



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:30 pm BST

PDB ID : 4ZIW  
Title : Crystal structure of AcrB deletion mutant in P21 space group  
Authors : Ababou, A.; Koronakis, V.  
Deposited on : 2015-04-28  
Resolution : 3.40 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

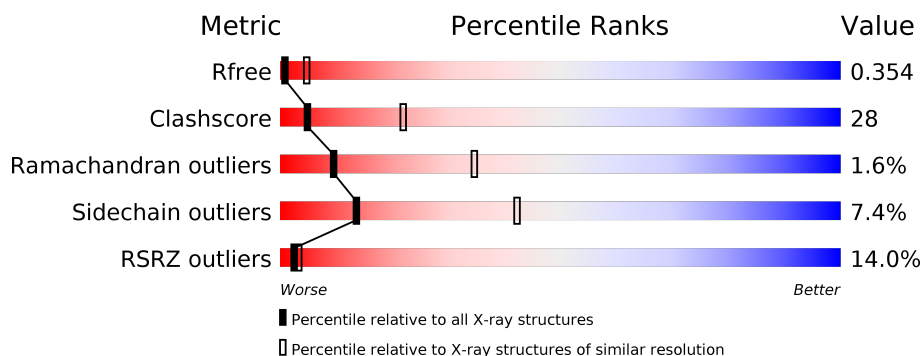
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1026 (3.48-3.32)                                      |
| Clashscore            | 141614                      | 1055 (3.48-3.32)                                      |
| Ramachandran outliers | 138981                      | 1038 (3.48-3.32)                                      |
| Sidechain outliers    | 138945                      | 1038 (3.48-3.32)                                      |
| RSRZ outliers         | 127900                      | 2173 (3.50-3.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 1044   | <div> <div>12%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div> |
| 1   | B     | 1044   | <div> <div>10%</div> <div>50%</div> <div>45%</div> <div>5%</div> </div> |
| 1   | C     | 1044   | <div> <div>12%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div> |
| 1   | D     | 1044   | <div> <div>16%</div> <div>44%</div> <div>50%</div> <div>5%</div> </div> |
| 1   | E     | 1044   | <div> <div>17%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div> |
| 1   | F     | 1044   | <div> <div>17%</div> <div>46%</div> <div>48%</div> <div>5%</div> </div> |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | LMT  | B     | 2000 | -         | -        | -       | X                |
| 2   | LMT  | D     | 2000 | X         | -        | -       | -                |
| 2   | LMT  | E     | 1101 | X         | -        | -       | X                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47532 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 Multidrug efflux pump subunit AcrB.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1038     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7893  | 5072 | 1306 | 1472 | 43 |         |         |       |
| 1   | B     | 1039     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7900  | 5076 | 1307 | 1474 | 43 |         |         |       |
| 1   | C     | 1035     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7867  | 5057 | 1299 | 1468 | 43 |         |         |       |
| 1   | D     | 1038     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7893  | 5072 | 1306 | 1472 | 43 |         |         |       |
| 1   | E     | 1037     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7883  | 5066 | 1303 | 1471 | 43 |         |         |       |
| 1   | F     | 1037     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7883  | 5066 | 1303 | 1471 | 43 |         |         |       |

There are 36 discrepancies between the modelled and reference sequences:

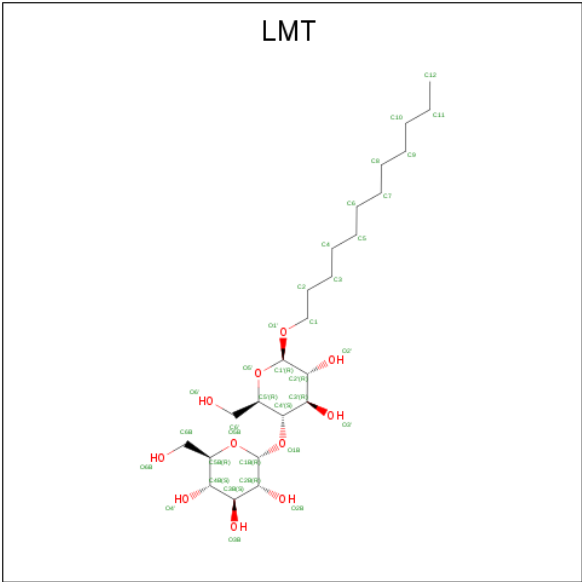
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 615     | GLY      | PHE    | engineered mutation | UNP P31224 |
| A     | ?       | -        | GLY    | deletion            | UNP P31224 |
| A     | ?       | -        | PHE    | deletion            | UNP P31224 |
| A     | ?       | -        | ALA    | deletion            | UNP P31224 |
| A     | ?       | -        | GLY    | deletion            | UNP P31224 |
| A     | ?       | -        | ARG    | deletion            | UNP P31224 |
| B     | 615     | GLY      | PHE    | engineered mutation | UNP P31224 |
| B     | ?       | -        | GLY    | deletion            | UNP P31224 |
| B     | ?       | -        | PHE    | deletion            | UNP P31224 |
| B     | ?       | -        | ALA    | deletion            | UNP P31224 |
| B     | ?       | -        | GLY    | deletion            | UNP P31224 |
| B     | ?       | -        | ARG    | deletion            | UNP P31224 |
| C     | 615     | GLY      | PHE    | engineered mutation | UNP P31224 |
| C     | ?       | -        | GLY    | deletion            | UNP P31224 |
| C     | ?       | -        | PHE    | deletion            | UNP P31224 |
| C     | ?       | -        | ALA    | deletion            | UNP P31224 |
| C     | ?       | -        | GLY    | deletion            | UNP P31224 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | ?       | -        | ARG    | deletion            | UNP P31224 |
| D     | 615     | GLY      | PHE    | engineered mutation | UNP P31224 |
| D     | ?       | -        | GLY    | deletion            | UNP P31224 |
| D     | ?       | -        | PHE    | deletion            | UNP P31224 |
| D     | ?       | -        | ALA    | deletion            | UNP P31224 |
| D     | ?       | -        | GLY    | deletion            | UNP P31224 |
| D     | ?       | -        | ARG    | deletion            | UNP P31224 |
| E     | 615     | GLY      | PHE    | engineered mutation | UNP P31224 |
| E     | ?       | -        | GLY    | deletion            | UNP P31224 |
| E     | ?       | -        | PHE    | deletion            | UNP P31224 |
| E     | ?       | -        | ALA    | deletion            | UNP P31224 |
| E     | ?       | -        | GLY    | deletion            | UNP P31224 |
| E     | ?       | -        | ARG    | deletion            | UNP P31224 |
| F     | 615     | GLY      | PHE    | engineered mutation | UNP P31224 |
| F     | ?       | -        | GLY    | deletion            | UNP P31224 |
| F     | ?       | -        | PHE    | deletion            | UNP P31224 |
| F     | ?       | -        | ALA    | deletion            | UNP P31224 |
| F     | ?       | -        | GLY    | deletion            | UNP P31224 |
| F     | ?       | -        | ARG    | deletion            | UNP P31224 |

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | C  | O       | 0       |
|     |       |          | 35    | 24 | 11      |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 2   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 2   | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 2   | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 2   | E     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 2   | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

