:C:455:THR:O    | 1:C:459:MET:HG2  | 2.22                     | 0.40              |
| 1:C:628:GLU:C    | 1:C:631:PRO:HD2  | 2.41                     | 0.40              |
| 1:D:244:ALA:CB   | 1:D:347:THR:HB   | 2.52                     | 0.40              |
| 1:A:467:HIS:O    | 1:A:469:PRO:HD3  | 2.22                     | 0.40              |
| 1:B:497:SER:C    | 1:B:499:PHE:N    | 2.75                     | 0.40              |
| 1:C:286:CYS:O    | 1:C:287:VAL:C    | 2.60                     | 0.40              |
| 1:C:331:LYS:HE3  | 1:C:332:TYR:CZ   | 2.55                     | 0.40              |
| 1:C:87:ALA:HA    | 1:C:88:PRO:HD3   | 1.97                     | 0.40              |
| 1:D:396:GLY:O    | 2:H:238:ASN:ND2  | 2.50                     | 0.40              |
| 2:E:238:ASN:O    | 2:E:239:SER:C    | 2.60                     | 0.40              |
| 2:E:261:LEU:HD12 | 2:E:262:TYR:N    | 2.35                     | 0.40              |
| 2:F:168:ILE:HD12 | 2:F:169:ASN:N    | 2.37                     | 0.40              |
| 2:F:118:SER:OG   | 2:F:257:GLN:HB2  | 2.22                     | 0.40              |
| 2:H:232:ARG:HG2  | 2:H:232:ARG:HH11 | 1.86                     | 0.40              |
| 1:A:186:ILE:O    | 1:A:186:ILE:HG23 | 2.22                     | 0.40              |
| 1:A:359:TYR:CD1  | 1:A:359:TYR:C    | 2.95                     | 0.40              |
| 1:B:359:TYR:CD1  | 1:B:359:TYR:C    | 2.95                     | 0.40              |
| 1:C:71:ASN:OD1   | 1:C:72:GLU:N     | 2.55                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 2:E:192:TRP:NE1 | 2:E:192:TRP:NE1[2_556] | 1.74                     | 0.46              |

## 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     | 525/574 (92%)   | 441 (84%)  | 62 (12%)  | 22 (4%)  | 3 23        |
| 1   | B     | 525/574 (92%)   | 441 (84%)  | 63 (12%)  | 21 (4%)  | 3 24        |
| 1   | C     | 525/574 (92%)   | 441 (84%)  | 63 (12%)  | 21 (4%)  | 3 24        |
| 1   | D     | 525/574 (92%)   | 441 (84%)  | 63 (12%)  | 21 (4%)  | 3 24        |
| 2   | E     | 175/243 (72%)   | 143 (82%)  | 23 (13%)  | 9 (5%)   | 2 19        |
| 2   | F     | 175/243 (72%)   | 143 (82%)  | 22 (13%)  | 10 (6%)  | 1 16        |
| 2   | G     | 175/243 (72%)   | 142 (81%)  | 23 (13%)  | 10 (6%)  | 1 16        |
| 2   | H     | 175/243 (72%)   | 143 (82%)  | 22 (13%)  | 10 (6%)  | 1 16        |
| All | All   | 2800/3268 (86%) | 2335 (83%) | 341 (12%) | 124 (4%) | 2 21        |

All (124) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 106 | ASP  |
| 1   | A     | 124 | GLY  |
| 1   | A     | 138 | ASN  |
| 1   | A     | 343 | ASN  |
| 1   | A     | 465 | ASP  |
| 1   | B     | 106 | ASP  |
| 1   | B     | 122 | ILE  |
| 1   | B     | 124 | GLY  |
| 1   | B     | 138 | ASN  |
| 1   | B     | 343 | ASN  |
| 1   | B     | 465 | ASP  |
| 1   | C     | 106 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 122 | ILE  |
| 1   | C     | 124 | GLY  |
| 1   | C     | 138 | ASN  |
| 1   | C     | 343 | ASN  |
| 1   | C     | 465 | ASP  |
| 1   | D     | 106 | ASP  |
| 1   | D     | 122 | ILE  |
| 1   | D     | 124 | GLY  |
| 1   | D     | 138 | ASN  |
| 1   | D     | 343 | ASN  |
| 1   | D     | 465 | ASP  |
| 2   | E     | 102 | PRO  |
| 2   | E     | 137 | ASP  |
| 2   | E     | 200 | ALA  |
| 2   | E     | 231 | GLY  |
| 2   | F     | 102 | PRO  |
| 2   | F     | 137 | ASP  |
| 2   | F     | 200 | ALA  |
| 2   | F     | 231 | GLY  |
| 2   | G     | 102 | PRO  |
| 2   | G     | 137 | ASP  |
| 2   | G     | 200 | ALA  |
| 2   | G     | 231 | GLY  |
| 2   | H     | 102 | PRO  |
| 2   | H     | 137 | ASP  |
| 2   | H     | 200 | ALA  |
| 2   | H     | 231 | GLY  |
| 1   | A     | 122 | ILE  |
| 1   | A     | 123 | ASP  |
| 1   | A     | 365 | GLN  |
| 1   | A     | 466 | ARG  |
| 1   | B     | 123 | ASP  |
| 1   | B     | 365 | GLN  |
| 1   | B     | 466 | ARG  |
| 1   | C     | 123 | ASP  |
| 1   | C     | 365 | GLN  |
| 1   | C     | 466 | ARG  |
| 1   | D     | 70  | ASN  |
| 1   | D     | 123 | ASP  |
| 1   | D     | 365 | GLN  |
| 1   | D     | 466 | ARG  |
| 1   | D     | 619 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 199 | PRO  |
| 2   | F     | 199 | PRO  |
| 2   | G     | 199 | PRO  |
| 2   | H     | 199 | PRO  |
| 1   | A     | 70  | ASN  |
| 1   | A     | 140 | ASP  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 546 | CYS  |
| 1   | B     | 70  | ASN  |
| 1   | B     | 140 | ASP  |
| 1   | B     | 154 | LEU  |
| 1   | B     | 546 | CYS  |
| 1   | C     | 70  | ASN  |
| 1   | C     | 140 | ASP  |
| 1   | C     | 154 | LEU  |
| 1   | C     | 546 | CYS  |
| 1   | C     | 619 | ARG  |
| 1   | D     | 140 | ASP  |
| 1   | D     | 154 | LEU  |
| 1   | D     | 342 | CYS  |
| 1   | D     | 546 | CYS  |
| 2   | E     | 103 | ASN  |
| 2   | E     | 239 | SER  |
| 2   | F     | 103 | ASN  |
| 2   | F     | 239 | SER  |
| 2   | G     | 103 | ASN  |
| 2   | G     | 239 | SER  |
| 2   | H     | 103 | ASN  |
| 2   | H     | 239 | SER  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 342 | CYS  |
| 1   | A     | 619 | ARG  |
| 1   | B     | 137 | ASN  |
| 1   | B     | 342 | CYS  |
| 1   | B     | 619 | ARG  |
| 1   | B     | 634 | HIS  |
| 1   | C     | 137 | ASN  |
| 1   | C     | 342 | CYS  |
| 1   | C     | 634 | HIS  |
| 1   | A     | 144 | SER  |
| 1   | A     | 421 | ASP  |
| 1   | A     | 498 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 634 | HIS  |
| 1   | C     | 144 | SER  |
| 1   | C     | 421 | ASP  |
| 1   | D     | 137 | ASN  |
| 1   | D     | 144 | SER  |
| 1   | D     | 421 | ASP  |
| 1   | D     | 634 | HIS  |
| 2   | E     | 132 | SER  |
| 2   | F     | 132 | SER  |
| 2   | G     | 132 | SER  |
| 2   | H     | 132 | SER  |
| 1   | B     | 144 | SER  |
| 1   | B     | 421 | ASP  |
| 1   | D     | 341 | GLY  |
| 2   | E     | 260 | GLY  |
| 2   | F     | 260 | GLY  |
| 2   | H     | 124 | ALA  |
| 1   | A     | 341 | GLY  |
| 1   | B     | 127 | PRO  |
| 1   | B     | 341 | GLY  |
| 1   | C     | 341 | GLY  |
| 1   | D     | 127 | PRO  |
| 2   | G     | 260 | GLY  |
| 2   | H     | 260 | GLY  |
| 1   | C     | 127 | PRO  |
| 2   | G     | 93  | GLY  |
| 1   | A     | 127 | PRO  |
| 2   | F     | 93  | GLY  |

