



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:08 AM EDT

PDB ID : 4XLQ / pdb\_00004xlq  
Title : Crystal structure of T.aquaticus transcription initiation complex containing upstream fork (-11 base-paired) promoter  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2015-01-13  
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

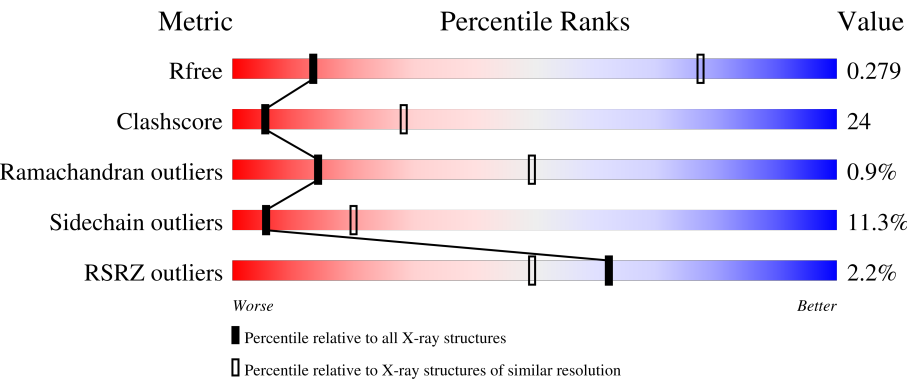
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1007 (5.28-3.92)                                      |
| Clashscore            | 190562                      | 1022 (5.26-3.94)                                      |
| Ramachandran outliers | 187476                      | 1069 (5.30-3.90)                                      |
| Sidechain outliers    | 187428                      | 1051 (5.30-3.90)                                      |
| RSRZ outliers         | 180081                      | 1002 (5.28-3.92)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                                 |
|-----|-------|--------|------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 314    | <div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>38%30%•28%</div></div>   |
| 1   | B     | 314    | <div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>32%33%7%28%</div></div>  |
| 1   | G     | 314    | <div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>35%32%5%28%</div></div> |
| 1   | H     | 314    | <div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>35%31%6%28%</div></div>  |
| 2   | C     | 1119   | <div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>43%49%8%•</div></div>   |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 2   | I     | 1119   | <div><div><div></div><div></div><div></div></div><div>3%44%47%8%•</div></div>  |
| 3   | D     | 1524   | <div><div><div></div><div></div><div></div></div><div>%47%44%7%•</div></div>   |
| 3   | J     | 1524   | <div><div><div></div><div></div><div></div></div><div>%44%39%7%10%</div></div> |
| 4   | E     | 99     | <div><div><div></div><div></div><div></div></div><div>3%58%32%•6%</div></div>  |
| 4   | K     | 99     | <div><div><div></div><div></div><div></div></div><div>2%64%27%•6%</div></div>  |
| 5   | F     | 347    | <div><div><div></div><div></div><div></div></div><div>3%54%43%••</div></div>   |
| 5   | L     | 347    | <div><div><div></div><div></div><div></div></div><div>5%53%42%••</div></div>   |
| 6   | O     | 30     | <div><div><div></div><div></div><div></div></div><div>17%83%</div></div>       |
| 6   | R     | 30     | <div><div><div></div><div></div><div></div></div><div>13%87%</div></div>       |
| 7   | P     | 26     | <div><div><div></div><div></div><div></div></div><div>8%88%•</div></div>       |
| 7   | S     | 26     | <div><div><div></div><div></div><div></div></div><div>4%12%88%</div></div>     |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56477 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 DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |
| 1   | B     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |
| 1   | G     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |
| 1   | H     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1112     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8739  | 5531 | 1553 | 1632 | 23 |         |         |       |
| 2   | I     | 1112     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8739  | 5531 | 1553 | 1632 | 23 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1490     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11761 | 7439 | 2088 | 2196 | 38 |         |         |       |
| 3   | J     | 1367     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10779 | 6810 | 1923 | 2010 | 36 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 768   | 490 | 136 | 138 | 4 |         |         |       |
| 4   | K     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 768   | 490 | 136 | 138 | 4 |         |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2787  | 1758 | 502 | 523 | 4 |         |         |       |
| 5   | L     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2787  | 1758 | 502 | 523 | 4 |         |         |       |

- Molecule 6 is a DNA chain called DNA (30-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 6   | O     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 613   | 296 | 109 | 179 | 29 |         |         |       |
| 6   | R     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 613   | 296 | 109 | 179 | 29 |         |         |       |

- Molecule 7 is a DNA chain called DNA (26-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 7   | P     | 25       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 510   | 245 | 91 | 149 | 25 |         |         |       |
| 7   | S     | 26       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 527   | 255 | 93 | 154 | 25 |         |         |       |

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

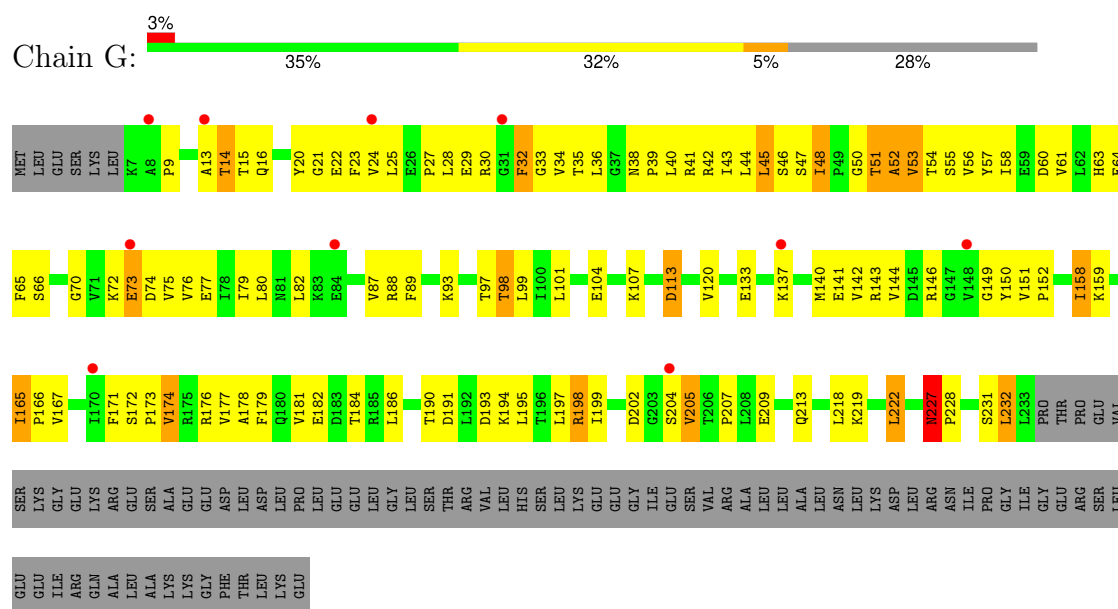
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 8   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 8   | J     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

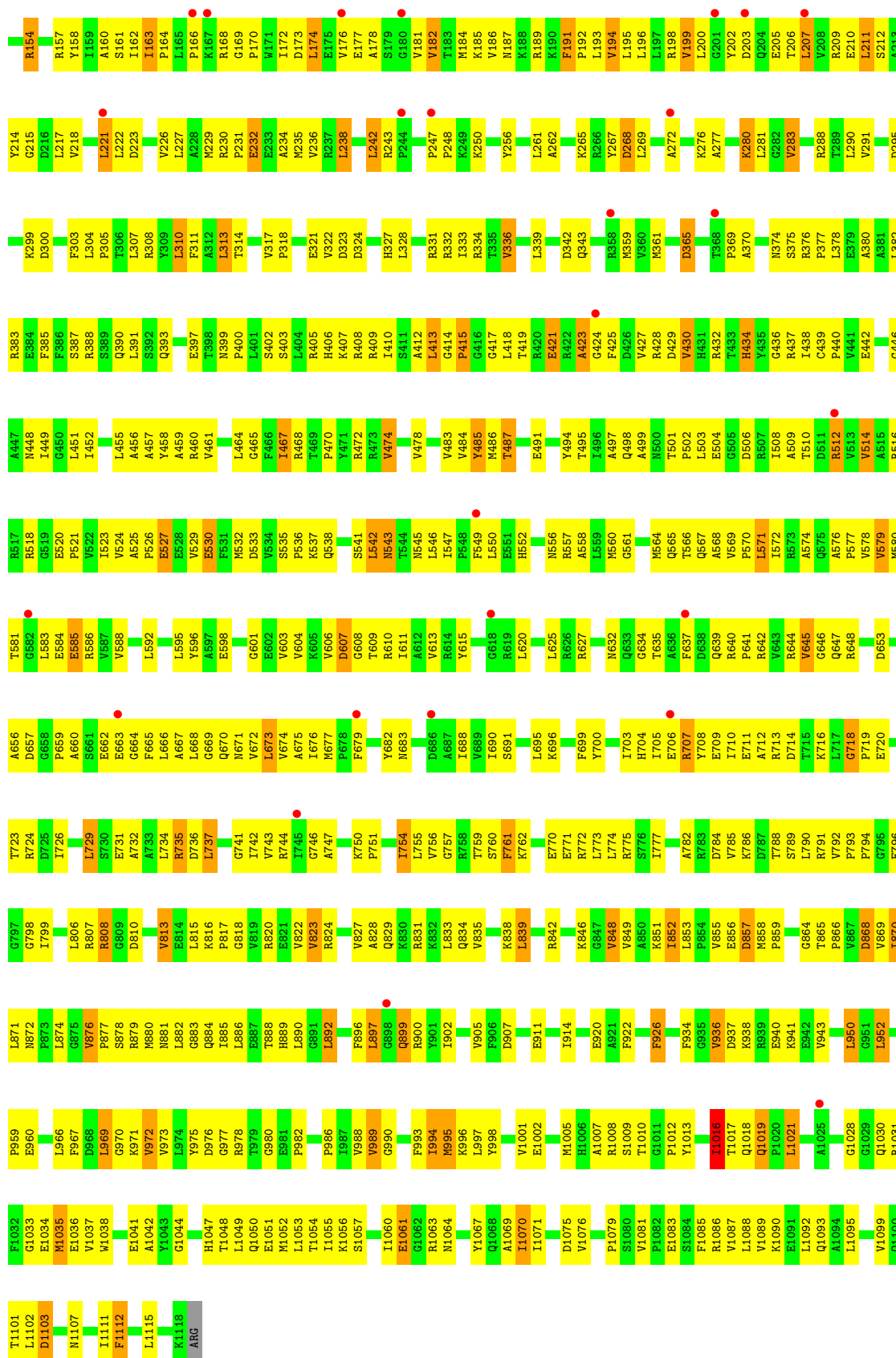
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |



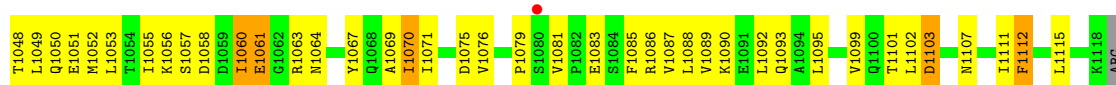
• Molecule 1: DNA-directed RNA polymerase subunit alpha



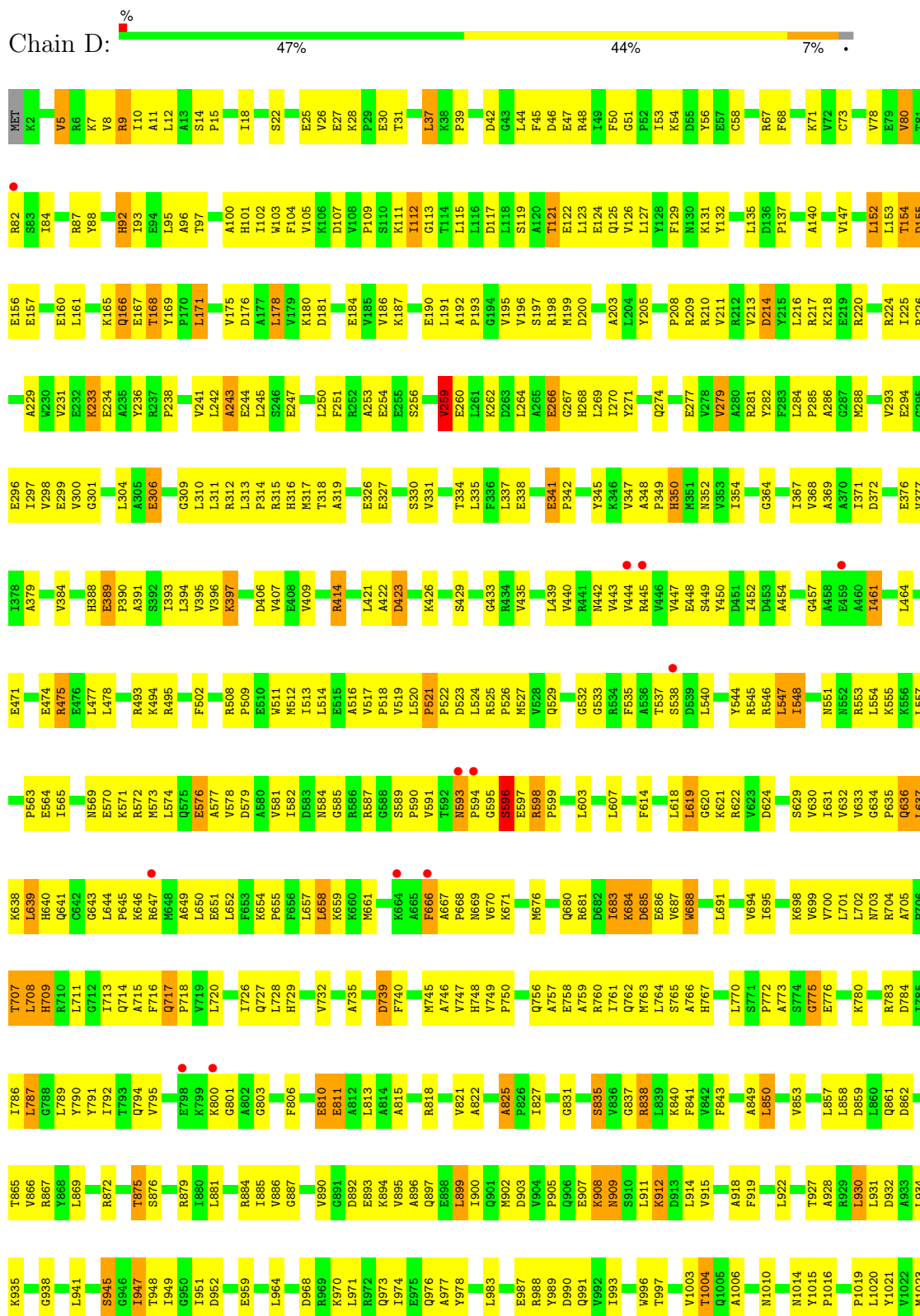


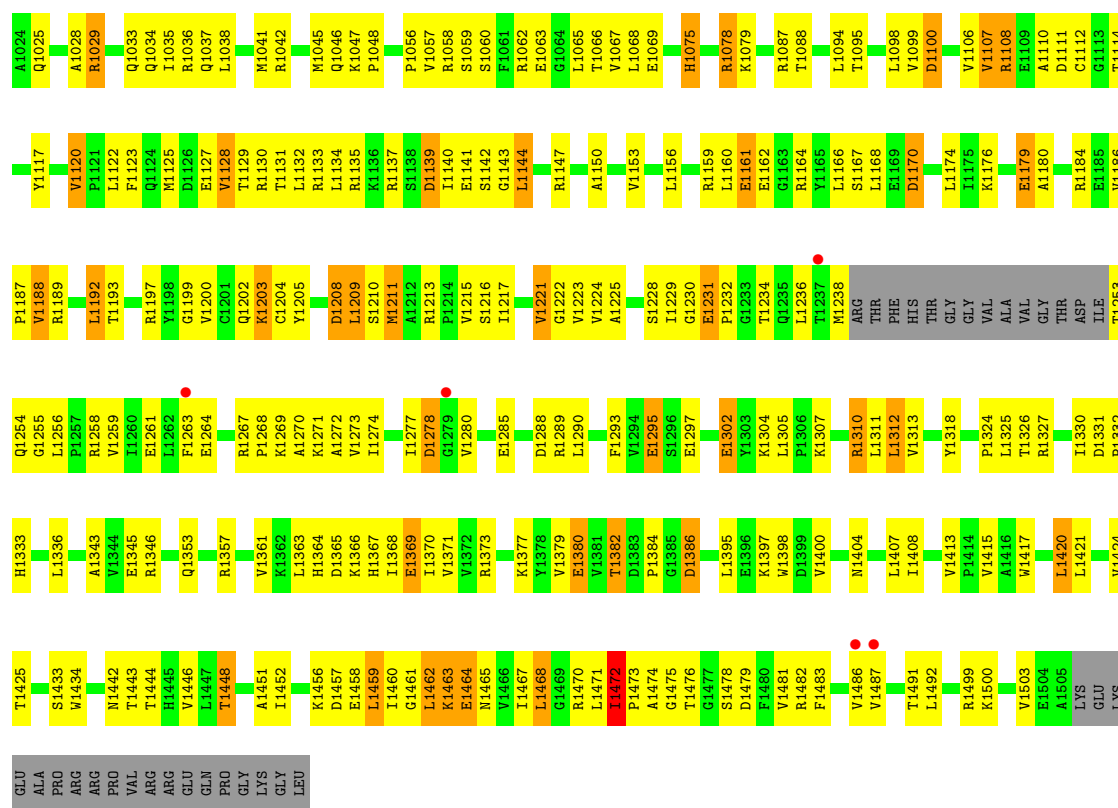




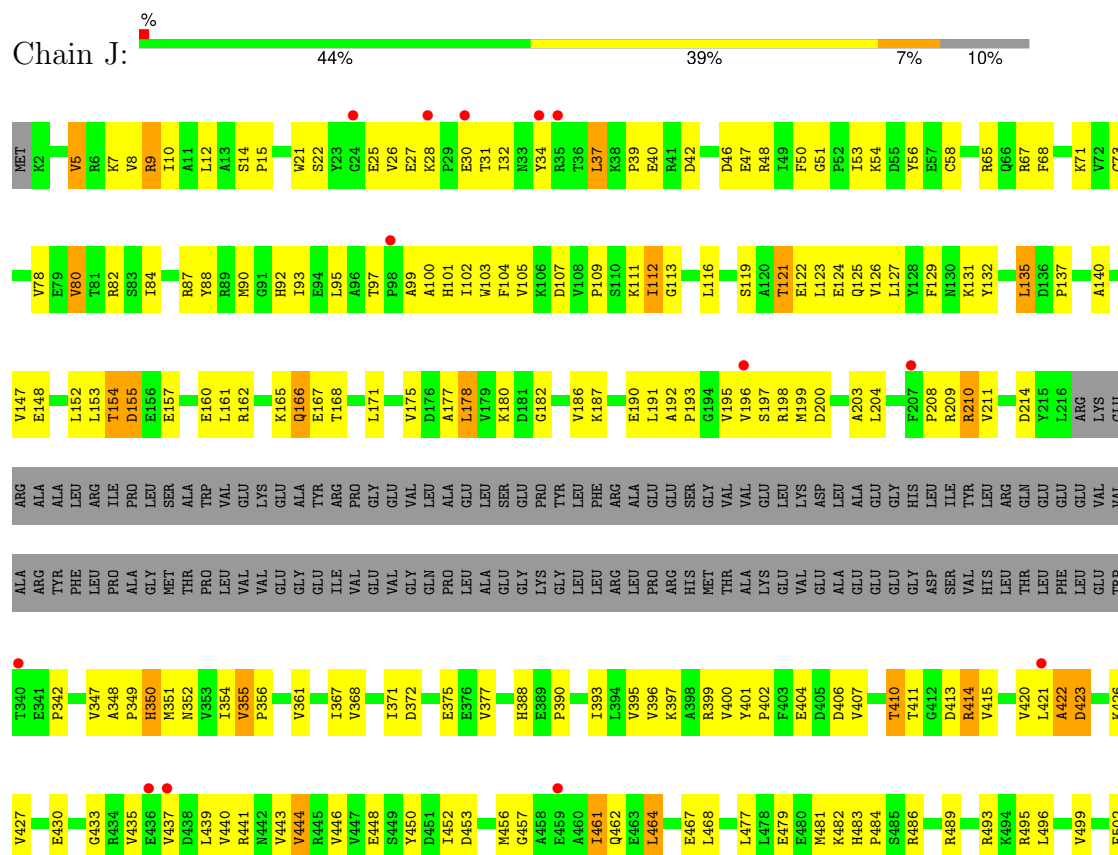


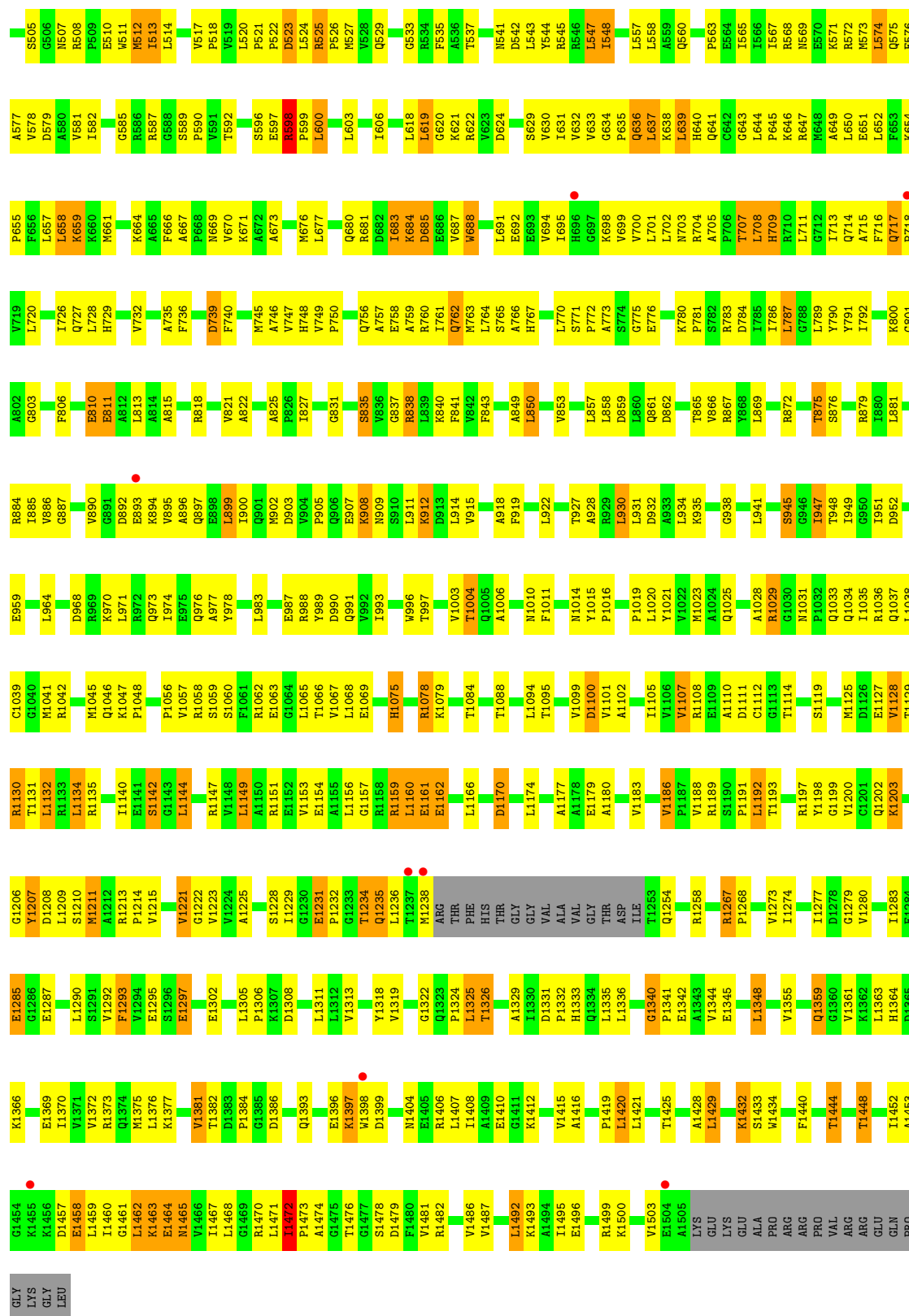
● Molecule 3: DNA-directed RNA polymerase subunit beta'





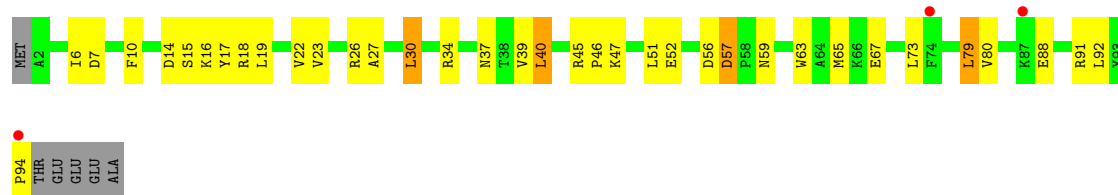
- Molecule 3: DNA-directed RNA polymerase subunit beta'





• Molecule 4: DNA-directed RNA polymerase subunit omega

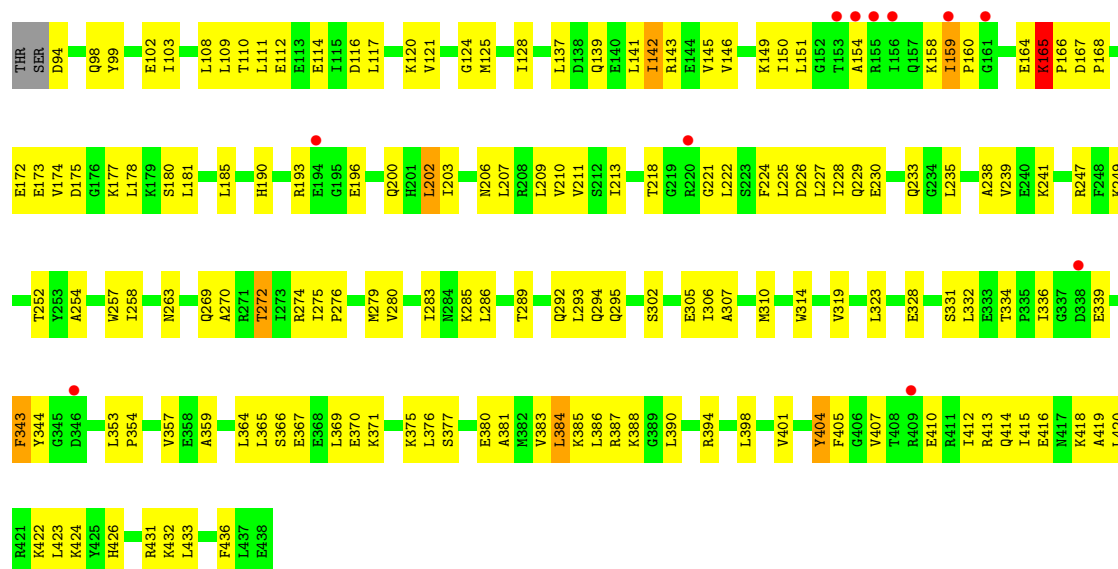
Chain E: 3% 58% 32% 6%



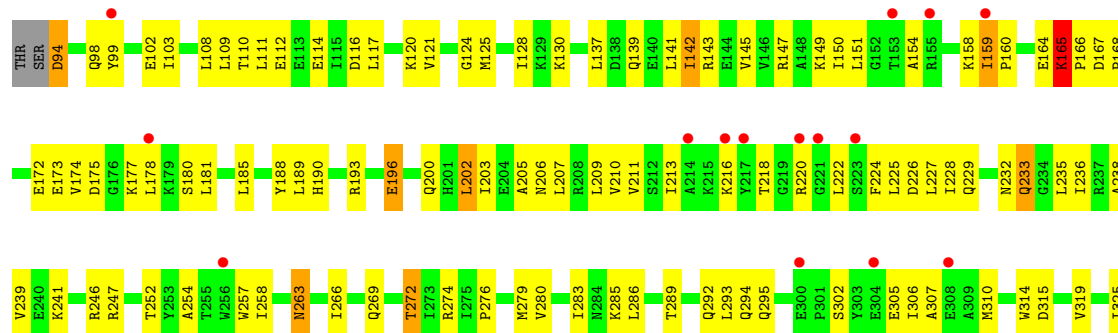
- Molecule 4: DNA-directed RNA polymerase subunit omega

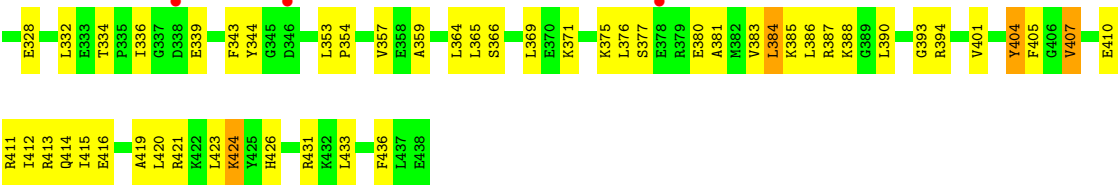


- Molecule 5: RNA polymerase sigma factor SigA

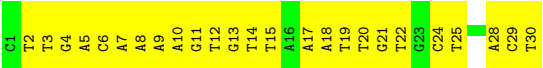
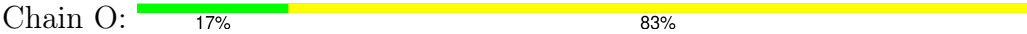


- Molecule 5: RNA polymerase sigma factor SigA





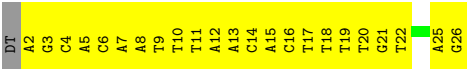
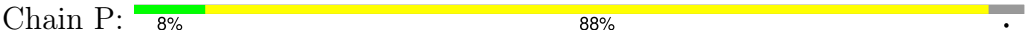
• Molecule 6: DNA (30-MER)



• Molecule 6: DNA (30-MER)



• Molecule 7: DNA (26-MER)



• Molecule 7: DNA (26-MER)



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 288.23Å 288.23Å 535.25Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.81 – 4.60<br>49.81 – 4.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (49.81-4.60)<br>98.5 (49.81-4.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.22                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.21 (at 4.64Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: dev_1839)                            | Depositor        |
| R, $R_{free}$                                                           | 0.245 , 0.281<br>0.247 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6224 reflections (2.79%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 154.6                                                       | Xtriage          |
| Anisotropy                                                              | 0.027                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 219.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.17$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 56477                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 175.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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: MG, ZN

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

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.45         | 0/1804  | 1.04        | 11/2455 (0.4%)   |
| 1   | B     | 0.43         | 0/1804  | 0.97        | 6/2455 (0.2%)    |
| 1   | G     | 0.45         | 0/1804  | 1.04        | 11/2455 (0.4%)   |
| 1   | H     | 0.44         | 0/1804  | 0.96        | 4/2455 (0.2%)    |
| 2   | C     | 0.38         | 0/8905  | 0.90        | 22/12040 (0.2%)  |
| 2   | I     | 0.38         | 0/8905  | 0.90        | 25/12040 (0.2%)  |
| 3   | D     | 0.39         | 0/11963 | 0.90        | 22/16165 (0.1%)  |
| 3   | J     | 0.39         | 0/10959 | 0.92        | 22/14802 (0.1%)  |
| 4   | E     | 0.32         | 0/783   | 0.85        | 2/1054 (0.2%)    |
| 4   | K     | 0.31         | 0/783   | 0.85        | 2/1054 (0.2%)    |
| 5   | F     | 0.36         | 0/2829  | 0.86        | 8/3804 (0.2%)    |
| 5   | L     | 0.36         | 0/2829  | 0.86        | 6/3804 (0.2%)    |
| 6   | O     | 0.18         | 0/687   | 0.44        | 0/1059           |
| 6   | R     | 0.18         | 0/687   | 0.45        | 0/1059           |
| 7   | P     | 0.22         | 0/571   | 0.47        | 0/878            |
| 7   | S     | 0.21         | 0/590   | 0.44        | 0/908            |
| All | All   | 0.38         | 0/57707 | 0.90        | 141/78487 (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 |
|-----|-------|---------------------|---------------------|
| 2   | C     | 0                   | 3                   |
| 2   | I     | 0                   | 3                   |
| 3   | D     | 0                   | 1                   |
| 3   | J     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

There are no bond length outliers.