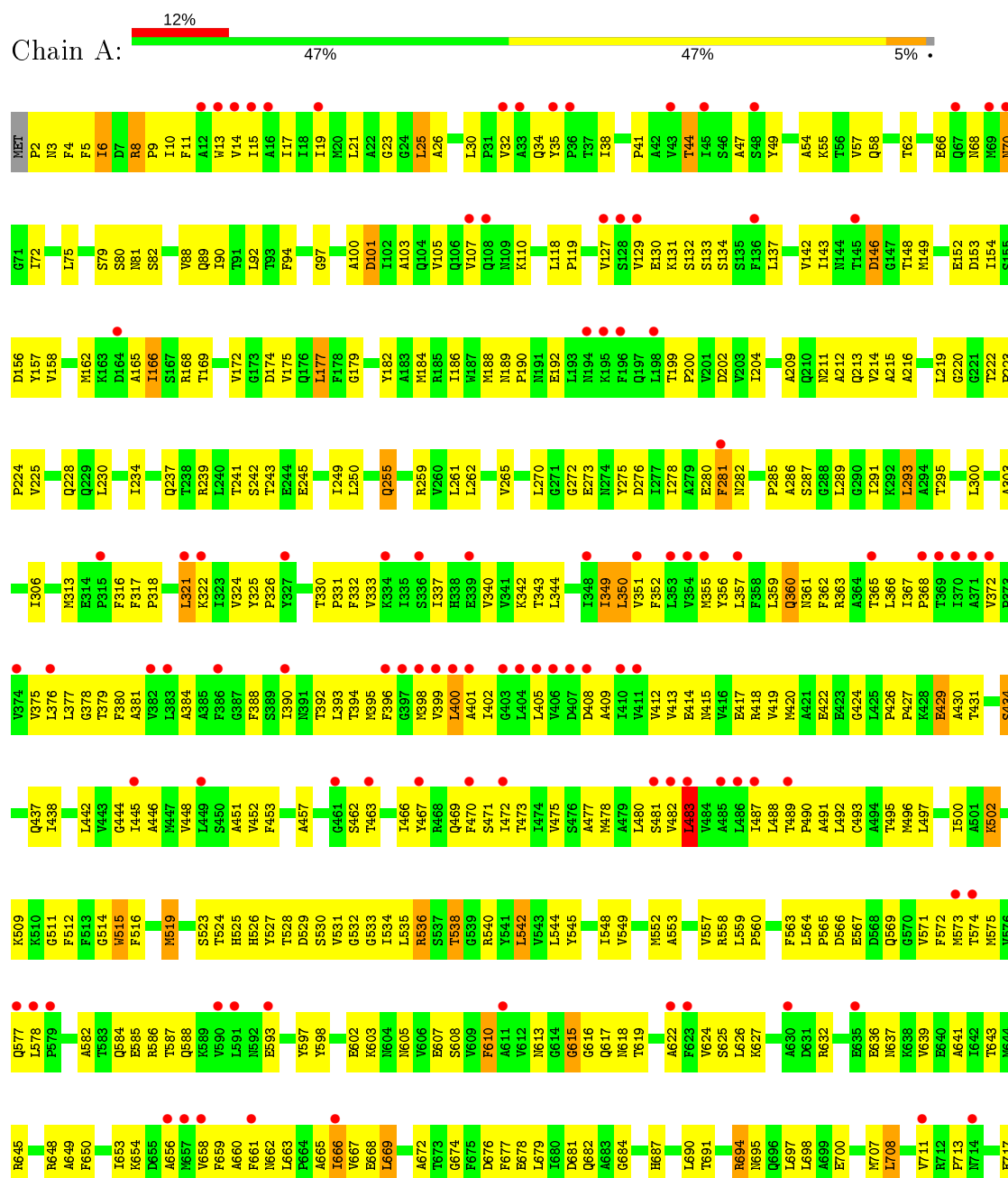
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

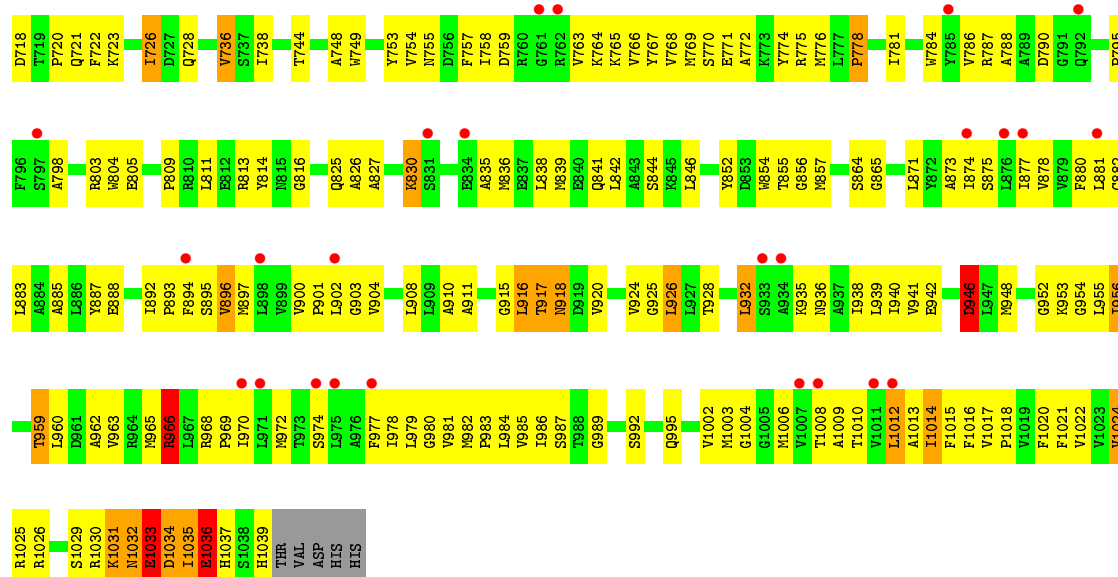
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Ni | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Ni | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Ni | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

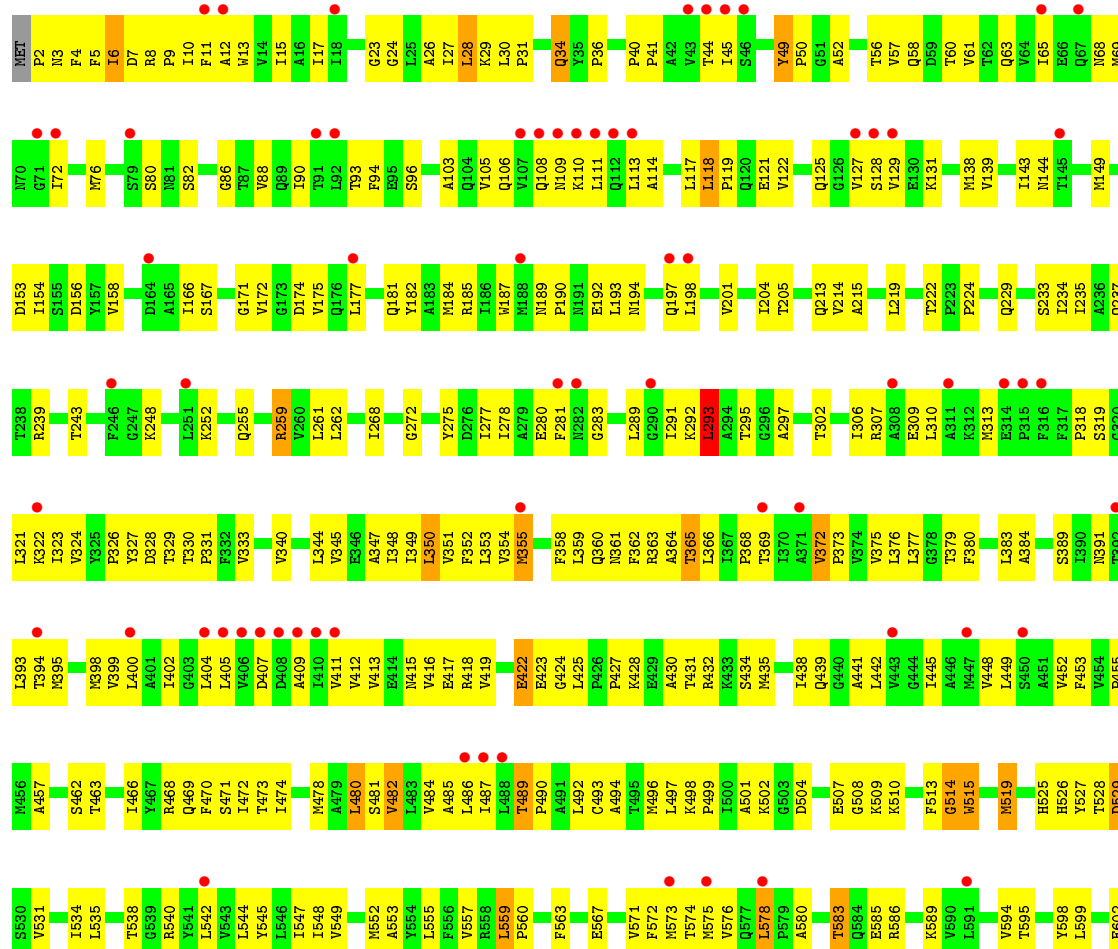
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Multidrug efflux pump subunit AcrB



