



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:31 am GMT

PDB ID : 4JTX  
Title : Crystal structure of 2009 pandemic influenza virus hemagglutinin mutant D225E  
Authors : Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.  
Deposited on : 2013-03-24  
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

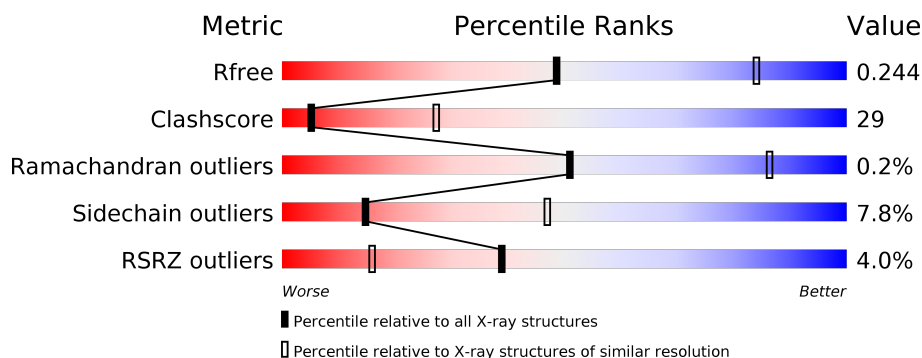
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1692 (3.00-3.00)                                      |
| Clashscore            | 112137                      | 2037 (3.00-3.00)                                      |
| Ramachandran outliers | 110173                      | 1973 (3.00-3.00)                                      |
| Sidechain outliers    | 110143                      | 1976 (3.00-3.00)                                      |
| RSRZ outliers         | 101464                      | 1716 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                                 |
|-----|-------|--------|--|
| 1   | A     | 323    | <div> <div>3%</div> <div>55% 38% 7%</div> </div> |
| 1   | C     | 323    | <div> <div>3%</div> <div>55% 39% 5%</div> </div> |
| 1   | E     | 323    | <div> <div>3%</div> <div>51% 43% 5%</div> </div> |
| 1   | G     | 323    | <div> <div>3%</div> <div>55% 40%</div> </div>    |
| 1   | I     | 323    | <div> <div>3%</div> <div>55% 39% 5%</div> </div> |
| 1   | K     | 323    | <div> <div>3%</div> <div>52% 42% 5%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B     | 166    |                  |
| 2   | D     | 166    |                  |
| 2   | F     | 166    |                  |
| 2   | H     | 166    |                  |
| 2   | J     | 166    |                  |
| 2   | L     | 166    |                  |

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  | K     | 601 | -         | -        | X       | X                |
| 4   | NAG  | I     | 601 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23277 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 323      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2525  | 1597 | 438 | 479 | 11 |         |         |       |
| 1   | C     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2517  | 1592 | 434 | 480 | 11 |         |         |       |
| 1   | E     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2510  | 1587 | 433 | 479 | 11 |         |         |       |
| 1   | G     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2513  | 1590 | 434 | 478 | 11 |         |         |       |
| 1   | I     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2517  | 1592 | 434 | 480 | 11 |         |         |       |
| 1   | K     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2517  | 1592 | 434 | 480 | 11 |         |         |       |

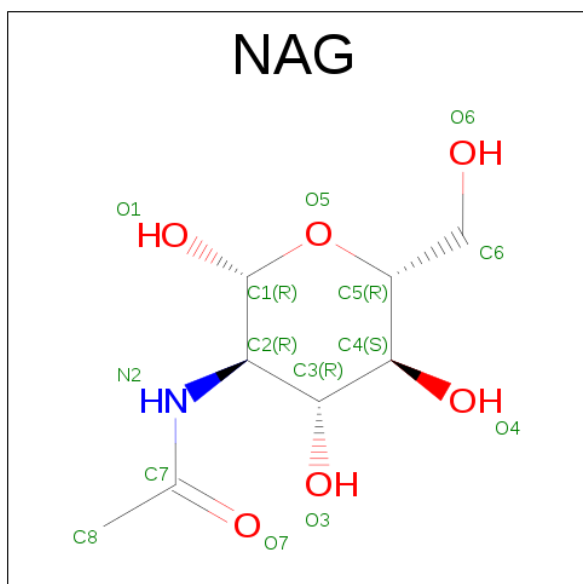
There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 6       | ARG      | -      | EXPRESSION TAG      | UNP C3W5S1 |
| A     | 228     | GLU      | ASP    | ENGINEERED MUTATION | UNP C3W5S1 |
| C     | 6       | ARG      | -      | EXPRESSION TAG      | UNP C3W5S1 |
| C     | 228     | GLU      | ASP    | ENGINEERED MUTATION | UNP C3W5S1 |
| E     | 6       | ARG      | -      | EXPRESSION TAG      | UNP C3W5S1 |
| E     | 228     | GLU      | ASP    | ENGINEERED MUTATION | UNP C3W5S1 |
| G     | 6       | ARG      | -      | EXPRESSION TAG      | UNP C3W5S1 |
| G     | 228     | GLU      | ASP    | ENGINEERED MUTATION | UNP C3W5S1 |
| I     | 6       | ARG      | -      | EXPRESSION TAG      | UNP C3W5S1 |
| I     | 228     | GLU      | ASP    | ENGINEERED MUTATION | UNP C3W5S1 |
| K     | 6       | ARG      | -      | EXPRESSION TAG      | UNP C3W5S1 |
| K     | 228     | GLU      | ASP    | ENGINEERED MUTATION | UNP C3W5S1 |

- Molecule 2 is a protein called Hemagglutinin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1305  | 822 | 220 | 257 | 6 |         |         |       |
| 2   | D     | 164      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1315  | 826 | 221 | 262 | 6 |         |         |       |
| 2   | F     | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1302  | 821 | 219 | 256 | 6 |         |         |       |
| 2   | H     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1305  | 822 | 220 | 257 | 6 |         |         |       |
| 2   | J     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1334  | 838 | 224 | 266 | 6 |         |         |       |
| 2   | L     | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1302  | 821 | 219 | 256 | 6 |         |         |       |

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 4   | A     | 2        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 28    | 16 | 2 | 10 |         |         |
| 4   | C     | 2        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 28    | 16 | 2 | 10 |         |         |
| 4   | I     | 2        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 28    | 16 | 2 | 10 |         |         |

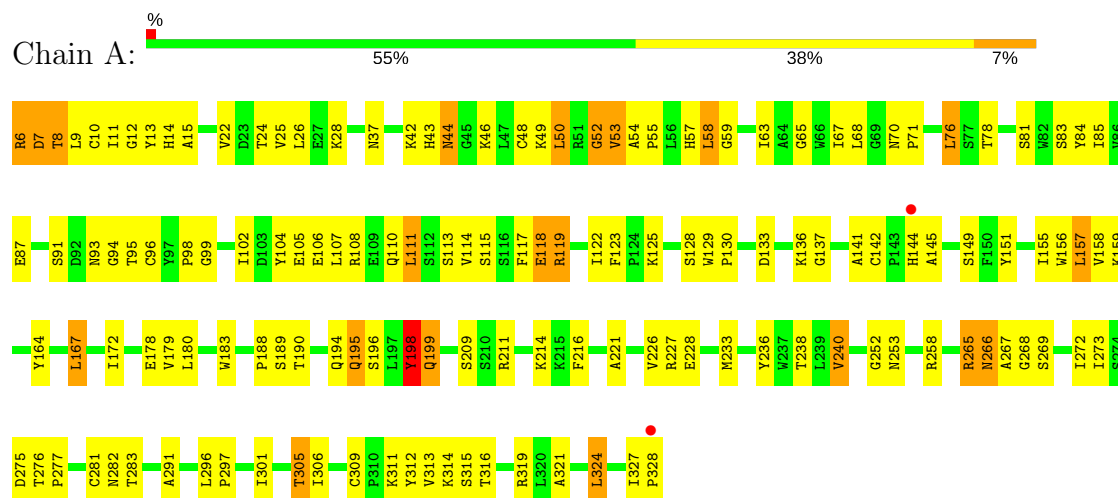
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 5   | B     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 5   | C     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 5   | D     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 5   | E     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 5   | F     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 5   | G     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 5   | H     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 5   | I     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 5   | J     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 5   | K     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 5   | L     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |

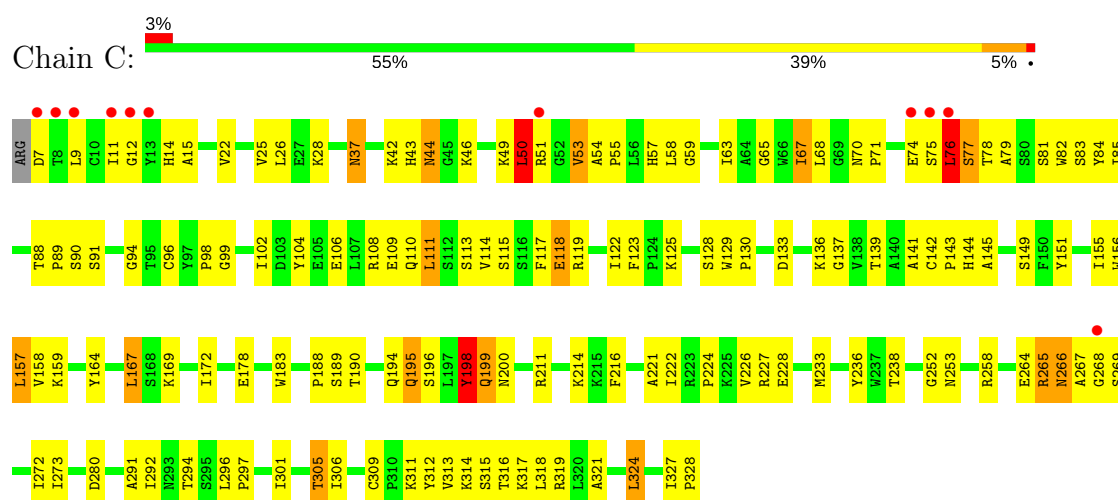
### 3 Residue-property plots

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

#### • Molecule 1: Hemagglutinin

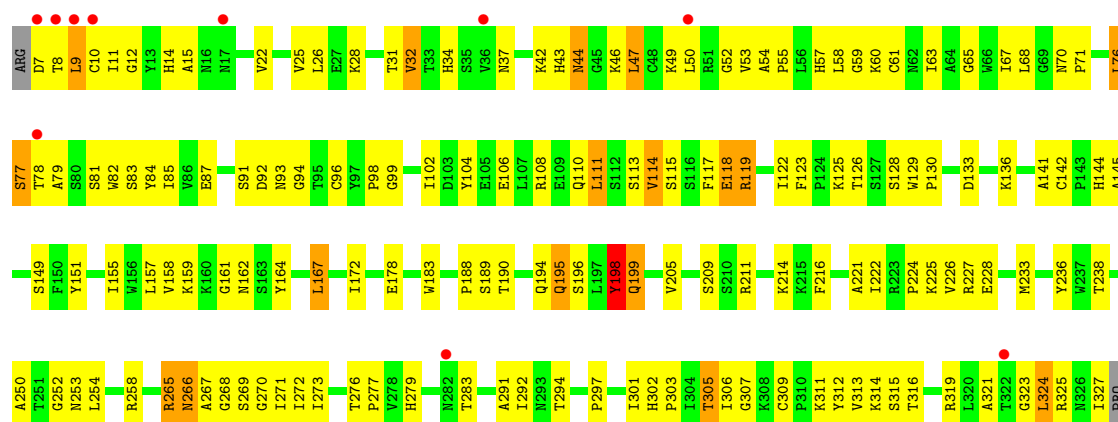


#### • Molecule 1: Hemagglutinin

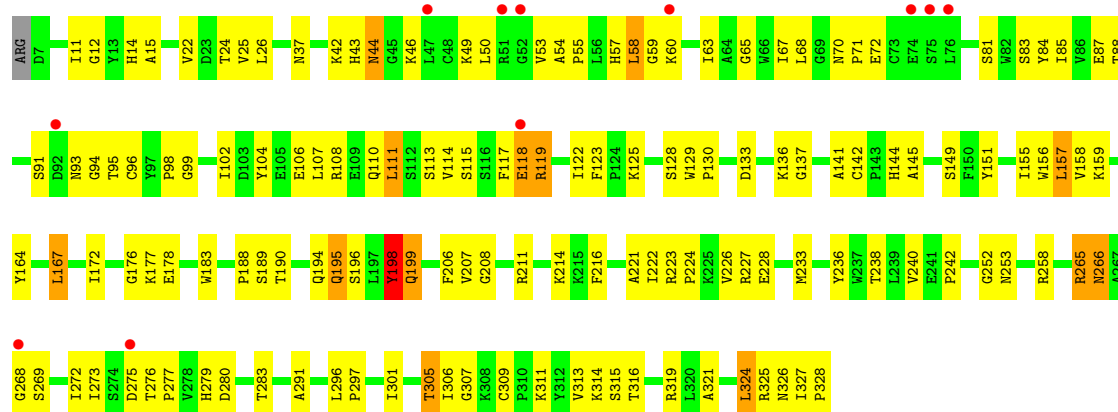


#### • Molecule 1: Hemagglutinin

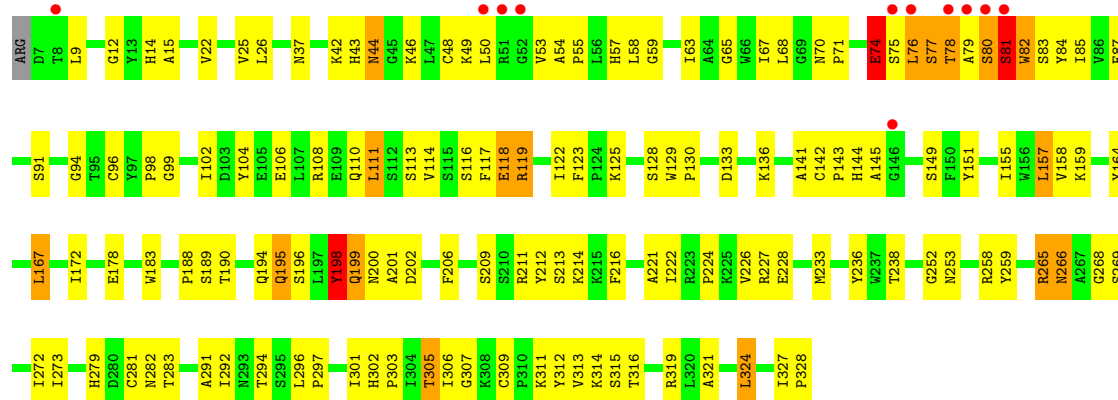




• Molecule 1: Hemagglutinin



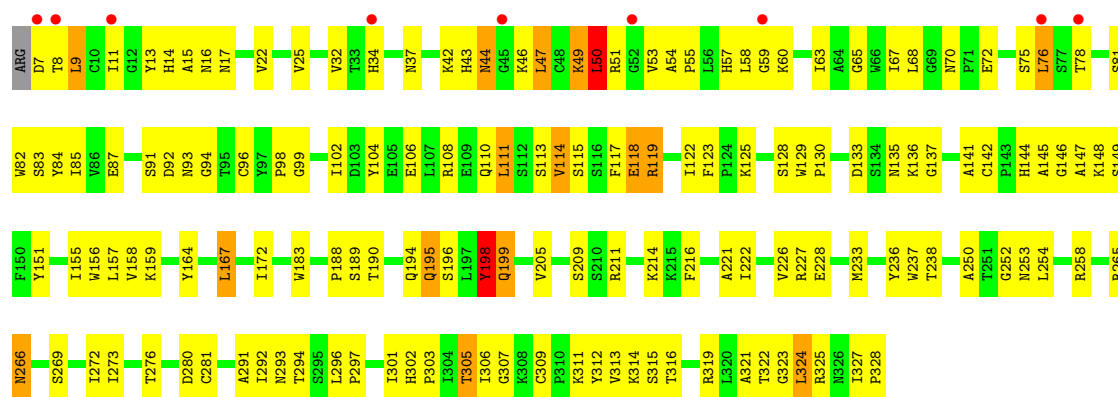
• Molecule 1: Hemagglutinin



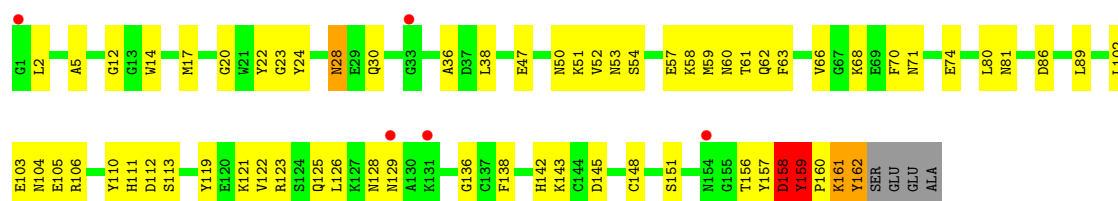
• Molecule 1: Hemagglutinin



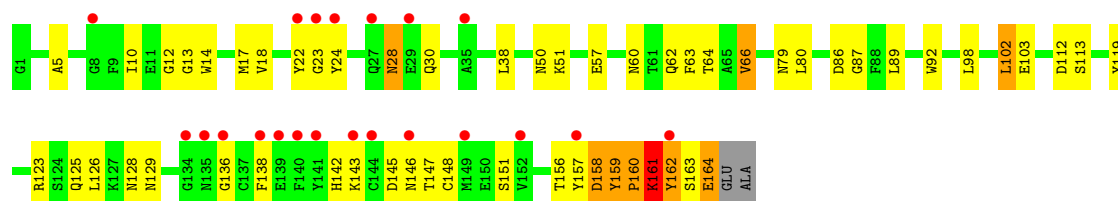




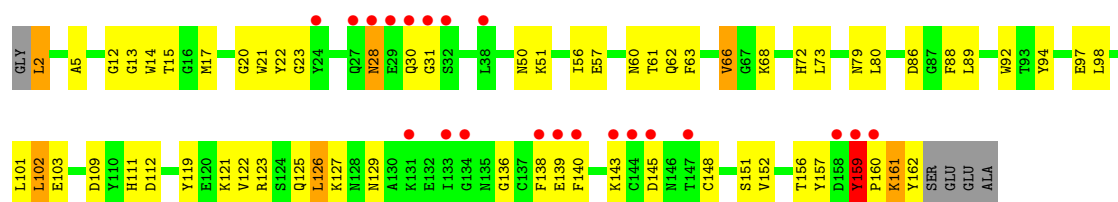
• Molecule 2: Hemagglutinin



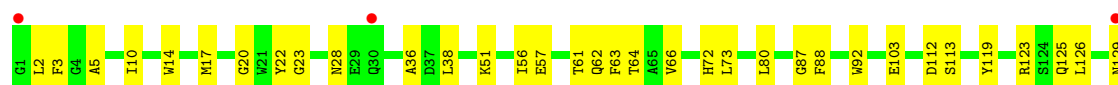
• Molecule 2: Hemagglutinin

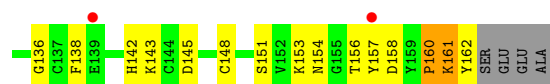


• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin

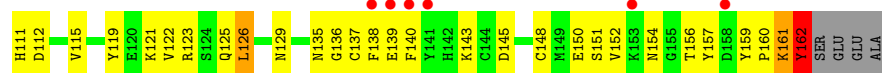




• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 67.69Å 119.01Å 123.61Å<br>115.14° 94.96° 96.78°             | Depositor        |
| Resolution (Å)  | 46.75 – 3.00<br>46.75 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.1 (46.75-3.00)<br>79.9 (46.75-3.00)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.08 (at 3.01Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.5_2)                               | Depositor        |
| R, $R_{free}$   | 0.210 , 0.243<br>0.212 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3273 reflections (5.09%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 54.4  | Xtriage          |
| Anisotropy  | 0.524   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 44.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | 0.004 for -h,-l,-k  | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 23277   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.27         | 0/2589      | 0.70        | 8/3517 (0.2%)   |
| 1   | C     | 0.27         | 0/2581      | 0.70        | 13/3506 (0.4%)  |
| 1   | E     | 0.25         | 0/2573      | 0.63        | 9/3494 (0.3%)   |
| 1   | G     | 0.25         | 0/2577      | 0.66        | 5/3501 (0.1%)   |
| 1   | I     | 0.29         | 0/2581      | 0.69        | 11/3506 (0.3%)  |
| 1   | K     | 0.26         | 0/2581      | 0.66        | 8/3506 (0.2%)   |
| 2   | B     | 0.25         | 0/1333      | 0.54        | 3/1797 (0.2%)   |
| 2   | D     | 0.24         | 0/1343      | 0.45        | 0/1811          |
| 2   | F     | 0.24         | 0/1330      | 0.49        | 1/1794 (0.1%)   |
| 2   | H     | 0.24         | 0/1333      | 0.48        | 1/1797 (0.1%)   |
| 2   | J     | 0.32         | 0/1362      | 0.58        | 3/1836 (0.2%)   |
| 2   | L     | 0.24         | 0/1330      | 0.53        | 1/1794 (0.1%)   |
| All | All   | 0.26         | 0/23513     | 0.62        | 63/31859 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | I     | 0                   | 1                   |

There are no bond length outliers.

All (63) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | G     | 119 | ARG  | NE-CZ-NH1 | -15.90 | 112.35      | 120.30   |
| 1   | A     | 119 | ARG  | NE-CZ-NH1 | -15.77 | 112.41      | 120.30   |
| 1   | G     | 119 | ARG  | NE-CZ-NH2 | 15.37  | 127.99      | 120.30   |
| 1   | A     | 119 | ARG  | NE-CZ-NH2 | 15.17  | 127.88      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | I     | 76  | LEU  | CB-CA-C   | -13.19 | 85.14       | 110.20   |
| 1   | C     | 78  | THR  | N-CA-CB   | -11.75 | 87.97       | 110.30   |
| 2   | J     | 162 | TYR  | N-CA-CB   | -10.98 | 90.83       | 110.60   |
| 1   | C     | 76  | LEU  | N-CA-CB   | -9.78  | 90.84       | 110.40   |
| 1   | C     | 50  | LEU  | N-CA-C    | 9.74   | 137.29      | 111.00   |
| 1   | K     | 76  | LEU  | N-CA-C    | 9.66   | 137.09      | 111.00   |
| 1   | I     | 76  | LEU  | N-CA-C    | 9.59   | 136.89      | 111.00   |
| 1   | C     | 79  | ALA  | CB-CA-C   | -8.74  | 96.99       | 110.10   |
| 1   | K     | 50  | LEU  | CB-CA-C   | -8.58  | 93.91       | 110.20   |
| 1   | A     | 52  | GLY  | N-CA-C    | -8.56  | 91.69       | 113.10   |
| 1   | E     | 76  | LEU  | N-CA-C    | 8.56   | 134.10      | 111.00   |
| 1   | E     | 119 | ARG  | NE-CZ-NH2 | -8.42  | 116.09      | 120.30   |
| 1   | I     | 75  | SER  | N-CA-CB   | -8.42  | 97.87       | 110.50   |
| 1   | C     | 119 | ARG  | NE-CZ-NH2 | -8.14  | 116.23      | 120.30   |
| 1   | I     | 119 | ARG  | NE-CZ-NH2 | -8.05  | 116.28      | 120.30   |
| 1   | C     | 119 | ARG  | NE-CZ-NH1 | 7.85   | 124.23      | 120.30   |
| 1   | K     | 199 | GLN  | N-CA-CB   | -7.79  | 96.59       | 110.60   |
| 1   | A     | 119 | ARG  | CD-NE-CZ  | 7.77   | 134.48      | 123.60   |
| 1   | G     | 119 | ARG  | CD-NE-CZ  | 7.76   | 134.46      | 123.60   |
| 1   | I     | 199 | GLN  | N-CA-CB   | -7.75  | 96.65       | 110.60   |
| 1   | E     | 199 | GLN  | N-CA-CB   | -7.72  | 96.71       | 110.60   |
| 1   | C     | 199 | GLN  | N-CA-CB   | -7.69  | 96.77       | 110.60   |
| 1   | A     | 199 | GLN  | N-CA-CB   | -7.68  | 96.78       | 110.60   |
| 1   | E     | 119 | ARG  | NE-CZ-NH1 | 7.66   | 124.13      | 120.30   |
| 1   | K     | 51  | ARG  | N-CA-C    | -7.64  | 90.38       | 111.00   |
| 1   | K     | 119 | ARG  | NE-CZ-NH2 | -7.56  | 116.52      | 120.30   |
| 1   | I     | 119 | ARG  | NE-CZ-NH1 | 7.55   | 124.07      | 120.30   |
| 1   | K     | 50  | LEU  | N-CA-C    | 7.54   | 131.36      | 111.00   |
| 1   | E     | 198 | TYR  | N-CA-C    | -7.51  | 90.72       | 111.00   |
| 1   | G     | 199 | GLN  | N-CA-CB   | -7.48  | 97.14       | 110.60   |
| 1   | I     | 198 | TYR  | N-CA-C    | -7.47  | 90.82       | 111.00   |
| 1   | K     | 198 | TYR  | N-CA-C    | -7.45  | 90.89       | 111.00   |
| 1   | C     | 198 | TYR  | N-CA-C    | -7.41  | 90.99       | 111.00   |
| 1   | A     | 198 | TYR  | N-CA-C    | -7.33  | 91.22       | 111.00   |
| 1   | K     | 119 | ARG  | NE-CZ-NH1 | 7.30   | 123.95      | 120.30   |
| 2   | J     | 164 | GLU  | N-CA-C    | -7.26  | 91.40       | 111.00   |
| 1   | C     | 51  | ARG  | N-CA-C    | -7.20  | 91.56       | 111.00   |
| 2   | B     | 158 | ASP  | CB-CA-C   | -7.16  | 96.09       | 110.40   |
| 1   | G     | 198 | TYR  | N-CA-C    | -7.01  | 92.07       | 111.00   |
| 1   | C     | 77  | SER  | N-CA-C    | -6.97  | 92.17       | 111.00   |
| 1   | I     | 82  | TRP  | N-CA-CB   | -6.95  | 98.09       | 110.60   |
| 1   | C     | 50  | LEU  | CB-CA-C   | -6.79  | 97.29       | 110.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 159 | TYR  | N-CA-CB    | -6.43 | 99.03       | 110.60   |
| 1   | I     | 76  | LEU  | N-CA-CB    | -6.42 | 97.56       | 110.40   |
| 2   | L     | 162 | TYR  | N-CA-C     | -6.17 | 94.33       | 111.00   |
| 1   | A     | 76  | LEU  | N-CA-C     | 5.85  | 126.80      | 111.00   |
| 1   | A     | 53  | VAL  | N-CA-C     | 5.79  | 126.62      | 111.00   |
| 1   | E     | 76  | LEU  | CB-CA-C    | -5.75 | 99.28       | 110.20   |
| 1   | I     | 75  | SER  | N-CA-C     | 5.64  | 126.22      | 111.00   |
| 1   | C     | 77  | SER  | CB-CA-C    | -5.56 | 99.53       | 110.10   |
| 1   | I     | 74  | GLU  | N-CA-C     | 5.54  | 125.96      | 111.00   |
| 1   | E     | 52  | GLY  | N-CA-C     | -5.47 | 99.41       | 113.10   |
| 2   | H     | 66  | VAL  | CB-CA-C    | -5.33 | 101.28      | 111.40   |
| 1   | E     | 77  | SER  | N-CA-CB    | 5.26  | 118.39      | 110.50   |
| 1   | C     | 78  | THR  | N-CA-C     | 5.24  | 125.15      | 111.00   |
| 2   | B     | 66  | VAL  | CB-CA-C    | -5.21 | 101.51      | 111.40   |
| 2   | F     | 159 | TYR  | N-CA-CB    | -5.17 | 101.29      | 110.60   |
| 2   | J     | 158 | ASP  | CB-CA-C    | -5.05 | 100.30      | 110.40   |
| 1   | E     | 32  | VAL  | CG1-CB-CG2 | 5.04  | 118.96      | 110.90   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | I     | 81  | SER  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2525  | 0        | 2471     | 157     | 0            |
| 1   | C     | 2517  | 0        | 2457     | 145     | 4            |
| 1   | E     | 2510  | 0        | 2452     | 181     | 5            |
| 1   | G     | 2513  | 0        | 2456     | 161     | 0            |
| 1   | I     | 2517  | 0        | 2458     | 158     | 0            |
| 1   | K     | 2517  | 0        | 2459     | 211     | 0            |
| 2   | B     | 1305  | 0        | 1228     | 105     | 0            |
| 2   | D     | 1315  | 0        | 1227     | 77      | 0            |
| 2   | F     | 1302  | 0        | 1226     | 97      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | H     | 1305  | 0        | 1228     | 44      | 0            |
| 2   | J     | 1334  | 0        | 1250     | 75      | 0            |
| 2   | L     | 1302  | 0        | 1226     | 96      | 0            |
| 3   | A     | 14    | 0        | 13       | 0       | 0            |
| 3   | C     | 14    | 0        | 13       | 0       | 0            |
| 3   | E     | 14    | 0        | 13       | 0       | 0            |
| 3   | G     | 14    | 0        | 13       | 0       | 0            |
| 3   | I     | 14    | 0        | 13       | 0       | 0            |
| 3   | K     | 14    | 0        | 13       | 9       | 0            |
| 4   | A     | 28    | 0        | 25       | 6       | 0            |
| 4   | C     | 28    | 0        | 25       | 4       | 0            |
| 4   | I     | 28    | 0        | 25       | 7       | 0            |
| 5   | A     | 18    | 0        | 0        | 23      | 0            |
| 5   | B     | 10    | 0        | 0        | 28      | 0            |
| 5   | C     | 16    | 0        | 0        | 33      | 0            |
| 5   | D     | 9     | 0        | 0        | 26      | 0            |
| 5   | E     | 14    | 0        | 0        | 37      | 0            |
| 5   | F     | 11    | 0        | 0        | 24      | 0            |
| 5   | G     | 14    | 0        | 0        | 46      | 0            |
| 5   | H     | 5     | 0        | 0        | 6       | 0            |
| 5   | I     | 11    | 0        | 0        | 15      | 1            |
| 5   | J     | 9     | 0        | 0        | 16      | 0            |
| 5   | K     | 21    | 0        | 0        | 65      | 0            |
| 5   | L     | 9     | 0        | 0        | 21      | 0            |
| All | All   | 23277 | 0        | 22291    | 1339    | 5            |