All (141) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | I     | 417  | GLY  | N-CA-C | 10.59 | 129.14      | 114.85   |
| 2   | C     | 417  | GLY  | N-CA-C | 10.55 | 129.09      | 114.85   |
| 2   | I     | 414  | GLY  | CA-C-N | 9.90  | 132.21      | 119.84   |
| 2   | I     | 414  | GLY  | C-N-CA | 9.90  | 132.21      | 119.84   |
| 2   | C     | 414  | GLY  | CA-C-N | 9.53  | 131.75      | 119.84   |
| 2   | C     | 414  | GLY  | C-N-CA | 9.53  | 131.75      | 119.84   |
| 3   | D     | 1472 | ILE  | CA-C-N | 9.30  | 128.93      | 119.82   |
| 3   | D     | 1472 | ILE  | C-N-CA | 9.30  | 128.93      | 119.82   |
| 3   | J     | 1472 | ILE  | CA-C-N | 8.96  | 128.60      | 119.82   |
| 3   | J     | 1472 | ILE  | C-N-CA | 8.96  | 128.60      | 119.82   |
| 2   | C     | 163  | ILE  | CA-C-N | 8.23  | 130.12      | 119.84   |
| 2   | C     | 163  | ILE  | C-N-CA | 8.23  | 130.12      | 119.84   |
| 2   | I     | 163  | ILE  | CA-C-N | 8.09  | 129.95      | 119.84   |
| 2   | I     | 163  | ILE  | C-N-CA | 8.09  | 129.95      | 119.84   |
| 1   | G     | 227  | ASN  | CA-C-N | 7.90  | 129.43      | 120.98   |
| 1   | G     | 227  | ASN  | C-N-CA | 7.90  | 129.43      | 120.98   |
| 1   | A     | 227  | ASN  | CA-C-N | 7.80  | 129.33      | 120.98   |
| 1   | A     | 227  | ASN  | C-N-CA | 7.80  | 129.33      | 120.98   |
| 1   | A     | 52   | ALA  | CA-C-N | 7.67  | 135.77      | 121.97   |
| 1   | A     | 52   | ALA  | C-N-CA | 7.67  | 135.77      | 121.97   |
| 3   | J     | 1186 | VAL  | CA-C-N | 7.56  | 129.29      | 119.84   |
| 3   | J     | 1186 | VAL  | C-N-CA | 7.56  | 129.29      | 119.84   |
| 1   | G     | 52   | ALA  | CA-C-N | 7.45  | 135.38      | 121.97   |
| 1   | G     | 52   | ALA  | C-N-CA | 7.45  | 135.38      | 121.97   |
| 3   | J     | 28   | LYS  | CA-C-N | 7.24  | 127.40      | 119.87   |
| 3   | J     | 28   | LYS  | C-N-CA | 7.24  | 127.40      | 119.87   |
| 3   | D     | 596  | SER  | N-CA-C | 7.17  | 119.48      | 108.30   |
| 5   | L     | 165  | LYS  | CA-C-N | 7.01  | 127.04      | 119.89   |
| 5   | L     | 165  | LYS  | C-N-CA | 7.01  | 127.04      | 119.89   |
| 5   | F     | 165  | LYS  | CA-C-N | 7.01  | 127.04      | 119.89   |
| 5   | F     | 165  | LYS  | C-N-CA | 7.01  | 127.04      | 119.89   |
| 1   | B     | 204  | SER  | N-CA-C | 6.98  | 118.54      | 111.07   |
| 2   | I     | 793  | PRO  | CA-C-N | 6.71  | 128.22      | 119.84   |
| 2   | I     | 793  | PRO  | C-N-CA | 6.71  | 128.22      | 119.84   |
| 1   | H     | 204  | SER  | N-CA-C | 6.69  | 118.23      | 111.07   |
| 2   | C     | 793  | PRO  | CA-C-N | 6.68  | 128.19      | 119.84   |
| 2   | C     | 793  | PRO  | C-N-CA | 6.68  | 128.19      | 119.84   |
| 3   | D     | 341  | GLU  | CA-C-N | 6.68  | 126.60      | 119.85   |
| 3   | D     | 341  | GLU  | C-N-CA | 6.68  | 126.60      | 119.85   |
| 2   | C     | 718  | GLY  | CA-C-N | 6.65  | 128.15      | 119.84   |
| 2   | C     | 718  | GLY  | C-N-CA | 6.65  | 128.15      | 119.84   |
| 2   | I     | 718  | GLY  | CA-C-N | 6.60  | 128.09      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | I     | 718  | GLY  | C-N-CA | 6.60  | 128.09      | 119.84   |
| 3   | J     | 355  | VAL  | N-CA-C | 6.54  | 114.55      | 109.19   |
| 3   | D     | 51   | GLY  | CA-C-N | 6.40  | 126.37      | 119.78   |
| 3   | D     | 51   | GLY  | C-N-CA | 6.40  | 126.37      | 119.78   |
| 3   | J     | 1235 | GLN  | CA-C-N | -6.40 | 113.19      | 123.23   |
| 3   | J     | 1235 | GLN  | C-N-CA | -6.40 | 113.19      | 123.23   |
| 3   | J     | 1340 | GLY  | CA-C-N | 6.34  | 126.09      | 119.05   |
| 3   | J     | 1340 | GLY  | C-N-CA | 6.34  | 126.09      | 119.05   |
| 3   | J     | 598  | ARG  | CA-C-N | 6.29  | 127.70      | 119.84   |
| 3   | J     | 598  | ARG  | C-N-CA | 6.29  | 127.70      | 119.84   |
| 2   | C     | 283  | VAL  | N-CA-C | 6.23  | 116.14      | 108.53   |
| 3   | D     | 521  | PRO  | CA-C-N | 6.18  | 125.40      | 118.97   |
| 3   | D     | 521  | PRO  | C-N-CA | 6.18  | 125.40      | 118.97   |
| 3   | J     | 775  | GLY  | N-CA-C | -6.16 | 106.61      | 114.37   |
| 3   | D     | 28   | LYS  | CA-C-N | 6.12  | 126.24      | 119.87   |
| 3   | D     | 28   | LYS  | C-N-CA | 6.12  | 126.24      | 119.87   |
| 2   | I     | 283  | VAL  | N-CA-C | 6.09  | 115.96      | 108.53   |
| 3   | J     | 51   | GLY  | CA-C-N | 6.08  | 126.05      | 119.78   |
| 3   | J     | 51   | GLY  | C-N-CA | 6.08  | 126.05      | 119.78   |
| 4   | K     | 57   | ASP  | CA-C-N | 6.05  | 125.75      | 119.82   |
| 4   | K     | 57   | ASP  | C-N-CA | 6.05  | 125.75      | 119.82   |
| 3   | J     | 1359 | GLN  | N-CA-C | 6.04  | 119.91      | 112.54   |
| 2   | I     | 1081 | VAL  | N-CA-C | 6.04  | 114.06      | 107.60   |
| 1   | A     | 172  | SER  | CA-C-N | 6.00  | 127.35      | 119.84   |
| 1   | A     | 172  | SER  | C-N-CA | 6.00  | 127.35      | 119.84   |
| 1   | G     | 172  | SER  | CA-C-N | 5.96  | 127.28      | 119.84   |
| 1   | G     | 172  | SER  | C-N-CA | 5.96  | 127.28      | 119.84   |
| 3   | D     | 775  | GLY  | N-CA-C | -5.93 | 106.89      | 114.37   |
| 4   | E     | 57   | ASP  | CA-C-N | 5.93  | 125.63      | 119.82   |
| 4   | E     | 57   | ASP  | C-N-CA | 5.93  | 125.63      | 119.82   |
| 3   | D     | 595  | GLY  | CA-C-N | -5.89 | 113.83      | 121.79   |
| 3   | D     | 595  | GLY  | C-N-CA | -5.89 | 113.83      | 121.79   |
| 1   | A     | 48   | ILE  | CA-C-N | 5.88  | 125.89      | 119.90   |
| 1   | A     | 48   | ILE  | C-N-CA | 5.88  | 125.89      | 119.90   |
| 2   | C     | 169  | GLY  | CA-C-N | 5.85  | 126.04      | 120.31   |
| 2   | C     | 169  | GLY  | C-N-CA | 5.85  | 126.04      | 120.31   |
| 2   | C     | 1081 | VAL  | N-CA-C | 5.83  | 113.84      | 107.60   |
| 5   | L     | 159  | ILE  | CA-C-N | -5.78 | 115.81      | 121.65   |
| 5   | L     | 159  | ILE  | C-N-CA | -5.78 | 115.81      | 121.65   |
| 3   | J     | 1381 | VAL  | N-CA-C | 5.76  | 116.49      | 108.89   |
| 3   | D     | 739  | ASP  | CA-C-N | -5.74 | 114.27      | 122.77   |
| 3   | D     | 739  | ASP  | C-N-CA | -5.74 | 114.27      | 122.77   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | J     | 739  | ASP  | CA-C-N | -5.72 | 114.30      | 122.77   |
| 3   | J     | 739  | ASP  | C-N-CA | -5.72 | 114.30      | 122.77   |
| 2   | C     | 1019 | GLN  | CA-C-N | 5.71  | 126.97      | 119.84   |
| 2   | C     | 1019 | GLN  | C-N-CA | 5.71  | 126.97      | 119.84   |
| 1   | G     | 48   | ILE  | CA-C-N | 5.67  | 125.69      | 119.90   |
| 1   | G     | 48   | ILE  | C-N-CA | 5.67  | 125.69      | 119.90   |
| 2   | I     | 1019 | GLN  | CA-C-N | 5.66  | 126.92      | 119.84   |
| 2   | I     | 1019 | GLN  | C-N-CA | 5.66  | 126.92      | 119.84   |
| 5   | F     | 159  | ILE  | CA-C-N | -5.64 | 115.95      | 121.65   |
| 5   | F     | 159  | ILE  | C-N-CA | -5.64 | 115.95      | 121.65   |
| 1   | A     | 61   | VAL  | N-CA-C | 5.63  | 116.05      | 108.17   |
| 1   | G     | 61   | VAL  | N-CA-C | 5.61  | 116.02      | 108.17   |
| 2   | I     | 1103 | ASP  | N-CA-C | 5.52  | 116.91      | 108.30   |
| 2   | I     | 169  | GLY  | CA-C-N | 5.50  | 125.70      | 120.31   |
| 2   | I     | 169  | GLY  | C-N-CA | 5.50  | 125.70      | 120.31   |
| 2   | C     | 1103 | ASP  | N-CA-C | 5.49  | 116.86      | 108.30   |
| 2   | I     | 191  | PHE  | CA-C-N | 5.38  | 125.37      | 119.89   |
| 2   | I     | 191  | PHE  | C-N-CA | 5.38  | 125.37      | 119.89   |
| 1   | B     | 189  | ARG  | N-CA-C | 5.36  | 118.28      | 109.76   |
| 1   | H     | 37   | GLY  | N-CA-C | 5.35  | 119.11      | 112.64   |
| 1   | H     | 189  | ARG  | N-CA-C | 5.32  | 118.21      | 109.76   |
| 3   | D     | 825  | ALA  | CA-C-N | 5.31  | 126.48      | 119.84   |
| 3   | D     | 825  | ALA  | C-N-CA | 5.31  | 126.48      | 119.84   |
| 1   | B     | 37   | GLY  | N-CA-C | 5.30  | 119.06      | 112.64   |
| 1   | B     | 55   | SER  | N-CA-C | 5.27  | 117.73      | 110.35   |
| 1   | H     | 55   | SER  | N-CA-C | 5.27  | 117.67      | 110.24   |
| 5   | L     | 94   | ASP  | CA-C-N | 5.26  | 124.77      | 119.19   |
| 5   | L     | 94   | ASP  | C-N-CA | 5.26  | 124.77      | 119.19   |
| 2   | C     | 76   | PRO  | CA-C-N | 5.23  | 124.41      | 118.97   |
| 2   | C     | 76   | PRO  | C-N-CA | 5.23  | 124.41      | 118.97   |
| 1   | A     | 165  | ILE  | CA-C-N | 5.23  | 125.17      | 119.78   |
| 1   | A     | 165  | ILE  | C-N-CA | 5.23  | 125.17      | 119.78   |
| 2   | I     | 76   | PRO  | CA-C-N | 5.21  | 124.39      | 118.97   |
| 2   | I     | 76   | PRO  | C-N-CA | 5.21  | 124.39      | 118.97   |
| 3   | D     | 1120 | VAL  | CA-C-N | 5.20  | 125.10      | 119.85   |
| 3   | D     | 1120 | VAL  | C-N-CA | 5.20  | 125.10      | 119.85   |
| 2   | C     | 191  | PHE  | CA-C-N | 5.19  | 125.18      | 119.89   |
| 2   | C     | 191  | PHE  | C-N-CA | 5.19  | 125.18      | 119.89   |
| 1   | G     | 165  | ILE  | CA-C-N | 5.16  | 125.09      | 119.78   |
| 1   | G     | 165  | ILE  | C-N-CA | 5.16  | 125.09      | 119.78   |
| 3   | J     | 1234 | THR  | N-CA-C | -5.14 | 102.88      | 110.48   |
| 3   | D     | 1365 | ASP  | N-CA-C | 5.13  | 117.53      | 111.33   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | F     | 275  | ILE  | CA-C-N  | 5.12  | 125.12      | 119.89   |
| 5   | F     | 275  | ILE  | C-N-CA  | 5.12  | 125.12      | 119.89   |
| 2   | C     | 735  | ARG  | CA-C-N  | -5.10 | 115.22      | 122.77   |
| 2   | C     | 735  | ARG  | C-N-CA  | -5.10 | 115.22      | 122.77   |
| 2   | I     | 303  | PHE  | N-CA-C  | 5.07  | 117.20      | 111.11   |
| 2   | I     | 816  | LYS  | CA-C-N  | 5.06  | 126.17      | 119.84   |
| 2   | I     | 816  | LYS  | C-N-CA  | 5.06  | 126.17      | 119.84   |
| 1   | B     | 159  | LYS  | CA-C-N  | -5.06 | 115.43      | 123.12   |
| 1   | B     | 159  | LYS  | C-N-CA  | -5.06 | 115.43      | 123.12   |
| 3   | J     | 1297 | GLU  | CB-CA-C | -5.04 | 110.74      | 116.54   |
| 3   | D     | 243  | ALA  | CB-CA-C | -5.03 | 109.81      | 115.79   |
| 5   | F     | 94   | ASP  | CA-C-N  | 5.02  | 124.52      | 119.19   |
| 5   | F     | 94   | ASP  | C-N-CA  | 5.02  | 124.52      | 119.19   |
| 2   | I     | 735  | ARG  | CA-C-N  | -5.00 | 115.35      | 122.41   |
| 2   | I     | 735  | ARG  | C-N-CA  | -5.00 | 115.35      | 122.41   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | C     | 415  | PRO  | Peptide |
| 2   | C     | 423  | ALA  | Peptide |
| 2   | C     | 737  | LEU  | Peptide |
| 3   | D     | 1208 | ASP  | Peptide |
| 2   | I     | 415  | PRO  | Peptide |
| 2   | I     | 423  | ALA  | Peptide |
| 2   | I     | 737  | LEU  | Peptide |
| 3   | J     | 1359 | GLN  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1770  | 0        | 1799     | 93      | 0            |
| 1   | B     | 1770  | 0        | 1799     | 102     | 0            |
| 1   | G     | 1770  | 0        | 1799     | 106     | 0            |
| 1   | H     | 1770  | 0        | 1799     | 95      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 8739  | 0        | 8841     | 521     | 0            |
| 2   | I     | 8739  | 0        | 8841     | 502     | 0            |
| 3   | D     | 11761 | 0        | 11976    | 607     | 0            |
| 3   | J     | 10779 | 0        | 10993    | 530     | 0            |
| 4   | E     | 768   | 0        | 784      | 38      | 0            |
| 4   | K     | 768   | 0        | 784      | 30      | 0            |
| 5   | F     | 2787  | 0        | 2866     | 123     | 0            |
| 5   | L     | 2787  | 0        | 2866     | 135     | 0            |
| 6   | O     | 613   | 0        | 343      | 27      | 0            |
| 6   | R     | 613   | 0        | 343      | 26      | 0            |
| 7   | P     | 510   | 0        | 284      | 27      | 0            |
| 7   | S     | 527   | 0        | 297      | 25      | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | J     | 2     | 0        | 0        | 0       | 0            |
| 9   | D     | 1     | 0        | 0        | 0       | 0            |
| 9   | J     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 56477 | 0        | 56414    | 2691    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2691) 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:C:707:ARG:HE  | 2:C:824:ARG:HE   | 1.17                     | 0.90              |
| 6:R:24:DC:H42   | 7:S:3:DG:H1      | 1.18                     | 0.90              |
| 2:C:995:MET:HE2 | 2:C:996:LYS:H    | 1.38                     | 0.88              |
| 3:D:105:VAL:HA  | 3:D:112:ILE:HD11 | 1.55                     | 0.88              |
| 4:E:30:LEU:HD12 | 4:E:37:ASN:HD21  | 1.39                     | 0.88              |
| 4:K:30:LEU:HD12 | 4:K:37:ASN:HD21  | 1.39                     | 0.87              |
| 2:I:537:LYS:HZ3 | 2:I:905:VAL:H    | 1.19                     | 0.87              |
| 1:A:158:ILE:HB  | 1:A:166:PRO:HG3  | 1.57                     | 0.86              |
| 2:I:707:ARG:HE  | 2:I:824:ARG:HE   | 1.17                     | 0.86              |
| 2:I:995:MET:HE2 | 2:I:996:LYS:H    | 1.39                     | 0.86              |
| 2:C:537:LYS:HZ3 | 2:C:905:VAL:H    | 1.21                     | 0.86              |
| 2:I:557:ARG:HG3 | 2:I:879:ARG:HB3  | 1.57                     | 0.86              |
| 3:J:105:VAL:HA  | 3:J:112:ILE:HD11 | 1.59                     | 0.85              |
| 2:C:557:ARG:HG3 | 2:C:879:ARG:HB3  | 1.59                     | 0.85              |
| 3:D:231:VAL:H   | 3:D:243:ALA:HA   | 1.43                     | 0.84              |
| 1:H:48:ILE:HA   | 1:H:213:GLN:HE22 | 1.44                     | 0.83              |
| 1:G:158:ILE:HB  | 1:G:166:PRO:HG3  | 1.58                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:313:LEU:HD13 | 2:C:321:GLU:HA   | 1.61                     | 0.83              |
| 2:I:313:LEU:HD13 | 2:I:321:GLU:HA   | 1.61                     | 0.82              |
| 2:C:857:ASP:HB3  | 2:C:978:ARG:HG2  | 1.62                     | 0.82              |
| 1:B:48:ILE:HA    | 1:B:213:GLN:HE22 | 1.44                     | 0.82              |
| 2:C:750:LYS:HD3  | 3:D:681:ARG:HG3  | 1.60                     | 0.82              |
| 2:I:857:ASP:HB3  | 2:I:978:ARG:HG2  | 1.62                     | 0.82              |
| 3:D:835:SER:HB3  | 3:D:838:ARG:HE   | 1.44                     | 0.81              |
| 2:C:716:LYS:HG3  | 3:D:37:LEU:HD11  | 1.62                     | 0.81              |
| 2:I:15:LEU:H     | 2:I:586:ARG:HH22 | 1.27                     | 0.81              |
| 2:C:494:TYR:HB3  | 2:C:530:GLU:HG3  | 1.62                     | 0.81              |
| 2:I:324:ASP:HB3  | 2:I:327:HIS:HB2  | 1.63                     | 0.80              |
| 2:I:1033:GLY:HA2 | 3:J:620:GLY:HA3  | 1.64                     | 0.80              |
| 2:C:15:LEU:H     | 2:C:586:ARG:HH22 | 1.29                     | 0.80              |
| 2:C:808:ARG:HH11 | 2:C:815:LEU:H    | 1.29                     | 0.80              |
| 2:C:1033:GLY:HA2 | 3:D:620:GLY:HA3  | 1.63                     | 0.80              |
| 2:I:716:LYS:HG3  | 3:J:37:LEU:HD11  | 1.63                     | 0.80              |
| 3:D:792:ILE:HG21 | 3:D:941:LEU:HD22 | 1.63                     | 0.80              |
| 2:I:808:ARG:HH11 | 2:I:815:LEU:H    | 1.30                     | 0.79              |
| 3:J:97:THR:HG21  | 3:J:571:LYS:HG3  | 1.64                     | 0.79              |
| 1:B:151:VAL:HG13 | 1:B:155:ARG:HB2  | 1.64                     | 0.79              |
| 3:J:1142:SER:O   | 3:J:1364:HIS:ND1 | 2.13                     | 0.79              |
| 3:D:166:GLN:HB3  | 3:D:396:VAL:HG13 | 1.64                     | 0.79              |
| 3:D:708:LEU:HD12 | 3:D:1231:GLU:HG2 | 1.66                     | 0.78              |
| 2:I:1036:GLU:HA  | 3:J:707:THR:HG21 | 1.66                     | 0.78              |
| 5:L:164:GLU:HG3  | 5:L:165:LYS:HD2  | 1.66                     | 0.78              |
| 2:C:1008:ARG:HD3 | 2:C:1028:GLY:HA2 | 1.66                     | 0.78              |
| 3:D:700:VAL:HG22 | 3:D:718:PRO:HG3  | 1.65                     | 0.78              |
| 1:G:97:THR:HG23  | 1:G:98:THR:H     | 1.49                     | 0.77              |
| 2:I:494:TYR:HB3  | 2:I:530:GLU:HG3  | 1.64                     | 0.77              |
| 3:J:700:VAL:HG22 | 3:J:718:PRO:HG3  | 1.64                     | 0.77              |
| 3:J:1202:GLN:NE2 | 3:J:1215:VAL:O   | 2.12                     | 0.77              |
| 2:C:324:ASP:HB3  | 2:C:327:HIS:HB2  | 1.66                     | 0.77              |
| 2:I:595:LEU:HD23 | 2:I:639:GLN:HE22 | 1.49                     | 0.77              |
| 3:J:47:GLU:HG3   | 3:J:53:ILE:HG13  | 1.67                     | 0.77              |
| 1:A:27:PRO:HD3   | 1:A:186:LEU:HD22 | 1.64                     | 0.77              |
| 2:I:129:ILE:HD13 | 2:I:134:ARG:HB2  | 1.66                     | 0.77              |
| 3:J:208:PRO:HA   | 3:J:390:PRO:HA   | 1.67                     | 0.77              |
| 3:J:563:PRO:HB3  | 5:L:200:GLN:HB3  | 1.66                     | 0.77              |
| 3:J:792:ILE:HG21 | 3:J:941:LEU:HD22 | 1.65                     | 0.77              |
| 1:A:222:LEU:HD13 | 1:B:218:LEU:HD23 | 1.66                     | 0.76              |
| 7:P:13:DA:H1'    | 7:P:14:DC:H5'    | 1.67                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:151:VAL:HG13  | 1:H:155:ARG:HB2   | 1.64                     | 0.76              |
| 7:P:15:DA:H1'     | 7:P:16:DC:H5'     | 1.66                     | 0.76              |
| 3:D:270:ILE:HB    | 3:D:282:TYR:HB2   | 1.67                     | 0.76              |
| 2:C:32:ALA:HA     | 2:C:73:ILE:HG21   | 1.67                     | 0.76              |
| 2:I:838:LYS:HB3   | 2:I:997:LEU:HB2   | 1.68                     | 0.76              |
| 2:I:32:ALA:HA     | 2:I:73:ILE:HG21   | 1.68                     | 0.76              |
| 3:D:47:GLU:HG3    | 3:D:53:ILE:HG13   | 1.68                     | 0.76              |
| 1:A:97:THR:HG23   | 1:A:98:THR:H      | 1.48                     | 0.76              |
| 3:D:879:ARG:HH12  | 3:D:905:PRO:HA    | 1.50                     | 0.76              |
| 2:I:710:ILE:HG21  | 2:I:756:VAL:HG21  | 1.66                     | 0.76              |
| 2:C:129:ILE:HD13  | 2:C:134:ARG:HB2   | 1.68                     | 0.76              |
| 5:F:164:GLU:HG3   | 5:F:165:LYS:HD2   | 1.66                     | 0.76              |
| 1:G:222:LEU:HD13  | 1:H:218:LEU:HD23  | 1.65                     | 0.76              |
| 3:J:1486:VAL:HG11 | 4:K:26:ARG:HB2    | 1.68                     | 0.75              |
| 5:L:203:ILE:HG12  | 5:L:239:VAL:HG21  | 1.68                     | 0.75              |
| 1:A:184:THR:HB    | 1:A:194:LYS:HB3   | 1.67                     | 0.75              |
| 5:F:203:ILE:HG12  | 5:F:239:VAL:HG21  | 1.67                     | 0.75              |
| 2:I:750:LYS:HD3   | 3:J:681:ARG:HG3   | 1.67                     | 0.75              |
| 3:J:1147:ARG:HB3  | 3:J:1188:VAL:HG11 | 1.66                     | 0.75              |
| 3:D:169:TYR:HE2   | 3:D:395:VAL:HG12  | 1.50                     | 0.75              |
| 1:G:27:PRO:HD3    | 1:G:186:LEU:HD22  | 1.66                     | 0.75              |
| 1:G:184:THR:HB    | 1:G:194:LYS:HB3   | 1.69                     | 0.75              |
| 7:S:12:DA:H1'     | 7:S:13:DA:H5'     | 1.68                     | 0.75              |
| 2:C:72:ARG:HB3    | 2:C:95:TYR:HB2    | 1.69                     | 0.75              |
| 1:G:55:SER:HB2    | 1:G:158:ILE:HG12  | 1.68                     | 0.74              |
| 3:D:1208:ASP:O    | 3:D:1210:SER:N    | 2.20                     | 0.74              |
| 2:C:580:MET:HE1   | 2:C:665:PHE:HB3   | 1.69                     | 0.74              |
| 2:C:595:LEU:HD23  | 2:C:639:GLN:HE22  | 1.50                     | 0.74              |
| 3:D:73:CYS:HB3    | 3:D:78:VAL:H      | 1.51                     | 0.74              |
| 3:J:73:CYS:HB3    | 3:J:78:VAL:H      | 1.52                     | 0.74              |
| 2:C:838:LYS:HB3   | 2:C:997:LEU:HB2   | 1.69                     | 0.74              |
| 1:A:53:VAL:HG22   | 1:A:54:THR:H      | 1.52                     | 0.74              |
| 1:A:205:VAL:HG13  | 1:A:209:GLU:HB2   | 1.69                     | 0.74              |
| 2:C:1036:GLU:HA   | 3:D:707:THR:HG21  | 1.70                     | 0.74              |
| 2:C:86:LYS:HE2    | 2:C:813:VAL:HG23  | 1.70                     | 0.74              |
| 3:D:1143:GLY:HA2  | 3:D:1364:HIS:CE1  | 2.22                     | 0.74              |
| 2:I:370:ALA:HB1   | 5:L:295:GLN:HE22  | 1.53                     | 0.74              |
| 2:C:419:THR:HG23  | 2:C:421:GLU:H     | 1.53                     | 0.74              |
| 7:P:2:DA:H1'      | 7:P:3:DG:H5'      | 1.70                     | 0.74              |
| 2:C:724:ARG:HG3   | 2:C:737:LEU:HD23  | 1.70                     | 0.73              |
| 3:D:39:PRO:HB3    | 3:D:46:ASP:HA     | 1.70                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1223:VAL:HG21 | 3:D:1462:LEU:HD21 | 1.69                     | 0.73              |
| 4:E:30:LEU:HD12   | 4:E:37:ASN:ND2    | 2.03                     | 0.73              |
| 1:G:53:VAL:HG22   | 1:G:54:THR:H      | 1.53                     | 0.73              |
| 2:I:601:GLY:HA2   | 2:I:615:TYR:HA    | 1.70                     | 0.73              |
| 3:D:191:LEU:HD11  | 3:D:197:SER:HB2   | 1.70                     | 0.73              |
| 3:D:1486:VAL:HG11 | 4:E:26:ARG:HB2    | 1.70                     | 0.73              |
| 1:H:57:TYR:CG     | 1:H:161:ARG:HG2   | 2.23                     | 0.73              |
| 2:I:1064:ASN:HD22 | 5:L:359:ALA:HB2   | 1.53                     | 0.73              |
| 3:J:165:LYS:H     | 3:J:397:LYS:HE2   | 1.52                     | 0.73              |
| 2:C:662:GLU:HG2   | 2:C:663:GLU:HG2   | 1.69                     | 0.73              |
| 2:C:498:GLN:HG3   | 3:D:1068:LEU:HD11 | 1.71                     | 0.73              |
| 2:C:710:ILE:HG21  | 2:C:756:VAL:HG21  | 1.69                     | 0.73              |
| 4:E:27:ALA:HA     | 4:E:30:LEU:HD22   | 1.71                     | 0.73              |
| 2:I:724:ARG:HG3   | 2:I:737:LEU:HD23  | 1.71                     | 0.73              |
| 2:I:662:GLU:HG2   | 2:I:663:GLU:HG2   | 1.71                     | 0.73              |
| 3:D:39:PRO:HG2    | 3:D:47:GLU:HB2    | 1.71                     | 0.73              |
| 2:I:1008:ARG:HD3  | 2:I:1028:GLY:HA2  | 1.71                     | 0.73              |
| 2:C:541:SER:O     | 2:C:545:ASN:ND2   | 2.22                     | 0.72              |
| 3:J:1336:LEU:HA   | 3:J:1344:VAL:HG21 | 1.71                     | 0.72              |
| 3:D:596:SER:OG    | 3:D:597:GLU:N     | 2.20                     | 0.72              |
| 3:J:680:GLN:HG2   | 3:J:681:ARG:H     | 1.54                     | 0.72              |
| 3:D:680:GLN:HG2   | 3:D:681:ARG:H     | 1.53                     | 0.72              |
| 1:A:55:SER:HB2    | 1:A:158:ILE:HG12  | 1.70                     | 0.72              |
| 1:B:57:TYR:CG     | 1:B:161:ARG:HG2   | 2.25                     | 0.72              |
| 2:I:541:SER:O     | 2:I:545:ASN:ND2   | 2.23                     | 0.72              |
| 3:J:39:PRO:HG2    | 3:J:47:GLU:HB2    | 1.71                     | 0.72              |
| 1:G:205:VAL:HG13  | 1:G:209:GLU:HB2   | 1.72                     | 0.72              |
| 5:L:376:LEU:HD11  | 5:L:423:LEU:HD11  | 1.72                     | 0.72              |
| 3:D:242:LEU:H     | 3:D:312:ARG:HA    | 1.53                     | 0.72              |
| 3:J:39:PRO:HB3    | 3:J:46:ASP:HA     | 1.72                     | 0.72              |
| 1:B:110:ARG:H     | 1:B:113:ASP:HB2   | 1.55                     | 0.72              |
| 2:I:146:VAL:HG12  | 2:I:162:ILE:HG13  | 1.72                     | 0.72              |
| 2:C:146:VAL:HG12  | 2:C:162:ILE:HG13  | 1.71                     | 0.71              |
| 3:D:97:THR:HG21   | 3:D:571:LYS:HG3   | 1.71                     | 0.71              |
| 3:J:410:THR:HG23  | 5:L:189:LEU:HD21  | 1.72                     | 0.71              |
| 3:J:879:ARG:HH12  | 3:J:905:PRO:HA    | 1.55                     | 0.71              |
| 3:J:1211:MET:HB3  | 3:J:1213:ARG:HG2  | 1.71                     | 0.71              |
| 2:C:163:ILE:HD12  | 2:C:164:PRO:HD2   | 1.71                     | 0.71              |
| 2:C:737:LEU:HG    | 2:C:741:GLY:HA2   | 1.72                     | 0.71              |
| 2:I:1053:LEU:HA   | 3:J:621:LYS:HE3   | 1.72                     | 0.71              |
| 6:O:7:DA:H61      | 7:P:20:DT:H3      | 1.38                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:214:ASP:OD1   | 3:D:214:ASP:N     | 2.22                     | 0.71              |
| 2:C:1053:LEU:HA   | 3:D:621:LYS:HE3   | 1.72                     | 0.71              |
| 3:D:226:PRO:HA    | 3:D:330:SER:HA    | 1.72                     | 0.71              |
| 3:D:1003:VAL:HG21 | 3:D:1041:MET:HG2  | 1.72                     | 0.71              |
| 2:I:419:THR:HG23  | 2:I:421:GLU:H     | 1.55                     | 0.71              |
| 2:I:737:LEU:HG    | 2:I:741:GLY:HA2   | 1.72                     | 0.71              |
| 3:D:618:LEU:HD23  | 3:D:1467:ILE:HG23 | 1.71                     | 0.71              |
| 2:I:163:ILE:HD12  | 2:I:164:PRO:HD2   | 1.71                     | 0.71              |
| 4:K:30:LEU:HD12   | 4:K:37:ASN:ND2    | 2.03                     | 0.71              |
| 5:F:376:LEU:HD11  | 5:F:423:LEU:HD11  | 1.71                     | 0.71              |
| 4:K:27:ALA:HA     | 4:K:30:LEU:HD22   | 1.72                     | 0.70              |
| 3:J:367:ILE:HB    | 3:J:377:VAL:HB    | 1.73                     | 0.70              |
| 2:C:601:GLY:HA2   | 2:C:615:TYR:HA    | 1.72                     | 0.70              |
| 1:G:219:LYS:HA    | 1:G:222:LEU:HD23  | 1.74                     | 0.70              |
| 1:B:186:LEU:HB2   | 1:B:192:LEU:HD11  | 1.72                     | 0.70              |
| 3:J:800:LYS:HB3   | 3:J:822:ALA:HB2   | 1.72                     | 0.70              |
| 3:J:1003:VAL:HG21 | 3:J:1041:MET:HG2  | 1.74                     | 0.70              |
| 3:J:1267:ARG:HE   | 3:J:1267:ARG:H    | 1.39                     | 0.70              |
| 3:D:214:ASP:HA    | 3:D:342:PRO:HA    | 1.74                     | 0.70              |
| 3:D:208:PRO:HA    | 3:D:390:PRO:HA    | 1.74                     | 0.70              |
| 3:J:361:VAL:HG21  | 3:J:367:ILE:HD11  | 1.74                     | 0.70              |
| 7:S:15:DA:H1'     | 7:S:16:DC:H5'     | 1.73                     | 0.70              |
| 3:D:9:ARG:HG3     | 3:D:1456:LYS:HG2  | 1.74                     | 0.70              |
| 3:J:371:ILE:HG21  | 5:L:247:ARG:HH22  | 1.53                     | 0.70              |
| 2:C:1101:THR:HG23 | 3:D:8:VAL:HG22    | 1.74                     | 0.69              |
| 3:D:1192:LEU:HA   | 3:D:1373:ARG:HG3  | 1.73                     | 0.69              |
| 2:I:498:GLN:HG3   | 3:J:1068:LEU:HD11 | 1.74                     | 0.69              |
| 3:J:191:LEU:HD11  | 3:J:197:SER:HB2   | 1.73                     | 0.69              |
| 6:O:17:DA:H1'     | 6:O:18:DA:H5'     | 1.73                     | 0.69              |
| 3:D:800:LYS:HB3   | 3:D:822:ALA:HB2   | 1.73                     | 0.69              |
| 3:J:1476:THR:HA   | 4:K:17:TYR:HB3    | 1.74                     | 0.69              |
| 3:D:563:PRO:HB3   | 5:F:200:GLN:HB3   | 1.74                     | 0.69              |
| 3:D:1272:ALA:HB3  | 3:D:1330:ILE:HD13 | 1.75                     | 0.69              |
| 3:J:371:ILE:HG23  | 3:J:372:ASP:H     | 1.55                     | 0.69              |
| 3:J:761:ILE:O     | 3:J:767:HIS:ND1   | 2.23                     | 0.69              |
| 2:I:72:ARG:HB3    | 2:I:95:TYR:HB2    | 1.75                     | 0.69              |
| 3:D:236:TYR:HB3   | 3:D:313:LEU:HD22  | 1.74                     | 0.69              |
| 1:H:110:ARG:H     | 1:H:113:ASP:HB2   | 1.58                     | 0.69              |
| 2:I:941:LYS:HZ2   | 2:I:959:PRO:HG2   | 1.58                     | 0.69              |
| 2:I:542:LEU:H     | 2:I:542:LEU:HD12  | 1.58                     | 0.69              |
| 3:J:1105:ILE:HD12 | 3:J:1373:ARG:HH12 | 1.58                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:715:ALA:HB3  | 3:D:764:LEU:HA    | 1.75                     | 0.69              |
| 2:I:468:ARG:HB3  | 2:I:485:TYR:O     | 1.93                     | 0.69              |
| 2:I:833:LEU:HD11 | 2:I:839:LEU:HD11  | 1.75                     | 0.69              |
| 3:D:93:ILE:HD13  | 3:D:548:ILE:HG23  | 1.75                     | 0.68              |
| 6:R:18:DA:H1'    | 6:R:19:DT:H5'     | 1.74                     | 0.68              |
| 2:C:880:MET:HE1  | 3:D:1037:GLN:HB2  | 1.73                     | 0.68              |
| 2:I:580:MET:HE1  | 2:I:665:PHE:HB3   | 1.75                     | 0.68              |
| 2:I:969:LEU:HD23 | 2:I:971:LYS:HE3   | 1.74                     | 0.68              |
| 6:O:10:DA:H1'    | 6:O:11:DG:H5'     | 1.75                     | 0.68              |
| 7:P:17:DT:H1'    | 7:P:18:DT:H5'     | 1.73                     | 0.68              |
| 3:J:560:GLN:O    | 5:L:147:ARG:NH1   | 2.26                     | 0.68              |
| 3:D:520:LEU:O    | 3:D:525:ARG:NH2   | 2.26                     | 0.68              |
| 2:I:880:MET:HE1  | 3:J:1037:GLN:HB2  | 1.75                     | 0.68              |
| 4:K:40:LEU:HD21  | 4:K:67:GLU:HA     | 1.75                     | 0.68              |
| 3:D:977:ALA:HB2  | 3:J:831:GLY:H     | 1.59                     | 0.68              |
| 1:B:59:GLU:HG3   | 1:B:139:TYR:HD2   | 1.57                     | 0.68              |
| 2:C:200:LEU:HG   | 2:C:300:ASP:HB2   | 1.76                     | 0.68              |
| 2:C:568:ALA:HB1  | 2:C:995:MET:SD    | 2.34                     | 0.68              |
| 3:D:93:ILE:HB    | 3:D:517:VAL:HB    | 1.75                     | 0.68              |
| 3:J:699:VAL:HG12 | 3:J:717:GLN:HG2   | 1.75                     | 0.68              |
| 5:L:222:LEU:HD11 | 5:L:269:GLN:HG2   | 1.76                     | 0.68              |
| 2:C:242:LEU:HD13 | 2:C:243:ARG:HB2   | 1.76                     | 0.68              |
| 3:D:1476:THR:HA  | 4:E:17:TYR:HB3    | 1.75                     | 0.68              |
| 3:J:8:VAL:HG21   | 3:J:1468:LEU:HD11 | 1.76                     | 0.68              |
| 3:D:371:ILE:HG23 | 3:D:372:ASP:H     | 1.59                     | 0.67              |
| 2:I:568:ALA:HB1  | 2:I:995:MET:SD    | 2.34                     | 0.67              |
| 3:D:45:PHE:HA    | 3:D:522:PRO:HB3   | 1.76                     | 0.67              |
| 2:I:439:CYS:HB2  | 2:I:541:SER:HB3   | 1.75                     | 0.67              |
| 7:P:25:DA:H1'    | 7:P:26:DG:H5'     | 1.76                     | 0.67              |
| 2:I:833:LEU:HD12 | 2:I:996:LYS:HE3   | 1.74                     | 0.67              |
| 2:C:261:LEU:HB3  | 2:C:291:VAL:HG22  | 1.77                     | 0.67              |
| 3:J:521:PRO:HD2  | 3:J:524:LEU:HD12  | 1.76                     | 0.67              |
| 3:J:783:ARG:HD3  | 3:J:1028:ALA:O    | 1.94                     | 0.67              |
| 2:C:230:ARG:HB3  | 2:C:231:PRO:HD2   | 1.76                     | 0.67              |
| 2:C:542:LEU:H    | 2:C:542:LEU:HD12  | 1.59                     | 0.67              |
| 1:G:39:PRO:HG2   | 1:H:39:PRO:HG3    | 1.76                     | 0.67              |
| 2:C:439:CYS:HB2  | 2:C:541:SER:HB3   | 1.77                     | 0.67              |
| 3:D:1202:GLN:NE2 | 3:D:1215:VAL:O    | 2.25                     | 0.67              |
| 3:J:1254:GLN:HB3 | 3:J:1258:ARG:HB2  | 1.77                     | 0.67              |
| 2:I:211:LEU:HD13 | 2:I:218:VAL:HA    | 1.76                     | 0.67              |
| 7:P:21:DG:H1'    | 7:P:22:DT:H5'     | 1.75                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1382:THR:HG23 | 3:D:1417:TRP:HA   | 1.77                     | 0.67              |
| 3:J:87:ARG:HG2    | 3:J:523:ASP:HB3   | 1.77                     | 0.67              |
| 3:J:1384:PRO:HA   | 3:J:1415:VAL:HG13 | 1.76                     | 0.67              |
| 5:L:164:GLU:O     | 5:L:166:PRO:HD3   | 1.95                     | 0.67              |
| 2:I:140:ILE:HG22  | 2:I:412:ALA:HA    | 1.76                     | 0.67              |
| 2:I:229:MET:HB3   | 2:I:234:ALA:HB2   | 1.76                     | 0.67              |
| 2:I:397:GLU:HB2   | 2:I:632:ASN:HB2   | 1.77                     | 0.67              |
| 3:J:618:LEU:HD23  | 3:J:1467:ILE:HG23 | 1.75                     | 0.67              |
| 3:J:1140:ILE:HG23 | 3:J:1144:LEU:HD23 | 1.77                     | 0.67              |
| 3:J:1273:VAL:HG22 | 3:J:1326:THR:HG22 | 1.77                     | 0.67              |
| 2:I:207:LEU:HD21  | 2:I:221:LEU:HB3   | 1.76                     | 0.66              |
| 6:O:9:DA:H1'      | 6:O:10:DA:H5'     | 1.77                     | 0.66              |
| 2:C:229:MET:HB3   | 2:C:234:ALA:HB2   | 1.75                     | 0.66              |
| 5:F:164:GLU:O     | 5:F:166:PRO:HD3   | 1.95                     | 0.66              |
| 3:J:100:ALA:HA    | 3:J:513:ILE:HA    | 1.77                     | 0.66              |
| 2:C:1042:ALA:HA   | 3:D:1224:VAL:HG22 | 1.75                     | 0.66              |
| 2:I:200:LEU:HG    | 2:I:300:ASP:HB2   | 1.77                     | 0.66              |
| 2:I:688:ILE:HB    | 2:I:849:VAL:HA    | 1.76                     | 0.66              |
| 3:D:783:ARG:HD3   | 3:D:1028:ALA:O    | 1.96                     | 0.66              |
| 2:I:172:ILE:HA    | 2:I:186:VAL:HG22  | 1.77                     | 0.66              |
| 3:J:423:ASP:HB3   | 3:J:426:LYS:HB3   | 1.76                     | 0.66              |
| 2:C:833:LEU:HD12  | 2:C:996:LYS:HE3   | 1.75                     | 0.66              |
| 3:D:569:ASN:HD22  | 5:F:229:GLN:HE21  | 1.44                     | 0.66              |
| 4:E:40:LEU:HD21   | 4:E:67:GLU:HA     | 1.76                     | 0.66              |
| 2:C:64:LEU:HD13   | 2:C:359:MET:HG2   | 1.78                     | 0.66              |
| 2:C:777:ILE:HA    | 5:F:420:LEU:HD11  | 1.77                     | 0.66              |
| 2:C:969:LEU:HD23  | 2:C:971:LYS:HE3   | 1.76                     | 0.66              |
| 2:I:230:ARG:HB3   | 2:I:231:PRO:HD2   | 1.76                     | 0.66              |
| 2:I:708:TYR:CE1   | 2:I:827:VAL:HB    | 2.31                     | 0.66              |
| 6:O:12:DT:H1'     | 6:O:13:DG:H5'     | 1.78                     | 0.66              |
| 2:C:468:ARG:HB3   | 2:C:485:TYR:O     | 1.95                     | 0.66              |
| 2:C:577:PRO:HA    | 2:C:671:ASN:HD21  | 1.61                     | 0.66              |
| 3:D:354:ILE:HD11  | 3:D:369:ALA:HB2   | 1.77                     | 0.66              |
| 2:I:242:LEU:HD13  | 2:I:243:ARG:HB2   | 1.76                     | 0.66              |
| 2:I:332:ARG:HB2   | 2:I:465:GLY:HA3   | 1.77                     | 0.66              |
| 2:I:1101:THR:HG23 | 3:J:8:VAL:HG22    | 1.78                     | 0.66              |
| 2:C:762:LYS:HB3   | 2:C:786:LYS:HB2   | 1.78                     | 0.66              |
| 2:I:458:TYR:HB3   | 2:I:470:PRO:HG2   | 1.77                     | 0.66              |
| 2:I:537:LYS:HZ3   | 2:I:905:VAL:N     | 1.91                     | 0.66              |
| 2:C:101:ILE:HG23  | 2:C:108:ILE:HA    | 1.77                     | 0.66              |
| 2:I:101:ILE:HG23  | 2:I:108:ILE:HA    | 1.79                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:O:24:DC:H42    | 7:P:3:DG:H1       | 1.43                     | 0.65              |
| 2:C:211:LEU:HD13 | 2:C:218:VAL:HA    | 1.77                     | 0.65              |
| 3:D:266:GLU:HG3  | 3:D:286:ALA:HB2   | 1.77                     | 0.65              |
| 3:D:594:PRO:HB3  | 5:F:221:GLY:HA2   | 1.78                     | 0.65              |
| 3:J:715:ALA:HB3  | 3:J:764:LEU:HA    | 1.78                     | 0.65              |
| 3:D:699:VAL:HG12 | 3:D:717:GLN:HG2   | 1.76                     | 0.65              |
| 1:A:219:LYS:HA   | 1:A:222:LEU:HD23  | 1.77                     | 0.65              |
| 2:C:140:ILE:HG22 | 2:C:412:ALA:HA    | 1.77                     | 0.65              |
| 3:J:582:ILE:HD13 | 3:J:603:LEU:HD12  | 1.79                     | 0.65              |
| 2:I:458:TYR:HD1  | 2:I:538:GLN:HB3   | 1.61                     | 0.65              |
| 3:J:100:ALA:HB2  | 3:J:513:ILE:HD13  | 1.78                     | 0.65              |
| 6:R:9:DA:H1'     | 6:R:10:DA:H5'     | 1.77                     | 0.65              |
| 3:D:224:ARG:NH2  | 3:D:254:GLU:OE2   | 2.29                     | 0.65              |
| 2:I:710:ILE:HB   | 2:I:790:LEU:HD22  | 1.79                     | 0.65              |
| 2:C:397:GLU:HB2  | 2:C:632:ASN:HB2   | 1.79                     | 0.65              |
| 2:C:1102:LEU:HB2 | 3:D:7:LYS:HB2     | 1.79                     | 0.65              |
| 4:K:67:GLU:HB3   | 4:K:73:LEU:HD11   | 1.79                     | 0.65              |
| 2:C:458:TYR:HB3  | 2:C:470:PRO:HG2   | 1.77                     | 0.65              |
| 1:B:24:VAL:HG22  | 1:B:196:THR:HG23  | 1.78                     | 0.65              |
| 3:D:8:VAL:HG21   | 3:D:1468:LEU:HD11 | 1.78                     | 0.65              |
| 6:R:10:DA:H1'    | 6:R:11:DG:H5'     | 1.78                     | 0.65              |
| 3:D:786:ILE:HD13 | 3:D:908:LYS:HG2   | 1.78                     | 0.64              |
| 5:F:222:LEU:HD11 | 5:F:269:GLN:HG2   | 1.79                     | 0.64              |
| 3:J:1285:GLU:HB3 | 3:J:1290:LEU:HA   | 1.79                     | 0.64              |
| 6:R:2:DT:H3      | 7:S:25:DA:H2      | 1.42                     | 0.64              |
| 2:C:207:LEU:HD21 | 2:C:221:LEU:HB3   | 1.77                     | 0.64              |
| 3:D:242:LEU:HD23 | 3:D:285:PRO:HB3   | 1.79                     | 0.64              |
| 3:D:260:GLU:HB3  | 3:D:271:TYR:HB2   | 1.79                     | 0.64              |
| 4:E:67:GLU:HB3   | 4:E:73:LEU:HD11   | 1.79                     | 0.64              |
| 2:I:576:ALA:HB1  | 2:I:580:MET:HE3   | 1.80                     | 0.64              |
| 2:C:1051:GLU:HG2 | 2:C:1055:ILE:HD12 | 1.79                     | 0.64              |
| 1:H:59:GLU:HB2   | 1:H:139:TYR:HB3   | 1.79                     | 0.64              |
| 7:S:13:DA:H1'    | 7:S:14:DC:H5'     | 1.78                     | 0.64              |
| 2:C:139:GLN:HB2  | 2:C:391:LEU:HD21  | 1.79                     | 0.64              |
| 3:D:268:HIS:HB2  | 3:D:284:LEU:HD22  | 1.78                     | 0.64              |
| 2:I:118:LEU:HD12 | 2:I:119:PRO:HD2   | 1.78                     | 0.64              |
| 2:C:217:LEU:HD13 | 2:C:311:PHE:HB3   | 1.80                     | 0.64              |
| 2:C:467:ILE:H    | 2:C:467:ILE:HD12  | 1.63                     | 0.64              |
| 2:I:773:LEU:HB2  | 5:L:388:LYS:HG3   | 1.80                     | 0.64              |
| 5:L:149:LYS:HD3  | 5:L:193:ARG:HH22  | 1.61                     | 0.64              |
| 3:D:573:MET:HA   | 3:D:576:GLU:HG2   | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:64:LEU:HD13   | 2:I:359:MET:HG2   | 1.80                     | 0.64              |
| 2:C:710:ILE:HB    | 2:C:790:LEU:HD22  | 1.80                     | 0.64              |
| 3:D:1048:PRO:HD3  | 3:D:1075:HIS:HB3  | 1.79                     | 0.64              |
| 3:J:67:ARG:HD2    | 5:L:394:ARG:HB2   | 1.78                     | 0.64              |
| 3:J:786:ILE:HD13  | 3:J:908:LYS:HG2   | 1.78                     | 0.64              |
| 1:H:186:LEU:HB2   | 1:H:192:LEU:HD11  | 1.79                     | 0.64              |
| 3:D:1274:ILE:HG22 | 3:D:1324:PRO:HA   | 1.80                     | 0.64              |
| 2:I:86:LYS:HE2    | 2:I:813:VAL:HG23  | 1.79                     | 0.64              |
| 2:I:139:GLN:HB2   | 2:I:391:LEU:HD21  | 1.80                     | 0.64              |
| 3:J:887:GLY:HA3   | 3:J:893:GLU:HA    | 1.79                     | 0.64              |
| 2:C:688:ILE:HB    | 2:C:849:VAL:HA    | 1.79                     | 0.63              |
| 1:H:24:VAL:HG22   | 1:H:196:THR:HG23  | 1.79                     | 0.63              |
| 2:I:261:LEU:HB3   | 2:I:291:VAL:HG22  | 1.80                     | 0.63              |
| 2:C:118:LEU:HD12  | 2:C:119:PRO:HD2   | 1.79                     | 0.63              |
| 2:C:458:TYR:HD1   | 2:C:538:GLN:HB3   | 1.62                     | 0.63              |
| 5:F:364:LEU:HD12  | 5:F:436:PHE:HZ    | 1.63                     | 0.63              |
| 2:I:101:ILE:HA    | 2:I:107:LEU:O     | 1.98                     | 0.63              |
| 2:I:577:PRO:HA    | 2:I:671:ASN:HD21  | 1.63                     | 0.63              |
| 3:D:618:LEU:HB3   | 3:D:1467:ILE:HG12 | 1.79                     | 0.63              |
| 3:J:102:ILE:HB    | 3:J:579:ASP:HB3   | 1.79                     | 0.63              |
| 6:O:18:DA:H1'     | 6:O:19:DT:H5'     | 1.78                     | 0.63              |
| 2:C:708:TYR:CE1   | 2:C:827:VAL:HB    | 2.33                     | 0.63              |
| 1:A:39:PRO:HG2    | 1:B:39:PRO:HG3    | 1.81                     | 0.63              |
| 2:C:1064:ASN:HD22 | 5:F:359:ALA:HB2   | 1.64                     | 0.63              |
| 2:C:576:ALA:HB1   | 2:C:580:MET:HE3   | 1.80                     | 0.63              |
| 3:D:887:GLY:HA3   | 3:D:893:GLU:HA    | 1.80                     | 0.63              |
| 3:J:65:ARG:NH1    | 5:L:393:GLY:O     | 2.32                     | 0.63              |
| 2:C:723:THR:O     | 2:C:757:GLY:HA3   | 1.99                     | 0.63              |
| 2:C:833:LEU:HD11  | 2:C:839:LEU:HD11  | 1.79                     | 0.63              |
| 2:I:217:LEU:HD13  | 2:I:311:PHE:HB3   | 1.81                     | 0.63              |
| 6:O:4:DG:H1'      | 6:O:5:DA:H5'      | 1.80                     | 0.63              |
| 2:C:1034:GLU:HG2  | 3:D:619:LEU:HB3   | 1.81                     | 0.63              |
| 3:D:1472:ILE:HG12 | 3:D:1474:ALA:H    | 1.63                     | 0.63              |
| 5:L:383:VAL:HA    | 5:L:386:LEU:HD12  | 1.79                     | 0.63              |
| 1:B:44:LEU:HD23   | 1:B:174:VAL:HG21  | 1.81                     | 0.63              |
| 1:B:73:GLU:HB2    | 1:B:78:ILE:HD11   | 1.80                     | 0.63              |
| 3:D:514:LEU:HD21  | 3:D:518:PRO:HD3   | 1.81                     | 0.63              |
| 3:D:701:LEU:HD21  | 3:D:763:MET:HG3   | 1.79                     | 0.63              |
| 3:D:703:ASN:HB2   | 3:D:713:ILE:HG12  | 1.80                     | 0.63              |
| 3:J:974:ILE:HG12  | 3:J:991:GLN:HE21  | 1.63                     | 0.63              |
| 2:C:172:ILE:HA    | 2:C:186:VAL:HG22  | 1.79                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:79:LEU:HG     | 4:E:80:VAL:HG13   | 1.80                     | 0.62              |
| 3:D:407:VAL:HG22  | 3:D:409:VAL:H     | 1.63                     | 0.62              |
| 2:I:467:ILE:H     | 2:I:467:ILE:HD12  | 1.63                     | 0.62              |
| 3:J:835:SER:HB3   | 3:J:838:ARG:HE    | 1.63                     | 0.62              |
| 3:D:761:ILE:O     | 3:D:767:HIS:ND1   | 2.26                     | 0.62              |
| 2:C:773:LEU:HB2   | 5:F:388:LYS:HG3   | 1.80                     | 0.62              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:HB    | 1.80                     | 0.62              |
| 5:F:383:VAL:HA    | 5:F:386:LEU:HD12  | 1.81                     | 0.62              |
| 2:I:607:ASP:O     | 2:I:609:THR:N     | 2.33                     | 0.62              |
| 2:C:370:ALA:HB1   | 5:F:295:GLN:HE22  | 1.64                     | 0.62              |
| 3:D:48:ARG:HA     | 3:D:78:VAL:HG22   | 1.81                     | 0.62              |
| 3:D:167:GLU:HB2   | 3:D:199:MET:HE3   | 1.81                     | 0.62              |
| 3:D:1384:PRO:HA   | 3:D:1415:VAL:HG13 | 1.82                     | 0.62              |
| 3:J:127:LEU:HD23  | 3:J:461:ILE:HG13  | 1.81                     | 0.62              |
| 3:J:1048:PRO:HD3  | 3:J:1075:HIS:HB3  | 1.81                     | 0.62              |
| 5:L:364:LEU:HD12  | 5:L:436:PHE:HZ    | 1.63                     | 0.62              |
| 2:C:537:LYS:HZ3   | 2:C:905:VAL:N     | 1.93                     | 0.62              |
| 2:I:123:GLU:HG2   | 2:I:592:LEU:HD13  | 1.81                     | 0.62              |
| 3:J:701:LEU:HD21  | 3:J:763:MET:HG3   | 1.80                     | 0.62              |
| 3:J:1472:ILE:HG12 | 3:J:1474:ALA:H    | 1.65                     | 0.62              |
| 5:F:180:SER:O     | 5:F:181:LEU:HD12  | 2.00                     | 0.62              |
| 2:I:691:SER:HB3   | 2:I:868:ASP:HA    | 1.82                     | 0.62              |
| 2:I:762:LYS:HB3   | 2:I:786:LYS:HB2   | 1.80                     | 0.62              |
| 2:I:502:PRO:HG3   | 2:I:510:THR:HG22  | 1.82                     | 0.62              |
| 2:C:101:ILE:HA    | 2:C:107:LEU:O     | 1.99                     | 0.62              |
| 3:J:1004:THR:HG23 | 3:J:1036:ARG:HB2  | 1.81                     | 0.62              |
| 1:B:59:GLU:HB2    | 1:B:139:TYR:HB3   | 1.82                     | 0.62              |
| 2:C:704:HIS:CD2   | 2:C:831:ARG:HD2   | 2.35                     | 0.62              |
| 3:D:137:PRO:HA    | 3:D:452:ILE:HG13  | 1.82                     | 0.62              |
| 1:G:46:SER:HB3    | 2:I:856:GLU:HG2   | 1.82                     | 0.62              |
| 2:I:839:LEU:HG    | 2:I:996:LYS:HA    | 1.81                     | 0.62              |
| 2:C:50:GLU:HA     | 2:C:265:LYS:HD2   | 1.82                     | 0.61              |
| 3:D:1202:GLN:HE21 | 3:D:1217:ILE:HG12 | 1.65                     | 0.61              |
| 1:H:73:GLU:HB2    | 1:H:78:ILE:HD11   | 1.82                     | 0.61              |
| 2:C:107:LEU:HD12  | 2:C:109:LYS:HB2   | 1.82                     | 0.61              |
| 3:D:168:THR:HA    | 3:D:394:LEU:HB2   | 1.81                     | 0.61              |
| 3:D:974:ILE:HG12  | 3:D:991:GLN:HE21  | 1.65                     | 0.61              |
| 1:H:44:LEU:HD23   | 1:H:174:VAL:HG21  | 1.82                     | 0.61              |
| 3:J:772:PRO:HA    | 3:J:1209:LEU:HB2  | 1.82                     | 0.61              |
| 6:R:10:DA:H2      | 7:S:17:DT:H3      | 1.47                     | 0.61              |
| 2:C:579:VAL:HG13  | 2:C:842:ARG:HH22  | 1.64                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:607:ASP:O     | 2:C:609:THR:N     | 2.32                     | 0.61              |
| 3:D:245:LEU:HB2   | 3:D:309:GLY:HA2   | 1.81                     | 0.61              |
| 2:C:174:LEU:HD13  | 2:C:310:LEU:HD22  | 1.81                     | 0.61              |
| 2:C:1090:LYS:NZ   | 2:C:1093:GLN:OE1  | 2.28                     | 0.61              |
| 3:D:192:ALA:HB1   | 3:D:193:PRO:HD2   | 1.81                     | 0.61              |
| 5:F:222:LEU:HB3   | 5:F:226:ASP:HB2   | 1.82                     | 0.61              |
| 2:I:36:PRO:HA     | 2:I:39:ARG:HD2    | 1.83                     | 0.61              |
| 2:I:723:THR:O     | 2:I:757:GLY:HA3   | 2.00                     | 0.61              |
| 3:J:112:ILE:HG23  | 3:J:512:MET:HG2   | 1.81                     | 0.61              |
| 3:J:1313:VAL:HG21 | 3:J:1325:LEU:HD12 | 1.81                     | 0.61              |
| 2:C:332:ARG:HB2   | 2:C:465:GLY:HA3   | 1.82                     | 0.61              |
| 3:D:1143:GLY:HA2  | 3:D:1364:HIS:HE1  | 1.65                     | 0.61              |
| 2:I:1016:ILE:O    | 3:J:87:ARG:NH2    | 2.34                     | 0.61              |
| 6:R:11:DG:N2      | 7:S:16:DC:O2      | 2.34                     | 0.61              |
| 2:C:571:LEU:HB2   | 2:C:574:ALA:HB2   | 1.81                     | 0.61              |
| 1:G:35:THR:HG21   | 1:H:43:ILE:HG13   | 1.81                     | 0.61              |
| 2:C:1037:VAL:HG13 | 2:C:1049:LEU:HD11 | 1.83                     | 0.61              |
| 3:D:1100:ASP:HA   | 3:D:1463:LYS:HE2  | 1.82                     | 0.61              |
| 1:H:59:GLU:HG3    | 1:H:139:TYR:HD2   | 1.66                     | 0.61              |
| 2:I:1102:LEU:HB2  | 3:J:7:LYS:HB2     | 1.83                     | 0.61              |
| 3:J:192:ALA:HB1   | 3:J:193:PRO:HD2   | 1.81                     | 0.61              |
| 2:C:36:PRO:HB2    | 2:C:70:GLU:HG2    | 1.83                     | 0.61              |
| 1:G:51:THR:HG23   | 1:G:146:ARG:HG2   | 1.83                     | 0.61              |
| 1:H:58:ILE:HD13   | 1:H:61:VAL:HB     | 1.82                     | 0.61              |
| 2:C:191:PHE:HB2   | 2:C:195:LEU:HD22  | 1.82                     | 0.61              |
| 2:I:262:ALA:HB2   | 2:I:291:VAL:HG23  | 1.83                     | 0.61              |
| 2:I:1034:GLU:HG2  | 3:J:619:LEU:HB3   | 1.82                     | 0.61              |
| 2:I:1037:VAL:HG13 | 2:I:1049:LEU:HD11 | 1.82                     | 0.61              |
| 3:J:557:LEU:HD21  | 5:L:233:GLN:HG2   | 1.83                     | 0.61              |
| 3:D:1208:ASP:HB2  | 3:D:1215:VAL:HA   | 1.81                     | 0.60              |
| 2:I:777:ILE:HA    | 5:L:420:LEU:HD11  | 1.83                     | 0.60              |
| 3:J:703:ASN:HB2   | 3:J:713:ILE:HG12  | 1.82                     | 0.60              |
| 4:K:79:LEU:HG     | 4:K:80:VAL:HG13   | 1.83                     | 0.60              |
| 3:D:1111:ASP:OD1  | 3:D:1203:LYS:NZ   | 2.35                     | 0.60              |
| 2:I:50:GLU:HA     | 2:I:265:LYS:HD2   | 1.83                     | 0.60              |
| 2:I:107:LEU:HD12  | 2:I:109:LYS:HB2   | 1.83                     | 0.60              |
| 3:J:165:LYS:HG3   | 3:J:199:MET:HE1   | 1.83                     | 0.60              |
| 2:I:36:PRO:HB2    | 2:I:70:GLU:HG2    | 1.83                     | 0.60              |
| 2:I:1089:VAL:HG21 | 2:I:1111:ILE:HG21 | 1.83                     | 0.60              |
| 2:C:1018:GLN:HB3  | 2:C:1063:ARG:NH1  | 2.15                     | 0.60              |
| 3:D:270:ILE:HG12  | 3:D:284:LEU:HD11  | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:174:LEU:HD13  | 2:I:310:LEU:HD22  | 1.82                     | 0.60              |
| 3:J:704:ARG:HB2   | 3:J:745:MET:HG2   | 1.83                     | 0.60              |
| 5:L:180:SER:O     | 5:L:181:LEU:HD12  | 2.00                     | 0.60              |
| 2:C:1016:ILE:HG13 | 2:C:1017:THR:H    | 1.66                     | 0.60              |
| 5:F:149:LYS:HD3   | 5:F:193:ARG:HH22  | 1.65                     | 0.60              |
| 3:J:407:VAL:HG23  | 3:J:422:ALA:HB2   | 1.84                     | 0.60              |
| 2:C:668:LEU:H     | 2:C:993:PHE:HZ    | 1.50                     | 0.60              |
| 3:D:514:LEU:HG    | 3:D:516:ALA:O     | 2.01                     | 0.60              |
| 2:I:876:VAL:HG11  | 2:I:885:ILE:HD11  | 1.82                     | 0.60              |
| 3:J:822:ALA:HB3   | 3:J:825:ALA:HB2   | 1.82                     | 0.60              |
| 5:L:222:LEU:HB3   | 5:L:226:ASP:HB2   | 1.83                     | 0.60              |
| 1:A:46:SER:HB3    | 2:C:856:GLU:HG2   | 1.84                     | 0.60              |
| 2:C:839:LEU:HG    | 2:C:996:LYS:HA    | 1.83                     | 0.60              |
| 2:C:876:VAL:HG11  | 2:C:885:ILE:HD11  | 1.83                     | 0.60              |
| 2:C:1005:MET:HG3  | 3:D:629:SER:HB2   | 1.83                     | 0.60              |
| 1:G:54:THR:HB     | 1:G:143:ARG:O     | 2.02                     | 0.60              |
| 1:H:51:THR:HB     | 1:H:87:VAL:O      | 2.01                     | 0.60              |
| 2:I:118:LEU:HD13  | 2:I:382:LEU:HD23  | 1.82                     | 0.60              |
| 3:J:1166:LEU:HD23 | 3:J:1174:LEU:HD11 | 1.81                     | 0.60              |
| 1:B:58:ILE:HD13   | 1:B:61:VAL:HB     | 1.81                     | 0.60              |
| 2:I:668:LEU:H     | 2:I:993:PHE:HZ    | 1.50                     | 0.60              |
| 2:I:1005:MET:HG3  | 3:J:629:SER:HB2   | 1.82                     | 0.60              |
| 3:J:573:MET:HE3   | 5:L:225:LEU:HB3   | 1.84                     | 0.60              |
| 2:I:1031:ARG:HG2  | 2:I:1033:GLY:H    | 1.67                     | 0.60              |
| 3:J:759:ALA:HA    | 3:J:763:MET:HB3   | 1.83                     | 0.60              |
| 3:D:1313:VAL:HG11 | 3:D:1325:LEU:HD23 | 1.83                     | 0.59              |
| 1:G:42:ARG:NH1    | 2:I:978:ARG:HA    | 2.17                     | 0.59              |
| 3:J:1105:ILE:HB   | 3:J:1222:GLY:HA3  | 1.83                     | 0.59              |
| 6:R:24:DC:N4      | 7:S:3:DG:H1       | 1.95                     | 0.59              |
| 2:I:571:LEU:HG    | 2:I:700:TYR:HA    | 1.84                     | 0.59              |
| 2:I:1051:GLU:HG2  | 2:I:1055:ILE:HD12 | 1.84                     | 0.59              |
| 3:J:27:GLU:H      | 3:J:42:ASP:HB3    | 1.67                     | 0.59              |
| 2:C:774:LEU:HG    | 5:F:365:LEU:HD21  | 1.84                     | 0.59              |
| 3:D:1189:ARG:HB3  | 3:D:1204:CYS:HA   | 1.84                     | 0.59              |
| 3:J:101:HIS:NE2   | 3:J:582:ILE:HG21  | 2.17                     | 0.59              |
| 3:D:919:PHE:HA    | 3:D:927:THR:HG21  | 1.85                     | 0.59              |
| 3:D:1139:ASP:O    | 3:D:1142:SER:HB2  | 2.02                     | 0.59              |
| 3:D:1188:VAL:HG12 | 3:D:1189:ARG:H    | 1.66                     | 0.59              |
| 1:G:13:ALA:HB3    | 1:H:228:PRO:HB3   | 1.83                     | 0.59              |
| 6:O:19:DT:H1'     | 6:O:20:DT:H5'     | 1.83                     | 0.59              |
| 3:D:92:HIS:HA     | 3:D:517:VAL:O     | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:433:GLY:HA2   | 3:D:449:SER:HB2   | 1.85                     | 0.59              |
| 2:I:571:LEU:HB2   | 2:I:574:ALA:HB2   | 1.83                     | 0.59              |
| 3:J:210:ARG:HD2   | 3:J:388:HIS:HB2   | 1.85                     | 0.59              |
| 3:J:708:LEU:HG    | 3:J:709:HIS:H     | 1.67                     | 0.59              |
| 3:J:978:TYR:HB2   | 3:J:988:ARG:HD3   | 1.83                     | 0.59              |
| 3:J:1487:VAL:HG21 | 3:J:1492:LEU:HD23 | 1.84                     | 0.59              |
| 2:C:408:ARG:NH2   | 2:C:456:ALA:O     | 2.35                     | 0.59              |
| 2:I:408:ARG:NH2   | 2:I:456:ALA:O     | 2.36                     | 0.59              |
| 3:J:48:ARG:HA     | 3:J:78:VAL:HG22   | 1.84                     | 0.59              |
| 3:J:714:GLN:HB3   | 3:J:765:SER:HB3   | 1.85                     | 0.59              |
| 1:B:51:THR:HB     | 1:B:87:VAL:O      | 2.02                     | 0.59              |
| 3:D:9:ARG:HG2     | 3:D:10:ILE:H      | 1.66                     | 0.59              |
| 3:D:129:PHE:CE1   | 3:D:457:GLY:HA3   | 2.37                     | 0.59              |
| 2:C:716:LYS:HD2   | 3:D:37:LEU:HD21   | 1.85                     | 0.59              |
| 3:D:1364:HIS:NE2  | 3:D:1366:LYS:HE2  | 2.17                     | 0.59              |
| 1:A:54:THR:HB     | 1:A:143:ARG:O     | 2.02                     | 0.59              |
| 2:C:911:GLU:OE1   | 3:D:1062:ARG:NH2  | 2.34                     | 0.59              |
| 3:D:1004:THR:HG23 | 3:D:1036:ARG:HB2  | 1.85                     | 0.59              |
| 3:D:1379:VAL:HG21 | 3:D:1400:VAL:HG11 | 1.85                     | 0.59              |
| 5:L:307:ALA:HB1   | 5:L:314:TRP:HB3   | 1.85                     | 0.59              |
| 2:C:941:LYS:HZ2   | 2:C:959:PRO:HG2   | 1.68                     | 0.59              |
| 3:D:245:LEU:HD12  | 3:D:311:LEU:HD21  | 1.84                     | 0.59              |
| 3:D:758:GLU:HG2   | 3:D:1476:THR:HG21 | 1.85                     | 0.59              |
| 3:D:1192:LEU:HD23 | 3:D:1373:ARG:HB2  | 1.85                     | 0.59              |
| 2:I:798:GLY:HA3   | 2:I:827:VAL:HG13  | 1.83                     | 0.59              |
| 3:J:698:LYS:HG3   | 4:K:59:ASN:HD21   | 1.68                     | 0.59              |
| 7:S:18:DT:H1'     | 7:S:19:DT:H5'     | 1.85                     | 0.59              |
| 2:C:413:LEU:H     | 2:C:413:LEU:HD12  | 1.68                     | 0.58              |
| 3:D:203:ALA:HA    | 3:D:395:VAL:HA    | 1.85                     | 0.58              |
| 1:G:53:VAL:HG22   | 1:G:54:THR:N      | 2.18                     | 0.58              |
| 2:I:704:HIS:CD2   | 2:I:831:ARG:HD2   | 2.37                     | 0.58              |
| 3:J:125:GLN:HB3   | 3:J:131:LYS:HB3   | 1.84                     | 0.58              |
| 2:C:15:LEU:HD11   | 2:C:457:ALA:HB1   | 1.85                     | 0.58              |
| 1:G:101:LEU:HB3   | 1:G:140:MET:HB3   | 1.85                     | 0.58              |
| 3:J:633:VAL:HG13  | 3:J:635:PRO:HD3   | 1.84                     | 0.58              |
| 3:J:1280:VAL:O    | 3:J:1295:GLU:N    | 2.35                     | 0.58              |
| 2:C:497:ALA:HB1   | 2:C:501:THR:HG21  | 1.85                     | 0.58              |
| 3:D:714:GLN:HB3   | 3:D:765:SER:HB3   | 1.86                     | 0.58              |
| 3:J:971:LEU:HA    | 3:J:974:ILE:HD12  | 1.85                     | 0.58              |
| 3:J:1111:ASP:OD1  | 3:J:1203:LYS:NZ   | 2.36                     | 0.58              |
| 2:C:207:LEU:HD13  | 2:C:222:LEU:HD23  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:532:MET:HG2   | 2:C:533:ASP:H     | 1.68                     | 0.58              |
| 2:C:584:GLU:H     | 2:C:584:GLU:CD    | 2.11                     | 0.58              |
| 3:D:125:GLN:HB3   | 3:D:131:LYS:HB3   | 1.85                     | 0.58              |
| 3:D:236:TYR:HB2   | 3:D:319:ALA:HB3   | 1.84                     | 0.58              |
| 3:D:407:VAL:HG23  | 3:D:422:ALA:HB2   | 1.86                     | 0.58              |
| 3:D:633:VAL:HG13  | 3:D:635:PRO:HD3   | 1.85                     | 0.58              |
| 3:D:801:GLY:HA2   | 3:D:821:VAL:HA    | 1.86                     | 0.58              |
| 3:D:907:GLU:O     | 3:D:911:LEU:HG    | 2.04                     | 0.58              |
| 3:D:978:TYR:HB2   | 3:D:988:ARG:HD3   | 1.85                     | 0.58              |
| 2:I:1016:ILE:HG13 | 2:I:1017:THR:H    | 1.68                     | 0.58              |
| 3:J:167:GLU:HB2   | 3:J:199:MET:HE3   | 1.85                     | 0.58              |
| 1:B:177:VAL:HG12  | 1:B:199:ILE:HG12  | 1.85                     | 0.58              |
| 3:D:262:LYS:HB2   | 3:D:269:LEU:HB2   | 1.85                     | 0.58              |
| 5:F:380:GLU:HB2   | 5:F:419:ALA:HB2   | 1.85                     | 0.58              |
| 2:I:236:VAL:HG21  | 2:I:250:LYS:HG2   | 1.86                     | 0.58              |
| 2:I:911:GLU:OE1   | 3:J:1062:ARG:NH2  | 2.36                     | 0.58              |
| 2:I:774:LEU:HG    | 5:L:365:LEU:HD21  | 1.84                     | 0.58              |
| 3:J:461:ILE:HB    | 3:J:513:ILE:HD11  | 1.85                     | 0.58              |
| 2:I:5:ARG:HA      | 2:I:902:ILE:HB    | 1.84                     | 0.58              |
| 6:R:19:DT:H1'     | 6:R:20:DT:H5'     | 1.85                     | 0.58              |
| 2:C:611:ILE:HG13  | 2:C:625:LEU:HD11  | 1.86                     | 0.58              |
| 3:D:772:PRO:HG3   | 3:D:1210:SER:HB3  | 1.86                     | 0.58              |
| 1:H:57:TYR:CD1    | 1:H:161:ARG:HG2   | 2.38                     | 0.58              |
| 3:J:671:LYS:HG3   | 5:L:436:PHE:CE2   | 2.39                     | 0.58              |
| 1:A:42:ARG:NH1    | 2:C:978:ARG:HA    | 2.18                     | 0.58              |
| 2:C:571:LEU:HG    | 2:C:700:TYR:HA    | 1.85                     | 0.58              |
| 2:C:1071:ILE:O    | 3:D:659:LYS:HG2   | 2.04                     | 0.58              |
| 3:D:165:LYS:HG3   | 3:D:199:MET:HE1   | 1.86                     | 0.58              |
| 3:J:137:PRO:HA    | 3:J:452:ILE:HG13  | 1.85                     | 0.58              |
| 3:J:1101:VAL:HB   | 3:J:1428:ALA:HB2  | 1.86                     | 0.58              |
| 3:D:12:LEU:HD21   | 3:D:1452:ILE:HD13 | 1.86                     | 0.58              |
| 2:I:579:VAL:HG13  | 2:I:842:ARG:HH22  | 1.69                     | 0.58              |
| 3:J:520:LEU:O     | 3:J:525:ARG:NH2   | 2.37                     | 0.58              |
| 6:R:17:DA:H1'     | 6:R:18:DA:H5'     | 1.86                     | 0.58              |
| 7:S:8:DA:H2''     | 7:S:9:DT:H5''     | 1.86                     | 0.58              |
| 1:A:51:THR:HG23   | 1:A:146:ARG:HG2   | 1.84                     | 0.57              |
| 2:C:691:SER:HB3   | 2:C:868:ASP:HA    | 1.86                     | 0.57              |
| 3:D:803:GLY:HA2   | 3:D:827:ILE:HG22  | 1.85                     | 0.57              |
| 3:D:822:ALA:HB3   | 3:D:825:ALA:HB2   | 1.86                     | 0.57              |
| 5:F:203:ILE:HG23  | 5:F:235:LEU:HD23  | 1.86                     | 0.57              |
| 1:H:177:VAL:HG12  | 1:H:199:ILE:HG12  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:9:ARG:HG2     | 3:J:10:ILE:H      | 1.68                     | 0.57              |
| 3:J:770:LEU:HB2   | 3:J:1210:SER:HA   | 1.85                     | 0.57              |
| 1:A:23:PHE:HE2    | 1:A:199:ILE:HD12  | 1.68                     | 0.57              |
| 2:C:236:VAL:HG21  | 2:C:250:LYS:HG2   | 1.86                     | 0.57              |
| 3:D:25:GLU:HG2    | 3:D:93:ILE:HA     | 1.86                     | 0.57              |
| 3:D:205:TYR:HD1   | 3:D:393:ILE:HG12  | 1.68                     | 0.57              |
| 3:D:502:PHE:HZ    | 3:D:512:MET:HE3   | 1.68                     | 0.57              |
| 2:I:637:PHE:HA    | 2:I:659:PRO:HG3   | 1.86                     | 0.57              |
| 5:L:225:LEU:HA    | 5:L:228:ILE:HD12  | 1.85                     | 0.57              |
| 2:C:1089:VAL:HG21 | 2:C:1111:ILE:HG21 | 1.86                     | 0.57              |
| 3:D:759:ALA:HA    | 3:D:763:MET:HB3   | 1.84                     | 0.57              |
| 2:I:191:PHE:HB2   | 2:I:195:LEU:HD22  | 1.86                     | 0.57              |
| 2:I:557:ARG:HB2   | 2:I:881:ASN:HD21  | 1.69                     | 0.57              |
| 2:I:584:GLU:H     | 2:I:584:GLU:CD    | 2.12                     | 0.57              |
| 2:I:732:ALA:O     | 2:I:735:ARG:HG3   | 2.04                     | 0.57              |
| 2:C:502:PRO:HG3   | 2:C:510:THR:HG22  | 1.87                     | 0.57              |
| 2:C:1031:ARG:HG2  | 2:C:1033:GLY:H    | 1.69                     | 0.57              |
| 3:D:443:VAL:HG22  | 3:D:445:ARG:H     | 1.69                     | 0.57              |
| 3:D:1087:ARG:NH2  | 3:D:1234:THR:O    | 2.37                     | 0.57              |
| 1:H:188:GLN:HA    | 3:J:688:TRP:HD1   | 1.69                     | 0.57              |
| 3:J:781:PRO:HD2   | 3:J:908:LYS:HZ1   | 1.69                     | 0.57              |
| 3:J:907:GLU:O     | 3:J:911:LEU:HG    | 2.05                     | 0.57              |
| 3:J:1042:ARG:HB3  | 3:J:1057:VAL:HG21 | 1.86                     | 0.57              |
| 2:C:162:ILE:HG22  | 2:C:172:ILE:HD13  | 1.85                     | 0.57              |
| 2:C:975:TYR:HA    | 2:C:982:PRO:HA    | 1.87                     | 0.57              |
| 2:C:1085:PHE:HA   | 3:D:618:LEU:HD21  | 1.87                     | 0.57              |
| 3:D:171:LEU:HD21  | 3:D:393:ILE:HD12  | 1.87                     | 0.57              |
| 2:I:532:MET:HG2   | 2:I:533:ASP:H     | 1.69                     | 0.57              |
| 3:J:881:LEU:O     | 3:J:885:ILE:HG13  | 2.05                     | 0.57              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:HG13   | 1.85                     | 0.57              |
| 1:A:53:VAL:HG22   | 1:A:54:THR:N      | 2.18                     | 0.57              |
| 3:D:843:PHE:HB2   | 3:D:866:VAL:HG23  | 1.86                     | 0.57              |
| 2:I:569:VAL:HB    | 2:I:635:THR:HG21  | 1.87                     | 0.57              |
| 1:A:14:THR:OG1    | 1:B:231:SER:OG    | 2.21                     | 0.57              |
| 2:C:5:ARG:HA      | 2:C:902:ILE:HB    | 1.86                     | 0.57              |
| 2:C:1037:VAL:O    | 2:C:1041:GLU:HG3  | 2.05                     | 0.57              |
| 3:D:1254:GLN:HB3  | 3:D:1258:ARG:CB   | 2.34                     | 0.57              |
| 1:H:218:LEU:O     | 1:H:222:LEU:HG    | 2.05                     | 0.57              |
| 2:C:1016:ILE:O    | 3:D:87:ARG:NH2    | 2.37                     | 0.57              |
| 3:D:244:GLU:O     | 3:D:310:LEU:N     | 2.36                     | 0.57              |
| 3:D:1042:ARG:HB3  | 3:D:1057:VAL:HG21 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1127:GLU:HG3  | 3:D:1128:VAL:HG23 | 1.85                     | 0.57              |
| 5:F:225:LEU:HA    | 5:F:228:ILE:HD12  | 1.85                     | 0.57              |
| 6:O:7:DA:H1'      | 6:O:8:DA:H5'      | 1.85                     | 0.57              |
| 3:D:299:GLU:CD    | 3:D:300:VAL:H     | 2.13                     | 0.57              |
| 3:D:669:ASN:ND2   | 5:F:364:LEU:HD11  | 2.20                     | 0.57              |
| 3:D:704:ARG:HB2   | 3:D:745:MET:HG2   | 1.85                     | 0.57              |
| 1:H:13:ALA:HB1    | 1:H:23:PHE:HD1    | 1.69                     | 0.57              |
| 5:F:307:ALA:HB1   | 5:F:314:TRP:HB3   | 1.87                     | 0.57              |
| 2:I:858:MET:H     | 2:I:977:GLY:HA3   | 1.70                     | 0.57              |
| 1:B:57:TYR:CD1    | 1:B:161:ARG:HG2   | 2.39                     | 0.56              |
| 3:D:95:LEU:HG     | 3:D:574:LEU:HD21  | 1.86                     | 0.56              |
| 5:F:98:GLN:O      | 5:F:102:GLU:HG3   | 2.04                     | 0.56              |
| 3:J:1100:ASP:HA   | 3:J:1463:LYS:HE2  | 1.86                     | 0.56              |
| 5:L:150:ILE:HG12  | 5:L:193:ARG:HH11  | 1.69                     | 0.56              |
| 3:D:56:TYR:HA     | 3:D:80:VAL:HG23   | 1.87                     | 0.56              |
| 2:I:567:GLN:O     | 2:I:998:TYR:N     | 2.38                     | 0.56              |
| 2:I:1060:ILE:HG13 | 2:I:1061:GLU:H    | 1.70                     | 0.56              |
| 7:P:8:DA:H2''     | 7:P:9:DT:H5''     | 1.87                     | 0.56              |
| 2:C:732:ALA:O     | 2:C:735:ARG:HG3   | 2.04                     | 0.56              |
| 3:D:900:ILE:HG12  | 3:D:914:LEU:HD21  | 1.87                     | 0.56              |
| 3:D:1176:LYS:HG3  | 3:J:1130:ARG:HD2  | 1.87                     | 0.56              |
| 1:G:23:PHE:HE2    | 1:G:199:ILE:HD12  | 1.69                     | 0.56              |
| 2:I:207:LEU:HD13  | 2:I:222:LEU:HD23  | 1.87                     | 0.56              |
| 2:I:639:GLN:HB3   | 2:I:656:ALA:HB1   | 1.88                     | 0.56              |
| 2:I:716:LYS:HD2   | 3:J:37:LEU:HD21   | 1.87                     | 0.56              |
| 3:J:14:SER:HB3    | 3:J:511:TRP:CE2   | 2.40                     | 0.56              |
| 3:J:758:GLU:HG2   | 3:J:1476:THR:HG21 | 1.87                     | 0.56              |
| 5:L:203:ILE:HG23  | 5:L:235:LEU:HD23  | 1.87                     | 0.56              |
| 2:C:262:ALA:HB2   | 2:C:291:VAL:HG23  | 1.87                     | 0.56              |
| 2:C:1069:ALA:HB3  | 2:C:1076:VAL:HG12 | 1.86                     | 0.56              |
| 3:D:698:LYS:HG3   | 4:E:59:ASN:HD21   | 1.69                     | 0.56              |
| 3:D:702:LEU:HG    | 3:D:745:MET:HE2   | 1.87                     | 0.56              |
| 3:D:881:LEU:O     | 3:D:885:ILE:HG13  | 2.05                     | 0.56              |
| 2:I:162:ILE:HG22  | 2:I:172:ILE:HD13  | 1.86                     | 0.56              |
| 2:I:497:ALA:HB1   | 2:I:501:THR:HG21  | 1.87                     | 0.56              |
| 2:I:926:PHE:HE2   | 2:I:960:GLU:HG3   | 1.69                     | 0.56              |
| 3:J:803:GLY:HA2   | 3:J:827:ILE:HG22  | 1.86                     | 0.56              |
| 3:J:919:PHE:HA    | 3:J:927:THR:HG21  | 1.86                     | 0.56              |
| 1:B:218:LEU:O     | 1:B:222:LEU:HG    | 2.05                     | 0.56              |
| 3:D:96:ALA:HB3    | 3:D:554:LEU:HD23  | 1.88                     | 0.56              |
| 3:D:191:LEU:HD13  | 3:D:195:VAL:HG12  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:770:LEU:HB2   | 3:D:1210:SER:HA   | 1.86                     | 0.56              |
| 3:D:1209:LEU:HD11 | 3:D:1364:HIS:CD2  | 2.40                     | 0.56              |
| 2:I:502:PRO:HB2   | 2:I:509:ALA:HB3   | 1.86                     | 0.56              |
| 2:I:774:LEU:HA    | 2:I:777:ILE:HD12  | 1.86                     | 0.56              |
| 3:J:56:TYR:HA     | 3:J:80:VAL:HG23   | 1.88                     | 0.56              |
| 3:J:699:VAL:HA    | 3:J:718:PRO:HD3   | 1.87                     | 0.56              |
| 6:O:2:DT:H2''     | 6:O:3:DT:H71      | 1.86                     | 0.56              |
| 3:D:773:ALA:HB2   | 3:D:1228:SER:HB3  | 1.86                     | 0.56              |
| 3:D:977:ALA:HB2   | 3:J:831:GLY:N     | 2.19                     | 0.56              |
| 3:D:1487:VAL:HG21 | 3:D:1492:LEU:HD23 | 1.87                     | 0.56              |
| 3:D:1500:LYS:HA   | 3:D:1503:VAL:HG22 | 1.88                     | 0.56              |
| 1:G:40:LEU:O      | 1:G:44:LEU:HB2    | 2.05                     | 0.56              |
| 7:S:17:DT:H1'     | 7:S:18:DT:H5'     | 1.87                     | 0.56              |
| 1:A:54:THR:HG22   | 1:A:158:ILE:HD11  | 1.87                     | 0.56              |
| 1:B:188:GLN:HA    | 3:D:688:TRP:HD1   | 1.71                     | 0.56              |
| 2:C:114:PHE:HB3   | 5:F:295:GLN:HA    | 1.88                     | 0.56              |
| 3:D:423:ASP:HB3   | 3:D:426:LYS:HB3   | 1.86                     | 0.56              |
| 3:D:684:LYS:HD3   | 3:D:685:ASP:H     | 1.71                     | 0.56              |
| 4:E:30:LEU:HD23   | 4:E:63:TRP:HB3    | 1.88                     | 0.56              |
| 2:I:146:VAL:HG21  | 2:I:281:LEU:HD21  | 1.88                     | 0.56              |
| 2:I:413:LEU:HD12  | 2:I:413:LEU:H     | 1.69                     | 0.56              |
| 2:I:611:ILE:HG13  | 2:I:625:LEU:HD11  | 1.88                     | 0.56              |
| 3:J:191:LEU:HD13  | 3:J:195:VAL:HG12  | 1.88                     | 0.56              |
| 3:J:974:ILE:HG22  | 3:J:988:ARG:HG3   | 1.86                     | 0.56              |
| 3:J:1088:THR:HA   | 3:J:1234:THR:HG22 | 1.87                     | 0.56              |
| 3:D:406:ASP:OD1   | 3:D:407:VAL:N     | 2.38                     | 0.56              |
| 4:K:30:LEU:HD23   | 4:K:63:TRP:HB3    | 1.86                     | 0.56              |
| 6:R:5:DA:H1'      | 6:R:6:DC:H5'      | 1.87                     | 0.56              |
| 1:A:40:LEU:O      | 1:A:44:LEU:HB2    | 2.06                     | 0.56              |
| 2:C:202:TYR:HD1   | 2:C:206:THR:HG21  | 1.70                     | 0.56              |
| 1:H:197:LEU:HG    | 1:H:199:ILE:HG13  | 1.88                     | 0.56              |
| 2:I:15:LEU:HD11   | 2:I:457:ALA:HB1   | 1.87                     | 0.56              |
| 2:I:560:MET:HB3   | 2:I:564:MET:HE2   | 1.87                     | 0.56              |
| 6:O:21:DG:H1'     | 6:O:22:DT:H5''    | 1.88                     | 0.56              |
| 1:A:13:ALA:HB3    | 1:B:228:PRO:HB3   | 1.87                     | 0.56              |
| 2:C:567:GLN:O     | 2:C:998:TYR:N     | 2.39                     | 0.56              |
| 2:C:831:ARG:HD3   | 2:C:1002:GLU:HG2  | 1.88                     | 0.56              |
| 3:D:585:GLY:HA3   | 3:D:590:PRO:HG3   | 1.88                     | 0.56              |
| 3:D:699:VAL:HA    | 3:D:718:PRO:HD3   | 1.88                     | 0.56              |
| 2:I:211:LEU:HB3   | 2:I:218:VAL:HG13  | 1.87                     | 0.56              |
| 3:J:529:GLN:HA    | 3:J:535:PHE:HA    | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:36:PRO:HA     | 2:C:39:ARG:HD2    | 1.88                     | 0.55              |
| 3:D:9:ARG:HG2     | 3:D:10:ILE:N      | 2.21                     | 0.55              |
| 3:D:671:LYS:HG3   | 5:F:436:PHE:CE2   | 2.41                     | 0.55              |
| 3:D:784:ASP:HA    | 3:D:787:LEU:HD23  | 1.88                     | 0.55              |
| 6:O:11:DG:N2      | 7:P:16:DC:O2      | 2.39                     | 0.55              |
| 1:B:68:ILE:HD12   | 1:B:69:PRO:HD2    | 1.88                     | 0.55              |
| 2:I:975:TYR:HA    | 2:I:982:PRO:HA    | 1.88                     | 0.55              |
| 7:S:2:DA:H1'      | 7:S:3:DG:H5'      | 1.88                     | 0.55              |
| 1:B:197:LEU:HG    | 1:B:199:ILE:HG13  | 1.88                     | 0.55              |
| 2:C:328:LEU:HD21  | 2:C:434:HIS:HA    | 1.89                     | 0.55              |
| 2:C:432:ARG:HH12  | 2:C:518:ARG:HE    | 1.53                     | 0.55              |
| 3:D:326:GLU:HB3   | 3:D:331:VAL:HG23  | 1.89                     | 0.55              |
| 3:D:708:LEU:HG    | 3:D:709:HIS:H     | 1.70                     | 0.55              |
| 3:D:947:ILE:HG22  | 3:D:1019:PRO:HB3  | 1.88                     | 0.55              |
| 3:J:1166:LEU:HD12 | 3:J:1166:LEU:H    | 1.70                     | 0.55              |
| 2:C:168:ARG:HD3   | 2:C:268:ASP:HB2   | 1.88                     | 0.55              |
| 3:D:87:ARG:HG2    | 3:D:523:ASP:HB3   | 1.86                     | 0.55              |
| 3:D:101:HIS:NE2   | 3:D:582:ILE:HG21  | 2.20                     | 0.55              |
| 3:D:238:PRO:HB3   | 3:D:315:ARG:HA    | 1.88                     | 0.55              |
| 3:D:683:ILE:HG22  | 3:D:687:VAL:HG21  | 1.89                     | 0.55              |
| 3:D:699:VAL:HG22  | 3:D:760:ARG:HG2   | 1.88                     | 0.55              |
| 3:D:1216:SER:HB2  | 4:E:15:SER:HB2    | 1.87                     | 0.55              |
| 1:B:182:GLU:HG3   | 1:B:194:LYS:HB3   | 1.89                     | 0.55              |
| 3:D:875:THR:HG21  | 3:D:879:ARG:HG2   | 1.89                     | 0.55              |
| 3:D:1448:THR:O    | 3:D:1452:ILE:HG12 | 2.07                     | 0.55              |
| 2:I:232:GLU:HA    | 2:I:235:MET:HE3   | 1.89                     | 0.55              |
| 3:J:702:LEU:HG    | 3:J:745:MET:HE2   | 1.87                     | 0.55              |
| 1:A:178:ALA:HB3   | 1:A:198:ARG:HG3   | 1.89                     | 0.55              |
| 1:G:54:THR:HG22   | 1:G:158:ILE:HD11  | 1.88                     | 0.55              |
| 1:H:68:ILE:HD12   | 1:H:69:PRO:HD2    | 1.88                     | 0.55              |
| 2:I:852:ILE:HG22  | 2:I:853:LEU:H     | 1.71                     | 0.55              |
| 2:I:1018:GLN:HB3  | 2:I:1063:ARG:NH1  | 2.22                     | 0.55              |
| 3:J:1331:ASP:O    | 3:J:1335:LEU:HD23 | 2.07                     | 0.55              |
| 3:D:27:GLU:H      | 3:D:42:ASP:HB3    | 1.72                     | 0.55              |
| 3:D:973:GLN:HG3   | 3:J:831:GLY:HA2   | 1.89                     | 0.55              |
| 3:D:1380:GLU:HB3  | 3:D:1420:LEU:HD13 | 1.89                     | 0.55              |
| 2:I:448:ASN:HA    | 2:I:451:LEU:HD22  | 1.89                     | 0.55              |
| 3:J:400:VAL:HB    | 3:J:443:VAL:HG21  | 1.88                     | 0.55              |
| 3:J:477:LEU:HD21  | 3:J:495:ARG:HD3   | 1.87                     | 0.55              |
| 3:J:784:ASP:HA    | 3:J:787:LEU:HD23  | 1.89                     | 0.55              |
| 3:J:843:PHE:HB2   | 3:J:866:VAL:HG23  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:911:LEU:O     | 3:J:915:VAL:HG23  | 2.05                     | 0.55              |
| 2:C:48:PHE:O      | 2:C:52:PHE:HB2    | 2.07                     | 0.55              |
| 2:C:123:GLU:HG2   | 2:C:592:LEU:HD13  | 1.87                     | 0.55              |
| 2:C:668:LEU:HB3   | 2:C:995:MET:CG    | 2.37                     | 0.55              |
| 3:D:260:GLU:HA    | 3:D:294:GLU:HG3   | 1.89                     | 0.55              |
| 3:D:1386:ASP:OD1  | 3:D:1386:ASP:N    | 2.39                     | 0.55              |
| 2:I:712:ALA:HB3   | 2:I:820:ARG:HB2   | 1.89                     | 0.55              |
| 6:R:12:DT:H1'     | 6:R:13:DG:H5'     | 1.89                     | 0.55              |
| 2:C:1060:ILE:HG13 | 2:C:1061:GLU:H    | 1.70                     | 0.55              |
| 3:D:238:PRO:HD3   | 3:D:318:THR:HG22  | 1.88                     | 0.55              |
| 1:G:178:ALA:HB3   | 1:G:198:ARG:HG3   | 1.88                     | 0.55              |
| 2:I:1037:VAL:O    | 2:I:1041:GLU:HG3  | 2.06                     | 0.55              |
| 3:J:630:VAL:HG22  | 3:J:631:ILE:H     | 1.72                     | 0.55              |
| 3:J:1345:GLU:HG2  | 3:J:1376:LEU:HD21 | 1.89                     | 0.55              |
| 4:K:45:ARG:HD2    | 4:K:63:TRP:CH2    | 2.42                     | 0.55              |
| 2:C:852:ILE:HG22  | 2:C:853:LEU:H     | 1.72                     | 0.55              |
| 2:C:858:MET:H     | 2:C:977:GLY:HA3   | 1.72                     | 0.55              |
| 3:D:31:THR:HG21   | 5:F:272:THR:HG22  | 1.89                     | 0.55              |
| 1:H:162:ILE:HG23  | 1:H:163:ASN:H     | 1.71                     | 0.55              |
| 2:I:408:ARG:NH1   | 2:I:455:LEU:O     | 2.39                     | 0.55              |
| 2:I:504:GLU:HG2   | 2:I:509:ALA:HB2   | 1.89                     | 0.55              |
| 3:J:31:THR:HG21   | 5:L:272:THR:HG22  | 1.89                     | 0.55              |
| 7:S:5:DA:H1'      | 7:S:6:DC:H5'      | 1.89                     | 0.55              |
| 1:B:111:ALA:HB2   | 1:B:127:LEU:HB3   | 1.87                     | 0.54              |
| 3:D:630:VAL:HG22  | 3:D:631:ILE:H     | 1.72                     | 0.54              |
| 2:I:202:TYR:HD1   | 2:I:206:THR:HG21  | 1.72                     | 0.54              |
| 3:J:708:LEU:HD12  | 3:J:1231:GLU:HG2  | 1.89                     | 0.54              |
| 3:J:875:THR:HG21  | 3:J:879:ARG:HG2   | 1.89                     | 0.54              |
| 3:J:900:ILE:HG12  | 3:J:914:LEU:HD21  | 1.89                     | 0.54              |
| 6:R:4:DG:H1       | 7:S:23:DC:H42     | 1.55                     | 0.54              |
| 1:A:101:LEU:HB3   | 1:A:140:MET:HB3   | 1.89                     | 0.54              |
| 2:C:232:GLU:HA    | 2:C:235:MET:HE3   | 1.89                     | 0.54              |
| 2:C:537:LYS:HD2   | 2:C:583:LEU:HD21  | 1.89                     | 0.54              |
| 2:C:713:ARG:HD3   | 3:D:532:GLY:H     | 1.71                     | 0.54              |
| 3:D:371:ILE:HG21  | 5:F:247:ARG:NH2   | 2.22                     | 0.54              |
| 3:D:1470:ARG:HG2  | 3:D:1471:LEU:H    | 1.72                     | 0.54              |
| 2:I:1103:ASP:OD1  | 2:I:1103:ASP:N    | 2.40                     | 0.54              |
| 3:J:371:ILE:HG21  | 5:L:247:ARG:NH2   | 2.21                     | 0.54              |
| 1:B:162:ILE:HG23  | 1:B:163:ASN:H     | 1.71                     | 0.54              |
| 2:C:90:TYR:O      | 2:C:119:PRO:HA    | 2.08                     | 0.54              |
| 2:C:798:GLY:HA2   | 2:C:829:GLN:HB3   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:371:ILE:HG21  | 5:F:247:ARG:HH22  | 1.72                     | 0.54              |
| 3:J:684:LYS:HD3   | 3:J:685:ASP:H     | 1.72                     | 0.54              |
| 2:C:194:VAL:HG23  | 2:C:195:LEU:HD12  | 1.88                     | 0.54              |
| 2:I:168:ARG:HD3   | 2:I:268:ASP:HB2   | 1.89                     | 0.54              |
| 2:I:754:ILE:HA    | 2:I:791:ARG:HA    | 1.88                     | 0.54              |
| 3:J:119:SER:HB3   | 3:J:122:GLU:HG2   | 1.90                     | 0.54              |
| 3:J:1208:ASP:HB2  | 3:J:1215:VAL:HA   | 1.89                     | 0.54              |
| 2:C:712:ALA:HB3   | 2:C:820:ARG:HB2   | 1.90                     | 0.54              |
| 2:C:1103:ASP:OD1  | 2:C:1103:ASP:N    | 2.40                     | 0.54              |
| 3:D:241:VAL:HG13  | 3:D:312:ARG:HG2   | 1.89                     | 0.54              |
| 3:D:569:ASN:HA    | 3:D:572:ARG:NH2   | 2.22                     | 0.54              |
| 2:I:149:THR:HA    | 2:I:322:VAL:HG13  | 1.88                     | 0.54              |
| 2:I:215:GLY:O     | 2:I:218:VAL:HG23  | 2.08                     | 0.54              |
| 2:I:537:LYS:HD2   | 2:I:583:LEU:HD21  | 1.89                     | 0.54              |
| 3:J:415:VAL:HG21  | 3:J:446:VAL:HG11  | 1.89                     | 0.54              |
| 5:L:280:VAL:HA    | 5:L:283:ILE:HD12  | 1.90                     | 0.54              |
| 1:B:13:ALA:HB1    | 1:B:23:PHE:HD1    | 1.73                     | 0.54              |
| 2:C:141:HIS:NE2   | 2:C:334:ARG:HD3   | 2.23                     | 0.54              |
| 2:C:215:GLY:O     | 2:C:218:VAL:HG23  | 2.07                     | 0.54              |
| 2:C:754:ILE:HG22  | 2:C:755:LEU:H     | 1.72                     | 0.54              |
| 3:D:547:LEU:HD13  | 3:D:578:VAL:HG22  | 1.88                     | 0.54              |
| 1:H:156:HIS:NE2   | 1:H:167:VAL:O     | 2.37                     | 0.54              |
| 2:I:969:LEU:HG    | 3:J:952:ASP:HB2   | 1.90                     | 0.54              |
| 3:J:1274:ILE:HG22 | 3:J:1324:PRO:HA   | 1.89                     | 0.54              |
| 3:J:1377:LYS:O    | 3:J:1397:LYS:N    | 2.40                     | 0.54              |
| 5:L:353:LEU:HD12  | 5:L:354:PRO:HD2   | 1.90                     | 0.54              |
| 5:L:380:GLU:O     | 5:L:384:LEU:HB2   | 2.08                     | 0.54              |
| 1:B:77:GLU:HB2    | 3:D:872:ARG:HH21  | 1.72                     | 0.54              |
| 2:C:115:LEU:HB3   | 2:C:378:LEU:HD23  | 1.90                     | 0.54              |
| 2:C:146:VAL:HG21  | 2:C:281:LEU:HD21  | 1.89                     | 0.54              |
| 2:C:754:ILE:HA    | 2:C:791:ARG:HA    | 1.90                     | 0.54              |
| 3:D:102:ILE:HD11  | 3:D:587:ARG:HB2   | 1.89                     | 0.54              |
| 3:D:1273:VAL:HG23 | 3:D:1325:LEU:HD12 | 1.90                     | 0.54              |
| 3:D:1434:TRP:CD1  | 3:D:1457:ASP:HB2  | 2.43                     | 0.54              |
| 5:F:154:ALA:O     | 5:F:158:LYS:HB2   | 2.07                     | 0.54              |
| 5:F:376:LEU:HB2   | 5:F:381:ALA:HB2   | 1.89                     | 0.54              |
| 1:H:62:LEU:HB3    | 1:H:163:ASN:ND2   | 2.23                     | 0.54              |
| 2:I:343:GLN:HG3   | 2:I:385:PHE:HB2   | 1.89                     | 0.54              |
| 3:J:1279:GLY:O    | 3:J:1319:VAL:HG22 | 2.08                     | 0.54              |
| 2:C:607:ASP:C     | 2:C:609:THR:H     | 2.15                     | 0.54              |
| 3:D:147:VAL:HG21  | 3:D:153:LEU:HD21  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:233:LYS:HE3   | 3:D:234:GLU:H     | 1.72                     | 0.54              |
| 3:D:1144:LEU:HD21 | 3:D:1186:VAL:HG21 | 1.89                     | 0.54              |
| 2:I:194:VAL:HG23  | 2:I:195:LEU:HD12  | 1.90                     | 0.54              |
| 2:I:1069:ALA:HB3  | 2:I:1076:VAL:HG12 | 1.88                     | 0.54              |
| 3:J:423:ASP:HB2   | 3:J:427:VAL:HG12  | 1.89                     | 0.54              |
| 2:C:206:THR:HG23  | 2:C:209:ARG:CZ    | 2.38                     | 0.54              |
| 2:C:468:ARG:HD3   | 2:C:487:THR:HG22  | 1.90                     | 0.54              |
| 2:C:504:GLU:HG2   | 2:C:509:ALA:HB2   | 1.90                     | 0.54              |
| 3:D:614:PHE:O     | 3:D:619:LEU:HB2   | 2.08                     | 0.54              |
| 5:F:150:ILE:HG12  | 5:F:193:ARG:HH11  | 1.72                     | 0.54              |
| 1:H:78:ILE:HD12   | 1:H:129:ILE:O     | 2.07                     | 0.54              |
| 3:J:647:ARG:HH12  | 3:J:683:ILE:HD11  | 1.73                     | 0.54              |
| 1:B:176:ARG:HH11  | 3:D:884:ARG:HH22  | 1.55                     | 0.54              |
| 2:C:971:LYS:HB3   | 2:C:986:PRO:HB2   | 1.90                     | 0.54              |
| 3:D:911:LEU:O     | 3:D:915:VAL:HG23  | 2.07                     | 0.54              |
| 1:G:14:THR:OG1    | 1:H:231:SER:OG    | 2.23                     | 0.54              |
| 1:H:161:ARG:HG3   | 1:H:162:ILE:N     | 2.23                     | 0.54              |
| 1:H:176:ARG:HH11  | 3:J:884:ARG:HH22  | 1.54                     | 0.54              |
| 2:I:668:LEU:HB3   | 2:I:995:MET:CG    | 2.38                     | 0.54              |
| 2:I:1112:PHE:HB3  | 3:J:88:TYR:CD2    | 2.43                     | 0.54              |
| 5:L:413:ARG:HE    | 7:S:22:DT:H2'     | 1.72                     | 0.54              |
| 2:C:889:HIS:CE1   | 2:C:970:GLY:HA3   | 2.43                     | 0.53              |
| 3:D:11:ALA:HA     | 3:D:1451:ALA:HA   | 1.90                     | 0.53              |
| 3:D:154:THR:HG22  | 3:D:157:GLU:HG2   | 1.90                     | 0.53              |
| 3:J:572:ARG:CZ    | 5:L:98:GLN:HG2    | 2.38                     | 0.53              |
| 5:L:376:LEU:HB2   | 5:L:381:ALA:HB2   | 1.90                     | 0.53              |
| 2:C:64:LEU:HD22   | 2:C:359:MET:SD    | 2.47                     | 0.53              |
| 2:C:114:PHE:HE1   | 5:F:294:GLN:HE21  | 1.55                     | 0.53              |
| 2:C:146:VAL:HG21  | 2:C:281:LEU:HD11  | 1.89                     | 0.53              |
| 2:C:668:LEU:HB3   | 2:C:995:MET:HG3   | 1.90                     | 0.53              |
| 2:C:759:THR:HB    | 2:C:785:VAL:HG21  | 1.90                     | 0.53              |
| 5:F:210:VAL:HA    | 5:F:213:ILE:HD12  | 1.89                     | 0.53              |
| 1:G:63:HIS:HA     | 1:G:165:ILE:HD11  | 1.88                     | 0.53              |
| 2:I:679:PHE:H     | 2:I:683:ASN:HD21  | 1.56                     | 0.53              |
| 2:I:950:LEU:HD21  | 2:I:952:LEU:HD22  | 1.90                     | 0.53              |
| 2:I:1071:ILE:O    | 3:J:659:LYS:HG2   | 2.08                     | 0.53              |
| 3:J:1336:LEU:HD22 | 3:J:1421:LEU:HB3  | 1.89                     | 0.53              |
| 2:C:926:PHE:HE2   | 2:C:960:GLU:HG3   | 1.72                     | 0.53              |
| 3:D:750:PRO:HG2   | 3:D:756:GLN:NE2   | 2.23                     | 0.53              |
| 3:D:1122:LEU:HD23 | 3:D:1140:ILE:HD13 | 1.91                     | 0.53              |
| 2:I:457:ALA:HB3   | 2:I:538:GLN:HA    | 1.89                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:726:ILE:HB    | 2:I:729:LEU:HB2  | 1.90                     | 0.53              |
| 2:I:889:HIS:CE1   | 2:I:970:GLY:HA3  | 2.44                     | 0.53              |
| 2:I:971:LYS:HB3   | 2:I:986:PRO:HB2  | 1.90                     | 0.53              |
| 2:I:1103:ASP:HA   | 3:J:5:VAL:HA     | 1.91                     | 0.53              |
| 3:J:147:VAL:HG21  | 3:J:153:LEU:HD21 | 1.90                     | 0.53              |
| 5:L:98:GLN:O      | 5:L:102:GLU:HG3  | 2.09                     | 0.53              |
| 7:S:7:DA:H1'      | 7:S:8:DA:H5'     | 1.90                     | 0.53              |
| 1:B:59:GLU:HG3    | 1:B:139:TYR:CD2  | 2.42                     | 0.53              |
| 3:D:229:ALA:HB1   | 3:D:245:LEU:H    | 1.74                     | 0.53              |
| 3:D:523:ASP:HA    | 3:D:526:PRO:HG3  | 1.90                     | 0.53              |
| 3:D:764:LEU:HD23  | 3:D:767:HIS:CD2  | 2.44                     | 0.53              |
| 5:F:207:LEU:O     | 5:F:211:VAL:HG23 | 2.08                     | 0.53              |
| 2:I:754:ILE:HG22  | 2:I:755:LEU:H    | 1.72                     | 0.53              |
| 2:I:759:THR:HB    | 2:I:785:VAL:HG21 | 1.91                     | 0.53              |
| 2:I:943:VAL:HG21  | 2:I:973:VAL:HG13 | 1.90                     | 0.53              |
| 2:C:408:ARG:NH1   | 2:C:455:LEU:O    | 2.41                     | 0.53              |
| 2:C:1086:ARG:HH11 | 2:C:1086:ARG:HG3 | 1.74                     | 0.53              |
| 5:F:145:VAL:HG21  | 5:F:174:VAL:HG11 | 1.91                     | 0.53              |
| 1:H:77:GLU:HB2    | 3:J:872:ARG:HH21 | 1.74                     | 0.53              |
| 2:I:432:ARG:HH12  | 2:I:518:ARG:HE   | 1.55                     | 0.53              |
| 2:I:1086:ARG:HH11 | 2:I:1086:ARG:HG3 | 1.73                     | 0.53              |
| 3:J:104:PHE:CD2   | 3:J:512:MET:HG3  | 2.43                     | 0.53              |
| 3:D:119:SER:HB3   | 3:D:122:GLU:HG2  | 1.91                     | 0.53              |
| 3:D:1114:THR:HG21 | 3:D:1193:THR:O   | 2.09                     | 0.53              |
| 3:D:1197:ARG:HE   | 3:D:1398:TRP:HB3 | 1.72                     | 0.53              |
| 3:D:1254:GLN:HB3  | 3:D:1258:ARG:HB2 | 1.91                     | 0.53              |
| 2:I:48:PHE:O      | 2:I:52:PHE:HB2   | 2.09                     | 0.53              |
| 3:J:140:ALA:HB1   | 3:J:161:LEU:HD23 | 1.91                     | 0.53              |
| 3:J:175:VAL:HG13  | 3:J:193:PRO:HD2  | 1.91                     | 0.53              |
| 3:J:947:ILE:HG22  | 3:J:1019:PRO:HB3 | 1.90                     | 0.53              |
| 1:A:23:PHE:CE2    | 1:A:199:ILE:HD12 | 2.44                     | 0.53              |
| 2:C:457:ALA:HB3   | 2:C:538:GLN:HA   | 1.90                     | 0.53              |
| 3:D:729:HIS:HB3   | 3:D:732:VAL:HG22 | 1.91                     | 0.53              |
| 4:E:45:ARG:HD2    | 4:E:63:TRP:CH2   | 2.43                     | 0.53              |
| 2:I:90:TYR:O      | 2:I:119:PRO:HA   | 2.07                     | 0.53              |
| 2:I:328:LEU:HD21  | 2:I:434:HIS:HA   | 1.91                     | 0.53              |
| 3:J:99:ALA:HB2    | 3:J:574:LEU:HD21 | 1.91                     | 0.53              |
| 3:J:166:GLN:HB3   | 3:J:396:VAL:HG13 | 1.91                     | 0.53              |
| 1:B:78:ILE:HD12   | 1:B:129:ILE:O    | 2.09                     | 0.53              |
| 2:C:149:THR:HA    | 2:C:322:VAL:HG13 | 1.91                     | 0.53              |
| 1:G:70:GLY:HA2    | 1:G:133:GLU:HG2  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:64:LEU:HD22   | 2:I:359:MET:SD    | 2.48                     | 0.53              |
| 3:J:750:PRO:HG2   | 3:J:756:GLN:NE2   | 2.24                     | 0.53              |
| 3:J:764:LEU:HD23  | 3:J:767:HIS:CD2   | 2.43                     | 0.53              |
| 1:B:62:LEU:HB3    | 1:B:163:ASN:ND2   | 2.24                     | 0.53              |
| 3:D:1147:ARG:NH2  | 3:D:1369:GLU:OE1  | 2.42                     | 0.53              |
| 5:F:380:GLU:O     | 5:F:384:LEU:HB2   | 2.09                     | 0.53              |
| 1:G:16:GLN:HB3    | 1:G:20:TYR:HB3    | 1.91                     | 0.53              |
| 3:J:131:LYS:HG3   | 3:J:153:LEU:O     | 2.09                     | 0.53              |
| 3:J:704:ARG:NE    | 3:J:705:ALA:O     | 2.42                     | 0.53              |
| 2:C:37:GLU:HG2    | 2:C:38:LYS:N      | 2.24                     | 0.53              |
| 2:C:448:ASN:HA    | 2:C:451:LEU:HD22  | 1.90                     | 0.53              |
| 3:D:205:TYR:CD1   | 3:D:390:PRO:HG2   | 2.44                     | 0.53              |
| 3:D:668:PRO:HB2   | 5:F:432:LYS:HD3   | 1.91                     | 0.53              |
| 3:D:704:ARG:NE    | 3:D:705:ALA:O     | 2.42                     | 0.53              |
| 3:D:757:ALA:O     | 3:D:761:ILE:HG13  | 2.09                     | 0.53              |
| 3:D:1366:LYS:O    | 3:D:1370:ILE:HG13 | 2.09                     | 0.53              |
| 1:G:27:PRO:HB3    | 1:G:186:LEU:O     | 2.09                     | 0.53              |
| 2:I:577:PRO:HG2   | 2:I:580:MET:HG2   | 1.91                     | 0.53              |
| 3:J:683:ILE:HG22  | 3:J:687:VAL:HG21  | 1.91                     | 0.53              |
| 5:L:154:ALA:O     | 5:L:158:LYS:HB2   | 2.08                     | 0.53              |
| 1:A:72:LYS:HG3    | 2:C:641:PRO:HB2   | 1.91                     | 0.52              |
| 5:F:137:LEU:HD22  | 5:F:178:LEU:HD11  | 1.91                     | 0.52              |
| 2:I:206:THR:HG23  | 2:I:209:ARG:CZ    | 2.39                     | 0.52              |
| 3:J:1293:PHE:HA   | 3:J:1302:GLU:HA   | 1.89                     | 0.52              |
| 5:L:207:LEU:O     | 5:L:211:VAL:HG23  | 2.09                     | 0.52              |
| 3:D:104:PHE:HB3   | 3:D:111:LYS:HB2   | 1.91                     | 0.52              |
| 3:D:928:ALA:HA    | 3:D:931:LEU:HD12  | 1.92                     | 0.52              |
| 1:G:53:VAL:HA     | 1:G:144:VAL:HG22  | 1.90                     | 0.52              |
| 3:J:7:LYS:NZ      | 3:J:1458:GLU:OE1  | 2.33                     | 0.52              |
| 3:J:1107:VAL:HG13 | 3:J:1200:VAL:HG23 | 1.91                     | 0.52              |
| 5:L:285:LYS:HD3   | 5:L:310:MET:HE1   | 1.90                     | 0.52              |
| 1:B:45:LEU:HD21   | 1:B:177:VAL:HG22  | 1.91                     | 0.52              |
| 1:B:77:GLU:HB2    | 3:D:872:ARG:NH2   | 2.25                     | 0.52              |
| 2:C:162:ILE:HB    | 2:C:172:ILE:HB    | 1.92                     | 0.52              |
| 2:C:304:LEU:HB2   | 2:C:305:PRO:HD3   | 1.92                     | 0.52              |
| 2:C:851:LYS:HG2   | 2:C:852:ILE:H     | 1.75                     | 0.52              |
| 3:D:264:LEU:HG    | 3:D:316:HIS:CE1   | 2.45                     | 0.52              |
| 3:D:780:LYS:HB3   | 3:D:912:LYS:HZ1   | 1.74                     | 0.52              |
| 3:D:831:GLY:HA3   | 3:J:977:ALA:HB2   | 1.91                     | 0.52              |
| 3:D:1311:LEU:HD23 | 3:D:1311:LEU:H    | 1.75                     | 0.52              |
| 3:J:154:THR:HG22  | 3:J:157:GLU:HG2   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:801:GLY:HA2   | 3:J:821:VAL:HA   | 1.92                     | 0.52              |
| 3:J:928:ALA:HA    | 3:J:931:LEU:HD12 | 1.92                     | 0.52              |
| 3:J:968:ASP:OD1   | 3:J:1058:ARG:NH2 | 2.43                     | 0.52              |
| 2:C:135:VAL:HG13  | 2:C:393:GLN:HG3  | 1.91                     | 0.52              |
| 5:F:280:VAL:HA    | 5:F:283:ILE:HD12 | 1.91                     | 0.52              |
| 2:I:468:ARG:HD3   | 2:I:487:THR:HG22 | 1.92                     | 0.52              |
| 2:I:607:ASP:C     | 2:I:609:THR:H    | 2.18                     | 0.52              |
| 2:I:708:TYR:HE1   | 2:I:827:VAL:HB   | 1.75                     | 0.52              |
| 3:J:1156:LEU:HD21 | 3:J:1177:ALA:HA  | 1.92                     | 0.52              |
| 1:A:16:GLN:HB3    | 1:A:20:TYR:HB3   | 1.90                     | 0.52              |
| 1:B:161:ARG:HG3   | 1:B:162:ILE:N    | 2.24                     | 0.52              |
| 2:I:162:ILE:HB    | 2:I:172:ILE:HB   | 1.91                     | 0.52              |
| 3:J:162:ARG:O     | 3:J:414:ARG:NH2  | 2.36                     | 0.52              |
| 3:J:657:LEU:HG    | 3:J:661:MET:SD   | 2.49                     | 0.52              |
| 3:J:1470:ARG:HG2  | 3:J:1471:LEU:H   | 1.73                     | 0.52              |
| 1:A:56:VAL:HG22   | 1:A:142:VAL:HG12 | 1.91                     | 0.52              |
| 2:C:290:LEU:HB3   | 2:C:303:PHE:CE1  | 2.45                     | 0.52              |
| 2:C:502:PRO:HB2   | 2:C:509:ALA:HB3  | 1.91                     | 0.52              |
| 2:C:798:GLY:HA3   | 2:C:827:VAL:HG13 | 1.91                     | 0.52              |
| 2:C:995:MET:HE2   | 2:C:996:LYS:N    | 2.17                     | 0.52              |
| 2:C:1044:GLY:HA3  | 4:E:17:TYR:CE1   | 2.45                     | 0.52              |
| 3:D:1491:THR:HG22 | 4:E:92:LEU:HD12  | 1.91                     | 0.52              |
| 2:I:304:LEU:HB2   | 2:I:305:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:27:PRO:HB3    | 1:A:186:LEU:O    | 2.09                     | 0.52              |
| 3:D:348:ALA:HB1   | 3:D:349:PRO:HD2  | 1.92                     | 0.52              |
| 3:D:650:LEU:HD11  | 3:D:688:TRP:CZ3  | 2.45                     | 0.52              |
| 5:F:387:ARG:HD3   | 5:F:401:VAL:HG21 | 1.90                     | 0.52              |
| 1:G:63:HIS:CE1    | 1:G:65:PHE:HB2   | 2.45                     | 0.52              |
| 2:I:115:LEU:HB3   | 2:I:378:LEU:HD23 | 1.91                     | 0.52              |
| 2:I:606:VAL:HG23  | 2:I:645:VAL:HA   | 1.91                     | 0.52              |
| 2:I:851:LYS:HG2   | 2:I:852:ILE:H    | 1.74                     | 0.52              |
| 3:J:791:TYR:CZ    | 3:J:945:SER:HB3  | 2.45                     | 0.52              |
| 3:J:1344:VAL:O    | 3:J:1348:LEU:HG  | 2.10                     | 0.52              |
| 5:L:383:VAL:HG13  | 5:L:401:VAL:HG11 | 1.91                     | 0.52              |
| 2:C:560:MET:HB3   | 2:C:564:MET:HE2  | 1.90                     | 0.52              |
| 2:C:577:PRO:HG2   | 2:C:580:MET:HG2  | 1.92                     | 0.52              |
| 3:D:224:ARG:HB3   | 3:D:251:PHE:CE2  | 2.44                     | 0.52              |
| 3:D:477:LEU:HD21  | 3:D:495:ARG:HD3  | 1.91                     | 0.52              |
| 3:D:639:LEU:HD22  | 3:D:766:ALA:HA   | 1.92                     | 0.52              |
| 3:D:1464:GLU:CD   | 3:D:1464:GLU:H   | 2.15                     | 0.52              |
| 2:I:37:GLU:HG2    | 2:I:38:LYS:N     | 2.25                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:995:MET:HE2   | 2:I:996:LYS:N     | 2.17                     | 0.52              |
| 7:P:18:DT:H1'     | 7:P:19:DT:H5'     | 1.92                     | 0.52              |
| 2:C:588:VAL:HG21  | 2:C:664:GLY:HA2   | 1.91                     | 0.52              |
| 2:C:674:VAL:O     | 2:C:989:VAL:HA    | 2.10                     | 0.52              |
| 2:C:848:VAL:CG2   | 3:D:740:PHE:HB3   | 2.40                     | 0.52              |
| 2:C:940:GLU:HA    | 2:C:973:VAL:HG11  | 1.91                     | 0.52              |
| 3:D:949:ILE:HD11  | 3:D:1023:MET:HE3  | 1.91                     | 0.52              |
| 1:H:100:ILE:HD12  | 1:H:141:GLU:HG2   | 1.91                     | 0.52              |
| 3:J:95:LEU:HG     | 3:J:574:LEU:HD11  | 1.91                     | 0.52              |
| 3:J:413:ASP:O     | 3:J:435:VAL:HG12  | 2.09                     | 0.52              |
| 3:J:757:ALA:O     | 3:J:761:ILE:HG13  | 2.10                     | 0.52              |
| 3:J:780:LYS:HB3   | 3:J:912:LYS:HZ1   | 1.74                     | 0.52              |
| 3:J:1102:ALA:HB1  | 3:J:1222:GLY:C    | 2.35                     | 0.52              |
| 1:B:156:HIS:NE2   | 1:B:167:VAL:O     | 2.38                     | 0.52              |
| 2:C:211:LEU:HB3   | 2:C:218:VAL:HG13  | 1.91                     | 0.52              |
| 2:C:484:VAL:HG12  | 2:C:486:MET:H     | 1.75                     | 0.52              |
| 2:C:704:HIS:HD2   | 2:C:831:ARG:HD2   | 1.74                     | 0.52              |
| 2:C:950:LEU:HD21  | 2:C:952:LEU:HD22  | 1.92                     | 0.52              |
| 2:C:976:ASP:O     | 2:C:980:GLY:N     | 2.43                     | 0.52              |
| 5:F:383:VAL:HG13  | 5:F:401:VAL:HG11  | 1.91                     | 0.52              |
| 2:I:135:VAL:HG11  | 2:I:406:HIS:CE1   | 2.45                     | 0.52              |
| 2:I:146:VAL:HG21  | 2:I:281:LEU:HD11  | 1.92                     | 0.52              |
| 2:I:184:MET:HE3   | 2:I:186:VAL:HG21  | 1.92                     | 0.52              |
| 2:I:195:LEU:HA    | 2:I:198:ARG:HD3   | 1.92                     | 0.52              |
| 2:I:1083:GLU:OE2  | 3:J:87:ARG:NH1    | 2.43                     | 0.52              |
| 3:J:542:ASP:OD1   | 3:J:545:ARG:NH2   | 2.43                     | 0.52              |
| 2:C:756:VAL:O     | 2:C:789:SER:HB2   | 2.11                     | 0.51              |
| 3:D:140:ALA:HB1   | 3:D:161:LEU:HD23  | 1.91                     | 0.51              |
| 3:D:1261:GLU:OE2  | 3:D:1268:PRO:HA   | 2.10                     | 0.51              |
| 3:D:1273:VAL:HG22 | 3:D:1326:THR:HG23 | 1.93                     | 0.51              |
| 1:H:111:ALA:HB2   | 1:H:127:LEU:HB3   | 1.91                     | 0.51              |
| 2:I:177:GLU:HG3   | 2:I:178:ALA:N     | 2.25                     | 0.51              |
| 2:I:756:VAL:O     | 2:I:789:SER:HB2   | 2.09                     | 0.51              |
| 2:C:706:GLU:HB3   | 2:C:708:TYR:CE1   | 2.44                     | 0.51              |
| 3:D:71:LYS:O      | 3:D:80:VAL:HG12   | 2.10                     | 0.51              |
| 3:D:1225:ALA:O    | 3:D:1229:ILE:HG13 | 2.09                     | 0.51              |
| 2:I:940:GLU:HA    | 2:I:973:VAL:HG11  | 1.92                     | 0.51              |
| 3:J:421:LEU:HD13  | 3:J:444:VAL:HB    | 1.92                     | 0.51              |
| 2:C:969:LEU:HG    | 3:D:952:ASP:HB2   | 1.92                     | 0.51              |
| 3:D:708:LEU:HD23  | 3:D:708:LEU:H     | 1.76                     | 0.51              |
| 3:D:894:LYS:HG3   | 3:D:895:VAL:H     | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:938:GLY:HA2  | 3:D:941:LEU:HD12 | 1.91                     | 0.51              |
| 5:F:249:LYS:HG2  | 6:O:29:DC:OP2    | 2.10                     | 0.51              |
| 5:F:353:LEU:HD12 | 5:F:354:PRO:HD2  | 1.91                     | 0.51              |
| 2:I:135:VAL:HG13 | 2:I:393:GLN:HG3  | 1.92                     | 0.51              |
| 2:I:136:ILE:HA   | 2:I:391:LEU:O    | 2.10                     | 0.51              |
| 3:J:502:PHE:HZ   | 3:J:512:MET:HE1  | 1.75                     | 0.51              |
| 3:J:938:GLY:HA2  | 3:J:941:LEU:HD12 | 1.91                     | 0.51              |
| 7:P:5:DA:H1'     | 7:P:6:DC:H5'     | 1.92                     | 0.51              |
| 2:C:343:GLN:HG3  | 2:C:385:PHE:HB2  | 1.92                     | 0.51              |
| 2:C:881:ASN:O    | 2:C:883:GLY:N    | 2.44                     | 0.51              |
| 2:C:1103:ASP:HA  | 3:D:5:VAL:HA     | 1.92                     | 0.51              |
| 3:D:131:LYS:HG3  | 3:D:153:LEU:O    | 2.10                     | 0.51              |
| 3:D:572:ARG:CZ   | 5:F:98:GLN:HG2   | 2.40                     | 0.51              |
| 1:G:87:VAL:HG11  | 1:G:144:VAL:HG11 | 1.92                     | 0.51              |
| 2:I:770:GLU:HG2  | 5:L:366:SER:HA   | 1.92                     | 0.51              |
| 2:I:876:VAL:HG13 | 2:I:884:GLN:HE21 | 1.76                     | 0.51              |
| 3:D:1047:LYS:HG2 | 3:D:1048:PRO:HD2 | 1.93                     | 0.51              |
| 3:D:1318:TYR:N   | 3:J:1157:GLY:O   | 2.43                     | 0.51              |
| 2:I:1044:GLY:HA3 | 4:K:17:TYR:CE1   | 2.45                     | 0.51              |
| 3:J:415:VAL:HG22 | 3:J:433:GLY:O    | 2.10                     | 0.51              |
| 3:J:1376:LEU:HA  | 3:J:1420:LEU:O   | 2.11                     | 0.51              |
| 1:A:53:VAL:HA    | 1:A:144:VAL:HG22 | 1.92                     | 0.51              |
| 2:C:408:ARG:HD3  | 2:C:542:LEU:HD21 | 1.92                     | 0.51              |
| 3:D:122:GLU:HB2  | 3:D:152:LEU:HD21 | 1.93                     | 0.51              |
| 2:I:18:LEU:HD22  | 2:I:18:LEU:H     | 1.75                     | 0.51              |
| 2:I:141:HIS:NE2  | 2:I:334:ARG:HD3  | 2.25                     | 0.51              |
| 2:I:290:LEU:HB3  | 2:I:303:PHE:CE1  | 2.45                     | 0.51              |
| 2:I:484:VAL:HG12 | 2:I:486:MET:H    | 1.75                     | 0.51              |
| 3:J:729:HIS:HB3  | 3:J:732:VAL:HG22 | 1.92                     | 0.51              |
| 5:L:110:THR:HG22 | 5:L:111:LEU:H    | 1.75                     | 0.51              |
| 5:L:137:LEU:HD22 | 5:L:178:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:181:VAL:HG12 | 1:B:195:LEU:HB2  | 1.93                     | 0.51              |
| 2:C:557:ARG:HB2  | 2:C:881:ASN:HD21 | 1.74                     | 0.51              |
| 2:C:637:PHE:HA   | 2:C:659:PRO:HG3  | 1.93                     | 0.51              |
| 2:C:943:VAL:HG21 | 2:C:973:VAL:HG13 | 1.91                     | 0.51              |
| 3:D:264:LEU:HG   | 3:D:316:HIS:NE2  | 2.26                     | 0.51              |
| 4:E:34:ARG:HH21  | 4:E:94:PRO:HG2   | 1.76                     | 0.51              |
| 5:F:285:LYS:HD3  | 5:F:310:MET:HE1  | 1.93                     | 0.51              |
| 2:I:114:PHE:HE1  | 5:L:294:GLN:HE21 | 1.57                     | 0.51              |
| 2:I:195:LEU:HD23 | 2:I:238:LEU:HG   | 1.91                     | 0.51              |
| 2:I:1035:MET:HB2 | 3:J:707:THR:HB   | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1110:ALA:O    | 3:J:1202:GLN:HB2  | 2.10                     | 0.51              |
| 5:L:145:VAL:HG21  | 5:L:174:VAL:HG11  | 1.92                     | 0.51              |
| 2:C:598:GLU:HG2   | 2:C:615:TYR:CZ    | 2.46                     | 0.51              |
| 3:D:1170:ASP:O    | 3:D:1174:LEU:HG   | 2.11                     | 0.51              |
| 3:D:1202:GLN:NE2  | 3:D:1217:ILE:HG12 | 2.26                     | 0.51              |
| 3:J:773:ALA:HB2   | 3:J:1228:SER:HB3  | 1.93                     | 0.51              |
| 3:J:1306:PRO:HB2  | 3:J:1308:ASP:OD1  | 2.11                     | 0.51              |
| 5:L:218:THR:HA    | 5:L:227:LEU:HD11  | 1.93                     | 0.51              |
| 5:L:380:GLU:HB2   | 5:L:419:ALA:HB2   | 1.93                     | 0.51              |
| 2:C:9:ILE:HD12    | 2:C:907:ASP:HB2   | 1.92                     | 0.51              |
| 2:C:195:LEU:HD23  | 2:C:238:LEU:HG    | 1.92                     | 0.51              |
| 2:C:198:ARG:HH22  | 2:C:238:LEU:HB2   | 1.75                     | 0.51              |
| 2:C:436:GLY:HA2   | 2:C:538:GLN:O     | 2.11                     | 0.51              |
| 2:C:606:VAL:HG23  | 2:C:645:VAL:HA    | 1.91                     | 0.51              |
| 2:C:708:TYR:HE1   | 2:C:827:VAL:HB    | 1.75                     | 0.51              |
| 3:D:1108:ARG:NH1  | 3:D:1108:ARG:HB2  | 2.26                     | 0.51              |
| 3:D:1336:LEU:HD22 | 3:D:1421:LEU:HB3  | 1.92                     | 0.51              |
| 5:F:110:THR:HG22  | 5:F:111:LEU:H     | 1.76                     | 0.51              |
| 1:H:49:PRO:HA     | 1:H:147:GLY:O     | 2.10                     | 0.51              |
| 2:I:135:VAL:HG23  | 2:I:407:LYS:HG2   | 1.92                     | 0.51              |
| 2:I:831:ARG:HD3   | 2:I:1002:GLU:HG2  | 1.93                     | 0.51              |
| 3:J:437:VAL:HG22  | 3:J:444:VAL:HG13  | 1.91                     | 0.51              |
| 3:D:111:LYS:HD2   | 3:D:1452:ILE:HG13 | 1.93                     | 0.51              |
| 3:D:647:ARG:HH12  | 3:D:683:ILE:HD11  | 1.76                     | 0.51              |
| 3:D:1095:THR:HG22 | 3:D:1230:GLY:HA3  | 1.93                     | 0.51              |
| 3:D:1135:ARG:HH21 | 3:D:1357:ARG:HH12 | 1.59                     | 0.51              |
| 5:F:412:ILE:HD13  | 5:F:415:ILE:HD12  | 1.93                     | 0.51              |
| 2:I:277:ALA:HA    | 2:I:280:LYS:HD3   | 1.93                     | 0.51              |
| 3:J:1047:LYS:HG2  | 3:J:1048:PRO:HD2  | 1.93                     | 0.51              |
| 5:L:116:ASP:O     | 5:L:120:LYS:HG3   | 2.10                     | 0.51              |
| 5:L:252:THR:HA    | 6:R:29:DC:H5      | 1.76                     | 0.51              |
| 3:D:896:ALA:O     | 3:D:900:ILE:HG13  | 2.11                     | 0.50              |
| 5:F:116:ASP:O     | 5:F:120:LYS:HG3   | 2.11                     | 0.50              |
| 5:F:254:ALA:O     | 5:F:258:ILE:HG12  | 2.11                     | 0.50              |
| 2:I:634:GLY:O     | 2:I:704:HIS:HA    | 2.11                     | 0.50              |
| 3:J:949:ILE:HD11  | 3:J:1023:MET:HE3  | 1.93                     | 0.50              |
| 3:J:1170:ASP:OD2  | 3:J:1170:ASP:N    | 2.43                     | 0.50              |
| 1:A:14:THR:HG23   | 1:B:231:SER:O     | 2.11                     | 0.50              |
| 1:B:149:GLY:O     | 1:B:171:PHE:HB2   | 2.12                     | 0.50              |
| 2:C:408:ARG:HG2   | 2:C:455:LEU:HB3   | 1.93                     | 0.50              |
| 3:D:657:LEU:HG    | 3:D:661:MET:SD    | 2.51                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:837:GLY:HA2   | 3:D:840:LYS:HB3   | 1.93                     | 0.50              |
| 3:D:1020:LEU:HD11 | 3:D:1035:ILE:HD12 | 1.94                     | 0.50              |
| 5:F:252:THR:OG1   | 6:O:28:DA:H2'     | 2.11                     | 0.50              |
| 1:G:14:THR:HG23   | 1:H:231:SER:O     | 2.11                     | 0.50              |
| 1:G:72:LYS:HG3    | 2:I:641:PRO:HB2   | 1.92                     | 0.50              |
| 2:I:408:ARG:HD3   | 2:I:542:LEU:HD21  | 1.94                     | 0.50              |
| 2:I:524:VAL:HG22  | 2:I:525:ALA:H     | 1.76                     | 0.50              |
| 3:J:1344:VAL:HG12 | 3:J:1348:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:88:ARG:HD2    | 1:A:204:SER:O     | 2.11                     | 0.50              |
| 2:C:18:LEU:HD22   | 2:C:18:LEU:H      | 1.76                     | 0.50              |
| 2:C:139:GLN:HB3   | 2:C:334:ARG:HB2   | 1.94                     | 0.50              |
| 2:C:184:MET:HE3   | 2:C:186:VAL:HG21  | 1.93                     | 0.50              |
| 3:D:1253:THR:HG22 | 3:D:1254:GLN:H    | 1.76                     | 0.50              |
| 3:D:1343:ALA:HA   | 3:D:1346:ARG:HG3  | 1.94                     | 0.50              |
| 5:F:410:GLU:O     | 5:F:413:ARG:HB3   | 2.10                     | 0.50              |
| 1:G:20:TYR:HD2    | 1:G:21:GLY:H      | 1.59                     | 0.50              |
| 1:H:45:LEU:HD21   | 1:H:177:VAL:HG22  | 1.94                     | 0.50              |
| 2:I:139:GLN:HB3   | 2:I:334:ARG:HB2   | 1.93                     | 0.50              |
| 2:I:668:LEU:HB3   | 2:I:995:MET:HG3   | 1.92                     | 0.50              |
| 2:I:683:ASN:HB2   | 2:I:872:ASN:H     | 1.77                     | 0.50              |
| 3:J:420:VAL:HG22  | 3:J:421:LEU:O     | 2.11                     | 0.50              |
| 3:J:479:GLU:O     | 3:J:482:LYS:HG2   | 2.12                     | 0.50              |
| 3:J:1285:GLU:HG2  | 3:J:1290:LEU:HG   | 1.93                     | 0.50              |
| 4:K:34:ARG:HH21   | 4:K:94:PRO:HG2    | 1.75                     | 0.50              |
| 5:L:165:LYS:HD2   | 5:L:165:LYS:H     | 1.76                     | 0.50              |
| 1:B:100:ILE:HD12  | 1:B:141:GLU:HG2   | 1.94                     | 0.50              |
| 1:G:218:LEU:HD21  | 1:H:222:LEU:HD22  | 1.94                     | 0.50              |
| 1:H:182:GLU:HG3   | 1:H:194:LYS:HB3   | 1.93                     | 0.50              |
| 2:I:508:ILE:HD11  | 2:I:529:VAL:HG11  | 1.93                     | 0.50              |
| 2:I:706:GLU:HB3   | 2:I:708:TYR:CE1   | 2.46                     | 0.50              |
| 3:J:543:LEU:HG    | 3:J:600:LEU:HD13  | 1.94                     | 0.50              |
| 3:J:989:TYR:O     | 3:J:993:ILE:HB    | 2.11                     | 0.50              |
| 1:B:89:PHE:HE1    | 1:B:97:THR:HG22   | 1.77                     | 0.50              |
| 3:D:791:TYR:CZ    | 3:D:945:SER:HB3   | 2.47                     | 0.50              |
| 2:I:501:THR:HG22  | 2:I:514:VAL:HG23  | 1.94                     | 0.50              |
| 3:J:633:VAL:C     | 3:J:635:PRO:HD3   | 2.36                     | 0.50              |
| 7:P:3:DG:H1'      | 7:P:4:DC:H5'      | 1.92                     | 0.50              |
| 2:C:113:VAL:HG12  | 2:C:370:ALA:HA    | 1.94                     | 0.50              |
| 2:C:403:SER:O     | 2:C:407:LYS:HE2   | 2.12                     | 0.50              |
| 1:G:23:PHE:CE2    | 1:G:199:ILE:HD12  | 2.45                     | 0.50              |
| 3:J:644:LEU:HG    | 3:J:649:ALA:HB2   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:650:LEU:HD11  | 3:J:688:TRP:CZ3   | 2.46                     | 0.50              |
| 3:J:654:LYS:O     | 3:J:658:LEU:HB2   | 2.11                     | 0.50              |
| 3:J:1231:GLU:HB3  | 3:J:1232:PRO:HD3  | 1.93                     | 0.50              |
| 7:P:8:DA:H1'      | 7:P:9:DT:H5''     | 1.93                     | 0.50              |
| 2:C:69:LEU:HG     | 2:C:98:LEU:HA     | 1.93                     | 0.50              |
| 2:C:195:LEU:HA    | 2:C:198:ARG:HD3   | 1.93                     | 0.50              |
| 2:C:770:GLU:HG2   | 5:F:366:SER:HA    | 1.93                     | 0.50              |
| 2:C:1112:PHE:HB3  | 3:D:88:TYR:CD2    | 2.46                     | 0.50              |
| 2:I:408:ARG:HG2   | 2:I:455:LEU:HB3   | 1.93                     | 0.50              |
| 3:J:1425:THR:HG22 | 3:J:1429:LEU:HD12 | 1.94                     | 0.50              |
| 5:L:431:ARG:HG2   | 5:L:431:ARG:O     | 2.12                     | 0.50              |
| 1:B:29:GLU:HB3    | 1:B:32:PHE:CD1    | 2.47                     | 0.50              |
| 2:C:726:ILE:HB    | 2:C:729:LEU:HB2   | 1.92                     | 0.50              |
| 3:D:112:ILE:HD12  | 3:D:113:GLY:N     | 2.27                     | 0.50              |
| 3:D:1473:PRO:O    | 3:D:1478:SER:HA   | 2.11                     | 0.50              |
| 2:I:173:ASP:O     | 2:I:184:MET:HG3   | 2.11                     | 0.50              |
| 3:J:631:ILE:HD11  | 3:J:739:ASP:O     | 2.12                     | 0.50              |
| 3:J:762:GLN:HB2   | 4:K:16:LYS:HZ1    | 1.77                     | 0.50              |
| 1:B:49:PRO:HA     | 1:B:147:GLY:O     | 2.12                     | 0.50              |
| 2:C:23:VAL:HA     | 2:C:121:MET:SD    | 2.52                     | 0.50              |
| 2:C:177:GLU:HG3   | 2:C:178:ALA:N     | 2.27                     | 0.50              |
| 2:C:627:ARG:HD2   | 2:C:639:GLN:H     | 1.76                     | 0.50              |
| 2:C:736:ASP:HB3   | 2:C:744:ARG:HG3   | 1.93                     | 0.50              |
| 2:C:885:ILE:HG22  | 2:C:889:HIS:CD2   | 2.47                     | 0.50              |
| 3:D:527:MET:HG3   | 3:D:537:THR:HB    | 1.92                     | 0.50              |
| 1:G:56:VAL:HG22   | 1:G:142:VAL:HG12  | 1.94                     | 0.50              |
| 1:H:149:GLY:O     | 1:H:171:PHE:HB2   | 2.11                     | 0.50              |
| 2:I:387:SER:HB2   | 2:I:388:ARG:NH1   | 2.27                     | 0.50              |
| 2:I:704:HIS:HD2   | 2:I:831:ARG:HD2   | 1.75                     | 0.50              |
| 2:I:881:ASN:O     | 2:I:883:GLY:N     | 2.45                     | 0.50              |
| 3:J:894:LYS:HG3   | 3:J:895:VAL:H     | 1.76                     | 0.50              |
| 3:J:896:ALA:O     | 3:J:900:ILE:HG13  | 2.12                     | 0.50              |
| 1:B:97:THR:OG1    | 1:B:98:THR:N      | 2.44                     | 0.49              |
| 2:C:448:ASN:O     | 2:C:451:LEU:HB2   | 2.12                     | 0.49              |
| 2:C:508:ILE:HD11  | 2:C:529:VAL:HG11  | 1.94                     | 0.49              |
| 3:D:274:GLN:HG3   | 3:D:279:VAL:HG21  | 1.94                     | 0.49              |
| 3:D:317:MET:SD    | 3:D:337:LEU:HD22  | 2.52                     | 0.49              |
| 3:D:780:LYS:HB2   | 3:D:908:LYS:HZ1   | 1.77                     | 0.49              |
| 3:D:1150:ALA:HB3  | 3:D:1187:PRO:HB2  | 1.93                     | 0.49              |
| 1:G:56:VAL:HG21   | 1:G:82:LEU:HD13   | 1.94                     | 0.49              |
| 1:H:77:GLU:HB2    | 3:J:872:ARG:NH2   | 2.26                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:121:MET:HE3  | 2:I:127:PHE:CE1   | 2.47                     | 0.49              |
| 2:I:537:LYS:HE3  | 2:I:583:LEU:HD11  | 1.94                     | 0.49              |
| 2:I:729:LEU:HD12 | 2:I:734:LEU:HD13  | 1.94                     | 0.49              |
| 2:I:848:VAL:HG11 | 3:J:630:VAL:HG21  | 1.94                     | 0.49              |
| 2:I:1085:PHE:HA  | 3:J:618:LEU:HD21  | 1.94                     | 0.49              |
| 3:J:402:PRO:HA   | 3:J:443:VAL:HA    | 1.93                     | 0.49              |
| 3:J:1225:ALA:O   | 3:J:1229:ILE:HG13 | 2.12                     | 0.49              |
| 6:R:7:DA:H61     | 7:S:20:DT:H3      | 1.60                     | 0.49              |
| 2:C:37:GLU:HG2   | 2:C:38:LYS:H      | 1.77                     | 0.49              |
| 2:C:214:TYR:HB3  | 2:C:217:LEU:HD12  | 1.94                     | 0.49              |
| 2:C:705:ILE:HG12 | 2:C:828:ALA:HB2   | 1.94                     | 0.49              |
| 2:C:708:TYR:OH   | 2:C:796:GLU:OE1   | 2.24                     | 0.49              |
| 3:D:112:ILE:HG23 | 3:D:512:MET:SD    | 2.52                     | 0.49              |
| 3:D:176:ASP:HA   | 3:D:389:GLU:HA    | 1.94                     | 0.49              |
| 3:D:815:ALA:HA   | 3:D:818:ARG:HE    | 1.77                     | 0.49              |
| 3:D:1110:ALA:O   | 3:D:1202:GLN:HB2  | 2.12                     | 0.49              |
| 3:D:1264:GLU:OE1 | 3:D:1425:THR:OG1  | 2.29                     | 0.49              |
| 1:H:159:LYS:HA   | 1:H:164:ALA:HB3   | 1.94                     | 0.49              |
| 2:I:976:ASP:O    | 2:I:980:GLY:N     | 2.44                     | 0.49              |
| 3:J:129:PHE:CE1  | 3:J:457:GLY:HA3   | 2.47                     | 0.49              |
| 1:A:63:HIS:HA    | 1:A:165:ILE:HD11  | 1.94                     | 0.49              |
| 1:A:218:LEU:HD21 | 1:B:222:LEU:HD22  | 1.95                     | 0.49              |
| 2:C:581:THR:OG1  | 2:C:584:GLU:OE2   | 2.30                     | 0.49              |
| 2:C:1083:GLU:O   | 2:C:1087:VAL:HG23 | 2.11                     | 0.49              |
| 3:D:18:ILE:HG12  | 3:D:518:PRO:HG3   | 1.94                     | 0.49              |
| 5:F:209:LEU:HB2  | 6:O:30:DT:C2      | 2.47                     | 0.49              |
| 5:F:289:THR:O    | 5:F:293:LEU:HG    | 2.12                     | 0.49              |
| 2:I:848:VAL:CG2  | 3:J:740:PHE:HB3   | 2.41                     | 0.49              |
| 3:J:160:GLU:CD   | 3:J:165:LYS:HD3   | 2.38                     | 0.49              |
| 3:J:650:LEU:HD21 | 3:J:683:ILE:HG21  | 1.94                     | 0.49              |
| 3:J:711:LEU:HB3  | 3:J:735:ALA:HB1   | 1.94                     | 0.49              |
| 2:C:277:ALA:HA   | 2:C:280:LYS:HD3   | 1.94                     | 0.49              |
| 2:C:390:GLN:HG2  | 2:C:415:PRO:HD3   | 1.94                     | 0.49              |
| 3:D:111:LYS:O    | 3:D:115:LEU:HB2   | 2.12                     | 0.49              |
| 3:D:633:VAL:C    | 3:D:635:PRO:HD3   | 2.37                     | 0.49              |
| 3:D:1231:GLU:HB3 | 3:D:1232:PRO:HD3  | 1.94                     | 0.49              |
| 2:I:1083:GLU:O   | 2:I:1087:VAL:HG23 | 2.11                     | 0.49              |
| 3:J:639:LEU:HD22 | 3:J:766:ALA:HA    | 1.94                     | 0.49              |
| 2:C:501:THR:HG22 | 2:C:514:VAL:HG23  | 1.94                     | 0.49              |
| 2:C:707:ARG:HB2  | 2:C:707:ARG:HH11  | 1.78                     | 0.49              |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:HD3   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:644:LEU:HG    | 3:D:649:ALA:HB2   | 1.95                     | 0.49              |
| 3:D:849:ALA:O     | 3:D:853:VAL:HG23  | 2.13                     | 0.49              |
| 4:E:19:LEU:O      | 4:E:23:VAL:HG23   | 2.13                     | 0.49              |
| 1:G:35:THR:HG23   | 1:H:42:ARG:HB2    | 1.94                     | 0.49              |
| 2:I:588:VAL:HG21  | 2:I:664:GLY:HA2   | 1.93                     | 0.49              |
| 3:J:132:TYR:HA    | 3:J:456:MET:HB3   | 1.94                     | 0.49              |
| 3:J:481:MET:HE1   | 3:J:493:ARG:HA    | 1.93                     | 0.49              |
| 2:C:1007:ALA:HB1  | 3:D:652:LEU:HD13  | 1.94                     | 0.49              |
| 3:D:245:LEU:CB    | 3:D:309:GLY:HA2   | 2.41                     | 0.49              |
| 3:D:638:LYS:HG3   | 3:D:639:LEU:N     | 2.27                     | 0.49              |
| 3:D:1434:TRP:NE1  | 3:D:1457:ASP:HB2  | 2.27                     | 0.49              |
| 2:I:64:LEU:HD21   | 2:I:66:LEU:HB2    | 1.95                     | 0.49              |
| 3:J:214:ASP:HA    | 3:J:342:PRO:HA    | 1.94                     | 0.49              |
| 3:J:577:ALA:O     | 3:J:581:VAL:HG23  | 2.12                     | 0.49              |
| 5:L:252:THR:HA    | 6:R:29:DC:C5      | 2.48                     | 0.49              |
| 2:C:524:VAL:HG22  | 2:C:525:ALA:H     | 1.76                     | 0.49              |
| 2:C:936:VAL:HB    | 2:C:941:LYS:HE2   | 1.95                     | 0.49              |
| 3:D:471:GLU:O     | 3:D:474:GLU:HB3   | 2.12                     | 0.49              |
| 5:F:149:LYS:HB2   | 5:F:193:ARG:HH12  | 1.78                     | 0.49              |
| 2:I:9:ILE:HD12    | 2:I:907:ASP:HB2   | 1.94                     | 0.49              |
| 2:I:598:GLU:HG2   | 2:I:615:TYR:CZ    | 2.47                     | 0.49              |
| 3:J:1361:VAL:HG12 | 3:J:1363:LEU:H    | 1.78                     | 0.49              |
| 5:L:241:LYS:HE2   | 6:R:24:DC:H3'     | 1.95                     | 0.49              |
| 5:L:254:ALA:O     | 5:L:258:ILE:HG12  | 2.13                     | 0.49              |
| 1:A:56:VAL:HG21   | 1:A:82:LEU:HD13   | 1.95                     | 0.49              |
| 2:C:729:LEU:HD12  | 2:C:734:LEU:HD13  | 1.94                     | 0.49              |
| 2:C:1067:TYR:O    | 2:C:1071:ILE:HB   | 2.12                     | 0.49              |
| 3:D:1046:GLN:HE22 | 3:D:1079:LYS:HE2  | 1.78                     | 0.49              |
| 3:D:1106:VAL:HB   | 3:D:1108:ARG:HH12 | 1.78                     | 0.49              |
| 3:D:1127:GLU:C    | 3:D:1129:THR:H    | 2.21                     | 0.49              |
| 2:I:69:LEU:C      | 2:I:70:GLU:HG3    | 2.37                     | 0.49              |
| 2:I:198:ARG:HH22  | 2:I:238:LEU:HB2   | 1.77                     | 0.49              |
| 2:I:272:ALA:O     | 2:I:276:LYS:N     | 2.39                     | 0.49              |
| 2:I:436:GLY:HA2   | 2:I:538:GLN:O     | 2.12                     | 0.49              |
| 2:I:572:ILE:HD11  | 2:I:703:ILE:HG13  | 1.93                     | 0.49              |
| 2:I:674:VAL:O     | 2:I:989:VAL:HA    | 2.12                     | 0.49              |
| 2:C:65:VAL:HG12   | 2:C:101:ILE:HB    | 1.95                     | 0.49              |
| 3:D:989:TYR:O     | 3:D:993:ILE:HB    | 2.12                     | 0.49              |
| 3:D:1131:THR:HA   | 3:J:1179:GLU:O    | 2.12                     | 0.49              |
| 5:F:103:ILE:HD13  | 5:F:211:VAL:HG21  | 1.95                     | 0.49              |
| 1:H:151:VAL:HG12  | 1:H:156:HIS:HD2   | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:193:LEU:HA    | 2:I:196:LEU:HD13  | 1.94                     | 0.49              |
| 3:J:815:ALA:HA    | 3:J:818:ARG:HE    | 1.78                     | 0.49              |
| 5:L:210:VAL:HA    | 5:L:213:ILE:HD12  | 1.95                     | 0.49              |
| 5:L:238:ALA:HB2   | 5:L:257:TRP:HB2   | 1.95                     | 0.49              |
| 5:L:387:ARG:HD3   | 5:L:401:VAL:HG21  | 1.95                     | 0.49              |
| 5:L:412:ILE:O     | 5:L:416:GLU:HG2   | 2.13                     | 0.49              |
| 1:A:87:VAL:HG11   | 1:A:144:VAL:HG11  | 1.95                     | 0.49              |
| 2:C:874:LEU:O     | 2:C:877:PRO:HD2   | 2.13                     | 0.49              |
| 3:D:1280:VAL:HG22 | 3:D:1295:GLU:O    | 2.12                     | 0.49              |
| 3:D:1459:LEU:HD23 | 3:D:1470:ARG:HE   | 1.78                     | 0.49              |
| 5:F:165:LYS:HD2   | 5:F:165:LYS:H     | 1.78                     | 0.49              |
| 5:F:292:GLN:O     | 5:F:295:GLN:HG3   | 2.13                     | 0.49              |
| 5:F:431:ARG:HG2   | 5:F:431:ARG:O     | 2.11                     | 0.49              |
| 1:H:176:ARG:HG3   | 3:J:850:LEU:HD22  | 1.94                     | 0.49              |
| 3:J:112:ILE:HD12  | 3:J:113:GLY:N     | 2.28                     | 0.49              |
| 3:J:644:LEU:HD12  | 3:J:645:PRO:HD2   | 1.94                     | 0.49              |
| 2:C:952:LEU:HD23  | 2:C:966:LEU:HD11  | 1.95                     | 0.48              |
| 3:D:112:ILE:HD12  | 3:D:113:GLY:H     | 1.78                     | 0.48              |
| 3:D:1377:LYS:O    | 3:D:1397:LYS:N    | 2.39                     | 0.48              |
| 1:G:15:THR:O      | 1:H:232:LEU:HD23  | 2.13                     | 0.48              |
| 2:I:65:VAL:HG12   | 2:I:101:ILE:HB    | 1.95                     | 0.48              |
| 2:I:497:ALA:HB3   | 2:I:532:MET:HG3   | 1.94                     | 0.48              |
| 2:I:853:LEU:HB3   | 2:I:858:MET:HE1   | 1.95                     | 0.48              |
| 3:J:638:LYS:HG3   | 3:J:639:LEU:N     | 2.28                     | 0.48              |
| 3:J:927:THR:HA    | 3:J:930:LEU:HB3   | 1.95                     | 0.48              |
| 3:J:1197:ARG:HE   | 3:J:1398:TRP:HB3  | 1.78                     | 0.48              |
| 5:L:124:GLY:O     | 5:L:128:ILE:HG13  | 2.13                     | 0.48              |
| 5:L:220:ARG:HH22  | 7:S:1:DT:H3'      | 1.78                     | 0.48              |
| 5:L:336:ILE:HD11  | 5:L:344:TYR:HA    | 1.95                     | 0.48              |
| 2:C:69:LEU:C      | 2:C:70:GLU:HG3    | 2.38                     | 0.48              |
| 3:D:974:ILE:HG22  | 3:D:988:ARG:HG3   | 1.94                     | 0.48              |
| 3:D:1107:VAL:HG13 | 3:D:1200:VAL:HG23 | 1.95                     | 0.48              |
| 3:D:1170:ASP:OD2  | 3:D:1170:ASP:N    | 2.43                     | 0.48              |
| 5:F:241:LYS:HE2   | 6:O:24:DC:H3'     | 1.96                     | 0.48              |
| 2:I:22:GLN:HA     | 2:I:336:VAL:HG21  | 1.95                     | 0.48              |