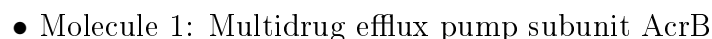


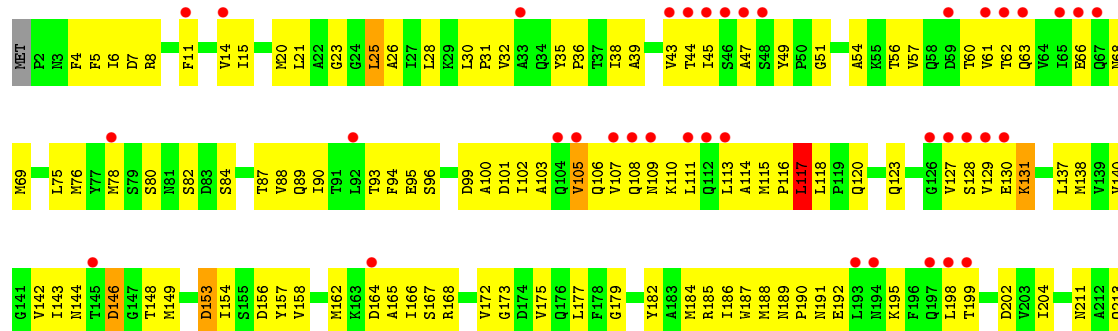
• Molecule 1: Multidrug efflux pump subunit AcrB

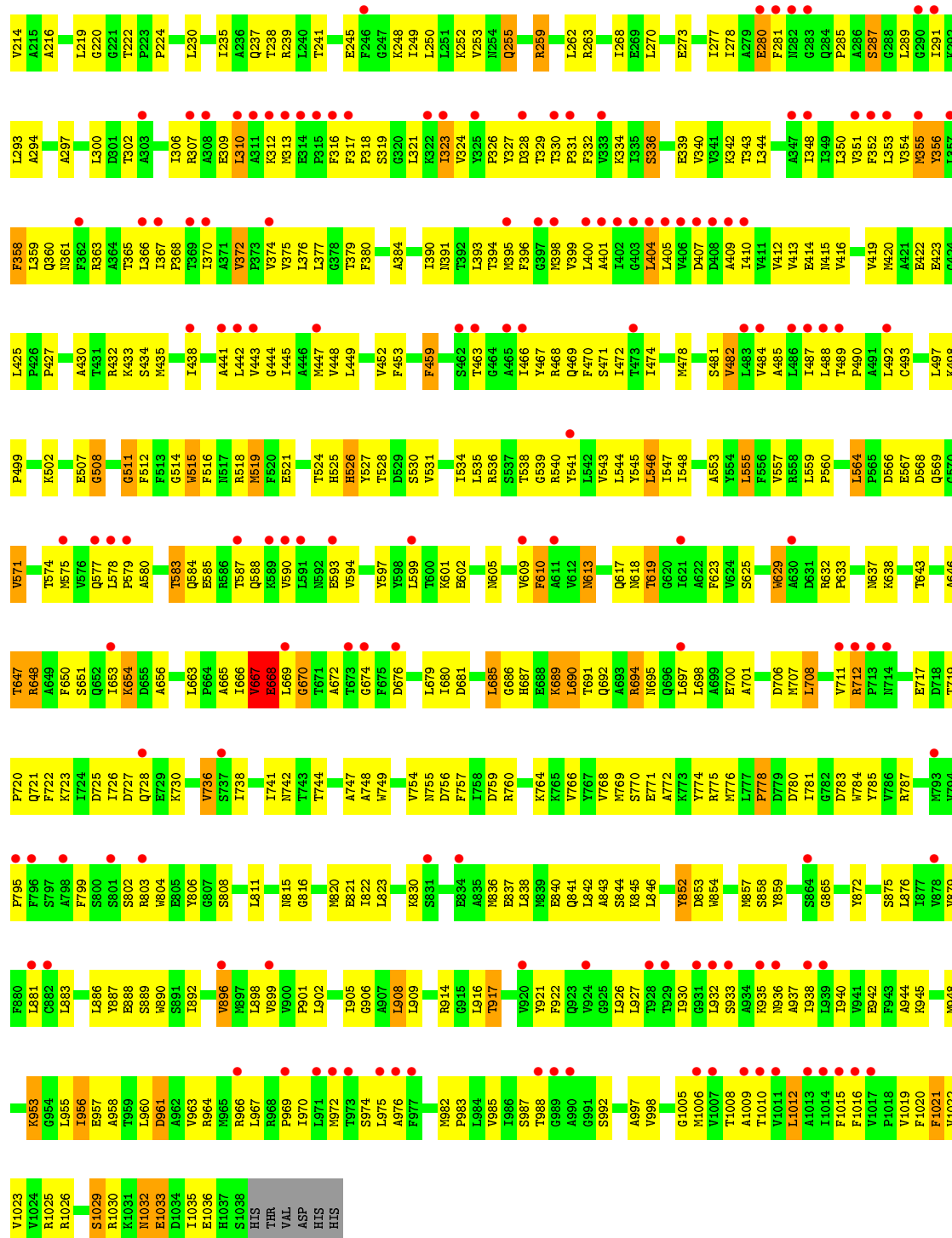






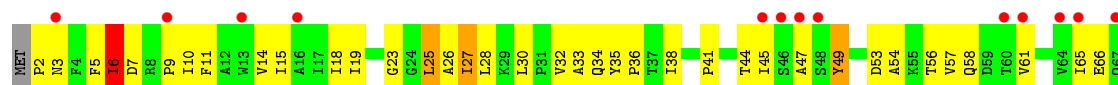


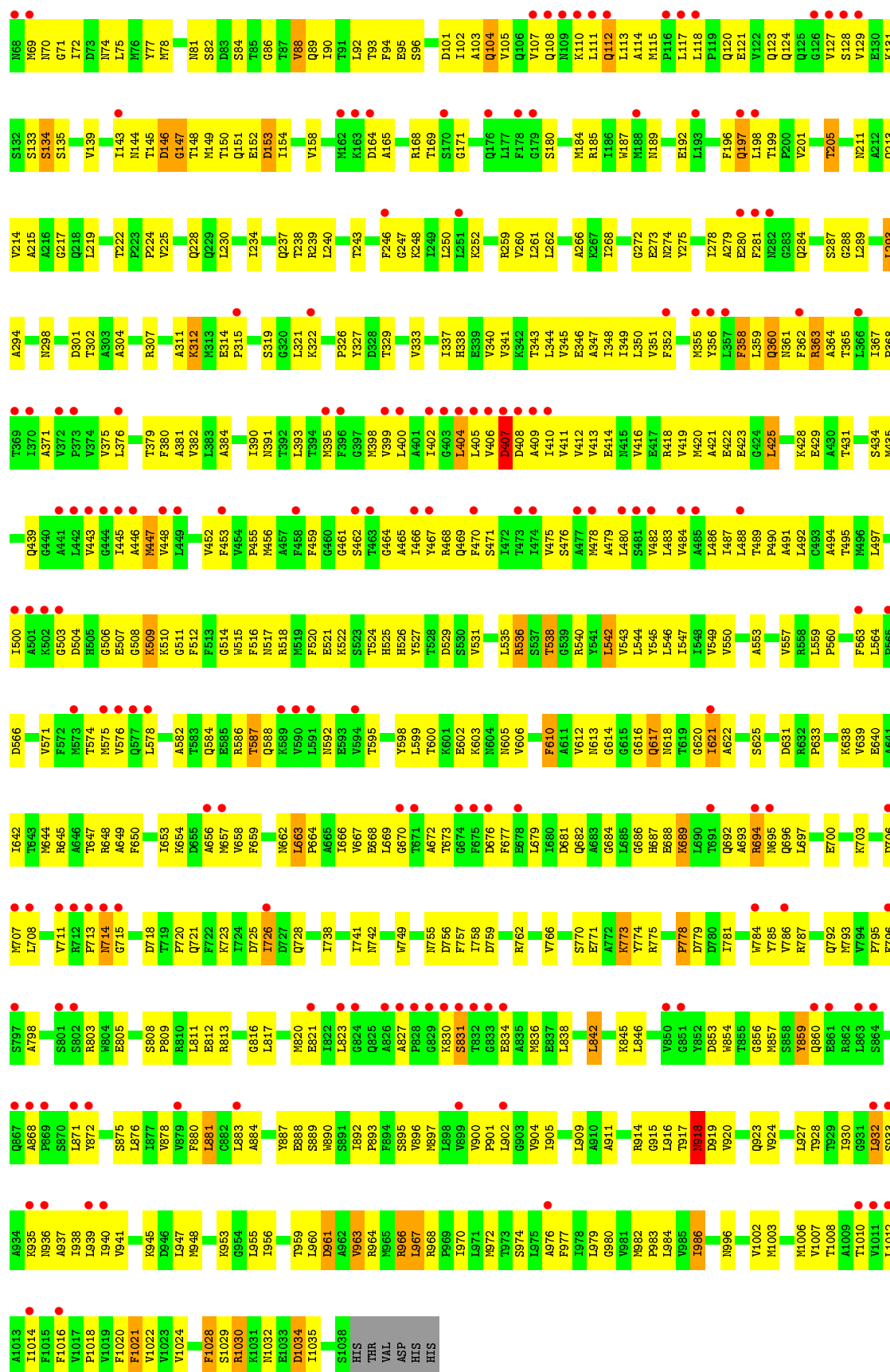




• Molecule 1: Multidrug efflux pump subunit AcrB

Chain F:





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 152.07Å 157.78Å 219.39Å<br>90.00° 93.14° 90.00°             | Depositor        |
| Resolution (Å)  | 20.00 – 3.40<br>109.53 – 3.40                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (20.00-3.40)<br>97.9 (109.53-3.40)                     | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.93 (at 3.41Å)   | Xtriage          |
| Refinement program  | PHENIX 1.8.2_1309   | Depositor        |
| R, $R_{free}$   | 0.275 , 0.349<br>0.285 , 0.354                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7110 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 98.9  | Xtriage          |
| Anisotropy  | 0.077   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 74.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.80  | EDS              |
| Total number of atoms   | 47532   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 77.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8623e-05.*

<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: NI, LMT

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     | 0.65         | 1/8043 (0.0%)  | 0.89        | 11/10922 (0.1%) |
| 1   | B     | 0.65         | 1/8050 (0.0%)  | 0.89        | 9/10932 (0.1%)  |
| 1   | C     | 0.67         | 1/8015 (0.0%)  | 0.91        | 9/10884 (0.1%)  |
| 1   | D     | 0.60         | 1/8043 (0.0%)  | 0.89        | 15/10922 (0.1%) |
| 1   | E     | 0.60         | 1/8032 (0.0%)  | 0.87        | 12/10907 (0.1%) |
| 1   | F     | 0.60         | 0/8032         | 0.89        | 7/10907 (0.1%)  |
| All | All   | 0.63         | 5/48215 (0.0%) | 0.89        | 63/65474 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 3                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | D     | 515 | TRP  | CB-CG | 7.50 | 1.63        | 1.50     |
| 1   | A     | 515 | TRP  | CB-CG | 6.68 | 1.62        | 1.50     |
| 1   | E     | 515 | TRP  | CB-CG | 5.77 | 1.60        | 1.50     |
| 1   | B     | 515 | TRP  | CB-CG | 5.72 | 1.60        | 1.50     |
| 1   | C     | 515 | TRP  | CB-CG | 5.07 | 1.59        | 1.50     |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | D     | 939  | LEU  | CA-CB-CG   | -8.38 | 96.02       | 115.30   |
| 1   | C     | 529  | ASP  | CB-CG-OD1  | 8.07  | 125.56      | 118.30   |
| 1   | F     | 529  | ASP  | CB-CG-OD1  | 7.98  | 125.48      | 118.30   |
| 1   | A     | 529  | ASP  | CB-CG-OD1  | 7.69  | 125.22      | 118.30   |
| 1   | D     | 350  | LEU  | CA-CB-CG   | -7.26 | 98.61       | 115.30   |
| 1   | B     | 480  | LEU  | CA-CB-CG   | -7.17 | 98.80       | 115.30   |
| 1   | D     | 979  | LEU  | CA-CB-CG   | -6.85 | 99.55       | 115.30   |
| 1   | E     | 670  | GLY  | N-CA-C     | 6.56  | 129.51      | 113.10   |
| 1   | E     | 908  | LEU  | CA-CB-CG   | 6.55  | 130.37      | 115.30   |
| 1   | B     | 529  | ASP  | CB-CG-OD1  | 6.52  | 124.17      | 118.30   |
| 1   | A     | 250  | LEU  | CA-CB-CG   | 6.50  | 130.25      | 115.30   |
| 1   | A     | 939  | LEU  | CA-CB-CG   | -6.47 | 100.42      | 115.30   |
| 1   | C     | 967  | LEU  | CA-CB-CG   | 6.47  | 130.18      | 115.30   |
| 1   | C     | 72   | ILE  | CG1-CB-CG2 | -6.41 | 97.31       | 111.40   |
| 1   | D     | 511  | GLY  | N-CA-C     | 6.28  | 128.79      | 113.10   |
| 1   | B     | 690  | LEU  | CA-CB-CG   | 6.24  | 129.65      | 115.30   |
| 1   | D     | 529  | ASP  | CB-CG-OD1  | 6.24  | 123.91      | 118.30   |
| 1   | F     | 425  | LEU  | CA-CB-CG   | 6.20  | 129.56      | 115.30   |
| 1   | D     | 198  | LEU  | CA-CB-CG   | 6.20  | 129.55      | 115.30   |
| 1   | E     | 519  | MET  | CB-CG-SD   | 6.13  | 130.78      | 112.40   |
| 1   | F     | 967  | LEU  | CA-CB-CG   | 6.11  | 129.36      | 115.30   |
| 1   | A     | 946  | ASP  | CB-CG-OD1  | 6.10  | 123.79      | 118.30   |
| 1   | D     | 75   | LEU  | CA-CB-CG   | 6.09  | 129.30      | 115.30   |
| 1   | B     | 293  | LEU  | CA-CB-CG   | 6.00  | 129.09      | 115.30   |
| 1   | B     | 519  | MET  | CB-CG-SD   | 5.96  | 130.28      | 112.40   |
| 1   | D     | 534  | ILE  | CG1-CB-CG2 | -5.96 | 98.30       | 111.40   |
| 1   | A     | 932  | LEU  | CA-CB-CG   | -5.93 | 101.67      | 115.30   |
| 1   | A     | 483  | LEU  | CA-CB-CG   | 5.92  | 128.92      | 115.30   |
| 1   | D     | 690  | LEU  | CA-CB-CG   | 5.92  | 128.92      | 115.30   |
| 1   | E     | 117  | LEU  | CA-CB-CG   | 5.82  | 128.69      | 115.30   |
| 1   | F     | 842  | LEU  | CA-CB-CG   | 5.80  | 128.64      | 115.30   |
| 1   | D     | 21   | LEU  | CA-CB-CG   | -5.71 | 102.17      | 115.30   |
| 1   | E     | 1032 | ASN  | C-N-CA     | 5.64  | 135.79      | 121.70   |
| 1   | C     | 979  | LEU  | CA-CB-CG   | -5.61 | 102.39      | 115.30   |
| 1   | D     | 967  | LEU  | CA-CB-CG   | 5.61  | 128.19      | 115.30   |
| 1   | E     | 546  | LEU  | CA-CB-CG   | 5.59  | 128.17      | 115.30   |
| 1   | D     | 293  | LEU  | CA-CB-CG   | 5.55  | 128.07      | 115.30   |
| 1   | B     | 118  | LEU  | CA-CB-CG   | 5.53  | 128.02      | 115.30   |
| 1   | C     | 534  | ILE  | CG1-CB-CG2 | -5.42 | 99.47       | 111.40   |
| 1   | E     | 674  | GLY  | N-CA-C     | 5.42  | 126.65      | 113.10   |
| 1   | B     | 555  | LEU  | CA-CB-CG   | -5.40 | 102.88      | 115.30   |
| 1   | C     | 542  | LEU  | CA-CB-CG   | -5.38 | 102.92      | 115.30   |
| 1   | C     | 30   | LEU  | CA-CB-CG   | 5.38  | 127.67      | 115.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | E     | 287  | SER  | C-N-CA    | -5.33 | 111.11      | 122.30   |
| 1   | A     | 321  | LEU  | CA-CB-CG  | 5.32  | 127.53      | 115.30   |
| 1   | E     | 449  | LEU  | CA-CB-CG  | -5.32 | 103.07      | 115.30   |
| 1   | F     | 536  | ARG  | CG-CD-NE  | 5.29  | 122.91      | 111.80   |
| 1   | C     | 1006 | MET  | CB-CG-SD  | 5.28  | 128.24      | 112.40   |
| 1   | E     | 407  | ASP  | CB-CG-OD2 | 5.25  | 123.03      | 118.30   |
| 1   | D     | 668  | GLU  | N-CA-C    | 5.25  | 125.17      | 111.00   |
| 1   | F     | 932  | LEU  | CA-CB-CG  | 5.22  | 127.30      | 115.30   |
| 1   | A     | 674  | GLY  | N-CA-C    | 5.21  | 126.13      | 113.10   |
| 1   | C     | 898  | LEU  | CB-CG-CD2 | -5.18 | 102.19      | 111.00   |
| 1   | E     | 293  | LEU  | CA-CB-CG  | 5.13  | 127.10      | 115.30   |
| 1   | A     | 8    | ARG  | CB-CG-CD  | -5.13 | 98.27       | 111.60   |
| 1   | D     | 1033 | GLU  | C-N-CA    | 5.11  | 134.47      | 121.70   |
| 1   | F     | 404  | LEU  | CB-CG-CD2 | -5.11 | 102.32      | 111.00   |
| 1   | B     | 902  | LEU  | CA-CB-CG  | 5.09  | 127.01      | 115.30   |
| 1   | B     | 28   | LEU  | CB-CG-CD2 | 5.03  | 119.56      | 111.00   |
| 1   | D     | 488  | LEU  | CA-CB-CG  | -5.03 | 103.74      | 115.30   |
| 1   | E     | 865  | GLY  | N-CA-C    | -5.02 | 100.54      | 113.10   |
| 1   | A     | 966  | ARG  | CB-CA-C   | 5.01  | 120.42      | 110.40   |
| 1   | A     | 357  | LEU  | CA-CB-CG  | 5.00  | 126.81      | 115.30   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1033 | GLU  | Peptide |
| 1   | A     | 1034 | ASP  | Peptide |
| 1   | A     | 1036 | GLU  | Peptide |
| 1   | B     | 1033 | GLU  | Peptide |
| 1   | B     | 1035 | ILE  | Peptide |
| 1   | C     | 6    | ILE  | Peptide |
| 1   | D     | 1035 | ILE  | Peptide |
| 1   | F     | 6    | ILE  | 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     | 7893  | 0        | 8034     | 457     | 0            |
| 1   | B     | 7900  | 0        | 8041     | 384     | 0            |
| 1   | C     | 7867  | 0        | 8015     | 444     | 0            |
| 1   | D     | 7893  | 0        | 8034     | 515     | 0            |
| 1   | E     | 7883  | 0        | 8027     | 461     | 0            |
| 1   | F     | 7883  | 0        | 8027     | 477     | 0            |
| 2   | A     | 35    | 0        | 46       | 4       | 0            |
| 2   | B     | 35    | 0        | 46       | 3       | 0            |
| 2   | C     | 35    | 0        | 46       | 1       | 0            |
| 2   | D     | 35    | 0        | 46       | 3       | 0            |
| 2   | E     | 35    | 0        | 46       | 8       | 0            |
| 2   | F     | 35    | 0        | 46       | 1       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 47532 | 0        | 48454    | 2651    | 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 28.