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

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|-------------|
| 1   | A     | 455/494 (92%) | 435 (96%) | 20 (4%)  | 28 62       |
| 1   | B     | 455/494 (92%) | 435 (96%) | 20 (4%)  | 28 62       |
| 1   | C     | 455/494 (92%) | 436 (96%) | 19 (4%)  | 30 63       |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1   | D     | 455/494 (92%)   | 436 (96%)  | 19 (4%)  | 30 63       |
| 2   | E     | 143/193 (74%)   | 131 (92%)  | 12 (8%)  | 11 40       |
| 2   | F     | 143/193 (74%)   | 132 (92%)  | 11 (8%)  | 13 42       |
| 2   | G     | 143/193 (74%)   | 132 (92%)  | 11 (8%)  | 13 42       |
| 2   | H     | 143/193 (74%)   | 132 (92%)  | 11 (8%)  | 13 42       |
| All | All   | 2392/2748 (87%) | 2269 (95%) | 123 (5%) | 24 57       |

All (123) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | ILE  |
| 1   | A     | 125 | ARG  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 206 | GLU  |
| 1   | A     | 278 | PHE  |
| 1   | A     | 288 | ASN  |
| 1   | A     | 297 | GLU  |
| 1   | A     | 323 | TRP  |
| 1   | A     | 359 | TYR  |
| 1   | A     | 379 | VAL  |
| 1   | A     | 405 | LEU  |
| 1   | A     | 438 | PHE  |
| 1   | A     | 451 | VAL  |
| 1   | A     | 466 | ARG  |
| 1   | A     | 494 | ASP  |
| 1   | A     | 555 | LEU  |
| 1   | A     | 592 | GLU  |
| 1   | A     | 593 | VAL  |
| 1   | A     | 597 | ARG  |
| 1   | A     | 624 | ASN  |
| 1   | B     | 65  | ILE  |
| 1   | B     | 125 | ARG  |
| 1   | B     | 126 | LEU  |
| 1   | B     | 206 | GLU  |
| 1   | B     | 278 | PHE  |
| 1   | B     | 288 | ASN  |
| 1   | B     | 297 | GLU  |
| 1   | B     | 323 | TRP  |
| 1   | B     | 379 | VAL  |
| 1   | B     | 405 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 438 | PHE  |
| 1   | B     | 451 | VAL  |
| 1   | B     | 466 | ARG  |
| 1   | B     | 494 | ASP  |
| 1   | B     | 555 | LEU  |
| 1   | B     | 592 | GLU  |
| 1   | B     | 593 | VAL  |
| 1   | B     | 597 | ARG  |
| 1   | B     | 612 | PRO  |
| 1   | B     | 624 | ASN  |
| 1   | C     | 65  | ILE  |
| 1   | C     | 125 | ARG  |
| 1   | C     | 126 | LEU  |
| 1   | C     | 206 | GLU  |
| 1   | C     | 278 | PHE  |
| 1   | C     | 288 | ASN  |
| 1   | C     | 297 | GLU  |
| 1   | C     | 323 | TRP  |
| 1   | C     | 379 | VAL  |
| 1   | C     | 405 | LEU  |
| 1   | C     | 438 | PHE  |
| 1   | C     | 451 | VAL  |
| 1   | C     | 466 | ARG  |
| 1   | C     | 494 | ASP  |
| 1   | C     | 555 | LEU  |
| 1   | C     | 592 | GLU  |
| 1   | C     | 593 | VAL  |
| 1   | C     | 597 | ARG  |
| 1   | C     | 624 | ASN  |
| 1   | D     | 65  | ILE  |
| 1   | D     | 125 | ARG  |
| 1   | D     | 126 | LEU  |
| 1   | D     | 206 | GLU  |
| 1   | D     | 278 | PHE  |
| 1   | D     | 288 | ASN  |
| 1   | D     | 297 | GLU  |
| 1   | D     | 323 | TRP  |
| 1   | D     | 359 | TYR  |
| 1   | D     | 379 | VAL  |
| 1   | D     | 405 | LEU  |
| 1   | D     | 438 | PHE  |
| 1   | D     | 451 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 466 | ARG  |
| 1   | D     | 494 | ASP  |
| 1   | D     | 555 | LEU  |
| 1   | D     | 592 | GLU  |
| 1   | D     | 593 | VAL  |
| 1   | D     | 624 | ASN  |
| 2   | E     | 100 | TRP  |
| 2   | E     | 102 | PRO  |
| 2   | E     | 106 | PRO  |
| 2   | E     | 129 | VAL  |
| 2   | E     | 157 | ASP  |
| 2   | E     | 173 | TYR  |
| 2   | E     | 179 | THR  |
| 2   | E     | 181 | SER  |
| 2   | E     | 186 | THR  |
| 2   | E     | 188 | GLN  |
| 2   | E     | 237 | PHE  |
| 2   | E     | 284 | ASN  |
| 2   | F     | 100 | TRP  |
| 2   | F     | 102 | PRO  |
| 2   | F     | 129 | VAL  |
| 2   | F     | 157 | ASP  |
| 2   | F     | 173 | TYR  |
| 2   | F     | 179 | THR  |
| 2   | F     | 181 | SER  |
| 2   | F     | 186 | THR  |
| 2   | F     | 188 | GLN  |
| 2   | F     | 237 | PHE  |
| 2   | F     | 284 | ASN  |
| 2   | G     | 100 | TRP  |
| 2   | G     | 102 | PRO  |
| 2   | G     | 129 | VAL  |
| 2   | G     | 157 | ASP  |
| 2   | G     | 173 | TYR  |
| 2   | G     | 179 | THR  |
| 2   | G     | 181 | SER  |
| 2   | G     | 186 | THR  |
| 2   | G     | 188 | GLN  |
| 2   | G     | 237 | PHE  |
| 2   | G     | 284 | ASN  |
| 2   | H     | 100 | TRP  |
| 2   | H     | 102 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 129 | VAL  |
| 2   | H     | 157 | ASP  |
| 2   | H     | 173 | TYR  |
| 2   | H     | 179 | THR  |
| 2   | H     | 181 | SER  |
| 2   | H     | 186 | THR  |
| 2   | H     | 188 | GLN  |
| 2   | H     | 237 | PHE  |
| 2   | H     | 284 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 624 | ASN  |
| 1   | B     | 437 | ASN  |
| 1   | B     | 624 | ASN  |
| 1   | C     | 120 | ASN  |
| 1   | C     | 437 | ASN  |
| 1   | D     | 120 | ASN  |
| 1   | D     | 437 | ASN  |
| 1   | D     | 624 | ASN  |