| 2:I:736:ASP:HB3   | 2:I:744:ARG:HG3   | 1.94                     | 0.48              |
| 2:I:751:PRO:HB3   | 2:I:794:PRO:HA    | 1.94                     | 0.48              |
| 3:J:122:GLU:O     | 3:J:126:VAL:HG23  | 2.12                     | 0.48              |
| 3:J:666:PHE:CE1   | 3:J:687:VAL:HG12  | 2.48                     | 0.48              |
| 3:J:702:LEU:HD12  | 3:J:746:ALA:O     | 2.12                     | 0.48              |
| 1:A:63:HIS:HB3    | 2:C:746:GLY:HA3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:11:GLU:HG3    | 2:C:535:SER:HB2  | 1.95                     | 0.48              |
| 2:C:410:ILE:O     | 2:C:452:ILE:HA   | 2.13                     | 0.48              |
| 5:F:336:ILE:HD11  | 5:F:344:TYR:HA   | 1.94                     | 0.48              |
| 2:I:713:ARG:NH1   | 3:J:533:GLY:HA2  | 2.28                     | 0.48              |
| 7:P:8:DA:C2'      | 7:P:9:DT:H5''    | 2.44                     | 0.48              |
| 1:B:151:VAL:HG12  | 1:B:156:HIS:HD2  | 1.79                     | 0.48              |
| 3:D:397:LYS:HE2   | 3:D:448:GLU:HB3  | 1.94                     | 0.48              |
| 3:D:421:LEU:HD11  | 3:D:429:SER:HB2  | 1.95                     | 0.48              |
| 3:D:806:PHE:CD1   | 3:D:811:GLU:HB3  | 2.48                     | 0.48              |
| 3:D:968:ASP:OD1   | 3:D:1058:ARG:NH2 | 2.46                     | 0.48              |
| 2:I:885:ILE:HG22  | 2:I:889:HIS:CD2  | 2.49                     | 0.48              |
| 2:I:936:VAL:HB    | 2:I:941:LYS:HE2  | 1.94                     | 0.48              |
| 3:J:15:PRO:HG3    | 3:J:514:LEU:HD12 | 1.95                     | 0.48              |
| 3:J:71:LYS:O      | 3:J:80:VAL:HG12  | 2.13                     | 0.48              |
| 6:O:14:DT:H1'     | 6:O:15:DT:H5'    | 1.95                     | 0.48              |
| 6:R:7:DA:H1'      | 6:R:8:DA:H5'     | 1.94                     | 0.48              |
| 1:B:176:ARG:HG3   | 3:D:850:LEU:HD22 | 1.94                     | 0.48              |
| 2:C:121:MET:HE3   | 2:C:127:PHE:CE1  | 2.48                     | 0.48              |
| 2:C:135:VAL:HG11  | 2:C:406:HIS:CE1  | 2.48                     | 0.48              |
| 2:C:816:LYS:HG3   | 2:C:817:PRO:HD2  | 1.94                     | 0.48              |
| 2:C:1035:MET:HB2  | 3:D:707:THR:HB   | 1.94                     | 0.48              |
| 3:D:1021:TYR:CE1  | 3:D:1025:GLN:HG3 | 2.49                     | 0.48              |
| 1:G:36:LEU:O      | 1:G:39:PRO:HD2   | 2.14                     | 0.48              |
| 1:H:156:HIS:ND1   | 1:H:156:HIS:O    | 2.46                     | 0.48              |
| 2:I:11:GLU:HG3    | 2:I:535:SER:HB2  | 1.94                     | 0.48              |
| 2:I:69:LEU:HG     | 2:I:98:LEU:HA    | 1.94                     | 0.48              |
| 2:I:572:ILE:HD12  | 2:I:572:ILE:H    | 1.77                     | 0.48              |
| 2:I:1112:PHE:HB2  | 2:I:1115:LEU:HB2 | 1.96                     | 0.48              |
| 1:A:30:ARG:HG3    | 2:C:938:LYS:NZ   | 2.28                     | 0.48              |
| 1:B:179:PHE:HB3   | 1:B:197:LEU:HD13 | 1.96                     | 0.48              |
| 2:C:124:ASP:HB2   | 2:C:407:LYS:HZ2  | 1.79                     | 0.48              |
| 2:C:679:PHE:H     | 2:C:683:ASN:HD21 | 1.60                     | 0.48              |
| 3:D:127:LEU:HD23  | 3:D:461:ILE:HG13 | 1.95                     | 0.48              |
| 3:D:1065:LEU:HB3  | 3:D:1069:GLU:HB2 | 1.95                     | 0.48              |
| 3:D:1098:LEU:HD11 | 3:D:1263:PHE:CD2 | 2.48                     | 0.48              |
| 2:I:37:GLU:HG2    | 2:I:38:LYS:H     | 1.78                     | 0.48              |
| 2:I:772:ARG:HG2   | 5:L:388:LYS:HD2  | 1.96                     | 0.48              |
| 2:I:816:LYS:HG3   | 2:I:817:PRO:HD2  | 1.95                     | 0.48              |
| 3:J:25:GLU:HG2    | 3:J:93:ILE:HA    | 1.94                     | 0.48              |
| 3:J:122:GLU:HB2   | 3:J:152:LEU:HD21 | 1.95                     | 0.48              |
| 3:J:699:VAL:HG22  | 3:J:760:ARG:HG2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:716:PHE:CZ    | 3:J:728:LEU:HD11  | 2.48                     | 0.48              |
| 3:J:862:ASP:O     | 3:J:876:SER:HA    | 2.13                     | 0.48              |
| 3:J:1283:ILE:HA   | 3:J:1292:VAL:HG22 | 1.96                     | 0.48              |
| 1:A:24:VAL:HA     | 1:A:195:LEU:O     | 2.14                     | 0.48              |
| 1:B:187:GLY:H     | 4:E:51:LEU:HD11   | 1.79                     | 0.48              |
| 2:C:71:TYR:HD1    | 2:C:94:LEU:HD11   | 1.78                     | 0.48              |
| 2:C:848:VAL:HG11  | 3:D:630:VAL:HG21  | 1.95                     | 0.48              |
| 2:C:1055:ILE:HD11 | 2:C:1079:PRO:HD3  | 1.95                     | 0.48              |
| 3:D:103:TRP:HE3   | 3:D:1448:THR:HG23 | 1.77                     | 0.48              |
| 3:D:521:PRO:HD2   | 3:D:524:LEU:HD12  | 1.95                     | 0.48              |
| 2:I:1089:VAL:HG11 | 2:I:1112:PHE:HE2  | 1.78                     | 0.48              |
| 3:J:1500:LYS:HA   | 3:J:1503:VAL:HG22 | 1.95                     | 0.48              |
| 5:L:165:LYS:O     | 5:L:165:LYS:HG2   | 2.13                     | 0.48              |
| 1:A:42:ARG:NH1    | 2:C:857:ASP:OD1   | 2.46                     | 0.48              |
| 1:A:57:TYR:HB3    | 1:A:141:GLU:HG3   | 1.95                     | 0.48              |
| 1:A:70:GLY:HA2    | 1:A:133:GLU:HG2   | 1.95                     | 0.48              |
| 2:C:157:ARG:CZ    | 2:C:314:THR:HB    | 2.43                     | 0.48              |
| 2:C:578:VAL:HG23  | 2:C:671:ASN:ND2   | 2.28                     | 0.48              |
| 2:C:1038:TRP:CE2  | 3:D:1099:VAL:HG11 | 2.49                     | 0.48              |
| 1:G:66:SER:O      | 1:G:75:VAL:HG23   | 2.14                     | 0.48              |
| 2:I:432:ARG:H     | 2:I:432:ARG:HG3   | 1.48                     | 0.48              |
| 2:I:448:ASN:O     | 2:I:451:LEU:HB2   | 2.14                     | 0.48              |
| 3:J:123:LEU:HG    | 3:J:127:LEU:HD11  | 1.96                     | 0.48              |
| 1:A:57:TYR:C      | 1:A:58:ILE:HD12   | 2.39                     | 0.48              |
| 1:A:63:HIS:CE1    | 1:A:65:PHE:HB2    | 2.48                     | 0.48              |
| 2:C:135:VAL:HG23  | 2:C:407:LYS:HG2   | 1.95                     | 0.48              |
| 2:C:660:ALA:O     | 2:C:667:ALA:N     | 2.41                     | 0.48              |
| 2:C:853:LEU:HB3   | 2:C:858:MET:HE1   | 1.96                     | 0.48              |
| 2:C:1050:GLN:HE22 | 3:D:1470:ARG:C    | 2.21                     | 0.48              |
| 3:D:1288:ASP:CG   | 3:D:1289:ARG:H    | 2.22                     | 0.48              |
| 2:I:113:VAL:HG12  | 2:I:370:ALA:HA    | 1.96                     | 0.48              |
| 2:I:627:ARG:HD2   | 2:I:639:GLN:H     | 1.79                     | 0.48              |
| 2:I:1055:ILE:HD11 | 2:I:1079:PRO:HD3  | 1.96                     | 0.48              |
| 3:J:876:SER:O     | 3:J:879:ARG:HB3   | 2.14                     | 0.48              |
| 3:J:1127:GLU:HG3  | 3:J:1128:VAL:HG23 | 1.96                     | 0.48              |
| 3:J:1473:PRO:O    | 3:J:1478:SER:HA   | 2.13                     | 0.48              |
| 2:C:173:ASP:O     | 2:C:184:MET:HG3   | 2.14                     | 0.48              |
| 2:C:387:SER:HB2   | 2:C:388:ARG:NH1   | 2.29                     | 0.48              |
| 2:C:399:ASN:HD21  | 2:C:566:THR:HA    | 1.79                     | 0.48              |
| 2:C:714:ASP:HA    | 2:C:719:PRO:HA    | 1.95                     | 0.48              |
| 2:C:886:LEU:HD21  | 3:D:951:ILE:HD13  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1052:MET:HE1  | 2:C:1056:LYS:HE3  | 1.96                     | 0.48              |
| 3:D:862:ASP:O     | 3:D:876:SER:HA    | 2.14                     | 0.48              |
| 4:E:26:ARG:O      | 4:E:30:LEU:HD13   | 2.14                     | 0.48              |
| 5:F:165:LYS:O     | 5:F:165:LYS:HG2   | 2.14                     | 0.48              |
| 1:G:42:ARG:NH1    | 2:I:857:ASP:OD1   | 2.47                     | 0.48              |
| 1:G:42:ARG:NH2    | 1:H:31:GLY:O      | 2.36                     | 0.48              |
| 2:I:798:GLY:HA3   | 2:I:827:VAL:CG1   | 2.43                     | 0.48              |
| 2:I:1047:HIS:HA   | 2:I:1050:GLN:HG2  | 1.94                     | 0.48              |
| 7:P:10:DT:H1'     | 7:P:11:DT:H5'     | 1.96                     | 0.48              |
| 1:A:36:LEU:O      | 1:A:39:PRO:HD2    | 2.14                     | 0.47              |
| 2:C:572:ILE:H     | 2:C:572:ILE:HD12  | 1.79                     | 0.47              |
| 3:D:46:ASP:O      | 3:D:50:PHE:HB2    | 2.14                     | 0.47              |
| 3:D:638:LYS:HG2   | 3:D:640:HIS:CE1   | 2.49                     | 0.47              |
| 3:D:661:MET:HG2   | 3:D:666:PHE:CZ    | 2.49                     | 0.47              |
| 1:G:88:ARG:HD2    | 1:G:204:SER:O     | 2.13                     | 0.47              |
| 1:H:64:GLU:HG3    | 1:H:165:ILE:HG21  | 1.96                     | 0.47              |
| 2:I:886:LEU:HD21  | 3:J:951:ILE:HD13  | 1.95                     | 0.47              |
| 3:J:406:ASP:CG    | 3:J:407:VAL:H     | 2.21                     | 0.47              |
| 3:J:760:ARG:HH21  | 4:K:65:MET:HG3    | 1.79                     | 0.47              |
| 3:J:1335:LEU:HD12 | 3:J:1344:VAL:HG22 | 1.96                     | 0.47              |
| 5:L:178:LEU:HA    | 5:L:181:LEU:HD13  | 1.96                     | 0.47              |
| 5:L:412:ILE:HD13  | 5:L:415:ILE:HD12  | 1.96                     | 0.47              |
| 1:B:64:GLU:HG3    | 1:B:165:ILE:HG21  | 1.96                     | 0.47              |
| 2:C:209:ARG:HG3   | 2:C:210:GLU:N     | 2.29                     | 0.47              |
| 2:C:569:VAL:HB    | 2:C:635:THR:HG21  | 1.96                     | 0.47              |
| 3:D:475:ARG:HA    | 3:D:478:LEU:HD12  | 1.96                     | 0.47              |
| 3:D:1238:MET:C    | 3:D:1253:THR:HB   | 2.38                     | 0.47              |
| 2:I:22:GLN:HG3    | 2:I:407:LYS:HB3   | 1.96                     | 0.47              |
| 2:I:705:ILE:HG12  | 2:I:828:ALA:HB2   | 1.96                     | 0.47              |
| 2:I:769:PRO:HG3   | 3:J:65:ARG:HH12   | 1.78                     | 0.47              |
| 2:I:1047:HIS:HA   | 2:I:1050:GLN:CG   | 2.43                     | 0.47              |
| 3:J:544:TYR:O     | 3:J:548:ILE:HG13  | 2.13                     | 0.47              |
| 3:J:560:GLN:HE22  | 5:L:236:ILE:HD13  | 1.79                     | 0.47              |
| 6:O:28:DA:H1'     | 6:O:29:DC:H5'     | 1.96                     | 0.47              |
| 1:A:20:TYR:HD2    | 1:A:21:GLY:H      | 1.62                     | 0.47              |
| 1:A:181:VAL:O     | 1:A:182:GLU:HG3   | 2.14                     | 0.47              |
| 2:C:876:VAL:HG13  | 2:C:884:GLN:HE21  | 1.79                     | 0.47              |
| 3:D:644:LEU:HD12  | 3:D:645:PRO:HD2   | 1.97                     | 0.47              |
| 3:D:650:LEU:HD21  | 3:D:683:ILE:HG21  | 1.95                     | 0.47              |
| 3:D:1225:ALA:HB1  | 3:D:1367:HIS:HB3  | 1.96                     | 0.47              |
| 1:G:44:LEU:HD13   | 1:G:177:VAL:HG21  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:177:VAL:HG13  | 1:G:199:ILE:HG12  | 1.95                     | 0.47              |
| 1:G:209:GLU:O     | 1:G:213:GLN:HG2   | 2.15                     | 0.47              |
| 2:I:157:ARG:CZ    | 2:I:314:THR:HB    | 2.44                     | 0.47              |
| 2:I:403:SER:O     | 2:I:407:LYS:HE2   | 2.13                     | 0.47              |
| 2:I:410:ILE:O     | 2:I:452:ILE:HA    | 2.14                     | 0.47              |
| 2:I:1085:PHE:HE2  | 3:J:1468:LEU:HD22 | 1.80                     | 0.47              |
| 3:J:977:ALA:HB3   | 3:J:983:LEU:HD12  | 1.96                     | 0.47              |
| 4:K:26:ARG:O      | 4:K:30:LEU:HD13   | 2.15                     | 0.47              |
| 5:L:125:MET:HE1   | 5:L:143:ARG:NH1   | 2.29                     | 0.47              |
| 2:C:374:ASN:OD1   | 2:C:375:SER:N     | 2.47                     | 0.47              |
| 2:C:700:TYR:HB3   | 2:C:833:LEU:HD13  | 1.96                     | 0.47              |
| 3:D:250:LEU:HD23  | 3:D:306:GLU:HG3   | 1.96                     | 0.47              |
| 3:D:517:VAL:O     | 3:D:519:VAL:HG23  | 2.15                     | 0.47              |
| 3:D:1153:VAL:O    | 3:D:1159:ARG:HB2  | 2.14                     | 0.47              |
| 3:D:1188:VAL:HG12 | 3:D:1189:ARG:N    | 2.30                     | 0.47              |
| 1:G:41:ARG:HD3    | 1:G:45:LEU:HD11   | 1.96                     | 0.47              |
| 2:I:209:ARG:HG3   | 2:I:210:GLU:N     | 2.29                     | 0.47              |
| 3:J:131:LYS:HE2   | 3:J:152:LEU:HB3   | 1.96                     | 0.47              |
| 3:J:708:LEU:HD23  | 3:J:708:LEU:H     | 1.79                     | 0.47              |
| 5:L:117:LEU:O     | 5:L:121:VAL:HG23  | 2.15                     | 0.47              |
| 2:C:578:VAL:HG13  | 2:C:900:ARG:HG2   | 1.97                     | 0.47              |
| 3:D:841:PHE:CE2   | 3:D:858:LEU:HD13  | 2.50                     | 0.47              |
| 3:D:918:ALA:O     | 3:D:922:LEU:HB2   | 2.15                     | 0.47              |
| 3:D:971:LEU:HA    | 3:D:974:ILE:HD12  | 1.95                     | 0.47              |
| 3:D:977:ALA:HB3   | 3:D:983:LEU:HD12  | 1.97                     | 0.47              |
| 3:D:1167:SER:H    | 3:D:1170:ASP:CG   | 2.22                     | 0.47              |
| 3:D:1302:GLU:OE2  | 3:D:1304:LYS:HE3  | 2.14                     | 0.47              |
| 1:H:150:TYR:HD2   | 3:J:857:LEU:HD12  | 1.80                     | 0.47              |
| 2:I:45:GLN:HA     | 2:I:45:GLN:HE21   | 1.79                     | 0.47              |
| 2:I:570:PRO:HD2   | 2:I:635:THR:HG21  | 1.97                     | 0.47              |
| 2:I:707:ARG:HH11  | 2:I:707:ARG:HB2   | 1.79                     | 0.47              |
| 3:J:9:ARG:HG2     | 3:J:10:ILE:N      | 2.28                     | 0.47              |
| 3:J:1114:THR:HG21 | 3:J:1193:THR:O    | 2.15                     | 0.47              |
| 3:J:1151:ARG:HA   | 3:J:1162:GLU:HG3  | 1.96                     | 0.47              |
| 3:J:1366:LYS:O    | 3:J:1370:ILE:HG13 | 2.14                     | 0.47              |
| 3:J:1495:ILE:HD13 | 4:K:80:VAL:HB     | 1.95                     | 0.47              |
| 5:L:286:LEU:HD23  | 5:L:310:MET:HG3   | 1.95                     | 0.47              |
| 5:L:383:VAL:HG22  | 5:L:404:TYR:HE2   | 1.77                     | 0.47              |
| 1:B:156:HIS:O     | 1:B:156:HIS:ND1   | 2.48                     | 0.47              |
| 2:C:64:LEU:HD21   | 2:C:66:LEU:HB2    | 1.95                     | 0.47              |
| 2:C:136:ILE:HA    | 2:C:391:LEU:O     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:772:ARG:HG2  | 5:F:388:LYS:HD2  | 1.96                     | 0.47              |
| 4:E:45:ARG:HD2   | 4:E:63:TRP:HH2   | 1.80                     | 0.47              |
| 5:F:238:ALA:HB2  | 5:F:257:TRP:HB2  | 1.96                     | 0.47              |
| 1:G:57:TYR:HB3   | 1:G:141:GLU:HG3  | 1.95                     | 0.47              |
| 1:H:54:THR:OG1   | 1:H:55:SER:N     | 2.47                     | 0.47              |
| 2:I:214:TYR:HB3  | 2:I:217:LEU:HD12 | 1.97                     | 0.47              |
| 2:I:669:GLY:HA2  | 2:I:995:MET:HE3  | 1.97                     | 0.47              |
| 2:I:874:LEU:O    | 2:I:877:PRO:HD2  | 2.14                     | 0.47              |
| 3:J:849:ALA:O    | 3:J:853:VAL:HG23 | 2.13                     | 0.47              |
| 3:J:1444:THR:O   | 3:J:1448:THR:OG1 | 2.33                     | 0.47              |
| 1:A:30:ARG:HG3   | 2:C:938:LYS:HZ3  | 1.80                     | 0.47              |
| 2:C:497:ALA:HB3  | 2:C:532:MET:HG3  | 1.97                     | 0.47              |
| 2:C:888:THR:HG22 | 2:C:989:VAL:O    | 2.15                     | 0.47              |
| 2:C:1048:THR:O   | 2:C:1052:MET:HG2 | 2.15                     | 0.47              |
| 3:D:25:GLU:HA    | 3:D:92:HIS:O     | 2.14                     | 0.47              |
| 3:D:122:GLU:O    | 3:D:126:VAL:HG23 | 2.15                     | 0.47              |
| 3:D:226:PRO:HD2  | 3:D:245:LEU:HD21 | 1.97                     | 0.47              |
| 3:D:517:VAL:HG11 | 3:D:547:LEU:HD21 | 1.96                     | 0.47              |
| 3:D:548:ILE:H    | 3:D:548:ILE:HG13 | 1.54                     | 0.47              |
| 3:D:557:LEU:HD11 | 5:F:229:GLN:OE1  | 2.14                     | 0.47              |
| 3:D:635:PRO:O    | 3:D:935:LYS:HE2  | 2.15                     | 0.47              |
| 3:D:711:LEU:HB3  | 3:D:735:ALA:HB1  | 1.95                     | 0.47              |
| 3:D:810:GLU:O    | 3:D:813:LEU:HB3  | 2.14                     | 0.47              |
| 3:D:930:LEU:O    | 3:D:934:LEU:HD12 | 2.15                     | 0.47              |
| 3:D:1117:TYR:HB2 | 3:D:1188:VAL:O   | 2.14                     | 0.47              |
| 3:D:1211:MET:HB3 | 3:D:1213:ARG:HG2 | 1.96                     | 0.47              |
| 5:F:124:GLY:O    | 5:F:128:ILE:HG13 | 2.13                     | 0.47              |
| 5:F:125:MET:HE1  | 5:F:143:ARG:NH1  | 2.30                     | 0.47              |
| 1:G:30:ARG:HG3   | 2:I:938:LYS:NZ   | 2.30                     | 0.47              |
| 1:H:34:VAL:HG11  | 2:I:978:ARG:HB3  | 1.97                     | 0.47              |
| 1:H:40:LEU:O     | 1:H:44:LEU:HB2   | 2.15                     | 0.47              |
| 1:H:187:GLY:H    | 4:K:51:LEU:HD11  | 1.79                     | 0.47              |
| 2:I:71:TYR:HD1   | 2:I:94:LEU:HD11  | 1.79                     | 0.47              |
| 2:I:754:ILE:HG12 | 2:I:791:ARG:HD3  | 1.95                     | 0.47              |
| 2:I:952:LEU:HD23 | 2:I:966:LEU:HD11 | 1.96                     | 0.47              |
| 2:I:1088:LEU:O   | 2:I:1092:LEU:HG  | 2.15                     | 0.47              |
| 3:J:46:ASP:O     | 3:J:50:PHE:HB2   | 2.13                     | 0.47              |
| 3:J:135:LEU:O    | 3:J:453:ASP:HB3  | 2.14                     | 0.47              |
| 3:J:698:LYS:HG3  | 4:K:59:ASN:ND2   | 2.29                     | 0.47              |
| 3:J:1459:LEU:HB3 | 3:J:1465:ASN:ND2 | 2.30                     | 0.47              |
| 6:O:5:DA:H1'     | 6:O:6:DC:H5'     | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:S:21:DG:H1'     | 7:S:22:DT:H5'     | 1.97                     | 0.47              |
| 1:B:159:LYS:HA    | 1:B:164:ALA:HB3   | 1.97                     | 0.47              |
| 2:C:430:VAL:HG12  | 2:C:434:HIS:CD2   | 2.50                     | 0.47              |
| 3:D:160:GLU:CD    | 3:D:165:LYS:HD3   | 2.40                     | 0.47              |
| 3:D:233:LYS:HB3   | 3:D:236:TYR:CE1   | 2.49                     | 0.47              |
| 3:D:1135:ARG:NH2  | 3:D:1357:ARG:HH22 | 2.13                     | 0.47              |
| 2:I:437:ARG:HH22  | 2:I:491:GLU:CD    | 2.21                     | 0.47              |
| 2:I:609:THR:O     | 2:I:625:LEU:HG    | 2.15                     | 0.47              |
| 3:J:486:ARG:HA    | 3:J:489:ARG:HG2   | 1.95                     | 0.47              |
| 3:J:1021:TYR:CE1  | 3:J:1025:GLN:HG3  | 2.50                     | 0.47              |
| 6:R:28:DA:H1'     | 6:R:29:DC:H5'     | 1.97                     | 0.47              |
| 1:A:177:VAL:HG13  | 1:A:199:ILE:HG12  | 1.96                     | 0.47              |
| 2:C:111:ASP:HB3   | 2:C:369:PRO:HG2   | 1.97                     | 0.47              |
| 2:C:202:TYR:CD1   | 2:C:206:THR:HG21  | 2.50                     | 0.47              |
| 2:C:456:ALA:HB1   | 2:C:538:GLN:O     | 2.15                     | 0.47              |
| 2:C:751:PRO:HB3   | 2:C:794:PRO:HA    | 1.96                     | 0.47              |
| 2:C:1019:GLN:OE1  | 2:C:1057:SER:OG   | 2.32                     | 0.47              |
| 3:D:1006:ALA:O    | 3:D:1010:ASN:HB2  | 2.15                     | 0.47              |
| 3:D:1087:ARG:NH1  | 3:D:1236:LEU:O    | 2.48                     | 0.47              |
| 1:G:35:THR:CG2    | 1:H:39:PRO:HA     | 2.45                     | 0.47              |
| 2:I:15:LEU:O      | 2:I:586:ARG:NH1   | 2.47                     | 0.47              |
| 2:I:299:LYS:HG3   | 2:I:300:ASP:H     | 1.80                     | 0.47              |
| 2:I:714:ASP:HA    | 2:I:719:PRO:HA    | 1.96                     | 0.47              |
| 2:I:1007:ALA:HB1  | 3:J:652:LEU:HD13  | 1.97                     | 0.47              |
| 2:I:1035:MET:HA   | 2:I:1038:TRP:CE3  | 2.50                     | 0.47              |
| 2:I:1050:GLN:HE22 | 3:J:1470:ARG:C    | 2.23                     | 0.47              |
| 3:J:918:ALA:O     | 3:J:922:LEU:HB2   | 2.14                     | 0.47              |
| 3:J:1209:LEU:HD12 | 3:J:1209:LEU:H    | 1.80                     | 0.47              |
| 3:J:1340:GLY:O    | 3:J:1344:VAL:HG23 | 2.15                     | 0.47              |
| 3:J:1341:PRO:O    | 3:J:1344:VAL:HB   | 2.15                     | 0.47              |
| 6:O:7:DA:N6       | 7:P:20:DT:H3      | 2.10                     | 0.47              |
| 1:B:54:THR:HG22   | 1:B:143:ARG:O     | 2.15                     | 0.47              |
| 2:C:118:LEU:HD13  | 2:C:382:LEU:HD23  | 1.96                     | 0.47              |
| 2:C:676:ILE:HA    | 2:C:871:LEU:O     | 2.14                     | 0.47              |
| 2:C:720:GLU:CD    | 2:C:760:SER:HB3   | 2.40                     | 0.47              |
| 2:C:829:GLN:OE1   | 2:C:831:ARG:NH2   | 2.43                     | 0.47              |
| 2:C:1047:HIS:HA   | 2:C:1050:GLN:CG   | 2.45                     | 0.47              |
| 3:D:123:LEU:HG    | 3:D:127:LEU:HD11  | 1.96                     | 0.47              |
| 3:D:632:VAL:O     | 3:D:727:GLN:HA    | 2.15                     | 0.47              |
| 3:D:767:HIS:CE1   | 4:E:6:ILE:HD13    | 2.50                     | 0.47              |
| 3:D:1373:ARG:O    | 3:D:1377:LYS:HB3  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1459:LEU:HB3  | 3:D:1465:ASN:ND2  | 2.30                     | 0.47              |
| 2:I:72:ARG:O      | 2:I:94:LEU:HD12   | 2.15                     | 0.47              |
| 2:I:456:ALA:HB1   | 2:I:538:GLN:O     | 2.15                     | 0.47              |
| 2:I:1038:TRP:CE2  | 3:J:1099:VAL:HG11 | 2.50                     | 0.47              |
| 2:I:1047:HIS:O    | 2:I:1051:GLU:HG3  | 2.15                     | 0.47              |
| 2:I:1048:THR:O    | 2:I:1052:MET:HG2  | 2.15                     | 0.47              |
| 3:J:560:GLN:NE2   | 5:L:236:ILE:HG21  | 2.30                     | 0.47              |
| 5:L:103:ILE:HD13  | 5:L:211:VAL:HG21  | 1.96                     | 0.47              |
| 1:A:55:SER:CB     | 1:A:158:ILE:HG12  | 2.44                     | 0.46              |
| 1:B:44:LEU:HA     | 1:B:48:ILE:HD13   | 1.96                     | 0.46              |
| 2:C:437:ARG:HH22  | 2:C:491:GLU:CD    | 2.21                     | 0.46              |
| 2:C:537:LYS:HE3   | 2:C:583:LEU:HD11  | 1.97                     | 0.46              |
| 2:C:720:GLU:HB2   | 2:C:759:THR:O     | 2.15                     | 0.46              |
| 2:C:1083:GLU:HA   | 2:C:1086:ARG:HG3  | 1.97                     | 0.46              |
| 3:D:1197:ARG:HG3  | 3:D:1398:TRP:CG   | 2.50                     | 0.46              |
| 1:G:24:VAL:HA     | 1:G:195:LEU:O     | 2.14                     | 0.46              |
| 2:I:1083:GLU:HA   | 2:I:1086:ARG:HG3  | 1.96                     | 0.46              |
| 3:J:514:LEU:HD21  | 3:J:518:PRO:HD3   | 1.96                     | 0.46              |
| 3:J:930:LEU:O     | 3:J:934:LEU:HD12  | 2.15                     | 0.46              |
| 3:J:996:TRP:CE2   | 3:J:1056:PRO:HD3  | 2.49                     | 0.46              |
| 1:A:63:HIS:CD2    | 1:A:66:SER:HB2    | 2.50                     | 0.46              |
| 2:C:890:LEU:HD21  | 2:C:914:ILE:HG12  | 1.97                     | 0.46              |
| 2:C:1102:LEU:HA   | 2:C:1107:ASN:O    | 2.15                     | 0.46              |
| 3:D:1465:ASN:HA   | 3:D:1468:LEU:HB2  | 1.96                     | 0.46              |
| 1:H:97:THR:OG1    | 1:H:98:THR:N      | 2.46                     | 0.46              |
| 2:I:23:VAL:HA     | 2:I:121:MET:SD    | 2.54                     | 0.46              |
| 3:J:1188:VAL:HG12 | 3:J:1189:ARG:H    | 1.80                     | 0.46              |
| 4:K:46:PRO:HB2    | 4:K:57:ASP:HB3    | 1.98                     | 0.46              |
| 7:S:3:DG:H1'      | 7:S:4:DC:H5'      | 1.97                     | 0.46              |
| 1:A:190:THR:OG1   | 1:A:191:ASP:N     | 2.47                     | 0.46              |
| 2:C:397:GLU:HG3   | 2:C:632:ASN:HD22  | 1.80                     | 0.46              |
| 2:C:532:MET:HG2   | 2:C:533:ASP:N     | 2.29                     | 0.46              |
| 2:C:537:LYS:NZ    | 2:C:905:VAL:H     | 2.02                     | 0.46              |
| 2:C:1047:HIS:HA   | 2:C:1050:GLN:HG2  | 1.97                     | 0.46              |
| 3:D:698:LYS:HG3   | 4:E:59:ASN:ND2    | 2.29                     | 0.46              |
| 3:D:876:SER:O     | 3:D:879:ARG:HB3   | 2.15                     | 0.46              |
| 3:D:1106:VAL:HG21 | 3:D:1474:ALA:HB2  | 1.96                     | 0.46              |
| 3:D:1331:ASP:HA   | 3:D:1332:PRO:HD3  | 1.82                     | 0.46              |
| 1:G:35:THR:HG22   | 1:H:39:PRO:HA     | 1.97                     | 0.46              |
| 1:H:59:GLU:HG3    | 1:H:139:TYR:CD2   | 2.47                     | 0.46              |
| 2:I:578:VAL:HG23  | 2:I:671:ASN:ND2   | 2.29                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:971:LYS:HG2   | 2:I:988:VAL:HG12  | 1.98                     | 0.46              |
| 3:J:1020:LEU:HD11 | 3:J:1035:ILE:HD12 | 1.95                     | 0.46              |
| 2:C:886:LEU:HA    | 2:C:889:HIS:HB2   | 1.97                     | 0.46              |
| 3:D:716:PHE:CZ    | 3:D:728:LEU:HD11  | 2.51                     | 0.46              |
| 4:E:46:PRO:HB2    | 4:E:57:ASP:HB3    | 1.97                     | 0.46              |
| 3:J:82:ARG:HB2    | 3:J:84:ILE:HG22   | 1.98                     | 0.46              |
| 3:J:1364:HIS:NE2  | 3:J:1366:LYS:HE3  | 2.31                     | 0.46              |
| 7:P:9:DT:H1'      | 7:P:10:DT:H5'     | 1.98                     | 0.46              |
| 1:B:185:ARG:NH2   | 1:B:187:GLY:O     | 2.49                     | 0.46              |
| 2:C:446:GLY:O     | 2:C:449:ILE:HG13  | 2.16                     | 0.46              |
| 3:D:264:LEU:HG    | 3:D:316:HIS:HE2   | 1.80                     | 0.46              |
| 3:D:646:LYS:HA    | 3:D:720:LEU:HD22  | 1.96                     | 0.46              |
| 3:D:1166:LEU:H    | 3:D:1166:LEU:HD12 | 1.80                     | 0.46              |
| 5:F:413:ARG:NH1   | 5:F:414:GLN:HG2   | 2.31                     | 0.46              |
| 3:J:592:THR:HB    | 3:J:598:ARG:O     | 2.14                     | 0.46              |
| 6:R:14:DT:H1'     | 6:R:15:DT:H5'     | 1.97                     | 0.46              |
| 1:B:89:PHE:CE1    | 1:B:97:THR:HG22   | 2.51                     | 0.46              |
| 2:C:151:ASP:HB2   | 2:C:154:ARG:O     | 2.14                     | 0.46              |
| 2:C:549:PHE:HB3   | 2:C:552:HIS:HD2   | 1.80                     | 0.46              |
| 2:C:718:GLY:HA2   | 2:C:719:PRO:HD3   | 1.78                     | 0.46              |
| 2:C:1035:MET:HA   | 2:C:1038:TRP:CE3  | 2.50                     | 0.46              |
| 3:D:253:ALA:HB2   | 3:D:304:LEU:HG    | 1.96                     | 0.46              |
| 3:D:493:ARG:HH11  | 3:D:494:LYS:HE3   | 1.81                     | 0.46              |
| 3:D:1045:MET:HA   | 3:D:1045:MET:HE2  | 1.98                     | 0.46              |
| 5:F:235:LEU:O     | 5:F:239:VAL:HG23  | 2.16                     | 0.46              |
| 5:F:413:ARG:HD2   | 7:P:22:DT:H72     | 1.98                     | 0.46              |
| 2:I:247:PRO:HA    | 2:I:248:PRO:HD3   | 1.84                     | 0.46              |
| 2:C:85:GLU:HA     | 2:C:824:ARG:HH22  | 1.79                     | 0.46              |
| 2:C:423:ALA:O     | 2:C:428:ARG:HG3   | 2.16                     | 0.46              |
| 2:C:798:GLY:HA3   | 2:C:827:VAL:CG1   | 2.45                     | 0.46              |
| 2:C:1085:PHE:HE2  | 3:D:1468:LEU:HD22 | 1.81                     | 0.46              |
| 3:D:927:THR:HA    | 3:D:930:LEU:HB3   | 1.97                     | 0.46              |
| 3:D:1205:TYR:O    | 3:D:1366:LYS:HD3  | 2.16                     | 0.46              |
| 5:F:178:LEU:HA    | 5:F:181:LEU:HD13  | 1.98                     | 0.46              |
| 1:G:29:GLU:O      | 1:G:32:PHE:HB2    | 2.15                     | 0.46              |
| 1:H:10:VAL:HG12   | 1:H:12:THR:HG23   | 1.98                     | 0.46              |
| 1:H:54:THR:HG22   | 1:H:143:ARG:O     | 2.16                     | 0.46              |
| 2:I:1056:LYS:O    | 3:J:624:ASP:N     | 2.35                     | 0.46              |
| 3:J:87:ARG:HG2    | 3:J:523:ASP:CB    | 2.45                     | 0.46              |
| 3:J:350:HIS:HB3   | 5:L:247:ARG:HH12  | 1.81                     | 0.46              |
| 3:J:646:LYS:HA    | 3:J:720:LEU:HD22  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:1154:GLU:HG2 | 3:J:1159:ARG:HB3  | 1.98                     | 0.46              |
| 3:J:1397:LYS:NZ  | 3:J:1397:LYS:HA   | 2.30                     | 0.46              |
| 2:C:15:LEU:O     | 2:C:586:ARG:NH1   | 2.48                     | 0.46              |
| 2:C:45:GLN:HA    | 2:C:45:GLN:HE21   | 1.80                     | 0.46              |
| 2:C:609:THR:O    | 2:C:625:LEU:HG    | 2.15                     | 0.46              |
| 2:C:897:LEU:HD23 | 2:C:899:GLN:H     | 1.80                     | 0.46              |
| 3:D:169:TYR:CE2  | 3:D:395:VAL:HG12  | 2.40                     | 0.46              |
| 3:D:474:GLU:O    | 3:D:478:LEU:HG    | 2.16                     | 0.46              |
| 5:F:319:VAL:O    | 5:F:323:LEU:HB2   | 2.15                     | 0.46              |
| 5:F:383:VAL:HG22 | 5:F:404:TYR:HE2   | 1.81                     | 0.46              |
| 2:I:405:ARG:O    | 2:I:409:ARG:HG3   | 2.16                     | 0.46              |
| 2:I:436:GLY:O    | 2:I:459:ALA:HB2   | 2.16                     | 0.46              |
| 2:I:532:MET:HG2  | 2:I:533:ASP:N     | 2.30                     | 0.46              |
| 2:I:660:ALA:O    | 2:I:667:ALA:N     | 2.41                     | 0.46              |
| 3:J:397:LYS:HE3  | 3:J:448:GLU:O     | 2.16                     | 0.46              |
| 3:J:527:MET:HG3  | 3:J:537:THR:HB    | 1.97                     | 0.46              |
| 3:J:1119:SER:HA  | 3:J:1186:VAL:O    | 2.16                     | 0.46              |
| 5:L:302:SER:O    | 5:L:306:ILE:HG22  | 2.16                     | 0.46              |
| 5:L:410:GLU:O    | 5:L:413:ARG:HB3   | 2.15                     | 0.46              |
| 1:A:66:SER:O     | 1:A:75:VAL:HG23   | 2.16                     | 0.46              |
| 5:F:376:LEU:HG   | 5:F:423:LEU:HD21  | 1.98                     | 0.46              |
| 3:J:93:ILE:HB    | 3:J:517:VAL:HB    | 1.98                     | 0.46              |
| 3:J:104:PHE:HB3  | 3:J:111:LYS:HB2   | 1.98                     | 0.46              |
| 3:J:1095:THR:O   | 3:J:1099:VAL:HG23 | 2.16                     | 0.46              |
| 3:J:1254:GLN:HB3 | 3:J:1258:ARG:CB   | 2.45                     | 0.46              |
| 5:L:235:LEU:O    | 5:L:239:VAL:HG23  | 2.16                     | 0.46              |
| 1:A:29:GLU:O     | 1:A:32:PHE:HB2    | 2.16                     | 0.46              |
| 1:B:150:TYR:HD2  | 3:D:857:LEU:HD12  | 1.80                     | 0.46              |
| 2:C:436:GLY:O    | 2:C:459:ALA:HB2   | 2.16                     | 0.46              |
| 3:D:414:ARG:HA   | 3:D:414:ARG:HD2   | 1.68                     | 0.46              |
| 3:D:584:ASN:OD1  | 3:D:591:VAL:HG12  | 2.16                     | 0.46              |
| 3:D:702:LEU:HD12 | 3:D:746:ALA:O     | 2.16                     | 0.46              |
| 5:F:412:ILE:O    | 5:F:416:GLU:HG2   | 2.16                     | 0.46              |
| 1:G:63:HIS:HB2   | 2:I:799:ILE:HD12  | 1.97                     | 0.46              |
| 2:I:744:ARG:NE   | 2:I:747:ALA:HB2   | 2.30                     | 0.46              |
| 2:I:1067:TYR:CE2 | 5:L:357:VAL:HA    | 2.52                     | 0.46              |
| 1:A:178:ALA:HB2  | 2:C:864:GLY:HA3   | 1.98                     | 0.45              |
| 2:C:711:GLU:HA   | 2:C:822:VAL:HG12  | 1.98                     | 0.45              |
| 2:C:880:MET:CE   | 3:D:1037:GLN:HB2  | 2.46                     | 0.45              |
| 2:C:922:PHE:HB2  | 2:C:967:PHE:CD2   | 2.52                     | 0.45              |
| 2:C:988:VAL:HG22 | 3:D:948:THR:OG1   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:175:VAL:HG13  | 3:D:193:PRO:HD2  | 1.99                     | 0.45              |
| 3:D:892:ASP:HB2   | 3:D:894:LYS:HG2  | 1.99                     | 0.45              |
| 5:F:202:LEU:HD21  | 5:F:239:VAL:HG22 | 1.98                     | 0.45              |
| 5:F:218:THR:HA    | 5:F:227:LEU:HD11 | 1.98                     | 0.45              |
| 1:H:29:GLU:HB3    | 1:H:32:PHE:CD1   | 2.51                     | 0.45              |
| 2:I:430:VAL:HG12  | 2:I:434:HIS:CD2  | 2.51                     | 0.45              |
| 2:I:1102:LEU:HA   | 2:I:1107:ASN:O   | 2.16                     | 0.45              |
| 3:J:483:HIS:CG    | 3:J:484:PRO:HD2  | 2.50                     | 0.45              |
| 3:J:522:PRO:HA    | 3:J:525:ARG:NH1  | 2.31                     | 0.45              |
| 3:J:565:ILE:HD12  | 3:J:565:ILE:H    | 1.80                     | 0.45              |
| 3:J:634:GLY:O     | 3:J:637:LEU:N    | 2.30                     | 0.45              |
| 1:B:176:ARG:HB3   | 1:B:200:TRP:CE3  | 2.51                     | 0.45              |
| 2:C:570:PRO:HD2   | 2:C:635:THR:HG21 | 1.99                     | 0.45              |
| 2:C:640:ARG:HG2   | 2:C:642:ARG:HH12 | 1.81                     | 0.45              |
| 2:C:1009:SER:HB3  | 3:D:651:GLU:O    | 2.17                     | 0.45              |
| 3:D:102:ILE:HB    | 3:D:579:ASP:HB3  | 1.98                     | 0.45              |
| 3:D:264:LEU:O     | 3:D:267:GLY:N    | 2.47                     | 0.45              |
| 3:D:293:VAL:HB    | 3:D:296:GLU:HB2  | 1.98                     | 0.45              |
| 3:D:388:HIS:C     | 3:D:389:GLU:HG3  | 2.41                     | 0.45              |
| 3:D:990:ASP:O     | 3:D:993:ILE:HG22 | 2.17                     | 0.45              |
| 3:D:1277:ILE:HG12 | 3:D:1278:ASP:H   | 1.81                     | 0.45              |
| 1:G:76:VAL:HA     | 1:G:79:ILE:HD12  | 1.98                     | 0.45              |
| 2:I:122:THR:HG23  | 2:I:128:ILE:HD11 | 1.98                     | 0.45              |
| 2:I:816:LYS:HA    | 2:I:817:PRO:HD3  | 1.83                     | 0.45              |
| 3:J:112:ILE:HD12  | 3:J:113:GLY:H    | 1.79                     | 0.45              |
| 3:J:1293:PHE:HD1  | 3:J:1293:PHE:H   | 1.63                     | 0.45              |
| 2:C:193:LEU:HA    | 2:C:196:LEU:HD13 | 1.97                     | 0.45              |
| 2:C:272:ALA:O     | 2:C:276:LYS:N    | 2.39                     | 0.45              |
| 2:C:677:MET:HE3   | 2:C:677:MET:HB2  | 1.84                     | 0.45              |
| 3:D:44:LEU:HG     | 3:D:525:ARG:HH12 | 1.81                     | 0.45              |
| 3:D:350:HIS:HB2   | 3:D:371:ILE:HG22 | 1.98                     | 0.45              |
| 3:D:698:LYS:HB3   | 3:D:756:GLN:NE2  | 2.31                     | 0.45              |
| 3:D:900:ILE:HB    | 3:D:902:MET:HE3  | 1.98                     | 0.45              |
| 3:D:1135:ARG:HB3  | 3:D:1139:ASP:HB3 | 1.98                     | 0.45              |
| 5:F:385:LYS:HA    | 5:F:390:LEU:HD12 | 1.98                     | 0.45              |
| 1:G:57:TYR:C      | 1:G:58:ILE:HD12  | 2.41                     | 0.45              |
| 1:H:179:PHE:HB3   | 1:H:197:LEU:HD13 | 1.99                     | 0.45              |
| 2:I:374:ASN:OD1   | 2:I:375:SER:N    | 2.47                     | 0.45              |
| 2:I:456:ALA:HB3   | 2:I:459:ALA:HB2  | 1.98                     | 0.45              |
| 2:I:640:ARG:HG2   | 2:I:642:ARG:HH12 | 1.82                     | 0.45              |
| 2:I:726:ILE:HD12  | 2:I:729:LEU:HG   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:102:ILE:HD11  | 3:J:587:ARG:HB2   | 1.97                     | 0.45              |
| 3:J:1046:GLN:HE22 | 3:J:1079:LYS:HE2  | 1.81                     | 0.45              |
| 3:J:1223:VAL:HG21 | 3:J:1462:LEU:HD21 | 1.98                     | 0.45              |
| 5:L:292:GLN:O     | 5:L:295:GLN:HG3   | 2.17                     | 0.45              |
| 5:L:376:LEU:HB3   | 5:L:380:GLU:HG3   | 1.98                     | 0.45              |
| 5:L:412:ILE:HA    | 5:L:415:ILE:HD12  | 1.97                     | 0.45              |
| 7:S:4:DC:H2"      | 7:S:5:DA:C8       | 2.51                     | 0.45              |
| 1:A:44:LEU:HD13   | 1:A:177:VAL:HG21  | 1.99                     | 0.45              |
| 2:C:16:PRO:HB2    | 2:C:460:ARG:NH2   | 2.31                     | 0.45              |
| 2:C:99:GLN:HB3    | 2:C:110:GLU:HG3   | 1.99                     | 0.45              |
| 2:C:185:LYS:HA    | 2:C:189:ARG:O     | 2.16                     | 0.45              |
| 2:C:242:LEU:HD11  | 2:C:256:TYR:CE2   | 2.52                     | 0.45              |
| 2:C:669:GLY:HA2   | 2:C:995:MET:HE3   | 1.98                     | 0.45              |
| 2:C:1056:LYS:NZ   | 3:D:748:HIS:HB3   | 2.32                     | 0.45              |
| 3:D:654:LYS:O     | 3:D:658:LEU:HB2   | 2.16                     | 0.45              |
| 3:D:974:ILE:HG12  | 3:D:991:GLN:HG2   | 1.97                     | 0.45              |
| 3:D:1088:THR:HA   | 3:D:1234:THR:HG22 | 1.99                     | 0.45              |
| 3:D:1482:ARG:HE   | 3:D:1483:PHE:HE1  | 1.65                     | 0.45              |
| 1:G:181:VAL:O     | 1:G:182:GLU:HG3   | 2.16                     | 0.45              |
| 2:I:357:GLU:HG2   | 5:L:216:LYS:HE2   | 1.99                     | 0.45              |
| 2:I:897:LEU:HD21  | 2:I:899:GLN:HG2   | 1.97                     | 0.45              |
| 3:J:990:ASP:O     | 3:J:993:ILE:HG22  | 2.16                     | 0.45              |
| 1:B:41:ARG:HG3    | 1:B:177:VAL:HG21  | 1.99                     | 0.45              |
| 1:B:211:LEU:O     | 1:B:215:VAL:HG13  | 2.15                     | 0.45              |
| 2:C:405:ARG:O     | 2:C:409:ARG:HG3   | 2.16                     | 0.45              |
| 2:C:639:GLN:HB3   | 2:C:656:ALA:HB1   | 1.99                     | 0.45              |
| 2:C:644:ARG:HD2   | 2:C:647:GLN:HB3   | 1.98                     | 0.45              |
| 3:D:187:LYS:N     | 3:D:200:ASP:OD2   | 2.49                     | 0.45              |
| 3:D:1095:THR:O    | 3:D:1099:VAL:HG23 | 2.16                     | 0.45              |
| 3:D:1221:VAL:HG23 | 3:D:1222:GLY:H    | 1.82                     | 0.45              |
| 4:E:18:ARG:O      | 4:E:22:VAL:HG23   | 2.17                     | 0.45              |
| 5:F:141:LEU:O     | 5:F:145:VAL:HG23  | 2.17                     | 0.45              |
| 1:G:104:GLU:HG3   | 1:G:137:LYS:HG2   | 1.97                     | 0.45              |
| 1:H:44:LEU:HA     | 1:H:48:ILE:HD13   | 1.98                     | 0.45              |
| 2:I:242:LEU:HD11  | 2:I:256:TYR:CE2   | 2.52                     | 0.45              |
| 2:I:897:LEU:HD23  | 2:I:899:GLN:H     | 1.80                     | 0.45              |
| 2:I:937:ASP:HB3   | 2:I:940:GLU:HG3   | 1.97                     | 0.45              |
| 3:J:356:PRO:HB3   | 3:J:441:ARG:HA    | 1.97                     | 0.45              |
| 3:J:684:LYS:O     | 3:J:687:VAL:HG22  | 2.17                     | 0.45              |
| 3:J:1135:ARG:HB2  | 3:J:1140:ILE:HD11 | 1.98                     | 0.45              |
| 3:J:1381:VAL:HG21 | 3:J:1393:GLN:HB3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:R:2:DT:H2''    | 6:R:3:DT:OP2      | 2.16                     | 0.45              |
| 1:B:23:PHE:HE2   | 1:B:199:ILE:HB    | 1.81                     | 0.45              |
| 1:B:48:ILE:HG22  | 1:B:173:PRO:HD2   | 1.99                     | 0.45              |
| 1:B:202:ASP:OD1  | 1:B:203:GLY:N     | 2.49                     | 0.45              |
| 2:C:166:PRO:C    | 2:C:168:ARG:H     | 2.25                     | 0.45              |
| 2:C:774:LEU:HA   | 2:C:777:ILE:HD12  | 1.97                     | 0.45              |
| 3:D:225:ILE:O    | 3:D:331:VAL:HG12  | 2.17                     | 0.45              |
| 3:D:522:PRO:HA   | 3:D:525:ARG:NH1   | 2.32                     | 0.45              |
| 3:D:593:ASN:ND2  | 5:F:331:SER:OG    | 2.50                     | 0.45              |
| 3:D:638:LYS:HG2  | 3:D:640:HIS:NE2   | 2.32                     | 0.45              |
| 3:D:1161:GLU:OE2 | 3:D:1164:ARG:HB2  | 2.16                     | 0.45              |
| 5:F:286:LEU:HD23 | 5:F:310:MET:HG3   | 1.98                     | 0.45              |
| 2:I:111:ASP:HB3  | 2:I:369:PRO:HG2   | 1.98                     | 0.45              |
| 2:I:140:ILE:HD12 | 2:I:332:ARG:O     | 2.17                     | 0.45              |
| 2:I:151:ASP:HB2  | 2:I:154:ARG:O     | 2.15                     | 0.45              |
| 2:I:878:SER:O    | 3:J:1034:GLN:NE2  | 2.49                     | 0.45              |
| 2:I:890:LEU:HD21 | 2:I:914:ILE:HG12  | 1.99                     | 0.45              |
| 2:I:1012:PRO:HB2 | 2:I:1021:LEU:HD11 | 1.98                     | 0.45              |
| 2:I:1044:GLY:HA3 | 4:K:17:TYR:HE1    | 1.81                     | 0.45              |
| 3:J:638:LYS:HG2  | 3:J:640:HIS:CE1   | 2.51                     | 0.45              |
| 3:J:1434:TRP:CD1 | 3:J:1457:ASP:HB2  | 2.52                     | 0.45              |
| 4:K:45:ARG:HD2   | 4:K:63:TRP:HH2    | 1.82                     | 0.45              |
| 5:L:413:ARG:NH1  | 5:L:414:GLN:HG2   | 2.31                     | 0.45              |
| 1:A:35:THR:HG23  | 1:B:42:ARG:HB2    | 1.99                     | 0.45              |
| 1:B:48:ILE:HA    | 1:B:49:PRO:HD2    | 1.79                     | 0.45              |
| 2:C:291:VAL:HG13 | 2:C:303:PHE:CE1   | 2.52                     | 0.45              |
| 2:C:440:PRO:O    | 3:D:1078:ARG:HG3  | 2.17                     | 0.45              |
| 3:D:300:VAL:HG12 | 3:D:301:GLY:H     | 1.82                     | 0.45              |
| 3:D:525:ARG:HG2  | 3:D:540:LEU:HD23  | 1.98                     | 0.45              |
| 3:D:815:ALA:HB1  | 3:D:821:VAL:HG23  | 1.99                     | 0.45              |
| 5:F:302:SER:O    | 5:F:306:ILE:HG22  | 2.16                     | 0.45              |
| 1:H:211:LEU:O    | 1:H:215:VAL:HG13  | 2.16                     | 0.45              |
| 2:I:440:PRO:O    | 3:J:1078:ARG:HG3  | 2.17                     | 0.45              |
| 2:I:1019:GLN:OE1 | 2:I:1057:SER:OG   | 2.34                     | 0.45              |
| 3:J:65:ARG:HG2   | 5:L:393:GLY:O     | 2.16                     | 0.45              |
| 3:J:767:HIS:CE1  | 4:K:6:ILE:HD13    | 2.52                     | 0.45              |
| 7:S:8:DA:C2'     | 7:S:9:DT:H5''     | 2.46                     | 0.45              |
| 1:B:62:LEU:H     | 1:B:62:LEU:HD12   | 1.82                     | 0.45              |
| 1:B:81:ASN:OD1   | 3:D:867:ARG:NH2   | 2.49                     | 0.45              |
| 1:B:87:VAL:HG12  | 1:B:122:ILE:HG12  | 1.97                     | 0.45              |
| 2:C:199:VAL:HA   | 2:C:231:PRO:HB3   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:584:GLU:HB3  | 2:C:666:LEU:HB3   | 1.99                     | 0.45              |
| 2:C:1067:TYR:CE2 | 5:F:357:VAL:HA    | 2.52                     | 0.45              |
| 3:D:14:SER:HB3   | 3:D:511:TRP:CD2   | 2.51                     | 0.45              |
| 3:D:22:SER:HB2   | 3:D:92:HIS:HB3    | 1.98                     | 0.45              |
| 3:D:684:LYS:O    | 3:D:687:VAL:HG22  | 2.17                     | 0.45              |
| 1:H:185:ARG:NH2  | 1:H:187:GLY:O     | 2.50                     | 0.45              |
| 2:I:207:LEU:HD13 | 2:I:227:LEU:HD11  | 1.97                     | 0.45              |
| 2:I:710:ILE:HD13 | 2:I:790:LEU:HD13  | 1.98                     | 0.45              |
| 3:J:597:GLU:O    | 3:J:599:PRO:HD3   | 2.17                     | 0.45              |
| 3:J:618:LEU:HB3  | 3:J:1467:ILE:HG12 | 1.98                     | 0.45              |
| 2:C:751:PRO:HA   | 2:C:792:VAL:HG13  | 1.99                     | 0.45              |
| 2:C:937:ASP:HB3  | 2:C:940:GLU:HG3   | 1.99                     | 0.45              |
| 3:D:129:PHE:CE1  | 3:D:571:LYS:HG2   | 2.52                     | 0.45              |
| 3:D:565:ILE:H    | 3:D:565:ILE:HD12  | 1.81                     | 0.45              |
| 3:D:701:LEU:HD21 | 3:D:763:MET:CG    | 2.46                     | 0.45              |
| 2:I:161:SER:C    | 2:I:162:ILE:HD12  | 2.41                     | 0.45              |
| 3:J:1045:MET:HE2 | 3:J:1045:MET:HA   | 1.97                     | 0.45              |
| 1:A:209:GLU:O    | 1:A:213:GLN:HG2   | 2.17                     | 0.45              |
| 2:C:634:GLY:O    | 2:C:704:HIS:HA    | 2.17                     | 0.45              |
| 2:C:673:LEU:HA   | 2:C:990:GLY:O     | 2.16                     | 0.45              |
| 2:C:771:GLU:O    | 2:C:775:ARG:HG3   | 2.17                     | 0.45              |
| 2:C:1088:LEU:O   | 2:C:1092:LEU:HG   | 2.17                     | 0.45              |
| 3:D:637:LEU:C    | 3:D:935:LYS:HZ1   | 2.25                     | 0.45              |
| 3:D:701:LEU:HD22 | 3:D:713:ILE:HG22  | 1.98                     | 0.45              |
| 3:D:794:GLN:HG3  | 3:D:795:VAL:N     | 2.32                     | 0.45              |
| 3:D:1125:MET:HE1 | 3:J:1180:ALA:O    | 2.17                     | 0.45              |
| 5:F:159:ILE:N    | 5:F:160:PRO:HD3   | 2.32                     | 0.45              |
| 1:G:231:SER:H    | 1:H:14:THR:HG22   | 1.81                     | 0.45              |
| 2:I:166:PRO:C    | 2:I:168:ARG:H     | 2.25                     | 0.45              |
| 2:I:429:ASP:OD1  | 2:I:430:VAL:N     | 2.43                     | 0.45              |
| 2:I:446:GLY:O    | 2:I:449:ILE:HG13  | 2.16                     | 0.45              |
| 2:I:1058:ASP:OD1 | 2:I:1058:ASP:N    | 2.49                     | 0.45              |
| 3:J:21:TRP:HE3   | 3:J:90:MET:HE1    | 1.82                     | 0.45              |
| 3:J:632:VAL:O    | 3:J:727:GLN:HA    | 2.17                     | 0.45              |
| 3:J:841:PHE:CE2  | 3:J:858:LEU:HD13  | 2.52                     | 0.45              |
| 4:K:79:LEU:HD23  | 4:K:80:VAL:HG22   | 1.99                     | 0.45              |
| 5:L:149:LYS:HB2  | 5:L:193:ARG:HH12  | 1.82                     | 0.45              |
| 5:L:202:LEU:HD21 | 5:L:239:VAL:HG22  | 1.98                     | 0.45              |
| 5:L:289:THR:O    | 5:L:293:LEU:HG    | 2.17                     | 0.45              |
| 7:P:19:DT:H1'    | 7:P:20:DT:H5'     | 1.99                     | 0.45              |
| 2:C:299:LYS:HG3  | 2:C:300:ASP:H     | 1.82                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:807:ARG:HB3  | 2:C:810:ASP:OD1   | 2.17                     | 0.44              |
| 3:D:259:VAL:HG13 | 3:D:298:VAL:HG21  | 2.00                     | 0.44              |
| 3:D:1179:GLU:HG2 | 3:J:1131:THR:HG22 | 1.99                     | 0.44              |
| 3:D:1364:HIS:CD2 | 3:D:1366:LYS:HE2  | 2.52                     | 0.44              |
| 5:F:181:LEU:HD23 | 5:F:185:LEU:HD13  | 1.98                     | 0.44              |
| 1:G:28:LEU:HD11  | 1:G:36:LEU:HD12   | 1.98                     | 0.44              |
| 2:I:549:PHE:HB3  | 2:I:552:HIS:HD2   | 1.82                     | 0.44              |
| 2:I:682:TYR:HA   | 3:J:633:VAL:HG11  | 1.98                     | 0.44              |
| 2:I:737:LEU:HD12 | 2:I:737:LEU:HA    | 1.61                     | 0.44              |
| 2:I:770:GLU:HB3  | 5:L:369:LEU:HD12  | 1.99                     | 0.44              |
| 2:I:1030:GLN:O   | 3:J:622:ARG:HA    | 2.17                     | 0.44              |
| 3:J:900:ILE:HB   | 3:J:902:MET:HE3   | 1.99                     | 0.44              |
| 3:J:1006:ALA:O   | 3:J:1010:ASN:HB2  | 2.16                     | 0.44              |
| 3:J:1479:ASP:HA  | 3:J:1482:ARG:HG2  | 1.99                     | 0.44              |
| 1:B:10:VAL:HG12  | 1:B:12:THR:HG23   | 1.99                     | 0.44              |
| 2:C:370:ALA:O    | 5:F:295:GLN:NE2   | 2.50                     | 0.44              |
| 2:C:432:ARG:HH12 | 2:C:518:ARG:NE    | 2.15                     | 0.44              |
| 3:D:352:ASN:C    | 3:D:368:VAL:HG13  | 2.42                     | 0.44              |
| 3:D:1144:LEU:HA  | 3:D:1144:LEU:HD12 | 1.53                     | 0.44              |
| 3:D:1312:LEU:HG  | 3:D:1325:LEU:O    | 2.17                     | 0.44              |
| 1:G:89:PHE:CE1   | 1:G:120:VAL:HG12  | 2.52                     | 0.44              |
| 2:I:142:ARG:HA   | 2:I:331:ARG:HA    | 2.00                     | 0.44              |
| 2:I:423:ALA:O    | 2:I:428:ARG:HG3   | 2.16                     | 0.44              |
| 2:I:564:MET:HG2  | 2:I:567:GLN:NE2   | 2.32                     | 0.44              |
| 2:I:1009:SER:HB3 | 3:J:651:GLU:O     | 2.18                     | 0.44              |
| 3:J:806:PHE:CD1  | 3:J:811:GLU:HB3   | 2.52                     | 0.44              |
| 3:J:810:GLU:O    | 3:J:813:LEU:HB3   | 2.17                     | 0.44              |
| 3:J:1191:PRO:O   | 3:J:1373:ARG:HD2  | 2.17                     | 0.44              |
| 3:J:1406:ARG:O   | 3:J:1410:GLU:HG3  | 2.16                     | 0.44              |
| 4:K:19:LEU:O     | 4:K:23:VAL:HG23   | 2.17                     | 0.44              |
| 1:A:28:LEU:HD22  | 1:A:32:PHE:HD2    | 1.82                     | 0.44              |
| 2:C:41:ASN:HA    | 2:C:45:GLN:HB3    | 1.99                     | 0.44              |
| 2:C:670:GLN:O    | 2:C:672:VAL:HG23  | 2.17                     | 0.44              |
| 2:C:744:ARG:NE   | 2:C:747:ALA:HB2   | 2.33                     | 0.44              |
| 2:C:971:LYS:HG2  | 2:C:988:VAL:HG12  | 1.99                     | 0.44              |
| 2:C:1030:GLN:O   | 3:D:622:ARG:HA    | 2.17                     | 0.44              |
| 3:D:638:LYS:HG3  | 3:D:640:HIS:H     | 1.81                     | 0.44              |
| 1:G:73:GLU:HB3   | 1:G:77:GLU:HG3    | 1.99                     | 0.44              |
| 1:H:87:VAL:HG12  | 1:H:122:ILE:HG12  | 1.99                     | 0.44              |
| 1:H:176:ARG:NH1  | 3:J:884:ARG:HH12  | 2.16                     | 0.44              |
| 2:I:16:PRO:HB2   | 2:I:460:ARG:NH2   | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:690:ILE:HG13  | 2:I:852:ILE:HG23  | 1.99                     | 0.44              |
| 2:I:880:MET:CE    | 3:J:1037:GLN:HB2  | 2.46                     | 0.44              |
| 5:L:159:ILE:N     | 5:L:160:PRO:HD3   | 2.33                     | 0.44              |
| 5:L:411:ARG:HD3   | 6:R:1:DC:C6       | 2.52                     | 0.44              |
| 1:A:22:GLU:HA     | 1:A:197:LEU:O     | 2.17                     | 0.44              |
| 1:A:79:ILE:HD13   | 1:A:167:VAL:HG12  | 2.00                     | 0.44              |
| 2:C:161:SER:C     | 2:C:162:ILE:HD12  | 2.42                     | 0.44              |
| 2:C:333:ILE:HB    | 2:C:461:VAL:HG11  | 2.00                     | 0.44              |
| 2:C:577:PRO:HB3   | 2:C:993:PHE:CG    | 2.52                     | 0.44              |
| 3:D:213:VAL:HB    | 3:D:345:TYR:HE1   | 1.82                     | 0.44              |
| 3:D:631:ILE:HD11  | 3:D:739:ASP:O     | 2.18                     | 0.44              |
| 3:D:1078:ARG:HB3  | 3:D:1078:ARG:HH11 | 1.82                     | 0.44              |
| 1:G:63:HIS:CD2    | 1:G:66:SER:HB2    | 2.53                     | 0.44              |
| 2:I:550:LEU:HD11  | 2:I:558:ALA:HB1   | 1.98                     | 0.44              |
| 3:J:701:LEU:HD22  | 3:J:713:ILE:HG22  | 1.98                     | 0.44              |
| 3:J:1293:PHE:CD1  | 3:J:1293:PHE:N    | 2.85                     | 0.44              |
| 6:O:2:DT:H2"      | 6:O:3:DT:OP2      | 2.18                     | 0.44              |
| 1:A:231:SER:H     | 1:B:14:THR:HG22   | 1.82                     | 0.44              |
| 2:C:97:ARG:HB2    | 2:C:112:GLU:HG3   | 1.99                     | 0.44              |
| 2:C:682:TYR:HA    | 3:D:633:VAL:HG11  | 2.00                     | 0.44              |
| 3:D:537:THR:C     | 5:F:332:LEU:HG    | 2.43                     | 0.44              |
| 3:D:634:GLY:O     | 3:D:637:LEU:N     | 2.28                     | 0.44              |
| 4:E:6:ILE:HG23    | 4:E:7:ASP:H       | 1.83                     | 0.44              |
| 2:I:194:VAL:O     | 2:I:198:ARG:HG3   | 2.17                     | 0.44              |
| 2:I:526:PRO:O     | 2:I:529:VAL:HG12  | 2.17                     | 0.44              |
| 2:I:644:ARG:HD2   | 2:I:647:GLN:HB3   | 2.00                     | 0.44              |
| 2:I:922:PHE:HB2   | 2:I:967:PHE:CD2   | 2.53                     | 0.44              |
| 3:J:22:SER:HB2    | 3:J:92:HIS:HB3    | 1.97                     | 0.44              |
| 3:J:107:ASP:CG    | 3:J:109:PRO:HD2   | 2.42                     | 0.44              |
| 3:J:661:MET:HG2   | 3:J:666:PHE:CZ    | 2.52                     | 0.44              |
| 3:J:1078:ARG:HB3  | 3:J:1078:ARG:HH11 | 1.83                     | 0.44              |
| 3:J:1144:LEU:HD13 | 3:J:1144:LEU:HA   | 1.77                     | 0.44              |
| 1:A:232:LEU:H     | 1:A:232:LEU:HD12  | 1.82                     | 0.44              |
| 1:B:23:PHE:HE1    | 1:B:208:LEU:HD12  | 1.82                     | 0.44              |
| 2:C:22:GLN:HG3    | 2:C:407:LYS:HB3   | 1.99                     | 0.44              |
| 2:C:878:SER:HB2   | 3:D:1029:ARG:HG3  | 1.99                     | 0.44              |
| 3:D:155:ASP:OD2   | 3:D:155:ASP:N     | 2.49                     | 0.44              |
| 1:H:202:ASP:OD1   | 1:H:203:GLY:N     | 2.51                     | 0.44              |
| 2:I:670:GLN:O     | 2:I:672:VAL:HG23  | 2.17                     | 0.44              |
| 2:I:761:PHE:HA    | 2:I:785:VAL:HA    | 1.99                     | 0.44              |
| 2:I:994:ILE:HG22  | 2:I:995:MET:H     | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1086:ARG:HG3  | 2:I:1086:ARG:NH1  | 2.32                     | 0.44              |
| 2:I:1090:LYS:NZ   | 2:I:1093:GLN:OE1  | 2.35                     | 0.44              |
| 3:J:84:ILE:HD11   | 3:J:88:TYR:HE1    | 1.83                     | 0.44              |
| 3:J:558:LEU:CD2   | 3:J:567:ILE:HG23  | 2.48                     | 0.44              |
| 5:L:99:TYR:O      | 5:L:103:ILE:HG12  | 2.17                     | 0.44              |
| 1:A:58:ILE:HG22   | 1:A:60:ASP:H      | 1.81                     | 0.44              |
| 1:A:227:ASN:HA    | 1:A:228:PRO:HD2   | 1.75                     | 0.44              |
| 3:D:117:ASP:HB2   | 3:D:495:ARG:CZ    | 2.47                     | 0.44              |
| 3:D:638:LYS:HB3   | 3:D:641:GLN:HE21  | 1.83                     | 0.44              |
| 3:D:1141:GLU:OE1  | 3:D:1168:LEU:HD11 | 2.18                     | 0.44              |
| 5:F:398:LEU:HB3   | 7:P:21:DG:OP2     | 2.18                     | 0.44              |
| 1:G:22:GLU:HA     | 1:G:197:LEU:O     | 2.18                     | 0.44              |
| 1:G:182:GLU:O     | 1:G:193:ASP:HA    | 2.18                     | 0.44              |
| 1:H:34:VAL:HG22   | 1:H:181:VAL:HG21  | 2.00                     | 0.44              |
| 1:H:41:ARG:HG3    | 1:H:177:VAL:HG21  | 2.00                     | 0.44              |
| 2:I:714:ASP:HB2   | 2:I:818:GLY:O     | 2.18                     | 0.44              |
| 2:I:834:GLN:HG2   | 2:I:835:VAL:H     | 1.82                     | 0.44              |
| 3:J:496:LEU:HD12  | 3:J:499:VAL:HB    | 1.99                     | 0.44              |
| 3:J:1202:GLN:O    | 3:J:1206:GLY:N    | 2.51                     | 0.44              |
| 3:J:1499:ARG:HH21 | 3:J:1500:LYS:HG3  | 1.83                     | 0.44              |
| 1:A:182:GLU:O     | 1:A:193:ASP:HA    | 2.18                     | 0.44              |
| 1:B:40:LEU:O      | 1:B:44:LEU:HB2    | 2.18                     | 0.44              |
| 1:B:78:ILE:O      | 1:B:82:LEU:HG     | 2.18                     | 0.44              |
| 2:C:588:VAL:HG23  | 2:C:596:TYR:OH    | 2.17                     | 0.44              |
| 2:C:834:GLN:HG2   | 2:C:835:VAL:H     | 1.82                     | 0.44              |
| 2:C:1112:PHE:HB2  | 2:C:1115:LEU:HB2  | 1.99                     | 0.44              |
| 3:D:107:ASP:CG    | 3:D:109:PRO:HD2   | 2.42                     | 0.44              |
| 3:D:209:ARG:HE    | 3:D:391:ALA:HB2   | 1.83                     | 0.44              |
| 3:D:1199:GLY:O    | 3:D:1373:ARG:NH1  | 2.51                     | 0.44              |
| 5:F:173:GLU:O     | 5:F:177:LYS:HB2   | 2.18                     | 0.44              |
| 2:I:269:LEU:HB2   | 2:I:288:ARG:O     | 2.18                     | 0.44              |
| 2:I:399:ASN:HD21  | 2:I:566:THR:HA    | 1.83                     | 0.44              |
| 2:I:1089:VAL:HG13 | 2:I:1099:VAL:HG11 | 2.00                     | 0.44              |
| 2:I:1115:LEU:HD21 | 3:J:84:ILE:HG23   | 2.00                     | 0.44              |
| 3:J:523:ASP:HA    | 3:J:526:PRO:HG3   | 2.00                     | 0.44              |
| 3:J:537:THR:O     | 5:L:332:LEU:HG    | 2.18                     | 0.44              |
| 3:J:568:ARG:HA    | 3:J:571:LYS:HE2   | 1.98                     | 0.44              |
| 3:J:1129:THR:C    | 3:J:1131:THR:H    | 2.25                     | 0.44              |
| 2:C:5:ARG:HE      | 2:C:5:ARG:HB2     | 1.70                     | 0.44              |
| 2:C:458:TYR:CD1   | 2:C:538:GLN:HB3   | 2.49                     | 0.44              |
| 3:D:529:GLN:HA    | 3:D:535:PHE:HA    | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1068:LEU:H    | 3:D:1068:LEU:HD12 | 1.83                     | 0.44              |
| 3:D:1189:ARG:HE   | 3:D:1203:LYS:HB2  | 1.82                     | 0.44              |
| 3:D:1258:ARG:O    | 3:D:1258:ARG:HG3  | 2.18                     | 0.44              |
| 3:D:1288:ASP:OD2  | 3:D:1288:ASP:N    | 2.50                     | 0.44              |
| 3:D:1370:ILE:HG13 | 3:D:1370:ILE:H    | 1.66                     | 0.44              |
| 2:I:537:LYS:NZ    | 2:I:905:VAL:H     | 2.01                     | 0.44              |
| 2:I:581:THR:OG1   | 2:I:584:GLU:OE2   | 2.36                     | 0.44              |
| 2:I:700:TYR:HB3   | 2:I:833:LEU:HD13  | 2.00                     | 0.44              |
| 2:I:988:VAL:HG22  | 3:J:948:THR:OG1   | 2.18                     | 0.44              |
| 3:J:439:LEU:HD21  | 5:L:190:HIS:HB3   | 2.00                     | 0.44              |
| 3:J:1033:GLN:O    | 3:J:1037:GLN:HG3  | 2.18                     | 0.44              |
| 3:J:1038:LEU:O    | 3:J:1060:SER:OG   | 2.22                     | 0.44              |
| 1:A:35:THR:CG2    | 1:B:39:PRO:HA     | 2.47                     | 0.43              |
| 1:A:44:LEU:HD11   | 1:A:199:ILE:HD13  | 1.99                     | 0.43              |
| 1:A:76:VAL:HA     | 1:A:79:ILE:HD12   | 1.99                     | 0.43              |
| 2:C:321:GLU:HG2   | 2:C:322:VAL:H     | 1.83                     | 0.43              |
| 2:C:675:ALA:O     | 2:C:870:ILE:HA    | 2.18                     | 0.43              |
| 2:C:714:ASP:HB2   | 2:C:818:GLY:O     | 2.18                     | 0.43              |
| 2:C:775:ARG:CZ    | 2:C:782:ALA:HB2   | 2.48                     | 0.43              |
| 2:C:1012:PRO:HB2  | 2:C:1021:LEU:HD11 | 2.00                     | 0.43              |
| 3:D:181:ASP:HB2   | 3:D:205:TYR:CD2   | 2.53                     | 0.43              |
| 3:D:701:LEU:HD11  | 3:D:763:MET:HG2   | 2.00                     | 0.43              |
| 3:D:1368:ILE:H    | 3:D:1368:ILE:HG13 | 1.67                     | 0.43              |
| 1:G:44:LEU:HD11   | 1:G:199:ILE:HD13  | 1.99                     | 0.43              |
| 2:I:332:ARG:HH11  | 2:I:334:ARG:HD2   | 1.82                     | 0.43              |
| 2:I:376:ARG:HB2   | 2:I:377:PRO:HD3   | 2.00                     | 0.43              |
| 2:I:588:VAL:HG23  | 2:I:596:TYR:OH    | 2.18                     | 0.43              |
| 2:I:709:GLU:HA    | 2:I:823:VAL:O     | 2.18                     | 0.43              |
| 2:I:807:ARG:HB3   | 2:I:810:ASP:OD1   | 2.18                     | 0.43              |
| 3:J:635:PRO:O     | 3:J:935:LYS:HE2   | 2.18                     | 0.43              |
| 3:J:638:LYS:HG2   | 3:J:640:HIS:NE2   | 2.33                     | 0.43              |
| 3:J:792:ILE:HD13  | 3:J:881:LEU:HD23  | 1.99                     | 0.43              |
| 2:C:140:ILE:HD12  | 2:C:332:ARG:O     | 2.17                     | 0.43              |
| 2:C:713:ARG:O     | 2:C:720:GLU:HG2   | 2.18                     | 0.43              |
| 3:D:154:THR:HG23  | 3:D:156:GLU:H     | 1.83                     | 0.43              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:HG3  | 2.18                     | 0.43              |
| 3:D:1180:ALA:O    | 3:J:1132:LEU:HD12 | 2.18                     | 0.43              |
| 1:G:28:LEU:HD22   | 1:G:32:PHE:HD2    | 1.83                     | 0.43              |
| 1:G:46:SER:OG     | 1:G:47:SER:N      | 2.51                     | 0.43              |
| 1:G:178:ALA:HB2   | 2:I:864:GLY:HA3   | 2.01                     | 0.43              |
| 2:I:269:LEU:H     | 2:I:288:ARG:HB3   | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:505:SER:HB3   | 3:J:1453:ALA:HA   | 1.99                     | 0.43              |
| 3:J:560:GLN:HE22  | 5:L:236:ILE:HG21  | 1.82                     | 0.43              |
| 3:J:637:LEU:HG    | 3:J:641:GLN:HB3   | 2.01                     | 0.43              |
| 3:J:1200:VAL:HG22 | 3:J:1221:VAL:HG21 | 1.99                     | 0.43              |
| 5:L:246:ARG:HD3   | 6:R:26:DA:C6      | 2.54                     | 0.43              |
| 5:L:407:VAL:HG12  | 6:R:1:DC:H3'      | 2.00                     | 0.43              |
| 1:B:51:THR:HG21   | 1:B:86:VAL:HG23   | 2.00                     | 0.43              |
| 1:B:107:LYS:O     | 1:B:132:LEU:HB2   | 2.17                     | 0.43              |
| 2:C:332:ARG:HH11  | 2:C:334:ARG:HD2   | 1.83                     | 0.43              |
| 2:C:897:LEU:HD21  | 2:C:899:GLN:HG2   | 1.99                     | 0.43              |
| 2:C:1047:HIS:O    | 2:C:1051:GLU:HG3  | 2.18                     | 0.43              |
| 2:C:1089:VAL:HG11 | 2:C:1112:PHE:HE2  | 1.82                     | 0.43              |
| 3:D:254:GLU:C     | 3:D:300:VAL:HG13  | 2.42                     | 0.43              |
| 3:D:1269:LYS:HG3  | 3:D:1270:ALA:H    | 1.82                     | 0.43              |
| 5:F:252:THR:HA    | 6:O:29:DC:H5      | 1.83                     | 0.43              |
| 5:F:377:SER:HB3   | 5:F:380:GLU:HG2   | 2.00                     | 0.43              |
| 2:I:390:GLN:HG2   | 2:I:415:PRO:HD3   | 1.99                     | 0.43              |
| 3:J:34:TYR:HB2    | 5:L:325:ILE:HG23  | 2.00                     | 0.43              |
| 3:J:1333:HIS:O    | 3:J:1336:LEU:HB3  | 2.18                     | 0.43              |
| 4:K:30:LEU:HA     | 4:K:37:ASN:HD21   | 1.83                     | 0.43              |
| 5:L:141:LEU:O     | 5:L:145:VAL:HG23  | 2.18                     | 0.43              |
| 1:B:7:LYS:C       | 1:B:9:PRO:HD3     | 2.44                     | 0.43              |
| 1:B:55:SER:HB2    | 1:B:166:PRO:HA    | 1.99                     | 0.43              |
| 2:C:65:VAL:CG1    | 2:C:101:ILE:HB    | 2.48                     | 0.43              |
| 2:C:84:ARG:HA     | 2:C:131:GLY:HA2   | 2.00                     | 0.43              |
| 2:C:122:THR:HG23  | 2:C:128:ILE:HD11  | 1.99                     | 0.43              |
| 2:C:994:ILE:HG22  | 2:C:995:MET:H     | 1.83                     | 0.43              |
| 3:D:67:ARG:HD2    | 5:F:394:ARG:HB2   | 1.99                     | 0.43              |
| 3:D:589:SER:HA    | 3:D:590:PRO:HD3   | 1.86                     | 0.43              |
| 3:D:790:TYR:CD1   | 3:D:907:GLU:HB3   | 2.54                     | 0.43              |
| 3:D:858:LEU:HD12  | 3:D:859:ASP:H     | 1.83                     | 0.43              |
| 3:D:996:TRP:CE2   | 3:D:1056:PRO:HD3  | 2.53                     | 0.43              |
| 5:F:276:PRO:HB2   | 5:F:279:MET:HG2   | 1.99                     | 0.43              |
| 1:H:37:GLY:HA3    | 1:H:179:PHE:CE1   | 2.53                     | 0.43              |
| 2:I:170:PRO:HD2   | 2:I:267:TYR:HD1   | 1.83                     | 0.43              |
| 2:I:202:TYR:CD1   | 2:I:206:THR:HG21  | 2.53                     | 0.43              |
| 2:I:327:HIS:O     | 2:I:331:ARG:HG3   | 2.18                     | 0.43              |
| 2:I:333:ILE:HB    | 2:I:461:VAL:HG11  | 2.00                     | 0.43              |
| 2:I:713:ARG:O     | 2:I:720:GLU:HG2   | 2.18                     | 0.43              |
| 3:J:32:ILE:HA     | 3:J:40:GLU:HG2    | 2.00                     | 0.43              |
| 3:J:592:THR:OG1   | 3:J:596:SER:O     | 2.29                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:661:MET:HE2   | 3:J:673:ALA:HB1   | 1.99                     | 0.43              |
| 3:J:892:ASP:HB2   | 3:J:894:LYS:HG2   | 2.01                     | 0.43              |
| 3:J:1042:ARG:HB3  | 3:J:1057:VAL:CG2  | 2.48                     | 0.43              |
| 3:J:1065:LEU:HB3  | 3:J:1069:GLU:HB2  | 1.99                     | 0.43              |
| 3:J:1068:LEU:H    | 3:J:1068:LEU:HD12 | 1.83                     | 0.43              |
| 3:J:1108:ARG:NH2  | 3:J:1198:TYR:O    | 2.50                     | 0.43              |
| 5:L:109:LEU:HD22  | 5:L:205:ALA:HB1   | 2.00                     | 0.43              |
| 5:L:376:LEU:HG    | 5:L:423:LEU:HD21  | 1.99                     | 0.43              |
| 6:O:5:DA:H2       | 7:P:22:DT:H3      | 1.65                     | 0.43              |
| 7:S:11:DT:H1'     | 7:S:12:DA:H5'     | 2.01                     | 0.43              |
| 1:A:42:ARG:NH2    | 1:B:31:GLY:O      | 2.41                     | 0.43              |
| 1:A:65:PHE:CD2    | 2:C:799:ILE:HD11  | 2.54                     | 0.43              |
| 1:B:160:ASP:O     | 1:B:161:ARG:HB2   | 2.18                     | 0.43              |
| 2:C:124:ASP:HB2   | 2:C:407:LYS:NZ    | 2.34                     | 0.43              |
| 2:C:269:LEU:HB2   | 2:C:288:ARG:O     | 2.18                     | 0.43              |
| 2:C:495:THR:H     | 2:C:530:GLU:CG    | 2.31                     | 0.43              |
| 2:C:710:ILE:HD13  | 2:C:790:LEU:HD13  | 2.00                     | 0.43              |
| 2:C:1018:GLN:HG2  | 2:C:1083:GLU:HG2  | 2.00                     | 0.43              |
| 3:D:30:GLU:HB3    | 5:F:274:ARG:HB2   | 2.00                     | 0.43              |
| 3:D:242:LEU:HB3   | 3:D:311:LEU:O     | 2.19                     | 0.43              |
| 3:D:970:LYS:O     | 3:D:973:GLN:HB3   | 2.18                     | 0.43              |
| 3:D:1142:SER:HB3  | 3:D:1353:GLN:NE2  | 2.33                     | 0.43              |
| 4:E:79:LEU:HD23   | 4:E:80:VAL:HG22   | 2.00                     | 0.43              |
| 1:G:20:TYR:C      | 1:G:207:PRO:HG2   | 2.44                     | 0.43              |
| 1:G:150:TYR:CZ    | 1:G:152:PRO:HG3   | 2.54                     | 0.43              |
| 1:G:232:LEU:H     | 1:G:232:LEU:HD12  | 1.83                     | 0.43              |
| 1:H:176:ARG:HB3   | 1:H:200:TRP:CE3   | 2.53                     | 0.43              |
| 1:H:213:GLN:HE21  | 1:H:217:ILE:HD11  | 1.83                     | 0.43              |
| 2:I:41:ASN:HA     | 2:I:45:GLN:HB3    | 2.01                     | 0.43              |
| 2:I:1056:LYS:NZ   | 3:J:748:HIS:HB3   | 2.34                     | 0.43              |
| 3:J:121:THR:O     | 3:J:124:GLU:HB3   | 2.18                     | 0.43              |
| 3:J:698:LYS:HB3   | 3:J:756:GLN:NE2   | 2.34                     | 0.43              |
| 2:C:390:GLN:CG    | 2:C:415:PRO:HD3   | 2.48                     | 0.43              |
| 2:C:1085:PHE:O    | 2:C:1089:VAL:HG23 | 2.18                     | 0.43              |
| 3:D:132:TYR:HB3   | 3:D:454:ALA:HB1   | 1.99                     | 0.43              |
| 3:D:1361:VAL:HG12 | 3:D:1363:LEU:H    | 1.84                     | 0.43              |
| 1:G:55:SER:CB     | 1:G:158:ILE:HG12  | 2.43                     | 0.43              |
| 1:G:64:GLU:HA     | 1:G:75:VAL:HG11   | 1.99                     | 0.43              |
| 2:I:160:ALA:HB3   | 2:I:174:LEU:HD11  | 2.01                     | 0.43              |
| 2:I:181:VAL:HG22  | 2:I:182:VAL:H     | 1.84                     | 0.43              |
| 2:I:321:GLU:HG2   | 2:I:322:VAL:H     | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:343:GLN:HG3   | 2:I:385:PHE:CB    | 2.48                     | 0.43              |
| 2:I:577:PRO:HB3   | 2:I:993:PHE:CG    | 2.53                     | 0.43              |
| 3:J:209:ARG:HA    | 3:J:347:VAL:HB    | 1.99                     | 0.43              |
| 3:J:354:ILE:HG23  | 3:J:355:VAL:HG13  | 2.01                     | 0.43              |
| 3:J:636:GLN:H     | 3:J:636:GLN:CD    | 2.26                     | 0.43              |
| 3:J:801:GLY:C     | 3:J:803:GLY:H     | 2.27                     | 0.43              |
| 3:J:1014:ASN:C    | 3:J:1016:PRO:HD3  | 2.43                     | 0.43              |
| 3:J:1059:SER:HB3  | 3:J:1063:GLU:HB2  | 1.99                     | 0.43              |
| 3:J:1149:LEU:HG   | 3:J:1160:LEU:HD12 | 2.01                     | 0.43              |
| 3:J:1336:LEU:HD11 | 3:J:1419:PRO:HB2  | 1.99                     | 0.43              |
| 3:J:1434:TRP:NE1  | 3:J:1457:ASP:HB2  | 2.33                     | 0.43              |
| 1:A:28:LEU:HD11   | 1:A:36:LEU:HD12   | 2.00                     | 0.43              |
| 1:A:89:PHE:CE1    | 1:A:120:VAL:HG12  | 2.54                     | 0.43              |
| 2:C:212:SER:C     | 2:C:214:TYR:H     | 2.25                     | 0.43              |
| 2:C:424:GLY:O     | 2:C:425:PHE:HD1   | 2.00                     | 0.43              |
| 2:C:690:ILE:HG13  | 2:C:852:ILE:HG23  | 2.00                     | 0.43              |
| 3:D:82:ARG:HB2    | 3:D:84:ILE:HG22   | 2.01                     | 0.43              |
| 3:D:1110:ALA:HB2  | 3:D:1217:ILE:HD13 | 2.01                     | 0.43              |
| 3:D:1192:LEU:HD13 | 3:D:1345:GLU:CD   | 2.44                     | 0.43              |
| 5:F:117:LEU:O     | 5:F:121:VAL:HG23  | 2.18                     | 0.43              |
| 1:H:89:PHE:HE1    | 1:H:97:THR:HG22   | 1.83                     | 0.43              |
| 2:I:676:ILE:O     | 2:I:987:ILE:HG23  | 2.18                     | 0.43              |
| 2:I:768:SER:O     | 2:I:772:ARG:N     | 2.50                     | 0.43              |
| 2:I:1067:TYR:O    | 2:I:1071:ILE:HB   | 2.19                     | 0.43              |
| 3:J:56:TYR:CA     | 3:J:80:VAL:HG23   | 2.49                     | 0.43              |
| 5:L:181:LEU:HD23  | 5:L:185:LEU:HD13  | 1.99                     | 0.43              |
| 5:L:263:ASN:HA    | 5:L:266:ILE:CD1   | 2.49                     | 0.43              |
| 2:C:537:LYS:CE    | 2:C:583:LEU:HD11  | 2.49                     | 0.43              |
| 3:D:56:TYR:CA     | 3:D:80:VAL:HG23   | 2.49                     | 0.43              |
| 3:D:187:LYS:HG2   | 3:D:198:ARG:C     | 2.44                     | 0.43              |
| 1:H:23:PHE:HE2    | 1:H:199:ILE:HB    | 1.83                     | 0.43              |
| 2:I:549:PHE:HB3   | 2:I:552:HIS:CD2   | 2.54                     | 0.43              |
| 3:J:187:LYS:N     | 3:J:200:ASP:OD2   | 2.49                     | 0.43              |
| 3:J:569:ASN:ND2   | 5:L:229:GLN:HE21  | 2.16                     | 0.43              |
| 3:J:585:GLY:CA    | 3:J:590:PRO:HG3   | 2.48                     | 0.43              |
| 3:J:1170:ASP:O    | 3:J:1174:LEU:HG   | 2.18                     | 0.43              |
| 4:K:6:ILE:HG23    | 4:K:7:ASP:H       | 1.82                     | 0.43              |
| 5:L:109:LEU:HD12  | 5:L:114:GLU:HA    | 2.01                     | 0.43              |
| 5:L:167:ASP:HB2   | 5:L:168:PRO:HD3   | 2.01                     | 0.43              |
| 5:L:377:SER:HB3   | 5:L:380:GLU:HG2   | 2.01                     | 0.43              |
| 2:C:64:LEU:HD21   | 2:C:66:LEU:CB     | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:160:ALA:HB3   | 2:C:174:LEU:HD11  | 2.01                     | 0.43              |
| 2:C:343:GLN:HG3   | 2:C:385:PHE:CB    | 2.49                     | 0.43              |
| 2:C:683:ASN:HB2   | 2:C:872:ASN:H     | 1.84                     | 0.43              |
| 2:C:1086:ARG:HG3  | 2:C:1086:ARG:NH1  | 2.33                     | 0.43              |
| 3:D:210:ARG:HD2   | 3:D:388:HIS:HB2   | 2.00                     | 0.43              |
| 3:D:553:ARG:HH11  | 5:F:230:GLU:HG2   | 1.83                     | 0.43              |
| 3:D:1042:ARG:HB3  | 3:D:1057:VAL:CG2  | 2.49                     | 0.43              |
| 3:D:1472:ILE:HA   | 3:D:1473:PRO:HD3  | 1.76                     | 0.43              |
| 1:G:53:VAL:CG2    | 1:G:54:THR:H      | 2.28                     | 0.43              |
| 1:H:101:LEU:HD22  | 1:H:102:ARG:H     | 1.84                     | 0.43              |
| 2:I:99:GLN:HB3    | 2:I:110:GLU:HG3   | 2.00                     | 0.43              |
| 2:I:124:ASP:HA    | 2:I:592:LEU:HD12  | 2.01                     | 0.43              |
| 2:I:495:THR:H     | 2:I:530:GLU:CG    | 2.32                     | 0.43              |
| 2:I:536:PRO:HB3   | 3:J:1067:VAL:HG11 | 2.01                     | 0.43              |
| 2:I:584:GLU:HB3   | 2:I:666:LEU:HB3   | 2.00                     | 0.43              |
| 3:J:155:ASP:N     | 3:J:155:ASP:OD2   | 2.52                     | 0.43              |
| 3:J:349:PRO:HB2   | 5:L:111:LEU:HD23  | 2.01                     | 0.43              |
| 3:J:354:ILE:HG22  | 3:J:367:ILE:O     | 2.19                     | 0.43              |
| 3:J:1192:LEU:HD23 | 3:J:1373:ARG:HB2  | 2.00                     | 0.43              |
| 2:C:182:VAL:O     | 2:C:192:PRO:HA    | 2.19                     | 0.43              |
| 2:C:543:ASN:HA    | 2:C:546:LEU:HD12  | 2.01                     | 0.43              |
| 2:C:564:MET:SD    | 2:C:846:LYS:HG2   | 2.59                     | 0.43              |
| 2:C:858:MET:SD    | 2:C:859:PRO:HD2   | 2.59                     | 0.43              |
| 2:C:892:LEU:HD13  | 2:C:970:GLY:HA2   | 2.01                     | 0.43              |
| 2:C:1035:MET:HE2  | 2:C:1035:MET:H    | 1.84                     | 0.43              |
| 3:D:84:ILE:HD11   | 3:D:88:TYR:HE1    | 1.84                     | 0.43              |
| 3:D:218:LYS:HA    | 3:D:337:LEU:O     | 2.19                     | 0.43              |
| 3:D:245:LEU:HD23  | 3:D:245:LEU:HA    | 1.75                     | 0.43              |
| 3:D:439:LEU:HD21  | 5:F:190:HIS:HB3   | 2.01                     | 0.43              |
| 3:D:792:ILE:HD13  | 3:D:881:LEU:HD23  | 2.00                     | 0.43              |
| 3:D:1289:ARG:HD3  | 3:D:1304:LYS:HD2  | 2.01                     | 0.43              |
| 3:D:1293:PHE:HA   | 3:D:1302:GLU:HA   | 2.01                     | 0.43              |
| 4:E:26:ARG:NH2    | 4:E:37:ASN:HD22   | 2.17                     | 0.43              |
| 1:H:160:ASP:O     | 1:H:161:ARG:HB2   | 2.19                     | 0.43              |
| 1:H:201:THR:HG21  | 1:H:205:VAL:HG23  | 2.01                     | 0.43              |
| 2:I:185:LYS:HA    | 2:I:189:ARG:O     | 2.19                     | 0.43              |
| 2:I:679:PHE:CE2   | 2:I:853:LEU:HD21  | 2.54                     | 0.43              |
| 2:I:1040:LEU:HG   | 3:J:763:MET:HE1   | 2.00                     | 0.43              |
| 3:J:791:TYR:CE2   | 3:J:945:SER:HB3   | 2.54                     | 0.43              |
| 3:J:1149:LEU:HD22 | 3:J:1166:LEU:HD11 | 2.00                     | 0.43              |
| 5:L:143:ARG:NH1   | 5:L:196:GLU:OE2   | 2.52                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:P:11:DT:H1'    | 7:P:12:DA:H5'     | 2.01                     | 0.43              |
| 6:R:21:DG:H1'    | 6:R:22:DT:H5''    | 2.00                     | 0.43              |
| 1:A:42:ARG:HH12  | 2:C:857:ASP:CG    | 2.27                     | 0.42              |
| 1:A:181:VAL:C    | 1:A:182:GLU:HG3   | 2.44                     | 0.42              |
| 1:B:34:VAL:HG11  | 2:C:978:ARG:HB3   | 2.01                     | 0.42              |
| 1:B:159:LYS:HG3  | 1:B:164:ALA:HB3   | 2.01                     | 0.42              |
| 2:C:181:VAL:HG22 | 2:C:182:VAL:H     | 1.83                     | 0.42              |
| 2:C:456:ALA:HB3  | 2:C:459:ALA:HB2   | 2.01                     | 0.42              |
| 3:D:369:ALA:HA   | 3:D:376:GLU:HG2   | 2.01                     | 0.42              |
| 3:D:397:LYS:O    | 3:D:447:VAL:HG23  | 2.19                     | 0.42              |
| 3:D:789:LEU:HD13 | 3:D:934:LEU:HD23  | 2.01                     | 0.42              |
| 5:F:167:ASP:HB2  | 5:F:168:PRO:HD3   | 2.01                     | 0.42              |
| 1:G:48:ILE:HG22  | 1:G:173:PRO:HD2   | 2.00                     | 0.42              |
| 1:G:97:THR:HG23  | 1:G:98:THR:N      | 2.27                     | 0.42              |
| 1:H:62:LEU:H     | 1:H:62:LEU:HD12   | 1.83                     | 0.42              |
| 2:I:397:GLU:HG3  | 2:I:632:ASN:HD22  | 1.84                     | 0.42              |
| 2:I:424:GLY:O    | 2:I:425:PHE:HD1   | 2.01                     | 0.42              |
| 2:I:711:GLU:HA   | 2:I:822:VAL:HG12  | 2.01                     | 0.42              |
| 2:I:720:GLU:HB2  | 2:I:759:THR:O     | 2.19                     | 0.42              |
| 2:I:878:SER:HB2  | 3:J:1029:ARG:HG3  | 2.00                     | 0.42              |
| 3:J:701:LEU:HD11 | 3:J:763:MET:HG2   | 2.01                     | 0.42              |
| 3:J:837:GLY:HA2  | 3:J:840:LYS:HB3   | 2.00                     | 0.42              |
| 3:J:1384:PRO:O   | 3:J:1415:VAL:HG22 | 2.19                     | 0.42              |
| 1:B:23:PHE:CE2   | 1:B:199:ILE:HB    | 2.54                     | 0.42              |
| 2:C:437:ARG:HD3  | 2:C:467:ILE:O     | 2.19                     | 0.42              |
| 2:C:547:ILE:HG21 | 2:C:550:LEU:HD13  | 2.02                     | 0.42              |
| 2:C:607:ASP:HB3  | 2:C:610:ARG:O     | 2.19                     | 0.42              |
| 2:C:737:LEU:HD12 | 2:C:737:LEU:HA    | 1.60                     | 0.42              |
| 3:D:573:MET:HE3  | 5:F:225:LEU:HB3   | 2.00                     | 0.42              |
| 3:D:576:GLU:HG3  | 3:D:577:ALA:N     | 2.35                     | 0.42              |
| 3:D:1433:SER:OG  | 3:D:1457:ASP:OD2  | 2.29                     | 0.42              |
| 5:F:142:ILE:HA   | 5:F:145:VAL:HB    | 2.02                     | 0.42              |
| 5:F:302:SER:H    | 5:F:305:GLU:CG    | 2.32                     | 0.42              |
| 1:G:43:ILE:HG13  | 1:H:35:THR:HG21   | 2.01                     | 0.42              |
| 1:H:55:SER:HB2   | 1:H:166:PRO:HA    | 2.00                     | 0.42              |
| 2:I:1019:GLN:HA  | 2:I:1020:PRO:HD3  | 1.87                     | 0.42              |
| 3:J:30:GLU:HB3   | 5:L:274:ARG:HB2   | 2.00                     | 0.42              |
| 3:J:1161:GLU:H   | 3:J:1161:GLU:HG2  | 1.58                     | 0.42              |
| 5:L:209:LEU:HB2  | 6:R:30:DT:C2      | 2.54                     | 0.42              |
| 1:A:34:VAL:HG22  | 1:A:181:VAL:HG21  | 2.02                     | 0.42              |
| 1:B:28:LEU:O     | 1:B:193:ASP:N     | 2.51                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:67:ASP:O      | 2:C:98:LEU:HB2    | 2.19                     | 0.42              |
| 2:C:564:MET:HG2   | 2:C:567:GLN:NE2   | 2.34                     | 0.42              |
| 3:D:14:SER:HB3    | 3:D:511:TRP:CE2   | 2.54                     | 0.42              |
| 3:D:100:ALA:HA    | 3:D:513:ILE:HA    | 2.02                     | 0.42              |
| 3:D:313:LEU:HD12  | 3:D:314:PRO:HD2   | 2.01                     | 0.42              |
| 3:D:698:LYS:HG2   | 3:D:756:GLN:HG2   | 2.01                     | 0.42              |
| 3:D:1122:LEU:HD12 | 3:D:1184:ARG:O    | 2.19                     | 0.42              |
| 2:I:212:SER:C     | 2:I:214:TYR:H     | 2.27                     | 0.42              |
| 2:I:328:LEU:HD23  | 2:I:437:ARG:HD2   | 2.01                     | 0.42              |
| 2:I:458:TYR:CD1   | 2:I:538:GLN:HB3   | 2.48                     | 0.42              |
| 2:I:537:LYS:CE    | 2:I:583:LEU:HD11  | 2.49                     | 0.42              |
| 3:J:58:CYS:HB2    | 3:J:78:VAL:HB     | 2.01                     | 0.42              |
| 3:J:103:TRP:O     | 3:J:107:ASP:HB2   | 2.19                     | 0.42              |
| 3:J:177:ALA:HB2   | 3:J:393:ILE:HD11  | 2.01                     | 0.42              |
| 3:J:508:ARG:HB3   | 3:J:510:GLU:CD    | 2.44                     | 0.42              |
| 3:J:603:LEU:O     | 3:J:606:ILE:HG22  | 2.19                     | 0.42              |
| 3:J:853:VAL:HG22  | 3:J:858:LEU:HD23  | 2.00                     | 0.42              |
| 3:J:1267:ARG:H    | 3:J:1267:ARG:NE   | 2.14                     | 0.42              |
| 3:J:1481:VAL:HG21 | 4:K:17:TYR:HB2    | 2.00                     | 0.42              |
| 1:A:173:PRO:HB3   | 1:A:202:ASP:OD1   | 2.20                     | 0.42              |
| 2:C:639:GLN:HA    | 2:C:657:ASP:O     | 2.20                     | 0.42              |
| 2:C:726:ILE:HD12  | 2:C:729:LEU:HG    | 2.01                     | 0.42              |
| 2:C:770:GLU:HB3   | 5:F:369:LEU:HD12  | 2.01                     | 0.42              |
| 2:C:806:LEU:HB2   | 2:C:822:VAL:HG22  | 2.01                     | 0.42              |
| 2:C:839:LEU:HA    | 2:C:995:MET:O     | 2.19                     | 0.42              |
| 3:D:544:TYR:O     | 3:D:548:ILE:HG13  | 2.20                     | 0.42              |
| 3:D:577:ALA:O     | 3:D:581:VAL:HG23  | 2.18                     | 0.42              |
| 3:D:643:GLY:O     | 3:D:726:ILE:HG23  | 2.19                     | 0.42              |
| 3:D:1021:TYR:O    | 3:D:1025:GLN:HB2  | 2.19                     | 0.42              |
| 3:D:1229:ILE:O    | 3:D:1232:PRO:HD2  | 2.19                     | 0.42              |
| 3:D:1404:ASN:O    | 3:D:1408:ILE:HG12 | 2.20                     | 0.42              |
| 3:D:1460:ILE:HG13 | 3:D:1461:GLY:N    | 2.33                     | 0.42              |
| 5:F:99:TYR:O      | 5:F:103:ILE:HG12  | 2.20                     | 0.42              |
| 1:G:20:TYR:HD2    | 1:G:21:GLY:N      | 2.17                     | 0.42              |
| 1:H:28:LEU:HB3    | 1:H:193:ASP:HB2   | 2.01                     | 0.42              |
| 2:I:751:PRO:HA    | 2:I:792:VAL:HG13  | 2.01                     | 0.42              |
| 2:I:775:ARG:CZ    | 2:I:782:ALA:HB2   | 2.49                     | 0.42              |
| 3:J:12:LEU:HD21   | 3:J:1452:ILE:HD13 | 2.01                     | 0.42              |
| 3:J:677:LEU:HD23  | 3:J:677:LEU:HA    | 1.87                     | 0.42              |
| 3:J:1229:ILE:O    | 3:J:1232:PRO:HD2  | 2.19                     | 0.42              |
| 3:J:1311:LEU:HD23 | 3:J:1311:LEU:H    | 1.83                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:L:421:ARG:HA    | 5:L:424:LYS:HG3  | 2.02                     | 0.42              |
| 1:B:101:LEU:HD22  | 1:B:102:ARG:H    | 1.85                     | 0.42              |
| 2:C:142:ARG:HA    | 2:C:331:ARG:HG2  | 2.01                     | 0.42              |
| 2:C:143:SER:H     | 2:C:331:ARG:HA   | 1.85                     | 0.42              |
| 2:C:194:VAL:O     | 2:C:198:ARG:HG3  | 2.19                     | 0.42              |
| 2:C:418:LEU:HD21  | 2:C:427:VAL:HG11 | 2.01                     | 0.42              |
| 2:C:572:ILE:HD11  | 2:C:703:ILE:HG13 | 2.00                     | 0.42              |
| 2:C:709:GLU:HA    | 2:C:823:VAL:O    | 2.19                     | 0.42              |
| 3:D:211:VAL:O     | 3:D:345:TYR:HD1  | 2.02                     | 0.42              |
| 3:D:220:ARG:O     | 3:D:281:ARG:HD3  | 2.20                     | 0.42              |
| 3:D:471:GLU:O     | 3:D:475:ARG:HG2  | 2.19                     | 0.42              |
| 3:D:909:ASN:O     | 3:D:912:LYS:HB3  | 2.20                     | 0.42              |
| 3:D:1047:LYS:CG   | 3:D:1048:PRO:HD2 | 2.49                     | 0.42              |
| 5:F:109:LEU:HD12  | 5:F:114:GLU:HA   | 2.02                     | 0.42              |
| 5:F:412:ILE:HA    | 5:F:415:ILE:HD12 | 2.00                     | 0.42              |
| 2:I:200:LEU:HD12  | 2:I:200:LEU:HA   | 1.69                     | 0.42              |
| 2:I:390:GLN:CG    | 2:I:415:PRO:HD3  | 2.49                     | 0.42              |
| 2:I:971:LYS:HA    | 2:I:988:VAL:HA   | 2.00                     | 0.42              |
| 3:J:1021:TYR:O    | 3:J:1025:GLN:HB2 | 2.19                     | 0.42              |
| 6:O:3:DT:H6       | 6:O:3:DT:H2'     | 1.65                     | 0.42              |
| 1:A:50:GLY:C      | 1:A:171:PHE:HD1  | 2.27                     | 0.42              |
| 1:B:37:GLY:HA3    | 1:B:179:PHE:CE1  | 2.54                     | 0.42              |
| 1:B:115:THR:HA    | 1:B:116:PRO:HD3  | 1.85                     | 0.42              |
| 2:C:549:PHE:HB3   | 2:C:552:HIS:CD2  | 2.53                     | 0.42              |
| 2:C:550:LEU:HD11  | 2:C:558:ALA:HB1  | 2.00                     | 0.42              |
| 2:C:1010:THR:HG23 | 2:C:1013:TYR:OH  | 2.20                     | 0.42              |
| 3:D:44:LEU:HG     | 3:D:525:ARG:NH1  | 2.35                     | 0.42              |
| 3:D:695:ILE:HG23  | 3:D:718:PRO:HB2  | 2.02                     | 0.42              |
| 4:E:30:LEU:HA     | 4:E:37:ASN:HD21  | 1.85                     | 0.42              |
| 5:F:376:LEU:HB3   | 5:F:380:GLU:HG3  | 2.01                     | 0.42              |
| 1:G:38:ASN:HB2    | 1:G:179:PHE:CZ   | 2.54                     | 0.42              |
| 1:G:58:ILE:HG22   | 1:G:60:ASP:H     | 1.84                     | 0.42              |
| 1:H:156:HIS:O     | 1:H:156:HIS:CG   | 2.72                     | 0.42              |
| 2:I:135:VAL:CG2   | 2:I:407:LYS:HG2  | 2.49                     | 0.42              |
| 2:I:399:ASN:HB2   | 2:I:400:PRO:HD2  | 2.00                     | 0.42              |
| 2:I:470:PRO:HA    | 2:I:484:VAL:O    | 2.20                     | 0.42              |
| 2:I:888:THR:HG22  | 2:I:989:VAL:O    | 2.19                     | 0.42              |
| 2:I:892:LEU:HD13  | 2:I:970:GLY:HA2  | 2.02                     | 0.42              |
| 3:J:95:LEU:HD12   | 3:J:95:LEU:HA    | 1.91                     | 0.42              |
| 5:L:142:ILE:HA    | 5:L:145:VAL:HB   | 2.02                     | 0.42              |
| 5:L:385:LYS:HA    | 5:L:390:LEU:HD12 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:156:HIS:O     | 1:B:156:HIS:CG   | 2.72                     | 0.42              |
| 2:C:22:GLN:HA     | 2:C:336:VAL:HG21 | 2.01                     | 0.42              |
| 2:C:498:GLN:H     | 2:C:501:THR:HG23 | 1.85                     | 0.42              |
| 2:C:569:VAL:O     | 2:C:995:MET:HE1  | 2.20                     | 0.42              |
| 2:C:926:PHE:CE2   | 2:C:960:GLU:HG3  | 2.55                     | 0.42              |
| 2:C:971:LYS:HA    | 2:C:988:VAL:HA   | 2.00                     | 0.42              |
| 3:D:218:LYS:NZ    | 3:D:338:GLU:HB3  | 2.35                     | 0.42              |
| 3:D:607:LEU:HB3   | 3:D:614:PHE:HE2  | 1.83                     | 0.42              |
| 3:D:637:LEU:HG    | 3:D:641:GLN:HB3  | 2.01                     | 0.42              |
| 3:D:1479:ASP:HA   | 3:D:1482:ARG:HG2 | 2.01                     | 0.42              |
| 3:D:1481:VAL:HG21 | 4:E:17:TYR:HB2   | 2.00                     | 0.42              |
| 5:F:375:LYS:HD3   | 5:F:426:HIS:CG   | 2.55                     | 0.42              |
| 2:I:607:ASP:C     | 2:I:609:THR:N    | 2.78                     | 0.42              |
| 2:I:708:TYR:OH    | 2:I:796:GLU:OE1  | 2.32                     | 0.42              |
| 2:I:858:MET:SD    | 2:I:859:PRO:HD2  | 2.60                     | 0.42              |
| 2:I:889:HIS:HA    | 2:I:892:LEU:HD12 | 2.01                     | 0.42              |
| 3:J:95:LEU:HD21   | 3:J:578:VAL:HG21 | 2.01                     | 0.42              |
| 3:J:116:LEU:HD23  | 3:J:468:LEU:HD22 | 2.00                     | 0.42              |
| 3:J:1188:VAL:HG12 | 3:J:1189:ARG:N   | 2.35                     | 0.42              |
| 5:L:302:SER:H     | 5:L:305:GLU:CG   | 2.33                     | 0.42              |
| 2:C:207:LEU:HD13  | 2:C:227:LEU:HD11 | 2.00                     | 0.42              |
| 2:C:526:PRO:O     | 2:C:529:VAL:HG12 | 2.19                     | 0.42              |
| 2:C:713:ARG:NH1   | 3:D:533:GLY:HA2  | 2.34                     | 0.42              |
| 2:C:816:LYS:HG3   | 2:C:817:PRO:CD   | 2.50                     | 0.42              |
| 2:C:1050:GLN:O    | 2:C:1054:THR:OG1 | 2.37                     | 0.42              |
| 3:D:217:ARG:HG3   | 3:D:341:GLU:OE1  | 2.20                     | 0.42              |
| 3:D:508:ARG:HB2   | 3:D:511:TRP:NE1  | 2.35                     | 0.42              |
| 3:D:646:LYS:HE3   | 3:D:688:TRP:CZ2  | 2.55                     | 0.42              |
| 3:D:1059:SER:HB3  | 3:D:1063:GLU:HB2 | 2.00                     | 0.42              |
| 3:D:1333:HIS:O    | 3:D:1336:LEU:HB3 | 2.19                     | 0.42              |
| 1:G:44:LEU:HD11   | 1:G:199:ILE:CD1  | 2.49                     | 0.42              |
| 1:G:88:ARG:HB2    | 1:G:204:SER:HA   | 2.02                     | 0.42              |
| 1:G:219:LYS:HE3   | 1:H:219:LYS:HD3  | 2.02                     | 0.42              |
| 2:I:603:VAL:O     | 2:I:646:GLY:HA2  | 2.19                     | 0.42              |
| 3:J:100:ALA:N     | 3:J:575:GLN:HE22 | 2.17                     | 0.42              |
| 3:J:666:PHE:CD1   | 3:J:676:MET:HE1  | 2.54                     | 0.42              |
| 3:J:789:LEU:O     | 3:J:792:ILE:HG13 | 2.19                     | 0.42              |
| 3:J:1011:PHE:HZ   | 3:J:1039:CYS:HG  | 1.64                     | 0.42              |
| 5:L:173:GLU:O     | 5:L:177:LYS:HB2  | 2.20                     | 0.42              |
| 5:L:334:THR:O     | 5:L:344:TYR:HB2  | 2.19                     | 0.42              |
| 1:A:104:GLU:HG3   | 1:A:137:LYS:HG2  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:54:THR:OG1    | 1:B:55:SER:N      | 2.50                     | 0.42              |
| 1:B:188:GLN:HA    | 3:D:688:TRP:CD1   | 2.54                     | 0.42              |
| 2:C:269:LEU:H     | 2:C:288:ARG:HB3   | 1.84                     | 0.42              |
| 2:C:376:ARG:HB2   | 2:C:377:PRO:HD3   | 2.01                     | 0.42              |
| 2:C:499:ALA:N     | 2:C:533:ASP:HB3   | 2.35                     | 0.42              |
| 2:C:603:VAL:O     | 2:C:646:GLY:HA2   | 2.19                     | 0.42              |
| 2:C:1056:LYS:O    | 3:D:624:ASP:N     | 2.35                     | 0.42              |
| 2:C:1102:LEU:HD12 | 2:C:1107:ASN:N    | 2.34                     | 0.42              |
| 3:D:643:GLY:HA3   | 3:D:727:GLN:HB2   | 2.02                     | 0.42              |
| 3:D:750:PRO:HG2   | 3:D:756:GLN:HE22  | 1.85                     | 0.42              |
| 3:D:895:VAL:O     | 3:D:899:LEU:HG    | 2.19                     | 0.42              |
| 3:D:1254:GLN:HG3  | 3:D:1258:ARG:HD3  | 2.01                     | 0.42              |
| 3:D:1255:GLY:O    | 3:D:1259:VAL:HG23 | 2.20                     | 0.42              |
| 4:E:88:GLU:HG2    | 4:E:91:ARG:NH2    | 2.35                     | 0.42              |
| 1:G:44:LEU:O      | 1:G:174:VAL:HG11  | 2.20                     | 0.42              |
| 1:G:89:PHE:HE1    | 1:G:120:VAL:HG12  | 1.85                     | 0.42              |
| 1:G:190:THR:OG1   | 1:G:191:ASP:N     | 2.48                     | 0.42              |
| 2:I:432:ARG:HH22  | 2:I:518:ARG:NH2   | 2.18                     | 0.42              |
| 2:I:926:PHE:O     | 2:I:930:GLN:HG2   | 2.19                     | 0.42              |
| 3:J:178:LEU:HD11  | 3:J:190:GLU:O     | 2.20                     | 0.42              |
| 5:L:206:ASN:O     | 5:L:209:LEU:HB3   | 2.20                     | 0.42              |
| 2:C:380:ALA:O     | 2:C:383:ARG:HG2   | 2.20                     | 0.42              |
| 2:C:399:ASN:HB2   | 2:C:400:PRO:HD2   | 2.01                     | 0.42              |
| 2:C:525:ALA:HB1   | 2:C:527:GLU:OE2   | 2.20                     | 0.42              |
| 2:C:679:PHE:CE2   | 2:C:853:LEU:HD21  | 2.55                     | 0.42              |
| 2:C:761:PHE:HA    | 2:C:785:VAL:HA    | 2.01                     | 0.42              |
| 3:D:205:TYR:CD1   | 3:D:393:ILE:HG12  | 2.53                     | 0.42              |
| 5:F:160:PRO:HG2   | 5:F:164:GLU:HG2   | 2.01                     | 0.42              |
| 1:G:42:ARG:HH12   | 2:I:857:ASP:CG    | 2.28                     | 0.42              |
| 1:G:50:GLY:C      | 1:G:171:PHE:HD1   | 2.27                     | 0.42              |
| 1:H:48:ILE:HG22   | 1:H:173:PRO:HD2   | 2.02                     | 0.42              |
| 2:I:549:PHE:HB3   | 2:I:886:LEU:HD12  | 2.01                     | 0.42              |
| 2:I:648:ARG:H     | 2:I:648:ARG:HG2   | 1.69                     | 0.42              |
| 2:I:720:GLU:CD    | 2:I:760:SER:HB3   | 2.44                     | 0.42              |
| 3:J:12:LEU:HD12   | 3:J:507:ASN:HB3   | 2.02                     | 0.42              |
| 3:J:790:TYR:CD1   | 3:J:907:GLU:HB3   | 2.55                     | 0.42              |
| 3:J:815:ALA:HB1   | 3:J:821:VAL:HG23  | 2.02                     | 0.42              |
| 1:A:44:LEU:HD11   | 1:A:199:ILE:CD1   | 2.49                     | 0.41              |
| 1:B:75:VAL:O      | 1:B:79:ILE:HG13   | 2.21                     | 0.41              |
| 2:C:170:PRO:HD2   | 2:C:267:TYR:HD1   | 1.85                     | 0.41              |
| 2:C:339:LEU:O     | 2:C:342:ASP:HB2   | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:15:PRO:HG3    | 3:D:514:LEU:HD12  | 2.02                     | 0.41              |
| 3:D:646:LYS:HE3   | 3:D:688:TRP:HZ2   | 1.84                     | 0.41              |
| 3:D:1215:VAL:HG21 | 3:D:1221:VAL:CG1  | 2.50                     | 0.41              |
| 3:D:1216:SER:HB2  | 4:E:16:LYS:H      | 1.85                     | 0.41              |
| 5:F:343:PHE:HD2   | 5:F:343:PHE:HA    | 1.75                     | 0.41              |
| 2:I:98:LEU:HD22   | 2:I:113:VAL:HG22  | 2.02                     | 0.41              |
| 2:I:950:LEU:HD11  | 2:I:952:LEU:HD13  | 2.02                     | 0.41              |
| 3:J:521:PRO:HA    | 3:J:522:PRO:HD3   | 1.95                     | 0.41              |
| 3:J:643:GLY:HA3   | 3:J:727:GLN:HB2   | 2.02                     | 0.41              |
| 3:J:643:GLY:O     | 3:J:726:ILE:HG23  | 2.20                     | 0.41              |
| 3:J:771:SER:HA    | 3:J:772:PRO:HD3   | 1.93                     | 0.41              |
| 3:J:1047:LYS:CG   | 3:J:1048:PRO:HD2  | 2.50                     | 0.41              |
| 3:J:1206:GLY:HA2  | 3:J:1215:VAL:HG12 | 2.02                     | 0.41              |
| 3:J:1274:ILE:HD12 | 3:J:1322:GLY:HA2  | 2.02                     | 0.41              |
| 4:K:10:PHE:CE1    | 4:K:16:LYS:HG2    | 2.55                     | 0.41              |
| 2:C:72:ARG:O      | 2:C:94:LEU:HD12   | 2.20                     | 0.41              |
| 2:C:191:PHE:HA    | 2:C:192:PRO:HD3   | 1.89                     | 0.41              |
| 2:C:399:ASN:O     | 2:C:402:SER:HB2   | 2.20                     | 0.41              |
| 2:C:535:SER:O     | 2:C:538:GLN:HG2   | 2.20                     | 0.41              |
| 3:D:216:LEU:HB3   | 3:D:218:LYS:HE2   | 2.01                     | 0.41              |
| 3:D:638:LYS:HB3   | 3:D:641:GLN:NE2   | 2.35                     | 0.41              |
| 3:D:666:PHE:CE1   | 3:D:687:VAL:HG12  | 2.55                     | 0.41              |
| 3:D:698:LYS:HG3   | 4:E:59:ASN:OD1    | 2.20                     | 0.41              |
| 3:D:1307:LYS:HE3  | 3:D:1307:LYS:HB3  | 1.76                     | 0.41              |
| 3:D:1475:GLY:HA2  | 4:E:17:TYR:CZ     | 2.55                     | 0.41              |
| 5:F:181:LEU:HB3   | 5:F:185:LEU:HB2   | 2.03                     | 0.41              |
| 1:G:181:VAL:C     | 1:G:182:GLU:HG3   | 2.45                     | 0.41              |
| 1:G:227:ASN:HA    | 1:G:228:PRO:HD2   | 1.75                     | 0.41              |
| 2:I:5:ARG:HE      | 2:I:5:ARG:HB2     | 1.72                     | 0.41              |
| 2:I:35:PRO:C      | 2:I:37:GLU:H      | 2.27                     | 0.41              |
| 2:I:291:VAL:HG13  | 2:I:303:PHE:CE1   | 2.56                     | 0.41              |
| 2:I:838:LYS:HG2   | 2:I:997:LEU:HD12  | 2.02                     | 0.41              |
| 2:I:1064:ASN:ND2  | 5:L:359:ALA:HB2   | 2.27                     | 0.41              |
| 3:J:1207:TYR:H    | 3:J:1214:PRO:HA   | 1.84                     | 0.41              |
| 3:J:1465:ASN:OD1  | 3:J:1470:ARG:HB3  | 2.20                     | 0.41              |
| 5:L:315:ASP:O     | 5:L:319:VAL:HG12  | 2.20                     | 0.41              |
| 1:A:53:VAL:CG2    | 1:A:54:THR:H      | 2.27                     | 0.41              |
| 1:A:99:LEU:HD13   | 1:A:144:VAL:HG23  | 2.02                     | 0.41              |
| 2:C:530:GLU:H     | 2:C:530:GLU:HG2   | 1.60                     | 0.41              |
| 3:D:58:CYS:HB2    | 3:D:78:VAL:HB     | 2.01                     | 0.41              |
| 3:D:502:PHE:CE1   | 3:D:509:PRO:HB3   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:869:LEU:HD21  | 3:D:893:GLU:HG3   | 2.02                     | 0.41              |
| 5:F:146:VAL:HG12  | 5:F:150:ILE:HG13  | 2.02                     | 0.41              |
| 5:F:398:LEU:HD12  | 5:F:412:ILE:HB    | 2.02                     | 0.41              |
| 1:H:80:LEU:HD23   | 3:J:867:ARG:HB2   | 2.02                     | 0.41              |
| 2:I:344:PHE:HA    | 2:I:382:LEU:HD11  | 2.01                     | 0.41              |
| 2:I:537:LYS:NZ    | 2:I:905:VAL:HG22  | 2.35                     | 0.41              |
| 2:I:1034:GLU:H    | 2:I:1034:GLU:HG3  | 1.69                     | 0.41              |
| 2:I:1085:PHE:CE2  | 3:J:1468:LEU:HD22 | 2.56                     | 0.41              |
| 2:I:1095:LEU:HD11 | 3:J:603:LEU:HB3   | 2.02                     | 0.41              |
| 3:J:203:ALA:HA    | 3:J:395:VAL:HA    | 2.02                     | 0.41              |
| 3:J:569:ASN:HD22  | 5:L:229:GLN:HE21  | 1.66                     | 0.41              |
| 3:J:1105:ILE:HG23 | 3:J:1199:GLY:HA2  | 2.02                     | 0.41              |
| 3:J:1236:LEU:HD22 | 3:J:1355:VAL:HG12 | 2.02                     | 0.41              |
| 1:B:49:PRO:HD2    | 1:B:213:GLN:HE22  | 1.86                     | 0.41              |
| 1:B:176:ARG:NH1   | 3:D:884:ARG:HH12  | 2.18                     | 0.41              |
| 2:C:35:PRO:C      | 2:C:37:GLU:H      | 2.27                     | 0.41              |
| 2:C:1044:GLY:HA3  | 4:E:17:TYR:HE1    | 1.84                     | 0.41              |
| 3:D:789:LEU:O     | 3:D:792:ILE:HG13  | 2.21                     | 0.41              |
| 3:D:801:GLY:C     | 3:D:803:GLY:H     | 2.28                     | 0.41              |
| 3:D:1147:ARG:HB3  | 3:D:1188:VAL:CG1  | 2.51                     | 0.41              |
| 4:E:52:GLU:H      | 4:E:52:GLU:HG3    | 1.59                     | 0.41              |
| 5:F:367:GLU:O     | 5:F:370:GLU:N     | 2.51                     | 0.41              |
| 2:I:89:THR:HB     | 2:I:91:GLN:NE2    | 2.35                     | 0.41              |
| 2:I:198:ARG:HE    | 2:I:198:ARG:HB2   | 1.50                     | 0.41              |
| 2:I:532:MET:HE2   | 2:I:532:MET:HB3   | 1.88                     | 0.41              |
| 2:I:673:LEU:HA    | 2:I:990:GLY:O     | 2.20                     | 0.41              |
| 2:I:839:LEU:HA    | 2:I:995:MET:O     | 2.20                     | 0.41              |
| 3:J:1386:ASP:HB2  | 3:J:1412:LYS:HB3  | 2.02                     | 0.41              |
| 5:L:94:ASP:O      | 5:L:98:GLN:HB2    | 2.21                     | 0.41              |
| 1:A:38:ASN:HB2    | 1:A:179:PHE:CZ    | 2.56                     | 0.41              |
| 2:C:429:ASP:OD1   | 2:C:430:VAL:N     | 2.43                     | 0.41              |
| 2:C:520:GLU:HA    | 2:C:521:PRO:HD3   | 1.92                     | 0.41              |
| 2:C:1095:LEU:HD11 | 3:D:603:LEU:HB3   | 2.02                     | 0.41              |
| 3:D:231:VAL:N     | 3:D:243:ALA:HA    | 2.23                     | 0.41              |
| 3:D:317:MET:HE2   | 3:D:337:LEU:HD13  | 2.03                     | 0.41              |
| 3:D:371:ILE:HG23  | 3:D:372:ASP:N     | 2.32                     | 0.41              |
| 3:D:886:VAL:O     | 3:D:890:VAL:HG23  | 2.20                     | 0.41              |
| 3:D:1263:PHE:CE2  | 3:D:1371:VAL:HG11 | 2.55                     | 0.41              |
| 3:D:1442:ASN:O    | 3:D:1446:VAL:HG23 | 2.20                     | 0.41              |
| 3:D:1460:ILE:HG13 | 3:D:1461:GLY:H    | 1.85                     | 0.41              |
| 1:H:51:THR:HG21   | 1:H:86:VAL:HG23   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:530:GLU:H     | 2:I:530:GLU:HG2   | 1.59                     | 0.41              |
| 2:I:676:ILE:HA    | 2:I:871:LEU:O     | 2.20                     | 0.41              |
| 3:J:187:LYS:HG2   | 3:J:198:ARG:C     | 2.45                     | 0.41              |
| 3:J:352:ASN:C     | 3:J:368:VAL:HG13  | 2.46                     | 0.41              |
| 3:J:401:TYR:HE1   | 3:J:446:VAL:HB    | 1.85                     | 0.41              |
| 3:J:525:ARG:HB2   | 3:J:541:ASN:OD1   | 2.20                     | 0.41              |
| 3:J:637:LEU:C     | 3:J:935:LYS:HZ1   | 2.26                     | 0.41              |
| 5:L:276:PRO:HB2   | 5:L:279:MET:HG2   | 2.03                     | 0.41              |
| 1:A:74:ASP:O      | 1:A:77:GLU:HB3    | 2.20                     | 0.41              |
| 1:B:201:THR:HG21  | 1:B:205:VAL:HG23  | 2.03                     | 0.41              |
| 2:C:215:GLY:O     | 2:C:217:LEU:N     | 2.54                     | 0.41              |
| 2:C:307:LEU:HD12  | 2:C:310:LEU:HD23  | 2.03                     | 0.41              |
| 2:C:508:ILE:HG21  | 2:C:526:PRO:HB3   | 2.02                     | 0.41              |
| 2:C:1070:ILE:H    | 2:C:1070:ILE:HG13 | 1.55                     | 0.41              |
| 2:C:1090:LYS:HE3  | 3:D:88:TYR:O      | 2.19                     | 0.41              |
| 3:D:775:GLY:HA2   | 3:D:1209:LEU:HB3  | 2.03                     | 0.41              |
| 3:D:1014:ASN:C    | 3:D:1016:PRO:HD3  | 2.45                     | 0.41              |
| 3:D:1310:ARG:HH21 | 3:D:1327:ARG:NH1  | 2.18                     | 0.41              |
| 1:G:48:ILE:HD13   | 1:G:48:ILE:HA     | 1.90                     | 0.41              |
| 1:G:63:HIS:HD2    | 1:G:66:SER:HB2    | 1.86                     | 0.41              |
| 1:G:149:GLY:O     | 1:G:171:PHE:HB2   | 2.21                     | 0.41              |
| 2:I:64:LEU:HD21   | 2:I:66:LEU:CB     | 2.50                     | 0.41              |
| 2:I:418:LEU:HD21  | 2:I:427:VAL:HG11  | 2.01                     | 0.41              |
| 2:I:718:GLY:HA2   | 2:I:719:PRO:HD3   | 1.78                     | 0.41              |
| 3:J:786:ILE:CD1   | 3:J:908:LYS:HG2   | 2.48                     | 0.41              |
| 3:J:1031:ASN:O    | 3:J:1034:GLN:HB3  | 2.20                     | 0.41              |
| 3:J:1127:GLU:C    | 3:J:1129:THR:H    | 2.29                     | 0.41              |
| 3:J:1382:THR:O    | 3:J:1416:ALA:HB3  | 2.20                     | 0.41              |
| 4:K:52:GLU:H      | 4:K:52:GLU:HG3    | 1.60                     | 0.41              |
| 5:L:421:ARG:O     | 5:L:424:LYS:HB2   | 2.21                     | 0.41              |
| 1:A:65:PHE:CE1    | 2:C:703:ILE:HD13  | 2.55                     | 0.41              |
| 1:B:32:PHE:O      | 1:B:36:LEU:HG     | 2.20                     | 0.41              |
| 2:C:98:LEU:HD22   | 2:C:113:VAL:HG22  | 2.01                     | 0.41              |
| 2:C:557:ARG:CG    | 2:C:879:ARG:HB3   | 2.40                     | 0.41              |
| 3:D:184:GLU:H     | 3:D:184:GLU:HG2   | 1.66                     | 0.41              |
| 3:D:354:ILE:HG13  | 3:D:369:ALA:H     | 1.85                     | 0.41              |
| 3:D:691:LEU:O     | 3:D:695:ILE:HG13  | 2.20                     | 0.41              |
| 3:D:750:PRO:HB2   | 3:D:756:GLN:HA    | 2.03                     | 0.41              |
| 3:D:1117:TYR:HA   | 3:D:1193:THR:HG21 | 2.02                     | 0.41              |
| 5:F:210:VAL:HG21  | 5:F:235:LEU:HD22  | 2.03                     | 0.41              |
| 2:I:167:LYS:HE3   | 2:I:167:LYS:HB3   | 1.93                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:237:ARG:HH22 | 2:I:241:LEU:HD21 | 1.86                     | 0.41              |
| 2:I:291:VAL:HB   | 2:I:299:LYS:O    | 2.20                     | 0.41              |
| 2:I:574:ALA:HA   | 2:I:670:GLN:CG   | 2.51                     | 0.41              |
| 2:I:744:ARG:NH1  | 2:I:746:GLY:O    | 2.54                     | 0.41              |
| 2:I:952:LEU:HD21 | 2:I:971:LYS:NZ   | 2.34                     | 0.41              |
| 3:J:67:ARG:HD2   | 5:L:394:ARG:CB   | 2.48                     | 0.41              |
| 3:J:650:LEU:HD21 | 3:J:688:TRP:HZ3  | 1.85                     | 0.41              |
| 3:J:669:ASN:HD22 | 5:L:364:LEU:HD11 | 1.86                     | 0.41              |
| 3:J:970:LYS:O    | 3:J:973:GLN:HB3  | 2.21                     | 0.41              |
| 3:J:1125:MET:HA  | 3:J:1132:LEU:HA  | 2.03                     | 0.41              |
| 3:J:1464:GLU:CD  | 3:J:1464:GLU:H   | 2.18                     | 0.41              |
| 3:J:1465:ASN:HA  | 3:J:1468:LEU:HB2 | 2.02                     | 0.41              |
| 5:L:232:ASN:O    | 5:L:236:ILE:HG13 | 2.20                     | 0.41              |
| 7:P:14:DC:H2"    | 7:P:15:DA:OP2    | 2.21                     | 0.41              |
| 1:A:149:GLY:O    | 1:A:171:PHE:HB2  | 2.21                     | 0.41              |
| 2:C:97:ARG:NH2   | 2:C:112:GLU:HB2  | 2.36                     | 0.41              |
| 2:C:607:ASP:C    | 2:C:609:THR:N    | 2.76                     | 0.41              |
| 2:C:696:LYS:NZ   | 2:C:855:VAL:HG11 | 2.36                     | 0.41              |
| 2:C:889:HIS:HA   | 2:C:892:LEU:HD12 | 2.02                     | 0.41              |
| 3:D:121:THR:O    | 3:D:124:GLU:HB3  | 2.20                     | 0.41              |
| 3:D:213:VAL:HG13 | 3:D:384:VAL:O    | 2.21                     | 0.41              |
| 3:D:760:ARG:HH21 | 4:E:65:MET:HG3   | 1.86                     | 0.41              |
| 5:F:207:LEU:HD23 | 5:F:207:LEU:HA   | 1.87                     | 0.41              |
| 1:G:99:LEU:HD13  | 1:G:144:VAL:HG23 | 2.02                     | 0.41              |
| 1:H:55:SER:HB2   | 1:H:158:ILE:HG23 | 2.03                     | 0.41              |
| 2:I:525:ALA:HA   | 2:I:526:PRO:HD3  | 1.91                     | 0.41              |
| 2:I:585:GLU:O    | 2:I:588:VAL:HG22 | 2.20                     | 0.41              |
| 2:I:677:MET:HE3  | 2:I:677:MET:HB2  | 1.91                     | 0.41              |
| 3:J:589:SER:HA   | 3:J:590:PRO:HD3  | 1.95                     | 0.41              |
| 3:J:638:LYS:HG3  | 3:J:640:HIS:H    | 1.86                     | 0.41              |
| 3:J:664:LYS:HE2  | 3:J:666:PHE:HE2  | 1.86                     | 0.41              |
| 3:J:858:LEU:HD12 | 3:J:859:ASP:H    | 1.86                     | 0.41              |
| 3:J:1366:LYS:O   | 3:J:1369:GLU:HB2 | 2.21                     | 0.41              |
| 3:J:1396:GLU:HB3 | 3:J:1399:ASP:OD1 | 2.21                     | 0.41              |
| 5:L:381:ALA:O    | 5:L:385:LYS:HG3  | 2.21                     | 0.41              |
| 7:S:14:DC:H2"    | 7:S:15:DA:OP2    | 2.20                     | 0.41              |
| 1:A:14:THR:O     | 1:A:14:THR:HG22  | 2.21                     | 0.41              |
| 2:C:45:GLN:HE21  | 2:C:48:PHE:HD2   | 1.69                     | 0.41              |
| 2:C:229:MET:CB   | 2:C:234:ALA:HB2  | 2.46                     | 0.41              |
| 2:C:328:LEU:HD23 | 2:C:437:ARG:HD2  | 2.03                     | 0.41              |
| 2:C:474:VAL:HG23 | 2:C:478:VAL:O    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:525:ALA:HA    | 2:C:526:PRO:HD3   | 1.92                     | 0.41              |
| 2:C:537:LYS:NZ    | 2:C:905:VAL:HG22  | 2.36                     | 0.41              |
| 2:C:648:ARG:H     | 2:C:648:ARG:HG2   | 1.67                     | 0.41              |
| 2:C:670:GLN:HE22  | 2:C:699:PHE:HA    | 1.85                     | 0.41              |
| 2:C:857:ASP:OD1   | 2:C:857:ASP:N     | 2.54                     | 0.41              |
| 2:C:1086:ARG:HB3  | 3:D:88:TYR:HE2    | 1.85                     | 0.41              |
| 2:C:1089:VAL:HG13 | 2:C:1099:VAL:HG11 | 2.03                     | 0.41              |
| 3:D:229:ALA:HB1   | 3:D:245:LEU:N     | 2.36                     | 0.41              |
| 3:D:1038:LEU:O    | 3:D:1060:SER:OG   | 2.23                     | 0.41              |
| 3:D:1271:LYS:HG3  | 3:D:1331:ASP:HB2  | 2.03                     | 0.41              |
| 4:E:10:PHE:CE1    | 4:E:16:LYS:HG2    | 2.56                     | 0.41              |
| 5:F:206:ASN:O     | 5:F:210:VAL:HG23  | 2.20                     | 0.41              |
| 5:F:334:THR:O     | 5:F:344:TYR:HB2   | 2.21                     | 0.41              |
| 1:G:14:THR:O      | 1:G:14:THR:HG22   | 2.21                     | 0.41              |
| 1:G:52:ALA:O      | 1:G:53:VAL:HG12   | 2.21                     | 0.41              |
| 1:H:13:ALA:CB     | 1:H:23:PHE:HD1    | 2.34                     | 0.41              |
| 2:I:55:GLU:HA     | 2:I:64:LEU:O      | 2.20                     | 0.41              |
| 2:I:93:PRO:HG3    | 2:I:117:HIS:NE2   | 2.36                     | 0.41              |
| 2:I:97:ARG:NH2    | 2:I:112:GLU:HB2   | 2.36                     | 0.41              |
| 2:I:215:GLY:O     | 2:I:217:LEU:N     | 2.54                     | 0.41              |
| 2:I:683:ASN:OD1   | 2:I:872:ASN:HB2   | 2.21                     | 0.41              |
| 2:I:872:ASN:ND2   | 3:J:784:ASP:OD2   | 2.54                     | 0.41              |
| 2:I:944:LEU:HD13  | 2:I:959:PRO:HB3   | 2.02                     | 0.41              |
| 2:I:1052:MET:HE1  | 2:I:1056:LYS:HE3  | 2.02                     | 0.41              |
| 2:I:1102:LEU:HD12 | 2:I:1107:ASN:N    | 2.35                     | 0.41              |
| 3:J:137:PRO:HG3   | 3:J:148:GLU:HA    | 2.02                     | 0.41              |
| 3:J:182:GLY:H     | 3:J:204:LEU:HD23  | 1.86                     | 0.41              |
| 3:J:542:ASP:O     | 3:J:545:ARG:HB3   | 2.20                     | 0.41              |
| 3:J:654:LYS:HB3   | 3:J:655:PRO:HD3   | 2.03                     | 0.41              |
| 3:J:657:LEU:HD22  | 3:J:691:LEU:HD13  | 2.03                     | 0.41              |
| 3:J:895:VAL:O     | 3:J:899:LEU:HG    | 2.20                     | 0.41              |
| 3:J:1084:THR:O    | 3:J:1088:THR:HG23 | 2.21                     | 0.41              |
| 3:J:1372:VAL:HA   | 3:J:1375:MET:SD   | 2.61                     | 0.41              |
| 3:J:1429:LEU:HG   | 3:J:1440:PHE:HD1  | 1.85                     | 0.41              |
| 5:L:160:PRO:HG2   | 5:L:164:GLU:HG2   | 2.03                     | 0.41              |
| 5:L:181:LEU:HB3   | 5:L:185:LEU:HB2   | 2.03                     | 0.41              |
| 5:L:375:LYS:HD3   | 5:L:426:HIS:CG    | 2.56                     | 0.41              |
| 6:O:24:DC:H1'     | 6:O:25:DT:H5'     | 2.01                     | 0.41              |
| 7:P:16:DC:H2''    | 7:P:17:DT:OP2     | 2.21                     | 0.41              |
| 1:A:33:GLY:O      | 1:A:195:LEU:HD21  | 2.21                     | 0.41              |
| 1:A:43:ILE:HG13   | 1:B:35:THR:HG21   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:46:SER:OG     | 1:A:47:SER:N      | 2.54                     | 0.41              |
| 2:C:291:VAL:HB    | 2:C:299:LYS:O     | 2.21                     | 0.41              |
| 2:C:472:ARG:HB3   | 2:C:532:MET:HE2   | 2.01                     | 0.41              |
| 2:C:536:PRO:HB3   | 3:D:1067:VAL:HG11 | 2.02                     | 0.41              |
| 2:C:603:VAL:HA    | 2:C:613:VAL:HG12  | 2.03                     | 0.41              |
| 2:C:941:LYS:NZ    | 2:C:959:PRO:HG2   | 2.35                     | 0.41              |
| 2:C:988:VAL:H     | 3:D:948:THR:HG21  | 1.85                     | 0.41              |
| 3:D:900:ILE:HG12  | 3:D:914:LEU:CD2   | 2.51                     | 0.41              |
| 5:F:154:ALA:HB1   | 5:F:158:LYS:HE2   | 2.02                     | 0.41              |
| 1:G:158:ILE:HG22  | 1:G:159:LYS:N     | 2.36                     | 0.41              |
| 2:I:639:GLN:HA    | 2:I:657:ASP:O     | 2.21                     | 0.41              |
| 2:I:1085:PHE:O    | 2:I:1089:VAL:HG23 | 2.21                     | 0.41              |
| 3:J:691:LEU:O     | 3:J:695:ILE:HG13  | 2.20                     | 0.41              |
| 3:J:886:VAL:O     | 3:J:890:VAL:HG23  | 2.21                     | 0.41              |
| 3:J:1460:ILE:HG13 | 3:J:1461:GLY:N    | 2.36                     | 0.41              |
| 6:O:6:DC:H2"      | 6:O:7:DA:OP2      | 2.21                     | 0.41              |
| 1:A:97:THR:HG23   | 1:A:98:THR:N      | 2.27                     | 0.40              |
| 1:A:107:LYS:HE2   | 1:A:113:ASP:OD2   | 2.21                     | 0.40              |
| 1:B:90:LEU:HB2    | 1:B:119:ASP:HB3   | 2.03                     | 0.40              |
| 2:C:215:GLY:C     | 2:C:217:LEU:H     | 2.29                     | 0.40              |
| 2:C:223:ASP:OD1   | 2:C:226:VAL:HG23  | 2.21                     | 0.40              |
| 2:C:317:VAL:HA    | 2:C:318:PRO:HD3   | 1.97                     | 0.40              |
| 2:C:512:ARG:H     | 2:C:512:ARG:HG2   | 1.54                     | 0.40              |
| 2:C:529:VAL:HG13  | 2:C:529:VAL:O     | 2.21                     | 0.40              |
| 2:C:585:GLU:O     | 2:C:588:VAL:HG22  | 2.22                     | 0.40              |
| 2:C:865:THR:HA    | 2:C:866:PRO:HD2   | 1.94                     | 0.40              |
| 2:C:1063:ARG:HH21 | 5:F:353:LEU:HD23  | 1.86                     | 0.40              |
| 3:D:666:PHE:CD1   | 3:D:676:MET:HE1   | 2.57                     | 0.40              |
| 3:D:698:LYS:H     | 4:E:59:ASN:ND2    | 2.19                     | 0.40              |
| 3:D:786:ILE:CD1   | 3:D:908:LYS:HG2   | 2.49                     | 0.40              |
| 3:D:1290:LEU:HB2  | 3:D:1307:LYS:HA   | 2.03                     | 0.40              |
| 5:F:99:TYR:HE2    | 5:F:211:VAL:HG22  | 1.86                     | 0.40              |
| 1:H:159:LYS:HG3   | 1:H:164:ALA:HB3   | 2.03                     | 0.40              |
| 1:H:188:GLN:HA    | 3:J:688:TRP:CD1   | 2.52                     | 0.40              |
| 2:I:6:PHE:HE1     | 2:I:901:TYR:HB3   | 1.86                     | 0.40              |
| 2:I:124:ASP:HB2   | 2:I:407:LYS:NZ    | 2.36                     | 0.40              |
| 2:I:352:ALA:O     | 2:I:356:ARG:HG3   | 2.20                     | 0.40              |
| 2:I:670:GLN:HE22  | 2:I:699:PHE:HA    | 1.86                     | 0.40              |
| 2:I:1010:THR:HG23 | 2:I:1013:TYR:OH   | 2.21                     | 0.40              |
| 3:J:547:LEU:HD13  | 3:J:578:VAL:HG22  | 2.03                     | 0.40              |
| 3:J:698:LYS:HG2   | 3:J:756:GLN:HG2   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:974:ILE:HG12  | 3:J:991:GLN:HG2   | 2.03                     | 0.40              |
| 3:J:1331:ASP:HA   | 3:J:1332:PRO:HD3  | 1.83                     | 0.40              |
| 5:L:206:ASN:O     | 5:L:210:VAL:HG23  | 2.22                     | 0.40              |
| 7:P:7:DA:H1'      | 7:P:8:DA:H5'      | 2.02                     | 0.40              |
| 7:S:19:DT:H1'     | 7:S:20:DT:H5'     | 2.02                     | 0.40              |
| 1:A:40:LEU:HG     | 1:A:218:LEU:HD22  | 2.03                     | 0.40              |
| 1:B:17:GLY:HA3    | 1:B:19:HIS:CE1    | 2.56                     | 0.40              |
| 1:B:79:ILE:HA     | 1:B:82:LEU:HD12   | 2.03                     | 0.40              |
| 2:C:56:GLU:OE1    | 2:C:359:MET:HE2   | 2.20                     | 0.40              |
| 2:C:247:PRO:HA    | 2:C:248:PRO:HD3   | 1.84                     | 0.40              |
| 2:C:561:GLY:O     | 2:C:565:GLN:HG2   | 2.21                     | 0.40              |
| 2:C:577:PRO:HD3   | 2:C:993:PHE:CZ    | 2.56                     | 0.40              |
| 2:C:1103:ASP:OD1  | 2:C:1107:ASN:HB2  | 2.21                     | 0.40              |
| 3:D:178:LEU:HD11  | 3:D:190:GLU:O     | 2.21                     | 0.40              |
| 3:D:285:PRO:HD2   | 3:D:288:MET:SD    | 2.61                     | 0.40              |
| 3:D:636:GLN:H     | 3:D:636:GLN:CD    | 2.29                     | 0.40              |
| 3:D:684:LYS:HB3   | 3:D:686:GLU:HG3   | 2.04                     | 0.40              |
| 3:D:1273:VAL:HG23 | 3:D:1325:LEU:HB2  | 2.03                     | 0.40              |
| 2:I:246:ASP:HA    | 2:I:247:PRO:HD3   | 1.94                     | 0.40              |
| 2:I:360:VAL:HG21  | 5:L:216:LYS:NZ    | 2.37                     | 0.40              |
| 2:I:399:ASN:O     | 2:I:402:SER:HB2   | 2.21                     | 0.40              |
| 2:I:498:GLN:H     | 2:I:501:THR:HG23  | 1.87                     | 0.40              |
| 2:I:1070:ILE:H    | 2:I:1070:ILE:HG13 | 1.58                     | 0.40              |
| 3:J:1268:PRO:HB3  | 3:J:1329:ALA:HB3  | 2.04                     | 0.40              |
| 1:B:182:GLU:CG    | 1:B:194:LYS:HB3   | 2.52                     | 0.40              |
| 3:D:131:LYS:HE2   | 3:D:152:LEU:HB3   | 2.04                     | 0.40              |
| 3:D:229:ALA:O     | 3:D:244:GLU:HB2   | 2.21                     | 0.40              |
| 3:D:256:SER:HB3   | 3:D:300:VAL:HG23  | 2.03                     | 0.40              |
| 3:D:545:ARG:NH1   | 5:F:269:GLN:O     | 2.54                     | 0.40              |
| 3:D:551:ASN:O     | 3:D:555:LYS:HG3   | 2.22                     | 0.40              |
| 3:D:640:HIS:O     | 3:D:717:GLN:HB2   | 2.21                     | 0.40              |
| 3:D:1107:VAL:HA   | 3:D:1200:VAL:O    | 2.21                     | 0.40              |
| 5:F:418:LYS:O     | 5:F:422:LYS:HB2   | 2.21                     | 0.40              |
| 1:G:34:VAL:HG22   | 1:G:181:VAL:HG21  | 2.03                     | 0.40              |
| 1:H:23:PHE:CE2    | 1:H:199:ILE:HB    | 2.55                     | 0.40              |
| 2:I:65:VAL:CG1    | 2:I:101:ILE:HB    | 2.50                     | 0.40              |
| 2:I:607:ASP:HB3   | 2:I:610:ARG:O     | 2.21                     | 0.40              |
| 2:I:1035:MET:HE2  | 2:I:1035:MET:H    | 1.86                     | 0.40              |
| 3:J:348:ALA:HB3   | 3:J:351:MET:HG3   | 2.03                     | 0.40              |
| 3:J:666:PHE:HD1   | 3:J:676:MET:HE1   | 1.86                     | 0.40              |
| 3:J:669:ASN:ND2   | 5:L:364:LEU:HD11  | 2.36                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:692:GLU:HA   | 3:J:695:ILE:HD12  | 2.04                     | 0.40              |
| 3:J:704:ARG:HB3  | 3:J:736:PHE:CD2   | 2.57                     | 0.40              |
| 3:J:869:LEU:HD21 | 3:J:893:GLU:HG3   | 2.03                     | 0.40              |
| 3:J:1207:TYR:HA  | 3:J:1213:ARG:O    | 2.21                     | 0.40              |
| 3:J:1396:GLU:OE2 | 3:J:1432:LYS:HD3  | 2.21                     | 0.40              |
| 2:C:158:TYR:HD1  | 2:C:314:THR:HA    | 1.86                     | 0.40              |
| 2:C:464:LEU:HD23 | 2:C:464:LEU:HA    | 1.95                     | 0.40              |
| 3:D:654:LYS:HB3  | 3:D:655:PRO:HD3   | 2.03                     | 0.40              |
| 3:D:1125:MET:N   | 3:D:1132:LEU:HD23 | 2.36                     | 0.40              |
| 4:E:65:MET:HE2   | 4:E:65:MET:HA     | 2.04                     | 0.40              |
| 1:G:9:PRO:HB2    | 1:G:25:LEU:HD11   | 2.03                     | 0.40              |
| 1:G:33:GLY:O     | 1:G:195:LEU:HD21  | 2.21                     | 0.40              |
| 1:G:79:ILE:HD13  | 1:G:167:VAL:HG12  | 2.02                     | 0.40              |
| 1:G:173:PRO:HB3  | 1:G:202:ASP:OD1   | 2.21                     | 0.40              |
| 1:G:195:LEU:HD23 | 1:G:195:LEU:HA    | 1.88                     | 0.40              |
| 1:H:192:LEU:HD23 | 1:H:192:LEU:N     | 2.36                     | 0.40              |
| 2:I:17:PRO:O     | 2:I:19:THR:N      | 2.55                     | 0.40              |
| 2:I:199:VAL:HA   | 2:I:231:PRO:HB3   | 2.02                     | 0.40              |
| 2:I:299:LYS:HG3  | 2:I:300:ASP:N     | 2.36                     | 0.40              |
| 2:I:341:ALA:O    | 2:I:345:ARG:HG2   | 2.21                     | 0.40              |
| 2:I:609:THR:O    | 2:I:625:LEU:N     | 2.54                     | 0.40              |
| 2:I:725:ASP:O    | 2:I:759:THR:HG21  | 2.21                     | 0.40              |
| 3:J:65:ARG:HA    | 3:J:65:ARG:HD3    | 1.93                     | 0.40              |
| 3:J:464:LEU:HA   | 3:J:467:GLU:CD    | 2.46                     | 0.40              |
| 3:J:701:LEU:HD21 | 3:J:763:MET:CG    | 2.48                     | 0.40              |
| 3:J:853:VAL:HA   | 3:J:858:LEU:HB3   | 2.04                     | 0.40              |
| 3:J:1153:VAL:HB  | 3:J:1160:LEU:HB3  | 2.04                     | 0.40              |
| 5:L:130:LYS:HG2  | 5:L:188:TYR:CZ    | 2.56                     | 0.40              |
| 7:P:15:DA:OP2    | 7:P:15:DA:H2'     | 2.22                     | 0.40              |
| 1:A:35:THR:HG22  | 1:B:39:PRO:HA     | 2.02                     | 0.40              |
| 1:B:192:LEU:HD23 | 1:B:192:LEU:N     | 2.36                     | 0.40              |
| 2:C:184:MET:HE1  | 2:C:196:LEU:HD21  | 2.03                     | 0.40              |
| 2:C:327:HIS:O    | 2:C:331:ARG:HG3   | 2.22                     | 0.40              |
| 2:C:627:ARG:HD3  | 2:C:639:GLN:O     | 2.21                     | 0.40              |
| 2:C:878:SER:O    | 3:D:1034:GLN:NE2  | 2.51                     | 0.40              |
| 3:D:364:GLY:HA2  | 3:D:379:ALA:O     | 2.21                     | 0.40              |
| 3:D:553:ARG:HB3  | 3:D:570:GLU:OE1   | 2.20                     | 0.40              |
| 3:D:598:ARG:HA   | 3:D:599:PRO:HD3   | 1.77                     | 0.40              |
| 3:D:711:LEU:HD13 | 3:D:711:LEU:HA    | 1.95                     | 0.40              |
| 3:D:1023:MET:HE2 | 3:D:1023:MET:HB2  | 1.87                     | 0.40              |
| 3:D:1267:ARG:HA  | 3:D:1268:PRO:HD3  | 1.93                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:107:LYS:HE2   | 1:G:113:ASP:OD2   | 2.22                     | 0.40              |
| 1:H:75:VAL:O      | 1:H:79:ILE:HG13   | 2.21                     | 0.40              |
| 1:H:129:ILE:HG22  | 1:H:130:ALA:N     | 2.37                     | 0.40              |
| 2:I:554:ASP:OD2   | 2:I:556:ASN:HB2   | 2.22                     | 0.40              |
| 2:I:585:GLU:HG2   | 2:I:665:PHE:CD1   | 2.56                     | 0.40              |
| 3:J:1041:MET:HE3  | 3:J:1041:MET:HB2  | 1.93                     | 0.40              |
| 3:J:1134:LEU:HD22 | 3:J:1135:ARG:N    | 2.37                     | 0.40              |
| 3:J:1404:ASN:O    | 3:J:1408:ILE:HG12 | 2.21                     | 0.40              |
| 5:L:145:VAL:HG21  | 5:L:174:VAL:CG1   | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 225/314 (72%)   | 200 (89%)  | 23 (10%)  | 2 (1%)   | 14          | 49  |
| 1   | B     | 225/314 (72%)   | 200 (89%)  | 20 (9%)   | 5 (2%)   | 5           | 29  |
| 1   | G     | 225/314 (72%)   | 200 (89%)  | 23 (10%)  | 2 (1%)   | 14          | 49  |
| 1   | H     | 225/314 (72%)   | 201 (89%)  | 18 (8%)   | 6 (3%)   | 4           | 25  |
| 2   | C     | 1108/1119 (99%) | 958 (86%)  | 139 (12%) | 11 (1%)  | 12          | 47  |
| 2   | I     | 1108/1119 (99%) | 956 (86%)  | 140 (13%) | 12 (1%)  | 11          | 45  |
| 3   | D     | 1486/1524 (98%) | 1315 (88%) | 162 (11%) | 9 (1%)   | 21          | 58  |
| 3   | J     | 1361/1524 (89%) | 1201 (88%) | 150 (11%) | 10 (1%)  | 18          | 55  |
| 4   | E     | 91/99 (92%)     | 75 (82%)   | 16 (18%)  | 0        | 100         | 100 |
| 4   | K     | 91/99 (92%)     | 75 (82%)   | 16 (18%)  | 0        | 100         | 100 |
| 5   | F     | 343/347 (99%)   | 299 (87%)  | 42 (12%)  | 2 (1%)   | 21          | 58  |
| 5   | L     | 343/347 (99%)   | 302 (88%)  | 40 (12%)  | 1 (0%)   | 36          | 71  |
| All | All   | 6831/7434 (92%) | 5982 (88%) | 789 (12%) | 60 (1%)  | 14          | 49  |