All (2651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:536:ARG:NE   | 2:E:1101:LMT:O3B | 1.81                     | 1.13              |
| 1:A:424:GLY:HA3  | 1:A:502:LYS:HG2  | 1.38                     | 1.04              |
| 1:D:954:GLY:HA2  | 1:D:1034:ASP:H   | 1.23                     | 1.03              |
| 1:C:686:GLY:HA3  | 1:C:689:LYS:HD3  | 1.42                     | 1.01              |
| 1:D:533:GLY:HA2  | 1:D:536:ARG:HD3  | 1.48                     | 0.95              |
| 1:D:113:LEU:HD11 | 1:F:128:SER:HB3  | 1.46                     | 0.94              |
| 1:A:41:PRO:HG2   | 1:A:94:PHE:HB2   | 1.50                     | 0.92              |
| 1:E:214:VAL:HG11 | 1:F:742:ASN:HB3  | 1.51                     | 0.91              |
| 1:F:340:VAL:HG11 | 1:F:395:MET:HB3  | 1.53                     | 0.91              |
| 1:E:239:ARG:NH1  | 1:E:756:ASP:O    | 2.04                     | 0.90              |
| 1:E:354:VAL:HG22 | 1:E:975:LEU:HD23 | 1.51                     | 0.90              |
| 1:C:151:GLN:NE2  | 1:C:286:ALA:O    | 2.05                     | 0.89              |
| 1:C:151:GLN:NE2  | 1:C:279:ALA:O    | 2.04                     | 0.89              |
| 1:D:571:VAL:HG22 | 1:D:625:SER:HA   | 1.54                     | 0.89              |
| 1:D:776:MET:HE1  | 1:F:225:VAL:H    | 1.37                     | 0.89              |
| 1:E:179:GLY:HA2  | 1:E:277:ILE:HD11 | 1.54                     | 0.89              |
| 1:E:355:MET:HG2  | 1:E:365:THR:HA   | 1.54                     | 0.88              |
| 1:B:34:GLN:HG3   | 1:B:333:VAL:HG22 | 1.55                     | 0.88              |
| 1:A:571:VAL:HG22 | 1:A:625:SER:HA   | 1.56                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:344:LEU:HD22 | 1:C:402:ILE:HD11 | 1.54                     | 0.88              |
| 1:C:61:VAL:HA    | 1:C:118:LEU:HD22 | 1.56                     | 0.87              |
| 1:E:211:ASN:O    | 1:E:755:ASN:ND2  | 2.07                     | 0.87              |
| 1:E:680:ILE:HD11 | 1:E:853:ASP:HB2  | 1.56                     | 0.87              |
| 1:D:446:ALA:HB2  | 1:D:482:VAL:HG21 | 1.56                     | 0.87              |
| 1:C:156:ASP:OD1  | 1:C:760:ARG:NH2  | 2.08                     | 0.87              |
| 1:B:350:LEU:HD22 | 1:B:979:LEU:HB3  | 1.57                     | 0.86              |
| 1:C:939:LEU:HB3  | 1:C:966:ARG:HD2  | 1.58                     | 0.86              |
| 1:D:70:ASN:O     | 1:D:110:LYS:NZ   | 2.09                     | 0.86              |
| 1:D:291:ILE:HD13 | 1:D:306:ILE:HD13 | 1.57                     | 0.85              |
| 1:C:653:ILE:HG13 | 1:C:654:LYS:HE2  | 1.58                     | 0.85              |
| 1:B:278:ILE:HG13 | 1:B:613:ASN:HB3  | 1.59                     | 0.85              |
| 1:A:723:LYS:NZ   | 1:C:236:ALA:O    | 2.09                     | 0.84              |
| 1:F:686:GLY:HA3  | 1:F:689:LYS:HD3  | 1.58                     | 0.84              |
| 1:D:159:ALA:HB2  | 1:D:177:LEU:HD11 | 1.57                     | 0.84              |
| 1:F:961:ASP:OD1  | 1:F:964:ARG:NH2  | 2.11                     | 0.83              |
| 1:A:574:THR:HG21 | 1:A:598:TYR:HE2  | 1.43                     | 0.83              |
| 1:C:264:ASP:OD1  | 1:C:264:ASP:N    | 2.12                     | 0.83              |
| 1:B:415:ASN:HD22 | 1:B:434:SER:HB2  | 1.42                     | 0.83              |
| 1:D:457:ALA:O    | 1:D:468:ARG:NE   | 2.10                     | 0.83              |
| 1:D:156:ASP:OD1  | 1:D:760:ARG:NH2  | 2.12                     | 0.83              |
| 1:D:41:PRO:HG2   | 1:D:94:PHE:HB2   | 1.59                     | 0.82              |
| 1:D:187:TRP:HB3  | 1:D:771:GLU:HA   | 1.59                     | 0.82              |
| 1:B:664:PRO:HB3  | 1:B:669:LEU:HD12 | 1.61                     | 0.82              |
| 1:D:706:ASP:O    | 1:D:830:LYS:NZ   | 2.11                     | 0.82              |
| 1:E:307:ARG:NH2  | 1:E:328:ASP:OD2  | 2.12                     | 0.82              |
| 1:D:400:LEU:HD23 | 1:D:924:VAL:HG12 | 1.61                     | 0.81              |
| 1:D:60:THR:HG23  | 1:D:61:VAL:HG23  | 1.62                     | 0.81              |
| 1:D:953:LYS:NZ   | 1:D:957:GLU:OE1  | 2.13                     | 0.80              |
| 1:E:149:MET:HB2  | 1:E:153:ASP:HB2  | 1.63                     | 0.80              |
| 1:A:237:GLN:OE1  | 1:B:742:ASN:ND2  | 2.14                     | 0.80              |
| 1:F:248:LYS:HA   | 1:F:261:LEU:HD13 | 1.63                     | 0.80              |
| 1:D:453:PHE:O    | 1:D:471:SER:OG   | 1.99                     | 0.80              |
| 1:A:691:THR:HG23 | 1:A:694:ARG:HH12 | 1.47                     | 0.79              |
| 1:D:455:PRO:HG2  | 1:D:875:SER:HB2  | 1.62                     | 0.79              |
| 1:E:1032:ASN:HB3 | 1:E:1033:GLU:HB3 | 1.64                     | 0.79              |
| 1:A:966:ARG:HE   | 1:A:970:ILE:HD11 | 1.46                     | 0.79              |
| 1:E:584:GLN:HB2  | 1:E:617:GLN:HG2  | 1.64                     | 0.79              |
| 1:F:34:GLN:HB2   | 1:F:333:VAL:HG22 | 1.64                     | 0.79              |
| 1:F:930:ILE:O    | 1:F:933:SER:OG   | 2.00                     | 0.79              |
| 1:D:139:VAL:HB   | 1:D:327:TYR:HB3  | 1.65                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:222:THR:HA   | 1:D:224:PRO:HD3  | 1.63                     | 0.79              |
| 1:A:153:ASP:OD2  | 1:A:182:TYR:OH   | 2.00                     | 0.78              |
| 1:C:914:ARG:O    | 1:C:916:LEU:N    | 2.16                     | 0.78              |
| 1:E:516:PHE:HA   | 1:E:519:MET:HG3  | 1.65                     | 0.78              |
| 1:C:262:LEU:HG   | 1:C:268:ILE:HD11 | 1.65                     | 0.78              |
| 1:F:356:TYR:HA   | 1:F:365:THR:HG21 | 1.65                     | 0.78              |
| 1:A:375:VAL:O    | 1:A:379:THR:OG1  | 2.01                     | 0.78              |
| 1:A:955:LEU:O    | 1:A:959:THR:OG1  | 2.01                     | 0.78              |
| 1:A:1034:ASP:HB3 | 1:A:1035:ILE:HA  | 1.66                     | 0.78              |