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

6 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$ |
| 3   | NAG  | I     | 1   | 3,2  | 14,14,15     | 1.18 | 1 (7%)      | 17,19,21    | 0.83 | 0           |
| 3   | NAG  | I     | 2   | 3    | 14,14,15     | 0.90 | 1 (7%)      | 17,19,21    | 0.66 | 0           |
| 3   | NAG  | J     | 1   | 3,2  | 14,14,15     | 1.20 | 1 (7%)      | 17,19,21    | 0.92 | 0           |
| 3   | NAG  | J     | 2   | 3    | 14,14,15     | 0.94 | 1 (7%)      | 17,19,21    | 0.65 | 0           |
| 3   | NAG  | K     | 1   | 3,2  | 14,14,15     | 1.16 | 1 (7%)      | 17,19,21    | 0.91 | 0           |
| 3   | NAG  | K     | 2   | 3    | 14,14,15     | 1.01 | 1 (7%)      | 17,19,21    | 0.63 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | I     | 1   | 3,2  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | I     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 1   | 3,2  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | K     | 1   | 3,2  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | K     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | J     | 1   | NAG  | C1-C2 | 3.40 | 1.57        | 1.52     |
| 3   | K     | 2   | NAG  | C1-C2 | 3.16 | 1.57        | 1.52     |
| 3   | I     | 1   | NAG  | C1-C2 | 3.12 | 1.57        | 1.52     |
| 3   | J     | 2   | NAG  | C1-C2 | 3.00 | 1.56        | 1.52     |
| 3   | K     | 1   | NAG  | C1-C2 | 2.93 | 1.56        | 1.52     |
| 3   | I     | 2   | NAG  | C1-C2 | 2.65 | 1.56        | 1.52     |

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | I     | 2   | NAG  | C3-C2-N2-C7 |

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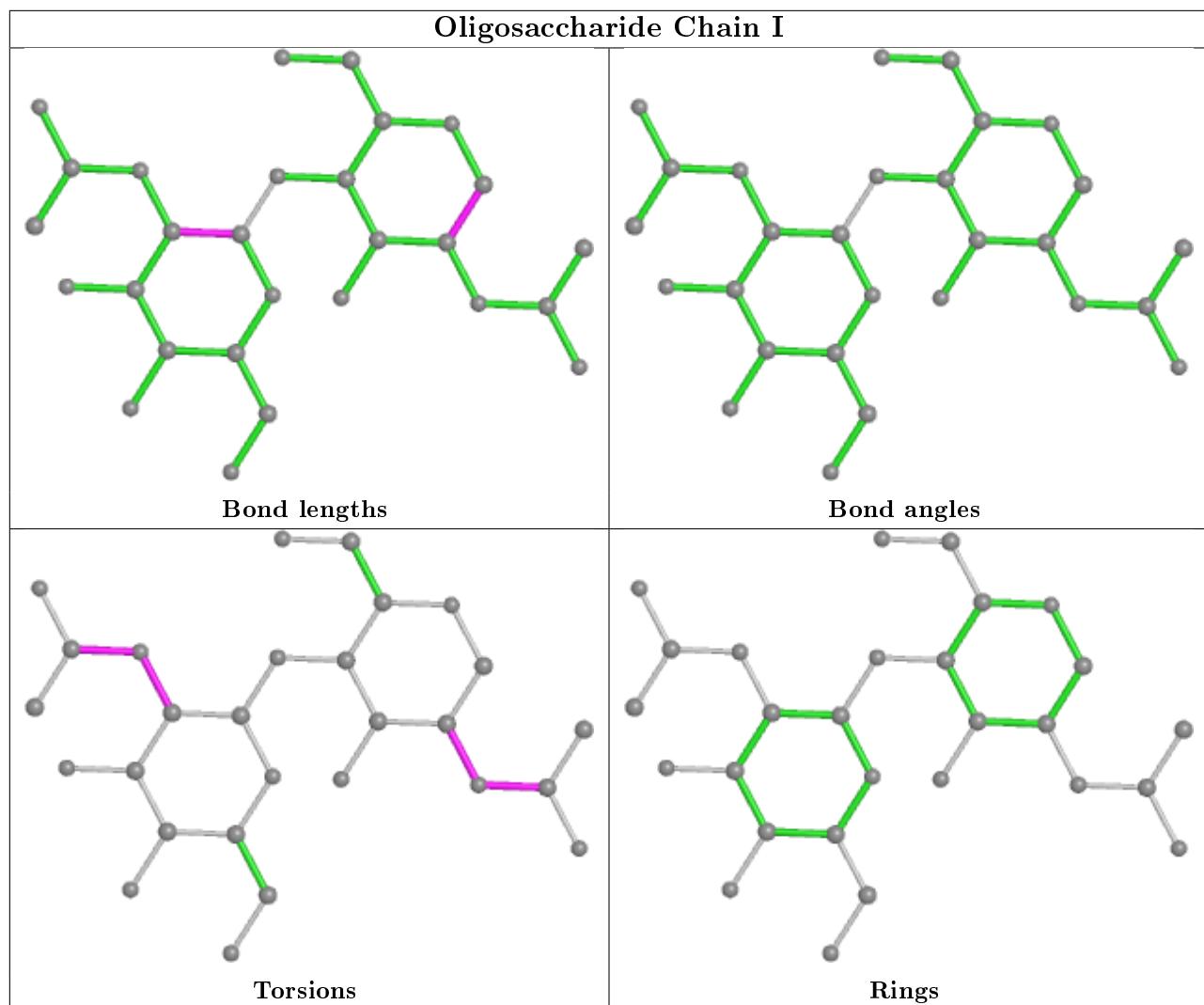
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | I     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | I     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | K     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | K     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | K     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | I     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | I     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | J     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | J     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | J     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | K     | 2   | NAG  | C3-C2-N2-C7 |
| 3   | K     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | K     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | J     | 2   | NAG  | C3-C2-N2-C7 |
| 3   | J     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | J     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | K     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | J     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | I     | 2   | NAG  | C1-C2-N2-C7 |
| 3   | J     | 2   | NAG  | C1-C2-N2-C7 |
| 3   | K     | 2   | NAG  | C1-C2-N2-C7 |