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 29.

All (1339) 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:B:145:ASP:HB2 | 5:B:204:HOH:O   | 1.29                     | 1.28              |
| 1:C:227:ARG:HD3 | 5:C:714:HOH:O   | 1.12                     | 1.27              |
| 1:K:238:THR:HB  | 5:K:718:HOH:O   | 1.10                     | 1.25              |
| 1:A:178:GLU:HA  | 5:A:713:HOH:O   | 1.10                     | 1.25              |
| 2:D:160:PRO:O   | 2:D:161:LYS:HG2 | 1.35                     | 1.24              |
| 1:G:242:PRO:HG3 | 5:G:708:HOH:O   | 1.34                     | 1.23              |
| 1:K:49:LYS:NZ   | 1:K:280:ASP:OD1 | 1.71                     | 1.21              |
| 2:F:15:THR:HG23 | 5:F:209:HOH:O   | 1.36                     | 1.20              |
| 2:L:137:CYS:SG  | 5:L:207:HOH:O   | 1.96                     | 1.19              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:74:GLU:HG2   | 1:I:74:GLU:O    | 1.39                     | 1.19              |
| 1:I:81:SER:O     | 1:I:82:TRP:CE3  | 1.96                     | 1.16              |
| 1:E:61:CYS:HA    | 5:E:711:HOH:O   | 1.45                     | 1.16              |
| 1:I:78:THR:HG23  | 1:I:79:ALA:N    | 1.62                     | 1.15              |
| 1:G:279:HIS:HB3  | 5:G:710:HOH:O   | 1.45                     | 1.14              |
| 1:K:309:CYS:SG   | 5:K:709:HOH:O   | 2.03                     | 1.14              |
| 1:A:6:ARG:HG2    | 1:A:6:ARG:NH1   | 1.63                     | 1.13              |
| 2:J:163:SER:O    | 5:J:209:HOH:O   | 1.64                     | 1.13              |
| 1:E:92:ASP:CA    | 5:E:709:HOH:O   | 1.92                     | 1.13              |
| 1:E:11:ILE:CA    | 5:E:706:HOH:O   | 1.95                     | 1.12              |
| 2:D:161:LYS:HD3  | 5:D:201:HOH:O   | 1.49                     | 1.11              |
| 1:K:148:LYS:N    | 5:K:712:HOH:O   | 1.83                     | 1.11              |
| 2:B:30:GLN:NE2   | 5:B:204:HOH:O   | 1.84                     | 1.10              |
| 1:C:169:LYS:NZ   | 5:C:716:HOH:O   | 1.80                     | 1.10              |
| 1:G:208:GLY:N    | 5:G:706:HOH:O   | 1.83                     | 1.10              |
| 1:A:6:ARG:HH11   | 1:A:6:ARG:HG2   | 1.15                     | 1.09              |
| 1:E:271:ILE:N    | 5:E:705:HOH:O   | 1.86                     | 1.09              |
| 1:K:292:ILE:CA   | 5:K:715:HOH:O   | 2.01                     | 1.09              |
| 1:C:194:GLN:HG3  | 5:C:707:HOH:O   | 1.51                     | 1.08              |
| 2:D:13:GLY:HA2   | 5:D:206:HOH:O   | 1.54                     | 1.08              |
| 2:J:160:PRO:N    | 5:J:203:HOH:O   | 1.87                     | 1.07              |
| 2:B:53:ASN:N     | 5:B:208:HOH:O   | 1.85                     | 1.07              |
| 1:K:15:ALA:HB1   | 5:K:716:HOH:O   | 1.52                     | 1.07              |
| 1:K:292:ILE:HG23 | 5:K:715:HOH:O   | 1.53                     | 1.07              |
| 1:E:10:CYS:C     | 5:E:706:HOH:O   | 1.92                     | 1.07              |
| 2:B:52:VAL:C     | 5:B:208:HOH:O   | 1.92                     | 1.07              |
| 2:D:161:LYS:CD   | 5:D:201:HOH:O   | 2.01                     | 1.06              |
| 1:I:327:ILE:C    | 5:I:706:HOH:O   | 1.92                     | 1.06              |
| 1:I:328:PRO:N    | 5:I:706:HOH:O   | 1.86                     | 1.06              |
| 1:K:16:ASN:N     | 5:K:716:HOH:O   | 1.85                     | 1.06              |
| 1:I:143:PRO:HD2  | 4:I:601:NAG:H83 | 1.37                     | 1.06              |
| 2:J:161:LYS:HE3  | 2:J:161:LYS:H   | 1.05                     | 1.06              |
| 2:B:110:TYR:C    | 5:B:210:HOH:O   | 1.92                     | 1.06              |
| 2:D:147:THR:N    | 5:D:209:HOH:O   | 1.86                     | 1.05              |
| 1:A:6:ARG:CG     | 1:A:6:ARG:HH11  | 1.63                     | 1.05              |
| 1:K:292:ILE:CG2  | 5:K:715:HOH:O   | 2.03                     | 1.05              |
| 2:B:60:ASN:HD21  | 1:E:314:LYS:HD2 | 1.19                     | 1.05              |
| 1:G:327:ILE:N    | 5:G:713:HOH:O   | 1.90                     | 1.04              |
| 1:G:206:PHE:CE1  | 5:G:706:HOH:O   | 2.10                     | 1.03              |
| 2:L:17:MET:HA    | 5:L:208:HOH:O   | 1.57                     | 1.03              |
| 1:G:208:GLY:HA3  | 5:G:706:HOH:O   | 1.55                     | 1.03              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:J:160:PRO:CA   | 5:J:203:HOH:O   | 2.04                     | 1.02              |
| 1:A:108:ARG:NH1  | 5:A:716:HOH:O   | 1.91                     | 1.02              |
| 1:A:7:ASP:O      | 1:A:8:THR:HG22  | 1.57                     | 1.02              |
| 1:C:318:LEU:N    | 5:C:712:HOH:O   | 1.81                     | 1.02              |
| 1:G:208:GLY:CA   | 5:G:706:HOH:O   | 2.01                     | 1.02              |
| 1:G:328:PRO:CD   | 5:G:711:HOH:O   | 2.07                     | 1.02              |
| 1:E:92:ASP:C     | 5:E:709:HOH:O   | 1.96                     | 1.02              |
| 1:G:328:PRO:HD2  | 5:G:711:HOH:O   | 1.59                     | 1.01              |
| 1:G:133:ASP:N    | 5:G:709:HOH:O   | 1.94                     | 1.01              |
| 1:K:133:ASP:C    | 5:K:719:HOH:O   | 2.00                     | 1.00              |
| 1:K:11:ILE:HD12  | 2:L:119:TYR:HA  | 1.43                     | 1.00              |
| 1:K:145:ALA:N    | 5:K:717:HOH:O   | 1.92                     | 1.00              |
| 1:A:180:LEU:N    | 5:A:708:HOH:O   | 1.91                     | 1.00              |
| 2:D:17:MET:HA    | 5:D:205:HOH:O   | 1.60                     | 1.00              |
| 1:C:313:VAL:HG12 | 1:C:315:SER:H   | 1.26                     | 0.99              |
| 2:D:30:GLN:HG2   | 5:D:203:HOH:O   | 1.60                     | 0.99              |
| 2:J:129:ASN:HD21 | 2:J:161:LYS:HG2 | 1.24                     | 0.99              |
| 2:B:52:VAL:HG12  | 5:B:208:HOH:O   | 1.60                     | 0.99              |
| 2:D:146:ASN:N    | 5:D:207:HOH:O   | 1.96                     | 0.99              |
| 1:G:328:PRO:O    | 5:G:711:HOH:O   | 1.80                     | 0.99              |
| 1:K:293:ASN:N    | 5:K:715:HOH:O   | 1.93                     | 0.99              |
| 1:A:179:VAL:C    | 5:A:708:HOH:O   | 2.01                     | 0.99              |
| 1:G:275:ASP:OD2  | 5:G:705:HOH:O   | 1.80                     | 0.99              |
| 1:I:14:HIS:O     | 5:I:707:HOH:O   | 1.81                     | 0.99              |
| 1:G:114:VAL:HG11 | 1:G:117:PHE:HB2 | 1.44                     | 0.99              |
| 1:I:114:VAL:HG11 | 1:I:117:PHE:HB2 | 1.45                     | 0.98              |
| 2:D:145:ASP:C    | 5:D:207:HOH:O   | 2.00                     | 0.98              |
| 1:E:313:VAL:HG12 | 1:E:315:SER:H   | 1.27                     | 0.98              |
| 1:I:259:TYR:OH   | 5:I:711:HOH:O   | 1.80                     | 0.98              |
| 1:A:240:VAL:O    | 5:A:713:HOH:O   | 1.81                     | 0.98              |
| 1:E:92:ASP:N     | 5:E:709:HOH:O   | 1.92                     | 0.98              |
| 1:E:91:SER:C     | 5:E:709:HOH:O   | 2.01                     | 0.98              |
| 1:G:313:VAL:HG12 | 1:G:315:SER:H   | 1.27                     | 0.98              |
| 1:C:114:VAL:HG11 | 1:C:117:PHE:HB2 | 1.45                     | 0.97              |
| 1:A:114:VAL:HG11 | 1:A:117:PHE:HB2 | 1.44                     | 0.97              |
| 1:E:78:THR:HG22  | 5:E:702:HOH:O   | 1.62                     | 0.97              |
| 1:I:313:VAL:HG12 | 1:I:315:SER:H   | 1.28                     | 0.97              |
| 2:J:161:LYS:C    | 2:J:161:LYS:HD2 | 1.84                     | 0.97              |
| 1:G:133:ASP:O    | 5:G:709:HOH:O   | 1.83                     | 0.97              |
| 1:A:313:VAL:HG12 | 1:A:315:SER:H   | 1.27                     | 0.96              |
| 2:J:161:LYS:CE   | 2:J:161:LYS:H   | 1.78                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:327:ILE:O    | 5:G:707:HOH:O    | 1.81                     | 0.96              |
| 1:K:130:PRO:C    | 5:K:705:HOH:O    | 2.04                     | 0.96              |
| 1:G:279:HIS:CB   | 5:G:710:HOH:O    | 2.03                     | 0.96              |
| 1:K:313:VAL:HG12 | 1:K:315:SER:H    | 1.27                     | 0.96              |
| 1:A:179:VAL:CA   | 5:A:708:HOH:O    | 2.14                     | 0.95              |
| 1:K:59:GLY:O     | 5:K:714:HOH:O    | 1.82                     | 0.95              |
| 1:E:11:ILE:N     | 5:E:706:HOH:O    | 1.90                     | 0.95              |
| 1:E:114:VAL:HG21 | 1:E:117:PHE:HB2  | 1.47                     | 0.95              |
| 1:G:280:ASP:N    | 5:G:710:HOH:O    | 1.98                     | 0.95              |
| 2:D:146:ASN:HA   | 5:D:207:HOH:O    | 1.67                     | 0.95              |
| 1:E:25:VAL:HG21  | 2:F:102:LEU:HD12 | 1.47                     | 0.95              |
| 1:C:143:PRO:HD2  | 4:C:602:NAG:H83  | 1.47                     | 0.95              |
| 1:C:264:GLU:OE2  | 5:C:713:HOH:O    | 1.85                     | 0.94              |
| 1:E:269:SER:O    | 5:E:714:HOH:O    | 1.85                     | 0.94              |
| 2:F:125:GLN:O    | 5:F:211:HOH:O    | 1.85                     | 0.94              |
| 1:E:31:THR:HG23  | 5:E:704:HOH:O    | 1.66                     | 0.94              |
| 1:K:114:VAL:HG21 | 1:K:117:PHE:HB2  | 1.47                     | 0.94              |
| 2:B:111:HIS:HA   | 5:B:210:HOH:O    | 1.67                     | 0.94              |
| 1:K:133:ASP:O    | 5:K:719:HOH:O    | 1.84                     | 0.94              |
| 2:F:127:LYS:HD2  | 5:F:201:HOH:O    | 1.69                     | 0.93              |
| 1:E:270:GLY:C    | 5:E:705:HOH:O    | 2.02                     | 0.93              |
| 1:G:177:LYS:N    | 5:G:708:HOH:O    | 2.01                     | 0.93              |
| 2:J:161:LYS:NZ   | 5:J:204:HOH:O    | 2.02                     | 0.93              |
| 2:J:60:ASN:O     | 5:J:205:HOH:O    | 1.85                     | 0.93              |
| 2:B:142:HIS:CG   | 2:B:161:LYS:HG2  | 2.03                     | 0.92              |
| 2:B:52:VAL:CB    | 5:B:208:HOH:O    | 2.17                     | 0.92              |
| 1:E:60:LYS:O     | 5:E:711:HOH:O    | 1.86                     | 0.92              |
| 1:G:177:LYS:CA   | 5:G:708:HOH:O    | 2.15                     | 0.92              |
| 2:L:150:GLU:O    | 5:L:209:HOH:O    | 1.86                     | 0.92              |
| 1:K:53:VAL:O     | 5:K:720:HOH:O    | 1.86                     | 0.92              |
| 1:E:31:THR:CG2   | 5:E:704:HOH:O    | 2.18                     | 0.91              |
| 1:C:200:ASN:O    | 5:C:707:HOH:O    | 1.86                     | 0.91              |
| 2:F:160:PRO:O    | 5:F:207:HOH:O    | 1.87                     | 0.91              |
| 2:B:60:ASN:ND2   | 1:E:314:LYS:HD2  | 1.84                     | 0.91              |
| 1:E:11:ILE:HD11  | 2:F:122:VAL:CG1  | 2.01                     | 0.91              |
| 4:A:602:NAG:H61  | 4:A:603:NAG:N2   | 1.86                     | 0.91              |
| 2:D:159:TYR:HB3  | 2:D:160:PRO:HD3  | 1.53                     | 0.91              |
| 1:C:96:CYS:O     | 5:C:714:HOH:O    | 1.87                     | 0.91              |
| 1:E:269:SER:N    | 5:E:703:HOH:O    | 1.91                     | 0.91              |
| 1:G:326:ASN:C    | 5:G:713:HOH:O    | 2.05                     | 0.91              |
| 1:K:147:ALA:C    | 5:K:712:HOH:O    | 2.05                     | 0.91              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:158:VAL:O   | 5:G:709:HOH:O    | 1.89                     | 0.90              |
| 1:G:269:SER:N   | 5:G:702:HOH:O    | 1.95                     | 0.90              |
| 1:K:269:SER:N   | 5:K:702:HOH:O    | 1.87                     | 0.90              |
| 4:A:602:NAG:H61 | 4:A:603:NAG:C7   | 2.01                     | 0.90              |
| 2:D:160:PRO:C   | 2:D:161:LYS:HG2  | 1.86                     | 0.90              |
| 2:D:161:LYS:CE  | 5:D:201:HOH:O    | 2.16                     | 0.90              |
| 1:I:81:SER:C    | 1:I:82:TRP:CE3   | 2.44                     | 0.90              |
| 2:D:146:ASN:C   | 5:D:209:HOH:O    | 2.10                     | 0.90              |
| 2:F:157:TYR:CD2 | 5:F:211:HOH:O    | 2.23                     | 0.90              |
| 3:K:601:NAG:C1  | 5:K:708:HOH:O    | 2.18                     | 0.90              |
| 1:K:93:ASN:N    | 5:K:721:HOH:O    | 2.04                     | 0.90              |
| 1:A:54:ALA:O    | 5:A:709:HOH:O    | 1.90                     | 0.90              |
| 2:F:159:TYR:HB3 | 2:F:161:LYS:HE2  | 1.54                     | 0.89              |
| 1:A:76:LEU:O    | 5:A:715:HOH:O    | 1.90                     | 0.89              |
| 2:L:161:LYS:HB3 | 2:L:161:LYS:NZ   | 1.86                     | 0.89              |
| 1:G:328:PRO:CB  | 5:G:711:HOH:O    | 2.21                     | 0.89              |
| 1:K:11:ILE:HD11 | 2:L:122:VAL:HG13 | 1.53                     | 0.88              |
| 1:K:237:TRP:O   | 5:K:718:HOH:O    | 1.92                     | 0.88              |
| 2:B:47:GLU:HB3  | 1:E:26:LEU:HB3   | 1.53                     | 0.88              |
| 2:D:146:ASN:CB  | 5:D:209:HOH:O    | 2.21                     | 0.88              |
| 2:J:164:GLU:HG3 | 2:J:164:GLU:O    | 1.73                     | 0.88              |
| 2:J:60:ASN:CG   | 5:J:208:HOH:O    | 2.11                     | 0.88              |
| 2:B:106:ARG:NH2 | 5:B:206:HOH:O    | 2.05                     | 0.88              |
| 2:D:12:GLY:O    | 5:D:206:HOH:O    | 1.92                     | 0.88              |
| 1:G:279:HIS:C   | 5:G:710:HOH:O    | 2.12                     | 0.87              |
| 2:J:159:TYR:O   | 2:J:161:LYS:CE   | 2.22                     | 0.87              |
| 1:I:305:THR:H   | 2:J:66:VAL:HG13  | 1.36                     | 0.87              |
| 2:D:30:GLN:CG   | 5:D:203:HOH:O    | 2.19                     | 0.87              |
| 1:I:74:GLU:O    | 1:I:74:GLU:CG    | 2.23                     | 0.87              |
| 1:I:78:THR:HG23 | 1:I:79:ALA:H     | 1.36                     | 0.87              |
| 2:B:30:GLN:CD   | 5:B:204:HOH:O    | 2.11                     | 0.87              |
| 1:C:268:GLY:N   | 5:C:710:HOH:O    | 2.08                     | 0.87              |
| 2:J:60:ASN:OD1  | 5:J:208:HOH:O    | 1.91                     | 0.87              |
| 1:C:128:SER:O   | 5:C:716:HOH:O    | 1.91                     | 0.86              |
| 1:C:194:GLN:CG  | 5:C:707:HOH:O    | 2.14                     | 0.86              |
| 1:C:77:SER:OG   | 1:C:77:SER:O     | 1.80                     | 0.86              |
| 2:F:157:TYR:CE2 | 5:F:211:HOH:O    | 2.27                     | 0.86              |
| 2:B:111:HIS:CA  | 5:B:210:HOH:O    | 2.23                     | 0.86              |
| 2:B:111:HIS:N   | 5:B:210:HOH:O    | 2.05                     | 0.86              |
| 1:K:11:ILE:HD11 | 2:L:122:VAL:CG1  | 2.05                     | 0.86              |
| 2:B:30:GLN:OE1  | 5:B:204:HOH:O    | 1.92                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:89:PRO:HD2   | 5:C:711:HOH:O    | 1.76                     | 0.86              |
| 2:J:161:LYS:N    | 2:J:161:LYS:HE3  | 1.91                     | 0.86              |
| 1:G:326:ASN:CA   | 5:G:713:HOH:O    | 2.24                     | 0.85              |
| 1:K:125:LYS:HB2  | 1:K:258:ARG:HH11 | 1.40                     | 0.85              |
| 1:A:125:LYS:HB2  | 1:A:258:ARG:HH11 | 1.41                     | 0.85              |
| 1:I:76:LEU:HD12  | 1:I:76:LEU:C     | 1.95                     | 0.85              |
| 2:J:129:ASN:HD21 | 2:J:161:LYS:CG   | 1.88                     | 0.85              |
| 1:A:6:ARG:HH11   | 1:A:6:ARG:CB     | 1.89                     | 0.85              |
| 2:J:60:ASN:CB    | 5:J:208:HOH:O    | 2.25                     | 0.85              |
| 2:B:162:TYR:N    | 2:B:162:TYR:CD2  | 2.44                     | 0.85              |
| 1:E:125:LYS:HB2  | 1:E:258:ARG:HH11 | 1.42                     | 0.85              |
| 1:C:125:LYS:HB2  | 1:C:258:ARG:HH11 | 1.42                     | 0.85              |
| 2:F:30:GLN:N     | 5:F:208:HOH:O    | 2.09                     | 0.85              |
| 1:G:327:ILE:C    | 5:G:707:HOH:O    | 2.14                     | 0.85              |
| 2:B:110:TYR:O    | 5:B:210:HOH:O    | 1.88                     | 0.84              |
| 2:B:70:PHE:N     | 5:B:205:HOH:O    | 2.10                     | 0.84              |
| 2:D:146:ASN:CA   | 5:D:207:HOH:O    | 2.20                     | 0.84              |
| 2:L:151:SER:HA   | 5:L:205:HOH:O    | 1.75                     | 0.84              |
| 1:K:292:ILE:C    | 5:K:715:HOH:O    | 2.05                     | 0.84              |
| 1:E:271:ILE:CA   | 5:E:705:HOH:O    | 2.19                     | 0.84              |
| 1:G:125:LYS:HB2  | 1:G:258:ARG:HH11 | 1.41                     | 0.84              |
| 1:I:328:PRO:CA   | 5:I:706:HOH:O    | 2.18                     | 0.84              |
| 2:D:30:GLN:OE1   | 5:D:203:HOH:O    | 1.96                     | 0.84              |
| 1:G:207:VAL:C    | 5:G:706:HOH:O    | 2.11                     | 0.84              |
| 1:E:91:SER:O     | 5:E:709:HOH:O    | 1.91                     | 0.84              |
| 1:A:281:CYS:HB2  | 5:A:718:HOH:O    | 1.77                     | 0.84              |
| 1:G:177:LYS:C    | 5:G:708:HOH:O    | 2.14                     | 0.83              |
| 2:L:126:LEU:N    | 5:L:206:HOH:O    | 2.10                     | 0.83              |
| 1:C:194:GLN:OE1  | 5:C:707:HOH:O    | 1.94                     | 0.83              |
| 1:I:125:LYS:HB2  | 1:I:258:ARG:HH11 | 1.42                     | 0.83              |
| 2:B:81:ASN:ND2   | 5:B:201:HOH:O    | 2.11                     | 0.83              |
| 1:K:327:ILE:HG23 | 1:K:328:PRO:HD2  | 1.61                     | 0.82              |
| 1:K:137:GLY:HA3  | 5:K:707:HOH:O    | 1.78                     | 0.82              |
| 1:C:305:THR:H    | 2:D:66:VAL:HG13  | 1.45                     | 0.82              |
| 1:G:328:PRO:CG   | 5:G:711:HOH:O    | 2.24                     | 0.82              |
| 4:I:601:NAG:H61  | 4:I:602:NAG:O5   | 1.80                     | 0.82              |
| 3:K:601:NAG:O5   | 5:K:708:HOH:O    | 1.96                     | 0.82              |
| 2:B:70:PHE:HB2   | 5:B:205:HOH:O    | 1.80                     | 0.82              |
| 2:B:51:LYS:HG3   | 1:E:25:VAL:CG1   | 2.09                     | 0.82              |
| 1:K:292:ILE:HA   | 5:K:715:HOH:O    | 1.72                     | 0.82              |
| 1:K:25:VAL:HG21  | 2:L:102:LEU:HD12 | 1.60                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:706:HOH:O    | 2:F:14:TRP:HH2   | 1.61                     | 0.81              |
| 1:I:78:THR:CG2   | 1:I:79:ALA:N     | 2.37                     | 0.81              |
| 1:A:327:ILE:HG23 | 1:A:328:PRO:HD2  | 1.63                     | 0.81              |
| 2:B:70:PHE:CB    | 5:B:205:HOH:O    | 2.29                     | 0.81              |
| 1:C:327:ILE:HG23 | 1:C:328:PRO:HD2  | 1.61                     | 0.81              |
| 1:C:7:ASP:OD2    | 5:C:705:HOH:O    | 1.97                     | 0.81              |
| 1:A:282:ASN:O    | 5:A:718:HOH:O    | 1.98                     | 0.80              |
| 1:C:89:PRO:CD    | 5:C:711:HOH:O    | 2.28                     | 0.80              |
| 1:C:89:PRO:N     | 5:C:711:HOH:O    | 2.13                     | 0.80              |
| 2:J:159:TYR:O    | 2:J:161:LYS:HE2  | 1.82                     | 0.80              |
| 2:L:126:LEU:CA   | 5:L:206:HOH:O    | 2.28                     | 0.80              |
| 1:I:327:ILE:HG23 | 1:I:328:PRO:HD2  | 1.64                     | 0.79              |
| 1:A:7:ASP:O      | 1:A:8:THR:CG2    | 2.30                     | 0.79              |
| 1:K:305:THR:H    | 2:L:66:VAL:HG13  | 1.45                     | 0.79              |
| 2:H:161:LYS:HA   | 5:H:202:HOH:O    | 1.83                     | 0.79              |
| 1:A:269:SER:N    | 5:A:712:HOH:O    | 2.13                     | 0.79              |
| 1:G:327:ILE:HG23 | 1:G:328:PRO:HD2  | 1.62                     | 0.79              |
| 1:E:161:GLY:HA2  | 5:E:707:HOH:O    | 1.83                     | 0.79              |
| 1:G:269:SER:HB3  | 5:G:702:HOH:O    | 1.83                     | 0.79              |
| 1:K:137:GLY:CA   | 5:K:707:HOH:O    | 2.28                     | 0.78              |
| 1:K:92:ASP:N     | 5:K:721:HOH:O    | 2.16                     | 0.78              |
| 1:I:50:LEU:HD11  | 1:I:306:ILE:HG22 | 1.65                     | 0.78              |
| 2:J:94:TYR:HB2   | 5:J:207:HOH:O    | 1.83                     | 0.78              |
| 1:C:90:SER:OG    | 5:C:709:HOH:O    | 2.01                     | 0.78              |
| 2:L:125:GLN:C    | 5:L:206:HOH:O    | 2.21                     | 0.78              |
| 1:I:80:SER:OG    | 1:I:116:SER:HA   | 1.83                     | 0.78              |
| 1:E:25:VAL:CG2   | 2:F:102:LEU:HD12 | 2.13                     | 0.78              |
| 2:B:58:LYS:HD2   | 2:F:97:GLU:HB3   | 1.66                     | 0.77              |
| 1:K:15:ALA:CB    | 5:K:716:HOH:O    | 2.20                     | 0.77              |
| 2:H:64:THR:HG21  | 5:L:204:HOH:O    | 1.83                     | 0.77              |
| 1:K:137:GLY:N    | 5:K:707:HOH:O    | 2.16                     | 0.77              |
| 1:E:10:CYS:O     | 5:E:706:HOH:O    | 1.96                     | 0.77              |
| 2:B:51:LYS:HG3   | 1:E:25:VAL:HG12  | 1.65                     | 0.77              |
| 2:D:158:ASP:OD2  | 2:D:160:PRO:HD2  | 1.85                     | 0.77              |
| 1:K:130:PRO:O    | 5:K:705:HOH:O    | 2.01                     | 0.77              |
| 2:L:86:ASP:OD2   | 5:L:204:HOH:O    | 2.03                     | 0.77              |
| 1:C:327:ILE:HG23 | 1:C:328:PRO:CD   | 2.15                     | 0.77              |
| 1:E:11:ILE:HD11  | 2:F:122:VAL:HG13 | 1.63                     | 0.77              |
| 2:B:70:PHE:CD2   | 5:B:205:HOH:O    | 2.37                     | 0.77              |
| 2:F:162:TYR:HD2  | 5:F:203:HOH:O    | 1.67                     | 0.76              |
| 2:F:28:ASN:ND2   | 5:F:210:HOH:O    | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:602:NAG:H3   | 4:C:603:NAG:O5   | 1.86                     | 0.76              |
| 1:A:188:PRO:HG2  | 1:A:194:GLN:NE2  | 2.01                     | 0.76              |
| 1:G:50:LEU:HD11  | 1:G:306:ILE:HG22 | 1.68                     | 0.76              |
| 1:I:202:ASP:N    | 5:I:709:HOH:O    | 2.16                     | 0.76              |
| 1:E:188:PRO:HG2  | 1:E:194:GLN:NE2  | 2.01                     | 0.76              |
| 1:I:188:PRO:HG2  | 1:I:194:GLN:NE2  | 2.00                     | 0.76              |
| 1:K:188:PRO:HG2  | 1:K:194:GLN:NE2  | 2.00                     | 0.76              |
| 2:B:162:TYR:H    | 2:B:162:TYR:HD2  | 1.31                     | 0.76              |
| 2:B:52:VAL:CG1   | 5:B:208:HOH:O    | 2.18                     | 0.76              |
| 1:C:188:PRO:HG2  | 1:C:194:GLN:NE2  | 2.00                     | 0.76              |
| 1:I:327:ILE:HG23 | 1:I:328:PRO:CD   | 2.15                     | 0.76              |
| 1:K:75:SER:CB    | 5:K:711:HOH:O    | 2.34                     | 0.76              |
| 1:G:269:SER:CB   | 5:G:702:HOH:O    | 2.34                     | 0.76              |
| 1:K:53:VAL:N     | 5:K:720:HOH:O    | 2.16                     | 0.76              |
| 1:G:327:ILE:HG23 | 1:G:328:PRO:CD   | 2.15                     | 0.76              |
| 1:K:8:THR:HG22   | 2:L:139:GLU:HA   | 1.67                     | 0.76              |
| 1:K:227:ARG:NH2  | 3:K:601:NAG:O3   | 2.20                     | 0.75              |
| 1:K:327:ILE:HG23 | 1:K:328:PRO:CD   | 2.15                     | 0.75              |
| 1:A:327:ILE:HG23 | 1:A:328:PRO:CD   | 2.16                     | 0.75              |
| 1:G:188:PRO:HG2  | 1:G:194:GLN:NE2  | 2.02                     | 0.75              |
| 2:L:156:THR:OG1  | 5:L:205:HOH:O    | 2.04                     | 0.75              |
| 2:D:18:VAL:N     | 5:D:205:HOH:O    | 2.03                     | 0.74              |
| 1:K:14:HIS:HB2   | 2:L:21:TRP:HA    | 1.69                     | 0.74              |
| 1:K:11:ILE:CD1   | 2:L:119:TYR:HA   | 2.15                     | 0.74              |
| 1:I:76:LEU:CD1   | 1:I:76:LEU:C     | 2.54                     | 0.74              |
| 1:C:139:THR:CG2  | 5:C:706:HOH:O    | 2.34                     | 0.74              |
| 2:J:129:ASN:ND2  | 2:J:161:LYS:HG2  | 2.02                     | 0.74              |
| 2:B:160:PRO:HD2  | 2:B:161:LYS:HE2  | 1.69                     | 0.74              |
| 2:D:159:TYR:H    | 2:D:160:PRO:HD2  | 1.53                     | 0.74              |
| 1:I:76:LEU:HD12  | 1:I:77:SER:CA    | 2.17                     | 0.74              |
| 1:K:156:TRP:O    | 5:K:707:HOH:O    | 2.05                     | 0.74              |
| 1:K:14:HIS:N     | 2:L:21:TRP:O     | 2.21                     | 0.74              |
| 1:I:58:LEU:HD11  | 1:I:63:ILE:HD13  | 1.70                     | 0.74              |
| 1:K:133:ASP:OD1  | 5:K:719:HOH:O    | 2.06                     | 0.73              |
| 2:L:160:PRO:O    | 2:L:161:LYS:HG2  | 1.89                     | 0.73              |
| 1:A:6:ARG:CG     | 1:A:6:ARG:NH1    | 2.30                     | 0.73              |
| 1:K:75:SER:HB3   | 5:K:711:HOH:O    | 1.88                     | 0.73              |
| 1:K:15:ALA:C     | 5:K:716:HOH:O    | 2.22                     | 0.73              |
| 2:D:160:PRO:O    | 2:D:161:LYS:CG   | 2.27                     | 0.73              |
| 1:E:11:ILE:HD11  | 2:F:122:VAL:HG11 | 1.68                     | 0.73              |
| 1:A:7:ASP:C      | 1:A:8:THR:CG2    | 2.57                     | 0.72              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:D:159:TYR:HB3  | 2:D:160:PRO:CD  | 2.17                     | 0.72              |
| 1:E:305:THR:H    | 2:F:66:VAL:HG13 | 1.52                     | 0.72              |
| 2:D:161:LYS:HE3  | 5:D:201:HOH:O   | 1.85                     | 0.72              |
| 1:K:133:ASP:OD1  | 5:K:713:HOH:O   | 2.07                     | 0.72              |
| 1:E:327:ILE:HG21 | 2:F:12:GLY:CA   | 2.19                     | 0.72              |
| 1:E:126:THR:CB   | 5:E:708:HOH:O   | 2.37                     | 0.72              |
| 1:G:133:ASP:CA   | 5:G:709:HOH:O   | 2.35                     | 0.72              |
| 1:I:76:LEU:HD12  | 1:I:76:LEU:O    | 1.88                     | 0.72              |
| 2:B:142:HIS:CE1  | 2:B:161:LYS:HZ2 | 2.08                     | 0.72              |
| 2:B:86:ASP:OD2   | 5:B:203:HOH:O   | 2.06                     | 0.72              |
| 1:E:11:ILE:HA    | 5:E:706:HOH:O   | 1.73                     | 0.72              |
| 1:E:327:ILE:CG2  | 2:F:13:GLY:H    | 2.03                     | 0.72              |
| 2:B:160:PRO:HD2  | 2:B:161:LYS:CE  | 2.20                     | 0.72              |
| 2:H:154:ASN:N    | 5:H:203:HOH:O   | 2.21                     | 0.72              |
| 1:C:50:LEU:HB2   | 1:C:83:SER:CB   | 2.20                     | 0.71              |
| 2:D:158:ASP:OD1  | 5:D:201:HOH:O   | 2.08                     | 0.71              |
| 1:E:11:ILE:HD12  | 2:F:119:TYR:HA  | 1.70                     | 0.71              |
| 1:E:31:THR:OG1   | 5:E:704:HOH:O   | 2.07                     | 0.71              |
| 2:L:126:LEU:HD23 | 5:L:206:HOH:O   | 1.89                     | 0.71              |
| 1:C:58:LEU:HD11  | 1:C:63:ILE:HD13 | 1.71                     | 0.71              |
| 1:K:58:LEU:HD11  | 1:K:63:ILE:HD13 | 1.70                     | 0.71              |
| 2:F:126:LEU:HA   | 5:F:211:HOH:O   | 1.89                     | 0.71              |
| 1:K:237:TRP:C    | 5:K:718:HOH:O   | 2.26                     | 0.71              |
| 1:K:63:ILE:O     | 1:K:67:ILE:HG13 | 1.91                     | 0.71              |
| 1:E:58:LEU:HD11  | 1:E:63:ILE:HD13 | 1.73                     | 0.71              |
| 1:E:161:GLY:CA   | 5:E:707:HOH:O   | 2.36                     | 0.71              |
| 1:K:34:HIS:CE1   | 2:L:21:TRP:HE1  | 2.09                     | 0.71              |
| 1:C:139:THR:HG23 | 5:C:706:HOH:O   | 1.91                     | 0.71              |
| 1:K:327:ILE:CG2  | 2:L:13:GLY:H    | 2.03                     | 0.71              |
| 1:I:76:LEU:HD12  | 1:I:77:SER:N    | 2.06                     | 0.70              |
| 2:H:153:LYS:CB   | 5:H:203:HOH:O   | 2.39                     | 0.70              |
| 1:E:228:GLU:CD   | 5:E:710:HOH:O   | 2.29                     | 0.70              |
| 1:G:177:LYS:O    | 5:G:708:HOH:O   | 2.07                     | 0.70              |
| 1:K:327:ILE:HG21 | 2:L:12:GLY:CA   | 2.22                     | 0.70              |
| 1:C:63:ILE:O     | 1:C:67:ILE:HG13 | 1.91                     | 0.70              |
| 1:I:81:SER:O     | 1:I:82:TRP:CZ3  | 2.44                     | 0.70              |
| 1:A:12:GLY:HA3   | 5:A:702:HOH:O   | 1.92                     | 0.69              |
| 1:C:90:SER:O     | 5:C:709:HOH:O   | 2.10                     | 0.69              |
| 2:D:159:TYR:O    | 2:D:161:LYS:CG  | 2.40                     | 0.69              |
| 2:J:158:ASP:HB3  | 2:J:160:PRO:HD3 | 1.74                     | 0.69              |
| 1:G:63:ILE:O     | 1:G:67:ILE:HG13 | 1.92                     | 0.69              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:C:602:NAG:C3  | 4:C:603:NAG:O5   | 2.39                     | 0.69              |
| 2:J:159:TYR:C   | 5:J:203:HOH:O    | 2.20                     | 0.69              |
| 1:E:63:ILE:O    | 1:E:67:ILE:HG13  | 1.93                     | 0.69              |
| 1:I:76:LEU:HD12 | 1:I:77:SER:HA    | 1.74                     | 0.69              |
| 1:G:58:LEU:HD21 | 1:G:63:ILE:HD13  | 1.73                     | 0.69              |
| 2:B:158:ASP:HB2 | 2:B:160:PRO:HD3  | 1.75                     | 0.69              |
| 2:B:86:ASP:HB2  | 5:B:203:HOH:O    | 1.92                     | 0.69              |
| 1:A:25:VAL:CG2  | 2:B:102:LEU:HD23 | 2.23                     | 0.69              |
| 1:E:188:PRO:HG2 | 1:E:194:GLN:HE21 | 1.58                     | 0.69              |
| 1:I:188:PRO:HG2 | 1:I:194:GLN:HE21 | 1.58                     | 0.69              |
| 1:I:63:ILE:O    | 1:I:67:ILE:HG13  | 1.93                     | 0.69              |
| 1:A:63:ILE:O    | 1:A:67:ILE:HG13  | 1.93                     | 0.68              |
| 1:K:44:ASN:HD21 | 1:K:291:ALA:H    | 1.42                     | 0.68              |
| 1:C:188:PRO:HG2 | 1:C:194:GLN:HE21 | 1.58                     | 0.68              |
| 2:B:68:LYS:HE3  | 2:F:79:ASN:HB2   | 1.76                     | 0.68              |
| 5:C:705:HOH:O   | 2:D:28:ASN:HB2   | 1.93                     | 0.68              |
| 1:K:125:LYS:HB2 | 1:K:258:ARG:NH1  | 2.09                     | 0.68              |
| 1:K:188:PRO:HG2 | 1:K:194:GLN:HE21 | 1.58                     | 0.68              |
| 2:B:52:VAL:HB   | 5:B:208:HOH:O    | 1.86                     | 0.68              |
| 2:B:142:HIS:CE1 | 2:B:161:LYS:NZ   | 2.62                     | 0.68              |
| 1:E:50:LEU:HD21 | 1:E:306:ILE:HG22 | 1.76                     | 0.68              |
| 1:C:44:ASN:HD21 | 1:C:291:ALA:H    | 1.42                     | 0.68              |
| 2:H:64:THR:CG2  | 5:L:204:HOH:O    | 2.41                     | 0.68              |
| 1:I:327:ILE:O   | 5:I:706:HOH:O    | 2.05                     | 0.68              |
| 1:A:93:ASN:ND2  | 4:A:602:NAG:O7   | 2.24                     | 0.67              |
| 1:A:188:PRO:HG2 | 1:A:194:GLN:HE21 | 1.58                     | 0.67              |
| 1:A:44:ASN:HD21 | 1:A:291:ALA:H    | 1.43                     | 0.67              |
| 1:E:93:ASN:N    | 5:E:711:HOH:O    | 2.24                     | 0.67              |
| 1:G:125:LYS:HB2 | 1:G:258:ARG:NH1  | 2.09                     | 0.67              |
| 1:A:58:LEU:HD21 | 1:A:63:ILE:HD13  | 1.76                     | 0.67              |
| 1:G:63:ILE:HG22 | 1:G:67:ILE:HD11  | 1.76                     | 0.67              |
| 2:L:86:ASP:CB   | 5:L:204:HOH:O    | 2.43                     | 0.67              |
| 1:E:268:GLY:N   | 5:E:703:HOH:O    | 2.28                     | 0.67              |
| 1:I:279:HIS:NE2 | 5:I:710:HOH:O    | 2.27                     | 0.67              |
| 1:A:63:ILE:HG22 | 1:A:67:ILE:HD11  | 1.77                     | 0.67              |
| 1:C:227:ARG:NH1 | 5:C:714:HOH:O    | 1.99                     | 0.67              |
| 2:D:164:GLU:N   | 5:D:204:HOH:O    | 2.27                     | 0.67              |
| 1:G:44:ASN:HD21 | 1:G:291:ALA:H    | 1.42                     | 0.67              |
| 1:A:125:LYS:HB2 | 1:A:258:ARG:NH1  | 2.10                     | 0.67              |
| 1:K:91:SER:HB3  | 5:K:714:HOH:O    | 1.93                     | 0.67              |
| 1:I:227:ARG:NH2 | 4:I:601:NAG:O3   | 2.28                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:8:THR:HG22   | 2:F:139:GLU:HA   | 1.77                     | 0.67              |
| 1:C:314:LYS:HD2  | 2:F:60:ASN:HD21  | 1.59                     | 0.66              |
| 1:E:44:ASN:HD21  | 1:E:291:ALA:H    | 1.43                     | 0.66              |
| 1:I:143:PRO:CD   | 4:I:601:NAG:H83  | 2.22                     | 0.66              |
| 1:K:155:ILE:HD11 | 1:K:258:ARG:HD2  | 1.78                     | 0.66              |
| 1:A:12:GLY:CA    | 5:A:702:HOH:O    | 2.43                     | 0.66              |
| 1:A:155:ILE:HD11 | 1:A:258:ARG:HD2  | 1.77                     | 0.66              |
| 1:I:25:VAL:HG21  | 2:J:102:LEU:HD12 | 1.77                     | 0.66              |
| 2:L:85:ASP:OD2   | 5:L:203:HOH:O    | 2.12                     | 0.66              |
| 1:A:11:ILE:HD11  | 2:B:122:VAL:HG21 | 1.77                     | 0.66              |
| 1:I:44:ASN:HD21  | 1:I:291:ALA:H    | 1.42                     | 0.66              |
| 1:C:50:LEU:HB2   | 1:C:83:SER:HB2   | 1.78                     | 0.66              |
| 2:J:129:ASN:ND2  | 2:J:161:LYS:CG   | 2.58                     | 0.66              |
| 1:C:194:GLN:CD   | 5:C:707:HOH:O    | 2.26                     | 0.66              |
| 1:E:167:LEU:C    | 1:E:167:LEU:HD23 | 2.15                     | 0.66              |
| 1:E:78:THR:HG22  | 1:E:78:THR:O     | 1.96                     | 0.66              |
| 1:I:125:LYS:HB2  | 1:I:258:ARG:NH1  | 2.10                     | 0.66              |
| 1:E:63:ILE:HG22  | 1:E:67:ILE:HD11  | 1.76                     | 0.66              |
| 1:E:78:THR:O     | 5:E:702:HOH:O    | 2.13                     | 0.66              |
| 1:G:188:PRO:HG2  | 1:G:194:GLN:HE21 | 1.60                     | 0.66              |
| 1:E:155:ILE:HD11 | 1:E:258:ARG:HD2  | 1.78                     | 0.66              |
| 2:L:86:ASP:HB2   | 5:L:204:HOH:O    | 1.95                     | 0.66              |
| 1:C:63:ILE:HG22  | 1:C:67:ILE:HD11  | 1.78                     | 0.65              |
| 1:C:25:VAL:HG21  | 2:D:102:LEU:HD12 | 1.78                     | 0.65              |
| 1:G:22:VAL:HG12  | 1:G:319:ARG:HG2  | 1.78                     | 0.65              |
| 2:B:162:TYR:N    | 2:B:162:TYR:HD2  | 1.87                     | 0.65              |
| 2:B:70:PHE:HD2   | 5:B:205:HOH:O    | 1.73                     | 0.65              |
| 1:G:133:ASP:C    | 5:G:709:HOH:O    | 2.28                     | 0.65              |
| 1:K:9:LEU:HD12   | 2:L:152:VAL:HG11 | 1.78                     | 0.65              |
| 1:C:167:LEU:O    | 1:C:167:LEU:HD12 | 1.96                     | 0.65              |
| 2:F:125:GLN:O    | 5:F:201:HOH:O    | 2.13                     | 0.65              |
| 2:F:161:LYS:HA   | 5:F:207:HOH:O    | 1.97                     | 0.65              |
| 1:E:14:HIS:N     | 2:F:21:TRP:O     | 2.29                     | 0.65              |
| 1:I:63:ILE:HG22  | 1:I:67:ILE:HD11  | 1.77                     | 0.65              |
| 1:I:155:ILE:HD11 | 1:I:258:ARG:HD2  | 1.77                     | 0.65              |
| 1:I:167:LEU:HD12 | 1:I:167:LEU:O    | 1.96                     | 0.65              |
| 2:D:159:TYR:O    | 2:D:160:PRO:C    | 2.36                     | 0.65              |
| 1:K:167:LEU:C    | 1:K:167:LEU:HD23 | 2.18                     | 0.65              |
| 1:A:22:VAL:HG12  | 1:A:319:ARG:HG2  | 1.79                     | 0.64              |
| 1:A:167:LEU:O    | 1:A:167:LEU:HD12 | 1.96                     | 0.64              |
| 1:G:155:ILE:HD11 | 1:G:258:ARG:HD2  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:159:TYR:CD1  | 2:J:161:LYS:HE2  | 2.32                     | 0.64              |
| 2:J:161:LYS:C    | 2:J:163:SER:N    | 2.48                     | 0.64              |
| 1:I:22:VAL:HG12  | 1:I:319:ARG:HG2  | 1.79                     | 0.64              |
| 2:J:90:ASP:O     | 5:J:207:HOH:O    | 2.15                     | 0.64              |
| 1:C:125:LYS:HB2  | 1:C:258:ARG:NH1  | 2.10                     | 0.64              |
| 1:C:167:LEU:HD12 | 1:C:167:LEU:C    | 2.18                     | 0.64              |
| 1:C:267:ALA:C    | 5:C:710:HOH:O    | 2.34                     | 0.64              |
| 1:E:125:LYS:HB2  | 1:E:258:ARG:NH1  | 2.11                     | 0.64              |
| 1:G:88:THR:HB    | 5:G:705:HOH:O    | 1.96                     | 0.64              |
| 1:K:75:SER:N     | 5:K:711:HOH:O    | 2.30                     | 0.64              |
| 1:A:102:ILE:HG13 | 1:A:236:TYR:CE2  | 2.33                     | 0.64              |
| 1:C:314:LYS:HD2  | 2:F:60:ASN:ND2   | 2.12                     | 0.64              |
| 2:F:161:LYS:CA   | 5:F:207:HOH:O    | 2.45                     | 0.64              |
| 1:K:327:ILE:HG21 | 2:L:12:GLY:HA2   | 1.80                     | 0.64              |
| 1:C:22:VAL:HG12  | 1:C:319:ARG:HG2  | 1.79                     | 0.64              |
| 1:E:292:ILE:HG22 | 1:E:294:THR:HG22 | 1.80                     | 0.64              |
| 1:G:269:SER:CA   | 5:G:702:HOH:O    | 2.39                     | 0.63              |
| 1:I:167:LEU:HD12 | 1:I:167:LEU:C    | 2.18                     | 0.63              |
| 1:A:50:LEU:HD11  | 1:A:306:ILE:HG22 | 1.78                     | 0.63              |
| 1:C:155:ILE:HD11 | 1:C:258:ARG:HD2  | 1.79                     | 0.63              |
| 1:I:102:ILE:HG13 | 1:I:236:TYR:CE2  | 2.33                     | 0.63              |
| 1:K:25:VAL:CG2   | 2:L:102:LEU:HD12 | 2.28                     | 0.63              |
| 2:L:154:ASN:HB2  | 5:L:205:HOH:O    | 1.98                     | 0.63              |
| 1:G:167:LEU:C    | 1:G:167:LEU:HD12 | 2.18                     | 0.63              |
| 1:I:292:ILE:HG22 | 1:I:294:THR:HG22 | 1.81                     | 0.63              |
| 1:I:212:TYR:C    | 5:I:708:HOH:O    | 2.37                     | 0.63              |
| 1:G:133:ASP:OD2  | 1:G:136:LYS:HE2  | 1.99                     | 0.63              |
| 1:K:22:VAL:HG12  | 1:K:319:ARG:HG2  | 1.79                     | 0.63              |
| 2:J:160:PRO:CG   | 5:J:203:HOH:O    | 2.45                     | 0.63              |
| 2:B:143:LYS:HA   | 2:B:143:LYS:HE2  | 1.81                     | 0.62              |
| 2:B:157:TYR:CE2  | 2:B:158:ASP:O    | 2.52                     | 0.62              |
| 1:E:313:VAL:HG12 | 1:E:315:SER:N    | 2.09                     | 0.62              |
| 1:G:167:LEU:HD12 | 1:G:167:LEU:O    | 1.98                     | 0.62              |
| 1:A:167:LEU:C    | 1:A:167:LEU:HD12 | 2.18                     | 0.62              |
| 1:A:54:ALA:C     | 5:A:709:HOH:O    | 2.36                     | 0.62              |
| 1:C:133:ASP:OD2  | 1:C:136:LYS:HE2  | 1.99                     | 0.62              |
| 1:E:102:ILE:HG13 | 1:E:236:TYR:CE2  | 2.34                     | 0.62              |
| 2:F:30:GLN:CG    | 5:F:208:HOH:O    | 2.47                     | 0.62              |
| 1:C:102:ILE:HG13 | 1:C:236:TYR:CE2  | 2.34                     | 0.62              |
| 1:I:313:VAL:HG12 | 1:I:315:SER:N    | 2.09                     | 0.62              |
| 1:E:22:VAL:HG12  | 1:E:319:ARG:HG2  | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:135:ASN:HB2  | 5:K:713:HOH:O    | 1.98                     | 0.62              |
| 1:A:25:VAL:HG21  | 2:B:102:LEU:CD2  | 2.30                     | 0.62              |
| 1:A:133:ASP:OD2  | 1:A:136:LYS:HE2  | 1.99                     | 0.62              |
| 1:G:102:ILE:HG13 | 1:G:236:TYR:CE2  | 2.34                     | 0.62              |
| 2:J:159:TYR:O    | 2:J:161:LYS:HE3  | 1.99                     | 0.62              |
| 1:K:63:ILE:HG22  | 1:K:67:ILE:HD11  | 1.80                     | 0.62              |
| 1:A:281:CYS:CB   | 5:A:718:HOH:O    | 2.41                     | 0.62              |
| 2:J:143:LYS:HE2  | 2:J:143:LYS:HA   | 1.82                     | 0.62              |
| 1:K:128:SER:O    | 1:K:130:PRO:HD3  | 2.00                     | 0.62              |
| 1:A:12:GLY:N     | 2:B:14:TRP:CH2   | 2.68                     | 0.62              |
| 1:I:133:ASP:OD2  | 1:I:136:LYS:HE2  | 1.99                     | 0.62              |
| 1:I:201:ALA:N    | 5:I:709:HOH:O    | 2.32                     | 0.62              |
| 2:F:143:LYS:HA   | 2:F:143:LYS:HE2  | 1.82                     | 0.61              |
| 1:I:81:SER:OG    | 1:I:82:TRP:HA    | 2.00                     | 0.61              |
| 1:E:93:ASN:N     | 5:E:709:HOH:O    | 2.24                     | 0.61              |
| 1:A:128:SER:O    | 1:A:130:PRO:HD3  | 2.01                     | 0.61              |
| 1:E:133:ASP:OD2  | 1:E:136:LYS:HE2  | 1.99                     | 0.61              |
| 1:E:327:ILE:HG21 | 2:F:12:GLY:HA2   | 1.80                     | 0.61              |
| 1:G:63:ILE:CG2   | 1:G:67:ILE:HD11  | 2.30                     | 0.61              |
| 1:K:133:ASP:OD2  | 1:K:136:LYS:HE2  | 2.00                     | 0.61              |
| 1:E:128:SER:O    | 1:E:130:PRO:HD3  | 2.00                     | 0.61              |
| 1:G:128:SER:O    | 1:G:130:PRO:HD3  | 2.01                     | 0.61              |
| 1:I:128:SER:O    | 1:I:130:PRO:HD3  | 2.00                     | 0.61              |
| 1:I:63:ILE:CG2   | 1:I:67:ILE:HD11  | 2.31                     | 0.61              |
| 1:I:81:SER:C     | 1:I:82:TRP:HE3   | 2.02                     | 0.61              |
| 2:L:143:LYS:HA   | 2:L:143:LYS:HE2  | 1.82                     | 0.61              |
| 1:K:102:ILE:HG13 | 1:K:236:TYR:CE2  | 2.36                     | 0.60              |
| 2:B:86:ASP:CB    | 5:B:203:HOH:O    | 2.48                     | 0.60              |
| 1:C:128:SER:O    | 1:C:130:PRO:HD3  | 2.01                     | 0.60              |
| 2:H:143:LYS:HE2  | 2:H:143:LYS:HA   | 1.82                     | 0.60              |
| 1:C:63:ILE:CG2   | 1:C:67:ILE:HD11  | 2.31                     | 0.60              |
| 2:D:143:LYS:HA   | 2:D:143:LYS:HE2  | 1.81                     | 0.60              |
| 1:A:43:HIS:HB3   | 1:A:301:ILE:HD13 | 1.83                     | 0.60              |
| 1:C:43:HIS:HB3   | 1:C:301:ILE:HD13 | 1.83                     | 0.60              |
| 2:D:146:ASN:HB3  | 5:D:209:HOH:O    | 1.90                     | 0.60              |
| 1:E:63:ILE:CG2   | 1:E:67:ILE:HD11  | 2.31                     | 0.60              |
| 1:E:14:HIS:HB2   | 2:F:21:TRP:HA    | 1.83                     | 0.60              |
| 2:J:163:SER:C    | 5:J:209:HOH:O    | 2.18                     | 0.60              |
| 2:F:31:GLY:O     | 5:F:210:HOH:O    | 2.17                     | 0.60              |
| 1:A:159:LYS:HE2  | 1:A:196:SER:O    | 2.02                     | 0.60              |
| 2:B:54:SER:HB3   | 2:F:101:LEU:HD13 | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:153:LYS:HB2  | 5:H:203:HOH:O    | 1.98                     | 0.60              |
| 1:A:13:TYR:N     | 5:A:702:HOH:O    | 2.16                     | 0.60              |
| 2:D:142:HIS:HB3  | 5:D:202:HOH:O    | 2.01                     | 0.60              |
| 1:A:313:VAL:HG12 | 1:A:315:SER:N    | 2.09                     | 0.60              |
| 1:K:311:LYS:HG3  | 2:L:92:TRP:CE2   | 2.37                     | 0.60              |
| 1:E:43:HIS:HB3   | 1:E:301:ILE:HD13 | 1.82                     | 0.59              |
| 1:A:179:VAL:HA   | 5:A:708:HOH:O    | 1.93                     | 0.59              |
| 2:J:60:ASN:HB2   | 5:J:208:HOH:O    | 1.95                     | 0.59              |
| 1:A:63:ILE:CG2   | 1:A:67:ILE:HD11  | 2.31                     | 0.59              |
| 1:G:328:PRO:CA   | 5:G:711:HOH:O    | 2.46                     | 0.59              |
| 1:K:238:THR:CB   | 5:K:718:HOH:O    | 1.93                     | 0.59              |
| 2:L:126:LEU:CB   | 5:L:206:HOH:O    | 2.48                     | 0.59              |
| 1:I:327:ILE:CG2  | 1:I:328:PRO:N    | 2.65                     | 0.59              |
| 1:C:88:THR:HB    | 5:C:711:HOH:O    | 2.02                     | 0.59              |
| 1:E:96:CYS:O     | 1:E:227:ARG:HD3  | 2.03                     | 0.59              |
| 1:G:327:ILE:CG2  | 1:G:328:PRO:N    | 2.65                     | 0.59              |
| 1:E:126:THR:OG1  | 5:E:708:HOH:O    | 2.17                     | 0.59              |
| 1:G:24:THR:O     | 5:G:714:HOH:O    | 2.17                     | 0.59              |
| 1:I:43:HIS:HB3   | 1:I:301:ILE:HD13 | 1.83                     | 0.59              |
| 2:B:51:LYS:HA    | 1:E:25:VAL:O     | 2.03                     | 0.59              |
| 1:C:159:LYS:HE2  | 1:C:196:SER:O    | 2.03                     | 0.59              |
| 2:F:51:LYS:HE3   | 2:F:103:GLU:OE1  | 2.03                     | 0.59              |
| 1:K:205:VAL:HB   | 1:K:250:ALA:HB2  | 1.85                     | 0.59              |
| 2:F:30:GLN:HG3   | 5:F:208:HOH:O    | 2.01                     | 0.59              |
| 1:I:279:HIS:CE1  | 5:I:710:HOH:O    | 2.55                     | 0.59              |
| 2:D:159:TYR:O    | 2:D:161:LYS:HG3  | 2.03                     | 0.59              |
| 1:E:106:GLU:O    | 1:E:110:GLN:HG2  | 2.03                     | 0.59              |
| 1:E:47:LEU:HD22  | 1:E:276:THR:O    | 2.03                     | 0.59              |
| 1:K:44:ASN:O     | 1:K:46:LYS:HG3   | 2.03                     | 0.59              |
| 1:A:275:ASP:OD2  | 5:A:707:HOH:O    | 2.17                     | 0.58              |
| 1:A:105:GLU:OE2  | 2:B:71:ASN:HB3   | 2.03                     | 0.58              |
| 1:I:159:LYS:HE2  | 1:I:196:SER:O    | 2.02                     | 0.58              |
| 1:I:96:CYS:O     | 1:I:227:ARG:HD3  | 2.02                     | 0.58              |
| 1:C:106:GLU:O    | 1:C:110:GLN:HG2  | 2.03                     | 0.58              |
| 1:C:313:VAL:HG12 | 1:C:315:SER:N    | 2.08                     | 0.58              |
| 1:G:44:ASN:O     | 1:G:46:LYS:HG3   | 2.03                     | 0.58              |
| 1:G:96:CYS:O     | 1:G:227:ARG:HD3  | 2.02                     | 0.58              |
| 1:A:327:ILE:CG2  | 1:A:328:PRO:N    | 2.66                     | 0.58              |
| 2:B:145:ASP:O    | 2:B:148:CYS:HB3  | 2.03                     | 0.58              |
| 2:L:161:LYS:HB3  | 2:L:161:LYS:HZ3  | 1.64                     | 0.58              |
| 1:C:96:CYS:O     | 1:C:227:ARG:HD3  | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:43:HIS:HB3   | 1:G:301:ILE:HD13 | 1.84                     | 0.58              |
| 1:K:106:GLU:O    | 1:K:110:GLN:HG2  | 2.03                     | 0.58              |
| 2:L:162:TYR:HD1  | 2:L:162:TYR:O    | 1.86                     | 0.58              |
| 1:E:44:ASN:O     | 1:E:46:LYS:HG3   | 2.03                     | 0.58              |
| 1:C:25:VAL:HG12  | 2:F:51:LYS:HG3   | 1.85                     | 0.58              |
| 1:G:159:LYS:HE2  | 1:G:196:SER:O    | 2.03                     | 0.58              |
| 2:H:162:TYR:N    | 5:H:202:HOH:O    | 2.31                     | 0.58              |
| 2:H:51:LYS:HE3   | 2:H:103:GLU:OE1  | 2.04                     | 0.58              |
| 1:K:96:CYS:O     | 1:K:227:ARG:HD3  | 2.03                     | 0.58              |
| 1:K:63:ILE:CG2   | 1:K:67:ILE:HD11  | 2.33                     | 0.58              |
| 5:B:206:HOH:O    | 2:F:109:ASP:OD2  | 2.17                     | 0.58              |
| 2:J:161:LYS:HD2  | 2:J:161:LYS:O    | 2.03                     | 0.58              |
| 1:K:11:ILE:HD11  | 2:L:122:VAL:HG11 | 1.86                     | 0.58              |
| 1:A:44:ASN:O     | 1:A:46:LYS:HG3   | 2.03                     | 0.58              |
| 1:G:313:VAL:HG12 | 1:G:315:SER:N    | 2.09                     | 0.58              |
| 1:I:82:TRP:N     | 1:I:82:TRP:CD2   | 2.64                     | 0.58              |
| 1:K:43:HIS:HB3   | 1:K:301:ILE:HD13 | 1.84                     | 0.58              |
| 2:L:145:ASP:O    | 2:L:148:CYS:HB3  | 2.04                     | 0.58              |
| 1:A:96:CYS:O     | 1:A:227:ARG:HD3  | 2.04                     | 0.58              |
| 1:A:25:VAL:HG21  | 2:B:102:LEU:HD23 | 1.85                     | 0.58              |
| 2:B:54:SER:HB3   | 2:F:101:LEU:CD1  | 2.33                     | 0.58              |
| 1:C:44:ASN:O     | 1:C:46:LYS:HG3   | 2.04                     | 0.58              |
| 2:F:15:THR:N     | 5:F:209:HOH:O    | 2.25                     | 0.58              |
| 1:I:44:ASN:O     | 1:I:46:LYS:HG3   | 2.03                     | 0.58              |
| 2:J:160:PRO:HA   | 5:J:203:HOH:O    | 1.83                     | 0.58              |
| 1:K:145:ALA:CA   | 5:K:717:HOH:O    | 2.44                     | 0.58              |
| 1:K:49:LYS:HB3   | 1:K:54:ALA:HA    | 1.86                     | 0.58              |
| 1:K:70:ASN:HD21  | 3:K:601:NAG:C7   | 2.17                     | 0.58              |
| 1:G:106:GLU:O    | 1:G:110:GLN:HG2  | 2.04                     | 0.57              |
| 2:J:161:LYS:C    | 2:J:163:SER:H    | 2.06                     | 0.57              |
| 1:I:314:LYS:HD2  | 2:L:60:ASN:HD21  | 1.69                     | 0.57              |
| 1:C:99:GLY:HA3   | 1:C:233:MET:O    | 2.04                     | 0.57              |
| 1:E:159:LYS:HE2  | 1:E:196:SER:O    | 2.03                     | 0.57              |
| 1:I:99:GLY:HA3   | 1:I:233:MET:O    | 2.04                     | 0.57              |
| 2:J:51:LYS:HE3   | 2:J:103:GLU:OE1  | 2.03                     | 0.57              |
| 1:K:8:THR:HA     | 2:L:138:PHE:O    | 2.03                     | 0.57              |
| 2:D:51:LYS:HE3   | 2:D:103:GLU:OE1  | 2.03                     | 0.57              |
| 1:E:162:ASN:N    | 5:E:707:HOH:O    | 2.23                     | 0.57              |
| 2:J:145:ASP:O    | 2:J:148:CYS:HB3  | 2.04                     | 0.57              |
| 2:B:128:ASN:HB2  | 2:B:159:TYR:OH   | 2.03                     | 0.57              |
| 2:B:68:LYS:HE3   | 2:F:79:ASN:CB    | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:99:GLY:HA3   | 1:G:233:MET:O    | 2.03                     | 0.57              |
| 2:B:51:LYS:HE3   | 2:B:103:GLU:OE1  | 2.04                     | 0.57              |
| 1:C:25:VAL:CG1   | 2:F:51:LYS:HG3   | 2.34                     | 0.57              |
| 2:L:129:ASN:OD1  | 2:L:160:PRO:HA   | 2.04                     | 0.57              |
| 2:D:145:ASP:O    | 2:D:148:CYS:HB3  | 2.05                     | 0.57              |
| 2:D:159:TYR:N    | 2:D:160:PRO:HD2  | 2.15                     | 0.57              |
| 1:E:34:HIS:CE1   | 2:F:21:TRP:HE1   | 2.23                     | 0.57              |
| 1:I:76:LEU:CG    | 1:I:77:SER:N     | 2.67                     | 0.57              |
| 1:K:324:LEU:HB3  | 2:L:111:HIS:CG   | 2.40                     | 0.57              |
| 1:E:205:VAL:HB   | 1:E:250:ALA:HB2  | 1.87                     | 0.57              |
| 1:K:159:LYS:HE2  | 1:K:196:SER:O    | 2.04                     | 0.57              |
| 1:A:312:TYR:CD2  | 2:B:89:LEU:HD13  | 2.40                     | 0.57              |
| 1:A:104:TYR:OH   | 5:A:716:HOH:O    | 1.90                     | 0.57              |
| 1:A:106:GLU:O    | 1:A:110:GLN:HG2  | 2.04                     | 0.57              |
| 2:F:145:ASP:O    | 2:F:148:CYS:HB3  | 2.05                     | 0.57              |
| 2:J:158:ASP:CB   | 2:J:160:PRO:HD3  | 2.35                     | 0.57              |
| 1:K:16:ASN:HB3   | 5:K:710:HOH:O    | 2.03                     | 0.57              |
| 2:L:51:LYS:HE3   | 2:L:103:GLU:OE1  | 2.04                     | 0.57              |
| 1:K:14:HIS:CD2   | 1:K:15:ALA:N     | 2.73                     | 0.57              |
| 1:C:327:ILE:CG2  | 1:C:328:PRO:N    | 2.67                     | 0.56              |
| 1:I:106:GLU:O    | 1:I:110:GLN:HG2  | 2.05                     | 0.56              |
| 2:L:150:GLU:HG3  | 5:L:209:HOH:O    | 2.05                     | 0.56              |
| 1:K:292:ILE:HG22 | 1:K:294:THR:HG22 | 1.88                     | 0.56              |
| 1:K:327:ILE:CG2  | 1:K:328:PRO:N    | 2.67                     | 0.56              |
| 1:A:11:ILE:HG12  | 2:B:24:TYR:CD2   | 2.39                     | 0.56              |
| 2:H:3:PHE:HZ     | 2:L:2:LEU:HD13   | 1.70                     | 0.56              |
| 2:H:51:LYS:HG3   | 1:K:25:VAL:CG1   | 2.35                     | 0.56              |
| 1:K:60:LYS:O     | 5:K:721:HOH:O    | 2.16                     | 0.56              |
| 1:A:78:THR:HG22  | 1:A:78:THR:O     | 2.04                     | 0.56              |
| 1:E:98:PRO:HG3   | 1:E:226:VAL:HG12 | 1.87                     | 0.56              |
| 1:E:11:ILE:CD1   | 2:F:122:VAL:HG13 | 2.34                     | 0.56              |
| 1:I:98:PRO:HG3   | 1:I:226:VAL:HG12 | 1.88                     | 0.56              |
| 1:K:14:HIS:CB    | 2:L:21:TRP:HA    | 2.35                     | 0.56              |
| 1:K:306:ILE:C    | 5:K:709:HOH:O    | 2.44                     | 0.56              |
| 2:B:119:TYR:CE1  | 2:B:136:GLY:HA2  | 2.41                     | 0.56              |
| 1:C:44:ASN:ND2   | 1:C:291:ALA:H    | 2.04                     | 0.56              |
| 1:E:11:ILE:C     | 5:E:706:HOH:O    | 2.32                     | 0.56              |
| 1:I:224:PRO:HG2  | 1:K:209:SER:HA   | 1.87                     | 0.56              |
| 1:C:114:VAL:CG1  | 1:C:117:PHE:HB2  | 2.30                     | 0.56              |
| 1:A:28:LYS:HD2   | 2:D:50:ASN:OD1   | 2.06                     | 0.56              |
| 1:K:313:VAL:HG12 | 1:K:315:SER:N    | 2.09                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:47:LEU:HD22  | 1:K:276:THR:O    | 2.05                     | 0.56              |
| 1:A:99:GLY:HA3   | 1:A:233:MET:O    | 2.05                     | 0.56              |
| 1:K:99:GLY:HA3   | 1:K:233:MET:O    | 2.05                     | 0.56              |
| 1:A:49:LYS:O     | 1:A:283:THR:HG22 | 2.06                     | 0.56              |
| 1:K:104:TYR:CZ   | 1:K:108:ARG:HD2  | 2.41                     | 0.56              |
| 1:A:98:PRO:HG3   | 1:A:226:VAL:HG12 | 1.88                     | 0.56              |
| 2:H:87:GLY:HA3   | 2:J:88:PHE:CZ    | 2.41                     | 0.56              |
| 2:H:145:ASP:O    | 2:H:148:CYS:HB3  | 2.05                     | 0.55              |
| 1:K:44:ASN:ND2   | 1:K:291:ALA:H    | 2.04                     | 0.55              |
| 1:C:292:ILE:HG22 | 1:C:294:THR:HG22 | 1.87                     | 0.55              |
| 1:G:57:HIS:CE1   | 1:G:59:GLY:HA2   | 2.41                     | 0.55              |
| 2:J:161:LYS:N    | 2:J:161:LYS:CE   | 2.59                     | 0.55              |
| 1:C:98:PRO:HG3   | 1:C:226:VAL:HG12 | 1.88                     | 0.55              |
| 1:C:15:ALA:HB1   | 1:C:327:ILE:O    | 2.07                     | 0.55              |
| 1:E:14:HIS:CD2   | 1:E:15:ALA:N     | 2.75                     | 0.55              |
| 1:I:57:HIS:CE1   | 1:I:59:GLY:HA2   | 2.41                     | 0.55              |
| 1:I:78:THR:HG21  | 1:I:81:SER:HB2   | 1.88                     | 0.55              |
| 2:L:119:TYR:CE1  | 2:L:136:GLY:HA2  | 2.41                     | 0.55              |
| 1:C:90:SER:N     | 5:C:711:HOH:O    | 2.26                     | 0.55              |
| 1:A:25:VAL:HG12  | 2:D:51:LYS:HG3   | 1.88                     | 0.55              |
| 1:G:25:VAL:CG1   | 2:J:51:LYS:HG3   | 2.36                     | 0.55              |
| 5:C:705:HOH:O    | 2:D:28:ASN:CB    | 2.52                     | 0.55              |
| 1:E:99:GLY:HA3   | 1:E:233:MET:O    | 2.06                     | 0.55              |
| 1:G:14:HIS:CD2   | 1:G:15:ALA:N     | 2.75                     | 0.55              |
| 1:G:328:PRO:HB2  | 5:G:711:HOH:O    | 1.94                     | 0.55              |
| 1:C:224:PRO:HG2  | 1:E:209:SER:HA   | 1.88                     | 0.55              |
| 2:J:119:TYR:CE1  | 2:J:136:GLY:HA2  | 2.42                     | 0.55              |
| 1:A:268:GLY:N    | 5:A:712:HOH:O    | 2.38                     | 0.55              |
| 2:D:123:ARG:HB2  | 2:D:138:PHE:HZ   | 1.71                     | 0.55              |
| 2:F:123:ARG:HB2  | 2:F:138:PHE:HZ   | 1.72                     | 0.55              |
| 1:I:15:ALA:HB1   | 1:I:327:ILE:O    | 2.06                     | 0.55              |
| 1:I:76:LEU:CD1   | 1:I:77:SER:N     | 2.70                     | 0.55              |
| 1:E:104:TYR:CZ   | 1:E:108:ARG:HD2  | 2.42                     | 0.55              |
| 1:C:104:TYR:CZ   | 1:C:108:ARG:HD2  | 2.42                     | 0.55              |
| 1:C:14:HIS:CD2   | 1:C:15:ALA:N     | 2.75                     | 0.55              |
| 2:D:119:TYR:CE1  | 2:D:136:GLY:HA2  | 2.42                     | 0.55              |
| 2:F:119:TYR:CE1  | 2:F:136:GLY:HA2  | 2.41                     | 0.55              |
| 2:F:159:TYR:HB3  | 2:F:161:LYS:CE   | 2.33                     | 0.55              |
| 1:G:44:ASN:ND2   | 1:G:291:ALA:H    | 2.04                     | 0.55              |
| 1:G:311:LYS:HG3  | 2:H:92:TRP:CE2   | 2.41                     | 0.55              |
| 1:I:49:LYS:O     | 1:I:283:THR:HG22 | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:68:LEU:O     | 1:I:151:TYR:HB3  | 2.07                     | 0.55              |
| 2:L:123:ARG:HB2  | 2:L:138:PHE:HZ   | 1.71                     | 0.55              |
| 1:I:76:LEU:HG    | 1:I:77:SER:N     | 2.22                     | 0.54              |