| 1:B:427:PRO:HD3  | 1:B:499:PRO:HB3  | 1.65                     | 0.78              |
| 1:F:45:ILE:HG12  | 1:F:129:VAL:HG13 | 1.66                     | 0.78              |
| 1:C:360:GLN:OE1  | 1:C:517:ASN:ND2  | 2.15                     | 0.78              |
| 1:D:414:GLU:OE1  | 1:D:968:ARG:NH1  | 2.17                     | 0.78              |
| 1:D:344:LEU:HD23 | 1:D:402:ILE:HD11 | 1.66                     | 0.78              |
| 1:D:211:ASN:O    | 1:D:755:ASN:ND2  | 2.18                     | 0.77              |
| 1:E:966:ARG:O    | 1:E:970:ILE:HG12 | 1.84                     | 0.77              |
| 1:C:3:ASN:N      | 1:C:3:ASN:OD1    | 2.16                     | 0.77              |
| 1:B:327:TYR:HB2  | 1:B:623:PHE:HE2  | 1.47                     | 0.77              |
| 1:F:82:SER:HB2   | 1:F:811:LEU:HB2  | 1.65                     | 0.77              |
| 1:D:457:ALA:HA   | 1:D:468:ARG:HG3  | 1.67                     | 0.77              |
| 1:E:156:ASP:OD1  | 1:E:760:ARG:NH2  | 2.18                     | 0.77              |
| 1:E:708:LEU:HD21 | 1:E:838:LEU:HD12 | 1.67                     | 0.77              |
| 1:B:602:GLU:HG3  | 1:B:605:ASN:HB2  | 1.66                     | 0.77              |
| 1:D:632:ARG:HH12 | 1:D:638:LYS:HA   | 1.50                     | 0.77              |
| 1:E:507:GLU:HG2  | 1:E:518:ARG:HA   | 1.66                     | 0.76              |
| 1:F:662:ASN:O    | 1:F:673:THR:OG1  | 2.03                     | 0.76              |
| 1:A:291:ILE:HD13 | 1:A:306:ILE:HD13 | 1.66                     | 0.76              |
| 1:C:427:PRO:O    | 1:C:431:THR:OG1  | 2.03                     | 0.76              |
| 1:A:344:LEU:HD23 | 1:A:402:ILE:HD11 | 1.67                     | 0.76              |
| 1:C:588:GLN:NE2  | 1:C:592:ASN:OD1  | 2.17                     | 0.76              |
| 1:C:940:ILE:HG12 | 1:C:966:ARG:CZ   | 2.15                     | 0.76              |
| 1:D:1036:GLU:HB3 | 1:D:1037:HIS:HB2 | 1.68                     | 0.76              |
| 1:E:144:ASN:ND2  | 1:E:319:SER:O    | 2.15                     | 0.76              |
| 1:E:415:ASN:HD22 | 1:E:434:SER:HB2  | 1.51                     | 0.76              |
| 1:A:214:VAL:HG11 | 1:B:742:ASN:HB3  | 1.68                     | 0.76              |
| 1:A:34:GLN:HE21  | 1:A:332:PHE:HE2  | 1.34                     | 0.76              |
| 1:A:491:ALA:O    | 1:A:495:THR:OG1  | 2.04                     | 0.76              |
| 1:A:605:ASN:HD21 | 1:A:637:ASN:HA   | 1.51                     | 0.75              |
| 1:E:340:VAL:HG11 | 1:E:395:MET:HB3  | 1.68                     | 0.75              |
| 1:E:343:THR:HG21 | 1:E:399:VAL:HG13 | 1.65                     | 0.75              |
| 1:E:241:THR:N    | 1:E:245:GLU:OE1  | 2.19                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:955:LEU:H    | 1:A:1033:GLU:HA   | 1.52                     | 0.75              |
| 1:C:632:ARG:NH1  | 1:C:637:ASN:O     | 2.19                     | 0.75              |
| 1:C:460:GLY:O    | 1:C:867:GLN:NE2   | 2.20                     | 0.75              |
| 1:E:115:MET:O    | 1:E:123:GLN:NE2   | 2.18                     | 0.75              |
| 1:A:687:HIS:NE2  | 1:A:718:ASP:OD1   | 2.19                     | 0.75              |
| 1:A:776:MET:HE1  | 1:C:225:VAL:H     | 1.50                     | 0.75              |
| 1:A:639:VAL:HG11 | 1:A:662:ASN:HB2   | 1.67                     | 0.75              |
| 1:D:11:PHE:N     | 1:E:888:GLU:OE1   | 2.17                     | 0.75              |
| 1:C:418:ARG:O    | 1:C:422:GLU:HB2   | 1.87                     | 0.75              |
| 1:A:415:ASN:HB3  | 1:A:434:SER:HB2   | 1.67                     | 0.75              |
| 1:E:23:GLY:HA3   | 1:E:377:LEU:HB3   | 1.68                     | 0.74              |
| 1:C:198:LEU:HD11 | 1:C:252:LYS:HB2   | 1.67                     | 0.74              |
| 1:C:708:LEU:HD23 | 1:C:711:VAL:HG21  | 1.69                     | 0.74              |
| 1:D:770:SER:HB3  | 1:D:775:ARG:HD3   | 1.68                     | 0.74              |
| 1:D:588:GLN:NE2  | 1:D:592:ASN:OD1   | 2.18                     | 0.74              |
| 1:B:930:ILE:O    | 1:B:933:SER:OG    | 2.05                     | 0.74              |
| 1:D:966:ARG:HE   | 1:D:970:ILE:HD11  | 1.50                     | 0.74              |
| 1:F:715:GLY:HA3  | 1:F:812:GLU:OE1   | 1.88                     | 0.74              |
| 1:A:955:LEU:HD21 | 1:A:1022:VAL:HG13 | 1.68                     | 0.74              |
| 1:F:598:TYR:HB3  | 1:F:606:VAL:HG21  | 1.68                     | 0.74              |
| 1:A:38:ILE:HD11  | 1:A:466:ILE:HD11  | 1.70                     | 0.74              |
| 1:E:39:ALA:HB2   | 1:E:668:GLU:HG3   | 1.70                     | 0.74              |
| 1:F:936:ASN:HD21 | 1:F:1010:THR:HG22 | 1.52                     | 0.74              |
| 1:A:175:VAL:HG11 | 1:A:289:LEU:HD13  | 1.68                     | 0.74              |
| 1:A:531:VAL:O    | 1:A:534:ILE:HG13  | 1.87                     | 0.74              |
| 1:F:165:ALA:O    | 1:F:169:THR:OG1   | 2.03                     | 0.74              |
| 1:A:707:MET:HG3  | 1:A:708:LEU:HD13  | 1.70                     | 0.73              |
| 1:D:448:VAL:HG22 | 1:D:882:CYS:HB3   | 1.69                     | 0.73              |
| 1:C:418:ARG:NH1  | 1:C:422:GLU:OE1   | 2.20                     | 0.73              |
| 1:C:420:MET:O    | 1:C:424:GLY:N     | 2.20                     | 0.73              |
| 1:F:887:TYR:O    | 1:F:889:SER:N     | 2.17                     | 0.73              |
| 1:A:101:ASP:OD1  | 1:A:101:ASP:N     | 2.20                     | 0.73              |
| 1:A:414:GLU:HG3  | 1:A:972:MET:HE1   | 1.70                     | 0.73              |
| 1:A:989:GLY:O    | 1:A:992:SER:OG    | 2.06                     | 0.73              |
| 1:B:372:VAL:HG23 | 1:B:373:PRO:HD3   | 1.71                     | 0.73              |
| 1:C:49:TYR:HD1   | 1:C:57:VAL:HG12   | 1.53                     | 0.73              |
| 1:A:186:ILE:HB   | 1:A:768:VAL:HG22  | 1.68                     | 0.73              |