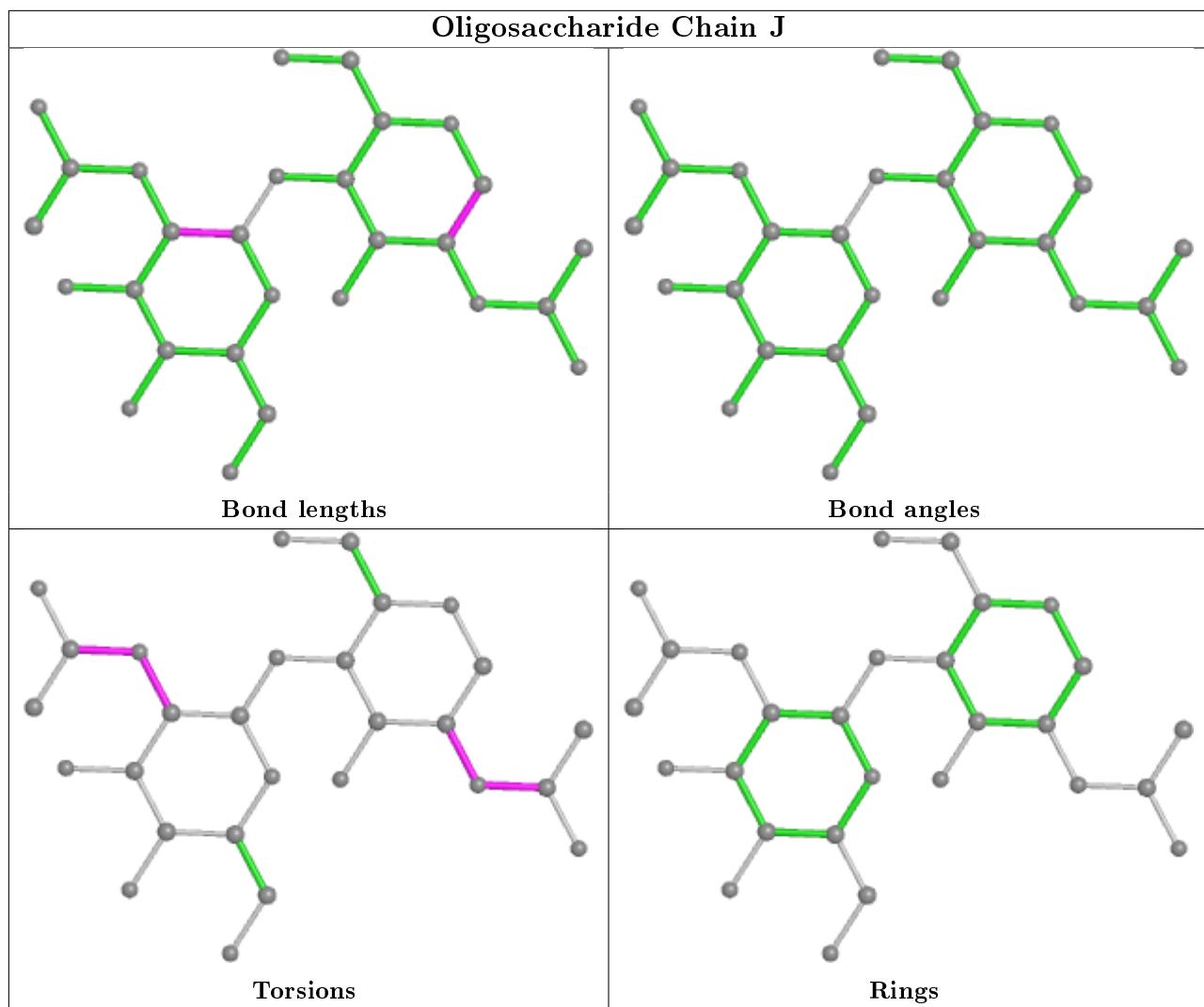
There are no ring outliers.

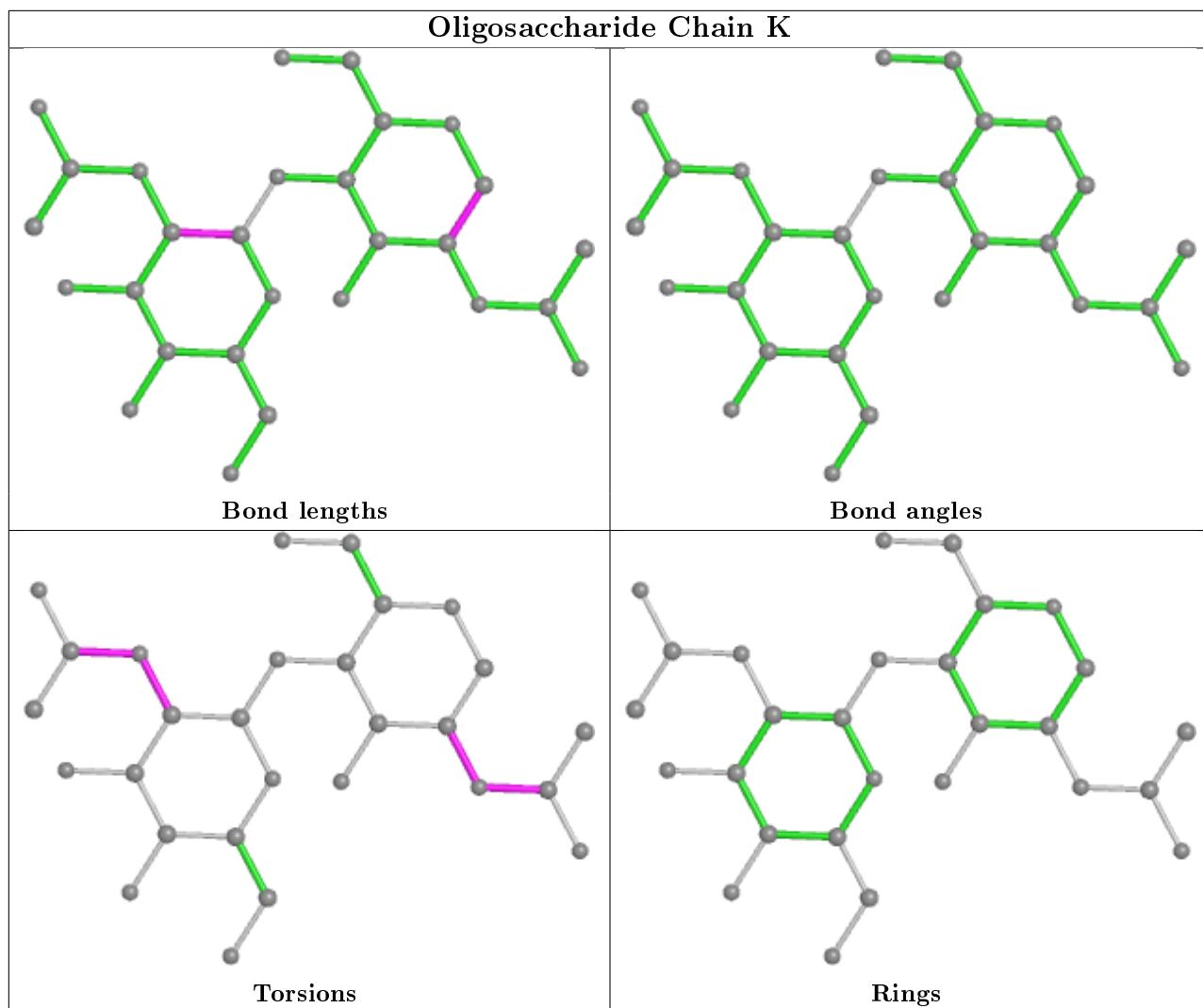
6 monomers are involved in 21 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | I     | 2   | NAG  | 4       | 0            |
| 3   | K     | 1   | NAG  | 7       | 0            |
| 3   | I     | 1   | NAG  | 7       | 0            |
| 3   | J     | 1   | NAG  | 7       | 0            |
| 3   | K     | 2   | NAG  | 4       | 0            |
| 3   | J     | 2   | NAG  | 4       | 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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | B     | 703 | 1    | 14,14,15     | 0.71 | 0        | 17,19,21    | 0.74 | 0        |
| 4   | NAG  | A     | 703 | 1    | 14,14,15     | 0.78 | 0        | 17,19,21    | 0.73 | 0        |
| 4   | NAG  | B     | 702 | 1    | 14,14,15     | 0.89 | 0        | 17,19,21    | 0.85 | 1 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | D     | 702 | 1    | 14,14,15     | 0.76 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 4   | NAG  | A     | 701 | 1    | 14,14,15     | 0.98 | 1 (7%)   | 17,19,21    | 0.59 | 0        |
| 4   | NAG  | D     | 701 | 1    | 14,14,15     | 0.74 | 0        | 17,19,21    | 0.48 | 0        |
| 4   | NAG  | B     | 701 | 1    | 14,14,15     | 0.94 | 1 (7%)   | 17,19,21    | 0.60 | 0        |
| 4   | NAG  | C     | 701 | 1    | 14,14,15     | 0.91 | 1 (7%)   | 17,19,21    | 0.61 | 0        |
| 4   | NAG  | A     | 702 | 1    | 14,14,15     | 1.03 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 4   | NAG  | C     | 702 | 1    | 14,14,15     | 0.86 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 4   | NAG  | D     | 703 | 1    | 14,14,15     | 0.67 | 0        | 17,19,21    | 0.68 | 0        |
| 4   | NAG  | C     | 703 | 1    | 14,14,15     | 0.76 | 0        | 17,19,21    | 0.74 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | B     | 703 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 703 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 702 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | D     | 702 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 701 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | D     | 701 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 701 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 701 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 702 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 702 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | D     | 703 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 703 | 1    | -       | 5/6/23/26 | 0/1/1/1 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | A     | 701 | NAG  | C1-C2 | 2.82 | 1.56        | 1.52     |
| 4   | B     | 701 | NAG  | C1-C2 | 2.68 | 1.56        | 1.52     |
| 4   | C     | 701 | NAG  | C1-C2 | 2.62 | 1.56        | 1.52     |
| 4   | A     | 702 | NAG  | C1-C2 | 2.24 | 1.55        | 1.52     |
| 4   | C     | 702 | NAG  | C1-C2 | 2.13 | 1.55        | 1.52     |
| 4   | D     | 702 | NAG  | C1-C2 | 2.01 | 1.55        | 1.52     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | B     | 702 | NAG  | C2-N2-C7 | -2.21 | 119.75      | 122.90   |
| 4   | C     | 702 | NAG  | C2-N2-C7 | -2.20 | 119.77      | 122.90   |
| 4   | D     | 702 | NAG  | C2-N2-C7 | -2.05 | 119.98      | 122.90   |
| 4   | A     | 702 | NAG  | C2-N2-C7 | -2.05 | 119.99      | 122.90   |