All (60) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 53   | VAL  |
| 3   | D     | 1128 | VAL  |
| 3   | D     | 1209 | LEU  |
| 1   | G     | 53   | VAL  |
| 3   | J     | 1128 | VAL  |
| 2   | C     | 608  | GLY  |
| 2   | C     | 972  | VAL  |
| 3   | D     | 666  | PHE  |
| 2   | I     | 608  | GLY  |
| 2   | I     | 972  | VAL  |
| 3   | J     | 1287 | GLU  |
| 1   | B     | 161  | ARG  |
| 2   | C     | 882  | LEU  |
| 1   | H     | 161  | ARG  |
| 2   | I     | 882  | LEU  |
| 3   | J     | 422  | ALA  |
| 1   | A     | 98   | THR  |
| 3   | J     | 1130 | ARG  |
| 1   | B     | 178  | ALA  |
| 2   | C     | 295  | ASP  |
| 2   | C     | 365  | ASP  |
| 2   | C     | 607  | ASP  |
| 3   | D     | 1075 | HIS  |
| 1   | G     | 98   | THR  |
| 1   | H     | 178  | ALA  |
| 2   | I     | 295  | ASP  |
| 2   | I     | 365  | ASP  |
| 2   | I     | 607  | ASP  |
| 3   | J     | 1075 | HIS  |
| 3   | J     | 1207 | TYR  |
| 1   | B     | 202  | ASP  |
| 3   | D     | 667  | ALA  |
| 5   | F     | 270  | ALA  |
| 1   | H     | 51   | THR  |
| 1   | H     | 202  | ASP  |
| 2   | C     | 870  | ILE  |
| 2   | C     | 1016 | ILE  |
| 3   | D     | 1221 | VAL  |
| 2   | I     | 870  | ILE  |
| 2   | I     | 1016 | ILE  |
| 3   | J     | 667  | ALA  |
| 3   | J     | 1221 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 989  | VAL  |
| 3   | D     | 670  | VAL  |
| 3   | D     | 947  | ILE  |
| 5   | F     | 407  | VAL  |
| 3   | J     | 947  | ILE  |
| 1   | H     | 116  | PRO  |
| 2   | I     | 989  | VAL  |
| 3   | J     | 670  | VAL  |
| 5   | L     | 407  | VAL  |
| 1   | B     | 48   | ILE  |
| 1   | B     | 116  | PRO  |
| 2   | C     | 17   | PRO  |
| 2   | C     | 852  | ILE  |
| 3   | D     | 259  | VAL  |
| 1   | H     | 48   | ILE  |
| 2   | I     | 17   | PRO  |
| 2   | I     | 852  | ILE  |
| 2   | I     | 1060 | ILE  |