| 1:D:587:THR:HB   | 1:D:613:ASN:ND2   | 2.02                     | 0.73              |
| 1:E:945:LYS:HA   | 1:E:948:MET:HE3   | 1.70                     | 0.73              |
| 1:D:587:THR:HB   | 1:D:613:ASN:HD21  | 1.53                     | 0.73              |
| 1:E:759:ASP:OD2  | 1:E:764:LYS:NZ    | 2.21                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:966:ARG:HB3  | 1:A:966:ARG:HH11  | 1.53                     | 0.73              |
| 1:A:584:GLN:HB2  | 1:A:617:GLN:HG2   | 1.71                     | 0.73              |
| 1:B:166:ILE:HD11 | 1:B:310:LEU:HD11  | 1.69                     | 0.73              |
| 1:E:445:ILE:HG22 | 1:E:938:ILE:HD13  | 1.69                     | 0.72              |
| 1:D:56:THR:OG1   | 1:F:213:GLN:NE2   | 2.22                     | 0.72              |
| 1:C:574:THR:HG21 | 1:C:598:TYR:HE2   | 1.53                     | 0.72              |
| 1:D:61:VAL:HA    | 1:D:118:LEU:HD22  | 1.70                     | 0.72              |
| 1:E:184:MET:HB3  | 1:E:766:VAL:HG13  | 1.71                     | 0.72              |
| 1:F:65:ILE:HG21  | 1:F:90:ILE:HD13   | 1.70                     | 0.72              |
| 1:C:49:TYR:CD1   | 1:C:57:VAL:HG12   | 2.25                     | 0.72              |
| 1:C:453:PHE:HD2  | 1:C:456:MET:HE1   | 1.55                     | 0.72              |
| 1:D:351:VAL:HG22 | 1:D:976:ALA:HB1   | 1.71                     | 0.72              |
| 1:E:448:VAL:HG13 | 1:E:879:VAL:HG13  | 1.72                     | 0.72              |
| 1:C:41:PRO:HG2   | 1:C:94:PHE:HB2    | 1.72                     | 0.72              |
| 1:C:853:ASP:OD2  | 1:C:862:ARG:NH2   | 2.23                     | 0.72              |
| 1:B:896:VAL:HG21 | 1:B:938:ILE:HG13  | 1.68                     | 0.72              |
| 1:D:225:VAL:HG22 | 1:E:776:MET:HE2   | 1.72                     | 0.72              |
| 1:E:375:VAL:O    | 1:E:379:THR:OG1   | 2.07                     | 0.72              |
| 1:F:47:ALA:HB3   | 1:F:88:VAL:HG13   | 1.71                     | 0.72              |
| 1:C:580:ALA:HB1  | 1:C:719:THR:HG22  | 1.69                     | 0.71              |
| 1:A:5:PHE:O      | 1:A:8:ARG:N       | 2.15                     | 0.71              |
| 1:D:137:LEU:HD23 | 1:D:291:ILE:HG22  | 1.69                     | 0.71              |
| 1:D:598:TYR:HB3  | 1:D:606:VAL:HG11  | 1.71                     | 0.71              |
| 1:D:602:GLU:OE2  | 1:D:645:ARG:NH1   | 2.23                     | 0.71              |
| 1:B:540:ARG:HH22 | 2:B:2000:LMT:H6'1 | 1.54                     | 0.71              |
| 1:E:351:VAL:HG22 | 1:E:976:ALA:HB1   | 1.72                     | 0.71              |
| 1:F:61:VAL:HA    | 1:F:118:LEU:HD22  | 1.72                     | 0.71              |
| 1:A:225:VAL:H    | 1:B:776:MET:HE1   | 1.54                     | 0.71              |
| 1:D:575:MET:HG2  | 1:D:661:PHE:HE1   | 1.54                     | 0.71              |
| 1:B:350:LEU:HD13 | 1:B:980:GLY:HA2   | 1.70                     | 0.71              |
| 1:B:985:VAL:O    | 1:B:996:ASN:ND2   | 2.23                     | 0.71              |
| 1:F:955:LEU:HD21 | 1:F:1022:VAL:HA   | 1.73                     | 0.71              |
| 1:C:896:VAL:HG23 | 1:C:937:ALA:HB3   | 1.71                     | 0.71              |
| 1:B:174:ASP:HB3  | 1:B:292:LYS:HB2   | 1.72                     | 0.71              |
| 1:B:375:VAL:O    | 1:B:379:THR:OG1   | 2.03                     | 0.71              |
| 1:D:574:THR:HG23 | 1:D:622:ALA:HB3   | 1.71                     | 0.71              |
| 1:B:309:GLU:HG3  | 1:B:313:MET:HE3   | 1.72                     | 0.71              |
| 1:C:2:PRO:O      | 1:C:6:ILE:HG12    | 1.90                     | 0.71              |
| 1:B:61:VAL:HG21  | 1:B:122:VAL:HG21  | 1.72                     | 0.70              |
| 1:C:61:VAL:HG13  | 1:C:118:LEU:HD13  | 1.71                     | 0.70              |
| 1:A:723:LYS:HG2  | 1:A:803:ARG:NH1   | 2.06                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:448:VAL:HG13 | 1:B:879:VAL:HG13  | 1.72                     | 0.70              |
| 1:D:32:VAL:HG22  | 1:D:390:ILE:HB    | 1.73                     | 0.70              |
| 1:D:375:VAL:HB   | 1:D:405:LEU:HD13  | 1.72                     | 0.70              |
| 1:D:880:PHE:CE1  | 1:D:893:PRO:HB2   | 2.26                     | 0.70              |
| 1:C:186:ILE:HG12 | 1:C:268:ILE:HG12  | 1.73                     | 0.70              |
| 1:F:45:ILE:HD11  | 1:F:107:VAL:HG12  | 1.72                     | 0.70              |
| 1:C:940:ILE:HG12 | 1:C:966:ARG:NH2   | 2.06                     | 0.70              |
| 1:F:544:LEU:HA   | 1:F:547:ILE:HD12  | 1.74                     | 0.70              |
| 1:F:892:ILE:HG23 | 1:F:941:VAL:HG11  | 1.72                     | 0.70              |
| 1:A:962:ALA:O    | 1:A:966:ARG:NH1   | 2.25                     | 0.70              |
| 1:B:974:SER:OG   | 1:B:1010:THR:HG21 | 1.92                     | 0.70              |
| 1:F:574:THR:HG23 | 1:F:622:ALA:HB3   | 1.73                     | 0.70              |
| 1:D:941:VAL:HG13 | 1:D:1021:PHE:CE1  | 2.26                     | 0.69              |
| 1:E:82:SER:HB2   | 1:E:811:LEU:HB2   | 1.73                     | 0.69              |
| 1:A:424:GLY:O    | 1:A:502:LYS:NZ    | 2.25                     | 0.69              |
| 1:A:415:ASN:OD1  | 1:A:418:ARG:NH2   | 2.25                     | 0.69              |
| 1:A:653:ILE:HG13 | 1:A:654:LYS:HE2   | 1.75                     | 0.69              |
| 1:B:149:MET:HG3  | 1:B:154:ILE:HG13  | 1.73                     | 0.69              |
| 1:C:248:LYS:HA   | 1:C:261:LEU:HD13  | 1.73                     | 0.69              |
| 1:D:6:ILE:HG22   | 1:D:490:PRO:HB2   | 1.75                     | 0.69              |
| 1:D:186:ILE:HG12 | 1:D:268:ILE:HG12  | 1.74                     | 0.69              |
| 1:F:714:ASN:HB3  | 1:F:821:GLU:HB3   | 1.73                     | 0.69              |
| 1:A:393:LEU:HD12 | 1:A:469:GLN:HG3   | 1.75                     | 0.69              |
| 1:A:1034:ASP:CB  | 1:A:1035:ILE:HA   | 2.22                     | 0.69              |