There are no chirality outliers.

All (51) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | B     | 703 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 703 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 703 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 703 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 702 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 702 | NAG  | O7-C7-N2-C2 |
| 4   | D     | 702 | NAG  | C8-C7-N2-C2 |
| 4   | D     | 702 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 701 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 701 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 701 | NAG  | O7-C7-N2-C2 |
| 4   | D     | 701 | NAG  | C8-C7-N2-C2 |
| 4   | D     | 701 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 701 | NAG  | C3-C2-N2-C7 |
| 4   | B     | 701 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 701 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 701 | NAG  | C3-C2-N2-C7 |
| 4   | C     | 701 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 701 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 702 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 702 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 702 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 702 | NAG  | O7-C7-N2-C2 |
| 4   | D     | 703 | NAG  | C3-C2-N2-C7 |
| 4   | D     | 703 | NAG  | C8-C7-N2-C2 |
| 4   | D     | 703 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 703 | NAG  | C8-C7-N2-C2 |
| 4   | C     | 703 | NAG  | O7-C7-N2-C2 |
| 4   | D     | 702 | NAG  | C4-C5-C6-O6 |
| 4   | D     | 702 | NAG  | O5-C5-C6-O6 |
| 4   | D     | 701 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 703 | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | C     | 703 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 703 | NAG  | C4-C5-C6-O6 |
| 4   | D     | 701 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 703 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 703 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 702 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 703 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 702 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 702 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 702 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 702 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 702 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 701 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 701 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 701 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 703 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 703 | NAG  | C3-C2-N2-C7 |
| 4   | D     | 701 | NAG  | C3-C2-N2-C7 |
| 4   | C     | 703 | NAG  | C3-C2-N2-C7 |

There are no ring outliers.

11 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | B     | 703 | NAG  | 1       | 0            |
| 4   | A     | 703 | NAG  | 1       | 0            |
| 4   | B     | 702 | NAG  | 1       | 0            |
| 4   | D     | 702 | NAG  | 1       | 0            |
| 4   | A     | 701 | NAG  | 1       | 0            |
| 4   | D     | 701 | NAG  | 1       | 0            |
| 4   | B     | 701 | NAG  | 1       | 0            |
| 4   | C     | 701 | NAG  | 1       | 0            |
| 4   | A     | 702 | NAG  | 1       | 0            |
| 4   | C     | 702 | NAG  | 1       | 0            |
| 4   | C     | 703 | NAG  | 1       | 0            |

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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     | 533/574 (92%)   | -0.25  | 2 (0%)   | 92  | 90                    | 63, 100, 139, 162  |
| 1   | B     | 533/574 (92%)   | -0.27  | 3 (0%)   | 89  | 86                    | 61, 96, 131, 178   |
| 1   | C     | 533/574 (92%)   | -0.12  | 6 (1%)   | 80  | 75                    | 72, 115, 153, 180  |
| 1   | D     | 533/574 (92%)   | 0.56   | 55 (10%) | 6   | 7                     | 75, 188, 282, 506  |
| 2   | E     | 177/243 (72%)   | -0.17  | 1 (0%)   | 89  | 86                    | 82, 120, 139, 154  |
| 2   | F     | 177/243 (72%)   | -0.42  | 0        | 100 | 100                   | 77, 95, 110, 122   |
| 2   | G     | 177/243 (72%)   | -0.14  | 2 (1%)   | 80  | 75                    | 78, 105, 130, 143  |
| 2   | H     | 177/243 (72%)   | 2.20   | 84 (47%) | 0   | 0                     | 146, 268, 426, 538 |
| All | All   | 2840/3268 (86%) | 0.08   | 153 (5%) | 25  | 23                    | 61, 112, 262, 538  |