| 1:G:68:LEU:O     | 1:G:151:TYR:HB3  | 2.08                     | 0.54              |
| 1:A:14:HIS:CD2   | 1:A:15:ALA:N     | 2.76                     | 0.54              |
| 1:A:282:ASN:N    | 5:A:718:HOH:O    | 2.41                     | 0.54              |
| 1:A:125:LYS:CB   | 1:A:258:ARG:NH1  | 2.71                     | 0.54              |
| 1:E:133:ASP:HB3  | 1:E:158:VAL:HG23 | 1.90                     | 0.54              |
| 1:K:13:TYR:CE2   | 2:L:6:ILE:HA     | 2.42                     | 0.54              |
| 1:K:68:LEU:O     | 1:K:151:TYR:HB3  | 2.08                     | 0.54              |
| 2:B:123:ARG:HB2  | 2:B:138:PHE:HZ   | 1.73                     | 0.54              |
| 2:H:153:LYS:C    | 5:H:203:HOH:O    | 2.45                     | 0.54              |
| 1:I:125:LYS:CB   | 1:I:258:ARG:NH1  | 2.71                     | 0.54              |
| 1:I:44:ASN:ND2   | 1:I:291:ALA:H    | 2.04                     | 0.54              |
| 1:K:125:LYS:CB   | 1:K:258:ARG:NH1  | 2.70                     | 0.54              |
| 2:L:135:ASN:HB3  | 5:L:207:HOH:O    | 2.06                     | 0.54              |
| 1:E:68:LEU:O     | 1:E:151:TYR:HB3  | 2.08                     | 0.54              |
| 1:G:49:LYS:O     | 1:G:283:THR:HG22 | 2.08                     | 0.54              |
| 1:I:314:LYS:HD2  | 2:L:60:ASN:ND2   | 2.23                     | 0.54              |
| 1:C:305:THR:HG21 | 1:C:309:CYS:HB2  | 1.90                     | 0.54              |
| 1:C:74:GLU:O     | 1:C:74:GLU:HG2   | 2.06                     | 0.54              |
| 1:E:49:LYS:O     | 1:E:283:THR:HG22 | 2.08                     | 0.54              |
| 2:F:127:LYS:CD   | 5:F:201:HOH:O    | 2.40                     | 0.54              |
| 2:F:127:LYS:N    | 5:F:201:HOH:O    | 2.41                     | 0.54              |
| 1:I:311:LYS:HG3  | 2:J:92:TRP:CE2   | 2.42                     | 0.54              |
| 1:A:44:ASN:ND2   | 1:A:291:ALA:H    | 2.05                     | 0.54              |
| 1:E:114:VAL:CG2  | 1:E:117:PHE:HB2  | 2.32                     | 0.54              |
| 1:E:14:HIS:HB2   | 2:F:20:GLY:O     | 2.08                     | 0.54              |
| 1:G:133:ASP:HB3  | 1:G:158:VAL:HG23 | 1.89                     | 0.54              |
| 2:H:51:LYS:HG3   | 1:K:25:VAL:HG12  | 1.89                     | 0.54              |
| 1:K:15:ALA:HB1   | 1:K:327:ILE:O    | 2.07                     | 0.54              |
| 1:A:57:HIS:CE1   | 1:A:59:GLY:HA2   | 2.42                     | 0.54              |
| 1:G:125:LYS:CB   | 1:G:258:ARG:NH1  | 2.70                     | 0.54              |
| 1:G:83:SER:HG    | 1:G:84:TYR:HD2   | 1.55                     | 0.54              |
| 1:G:98:PRO:HG3   | 1:G:226:VAL:HG12 | 1.89                     | 0.54              |
| 2:H:119:TYR:CE1  | 2:H:136:GLY:HA2  | 2.42                     | 0.54              |
| 1:K:57:HIS:CE1   | 1:K:59:GLY:HA2   | 2.43                     | 0.54              |
| 1:A:68:LEU:O     | 1:A:151:TYR:HB3  | 2.08                     | 0.53              |
| 1:E:273:ILE:N    | 1:E:273:ILE:HD12 | 2.24                     | 0.53              |
| 1:E:57:HIS:CE1   | 1:E:59:GLY:HA2   | 2.43                     | 0.53              |
| 2:H:123:ARG:HB2  | 2:H:138:PHE:HZ   | 1.73                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:83:SER:HG    | 1:I:84:TYR:HD2   | 1.55                     | 0.53              |
| 1:C:9:LEU:HD11   | 2:D:24:TYR:HB3   | 1.90                     | 0.53              |
| 2:F:159:TYR:O    | 2:F:161:LYS:HG2  | 2.08                     | 0.53              |
| 1:I:104:TYR:CZ   | 1:I:108:ARG:HD2  | 2.44                     | 0.53              |
| 1:C:167:LEU:CD1  | 1:C:167:LEU:C    | 2.77                     | 0.53              |
| 1:C:49:LYS:CE    | 1:C:280:ASP:OD1  | 2.56                     | 0.53              |
| 1:C:57:HIS:CE1   | 1:C:59:GLY:HA2   | 2.43                     | 0.53              |
| 1:G:104:TYR:CZ   | 1:G:108:ARG:HD2  | 2.43                     | 0.53              |
| 1:G:15:ALA:HB1   | 1:G:327:ILE:O    | 2.09                     | 0.53              |
| 1:I:14:HIS:CD2   | 1:I:15:ALA:N     | 2.77                     | 0.53              |
| 1:I:305:THR:HG21 | 1:I:309:CYS:HB2  | 1.90                     | 0.53              |
| 1:A:118:GLU:HG3  | 1:A:118:GLU:O    | 2.09                     | 0.53              |
| 1:A:54:ALA:HB1   | 1:A:55:PRO:HD2   | 1.91                     | 0.53              |
| 2:F:125:GLN:HE21 | 2:F:157:TYR:H    | 1.57                     | 0.53              |
| 1:I:167:LEU:C    | 1:I:167:LEU:CD1  | 2.77                     | 0.53              |
| 1:K:98:PRO:HG3   | 1:K:226:VAL:HG12 | 1.90                     | 0.53              |
| 1:A:104:TYR:CZ   | 1:A:108:ARG:HD2  | 2.44                     | 0.53              |
| 2:D:146:ASN:N    | 5:D:208:HOH:O    | 2.42                     | 0.53              |
| 2:F:30:GLN:NE2   | 5:F:208:HOH:O    | 2.15                     | 0.53              |
| 1:G:305:THR:HG21 | 1:G:309:CYS:HB2  | 1.91                     | 0.53              |
| 1:K:114:VAL:CG2  | 1:K:117:PHE:HB2  | 2.31                     | 0.53              |
| 1:K:118:GLU:HG3  | 1:K:118:GLU:O    | 2.08                     | 0.53              |
| 2:B:159:TYR:O    | 2:B:159:TYR:CD2  | 2.62                     | 0.53              |
| 1:E:167:LEU:CD2  | 1:E:167:LEU:C    | 2.77                     | 0.53              |
| 1:E:324:LEU:HB3  | 2:F:111:HIS:CG   | 2.44                     | 0.53              |
| 1:I:76:LEU:CD1   | 1:I:77:SER:HA    | 2.39                     | 0.53              |
| 1:K:91:SER:CB    | 5:K:714:HOH:O    | 2.55                     | 0.53              |
| 1:K:327:ILE:HG22 | 2:L:13:GLY:H     | 1.73                     | 0.53              |
| 1:A:15:ALA:HB1   | 1:A:327:ILE:O    | 2.08                     | 0.53              |
| 1:A:167:LEU:C    | 1:A:167:LEU:CD1  | 2.77                     | 0.53              |
| 1:C:68:LEU:O     | 1:C:151:TYR:HB3  | 2.08                     | 0.53              |
| 1:E:125:LYS:CB   | 1:E:258:ARG:NH1  | 2.72                     | 0.53              |
| 1:G:118:GLU:O    | 1:G:118:GLU:HG3  | 2.09                     | 0.53              |
| 1:I:118:GLU:HG3  | 1:I:118:GLU:O    | 2.09                     | 0.52              |
| 1:K:54:ALA:HB1   | 1:K:55:PRO:HD2   | 1.91                     | 0.52              |
| 1:A:305:THR:HG21 | 1:A:309:CYS:HB2  | 1.91                     | 0.52              |
| 1:E:15:ALA:HB1   | 1:E:327:ILE:O    | 2.10                     | 0.52              |
| 1:G:129:TRP:C    | 5:G:712:HOH:O    | 2.47                     | 0.52              |
| 1:K:133:ASP:HB3  | 1:K:158:VAL:HG23 | 1.90                     | 0.52              |
| 1:K:305:THR:HG21 | 1:K:309:CYS:HB2  | 1.90                     | 0.52              |
| 2:L:161:LYS:HB3  | 2:L:161:LYS:HZ2  | 1.73                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:25:VAL:HG22  | 2:B:102:LEU:HD23 | 1.90                     | 0.52              |
| 1:A:7:ASP:C      | 1:A:8:THR:HG23   | 2.29                     | 0.52              |
| 1:C:44:ASN:HD22  | 1:C:44:ASN:C     | 2.12                     | 0.52              |
| 1:K:307:GLY:CA   | 5:K:709:HOH:O    | 2.56                     | 0.52              |
| 1:E:44:ASN:ND2   | 1:E:291:ALA:H    | 2.05                     | 0.52              |
| 1:E:50:LEU:CD2   | 1:E:306:ILE:HG22 | 2.39                     | 0.52              |
| 1:K:65:GLY:HA3   | 1:K:94:GLY:HA2   | 1.92                     | 0.52              |
| 1:A:189:SER:HA   | 1:A:221:ALA:O    | 2.10                     | 0.52              |
| 1:C:65:GLY:HA3   | 1:C:94:GLY:HA2   | 1.92                     | 0.52              |
| 2:D:163:SER:N    | 5:D:202:HOH:O    | 2.43                     | 0.52              |
| 1:I:133:ASP:HB3  | 1:I:158:VAL:HG23 | 1.90                     | 0.52              |
| 1:I:44:ASN:C     | 1:I:44:ASN:HD22  | 2.13                     | 0.52              |
| 1:K:44:ASN:C     | 1:K:44:ASN:HD22  | 2.11                     | 0.52              |
| 1:K:96:CYS:HB3   | 3:K:601:NAG:H81  | 1.90                     | 0.52              |
| 1:C:269:SER:N    | 5:C:710:HOH:O    | 2.22                     | 0.52              |
| 1:C:37:ASN:ND2   | 5:C:712:HOH:O    | 2.38                     | 0.52              |
| 1:E:44:ASN:HD22  | 1:E:44:ASN:C     | 2.11                     | 0.52              |
| 2:B:62:GLN:HG3   | 2:F:86:ASP:HB3   | 1.91                     | 0.52              |
| 1:G:326:ASN:HA   | 5:G:713:HOH:O    | 1.97                     | 0.52              |
| 1:G:44:ASN:C     | 1:G:44:ASN:HD22  | 2.13                     | 0.52              |
| 2:J:123:ARG:HB2  | 2:J:138:PHE:HZ   | 1.74                     | 0.52              |
| 2:L:125:GLN:HE21 | 2:L:157:TYR:H    | 1.58                     | 0.52              |
| 1:C:125:LYS:CB   | 1:C:258:ARG:NH1  | 2.71                     | 0.52              |
| 1:C:133:ASP:HB3  | 1:C:158:VAL:HG23 | 1.90                     | 0.52              |
| 1:E:65:GLY:HA3   | 1:E:94:GLY:HA2   | 1.90                     | 0.52              |
| 1:I:143:PRO:HD2  | 4:I:601:NAG:C8   | 2.25                     | 0.52              |
| 1:K:273:ILE:N    | 1:K:273:ILE:HD12 | 2.24                     | 0.52              |
| 1:E:305:THR:HG21 | 1:E:309:CYS:HB2  | 1.90                     | 0.52              |
| 1:G:167:LEU:C    | 1:G:167:LEU:CD1  | 2.78                     | 0.52              |
| 1:I:25:VAL:HG12  | 2:L:51:LYS:HG3   | 1.91                     | 0.52              |
| 1:A:25:VAL:CG1   | 2:D:51:LYS:HG3   | 2.40                     | 0.52              |
| 2:J:87:GLY:HA3   | 2:L:88:PHE:CZ    | 2.45                     | 0.52              |
| 1:A:44:ASN:C     | 1:A:44:ASN:HD22  | 2.13                     | 0.52              |
| 1:A:9:LEU:HD11   | 2:B:24:TYR:HB3   | 1.91                     | 0.52              |
| 1:C:49:LYS:HE3   | 1:C:280:ASP:OD1  | 2.10                     | 0.52              |
| 1:C:54:ALA:HB1   | 1:C:55:PRO:HD2   | 1.92                     | 0.52              |
| 1:I:142:CYS:HB2  | 1:I:149:SER:O    | 2.11                     | 0.52              |
| 1:E:96:CYS:HB2   | 1:E:141:ALA:O    | 2.11                     | 0.51              |
| 2:F:126:LEU:CA   | 5:F:211:HOH:O    | 2.54                     | 0.51              |
| 1:A:311:LYS:HE2  | 2:B:61:THR:HG22  | 1.92                     | 0.51              |
| 1:I:252:GLY:C    | 1:I:253:ASN:HD22 | 2.14                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:146:GLY:N    | 5:K:717:HOH:O    | 2.29                     | 0.51              |
| 1:A:133:ASP:HB3  | 1:A:158:VAL:HG23 | 1.91                     | 0.51              |
| 1:C:273:ILE:N    | 1:C:273:ILE:HD12 | 2.25                     | 0.51              |
| 1:E:65:GLY:CA    | 1:E:94:GLY:HA2   | 2.40                     | 0.51              |
| 1:E:327:ILE:HG22 | 2:F:13:GLY:H     | 1.75                     | 0.51              |
| 1:I:189:SER:HA   | 1:I:221:ALA:O    | 2.10                     | 0.51              |
| 1:I:273:ILE:HD12 | 1:I:273:ILE:N    | 2.24                     | 0.51              |
| 1:G:65:GLY:HA3   | 1:G:94:GLY:HA2   | 1.92                     | 0.51              |
| 1:G:96:CYS:HB2   | 1:G:141:ALA:O    | 2.11                     | 0.51              |
| 1:K:7:ASP:O      | 2:L:140:PHE:N    | 2.31                     | 0.51              |
| 1:C:311:LYS:HG3  | 2:D:92:TRP:CE2   | 2.45                     | 0.51              |
| 1:G:54:ALA:HB1   | 1:G:55:PRO:HD2   | 1.93                     | 0.51              |
| 1:K:325:ARG:O    | 5:K:706:HOH:O    | 2.19                     | 0.51              |
| 1:C:227:ARG:O    | 1:C:228:GLU:HB2  | 2.11                     | 0.51              |
| 1:E:227:ARG:O    | 1:E:228:GLU:HB2  | 2.11                     | 0.51              |
| 1:K:15:ALA:CA    | 5:K:716:HOH:O    | 2.50                     | 0.51              |
| 2:L:122:VAL:HG22 | 2:L:138:PHE:CE1  | 2.46                     | 0.51              |
| 1:I:65:GLY:HA3   | 1:I:94:GLY:HA2   | 1.93                     | 0.51              |
| 2:H:2:LEU:HG     | 2:J:3:PHE:CZ     | 2.46                     | 0.51              |
| 1:K:167:LEU:CD2  | 1:K:167:LEU:C    | 2.79                     | 0.51              |
| 1:K:307:GLY:HA2  | 2:L:63:PHE:CE1   | 2.46                     | 0.51              |
| 1:A:114:VAL:CG1  | 1:A:117:PHE:HB2  | 2.30                     | 0.51              |
| 1:G:252:GLY:C    | 1:G:253:ASN:HD22 | 2.14                     | 0.51              |
| 1:I:213:SER:HB2  | 5:I:708:HOH:O    | 2.09                     | 0.51              |
| 1:K:252:GLY:C    | 1:K:253:ASN:HD22 | 2.15                     | 0.51              |
| 1:G:273:ILE:N    | 1:G:273:ILE:HD12 | 2.26                     | 0.51              |
| 4:I:601:NAG:H61  | 4:I:602:NAG:C1   | 2.40                     | 0.51              |
| 1:I:96:CYS:HB2   | 1:I:141:ALA:O    | 2.11                     | 0.51              |
| 2:L:154:ASN:HB2  | 5:L:209:HOH:O    | 2.10                     | 0.51              |
| 1:A:273:ILE:N    | 1:A:273:ILE:HD12 | 2.26                     | 0.51              |
| 1:A:65:GLY:HA3   | 1:A:94:GLY:HA2   | 1.93                     | 0.51              |
| 1:C:118:GLU:O    | 1:C:118:GLU:HG3  | 2.10                     | 0.51              |
| 2:L:150:GLU:C    | 5:L:209:HOH:O    | 2.43                     | 0.51              |
| 1:C:49:LYS:NZ    | 1:C:280:ASP:OD1  | 2.42                     | 0.50              |
| 2:D:128:ASN:HB3  | 2:D:162:TYR:CZ   | 2.46                     | 0.50              |
| 1:G:25:VAL:HG12  | 2:J:51:LYS:HG3   | 1.94                     | 0.50              |
| 1:I:327:ILE:CG2  | 1:I:328:PRO:CD   | 2.89                     | 0.50              |
| 1:I:54:ALA:HB1   | 1:I:55:PRO:HD2   | 1.92                     | 0.50              |
| 3:K:601:NAG:H2   | 5:K:708:HOH:O    | 2.11                     | 0.50              |
| 2:F:122:VAL:HG22 | 2:F:138:PHE:CE1  | 2.47                     | 0.50              |
| 1:G:223:ARG:HG3  | 1:I:206:PHE:HZ   | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:227:ARG:O    | 1:G:228:GLU:HB2  | 2.10                     | 0.50              |
| 1:C:142:CYS:HB2  | 1:C:149:SER:O    | 2.11                     | 0.50              |
| 2:D:123:ARG:HB2  | 2:D:138:PHE:CZ   | 2.47                     | 0.50              |
| 1:E:252:GLY:C    | 1:E:253:ASN:HD22 | 2.14                     | 0.50              |
| 1:I:12:GLY:N     | 2:J:14:TRP:CH2   | 2.80                     | 0.50              |
| 1:K:17:ASN:ND2   | 5:K:704:HOH:O    | 2.12                     | 0.50              |
| 1:A:252:GLY:C    | 1:A:253:ASN:HD22 | 2.15                     | 0.50              |
| 2:D:160:PRO:C    | 2:D:161:LYS:CG   | 2.71                     | 0.50              |
| 1:G:189:SER:HA   | 1:G:221:ALA:O    | 2.10                     | 0.50              |
| 1:I:9:LEU:HD11   | 2:J:24:TYR:HB3   | 1.94                     | 0.50              |
| 1:K:324:LEU:HB3  | 2:L:111:HIS:CD2  | 2.47                     | 0.50              |
| 1:A:142:CYS:HB2  | 1:A:149:SER:O    | 2.12                     | 0.50              |
| 2:H:5:ALA:HB3    | 2:H:112:ASP:OD2  | 2.12                     | 0.50              |
| 1:K:189:SER:HA   | 1:K:221:ALA:O    | 2.11                     | 0.50              |
| 1:K:83:SER:HG    | 1:K:84:TYR:HD2   | 1.56                     | 0.50              |
| 1:C:252:GLY:C    | 1:C:253:ASN:HD22 | 2.15                     | 0.50              |
| 2:B:125:GLN:HE21 | 2:B:157:TYR:H    | 1.60                     | 0.50              |
| 1:C:90:SER:CB    | 5:C:709:HOH:O    | 2.57                     | 0.50              |
| 2:D:151:SER:HB2  | 2:D:156:THR:O    | 2.11                     | 0.50              |
| 1:E:159:LYS:HD2  | 1:E:199:GLN:HG2  | 1.94                     | 0.50              |
| 2:H:125:GLN:HE21 | 2:H:157:TYR:H    | 1.58                     | 0.50              |
| 1:C:12:GLY:N     | 2:D:14:TRP:CH2   | 2.79                     | 0.50              |
| 2:H:151:SER:HB2  | 2:H:156:THR:O    | 2.12                     | 0.50              |
| 1:I:227:ARG:O    | 1:I:228:GLU:HB2  | 2.12                     | 0.50              |
| 1:I:307:GLY:HA2  | 2:J:63:PHE:CE1   | 2.46                     | 0.50              |
| 2:J:151:SER:HB2  | 2:J:156:THR:O    | 2.12                     | 0.50              |
| 1:K:65:GLY:CA    | 1:K:94:GLY:HA2   | 2.42                     | 0.50              |
| 1:A:159:LYS:HD2  | 1:A:199:GLN:HG2  | 1.94                     | 0.49              |
| 1:C:159:LYS:HD2  | 1:C:199:GLN:HG2  | 1.94                     | 0.49              |
| 1:E:118:GLU:O    | 1:E:118:GLU:HG3  | 2.10                     | 0.49              |
| 1:E:142:CYS:HB2  | 1:E:149:SER:O    | 2.12                     | 0.49              |
| 2:F:17:MET:SD    | 2:F:23:GLY:HA3   | 2.52                     | 0.49              |
| 1:G:142:CYS:HB2  | 1:G:149:SER:O    | 2.12                     | 0.49              |
| 1:G:307:GLY:HA2  | 2:H:63:PHE:CE1   | 2.46                     | 0.49              |
| 2:J:125:GLN:HE21 | 2:J:157:TYR:H    | 1.58                     | 0.49              |
| 1:A:96:CYS:HB2   | 1:A:141:ALA:O    | 2.12                     | 0.49              |
| 2:H:113:SER:CB   | 2:L:2:LEU:HD22   | 2.42                     | 0.49              |
| 1:I:159:LYS:HD2  | 1:I:199:GLN:HG2  | 1.94                     | 0.49              |
| 2:L:123:ARG:HB2  | 2:L:138:PHE:CZ   | 2.47                     | 0.49              |
| 1:G:65:GLY:CA    | 1:G:94:GLY:HA2   | 2.42                     | 0.49              |
| 1:E:54:ALA:HB1   | 1:E:55:PRO:HD2   | 1.93                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:159:LYS:HD2  | 1:G:199:GLN:HG2 | 1.94                     | 0.49              |
| 1:I:214:LYS:HE3  | 1:I:216:PHE:CE2 | 2.48                     | 0.49              |
| 1:C:189:SER:HA   | 1:C:221:ALA:O   | 2.12                     | 0.49              |
| 2:B:151:SER:HB2  | 2:B:156:THR:O   | 2.12                     | 0.49              |
| 1:C:312:TYR:CD2  | 2:D:89:LEU:HD13 | 2.48                     | 0.49              |
| 2:B:50:ASN:OD1   | 1:E:28:LYS:HD2  | 2.12                     | 0.49              |
| 1:E:297:PRO:HG3  | 2:F:56:ILE:HA   | 1.94                     | 0.49              |
| 2:F:151:SER:HB2  | 2:F:156:THR:O   | 2.13                     | 0.49              |
| 1:K:11:ILE:O     | 2:L:10:ILE:HD13 | 2.11                     | 0.49              |
| 1:I:25:VAL:CG1   | 2:L:51:LYS:HG3  | 2.43                     | 0.49              |
| 2:J:79:ASN:HB2   | 2:L:68:LYS:HE3  | 1.94                     | 0.49              |
| 2:D:125:GLN:HE21 | 2:D:157:TYR:H   | 1.59                     | 0.49              |
| 1:E:67:ILE:HD13  | 1:E:111:LEU:CD2 | 2.43                     | 0.49              |
| 2:F:123:ARG:HB2  | 2:F:138:PHE:CZ  | 2.47                     | 0.49              |
| 1:G:327:ILE:CG2  | 1:G:328:PRO:CD  | 2.90                     | 0.49              |
| 1:G:224:PRO:HG2  | 1:I:209:SER:HA  | 1.95                     | 0.49              |
| 2:L:5:ALA:HB3    | 2:L:112:ASP:OD2 | 2.12                     | 0.49              |
| 1:A:327:ILE:CG2  | 1:A:328:PRO:CD  | 2.90                     | 0.49              |
| 2:B:142:HIS:CD2  | 2:B:161:LYS:HG2 | 2.43                     | 0.49              |
| 1:K:142:CYS:HB2  | 1:K:149:SER:O   | 2.12                     | 0.49              |
| 2:L:151:SER:HB2  | 2:L:156:THR:O   | 2.13                     | 0.49              |
| 1:E:307:GLY:HA2  | 2:F:63:PHE:CE1  | 2.48                     | 0.49              |
| 1:G:328:PRO:C    | 5:G:711:HOH:O   | 2.35                     | 0.49              |
| 1:K:159:LYS:HD2  | 1:K:199:GLN:HG2 | 1.94                     | 0.49              |
| 1:C:96:CYS:HB2   | 1:C:141:ALA:O   | 2.11                     | 0.48              |
| 1:C:65:GLY:CA    | 1:C:94:GLY:HA2  | 2.43                     | 0.48              |
| 2:D:17:MET:SD    | 2:D:23:GLY:HA3  | 2.53                     | 0.48              |
| 1:G:114:VAL:CG1  | 1:G:117:PHE:HB2 | 2.30                     | 0.48              |
| 1:C:67:ILE:HD13  | 1:C:111:LEU:CD2 | 2.43                     | 0.48              |
| 2:F:5:ALA:HB3    | 2:F:112:ASP:OD2 | 2.12                     | 0.48              |
| 1:K:324:LEU:HD23 | 1:K:324:LEU:N   | 2.29                     | 0.48              |
| 2:L:162:TYR:HD1  | 2:L:162:TYR:C   | 2.16                     | 0.48              |
| 2:B:47:GLU:HA    | 1:E:26:LEU:O    | 2.13                     | 0.48              |
| 1:G:63:ILE:HD11  | 1:G:85:ILE:HG21 | 1.95                     | 0.48              |
| 1:K:81:SER:HB3   | 1:K:115:SER:O   | 2.14                     | 0.48              |
| 1:A:65:GLY:CA    | 1:A:94:GLY:HA2  | 2.43                     | 0.48              |
| 1:A:81:SER:HB3   | 1:A:115:SER:O   | 2.13                     | 0.48              |
| 2:B:5:ALA:HB3    | 2:B:112:ASP:OD2 | 2.12                     | 0.48              |
| 2:B:123:ARG:HB2  | 2:B:138:PHE:CZ  | 2.48                     | 0.48              |
| 2:B:51:LYS:HG3   | 1:E:25:VAL:HG11 | 1.93                     | 0.48              |
| 1:E:189:SER:HA   | 1:E:221:ALA:O   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:313:VAL:CG1  | 1:E:315:SER:H    | 2.14                     | 0.48              |
| 2:H:2:LEU:HG     | 2:J:3:PHE:HZ     | 1.78                     | 0.48              |
| 2:L:17:MET:SD    | 2:L:23:GLY:HA3   | 2.54                     | 0.48              |
| 2:D:5:ALA:HB3    | 2:D:112:ASP:OD2  | 2.13                     | 0.48              |
| 1:G:297:PRO:HG3  | 2:H:56:ILE:HA    | 1.95                     | 0.48              |
| 1:I:65:GLY:CA    | 1:I:94:GLY:HA2   | 2.43                     | 0.48              |
| 1:I:76:LEU:CD1   | 1:I:76:LEU:O     | 2.59                     | 0.48              |
| 1:K:133:ASP:CB   | 5:K:719:HOH:O    | 2.61                     | 0.48              |
| 1:K:238:THR:CA   | 5:K:718:HOH:O    | 2.49                     | 0.48              |
| 1:K:327:ILE:CG2  | 1:K:328:PRO:CD   | 2.89                     | 0.48              |
| 1:K:67:ILE:HD13  | 1:K:111:LEU:CD2  | 2.43                     | 0.48              |
| 1:K:11:ILE:CD1   | 2:L:122:VAL:HG13 | 2.34                     | 0.48              |
| 1:A:8:THR:HB     | 2:B:138:PHE:O    | 2.14                     | 0.48              |
| 1:E:311:LYS:HG3  | 2:F:92:TRP:CE2   | 2.48                     | 0.48              |
| 1:E:77:SER:C     | 1:E:79:ALA:H     | 2.16                     | 0.48              |
| 2:H:123:ARG:HB2  | 2:H:138:PHE:CZ   | 2.48                     | 0.48              |
| 2:H:142:HIS:CE1  | 2:H:161:LYS:NZ   | 2.81                     | 0.48              |
| 1:I:67:ILE:HD13  | 1:I:111:LEU:CD2  | 2.43                     | 0.48              |
| 1:C:214:LYS:HE3  | 1:C:216:PHE:CE2  | 2.49                     | 0.48              |
| 1:E:129:TRP:CD2  | 1:E:157:LEU:HD11 | 2.49                     | 0.48              |
| 1:G:68:LEU:CD1   | 1:G:95:THR:HG22  | 2.44                     | 0.48              |
| 1:K:96:CYS:HB2   | 1:K:141:ALA:O    | 2.13                     | 0.48              |
| 2:D:87:GLY:HA3   | 2:F:88:PHE:CZ    | 2.49                     | 0.48              |
| 2:H:17:MET:SD    | 2:H:23:GLY:HA3   | 2.53                     | 0.48              |
| 2:L:162:TYR:CD1  | 2:L:162:TYR:C    | 2.87                     | 0.48              |
| 2:B:58:LYS:HD2   | 2:F:97:GLU:CB    | 2.41                     | 0.48              |
| 2:J:5:ALA:HB3    | 2:J:112:ASP:OD2  | 2.13                     | 0.48              |
| 1:K:16:ASN:ND2   | 5:K:710:HOH:O    | 2.09                     | 0.48              |
| 1:A:68:LEU:CD1   | 1:A:95:THR:HG22  | 2.44                     | 0.47              |
| 1:C:83:SER:HG    | 1:C:84:TYR:HD2   | 1.61                     | 0.47              |
| 5:B:203:HOH:O    | 2:D:64:THR:HG21  | 2.14                     | 0.47              |
| 1:E:324:LEU:N    | 1:E:324:LEU:HD23 | 2.29                     | 0.47              |
| 1:C:28:LYS:HD2   | 2:F:50:ASN:OD1   | 2.14                     | 0.47              |
| 2:J:17:MET:SD    | 2:J:23:GLY:HA3   | 2.54                     | 0.47              |
| 1:A:67:ILE:HD13  | 1:A:111:LEU:CD2  | 2.44                     | 0.47              |
| 2:B:17:MET:SD    | 2:B:23:GLY:HA3   | 2.54                     | 0.47              |
| 1:C:272:ILE:HD11 | 1:C:306:ILE:HD12 | 1.96                     | 0.47              |
| 1:E:195:GLN:HA   | 1:E:198:TYR:O    | 2.14                     | 0.47              |
| 1:G:67:ILE:HD13  | 1:G:111:LEU:CD2  | 2.43                     | 0.47              |
| 1:I:63:ILE:HD11  | 1:I:85:ILE:HG21  | 1.96                     | 0.47              |
| 1:E:325:ARG:HG3  | 5:E:701:HOH:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:63:PHE:C     | 2:H:63:PHE:CD2   | 2.88                     | 0.47              |
| 1:I:114:VAL:CG1  | 1:I:117:PHE:HB2  | 2.30                     | 0.47              |
| 2:H:62:GLN:HG3   | 2:L:86:ASP:HB3   | 1.95                     | 0.47              |
| 2:B:63:PHE:C     | 2:B:63:PHE:CD2   | 2.87                     | 0.47              |
| 1:C:317:LYS:CA   | 5:C:712:HOH:O    | 2.60                     | 0.47              |
| 1:E:81:SER:HB3   | 1:E:115:SER:O    | 2.14                     | 0.47              |
| 1:E:214:LYS:HE3  | 1:E:216:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:9:LEU:HD12   | 2:F:152:VAL:HG11 | 1.96                     | 0.47              |
| 1:K:133:ASP:CG   | 5:K:713:HOH:O    | 2.49                     | 0.47              |
| 1:K:44:ASN:C     | 1:K:44:ASN:ND2   | 2.67                     | 0.47              |
| 1:G:11:ILE:HD12  | 2:H:119:TYR:HA   | 1.95                     | 0.47              |
| 1:K:214:LYS:HE3  | 1:K:216:PHE:CE2  | 2.50                     | 0.47              |
| 1:K:269:SER:CB   | 5:K:702:HOH:O    | 2.63                     | 0.47              |
| 1:C:63:ILE:HD11  | 1:C:85:ILE:HG21  | 1.97                     | 0.47              |
| 1:E:44:ASN:ND2   | 1:E:44:ASN:C     | 2.68                     | 0.47              |
| 1:G:214:LYS:HE3  | 1:G:216:PHE:CE2  | 2.49                     | 0.47              |
| 1:G:93:ASN:ND2   | 5:G:703:HOH:O    | 2.43                     | 0.47              |
| 1:K:195:GLN:HA   | 1:K:198:TYR:O    | 2.15                     | 0.47              |
| 1:E:323:GLY:O    | 2:F:111:HIS:CD2  | 2.68                     | 0.47              |
| 2:F:125:GLN:NE2  | 2:F:157:TYR:H    | 2.13                     | 0.47              |
| 1:G:268:GLY:O    | 2:H:63:PHE:HE2   | 1.97                     | 0.47              |
| 2:J:63:PHE:CD2   | 2:J:63:PHE:C     | 2.87                     | 0.47              |
| 1:K:129:TRP:CD2  | 1:K:157:LEU:HD11 | 2.50                     | 0.47              |
| 1:K:227:ARG:O    | 1:K:228:GLU:HB2  | 2.14                     | 0.47              |
| 2:B:123:ARG:HH22 | 2:D:123:ARG:HH22 | 1.62                     | 0.47              |
| 2:D:63:PHE:CD2   | 2:D:63:PHE:C     | 2.87                     | 0.47              |
| 1:I:195:GLN:HA   | 1:I:198:TYR:O    | 2.15                     | 0.47              |
| 2:J:161:LYS:CD   | 2:J:161:LYS:H    | 2.27                     | 0.47              |
| 1:K:72:GLU:HG3   | 3:K:601:NAG:N2   | 2.30                     | 0.47              |
| 1:K:7:ASP:HB2    | 2:L:140:PHE:HB2  | 1.97                     | 0.47              |
| 1:C:195:GLN:HA   | 1:C:198:TYR:O    | 2.15                     | 0.47              |
| 1:E:311:LYS:HE2  | 2:F:61:THR:HG22  | 1.97                     | 0.47              |
| 1:G:81:SER:HB3   | 1:G:115:SER:O    | 2.14                     | 0.47              |
| 1:G:242:PRO:CG   | 5:G:708:HOH:O    | 2.18                     | 0.47              |
| 1:G:324:LEU:HD23 | 1:G:324:LEU:N    | 2.29                     | 0.47              |
| 1:A:272:ILE:HD11 | 1:A:306:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:324:LEU:N    | 1:A:324:LEU:HD23 | 2.30                     | 0.46              |
| 2:B:60:ASN:HD21  | 1:E:314:LYS:CD   | 2.08                     | 0.46              |
| 1:C:266:ASN:H    | 1:C:266:ASN:ND2  | 2.14                     | 0.46              |
| 2:D:79:ASN:HB2   | 2:F:68:LYS:HE3   | 1.96                     | 0.46              |
| 1:E:63:ILE:HD11  | 1:E:85:ILE:HG21  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:91:SER:C     | 5:K:721:HOH:O    | 2.46                     | 0.46              |
| 1:C:317:LYS:HA   | 5:C:712:HOH:O    | 2.14                     | 0.46              |
| 1:C:327:ILE:CG2  | 1:C:328:PRO:CD   | 2.89                     | 0.46              |
| 1:C:81:SER:HB3   | 1:C:115:SER:O    | 2.15                     | 0.46              |
| 2:D:159:TYR:O    | 2:D:161:LYS:N    | 2.48                     | 0.46              |
| 2:F:63:PHE:C     | 2:F:63:PHE:CD2   | 2.88                     | 0.46              |
| 2:L:63:PHE:C     | 2:L:63:PHE:CD2   | 2.88                     | 0.46              |
| 2:H:129:ASN:N    | 2:H:129:ASN:HD22 | 2.14                     | 0.46              |
| 1:I:81:SER:C     | 1:I:82:TRP:CD2   | 2.88                     | 0.46              |
| 2:J:123:ARG:HB2  | 2:J:138:PHE:CZ   | 2.49                     | 0.46              |
| 1:K:49:LYS:HG3   | 1:K:281:CYS:O    | 2.15                     | 0.46              |
| 1:A:44:ASN:C     | 1:A:44:ASN:ND2   | 2.69                     | 0.46              |
| 1:G:266:ASN:H    | 1:G:266:ASN:ND2  | 2.14                     | 0.46              |
| 1:A:10:CYS:O     | 2:B:24:TYR:HA    | 2.16                     | 0.46              |
| 1:A:144:HIS:O    | 1:A:145:ALA:HB3  | 2.16                     | 0.46              |
| 1:A:63:ILE:HD11  | 1:A:85:ILE:HG21  | 1.97                     | 0.46              |
| 1:A:327:ILE:HG21 | 2:B:12:GLY:CA    | 2.46                     | 0.46              |
| 1:C:324:LEU:HD23 | 1:C:324:LEU:N    | 2.30                     | 0.46              |
| 1:G:26:LEU:HB3   | 2:J:47:GLU:HB3   | 1.97                     | 0.46              |
| 1:G:58:LEU:CD2   | 1:G:63:ILE:HD13  | 2.42                     | 0.46              |
| 1:I:44:ASN:ND2   | 1:I:44:ASN:C     | 2.69                     | 0.46              |
| 1:K:272:ILE:HD11 | 1:K:306:ILE:HD12 | 1.97                     | 0.46              |
| 1:K:322:THR:HB   | 2:L:48:ILE:HG21  | 1.98                     | 0.46              |
| 1:K:323:GLY:O    | 2:L:111:HIS:CD2  | 2.69                     | 0.46              |
| 1:A:11:ILE:HG12  | 2:B:24:TYR:HD2   | 1.80                     | 0.46              |
| 1:A:122:ILE:HG23 | 1:A:123:PHE:N    | 2.31                     | 0.46              |
| 1:E:312:TYR:CD2  | 2:F:89:LEU:HD13  | 2.51                     | 0.46              |
| 1:G:12:GLY:N     | 2:H:14:TRP:CH2   | 2.84                     | 0.46              |
| 1:G:50:LEU:CD1   | 1:G:306:ILE:HG22 | 2.43                     | 0.46              |
| 1:I:266:ASN:H    | 1:I:266:ASN:ND2  | 2.14                     | 0.46              |
| 1:I:324:LEU:N    | 1:I:324:LEU:HD23 | 2.31                     | 0.46              |
| 1:A:209:SER:HA   | 1:E:224:PRO:HG2  | 1.97                     | 0.46              |
| 1:E:266:ASN:H    | 1:E:266:ASN:ND2  | 2.14                     | 0.46              |
| 1:E:83:SER:HG    | 1:E:84:TYR:HD2   | 1.60                     | 0.46              |
| 1:K:63:ILE:HD11  | 1:K:85:ILE:HG21  | 1.97                     | 0.46              |
| 1:K:14:HIS:HB2   | 2:L:20:GLY:O     | 2.15                     | 0.46              |
| 1:A:266:ASN:ND2  | 1:A:266:ASN:H    | 2.15                     | 0.45              |
| 2:B:121:LYS:HB3  | 2:B:121:LYS:HE2  | 1.75                     | 0.45              |
| 2:B:129:ASN:HD22 | 2:B:129:ASN:N    | 2.14                     | 0.45              |
| 1:C:44:ASN:C     | 1:C:44:ASN:ND2   | 2.69                     | 0.45              |
| 2:D:146:ASN:HB2  | 5:D:209:HOH:O    | 2.02                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:195:GLN:HA   | 1:A:198:TYR:O    | 2.15                     | 0.45              |
| 1:C:227:ARG:CB   | 5:C:714:HOH:O    | 2.63                     | 0.45              |
| 1:E:327:ILE:HG21 | 2:F:12:GLY:HA3   | 1.96                     | 0.45              |
| 1:K:8:THR:HG22   | 2:L:139:GLU:CA   | 2.42                     | 0.45              |
| 2:L:125:GLN:NE2  | 2:L:157:TYR:H    | 2.14                     | 0.45              |
| 1:I:129:TRP:CD2  | 1:I:157:LEU:HD21 | 2.51                     | 0.45              |
| 1:K:183:TRP:HZ3  | 1:K:238:THR:HG22 | 1.82                     | 0.45              |
| 1:G:44:ASN:C     | 1:G:44:ASN:ND2   | 2.69                     | 0.45              |
| 2:J:164:GLU:O    | 2:J:165:GLU:CG   | 2.65                     | 0.45              |
| 1:K:313:VAL:CG1  | 1:K:315:SER:H    | 2.14                     | 0.45              |
| 1:A:214:LYS:HE3  | 1:A:216:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:78:THR:CG2   | 1:A:78:THR:O     | 2.64                     | 0.45              |
| 2:D:159:TYR:O    | 2:D:161:LYS:HG2  | 2.15                     | 0.45              |
| 2:F:129:ASN:HD22 | 2:F:129:ASN:N    | 2.14                     | 0.45              |
| 2:B:113:SER:CB   | 2:F:2:LEU:HD22   | 2.47                     | 0.45              |
| 2:D:86:ASP:HB3   | 2:F:62:GLN:HG3   | 1.98                     | 0.45              |
| 2:J:129:ASN:N    | 2:J:129:ASN:HD22 | 2.15                     | 0.45              |
| 2:J:161:LYS:CD   | 2:J:161:LYS:N    | 2.80                     | 0.45              |
| 1:K:144:HIS:O    | 1:K:145:ALA:HB3  | 2.17                     | 0.45              |
| 1:K:164:TYR:CZ   | 1:K:252:GLY:HA2  | 2.52                     | 0.45              |
| 1:E:122:ILE:HG23 | 1:E:123:PHE:N    | 2.32                     | 0.45              |
| 1:G:122:ILE:HG23 | 1:G:123:PHE:N    | 2.32                     | 0.45              |
| 1:K:266:ASN:ND2  | 1:K:266:ASN:H    | 2.15                     | 0.45              |
| 2:L:129:ASN:HD22 | 2:L:129:ASN:N    | 2.13                     | 0.45              |
| 1:A:83:SER:HG    | 1:A:84:TYR:HD2   | 1.65                     | 0.45              |
| 2:D:129:ASN:N    | 2:D:129:ASN:HD22 | 2.14                     | 0.45              |
| 1:G:327:ILE:HD12 | 5:G:713:HOH:O    | 2.17                     | 0.45              |
| 1:I:312:TYR:CD2  | 2:J:89:LEU:HD13  | 2.52                     | 0.45              |
| 2:J:164:GLU:CG   | 2:J:164:GLU:O    | 2.49                     | 0.45              |
| 1:C:164:TYR:CZ   | 1:C:252:GLY:HA2  | 2.52                     | 0.45              |
| 1:C:59:GLY:O     | 1:C:91:SER:HB3   | 2.17                     | 0.45              |
| 1:I:143:PRO:O    | 4:I:601:NAG:H82  | 2.17                     | 0.45              |
| 2:J:159:TYR:CD1  | 2:J:161:LYS:CE   | 3.00                     | 0.45              |
| 2:B:157:TYR:CD2  | 2:B:158:ASP:O    | 2.70                     | 0.45              |
| 2:D:159:TYR:N    | 2:D:160:PRO:CD   | 2.80                     | 0.45              |
| 1:E:272:ILE:HD11 | 1:E:306:ILE:HD12 | 1.98                     | 0.45              |
| 1:G:129:TRP:CD2  | 1:G:157:LEU:HD21 | 2.51                     | 0.45              |
| 1:I:328:PRO:HA   | 5:I:706:HOH:O    | 1.99                     | 0.45              |
| 1:A:227:ARG:O    | 1:A:228:GLU:HB2  | 2.17                     | 0.44              |
| 1:E:268:GLY:O    | 2:F:63:PHE:HE2   | 2.01                     | 0.44              |
| 2:B:59:MET:HB2   | 2:F:94:TYR:CE1   | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:268:GLY:O    | 2:J:63:PHE:HE2   | 2.01                     | 0.44              |
| 1:K:59:GLY:O     | 1:K:91:SER:HB3   | 2.17                     | 0.44              |
| 1:A:129:TRP:CD2  | 1:A:157:LEU:HD21 | 2.52                     | 0.44              |
| 1:A:179:VAL:N    | 5:A:708:HOH:O    | 2.46                     | 0.44              |
| 1:A:26:LEU:HD12  | 2:B:105:GLU:OE2  | 2.17                     | 0.44              |
| 1:K:122:ILE:HG23 | 1:K:123:PHE:N    | 2.31                     | 0.44              |
| 1:K:172:ILE:O    | 1:K:172:ILE:HG23 | 2.18                     | 0.44              |
| 1:A:267:ALA:C    | 5:A:712:HOH:O    | 2.54                     | 0.44              |
| 1:A:313:VAL:CG1  | 1:A:315:SER:H    | 2.14                     | 0.44              |
| 1:A:57:HIS:O     | 1:A:76:LEU:HD22  | 2.18                     | 0.44              |
| 2:B:159:TYR:O    | 2:B:159:TYR:HD2  | 1.99                     | 0.44              |
| 1:E:14:HIS:CB    | 2:F:21:TRP:HA    | 2.47                     | 0.44              |
| 1:I:122:ILE:HG23 | 1:I:123:PHE:N    | 2.32                     | 0.44              |
| 1:K:93:ASN:CG    | 5:K:708:HOH:O    | 2.56                     | 0.44              |
| 1:K:327:ILE:HG21 | 2:L:13:GLY:H     | 1.80                     | 0.44              |
| 1:A:172:ILE:O    | 1:A:172:ILE:HG23 | 2.18                     | 0.44              |
| 4:A:602:NAG:C6   | 4:A:603:NAG:N2   | 2.71                     | 0.44              |
| 1:I:302:HIS:HA   | 1:I:303:PRO:HD3  | 1.79                     | 0.44              |
| 1:I:57:HIS:HE1   | 1:I:59:GLY:HA2   | 1.83                     | 0.44              |
| 1:A:113:SER:HB2  | 1:A:269:SER:HB3  | 1.99                     | 0.44              |
| 1:A:314:LYS:HD2  | 2:D:60:ASN:ND2   | 2.32                     | 0.44              |
| 1:E:144:HIS:O    | 1:E:145:ALA:HB3  | 2.17                     | 0.44              |
| 1:G:183:TRP:HZ3  | 1:G:238:THR:HG22 | 1.82                     | 0.44              |
| 1:I:159:LYS:NZ   | 1:I:199:GLN:HE21 | 2.15                     | 0.44              |
| 1:I:272:ILE:HD11 | 1:I:306:ILE:HD12 | 1.99                     | 0.44              |
| 1:K:205:VAL:HG21 | 1:K:254:LEU:HD13 | 1.99                     | 0.44              |
| 1:K:307:GLY:N    | 5:K:709:HOH:O    | 2.51                     | 0.44              |
| 1:C:129:TRP:CD2  | 1:C:157:LEU:HD21 | 2.53                     | 0.44              |
| 1:E:113:SER:HB2  | 1:E:269:SER:HB3  | 1.99                     | 0.44              |
| 1:G:57:HIS:HE1   | 1:G:59:GLY:HA2   | 1.82                     | 0.44              |
| 2:B:159:TYR:C    | 2:B:159:TYR:HD2  | 2.21                     | 0.44              |
| 1:C:296:LEU:HA   | 1:C:297:PRO:HD3  | 1.82                     | 0.44              |
| 5:B:203:HOH:O    | 2:D:64:THR:CG2   | 2.65                     | 0.44              |
| 1:E:183:TRP:HZ3  | 1:E:238:THR:HG22 | 1.82                     | 0.44              |
| 1:G:172:ILE:O    | 1:G:172:ILE:HG23 | 2.17                     | 0.44              |
| 1:I:327:ILE:HG22 | 1:I:328:PRO:N    | 2.31                     | 0.44              |
| 1:A:164:TYR:CZ   | 1:A:252:GLY:HA2  | 2.53                     | 0.44              |
| 1:A:296:LEU:HA   | 1:A:297:PRO:HD3  | 1.82                     | 0.44              |
| 2:B:86:ASP:HB3   | 2:D:62:GLN:HG3   | 1.98                     | 0.44              |
| 1:E:267:ALA:C    | 5:E:703:HOH:O    | 2.56                     | 0.44              |
| 1:K:113:SER:HB2  | 1:K:269:SER:HB3  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:78:THR:HG22  | 1:K:78:THR:O     | 2.18                     | 0.44              |
| 1:A:183:TRP:HZ3  | 1:A:238:THR:HG22 | 1.82                     | 0.44              |
| 2:F:159:TYR:CB   | 2:F:161:LYS:HE2  | 2.37                     | 0.44              |
| 1:G:164:TYR:CZ   | 1:G:252:GLY:HA2  | 2.52                     | 0.44              |
| 1:I:183:TRP:HZ3  | 1:I:238:THR:HG22 | 1.83                     | 0.44              |
| 1:I:113:SER:HB2  | 1:I:269:SER:HB3  | 1.99                     | 0.44              |
| 1:A:25:VAL:HG21  | 2:B:102:LEU:HD22 | 1.98                     | 0.43              |
| 1:A:59:GLY:O     | 1:A:91:SER:HB3   | 2.17                     | 0.43              |
| 1:C:70:ASN:OD1   | 1:C:71:PRO:HD2   | 2.18                     | 0.43              |
| 1:G:144:HIS:O    | 1:G:145:ALA:HB3  | 2.17                     | 0.43              |
| 1:G:50:LEU:HD23  | 1:G:50:LEU:HA    | 1.87                     | 0.43              |
| 2:J:160:PRO:HG3  | 5:J:203:HOH:O    | 2.15                     | 0.43              |
| 1:K:82:TRP:CZ2   | 1:K:114:VAL:HG13 | 2.53                     | 0.43              |
| 1:K:72:GLU:HG3   | 3:K:601:NAG:HN2  | 1.83                     | 0.43              |
| 1:A:312:TYR:HD2  | 2:B:89:LEU:HD13  | 1.82                     | 0.43              |
| 1:G:113:SER:HB2  | 1:G:269:SER:HB3  | 1.99                     | 0.43              |
| 1:I:164:TYR:CZ   | 1:I:252:GLY:HA2  | 2.53                     | 0.43              |
| 2:J:121:LYS:HE2  | 2:J:121:LYS:HB3  | 1.76                     | 0.43              |
| 1:A:57:HIS:HE1   | 1:A:59:GLY:HA2   | 1.84                     | 0.43              |
| 1:C:172:ILE:HG23 | 1:C:172:ILE:O    | 2.18                     | 0.43              |
| 1:E:59:GLY:O     | 1:E:91:SER:HB3   | 2.18                     | 0.43              |
| 1:G:59:GLY:O     | 1:G:91:SER:HB3   | 2.17                     | 0.43              |
| 1:G:11:ILE:O     | 2:H:10:ILE:HD13  | 2.19                     | 0.43              |
| 1:K:141:ALA:O    | 1:K:227:ARG:NH1  | 2.51                     | 0.43              |
| 1:C:144:HIS:O    | 1:C:145:ALA:HB3  | 2.18                     | 0.43              |
| 1:C:113:SER:HB2  | 1:C:269:SER:HB3  | 2.00                     | 0.43              |
| 1:G:22:VAL:HG21  | 1:G:321:ALA:HB2  | 2.00                     | 0.43              |
| 1:I:22:VAL:HG21  | 1:I:321:ALA:HB2  | 2.01                     | 0.43              |
| 1:C:122:ILE:HG23 | 1:C:123:PHE:N    | 2.33                     | 0.43              |
| 1:C:266:ASN:O    | 1:C:266:ASN:ND2  | 2.50                     | 0.43              |
| 1:G:176:GLY:C    | 5:G:708:HOH:O    | 2.44                     | 0.43              |
| 2:B:159:TYR:C    | 2:B:159:TYR:CD2  | 2.92                     | 0.43              |
| 2:H:158:ASP:C    | 2:H:160:PRO:HD3  | 2.39                     | 0.43              |
| 1:I:50:LEU:HD23  | 1:I:50:LEU:HA    | 1.87                     | 0.43              |
| 1:A:327:ILE:HG22 | 1:A:328:PRO:N    | 2.34                     | 0.43              |
| 1:A:68:LEU:HD12  | 1:A:95:THR:HG22  | 2.01                     | 0.43              |
| 1:E:104:TYR:CE2  | 1:E:108:ARG:HD2  | 2.54                     | 0.43              |
| 1:K:104:TYR:CE2  | 1:K:108:ARG:HD2  | 2.53                     | 0.43              |
| 1:A:276:THR:HA   | 1:A:277:PRO:HD3  | 1.85                     | 0.43              |
| 1:A:58:LEU:CD2   | 1:A:63:ILE:HD13  | 2.45                     | 0.43              |
| 1:C:136:LYS:HB2  | 1:C:158:VAL:HG21 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:155:ILE:HG22 | 1:C:157:LEU:HD13 | 2.01                     | 0.43              |
| 1:C:141:ALA:O    | 1:C:227:ARG:NH1  | 2.52                     | 0.43              |
| 1:C:183:TRP:HZ3  | 1:C:238:THR:HG22 | 1.82                     | 0.43              |
| 1:E:164:TYR:CZ   | 1:E:252:GLY:HA2  | 2.54                     | 0.43              |
| 1:E:324:LEU:HB3  | 2:F:111:HIS:CD2  | 2.54                     | 0.43              |
| 1:E:327:ILE:HG21 | 2:F:13:GLY:H     | 1.81                     | 0.43              |
| 1:I:136:LYS:HB2  | 1:I:158:VAL:HG21 | 2.01                     | 0.43              |
| 1:K:159:LYS:NZ   | 1:K:199:GLN:HE21 | 2.16                     | 0.43              |
| 1:K:189:SER:HB2  | 1:K:222:ILE:HD13 | 2.01                     | 0.43              |
| 1:K:22:VAL:HG21  | 1:K:321:ALA:HB2  | 2.01                     | 0.43              |
| 1:K:7:ASP:O      | 2:L:140:PHE:HB2  | 2.19                     | 0.43              |
| 1:K:13:TYR:CD2   | 2:L:6:ILE:HG12   | 2.54                     | 0.43              |
| 1:A:63:ILE:HG12  | 1:A:87:GLU:OE1   | 2.19                     | 0.43              |
| 1:C:11:ILE:O     | 2:D:10:ILE:HD13  | 2.19                     | 0.43              |
| 1:E:141:ALA:O    | 1:E:227:ARG:NH1  | 2.52                     | 0.43              |
| 1:K:269:SER:HB3  | 5:K:702:HOH:O    | 2.19                     | 0.43              |
| 1:A:104:TYR:CE2  | 1:A:108:ARG:HD2  | 2.54                     | 0.42              |
| 1:A:141:ALA:O    | 1:A:227:ARG:NH1  | 2.51                     | 0.42              |
| 1:A:268:GLY:O    | 2:B:63:PHE:HE2   | 2.01                     | 0.42              |
| 1:C:314:LYS:HB2  | 1:C:314:LYS:HE3  | 1.80                     | 0.42              |
| 1:E:12:GLY:N     | 5:E:706:HOH:O    | 2.51                     | 0.42              |
| 1:I:141:ALA:O    | 1:I:227:ARG:NH1  | 2.52                     | 0.42              |
| 1:K:16:ASN:CB    | 5:K:710:HOH:O    | 2.62                     | 0.42              |
| 1:E:205:VAL:HG21 | 1:E:254:LEU:HD13 | 2.01                     | 0.42              |
| 1:E:22:VAL:HG21  | 1:E:321:ALA:HB2  | 2.01                     | 0.42              |
| 1:G:136:LYS:HB2  | 1:G:158:VAL:HG21 | 2.01                     | 0.42              |
| 1:G:272:ILE:HD11 | 1:G:306:ILE:HD12 | 2.00                     | 0.42              |
| 2:J:164:GLU:O    | 2:J:165:GLU:HG2  | 2.19                     | 0.42              |
| 4:A:602:NAG:C6   | 4:A:603:NAG:H82  | 2.49                     | 0.42              |
| 4:C:602:NAG:H61  | 4:C:603:NAG:H2   | 2.01                     | 0.42              |
| 1:E:11:ILE:CD1   | 2:F:119:TYR:HA   | 2.44                     | 0.42              |
| 1:K:50:LEU:HD21  | 1:K:306:ILE:HG22 | 2.02                     | 0.42              |
| 1:A:53:VAL:HG23  | 1:A:53:VAL:H     | 1.51                     | 0.42              |
| 1:C:268:GLY:O    | 2:D:63:PHE:HE2   | 2.03                     | 0.42              |
| 2:B:58:LYS:CD    | 2:F:97:GLU:HB3   | 2.44                     | 0.42              |
| 1:G:68:LEU:HD12  | 1:G:95:THR:HG22  | 2.01                     | 0.42              |
| 1:G:11:ILE:CD1   | 2:H:119:TYR:HA   | 2.49                     | 0.42              |
| 1:I:144:HIS:O    | 1:I:145:ALA:HB3  | 2.19                     | 0.42              |
| 1:I:296:LEU:HA   | 1:I:297:PRO:HD3  | 1.82                     | 0.42              |
| 1:K:227:ARG:HH22 | 3:K:601:NAG:HO3  | 1.55                     | 0.42              |
| 1:K:327:ILE:HG22 | 1:K:328:PRO:N    | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:104:TYR:CE2  | 1:C:108:ARG:HD2  | 2.54                     | 0.42              |
| 1:C:159:LYS:NZ   | 1:C:199:GLN:HE21 | 2.17                     | 0.42              |
| 1:E:136:LYS:HB2  | 1:E:158:VAL:HG21 | 2.02                     | 0.42              |
| 1:G:327:ILE:HG22 | 1:G:328:PRO:N    | 2.33                     | 0.42              |
| 1:G:55:PRO:HB3   | 1:G:84:TYR:CZ    | 2.55                     | 0.42              |
| 1:I:59:GLY:O     | 1:I:91:SER:HB3   | 2.18                     | 0.42              |
| 2:L:121:LYS:HB3  | 2:L:121:LYS:HE2  | 1.76                     | 0.42              |
| 1:A:50:LEU:HB2   | 1:A:83:SER:HB2   | 2.02                     | 0.42              |
| 1:C:327:ILE:HG22 | 1:C:328:PRO:N    | 2.35                     | 0.42              |
| 1:C:55:PRO:HB3   | 1:C:84:TYR:CZ    | 2.54                     | 0.42              |
| 1:E:266:ASN:ND2  | 1:E:266:ASN:O    | 2.52                     | 0.42              |
| 1:E:276:THR:HA   | 1:E:277:PRO:HD3  | 1.85                     | 0.42              |
| 1:E:63:ILE:HG12  | 1:E:87:GLU:OE1   | 2.20                     | 0.42              |
| 2:F:121:LYS:HE2  | 2:F:121:LYS:HB3  | 1.76                     | 0.42              |
| 1:G:195:GLN:HA   | 1:G:198:TYR:O    | 2.20                     | 0.42              |
| 1:A:155:ILE:HG22 | 1:A:157:LEU:HD13 | 2.01                     | 0.42              |
| 1:E:55:PRO:HB3   | 1:E:84:TYR:CZ    | 2.55                     | 0.42              |
| 1:K:136:LYS:HB2  | 1:K:158:VAL:HG21 | 2.01                     | 0.42              |
| 1:K:14:HIS:CG    | 1:K:15:ALA:N     | 2.88                     | 0.42              |
| 1:A:55:PRO:HB3   | 1:A:84:TYR:CZ    | 2.54                     | 0.42              |
| 2:D:145:ASP:HB2  | 5:D:208:HOH:O    | 2.18                     | 0.42              |
| 1:G:189:SER:HB2  | 1:G:222:ILE:HD13 | 2.02                     | 0.42              |
| 1:E:155:ILE:HG22 | 1:E:157:LEU:HD23 | 2.01                     | 0.42              |
| 1:E:189:SER:HB2  | 1:E:222:ILE:HD13 | 2.02                     | 0.42              |
| 1:G:63:ILE:HG12  | 1:G:87:GLU:OE1   | 2.19                     | 0.42              |
| 1:G:72:GLU:HG3   | 1:G:93:ASN:HD22  | 1.84                     | 0.42              |
| 1:C:109:GLU:OE1  | 5:C:715:HOH:O    | 2.21                     | 0.42              |
| 1:E:53:VAL:HG12  | 1:E:54:ALA:O     | 2.20                     | 0.42              |
| 1:G:137:GLY:HA3  | 1:G:156:TRP:HB3  | 2.02                     | 0.42              |
| 1:G:159:LYS:NZ   | 1:G:199:GLN:HE21 | 2.18                     | 0.42              |
| 1:G:266:ASN:O    | 1:G:266:ASN:ND2  | 2.49                     | 0.42              |
| 1:G:309:CYS:O    | 2:H:61:THR:HG21  | 2.20                     | 0.42              |
| 1:K:296:LEU:HA   | 1:K:297:PRO:HD3  | 1.84                     | 0.42              |
| 2:L:20:GLY:HA3   | 2:L:36:ALA:HB1   | 2.02                     | 0.42              |
| 1:A:136:LYS:HB2  | 1:A:158:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:178:GLU:OE1  | 1:A:265:ARG:NH1  | 2.52                     | 0.41              |
| 4:A:602:NAG:H61  | 4:A:603:NAG:C8   | 2.48                     | 0.41              |
| 1:E:7:ASP:O      | 2:F:140:PHE:HB2  | 2.20                     | 0.41              |
| 1:I:172:ILE:HG23 | 1:I:172:ILE:O    | 2.18                     | 0.41              |
| 1:K:53:VAL:HG12  | 1:K:54:ALA:O     | 2.20                     | 0.41              |
| 1:C:178:GLU:OE1  | 1:C:265:ARG:NH1  | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:72:HIS:CD2   | 2:F:73:LEU:HG    | 2.55                     | 0.41              |
| 1:G:178:GLU:OE1  | 1:G:265:ARG:NH1  | 2.53                     | 0.41              |
| 1:G:307:GLY:HA2  | 2:H:63:PHE:CD1   | 2.55                     | 0.41              |
| 1:G:325:ARG:C    | 5:G:713:HOH:O    | 2.59                     | 0.41              |
| 1:I:55:PRO:HB3   | 1:I:84:TYR:CZ    | 2.55                     | 0.41              |
| 2:J:159:TYR:N    | 2:J:160:PRO:HD3  | 2.35                     | 0.41              |
| 2:B:2:LEU:O      | 2:D:113:SER:OG   | 2.30                     | 0.41              |
| 1:C:70:ASN:HA    | 1:C:71:PRO:HD3   | 1.94                     | 0.41              |
| 1:G:314:LYS:HE3  | 1:G:314:LYS:HB2  | 1.79                     | 0.41              |
| 1:I:189:SER:HB2  | 1:I:222:ILE:HD13 | 2.02                     | 0.41              |
| 2:J:70:PHE:HB3   | 2:J:74:GLU:HB2   | 2.02                     | 0.41              |
| 1:K:8:THR:CA     | 2:L:138:PHE:O    | 2.67                     | 0.41              |
| 2:H:88:PHE:CZ    | 2:L:87:GLY:HA3   | 2.56                     | 0.41              |
| 1:A:159:LYS:NZ   | 1:A:199:GLN:HE21 | 2.17                     | 0.41              |
| 1:C:137:GLY:HA3  | 1:C:156:TRP:HB3  | 2.02                     | 0.41              |
| 2:F:160:PRO:C    | 5:F:207:HOH:O    | 2.49                     | 0.41              |
| 1:G:141:ALA:O    | 1:G:227:ARG:NH1  | 2.52                     | 0.41              |
| 1:G:296:LEU:HA   | 1:G:297:PRO:HD3  | 1.83                     | 0.41              |
| 1:K:155:ILE:HG22 | 1:K:157:LEU:HD23 | 2.01                     | 0.41              |
| 1:K:63:ILE:HG12  | 1:K:87:GLU:OE1   | 2.20                     | 0.41              |
| 1:A:24:THR:HG22  | 2:B:104:ASN:HB3  | 2.02                     | 0.41              |
| 1:E:167:LEU:HD23 | 1:E:167:LEU:O    | 2.21                     | 0.41              |
| 1:E:159:LYS:NZ   | 1:E:199:GLN:HE21 | 2.18                     | 0.41              |
| 2:B:51:LYS:CG    | 1:E:25:VAL:HG12  | 2.41                     | 0.41              |
| 1:G:70:ASN:OD1   | 1:G:71:PRO:HD2   | 2.21                     | 0.41              |
| 1:I:200:ASN:HB3  | 5:I:709:HOH:O    | 2.20                     | 0.41              |
| 1:I:48:CYS:HB3   | 1:I:281:CYS:O    | 2.21                     | 0.41              |
| 1:A:137:GLY:HA3  | 1:A:156:TRP:HB3  | 2.02                     | 0.41              |
| 2:B:160:PRO:HD2  | 2:B:161:LYS:HD2  | 2.02                     | 0.41              |
| 2:B:20:GLY:HA3   | 2:B:36:ALA:HB1   | 2.03                     | 0.41              |
| 2:B:60:ASN:O     | 1:E:314:LYS:NZ   | 2.49                     | 0.41              |
| 2:D:158:ASP:OD2  | 2:D:159:TYR:N    | 2.54                     | 0.41              |
| 1:E:302:HIS:HA   | 1:E:303:PRO:HD3  | 1.79                     | 0.41              |
| 2:H:72:HIS:CD2   | 2:H:73:LEU:HG    | 2.55                     | 0.41              |
| 1:I:282:ASN:N    | 1:I:282:ASN:OD1  | 2.53                     | 0.41              |
| 1:K:302:HIS:HA   | 1:K:303:PRO:HD3  | 1.79                     | 0.41              |
| 1:C:22:VAL:HG21  | 1:C:321:ALA:HB2  | 2.02                     | 0.41              |
| 2:F:162:TYR:HD1  | 5:F:207:HOH:O    | 2.03                     | 0.41              |
| 1:I:283:THR:OG1  | 1:I:291:ALA:HB1  | 2.20                     | 0.41              |
| 1:K:148:LYS:CA   | 5:K:712:HOH:O    | 2.48                     | 0.41              |
| 1:K:266:ASN:ND2  | 1:K:266:ASN:O    | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:VAL:HG12  | 1:A:54:ALA:O     | 2.21                     | 0.41              |
| 1:E:283:THR:OG1  | 1:E:291:ALA:HB1  | 2.21                     | 0.41              |
| 1:E:314:LYS:HE3  | 1:E:314:LYS:HB2  | 1.80                     | 0.41              |
| 1:I:292:ILE:CG2  | 1:I:294:THR:HG22 | 2.51                     | 0.41              |
| 1:I:63:ILE:HG12  | 1:I:87:GLU:OE1   | 2.19                     | 0.41              |
| 1:K:133:ASP:CG   | 5:K:719:HOH:O    | 2.56                     | 0.41              |
| 1:K:307:GLY:C    | 5:K:709:HOH:O    | 2.59                     | 0.41              |
| 1:K:55:PRO:HB3   | 1:K:84:TYR:CZ    | 2.56                     | 0.41              |
| 1:C:63:ILE:HG13  | 1:C:108:ARG:HG2  | 2.01                     | 0.41              |
| 1:E:172:ILE:HG23 | 1:E:172:ILE:O    | 2.21                     | 0.41              |
| 1:E:324:LEU:H    | 1:E:324:LEU:HD23 | 1.86                     | 0.41              |
| 1:G:53:VAL:HG12  | 1:G:54:ALA:O     | 2.20                     | 0.41              |
| 2:H:142:HIS:CE1  | 2:H:161:LYS:HZ2  | 2.39                     | 0.41              |
| 1:C:14:HIS:CG    | 1:C:15:ALA:N     | 2.89                     | 0.41              |
| 1:C:49:LYS:HD3   | 1:C:54:ALA:HB2   | 2.03                     | 0.41              |
| 1:E:63:ILE:HG13  | 1:E:108:ARG:HG2  | 2.03                     | 0.41              |
| 1:E:82:TRP:CZ2   | 1:E:114:VAL:HG13 | 2.55                     | 0.41              |
| 2:F:151:SER:O    | 2:F:157:TYR:N    | 2.54                     | 0.41              |
| 1:G:155:ILE:HG22 | 1:G:157:LEU:HD13 | 2.02                     | 0.41              |
| 1:I:155:ILE:HG22 | 1:I:157:LEU:HD13 | 2.03                     | 0.41              |
| 2:B:28:ASN:HD22  | 2:B:28:ASN:H     | 1.69                     | 0.41              |
| 1:E:14:HIS:CG    | 1:E:15:ALA:N     | 2.89                     | 0.41              |
| 1:E:292:ILE:CG2  | 1:E:294:THR:HG22 | 2.49                     | 0.41              |
| 1:I:178:GLU:OE1  | 1:I:265:ARG:NH1  | 2.54                     | 0.41              |
| 1:I:70:ASN:OD1   | 1:I:71:PRO:HD2   | 2.21                     | 0.41              |
| 1:I:25:VAL:CG2   | 2:J:102:LEU:HD12 | 2.49                     | 0.41              |
| 1:K:297:PRO:HG3  | 2:L:56:ILE:HA    | 2.03                     | 0.41              |
| 1:C:53:VAL:CG2   | 1:C:82:TRP:HA    | 2.51                     | 0.40              |
| 1:E:271:ILE:C    | 5:E:705:HOH:O    | 2.51                     | 0.40              |
| 2:F:161:LYS:C    | 5:F:207:HOH:O    | 2.57                     | 0.40              |
| 1:G:283:THR:OG1  | 1:G:291:ALA:HB1  | 2.21                     | 0.40              |
| 1:I:50:LEU:CD1   | 1:I:306:ILE:HG22 | 2.42                     | 0.40              |
| 1:K:13:TYR:CD2   | 2:L:115:VAL:HG21 | 2.56                     | 0.40              |
| 1:K:312:TYR:CD2  | 2:L:89:LEU:HD13  | 2.56                     | 0.40              |
| 1:A:22:VAL:HG21  | 1:A:321:ALA:HB2  | 2.02                     | 0.40              |
| 1:A:70:ASN:OD1   | 1:A:71:PRO:HD2   | 2.21                     | 0.40              |
| 1:G:60:LYS:HB2   | 1:G:60:LYS:HE3   | 1.88                     | 0.40              |
| 1:I:195:GLN:HB2  | 1:I:195:GLN:HE21 | 1.70                     | 0.40              |
| 1:K:314:LYS:HE3  | 1:K:314:LYS:HB2  | 1.79                     | 0.40              |
| 2:L:28:ASN:HD22  | 2:L:28:ASN:H     | 1.69                     | 0.40              |
| 1:A:48:CYS:HB3   | 1:A:281:CYS:O    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:70:PHE:HB3   | 2:B:74:GLU:HB2   | 2.03                     | 0.40              |
| 1:C:189:SER:HB2  | 1:C:222:ILE:HD13 | 2.02                     | 0.40              |
| 1:E:178:GLU:OE1  | 1:E:265:ARG:NH1  | 2.55                     | 0.40              |
| 1:G:276:THR:HA   | 1:G:277:PRO:HD3  | 1.84                     | 0.40              |
| 2:H:20:GLY:HA3   | 2:H:36:ALA:HB1   | 2.03                     | 0.40              |
| 1:I:212:TYR:O    | 5:I:708:HOH:O    | 2.22                     | 0.40              |
| 2:J:129:ASN:OD1  | 2:J:161:LYS:HB3  | 2.21                     | 0.40              |
| 1:K:324:LEU:HD23 | 1:K:324:LEU:H    | 1.87                     | 0.40              |
| 1:K:58:LEU:CD1   | 1:K:63:ILE:HD13  | 2.46                     | 0.40              |
| 1:E:70:ASN:OD1   | 1:E:71:PRO:HD2   | 2.21                     | 0.40              |
| 1:I:58:LEU:CD1   | 1:I:63:ILE:HD13  | 2.46                     | 0.40              |
| 1:I:297:PRO:HG3  | 2:J:56:ILE:HA    | 2.04                     | 0.40              |
| 1:K:13:TYR:CZ    | 2:L:6:ILE:HG23   | 2.56                     | 0.40              |
| 2:L:72:HIS:CD2   | 2:L:73:LEU:HG    | 2.57                     | 0.40              |
| 2:B:129:ASN:ND2  | 2:B:159:TYR:CE2  | 2.86                     | 0.40              |
| 1:G:104:TYR:CE2  | 1:G:108:ARG:HD2  | 2.55                     | 0.40              |
| 1:I:104:TYR:CE2  | 1:I:108:ARG:HD2  | 2.56                     | 0.40              |
| 1:K:9:LEU:CD1    | 2:L:152:VAL:HG11 | 2.49                     | 0.40              |