### 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     | 194/270 (72%)   | 176 (91%)  | 18 (9%)   | 8           | 26 |
| 1   | B     | 194/270 (72%)   | 173 (89%)  | 21 (11%)  | 6           | 22 |
| 1   | G     | 194/270 (72%)   | 176 (91%)  | 18 (9%)   | 8           | 26 |
| 1   | H     | 194/270 (72%)   | 172 (89%)  | 22 (11%)  | 5           | 20 |
| 2   | C     | 931/936 (100%)  | 822 (88%)  | 109 (12%) | 5           | 19 |
| 2   | I     | 931/936 (100%)  | 821 (88%)  | 110 (12%) | 5           | 19 |
| 3   | D     | 1252/1281 (98%) | 1097 (88%) | 155 (12%) | 4           | 18 |
| 3   | J     | 1150/1281 (90%) | 1008 (88%) | 142 (12%) | 4           | 18 |
| 4   | E     | 83/88 (94%)     | 76 (92%)   | 7 (8%)    | 10          | 30 |
| 4   | K     | 83/88 (94%)     | 77 (93%)   | 6 (7%)    | 13          | 35 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 5   | F     | 296/299 (99%)   | 273 (92%)  | 23 (8%)   | 11          | 32 |
| 5   | L     | 296/299 (99%)   | 273 (92%)  | 23 (8%)   | 11          | 32 |
| All | All   | 5798/6288 (92%) | 5144 (89%) | 654 (11%) | 5           | 20 |