All (153) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 260 | GLY  | 11.5 |
| 2   | H     | 263 | TYR  | 8.1  |
| 2   | H     | 164 | SER  | 7.6  |
| 2   | H     | 127 | VAL  | 6.8  |
| 1   | D     | 80  | PHE  | 6.8  |
| 1   | D     | 79  | GLN  | 6.7  |
| 2   | H     | 126 | LEU  | 6.6  |
| 2   | H     | 285 | VAL  | 6.3  |
| 2   | H     | 139 | LEU  | 5.9  |
| 2   | H     | 269 | LEU  | 5.9  |
| 1   | D     | 387 | ASP  | 5.8  |
| 1   | D     | 214 | GLY  | 5.8  |
| 2   | H     | 259 | SER  | 5.7  |
| 2   | H     | 85  | THR  | 5.6  |
| 2   | H     | 149 | GLY  | 5.5  |
| 2   | H     | 279 | ILE  | 5.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 250 | GLN  | 5.0  |
| 2   | H     | 261 | LEU  | 5.0  |
| 2   | H     | 288 | VAL  | 4.9  |
| 2   | H     | 254 | PHE  | 4.9  |
| 2   | H     | 196 | GLU  | 4.8  |
| 2   | H     | 129 | VAL  | 4.8  |
| 1   | D     | 272 | PRO  | 4.7  |
| 2   | H     | 264 | ASN  | 4.6  |
| 1   | D     | 201 | GLY  | 4.6  |
| 2   | H     | 141 | LEU  | 4.6  |
| 2   | H     | 160 | ALA  | 4.6  |
| 2   | H     | 232 | ARG  | 4.5  |
| 1   | D     | 398 | PHE  | 4.4  |
| 1   | D     | 279 | GLY  | 4.4  |
| 1   | D     | 53  | PRO  | 4.3  |
| 2   | H     | 276 | ASP  | 4.3  |
| 2   | H     | 245 | ILE  | 4.2  |
| 2   | H     | 249 | GLU  | 4.2  |
| 2   | H     | 268 | VAL  | 4.1  |
| 1   | D     | 270 | GLY  | 4.0  |
| 1   | D     | 113 | PHE  | 4.0  |
| 1   | D     | 158 | ILE  | 3.9  |
| 2   | H     | 148 | ILE  | 3.8  |
| 1   | D     | 402 | ASP  | 3.8  |
| 1   | D     | 496 | HIS  | 3.7  |
| 1   | D     | 69  | LEU  | 3.7  |
| 2   | H     | 111 | ASP  | 3.7  |
| 2   | H     | 108 | THR  | 3.7  |
| 2   | H     | 114 | ALA  | 3.7  |
| 2   | H     | 243 | ILE  | 3.7  |
| 2   | H     | 262 | TYR  | 3.7  |
| 2   | H     | 193 | PRO  | 3.7  |
| 2   | H     | 165 | ASN  | 3.6  |
| 2   | H     | 270 | ASN  | 3.6  |
| 1   | D     | 268 | PHE  | 3.5  |
| 2   | H     | 163 | GLU  | 3.5  |
| 2   | H     | 115 | ILE  | 3.4  |
| 2   | H     | 166 | ALA  | 3.4  |
| 1   | D     | 595 | TRP  | 3.4  |
| 2   | H     | 96  | ILE  | 3.4  |
| 1   | D     | 267 | PHE  | 3.4  |
| 1   | D     | 81  | LEU  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 238 | ASN  | 3.3  |
| 2   | H     | 194 | VAL  | 3.3  |
| 1   | D     | 139 | LEU  | 3.2  |
| 2   | H     | 122 | LYS  | 3.2  |
| 1   | D     | 65  | ILE  | 3.2  |
| 2   | H     | 176 | VAL  | 3.1  |
| 2   | H     | 140 | GLU  | 3.1  |
| 1   | D     | 404 | MET  | 3.0  |
| 2   | H     | 110 | ALA  | 3.0  |
| 2   | H     | 177 | ARG  | 3.0  |
| 2   | H     | 98  | TYR  | 3.0  |
| 2   | H     | 266 | LEU  | 3.0  |
| 2   | H     | 150 | VAL  | 3.0  |
| 2   | G     | 94  | GLY  | 3.0  |
| 2   | H     | 121 | GLN  | 3.0  |
| 1   | D     | 594 | ALA  | 2.9  |
| 2   | H     | 95  | GLN  | 2.9  |
| 1   | D     | 66  | LYS  | 2.9  |
| 1   | D     | 271 | ASP  | 2.9  |
| 1   | D     | 247 | GLY  | 2.8  |
| 2   | H     | 283 | GLY  | 2.8  |
| 2   | H     | 131 | SER  | 2.8  |
| 1   | D     | 248 | ASN  | 2.8  |
| 1   | D     | 213 | ASP  | 2.8  |
| 2   | H     | 183 | GLY  | 2.8  |
| 2   | H     | 86  | THR  | 2.8  |
| 2   | H     | 198 | TYR  | 2.8  |
| 1   | D     | 262 | SER  | 2.8  |
| 1   | A     | 592 | GLU  | 2.8  |
| 1   | D     | 157 | ASN  | 2.8  |
| 2   | H     | 89  | PHE  | 2.7  |
| 2   | H     | 88  | ILE  | 2.7  |
| 1   | D     | 64  | GLY  | 2.7  |
| 2   | G     | 285 | VAL  | 2.7  |
| 1   | D     | 537 | MET  | 2.7  |
| 2   | H     | 286 | ARG  | 2.7  |
| 1   | C     | 201 | GLY  | 2.7  |
| 1   | C     | 187 | ARG  | 2.7  |
| 2   | H     | 195 | ILE  | 2.7  |
| 1   | D     | 196 | MET  | 2.7  |
| 1   | D     | 256 | GLN  | 2.6  |
| 1   | B     | 187 | ARG  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 188 | ASP  | 2.6  |
| 1   | D     | 95  | PHE  | 2.6  |
| 1   | B     | 188 | ASP  | 2.6  |
| 1   | D     | 365 | GLN  | 2.6  |
| 2   | H     | 159 | ILE  | 2.6  |
| 1   | D     | 244 | ALA  | 2.6  |
| 2   | H     | 130 | ASP  | 2.6  |
| 1   | D     | 68  | GLU  | 2.6  |
| 1   | D     | 138 | ASN  | 2.6  |
| 2   | E     | 83  | ALA  | 2.6  |
| 1   | D     | 67  | LYS  | 2.6  |
| 2   | H     | 237 | PHE  | 2.6  |
| 1   | D     | 219 | SER  | 2.6  |
| 1   | C     | 189 | SER  | 2.6  |
| 2   | H     | 142 | HIS  | 2.6  |
| 1   | D     | 284 | GLY  | 2.6  |
| 2   | H     | 151 | LYS  | 2.5  |
| 2   | H     | 235 | THR  | 2.5  |
| 1   | C     | 107 | ILE  | 2.5  |
| 2   | H     | 182 | GLY  | 2.5  |
| 1   | D     | 187 | ARG  | 2.5  |
| 2   | H     | 116 | GLY  | 2.5  |
| 2   | H     | 181 | SER  | 2.5  |
| 2   | H     | 244 | ILE  | 2.4  |
| 2   | H     | 287 | LEU  | 2.4  |
| 1   | D     | 240 | THR  | 2.4  |
| 1   | D     | 207 | GLY  | 2.4  |
| 1   | D     | 112 | GLN  | 2.4  |
| 1   | D     | 265 | ILE  | 2.4  |
| 2   | H     | 192 | TRP  | 2.3  |
| 2   | H     | 278 | ASN  | 2.3  |
| 1   | A     | 424 | ASP  | 2.3  |
| 1   | D     | 596 | THR  | 2.3  |
| 2   | H     | 200 | ALA  | 2.3  |
| 1   | D     | 425 | GLY  | 2.3  |
| 1   | D     | 200 | HIS  | 2.2  |
| 1   | D     | 215 | SER  | 2.2  |
| 1   | D     | 568 | LYS  | 2.2  |
| 2   | H     | 197 | ARG  | 2.2  |
| 2   | H     | 93  | GLY  | 2.2  |
| 2   | H     | 239 | SER  | 2.2  |
| 2   | H     | 94  | GLY  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 283 | GLY  | 2.2  |
| 2   | H     | 258 | LEU  | 2.2  |
| 2   | H     | 199 | PRO  | 2.1  |
| 2   | H     | 133 | SER  | 2.1  |
| 1   | C     | 61  | LYS  | 2.1  |
| 1   | D     | 281 | GLY  | 2.1  |
| 2   | H     | 152 | PHE  | 2.1  |
| 1   | D     | 280 | SER  | 2.1  |
| 2   | H     | 277 | ALA  | 2.0  |
| 2   | H     | 92  | GLY  | 2.0  |
| 1   | B     | 634 | HIS  | 2.0  |