All (5) 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) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:C:76:LEU:CG   | 1:E:225:LYS:CE[1_455] | 1.33                     | 0.87              |
| 1:C:76:LEU:CG   | 1:E:225:LYS:NZ[1_455] | 1.38                     | 0.82              |
| 1:C:76:LEU:CD1  | 1:E:225:LYS:NZ[1_455] | 1.73                     | 0.47              |
| 1:C:76:LEU:CD2  | 1:E:225:LYS:CE[1_455] | 1.86                     | 0.34              |
| 1:E:279:HIS:NE2 | 5:I:710:HOH:O[1_655]  | 2.17                     | 0.03              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 321/323 (99%)   | 304 (95%)  | 16 (5%)  | 1 (0%)   | 44          | 81  |
| 1   | C     | 320/323 (99%)   | 300 (94%)  | 19 (6%)  | 1 (0%)   | 44          | 81  |
| 1   | E     | 319/323 (99%)   | 300 (94%)  | 19 (6%)  | 0        | 100         | 100 |
| 1   | G     | 320/323 (99%)   | 299 (93%)  | 21 (7%)  | 0        | 100         | 100 |
| 1   | I     | 320/323 (99%)   | 299 (93%)  | 21 (7%)  | 0        | 100         | 100 |
| 1   | K     | 320/323 (99%)   | 303 (95%)  | 17 (5%)  | 0        | 100         | 100 |
| 2   | B     | 160/166 (96%)   | 151 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| 2   | D     | 162/166 (98%)   | 149 (92%)  | 10 (6%)  | 3 (2%)   | 9           | 41  |
| 2   | F     | 159/166 (96%)   | 150 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| 2   | H     | 160/166 (96%)   | 150 (94%)  | 9 (6%)   | 1 (1%)   | 28          | 70  |
| 2   | J     | 164/166 (99%)   | 151 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 2   | L     | 159/166 (96%)   | 149 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| All | All   | 2884/2934 (98%) | 2705 (94%) | 173 (6%) | 6 (0%)   | 51          | 86  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 159 | TYR  |
| 2   | D     | 160 | PRO  |
| 2   | H     | 160 | PRO  |
| 1   | C     | 75  | SER  |
| 2   | D     | 161 | LYS  |
| 1   | A     | 52  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 283/284 (100%) | 259 (92%) | 24 (8%)  | 12          | 43 |
| 1   | C     | 283/284 (100%) | 262 (93%) | 21 (7%)  | 16          | 49 |
| 1   | E     | 282/284 (99%)  | 261 (93%) | 21 (7%)  | 16          | 49 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | G     | 282/284 (99%)   | 262 (93%)  | 20 (7%)  | 17          | 52 |
| 1   | I     | 283/284 (100%)  | 259 (92%)  | 24 (8%)  | 12          | 43 |
| 1   | K     | 283/284 (100%)  | 260 (92%)  | 23 (8%)  | 14          | 45 |
| 2   | B     | 139/142 (98%)   | 129 (93%)  | 10 (7%)  | 17          | 51 |
| 2   | D     | 140/142 (99%)   | 127 (91%)  | 13 (9%)  | 10          | 38 |
| 2   | F     | 139/142 (98%)   | 128 (92%)  | 11 (8%)  | 14          | 46 |
| 2   | H     | 139/142 (98%)   | 132 (95%)  | 7 (5%)   | 28          | 67 |
| 2   | J     | 142/142 (100%)  | 130 (92%)  | 12 (8%)  | 12          | 43 |
| 2   | L     | 139/142 (98%)   | 127 (91%)  | 12 (9%)  | 12          | 42 |
| All | All   | 2534/2556 (99%) | 2336 (92%) | 198 (8%) | 15          | 47 |