All (654) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | THR  |
| 1   | A     | 32  | PHE  |
| 1   | A     | 45  | LEU  |
| 1   | A     | 51  | THR  |
| 1   | A     | 73  | GLU  |
| 1   | A     | 74  | ASP  |
| 1   | A     | 80  | LEU  |
| 1   | A     | 93  | LYS  |
| 1   | A     | 113 | ASP  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 158 | ILE  |
| 1   | A     | 174 | VAL  |
| 1   | A     | 176 | ARG  |
| 1   | A     | 198 | ARG  |
| 1   | A     | 205 | VAL  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 227 | ASN  |
| 1   | A     | 232 | LEU  |
| 1   | B     | 7   | LYS  |
| 1   | B     | 23  | PHE  |
| 1   | B     | 38  | ASN  |
| 1   | B     | 44  | LEU  |
| 1   | B     | 51  | THR  |
| 1   | B     | 58  | ILE  |
| 1   | B     | 62  | LEU  |
| 1   | B     | 74  | ASP  |
| 1   | B     | 75  | VAL  |
| 1   | B     | 104 | GLU  |
| 1   | B     | 113 | ASP  |
| 1   | B     | 129 | ILE  |
| 1   | B     | 131 | THR  |
| 1   | B     | 158 | ILE  |
| 1   | B     | 177 | VAL  |
| 1   | B     | 189 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 192 | LEU  |
| 1   | B     | 201 | THR  |
| 1   | B     | 215 | VAL  |
| 1   | B     | 219 | LYS  |
| 1   | B     | 227 | ASN  |
| 2   | C     | 12  | VAL  |
| 2   | C     | 20  | GLU  |
| 2   | C     | 30  | LEU  |
| 2   | C     | 41  | ASN  |
| 2   | C     | 45  | GLN  |
| 2   | C     | 55  | GLU  |
| 2   | C     | 75  | ASP  |
| 2   | C     | 98  | LEU  |
| 2   | C     | 101 | ILE  |
| 2   | C     | 104 | ASP  |
| 2   | C     | 107 | LEU  |
| 2   | C     | 112 | GLU  |
| 2   | C     | 148 | PHE  |
| 2   | C     | 154 | ARG  |
| 2   | C     | 174 | LEU  |
| 2   | C     | 176 | VAL  |
| 2   | C     | 182 | VAL  |
| 2   | C     | 187 | ASN  |
| 2   | C     | 194 | VAL  |
| 2   | C     | 199 | VAL  |
| 2   | C     | 203 | ASP  |
| 2   | C     | 205 | GLU  |
| 2   | C     | 207 | LEU  |
| 2   | C     | 211 | LEU  |
| 2   | C     | 221 | LEU  |
| 2   | C     | 232 | GLU  |
| 2   | C     | 238 | LEU  |
| 2   | C     | 242 | LEU  |
| 2   | C     | 268 | ASP  |
| 2   | C     | 280 | LYS  |
| 2   | C     | 283 | VAL  |
| 2   | C     | 308 | ARG  |
| 2   | C     | 310 | LEU  |
| 2   | C     | 313 | LEU  |
| 2   | C     | 323 | ASP  |
| 2   | C     | 336 | VAL  |
| 2   | C     | 361 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 365 | ASP  |
| 2   | C     | 413 | LEU  |
| 2   | C     | 421 | GLU  |
| 2   | C     | 430 | VAL  |
| 2   | C     | 434 | HIS  |
| 2   | C     | 438 | ILE  |
| 2   | C     | 442 | GLU  |
| 2   | C     | 467 | ILE  |
| 2   | C     | 474 | VAL  |
| 2   | C     | 483 | VAL  |
| 2   | C     | 485 | TYR  |
| 2   | C     | 487 | THR  |
| 2   | C     | 503 | LEU  |
| 2   | C     | 506 | ASP  |
| 2   | C     | 512 | ARG  |
| 2   | C     | 514 | VAL  |
| 2   | C     | 516 | ARG  |
| 2   | C     | 523 | ILE  |
| 2   | C     | 527 | GLU  |
| 2   | C     | 530 | GLU  |
| 2   | C     | 542 | LEU  |
| 2   | C     | 543 | ASN  |
| 2   | C     | 556 | ASN  |
| 2   | C     | 571 | LEU  |
| 2   | C     | 579 | VAL  |
| 2   | C     | 585 | GLU  |
| 2   | C     | 604 | VAL  |
| 2   | C     | 620 | LEU  |
| 2   | C     | 645 | VAL  |
| 2   | C     | 653 | ASP  |
| 2   | C     | 673 | LEU  |
| 2   | C     | 695 | LEU  |
| 2   | C     | 707 | ARG  |
| 2   | C     | 729 | LEU  |
| 2   | C     | 731 | GLU  |
| 2   | C     | 742 | ILE  |
| 2   | C     | 743 | VAL  |
| 2   | C     | 754 | ILE  |
| 2   | C     | 761 | PHE  |
| 2   | C     | 784 | ASP  |
| 2   | C     | 788 | THR  |
| 2   | C     | 808 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 813  | VAL  |
| 2   | C     | 823  | VAL  |
| 2   | C     | 839  | LEU  |
| 2   | C     | 848  | VAL  |
| 2   | C     | 857  | ASP  |
| 2   | C     | 868  | ASP  |
| 2   | C     | 869  | VAL  |
| 2   | C     | 876  | VAL  |
| 2   | C     | 892  | LEU  |
| 2   | C     | 896  | PHE  |
| 2   | C     | 897  | LEU  |
| 2   | C     | 899  | GLN  |
| 2   | C     | 920  | GLU  |
| 2   | C     | 926  | PHE  |
| 2   | C     | 934  | PHE  |
| 2   | C     | 936  | VAL  |
| 2   | C     | 950  | LEU  |
| 2   | C     | 952  | LEU  |
| 2   | C     | 969  | LEU  |
| 2   | C     | 972  | VAL  |
| 2   | C     | 994  | ILE  |
| 2   | C     | 995  | MET  |
| 2   | C     | 1001 | VAL  |
| 2   | C     | 1016 | ILE  |
| 2   | C     | 1021 | LEU  |
| 2   | C     | 1035 | MET  |
| 2   | C     | 1061 | GLU  |
| 2   | C     | 1070 | ILE  |
| 2   | C     | 1075 | ASP  |
| 2   | C     | 1112 | PHE  |
| 3   | D     | 5    | VAL  |
| 3   | D     | 9    | ARG  |
| 3   | D     | 26   | VAL  |
| 3   | D     | 37   | LEU  |
| 3   | D     | 54   | LYS  |
| 3   | D     | 68   | PHE  |
| 3   | D     | 80   | VAL  |
| 3   | D     | 92   | HIS  |
| 3   | D     | 112  | ILE  |
| 3   | D     | 121  | THR  |
| 3   | D     | 135  | LEU  |
| 3   | D     | 152  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 154 | THR  |
| 3   | D     | 155 | ASP  |
| 3   | D     | 166 | GLN  |
| 3   | D     | 168 | THR  |
| 3   | D     | 171 | LEU  |
| 3   | D     | 178 | LEU  |
| 3   | D     | 180 | LYS  |
| 3   | D     | 186 | VAL  |
| 3   | D     | 196 | VAL  |
| 3   | D     | 214 | ASP  |
| 3   | D     | 233 | LYS  |
| 3   | D     | 247 | GLU  |
| 3   | D     | 259 | VAL  |
| 3   | D     | 266 | GLU  |
| 3   | D     | 277 | GLU  |
| 3   | D     | 279 | VAL  |
| 3   | D     | 297 | ILE  |
| 3   | D     | 306 | GLU  |
| 3   | D     | 327 | GLU  |
| 3   | D     | 334 | THR  |
| 3   | D     | 335 | LEU  |
| 3   | D     | 347 | VAL  |
| 3   | D     | 350 | HIS  |
| 3   | D     | 389 | GLU  |
| 3   | D     | 397 | LYS  |
| 3   | D     | 414 | ARG  |
| 3   | D     | 423 | ASP  |
| 3   | D     | 435 | VAL  |
| 3   | D     | 440 | VAL  |
| 3   | D     | 442 | ASN  |
| 3   | D     | 444 | VAL  |
| 3   | D     | 450 | TYR  |
| 3   | D     | 461 | ILE  |
| 3   | D     | 464 | LEU  |
| 3   | D     | 475 | ARG  |
| 3   | D     | 538 | SER  |
| 3   | D     | 546 | ARG  |
| 3   | D     | 547 | LEU  |
| 3   | D     | 548 | ILE  |
| 3   | D     | 564 | GLU  |
| 3   | D     | 576 | GLU  |
| 3   | D     | 593 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 596 | SER  |
| 3   | D     | 598 | ARG  |
| 3   | D     | 619 | LEU  |
| 3   | D     | 636 | GLN  |
| 3   | D     | 637 | LEU  |
| 3   | D     | 639 | LEU  |
| 3   | D     | 658 | LEU  |
| 3   | D     | 683 | ILE  |
| 3   | D     | 684 | LYS  |
| 3   | D     | 685 | ASP  |
| 3   | D     | 688 | TRP  |
| 3   | D     | 694 | VAL  |
| 3   | D     | 707 | THR  |
| 3   | D     | 708 | LEU  |
| 3   | D     | 709 | HIS  |
| 3   | D     | 717 | GLN  |
| 3   | D     | 747 | VAL  |
| 3   | D     | 749 | VAL  |
| 3   | D     | 762 | GLN  |
| 3   | D     | 776 | GLU  |
| 3   | D     | 787 | LEU  |
| 3   | D     | 810 | GLU  |
| 3   | D     | 811 | GLU  |
| 3   | D     | 835 | SER  |
| 3   | D     | 838 | ARG  |
| 3   | D     | 850 | LEU  |
| 3   | D     | 861 | GLN  |
| 3   | D     | 865 | THR  |
| 3   | D     | 875 | THR  |
| 3   | D     | 897 | GLN  |
| 3   | D     | 899 | LEU  |
| 3   | D     | 903 | ASP  |
| 3   | D     | 908 | LYS  |
| 3   | D     | 909 | ASN  |
| 3   | D     | 912 | LYS  |
| 3   | D     | 930 | LEU  |
| 3   | D     | 932 | ASP  |
| 3   | D     | 945 | SER  |
| 3   | D     | 959 | GLU  |
| 3   | D     | 964 | LEU  |
| 3   | D     | 976 | GLN  |
| 3   | D     | 987 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 997  | THR  |
| 3   | D     | 1004 | THR  |
| 3   | D     | 1015 | TYR  |
| 3   | D     | 1029 | ARG  |
| 3   | D     | 1066 | THR  |
| 3   | D     | 1078 | ARG  |
| 3   | D     | 1094 | LEU  |
| 3   | D     | 1100 | ASP  |
| 3   | D     | 1107 | VAL  |
| 3   | D     | 1108 | ARG  |
| 3   | D     | 1112 | CYS  |
| 3   | D     | 1120 | VAL  |
| 3   | D     | 1123 | PHE  |
| 3   | D     | 1130 | ARG  |
| 3   | D     | 1133 | ARG  |
| 3   | D     | 1134 | LEU  |
| 3   | D     | 1137 | ARG  |
| 3   | D     | 1139 | ASP  |
| 3   | D     | 1144 | LEU  |
| 3   | D     | 1156 | LEU  |
| 3   | D     | 1160 | LEU  |
| 3   | D     | 1161 | GLU  |
| 3   | D     | 1162 | GLU  |
| 3   | D     | 1170 | ASP  |
| 3   | D     | 1179 | GLU  |
| 3   | D     | 1188 | VAL  |
| 3   | D     | 1192 | LEU  |
| 3   | D     | 1203 | LYS  |
| 3   | D     | 1211 | MET  |
| 3   | D     | 1231 | GLU  |
| 3   | D     | 1256 | LEU  |
| 3   | D     | 1278 | ASP  |
| 3   | D     | 1285 | GLU  |
| 3   | D     | 1295 | GLU  |
| 3   | D     | 1297 | GLU  |
| 3   | D     | 1302 | GLU  |
| 3   | D     | 1305 | LEU  |
| 3   | D     | 1310 | ARG  |
| 3   | D     | 1312 | LEU  |
| 3   | D     | 1369 | GLU  |
| 3   | D     | 1380 | GLU  |
| 3   | D     | 1382 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1386 | ASP  |
| 3   | D     | 1395 | LEU  |
| 3   | D     | 1407 | LEU  |
| 3   | D     | 1413 | VAL  |
| 3   | D     | 1420 | LEU  |
| 3   | D     | 1424 | VAL  |
| 3   | D     | 1443 | THR  |
| 3   | D     | 1444 | THR  |
| 3   | D     | 1448 | THR  |
| 3   | D     | 1458 | GLU  |
| 3   | D     | 1459 | LEU  |
| 3   | D     | 1462 | LEU  |
| 3   | D     | 1463 | LYS  |
| 3   | D     | 1464 | GLU  |
| 3   | D     | 1468 | LEU  |
| 3   | D     | 1472 | ILE  |
| 3   | D     | 1499 | ARG  |
| 4   | E     | 14   | ASP  |
| 4   | E     | 30   | LEU  |
| 4   | E     | 39   | VAL  |
| 4   | E     | 40   | LEU  |
| 4   | E     | 47   | LYS  |
| 4   | E     | 56   | ASP  |
| 4   | E     | 79   | LEU  |
| 5   | F     | 108  | LEU  |
| 5   | F     | 112  | GLU  |
| 5   | F     | 139  | GLN  |
| 5   | F     | 142  | ILE  |
| 5   | F     | 151  | LEU  |
| 5   | F     | 165  | LYS  |
| 5   | F     | 172  | GLU  |
| 5   | F     | 175  | ASP  |
| 5   | F     | 196  | GLU  |
| 5   | F     | 202  | LEU  |
| 5   | F     | 224  | PHE  |
| 5   | F     | 233  | GLN  |
| 5   | F     | 263  | ASN  |
| 5   | F     | 272  | THR  |
| 5   | F     | 328  | GLU  |
| 5   | F     | 339  | GLU  |
| 5   | F     | 343  | PHE  |
| 5   | F     | 371  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 384 | LEU  |
| 5   | F     | 404 | TYR  |
| 5   | F     | 405 | PHE  |
| 5   | F     | 424 | LYS  |
| 5   | F     | 433 | LEU  |
| 1   | G     | 14  | THR  |
| 1   | G     | 32  | PHE  |
| 1   | G     | 45  | LEU  |
| 1   | G     | 51  | THR  |
| 1   | G     | 73  | GLU  |
| 1   | G     | 74  | ASP  |
| 1   | G     | 80  | LEU  |
| 1   | G     | 93  | LYS  |
| 1   | G     | 113 | ASP  |
| 1   | G     | 151 | VAL  |
| 1   | G     | 158 | ILE  |
| 1   | G     | 174 | VAL  |
| 1   | G     | 176 | ARG  |
| 1   | G     | 198 | ARG  |
| 1   | G     | 205 | VAL  |
| 1   | G     | 222 | LEU  |
| 1   | G     | 227 | ASN  |
| 1   | G     | 232 | LEU  |
| 1   | H     | 7   | LYS  |
| 1   | H     | 23  | PHE  |
| 1   | H     | 38  | ASN  |
| 1   | H     | 44  | LEU  |
| 1   | H     | 51  | THR  |
| 1   | H     | 58  | ILE  |
| 1   | H     | 62  | LEU  |
| 1   | H     | 74  | ASP  |
| 1   | H     | 75  | VAL  |
| 1   | H     | 104 | GLU  |
| 1   | H     | 113 | ASP  |
| 1   | H     | 129 | ILE  |
| 1   | H     | 131 | THR  |
| 1   | H     | 140 | MET  |
| 1   | H     | 158 | ILE  |
| 1   | H     | 177 | VAL  |
| 1   | H     | 189 | ARG  |
| 1   | H     | 192 | LEU  |
| 1   | H     | 201 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 215 | VAL  |
| 1   | H     | 219 | LYS  |
| 1   | H     | 227 | ASN  |
| 2   | I     | 12  | VAL  |
| 2   | I     | 20  | GLU  |
| 2   | I     | 30  | LEU  |
| 2   | I     | 41  | ASN  |
| 2   | I     | 45  | GLN  |
| 2   | I     | 55  | GLU  |
| 2   | I     | 70  | GLU  |
| 2   | I     | 75  | ASP  |
| 2   | I     | 98  | LEU  |
| 2   | I     | 101 | ILE  |
| 2   | I     | 104 | ASP  |
| 2   | I     | 107 | LEU  |
| 2   | I     | 112 | GLU  |
| 2   | I     | 134 | ARG  |
| 2   | I     | 148 | PHE  |
| 2   | I     | 154 | ARG  |
| 2   | I     | 174 | LEU  |
| 2   | I     | 176 | VAL  |
| 2   | I     | 182 | VAL  |
| 2   | I     | 187 | ASN  |
| 2   | I     | 194 | VAL  |
| 2   | I     | 199 | VAL  |
| 2   | I     | 203 | ASP  |
| 2   | I     | 205 | GLU  |
| 2   | I     | 207 | LEU  |
| 2   | I     | 211 | LEU  |
| 2   | I     | 221 | LEU  |
| 2   | I     | 232 | GLU  |
| 2   | I     | 238 | LEU  |
| 2   | I     | 242 | LEU  |
| 2   | I     | 268 | ASP  |
| 2   | I     | 280 | LYS  |
| 2   | I     | 283 | VAL  |
| 2   | I     | 308 | ARG  |
| 2   | I     | 310 | LEU  |
| 2   | I     | 313 | LEU  |
| 2   | I     | 323 | ASP  |
| 2   | I     | 336 | VAL  |
| 2   | I     | 361 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 365 | ASP  |
| 2   | I     | 413 | LEU  |
| 2   | I     | 421 | GLU  |
| 2   | I     | 430 | VAL  |
| 2   | I     | 434 | HIS  |
| 2   | I     | 438 | ILE  |
| 2   | I     | 442 | GLU  |
| 2   | I     | 467 | ILE  |
| 2   | I     | 474 | VAL  |
| 2   | I     | 485 | TYR  |
| 2   | I     | 487 | THR  |
| 2   | I     | 503 | LEU  |
| 2   | I     | 506 | ASP  |
| 2   | I     | 512 | ARG  |
| 2   | I     | 514 | VAL  |
| 2   | I     | 523 | ILE  |
| 2   | I     | 527 | GLU  |
| 2   | I     | 530 | GLU  |
| 2   | I     | 542 | LEU  |
| 2   | I     | 543 | ASN  |
| 2   | I     | 556 | ASN  |
| 2   | I     | 571 | LEU  |
| 2   | I     | 579 | VAL  |
| 2   | I     | 585 | GLU  |
| 2   | I     | 604 | VAL  |
| 2   | I     | 620 | LEU  |
| 2   | I     | 645 | VAL  |
| 2   | I     | 653 | ASP  |
| 2   | I     | 673 | LEU  |
| 2   | I     | 695 | LEU  |
| 2   | I     | 707 | ARG  |
| 2   | I     | 729 | LEU  |
| 2   | I     | 731 | GLU  |
| 2   | I     | 742 | ILE  |
| 2   | I     | 743 | VAL  |
| 2   | I     | 754 | ILE  |
| 2   | I     | 761 | PHE  |
| 2   | I     | 784 | ASP  |
| 2   | I     | 788 | THR  |
| 2   | I     | 808 | ARG  |
| 2   | I     | 813 | VAL  |
| 2   | I     | 823 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 839  | LEU  |
| 2   | I     | 848  | VAL  |
| 2   | I     | 852  | ILE  |
| 2   | I     | 857  | ASP  |
| 2   | I     | 868  | ASP  |
| 2   | I     | 869  | VAL  |
| 2   | I     | 876  | VAL  |
| 2   | I     | 892  | LEU  |
| 2   | I     | 896  | PHE  |
| 2   | I     | 897  | LEU  |
| 2   | I     | 899  | GLN  |
| 2   | I     | 920  | GLU  |
| 2   | I     | 926  | PHE  |
| 2   | I     | 934  | PHE  |
| 2   | I     | 936  | VAL  |
| 2   | I     | 950  | LEU  |
| 2   | I     | 952  | LEU  |
| 2   | I     | 969  | LEU  |
| 2   | I     | 972  | VAL  |
| 2   | I     | 994  | ILE  |
| 2   | I     | 995  | MET  |
| 2   | I     | 1001 | VAL  |
| 2   | I     | 1016 | ILE  |
| 2   | I     | 1021 | LEU  |
| 2   | I     | 1035 | MET  |
| 2   | I     | 1061 | GLU  |
| 2   | I     | 1070 | ILE  |
| 2   | I     | 1075 | ASP  |
| 2   | I     | 1112 | PHE  |
| 3   | J     | 5    | VAL  |
| 3   | J     | 9    | ARG  |
| 3   | J     | 26   | VAL  |
| 3   | J     | 37   | LEU  |
| 3   | J     | 54   | LYS  |
| 3   | J     | 68   | PHE  |
| 3   | J     | 80   | VAL  |
| 3   | J     | 112  | ILE  |
| 3   | J     | 121  | THR  |
| 3   | J     | 135  | LEU  |
| 3   | J     | 154  | THR  |
| 3   | J     | 155  | ASP  |
| 3   | J     | 166  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | J     | 168 | THR  |
| 3   | J     | 171 | LEU  |
| 3   | J     | 178 | LEU  |
| 3   | J     | 180 | LYS  |
| 3   | J     | 186 | VAL  |
| 3   | J     | 196 | VAL  |
| 3   | J     | 210 | ARG  |
| 3   | J     | 211 | VAL  |
| 3   | J     | 350 | HIS  |
| 3   | J     | 375 | GLU  |
| 3   | J     | 399 | ARG  |
| 3   | J     | 404 | GLU  |
| 3   | J     | 410 | THR  |
| 3   | J     | 411 | THR  |
| 3   | J     | 414 | ARG  |
| 3   | J     | 423 | ASP  |
| 3   | J     | 430 | GLU  |
| 3   | J     | 440 | VAL  |
| 3   | J     | 444 | VAL  |
| 3   | J     | 450 | TYR  |
| 3   | J     | 461 | ILE  |
| 3   | J     | 462 | GLN  |
| 3   | J     | 464 | LEU  |
| 3   | J     | 512 | MET  |
| 3   | J     | 513 | ILE  |
| 3   | J     | 523 | ASP  |
| 3   | J     | 525 | ARG  |
| 3   | J     | 547 | LEU  |
| 3   | J     | 548 | ILE  |
| 3   | J     | 574 | LEU  |
| 3   | J     | 576 | GLU  |
| 3   | J     | 598 | ARG  |
| 3   | J     | 600 | LEU  |
| 3   | J     | 619 | LEU  |
| 3   | J     | 636 | GLN  |
| 3   | J     | 637 | LEU  |
| 3   | J     | 639 | LEU  |
| 3   | J     | 658 | LEU  |
| 3   | J     | 659 | LYS  |
| 3   | J     | 683 | ILE  |
| 3   | J     | 684 | LYS  |
| 3   | J     | 685 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 688  | TRP  |
| 3   | J     | 694  | VAL  |
| 3   | J     | 707  | THR  |
| 3   | J     | 708  | LEU  |
| 3   | J     | 709  | HIS  |
| 3   | J     | 717  | GLN  |
| 3   | J     | 747  | VAL  |
| 3   | J     | 749  | VAL  |
| 3   | J     | 762  | GLN  |
| 3   | J     | 776  | GLU  |
| 3   | J     | 787  | LEU  |
| 3   | J     | 810  | GLU  |
| 3   | J     | 811  | GLU  |
| 3   | J     | 835  | SER  |
| 3   | J     | 838  | ARG  |
| 3   | J     | 850  | LEU  |
| 3   | J     | 861  | GLN  |
| 3   | J     | 865  | THR  |
| 3   | J     | 875  | THR  |
| 3   | J     | 897  | GLN  |
| 3   | J     | 899  | LEU  |
| 3   | J     | 903  | ASP  |
| 3   | J     | 908  | LYS  |
| 3   | J     | 909  | ASN  |
| 3   | J     | 912  | LYS  |
| 3   | J     | 930  | LEU  |
| 3   | J     | 932  | ASP  |
| 3   | J     | 945  | SER  |
| 3   | J     | 959  | GLU  |
| 3   | J     | 964  | LEU  |
| 3   | J     | 976  | GLN  |
| 3   | J     | 987  | GLU  |
| 3   | J     | 997  | THR  |
| 3   | J     | 1004 | THR  |
| 3   | J     | 1015 | TYR  |
| 3   | J     | 1029 | ARG  |
| 3   | J     | 1066 | THR  |
| 3   | J     | 1078 | ARG  |
| 3   | J     | 1094 | LEU  |
| 3   | J     | 1100 | ASP  |
| 3   | J     | 1107 | VAL  |
| 3   | J     | 1112 | CYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 1132 | LEU  |
| 3   | J     | 1134 | LEU  |
| 3   | J     | 1142 | SER  |
| 3   | J     | 1144 | LEU  |
| 3   | J     | 1149 | LEU  |
| 3   | J     | 1159 | ARG  |
| 3   | J     | 1160 | LEU  |
| 3   | J     | 1161 | GLU  |
| 3   | J     | 1162 | GLU  |
| 3   | J     | 1170 | ASP  |
| 3   | J     | 1183 | VAL  |
| 3   | J     | 1192 | LEU  |
| 3   | J     | 1203 | LYS  |
| 3   | J     | 1211 | MET  |
| 3   | J     | 1231 | GLU  |
| 3   | J     | 1235 | GLN  |
| 3   | J     | 1238 | MET  |
| 3   | J     | 1267 | ARG  |
| 3   | J     | 1277 | ILE  |
| 3   | J     | 1285 | GLU  |
| 3   | J     | 1293 | PHE  |
| 3   | J     | 1297 | GLU  |
| 3   | J     | 1305 | LEU  |
| 3   | J     | 1318 | TYR  |
| 3   | J     | 1325 | LEU  |
| 3   | J     | 1326 | THR  |
| 3   | J     | 1342 | GLU  |
| 3   | J     | 1348 | LEU  |
| 3   | J     | 1397 | LYS  |
| 3   | J     | 1407 | LEU  |
| 3   | J     | 1420 | LEU  |
| 3   | J     | 1429 | LEU  |
| 3   | J     | 1432 | LYS  |
| 3   | J     | 1433 | SER  |
| 3   | J     | 1444 | THR  |
| 3   | J     | 1448 | THR  |
| 3   | J     | 1458 | GLU  |
| 3   | J     | 1462 | LEU  |
| 3   | J     | 1463 | LYS  |
| 3   | J     | 1464 | GLU  |
| 3   | J     | 1465 | ASN  |
| 3   | J     | 1472 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 1492 | LEU  |
| 3   | J     | 1493 | LYS  |
| 3   | J     | 1496 | GLU  |
| 4   | K     | 14   | ASP  |
| 4   | K     | 30   | LEU  |
| 4   | K     | 39   | VAL  |
| 4   | K     | 47   | LYS  |
| 4   | K     | 56   | ASP  |
| 4   | K     | 79   | LEU  |
| 5   | L     | 108  | LEU  |
| 5   | L     | 112  | GLU  |
| 5   | L     | 139  | GLN  |
| 5   | L     | 142  | ILE  |
| 5   | L     | 151  | LEU  |
| 5   | L     | 165  | LYS  |
| 5   | L     | 172  | GLU  |
| 5   | L     | 175  | ASP  |
| 5   | L     | 196  | GLU  |
| 5   | L     | 202  | LEU  |
| 5   | L     | 224  | PHE  |
| 5   | L     | 233  | GLN  |
| 5   | L     | 263  | ASN  |
| 5   | L     | 272  | THR  |
| 5   | L     | 328  | GLU  |
| 5   | L     | 339  | GLU  |
| 5   | L     | 343  | PHE  |
| 5   | L     | 371  | LYS  |
| 5   | L     | 384  | LEU  |
| 5   | L     | 404  | TYR  |
| 5   | L     | 405  | PHE  |
| 5   | L     | 424  | LYS  |
| 5   | L     | 433  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | HIS  |
| 1   | A     | 212 | ASN  |
| 1   | B     | 128 | HIS  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 213 | GLN  |
| 2   | C     | 22  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 41   | ASN  |
| 2   | C     | 45   | GLN  |
| 2   | C     | 393  | GLN  |
| 2   | C     | 434  | HIS  |
| 2   | C     | 498  | GLN  |
| 2   | C     | 538  | GLN  |
| 2   | C     | 567  | GLN  |
| 2   | C     | 575  | GLN  |
| 2   | C     | 639  | GLN  |
| 2   | C     | 671  | ASN  |
| 2   | C     | 765  | GLN  |
| 2   | C     | 845  | ASN  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 962  | GLN  |
| 2   | C     | 991  | GLN  |
| 2   | C     | 999  | HIS  |
| 2   | C     | 1006 | HIS  |
| 2   | C     | 1050 | GLN  |
| 2   | C     | 1100 | GLN  |
| 2   | C     | 1107 | ASN  |
| 3   | D     | 66   | GLN  |
| 3   | D     | 130  | ASN  |
| 3   | D     | 151  | GLN  |
| 3   | D     | 274  | GLN  |
| 3   | D     | 350  | HIS  |
| 3   | D     | 462  | GLN  |
| 3   | D     | 569  | ASN  |
| 3   | D     | 593  | ASN  |
| 3   | D     | 640  | HIS  |
| 3   | D     | 641  | GLN  |
| 3   | D     | 669  | ASN  |
| 3   | D     | 680  | GLN  |
| 3   | D     | 756  | GLN  |
| 3   | D     | 762  | GLN  |
| 3   | D     | 794  | GLN  |
| 3   | D     | 897  | GLN  |
| 3   | D     | 991  | GLN  |
| 3   | D     | 1010 | ASN  |
| 3   | D     | 1046 | GLN  |
| 3   | D     | 1116 | ASN  |
| 3   | D     | 1235 | GLN  |
| 3   | D     | 1359 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | E     | 37   | ASN  |
| 4   | E     | 59   | ASN  |
| 5   | F     | 206  | ASN  |
| 5   | F     | 233  | GLN  |
| 5   | F     | 263  | ASN  |
| 5   | F     | 269  | GLN  |
| 5   | F     | 294  | GLN  |
| 5   | F     | 295  | GLN  |
| 5   | F     | 396  | HIS  |
| 5   | F     | 417  | ASN  |
| 5   | F     | 426  | HIS  |
| 1   | G     | 63   | HIS  |
| 1   | G     | 212  | ASN  |
| 1   | H     | 163  | ASN  |
| 1   | H     | 213  | GLN  |
| 2   | I     | 22   | GLN  |
| 2   | I     | 41   | ASN  |
| 2   | I     | 45   | GLN  |
| 2   | I     | 393  | GLN  |
| 2   | I     | 434  | HIS  |
| 2   | I     | 498  | GLN  |
| 2   | I     | 538  | GLN  |
| 2   | I     | 567  | GLN  |
| 2   | I     | 575  | GLN  |
| 2   | I     | 639  | GLN  |
| 2   | I     | 671  | ASN  |
| 2   | I     | 765  | GLN  |
| 2   | I     | 841  | ASN  |
| 2   | I     | 881  | ASN  |
| 2   | I     | 884  | GLN  |
| 2   | I     | 962  | GLN  |
| 2   | I     | 991  | GLN  |
| 2   | I     | 999  | HIS  |
| 2   | I     | 1050 | GLN  |
| 2   | I     | 1100 | GLN  |
| 2   | I     | 1107 | ASN  |
| 3   | J     | 66   | GLN  |
| 3   | J     | 130  | ASN  |
| 3   | J     | 151  | GLN  |
| 3   | J     | 386  | HIS  |
| 3   | J     | 442  | ASN  |
| 3   | J     | 560  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 593  | ASN  |
| 3   | J     | 640  | HIS  |
| 3   | J     | 641  | GLN  |
| 3   | J     | 669  | ASN  |
| 3   | J     | 680  | GLN  |
| 3   | J     | 703  | ASN  |
| 3   | J     | 756  | GLN  |
| 3   | J     | 762  | GLN  |
| 3   | J     | 794  | GLN  |
| 3   | J     | 897  | GLN  |
| 3   | J     | 991  | GLN  |
| 3   | J     | 1046 | GLN  |
| 3   | J     | 1334 | GLN  |
| 3   | J     | 1393 | GLN  |
| 3   | J     | 1441 | GLN  |
| 4   | K     | 29   | GLN  |
| 4   | K     | 37   | ASN  |
| 4   | K     | 59   | ASN  |
| 5   | L     | 190  | HIS  |
| 5   | L     | 206  | ASN  |
| 5   | L     | 229  | GLN  |
| 5   | L     | 269  | GLN  |
| 5   | L     | 294  | GLN  |
| 5   | L     | 295  | GLN  |
| 5   | L     | 327  | GLN  |
| 5   | L     | 396  | HIS  |
| 5   | L     | 417  | ASN  |
| 5   | L     | 426  | HIS  |