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

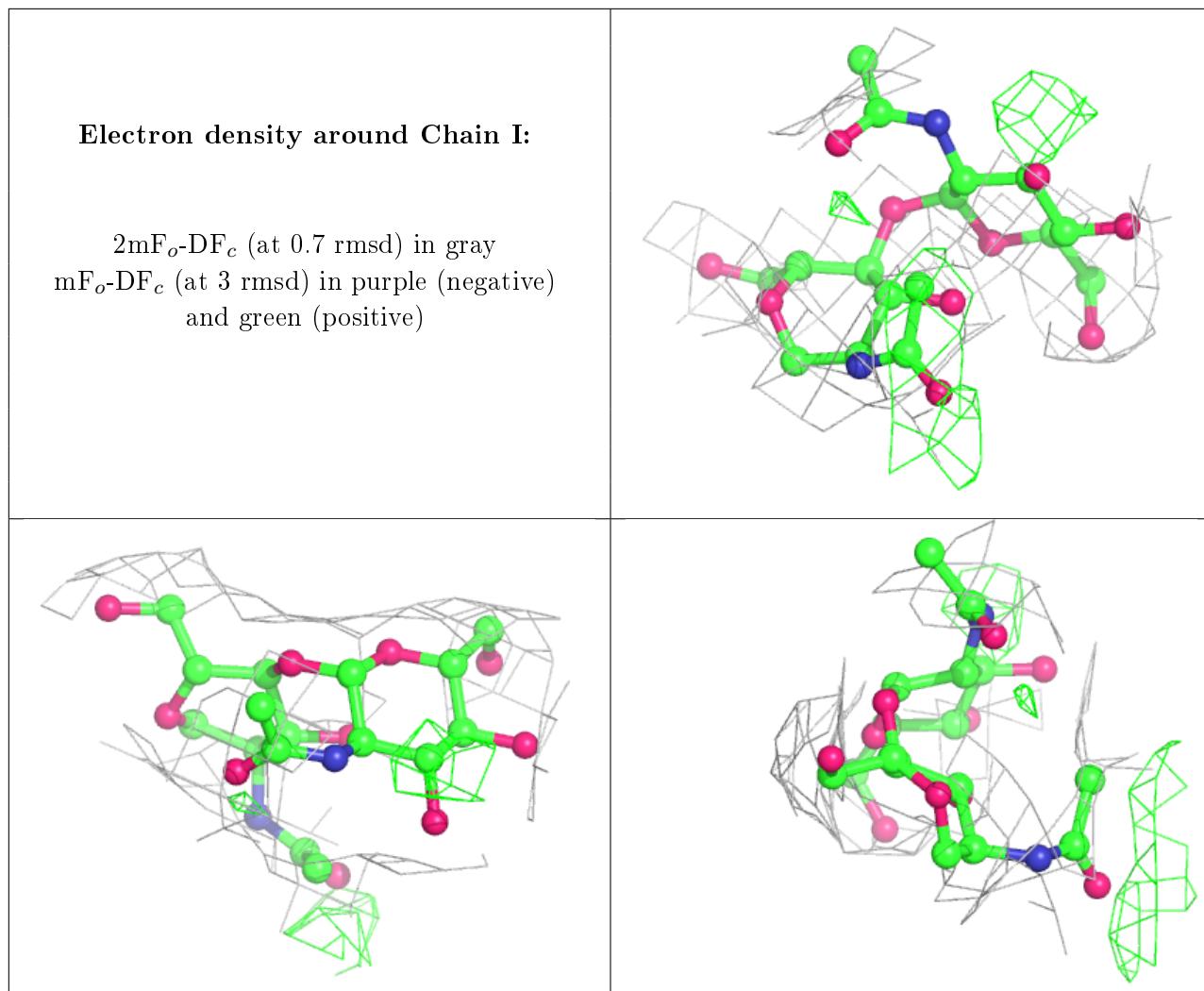
There are no non-standard protein/DNA/RNA residues in this entry.

## 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.

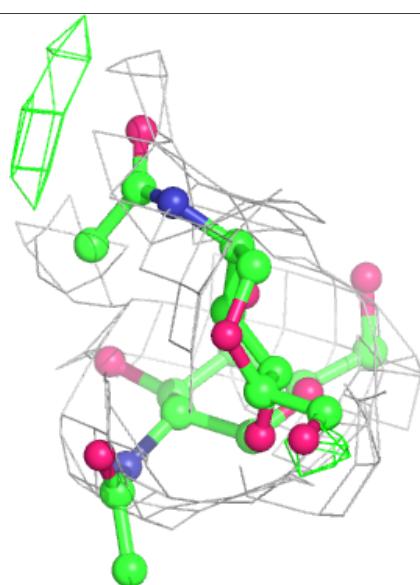
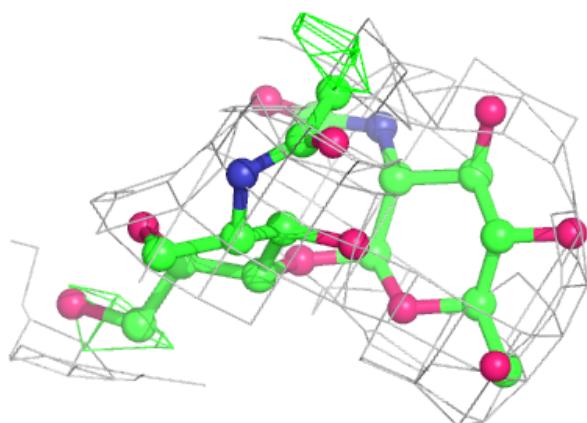
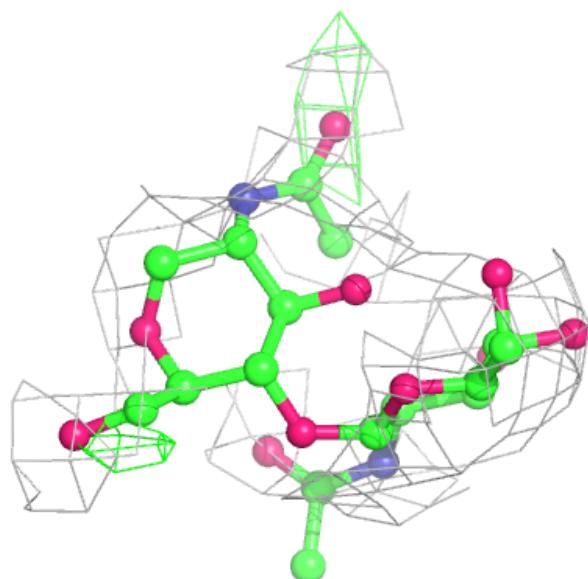
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | NAG  | K     | 1   | 14/15 | 0.69 | 0.28 | 127,133,136,142            | 0     |
| 3   | NAG  | I     | 1   | 14/15 | 0.69 | 0.20 | 146,152,154,157            | 0     |
| 3   | NAG  | J     | 1   | 14/15 | 0.70 | 0.22 | 122,130,133,141            | 0     |
| 3   | NAG  | K     | 2   | 14/15 | 0.83 | 0.30 | 154,158,159,159            | 0     |
| 3   | NAG  | I     | 2   | 14/15 | 0.86 | 0.17 | 146,150,151,152            | 0     |
| 3   | NAG  | J     | 2   | 14/15 | 0.91 | 0.23 | 172,174,177,178            | 0     |