All (198) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ARG  |
| 1   | A     | 7   | ASP  |
| 1   | A     | 8   | THR  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 42  | LYS  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 50  | LEU  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 107 | LEU  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 118 | GLU  |
| 1   | A     | 119 | ARG  |
| 1   | A     | 157 | LEU  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 190 | THR  |
| 1   | A     | 195 | GLN  |
| 1   | A     | 198 | TYR  |
| 1   | A     | 211 | ARG  |
| 1   | A     | 240 | VAL  |
| 1   | A     | 265 | ARG  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 305 | THR  |
| 1   | A     | 316 | THR  |
| 1   | A     | 324 | LEU  |
| 2   | B     | 22  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 28  | ASN  |
| 2   | B     | 38  | LEU  |
| 2   | B     | 57  | GLU  |
| 2   | B     | 80  | LEU  |
| 2   | B     | 126 | LEU  |
| 2   | B     | 158 | ASP  |
| 2   | B     | 159 | TYR  |
| 2   | B     | 161 | LYS  |
| 2   | B     | 162 | TYR  |
| 1   | C     | 26  | LEU  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 42  | LYS  |
| 1   | C     | 44  | ASN  |
| 1   | C     | 50  | LEU  |
| 1   | C     | 53  | VAL  |
| 1   | C     | 67  | ILE  |
| 1   | C     | 76  | LEU  |
| 1   | C     | 111 | LEU  |
| 1   | C     | 118 | GLU  |
| 1   | C     | 157 | LEU  |
| 1   | C     | 167 | LEU  |
| 1   | C     | 190 | THR  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 198 | TYR  |
| 1   | C     | 211 | ARG  |
| 1   | C     | 265 | ARG  |
| 1   | C     | 266 | ASN  |
| 1   | C     | 305 | THR  |
| 1   | C     | 316 | THR  |
| 1   | C     | 324 | LEU  |
| 2   | D     | 22  | TYR  |
| 2   | D     | 28  | ASN  |
| 2   | D     | 38  | LEU  |
| 2   | D     | 57  | GLU  |
| 2   | D     | 66  | VAL  |
| 2   | D     | 80  | LEU  |
| 2   | D     | 98  | LEU  |
| 2   | D     | 102 | LEU  |
| 2   | D     | 126 | LEU  |
| 2   | D     | 158 | ASP  |
| 2   | D     | 161 | LYS  |
| 2   | D     | 162 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 164 | GLU  |
| 1   | E     | 9   | LEU  |
| 1   | E     | 32  | VAL  |
| 1   | E     | 37  | ASN  |
| 1   | E     | 42  | LYS  |
| 1   | E     | 44  | ASN  |
| 1   | E     | 47  | LEU  |
| 1   | E     | 76  | LEU  |
| 1   | E     | 111 | LEU  |
| 1   | E     | 114 | VAL  |
| 1   | E     | 118 | GLU  |
| 1   | E     | 119 | ARG  |
| 1   | E     | 167 | LEU  |
| 1   | E     | 190 | THR  |
| 1   | E     | 195 | GLN  |
| 1   | E     | 198 | TYR  |
| 1   | E     | 211 | ARG  |
| 1   | E     | 265 | ARG  |
| 1   | E     | 266 | ASN  |
| 1   | E     | 305 | THR  |
| 1   | E     | 316 | THR  |
| 1   | E     | 324 | LEU  |
| 2   | F     | 2   | LEU  |
| 2   | F     | 22  | TYR  |
| 2   | F     | 28  | ASN  |
| 2   | F     | 57  | GLU  |
| 2   | F     | 66  | VAL  |
| 2   | F     | 80  | LEU  |
| 2   | F     | 98  | LEU  |
| 2   | F     | 102 | LEU  |
| 2   | F     | 126 | LEU  |
| 2   | F     | 159 | TYR  |
| 2   | F     | 161 | LYS  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 42  | LYS  |
| 1   | G     | 44  | ASN  |
| 1   | G     | 58  | LEU  |
| 1   | G     | 107 | LEU  |
| 1   | G     | 111 | LEU  |
| 1   | G     | 118 | GLU  |
| 1   | G     | 119 | ARG  |
| 1   | G     | 157 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 167 | LEU  |
| 1   | G     | 190 | THR  |
| 1   | G     | 195 | GLN  |
| 1   | G     | 198 | TYR  |
| 1   | G     | 211 | ARG  |
| 1   | G     | 240 | VAL  |
| 1   | G     | 265 | ARG  |
| 1   | G     | 266 | ASN  |
| 1   | G     | 305 | THR  |
| 1   | G     | 316 | THR  |
| 1   | G     | 324 | LEU  |
| 2   | H     | 22  | TYR  |
| 2   | H     | 28  | ASN  |
| 2   | H     | 38  | LEU  |
| 2   | H     | 57  | GLU  |
| 2   | H     | 80  | LEU  |
| 2   | H     | 126 | LEU  |
| 2   | H     | 161 | LYS  |
| 1   | I     | 26  | LEU  |
| 1   | I     | 37  | ASN  |
| 1   | I     | 42  | LYS  |
| 1   | I     | 44  | ASN  |
| 1   | I     | 53  | VAL  |
| 1   | I     | 74  | GLU  |
| 1   | I     | 77  | SER  |
| 1   | I     | 78  | THR  |
| 1   | I     | 80  | SER  |
| 1   | I     | 81  | SER  |
| 1   | I     | 111 | LEU  |
| 1   | I     | 118 | GLU  |
| 1   | I     | 119 | ARG  |
| 1   | I     | 157 | LEU  |
| 1   | I     | 167 | LEU  |
| 1   | I     | 190 | THR  |
| 1   | I     | 195 | GLN  |
| 1   | I     | 198 | TYR  |
| 1   | I     | 211 | ARG  |
| 1   | I     | 265 | ARG  |
| 1   | I     | 266 | ASN  |
| 1   | I     | 305 | THR  |
| 1   | I     | 316 | THR  |
| 1   | I     | 324 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 22  | TYR  |
| 2   | J     | 28  | ASN  |
| 2   | J     | 38  | LEU  |
| 2   | J     | 57  | GLU  |
| 2   | J     | 66  | VAL  |
| 2   | J     | 80  | LEU  |
| 2   | J     | 98  | LEU  |
| 2   | J     | 102 | LEU  |
| 2   | J     | 126 | LEU  |
| 2   | J     | 158 | ASP  |
| 2   | J     | 161 | LYS  |
| 2   | J     | 163 | SER  |
| 1   | K     | 9   | LEU  |
| 1   | K     | 32  | VAL  |
| 1   | K     | 37  | ASN  |
| 1   | K     | 42  | LYS  |
| 1   | K     | 44  | ASN  |
| 1   | K     | 47  | LEU  |
| 1   | K     | 49  | LYS  |
| 1   | K     | 50  | LEU  |
| 1   | K     | 76  | LEU  |
| 1   | K     | 111 | LEU  |
| 1   | K     | 114 | VAL  |
| 1   | K     | 118 | GLU  |
| 1   | K     | 119 | ARG  |
| 1   | K     | 167 | LEU  |
| 1   | K     | 190 | THR  |
| 1   | K     | 195 | GLN  |
| 1   | K     | 198 | TYR  |
| 1   | K     | 211 | ARG  |
| 1   | K     | 265 | ARG  |
| 1   | K     | 266 | ASN  |
| 1   | K     | 305 | THR  |
| 1   | K     | 316 | THR  |
| 1   | K     | 324 | LEU  |
| 2   | L     | 2   | LEU  |
| 2   | L     | 22  | TYR  |
| 2   | L     | 28  | ASN  |
| 2   | L     | 57  | GLU  |
| 2   | L     | 66  | VAL  |
| 2   | L     | 80  | LEU  |
| 2   | L     | 98  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 102 | LEU  |
| 2   | L     | 126 | LEU  |
| 2   | L     | 159 | TYR  |
| 2   | L     | 161 | LYS  |
| 2   | L     | 162 | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | HIS  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 132 | HIS  |
| 1   | A     | 144 | HIS  |
| 1   | A     | 162 | ASN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 195 | GLN  |
| 1   | A     | 199 | GLN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 279 | HIS  |
| 2   | B     | 28  | ASN  |
| 2   | B     | 30  | GLN  |
| 2   | B     | 60  | ASN  |
| 2   | B     | 125 | GLN  |
| 2   | B     | 129 | ASN  |
| 2   | B     | 142 | HIS  |
| 2   | B     | 146 | ASN  |
| 1   | C     | 14  | HIS  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 44  | ASN  |
| 1   | C     | 132 | HIS  |
| 1   | C     | 162 | ASN  |
| 1   | C     | 194 | GLN  |
| 1   | C     | 195 | GLN  |
| 1   | C     | 199 | GLN  |
| 1   | C     | 253 | ASN  |
| 1   | C     | 266 | ASN  |
| 1   | C     | 279 | HIS  |
| 2   | D     | 28  | ASN  |
| 2   | D     | 30  | GLN  |
| 2   | D     | 60  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 125 | GLN  |
| 2   | D     | 129 | ASN  |
| 2   | D     | 146 | ASN  |
| 1   | E     | 37  | ASN  |
| 1   | E     | 44  | ASN  |
| 1   | E     | 132 | HIS  |
| 1   | E     | 144 | HIS  |
| 1   | E     | 162 | ASN  |
| 1   | E     | 194 | GLN  |
| 1   | E     | 195 | GLN  |
| 1   | E     | 199 | GLN  |
| 1   | E     | 253 | ASN  |
| 1   | E     | 266 | ASN  |
| 1   | E     | 279 | HIS  |
| 2   | F     | 28  | ASN  |
| 2   | F     | 30  | GLN  |
| 2   | F     | 60  | ASN  |
| 2   | F     | 125 | GLN  |
| 2   | F     | 129 | ASN  |
| 2   | F     | 146 | ASN  |
| 1   | G     | 14  | HIS  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 44  | ASN  |
| 1   | G     | 132 | HIS  |
| 1   | G     | 144 | HIS  |
| 1   | G     | 162 | ASN  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 195 | GLN  |
| 1   | G     | 199 | GLN  |
| 1   | G     | 253 | ASN  |
| 1   | G     | 266 | ASN  |
| 1   | G     | 279 | HIS  |
| 2   | H     | 28  | ASN  |
| 2   | H     | 30  | GLN  |
| 2   | H     | 60  | ASN  |
| 2   | H     | 125 | GLN  |
| 2   | H     | 142 | HIS  |
| 2   | H     | 146 | ASN  |
| 1   | I     | 14  | HIS  |
| 1   | I     | 37  | ASN  |
| 1   | I     | 44  | ASN  |
| 1   | I     | 132 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 162 | ASN  |
| 1   | I     | 194 | GLN  |
| 1   | I     | 195 | GLN  |
| 1   | I     | 199 | GLN  |
| 1   | I     | 253 | ASN  |
| 1   | I     | 266 | ASN  |
| 1   | I     | 279 | HIS  |
| 2   | J     | 28  | ASN  |
| 2   | J     | 30  | GLN  |
| 2   | J     | 60  | ASN  |
| 2   | J     | 125 | GLN  |
| 2   | J     | 129 | ASN  |
| 2   | J     | 146 | ASN  |
| 1   | K     | 37  | ASN  |
| 1   | K     | 44  | ASN  |
| 1   | K     | 132 | HIS  |
| 1   | K     | 144 | HIS  |
| 1   | K     | 162 | ASN  |
| 1   | K     | 194 | GLN  |
| 1   | K     | 195 | GLN  |
| 1   | K     | 199 | GLN  |
| 1   | K     | 253 | ASN  |
| 1   | K     | 266 | ASN  |
| 1   | K     | 279 | HIS  |
| 2   | L     | 28  | ASN  |
| 2   | L     | 30  | GLN  |
| 2   | L     | 60  | ASN  |
| 2   | L     | 125 | GLN  |
| 2   | L     | 146 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