### 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 ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 227/314 (72%)   | 0.24   | 4 (1%) 67 54   | 107, 189, 236, 264    | 0     |
| 1   | B     | 227/314 (72%)   | 0.14   | 2 (0%) 81 66   | 94, 161, 214, 264     | 0     |
| 1   | G     | 227/314 (72%)   | 0.46   | 10 (4%) 39 35  | 116, 199, 240, 276    | 0     |
| 1   | H     | 227/314 (72%)   | 0.26   | 4 (1%) 67 54   | 116, 173, 216, 267    | 0     |
| 2   | C     | 1112/1119 (99%) | 0.25   | 29 (2%) 57 45  | 90, 179, 243, 314     | 0     |
| 2   | I     | 1112/1119 (99%) | 0.29   | 32 (2%) 53 43  | 94, 185, 244, 315     | 0     |
| 3   | D     | 1490/1524 (97%) | 0.08   | 17 (1%) 78 62  | 64, 149, 204, 259     | 0     |
| 3   | J     | 1367/1524 (89%) | 0.16   | 21 (1%) 72 57  | 79, 159, 217, 264     | 0     |
| 4   | E     | 93/99 (93%)     | 0.27   | 3 (3%) 50 41   | 100, 159, 205, 238    | 0     |
| 4   | K     | 93/99 (93%)     | 0.42   | 2 (2%) 62 49   | 112, 168, 216, 253    | 0     |
| 5   | F     | 345/347 (99%)   | 0.31   | 11 (3%) 50 41  | 115, 185, 255, 300    | 0     |
| 5   | L     | 345/347 (99%)   | 0.44   | 18 (5%) 33 31  | 121, 188, 252, 300    | 0     |
| 6   | O     | 30/30 (100%)    | 0.18   | 0 100 100      | 154, 221, 293, 311    | 0     |
| 6   | R     | 30/30 (100%)    | 0.16   | 0 100 100      | 164, 221, 257, 267    | 0     |
| 7   | P     | 25/26 (96%)     | 0.29   | 0 100 100      | 172, 235, 306, 326    | 0     |
| 7   | S     | 26/26 (100%)    | 0.42   | 1 (3%) 44 38   | 184, 224, 263, 283    | 0     |
| All | All   | 6976/7546 (92%) | 0.22   | 154 (2%) 62 49 | 64, 171, 235, 326     | 0     |