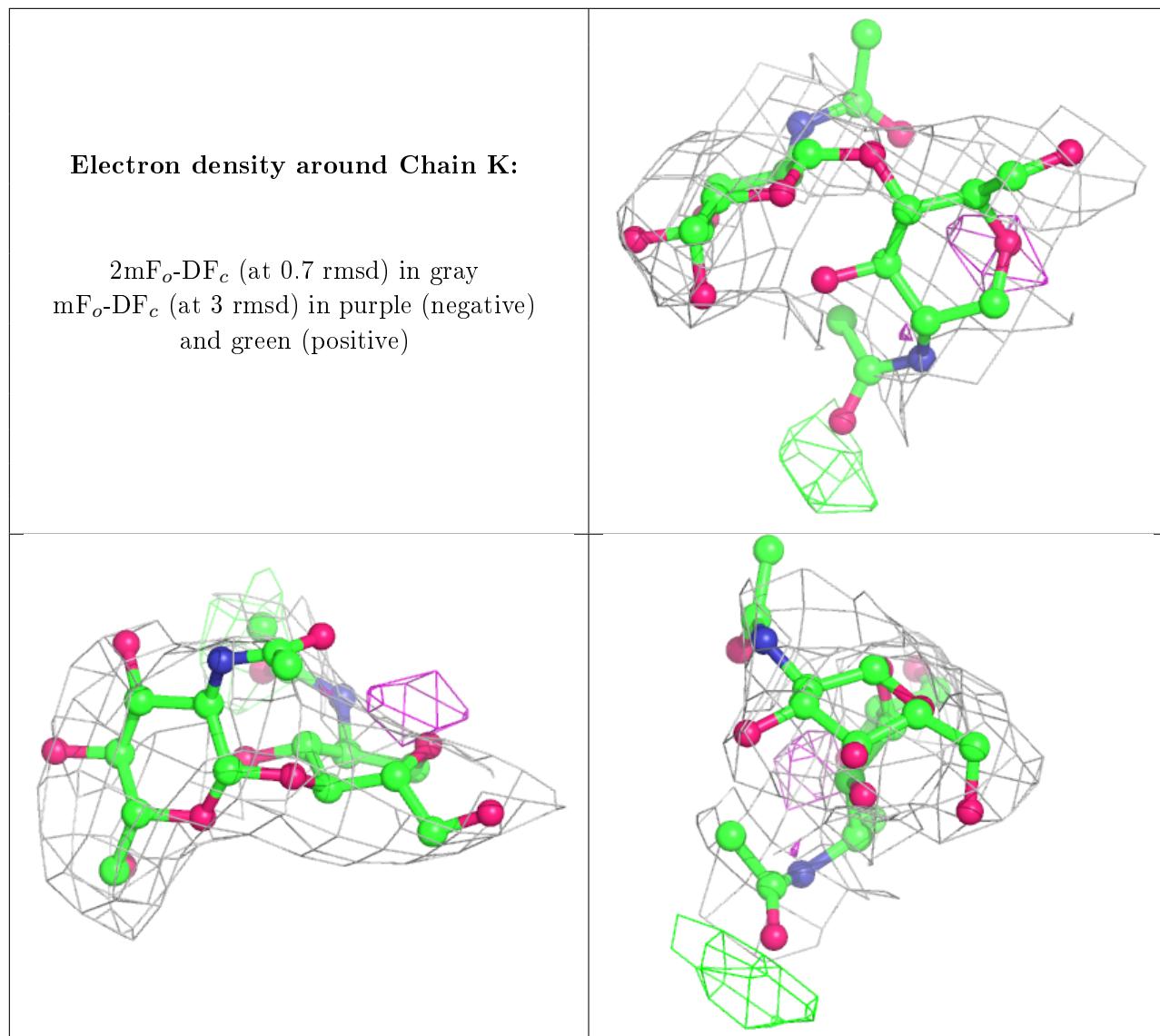
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain J:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (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 |
|-----|------|-------|-----|-------|-------|------|----------------------------|-------|
| 4   | NAG  | C     | 703 | 14/15 | -0.02 | 0.84 | 218,222,222,222            | 0     |
| 4   | NAG  | D     | 703 | 14/15 | 0.30  | 0.45 | 251,251,251,251            | 0     |
| 4   | NAG  | D     | 702 | 14/15 | 0.38  | 0.81 | 205,205,205,205            | 0     |
| 4   | NAG  | D     | 701 | 14/15 | 0.40  | 0.44 | 219,219,219,219            | 0     |
| 4   | NAG  | B     | 701 | 14/15 | 0.44  | 0.40 | 184,187,191,192            | 0     |
| 4   | NAG  | C     | 701 | 14/15 | 0.46  | 0.25 | 216,218,219,219            | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | NAG  | A     | 703 | 14/15 | 0.50 | 0.36 | 218,222,225,225            | 0     |
| 4   | NAG  | B     | 703 | 14/15 | 0.57 | 0.38 | 236,240,241,242            | 0     |
| 4   | NAG  | B     | 702 | 14/15 | 0.59 | 0.28 | 136,138,139,140            | 0     |
| 4   | NAG  | A     | 701 | 14/15 | 0.67 | 0.29 | 152,155,156,157            | 0     |
| 5   | CA   | G     | 402 | 1/1   | 0.69 | 0.29 | 111,111,111,111            | 0     |
| 4   | NAG  | A     | 702 | 14/15 | 0.72 | 0.25 | 145,147,148,148            | 0     |
| 4   | NAG  | C     | 702 | 14/15 | 0.74 | 0.51 | 186,187,189,189            | 0     |
| 5   | CA   | F     | 402 | 1/1   | 0.85 | 0.27 | 96,96,96,96                | 0     |
| 5   | CA   | E     | 402 | 1/1   | 0.90 | 0.31 | 96,96,96,96                | 0     |
| 5   | CA   | F     | 401 | 1/1   | 0.95 | 0.20 | 76,76,76,76                | 0     |
| 5   | CA   | E     | 401 | 1/1   | 0.97 | 0.23 | 89,89,89,89                | 0     |
| 5   | CA   | G     | 401 | 1/1   | 0.99 | 0.16 | 79,79,79,79                | 0     |

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.