6 carbohydrates are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | NAG  | A     | 602 | 1,4  | 14,14,15     | 0.66 | 0           | 15,19,21    | 1.97 | 2 (13%)     |
| 4   | NAG  | A     | 603 | 4    | 14,14,15     | 0.45 | 0           | 15,19,21    | 2.01 | 4 (26%)     |
| 4   | NAG  | C     | 602 | 1,4  | 14,14,15     | 0.91 | 1 (7%)      | 15,19,21    | 2.01 | 6 (40%)     |
| 4   | NAG  | C     | 603 | 4    | 14,14,15     | 0.49 | 0           | 15,19,21    | 1.30 | 1 (6%)      |
| 4   | NAG  | I     | 601 | 1,4  | 14,14,15     | 0.82 | 1 (7%)      | 15,19,21    | 2.34 | 5 (33%)     |
| 4   | NAG  | I     | 602 | 4    | 14,14,15     | 0.61 | 0           | 15,19,21    | 0.91 | 1 (6%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | A     | 602 | 1,4  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 603 | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 602 | 1,4  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 603 | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | I     | 601 | 1,4  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | I     | 602 | 4    | -       | 0/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | I     | 601 | NAG  | C1-C2 | 2.44 | 1.55        | 1.52     |
| 4   | C     | 602 | NAG  | C1-C2 | 3.13 | 1.56        | 1.52     |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | A     | 603 | NAG  | C2-N2-C7 | -5.79 | 114.49      | 122.94   |
| 4   | A     | 602 | NAG  | C2-N2-C7 | -4.77 | 115.98      | 122.94   |
| 4   | C     | 602 | NAG  | C4-C3-C2 | -3.69 | 105.60      | 111.02   |
| 4   | C     | 603 | NAG  | C1-O5-C5 | -3.61 | 107.19      | 112.17   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | C     | 602 | NAG  | C2-N2-C7 | -2.98 | 118.59      | 122.94   |
| 4   | I     | 601 | NAG  | O4-C4-C3 | -2.73 | 104.42      | 110.36   |
| 4   | C     | 602 | NAG  | C3-C4-C5 | -2.41 | 105.97      | 110.22   |
| 4   | I     | 602 | NAG  | C2-N2-C7 | -2.37 | 119.48      | 122.94   |
| 4   | I     | 601 | NAG  | C2-N2-C7 | -2.13 | 119.83      | 122.94   |
| 4   | A     | 603 | NAG  | C4-C3-C2 | -2.07 | 107.99      | 111.02   |
| 4   | A     | 603 | NAG  | C1-C2-N2 | 2.11  | 114.09      | 110.49   |
| 4   | I     | 601 | NAG  | O3-C3-C2 | 2.18  | 114.06      | 109.39   |
| 4   | C     | 602 | NAG  | O4-C4-C5 | 2.34  | 115.18      | 109.28   |
| 4   | A     | 603 | NAG  | C1-O5-C5 | 2.78  | 115.99      | 112.17   |
| 4   | C     | 602 | NAG  | O4-C4-C3 | 2.79  | 116.42      | 110.36   |
| 4   | I     | 601 | NAG  | C4-C3-C2 | 3.41  | 116.01      | 111.02   |
| 4   | C     | 602 | NAG  | C1-O5-C5 | 4.05  | 117.75      | 112.17   |
| 4   | A     | 602 | NAG  | C1-O5-C5 | 4.92  | 118.95      | 112.17   |
| 4   | I     | 601 | NAG  | C1-O5-C5 | 6.58  | 121.23      | 112.17   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 602 | NAG  | 6       | 0            |
| 4   | A     | 603 | NAG  | 5       | 0            |
| 4   | C     | 602 | NAG  | 4       | 0            |
| 4   | C     | 603 | NAG  | 3       | 0            |
| 4   | I     | 601 | NAG  | 7       | 0            |
| 4   | I     | 602 | NAG  | 2       | 0            |