All (154) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | F     | 153 | THR  | 4.8  |
| 7   | S     | 1   | DT   | 4.8  |
| 1   | G     | 170 | ILE  | 4.5  |
| 3   | J     | 30  | GLU  | 3.8  |
| 2   | I     | 203 | ASP  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | I     | 247  | PRO  | 3.5  |
| 2   | C     | 221  | LEU  | 3.5  |
| 3   | D     | 666  | PHE  | 3.5  |
| 5   | L     | 159  | ILE  | 3.4  |
| 5   | L     | 378  | GLU  | 3.4  |
| 3   | D     | 1237 | THR  | 3.3  |
| 2   | C     | 176  | VAL  | 3.3  |
| 5   | F     | 155  | ARG  | 3.2  |
| 5   | L     | 153  | THR  | 3.2  |
| 1   | G     | 24   | VAL  | 3.2  |
| 3   | D     | 459  | GLU  | 3.1  |
| 1   | G     | 13   | ALA  | 3.1  |
| 3   | J     | 1237 | THR  | 3.1  |
| 5   | L     | 338  | ASP  | 3.1  |
| 5   | F     | 161  | GLY  | 3.0  |
| 5   | F     | 194  | GLU  | 3.0  |
| 5   | L     | 220  | ARG  | 3.0  |
| 1   | H     | 194  | LYS  | 3.0  |
| 5   | L     | 217  | TYR  | 2.9  |
| 2   | I     | 62   | GLY  | 2.9  |
| 2   | I     | 244  | PRO  | 2.9  |
| 2   | I     | 217  | LEU  | 2.9  |
| 3   | D     | 82   | ARG  | 2.8  |
| 1   | H     | 67   | THR  | 2.8  |
| 3   | J     | 459  | GLU  | 2.8  |
| 3   | D     | 538  | SER  | 2.8  |
| 1   | G     | 84   | GLU  | 2.8  |
| 5   | L     | 99   | TYR  | 2.8  |
| 3   | J     | 1455 | LYS  | 2.8  |
| 2   | I     | 292  | ARG  | 2.7  |
| 3   | J     | 1238 | MET  | 2.7  |
| 2   | I     | 628  | TYR  | 2.7  |
| 4   | K     | 74   | PHE  | 2.7  |
| 3   | J     | 340  | THR  | 2.7  |
| 2   | C     | 166  | PRO  | 2.7  |
| 2   | C     | 745  | ILE  | 2.7  |
| 2   | I     | 287  | GLY  | 2.6  |
| 2   | I     | 319  | GLY  | 2.6  |
| 5   | F     | 159  | ILE  | 2.6  |
| 2   | I     | 368  | THR  | 2.6  |
| 5   | L     | 155  | ARG  | 2.6  |
| 2   | I     | 166  | PRO  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 167  | LYS  | 2.6  |
| 5   | F     | 154  | ALA  | 2.6  |
| 4   | K     | 94   | PRO  | 2.6  |
| 2   | I     | 180  | GLY  | 2.5  |
| 2   | C     | 247  | PRO  | 2.5  |
| 5   | F     | 409  | ARG  | 2.5  |
| 1   | G     | 8    | ALA  | 2.5  |
| 2   | I     | 245  | GLY  | 2.5  |
| 1   | G     | 31   | GLY  | 2.5  |
| 3   | J     | 35   | ARG  | 2.5  |
| 3   | D     | 445  | ARG  | 2.5  |
| 2   | I     | 213  | ALA  | 2.5  |
| 5   | F     | 156  | ILE  | 2.5  |
| 1   | B     | 233  | LEU  | 2.4  |
| 3   | D     | 1263 | PHE  | 2.4  |
| 5   | F     | 338  | ASP  | 2.4  |
| 2   | C     | 1025 | ALA  | 2.4  |
| 2   | I     | 447  | ALA  | 2.4  |
| 3   | J     | 696  | HIS  | 2.4  |
| 2   | C     | 663  | GLU  | 2.4  |
| 2   | I     | 906  | PHE  | 2.4  |
| 1   | H     | 66   | SER  | 2.4  |
| 2   | I     | 738  | ASP  | 2.4  |
| 2   | C     | 244  | PRO  | 2.4  |
| 5   | F     | 220  | ARG  | 2.4  |
| 1   | B     | 188  | GLN  | 2.3  |
| 3   | D     | 1486 | VAL  | 2.3  |
| 3   | D     | 800  | LYS  | 2.3  |
| 2   | I     | 801  | VAL  | 2.3  |
| 2   | C     | 203  | ASP  | 2.3  |
| 2   | C     | 207  | LEU  | 2.3  |
| 2   | C     | 686  | ASP  | 2.3  |
| 2   | I     | 1080 | SER  | 2.3  |
| 4   | E     | 74   | PHE  | 2.3  |
| 2   | C     | 898  | GLY  | 2.3  |
| 3   | J     | 98   | PRO  | 2.3  |
| 3   | D     | 1487 | VAL  | 2.3  |
| 2   | C     | 62   | GLY  | 2.2  |
| 2   | C     | 582  | GLY  | 2.2  |
| 3   | J     | 421  | LEU  | 2.2  |
| 5   | L     | 256  | TRP  | 2.2  |
| 3   | D     | 444  | VAL  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 1279 | GLY  | 2.2  |
| 2   | I     | 567  | GLN  | 2.2  |
| 5   | F     | 346  | ASP  | 2.2  |
| 5   | L     | 308  | GLU  | 2.2  |
| 1   | A     | 162  | ILE  | 2.2  |
| 5   | L     | 214  | ALA  | 2.2  |
| 5   | L     | 221  | GLY  | 2.2  |
| 3   | J     | 436  | GLU  | 2.2  |
| 5   | L     | 304  | GLU  | 2.2  |
| 2   | I     | 416  | GLY  | 2.2  |
| 2   | C     | 424  | GLY  | 2.2  |
| 5   | L     | 223  | SER  | 2.2  |
| 2   | I     | 221  | LEU  | 2.2  |
| 5   | L     | 216  | LYS  | 2.2  |
| 2   | C     | 706  | GLU  | 2.2  |
| 3   | J     | 24   | GLY  | 2.2  |
| 2   | C     | 679  | PHE  | 2.2  |
| 1   | G     | 137  | LYS  | 2.2  |
| 1   | G     | 148  | VAL  | 2.2  |
| 1   | G     | 73   | GLU  | 2.1  |
| 2   | I     | 626  | ARG  | 2.1  |
| 3   | J     | 34   | TYR  | 2.1  |
| 2   | I     | 1023 | GLY  | 2.1  |
| 3   | J     | 1504 | GLU  | 2.1  |
| 3   | J     | 1398 | TRP  | 2.1  |
| 2   | I     | 896  | PHE  | 2.1  |
| 2   | I     | 181  | VAL  | 2.1  |
| 2   | C     | 180  | GLY  | 2.1  |
| 3   | J     | 718  | PRO  | 2.1  |
| 4   | E     | 87   | LYS  | 2.1  |
| 5   | L     | 300  | GLU  | 2.1  |
| 2   | I     | 214  | TYR  | 2.1  |
| 2   | C     | 272  | ALA  | 2.1  |
| 2   | C     | 368  | THR  | 2.1  |
| 2   | C     | 637  | PHE  | 2.1  |
| 2   | I     | 637  | PHE  | 2.1  |
| 2   | I     | 844  | GLY  | 2.1  |
| 3   | D     | 664  | LYS  | 2.1  |
| 1   | G     | 204  | SER  | 2.1  |
| 3   | J     | 196  | VAL  | 2.1  |
| 3   | J     | 437  | VAL  | 2.1  |
| 2   | C     | 10   | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 358 | ARG  | 2.1  |
| 3   | D     | 647 | ARG  | 2.1  |
| 1   | A     | 14  | THR  | 2.1  |
| 1   | A     | 67  | THR  | 2.1  |
| 2   | I     | 693 | GLU  | 2.1  |
| 5   | L     | 178 | LEU  | 2.0  |
| 2   | I     | 228 | ALA  | 2.0  |
| 3   | D     | 593 | ASN  | 2.0  |
| 2   | C     | 618 | GLY  | 2.0  |
| 2   | I     | 246 | ASP  | 2.0  |
| 5   | L     | 346 | ASP  | 2.0  |
| 1   | A     | 163 | ASN  | 2.0  |
| 4   | E     | 94  | PRO  | 2.0  |
| 2   | C     | 11  | GLU  | 2.0  |
| 2   | C     | 512 | ARG  | 2.0  |
| 3   | J     | 893 | GLU  | 2.0  |
| 3   | J     | 28  | LYS  | 2.0  |
| 3   | J     | 207 | PHE  | 2.0  |
| 2   | C     | 201 | GLY  | 2.0  |
| 1   | H     | 60  | ASP  | 2.0  |
| 3   | D     | 594 | PRO  | 2.0  |
| 3   | D     | 798 | GLU  | 2.0  |
| 2   | C     | 549 | PHE  | 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](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 9   | MG   | D     | 2003 | 1/1   | 0.78 | 0.14 | 286,286,286,286             | 0     |
| 9   | MG   | J     | 2003 | 1/1   | 0.78 | 0.17 | 331,331,331,331             | 0     |
| 8   | ZN   | J     | 2002 | 1/1   | 0.99 | 0.03 | 147,147,147,147             | 0     |
| 8   | ZN   | D     | 2002 | 1/1   | 0.99 | 0.07 | 182,182,182,182             | 0     |
| 8   | ZN   | J     | 2001 | 1/1   | 0.99 | 0.05 | 166,166,166,166             | 0     |
| 8   | ZN   | D     | 2001 | 1/1   | 1.00 | 0.04 | 107,107,107,107             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.