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | A     | 601 | 1    | 14,14,15     | 0.63 | 0        | 15,19,21    | 2.74 | 4 (26%)  |
| 3   | NAG  | C     | 601 | 1    | 14,14,15     | 0.63 | 0        | 15,19,21    | 2.02 | 4 (26%)  |
| 3   | NAG  | E     | 601 | 1    | 14,14,15     | 0.76 | 1 (7%)   | 15,19,21    | 1.16 | 1 (6%)   |
| 3   | NAG  | G     | 601 | 1    | 14,14,15     | 0.50 | 0        | 15,19,21    | 1.53 | 3 (20%)  |
| 3   | NAG  | I     | 603 | 1    | 14,14,15     | 0.79 | 1 (7%)   | 15,19,21    | 2.52 | 4 (26%)  |
| 3   | NAG  | K     | 601 | 1    | 14,14,15     | 0.42 | 0        | 15,19,21    | 2.19 | 1 (6%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | A     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | G     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | I     | 603 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | K     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | E     | 601 | NAG  | C1-C2 | 2.18 | 1.55        | 1.52     |
| 3   | I     | 603 | NAG  | C1-C2 | 2.63 | 1.56        | 1.52     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | K     | 601 | NAG  | C2-N2-C7 | -7.80 | 111.56      | 122.94   |
| 3   | I     | 603 | NAG  | C4-C3-C2 | -4.01 | 105.14      | 111.02   |
| 3   | A     | 601 | NAG  | C2-N2-C7 | -3.79 | 117.42      | 122.94   |
| 3   | E     | 601 | NAG  | C2-N2-C7 | -2.40 | 119.44      | 122.94   |
| 3   | I     | 603 | NAG  | C3-C4-C5 | -2.39 | 106.01      | 110.22   |
| 3   | A     | 601 | NAG  | C6-C5-C4 | -2.37 | 107.46      | 113.00   |
| 3   | G     | 601 | NAG  | C4-C3-C2 | 2.08  | 114.06      | 111.02   |
| 3   | I     | 603 | NAG  | O5-C1-C2 | 2.43  | 114.86      | 111.47   |
| 3   | C     | 601 | NAG  | C3-C4-C5 | 2.68  | 114.93      | 110.22   |
| 3   | G     | 601 | NAG  | O5-C1-C2 | 2.85  | 115.44      | 111.47   |
| 3   | C     | 601 | NAG  | C4-C3-C2 | 3.54  | 116.21      | 111.02   |
| 3   | C     | 601 | NAG  | O5-C1-C2 | 3.84  | 116.81      | 111.47   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | G     | 601 | NAG  | C1-O5-C5 | 3.93 | 117.58      | 112.17   |
| 3   | C     | 601 | NAG  | C1-O5-C5 | 4.05 | 117.75      | 112.17   |
| 3   | A     | 601 | NAG  | O5-C1-C2 | 5.01 | 118.45      | 111.47   |
| 3   | I     | 603 | NAG  | C1-O5-C5 | 7.09 | 121.94      | 112.17   |
| 3   | A     | 601 | NAG  | C1-O5-C5 | 7.83 | 122.96      | 112.17   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | K     | 601 | NAG  | 9       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 323/323 (100%)  | -0.03  | 2 (0%) 89 71   | 20, 50, 95, 142       | 0     |
| 1   | C     | 322/323 (99%)   | 0.03   | 11 (3%) 46 20  | 17, 47, 94, 172       | 0     |
| 1   | E     | 321/323 (99%)   | 0.11   | 10 (3%) 49 22  | 22, 48, 88, 152       | 0     |
| 1   | G     | 322/323 (99%)   | 0.14   | 11 (3%) 46 20  | 23, 54, 99, 155       | 0     |
| 1   | I     | 322/323 (99%)   | 0.05   | 11 (3%) 46 20  | 22, 52, 87, 212       | 0     |
| 1   | K     | 322/323 (99%)   | 0.00   | 9 (2%) 53 25   | 23, 52, 98, 160       | 0     |
| 2   | B     | 162/166 (97%)   | 0.26   | 5 (3%) 49 22   | 21, 60, 109, 160      | 0     |
| 2   | D     | 164/166 (98%)   | 0.61   | 21 (12%) 4 2   | 20, 71, 137, 180      | 0     |
| 2   | F     | 161/166 (96%)   | 0.52   | 21 (13%) 4 1   | 23, 73, 141, 203      | 0     |
| 2   | H     | 162/166 (97%)   | 0.11   | 5 (3%) 49 22   | 24, 61, 116, 160      | 0     |
| 2   | J     | 166/166 (100%)  | 0.17   | 2 (1%) 79 53   | 19, 58, 102, 132      | 0     |
| 2   | L     | 161/166 (96%)   | 0.38   | 9 (5%) 25 10   | 26, 68, 132, 199      | 0     |
| All | All   | 2908/2934 (99%) | 0.15   | 117 (4%) 39 16 | 17, 54, 115, 212      | 0     |

All (117) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 79  | ALA  | 9.7  |
| 1   | C     | 8   | THR  | 6.3  |
| 1   | C     | 76  | LEU  | 6.3  |
| 2   | D     | 24  | TYR  | 6.2  |
| 1   | E     | 9   | LEU  | 6.2  |
| 1   | I     | 81  | SER  | 5.8  |
| 2   | F     | 159 | TYR  | 5.7  |
| 2   | D     | 29  | GLU  | 5.1  |
| 1   | I     | 75  | SER  | 5.0  |
| 2   | L     | 158 | ASP  | 5.0  |
| 2   | L     | 140 | PHE  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 9   | LEU  | 4.6  |
| 2   | F     | 139 | GLU  | 4.6  |
| 2   | D     | 35  | ALA  | 4.5  |
| 1   | A     | 144 | HIS  | 4.4  |
| 1   | G     | 74  | GLU  | 4.3  |
| 2   | D     | 139 | GLU  | 3.9  |
| 2   | D     | 140 | PHE  | 3.9  |
| 1   | E     | 78  | THR  | 3.9  |
| 1   | I     | 78  | THR  | 3.9  |
| 2   | F     | 29  | GLU  | 3.8  |
| 1   | K     | 7   | ASP  | 3.7  |
| 2   | F     | 27  | GLN  | 3.6  |
| 2   | D     | 23  | GLY  | 3.6  |
| 2   | F     | 145 | ASP  | 3.6  |
| 2   | F     | 158 | ASP  | 3.5  |
| 2   | L     | 139 | GLU  | 3.5  |
| 2   | D     | 138 | PHE  | 3.5  |
| 1   | K     | 11  | ILE  | 3.4  |
| 2   | L     | 38  | LEU  | 3.4  |
| 2   | D     | 22  | TYR  | 3.4  |
| 1   | I     | 76  | LEU  | 3.4  |
| 2   | D     | 141 | TYR  | 3.4  |
| 1   | C     | 51  | ARG  | 3.3  |
| 1   | I     | 52  | GLY  | 3.3  |
| 2   | F     | 24  | TYR  | 3.3  |
| 2   | F     | 38  | LEU  | 3.3  |
| 1   | G     | 52  | GLY  | 3.3  |
| 2   | L     | 27  | GLN  | 3.3  |
| 2   | H     | 139 | GLU  | 3.2  |
| 2   | D     | 135 | ASN  | 3.2  |
| 2   | D     | 162 | TYR  | 3.2  |
| 2   | F     | 143 | LYS  | 3.2  |
| 2   | F     | 131 | LYS  | 3.1  |
| 2   | D     | 136 | GLY  | 3.1  |
| 2   | D     | 144 | CYS  | 3.1  |
| 1   | E     | 7   | ASP  | 3.0  |
| 2   | B     | 154 | ASN  | 3.0  |
| 2   | D     | 143 | LYS  | 3.0  |
| 1   | K     | 8   | THR  | 3.0  |
| 2   | D     | 149 | MET  | 2.9  |
| 2   | F     | 138 | PHE  | 2.9  |
| 2   | D     | 134 | GLY  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 1   | GLY  | 2.8  |
| 2   | F     | 30  | GLN  | 2.8  |
| 2   | F     | 28  | ASN  | 2.8  |
| 1   | C     | 74  | GLU  | 2.8  |
| 1   | G     | 92  | ASP  | 2.7  |
| 1   | E     | 10  | CYS  | 2.7  |
| 1   | G     | 76  | LEU  | 2.7  |
| 2   | F     | 147 | THR  | 2.7  |
| 1   | C     | 75  | SER  | 2.7  |
| 1   | C     | 12  | GLY  | 2.7  |
| 2   | D     | 8   | GLY  | 2.7  |
| 1   | I     | 51  | ARG  | 2.6  |
| 2   | L     | 141 | TYR  | 2.6  |
| 1   | C     | 7   | ASP  | 2.6  |
| 1   | I     | 8   | THR  | 2.6  |
| 1   | G     | 60  | LYS  | 2.6  |
| 2   | J     | 143 | LYS  | 2.6  |
| 1   | E     | 17  | ASN  | 2.6  |
| 2   | D     | 27  | GLN  | 2.5  |
| 2   | H     | 30  | GLN  | 2.5  |
| 1   | E     | 8   | THR  | 2.5  |
| 1   | I     | 146 | GLY  | 2.5  |
| 2   | F     | 144 | CYS  | 2.5  |
| 1   | K     | 52  | GLY  | 2.5  |
| 2   | F     | 31  | GLY  | 2.5  |
| 2   | F     | 133 | ILE  | 2.5  |
| 1   | K     | 59  | GLY  | 2.4  |
| 2   | F     | 32  | SER  | 2.4  |
| 2   | L     | 138 | PHE  | 2.4  |
| 1   | E     | 322 | THR  | 2.4  |
| 2   | L     | 32  | SER  | 2.4  |
| 1   | K     | 45  | GLY  | 2.4  |
| 1   | C     | 268 | GLY  | 2.4  |
| 2   | F     | 140 | PHE  | 2.3  |
| 1   | K     | 76  | LEU  | 2.3  |
| 2   | D     | 146 | ASN  | 2.3  |
| 2   | B     | 131 | LYS  | 2.3  |
| 1   | G     | 47  | LEU  | 2.3  |
| 2   | D     | 152 | VAL  | 2.3  |
| 2   | D     | 157 | TYR  | 2.3  |
| 1   | I     | 80  | SER  | 2.3  |
| 2   | B     | 129 | ASN  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 50  | LEU  | 2.3  |
| 1   | K     | 34  | HIS  | 2.3  |
| 2   | F     | 160 | PRO  | 2.2  |
| 1   | G     | 268 | GLY  | 2.2  |
| 1   | E     | 50  | LEU  | 2.1  |
| 2   | B     | 33  | GLY  | 2.1  |
| 1   | C     | 11  | ILE  | 2.1  |
| 2   | H     | 157 | TYR  | 2.1  |
| 2   | B     | 1   | GLY  | 2.1  |
| 1   | K     | 78  | THR  | 2.1  |
| 2   | L     | 153 | LYS  | 2.1  |
| 1   | G     | 118 | GLU  | 2.1  |
| 1   | G     | 275 | ASP  | 2.1  |
| 1   | A     | 328 | PRO  | 2.1  |
| 1   | E     | 36  | VAL  | 2.1  |
| 1   | G     | 75  | SER  | 2.1  |
| 1   | C     | 13  | TYR  | 2.1  |
| 1   | G     | 51  | ARG  | 2.1  |
| 2   | H     | 129 | ASN  | 2.1  |
| 1   | E     | 282 | ASN  | 2.1  |
| 2   | F     | 134 | GLY  | 2.0  |
| 2   | H     | 1   | GLY  | 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | NAG  | I     | 601 | 14/15 | 0.88 | 0.23 | 1.89  | 54,67,82,89                | 0     |
| 4   | NAG  | A     | 602 | 14/15 | 0.90 | 0.21 | 0.24  | 50,55,73,87                | 0     |
| 4   | NAG  | C     | 602 | 14/15 | 0.85 | 0.18 | -0.28 | 61,91,103,103              | 0     |
| 4   | NAG  | C     | 603 | 14/15 | 0.65 | 0.34 | -     | 119,145,155,170            | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 4   | NAG  | A     | 603 | 14/15 | 0.82 | 0.24 | -    | 70,99,123,128               | 0     |
| 4   | NAG  | I     | 602 | 14/15 | 0.76 | 0.28 | -    | 65,96,112,114               | 0     |

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 3   | NAG  | K     | 601 | 14/15 | 0.79 | 0.28 | 4.28 | 69,93,112,117               | 0     |
| 3   | NAG  | C     | 601 | 14/15 | 0.73 | 0.33 | -    | 108,149,162,165             | 0     |
| 3   | NAG  | E     | 601 | 14/15 | 0.69 | 0.35 | -    | 127,145,172,172             | 0     |
| 3   | NAG  | I     | 603 | 14/15 | 0.78 | 0.27 | -    | 67,95,120,122               | 0     |
| 3   | NAG  | G     | 601 | 14/15 | 0.76 | 0.25 | -    | 67,103,119,122              | 0     |
| 3   | NAG  | A     | 601 | 14/15 | 0.84 | 0.33 | -    | 111,124,137,141             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.