| 1:B:239:ARG:NH1  | 1:B:756:ASP:HB2   | 2.08                     | 0.69              |
| 1:F:531:VAL:O    | 1:F:535:LEU:HG    | 1.92                     | 0.69              |
| 1:B:144:ASN:ND2  | 1:B:319:SER:O     | 2.23                     | 0.69              |
| 1:B:184:MET:HB2  | 1:B:757:PHE:CE2   | 2.28                     | 0.69              |
| 1:C:144:ASN:HB3  | 1:C:148:THR:HG23  | 1.75                     | 0.69              |
| 1:B:422:GLU:OE2  | 1:B:964:ARG:NH1   | 2.26                     | 0.68              |
| 1:C:326:PRO:O    | 1:C:625:SER:OG    | 2.11                     | 0.68              |
| 1:C:587:THR:OG1  | 1:C:613:ASN:ND2   | 2.26                     | 0.68              |
| 1:D:209:ALA:O    | 1:D:237:GLN:NE2   | 2.23                     | 0.68              |
| 1:D:899:VAL:O    | 1:D:902:LEU:HB2   | 1.93                     | 0.68              |
| 1:E:185:ARG:NH2  | 1:E:273:GLU:O     | 2.24                     | 0.68              |
| 1:C:456:MET:HE3  | 1:C:467:TYR:O     | 1.92                     | 0.68              |
| 1:D:254:ASN:ND2  | 1:D:258:SER:OG    | 2.20                     | 0.68              |
| 1:B:259:ARG:HD3  | 1:B:259:ARG:H     | 1.57                     | 0.68              |
| 1:C:45:ILE:HB    | 1:C:90:ILE:HD12   | 1.75                     | 0.68              |
| 1:D:274:ASN:ND2  | 1:D:276:ASP:OD2   | 2.26                     | 0.68              |
| 1:E:192:GLU:HA   | 1:E:195:LYS:HE3   | 1.74                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:422:GLU:O    | 1:E:502:LYS:NZ    | 2.22                     | 0.68              |
| 1:F:368:PRO:HG3  | 1:F:413:VAL:HG21  | 1.75                     | 0.68              |
| 1:B:383:LEU:HD11 | 1:B:473:THR:HA    | 1.74                     | 0.68              |
| 1:D:914:ARG:O    | 1:D:916:LEU:N     | 2.27                     | 0.68              |
| 1:F:149:MET:HG3  | 1:F:154:ILE:HG13  | 1.75                     | 0.68              |
| 1:F:741:ILE:HG22 | 1:F:786:VAL:HG21  | 1.75                     | 0.68              |
| 1:B:602:GLU:OE2  | 1:B:645:ARG:NH1   | 2.26                     | 0.68              |
| 1:C:278:ILE:HG13 | 1:C:613:ASN:HB3   | 1.75                     | 0.68              |
| 1:A:636:GLU:HB2  | 1:A:645:ARG:HH22  | 1.59                     | 0.68              |
| 1:D:700:GLU:HB3  | 1:D:842:LEU:HD22  | 1.74                     | 0.68              |
| 1:A:511:GLY:HA2  | 1:A:515:TRP:HD1   | 1.57                     | 0.68              |
| 1:B:559:LEU:HD12 | 1:B:918:ASN:HB2   | 1.76                     | 0.68              |
| 1:E:908:LEU:HD23 | 1:E:922:PHE:HZ    | 1.59                     | 0.68              |
| 1:A:367:ILE:HB   | 1:A:368:PRO:HD3   | 1.76                     | 0.67              |
| 1:A:892:ILE:HG12 | 1:A:1025:ARG:HD3  | 1.75                     | 0.67              |
| 1:C:3:ASN:ND2    | 1:C:486:LEU:O     | 2.28                     | 0.67              |
| 1:D:250:LEU:HD13 | 1:D:259:ARG:HB3   | 1.75                     | 0.67              |
| 1:D:707:MET:HG3  | 1:D:708:LEU:HD13  | 1.77                     | 0.67              |
| 1:E:184:MET:HB2  | 1:E:757:PHE:CE2   | 2.29                     | 0.67              |
| 1:C:5:PHE:O      | 1:C:7:ASP:N       | 2.27                     | 0.67              |
| 1:B:219:LEU:HG   | 1:B:234:ILE:HD11  | 1.74                     | 0.67              |
| 1:C:453:PHE:HD2  | 1:C:456:MET:CE    | 2.07                     | 0.67              |
| 1:C:112:GLN:HG3  | 1:C:115:MET:HG3   | 1.77                     | 0.67              |
| 1:C:696:GLN:HE21 | 1:C:845:LYS:HE3   | 1.59                     | 0.67              |
| 1:D:884:ALA:HA   | 1:D:889:SER:O     | 1.94                     | 0.67              |
| 1:F:239:ARG:HB2  | 1:F:758:ILE:HD12  | 1.75                     | 0.67              |
| 1:A:697:LEU:HD12 | 1:A:846:LEU:HD21  | 1.75                     | 0.67              |
| 1:C:942:GLU:HG3  | 1:C:943:PHE:N     | 2.09                     | 0.67              |
| 1:D:47:ALA:HB2   | 1:D:127:VAL:HG13  | 1.76                     | 0.67              |
| 1:E:536:ARG:HE   | 2:E:1101:LMT:H3O1 | 1.39                     | 0.67              |
| 1:E:906:GLY:HA3  | 1:E:1008:THR:HG21 | 1.76                     | 0.67              |
| 1:A:1026:ARG:NH1 | 1:A:1033:GLU:OE1  | 2.27                     | 0.67              |
| 1:A:129:VAL:HG23 | 1:B:113:LEU:HD11  | 1.77                     | 0.67              |
| 1:D:375:VAL:O    | 1:D:379:THR:OG1   | 2.11                     | 0.67              |
| 1:F:211:ASN:O    | 1:F:755:ASN:ND2   | 2.28                     | 0.67              |
| 1:B:156:ASP:OD1  | 1:B:760:ARG:NH2   | 2.27                     | 0.67              |
| 1:D:954:GLY:HA2  | 1:D:1034:ASP:N    | 2.05                     | 0.67              |
| 1:E:1021:PHE:HE2 | 1:E:1025:ARG:HD3  | 1.58                     | 0.67              |
| 1:B:770:SER:HB3  | 1:B:775:ARG:HD3   | 1.77                     | 0.67              |
| 1:D:400:LEU:HD21 | 1:D:925:GLY:HA2   | 1.77                     | 0.67              |
| 1:F:418:ARG:O    | 1:F:422:GLU:HB2   | 1.94                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:443:VAL:O    | 1:F:447:MET:HB3   | 1.95                     | 0.67              |
| 1:B:982:MET:HB3  | 1:B:983:PRO:HD3   | 1.77                     | 0.66              |
| 1:C:855:THR:HA   | 1:C:859:TYR:HB2   | 1.77                     | 0.66              |
| 1:D:545:TYR:HD1  | 1:D:546:LEU:HD23  | 1.60                     | 0.66              |
| 1:D:452:VAL:HA   | 1:D:875:SER:OG    | 1.95                     | 0.66              |
| 1:F:27:ILE:HG22  | 1:F:380:PHE:HB3   | 1.77                     | 0.66              |
| 1:A:511:GLY:HA2  | 1:A:515:TRP:CD1   | 2.31                     | 0.66              |
| 1:A:645:ARG:O    | 1:A:648:ARG:HB3   | 1.95                     | 0.66              |
| 1:B:24:GLY:O     | 1:B:27:ILE:HG22   | 1.95                     | 0.66              |
| 1:B:966:ARG:O    | 1:B:970:ILE:HG12  | 1.96                     | 0.66              |
| 1:D:343:THR:O    | 1:D:346:GLU:N     | 2.28                     | 0.66              |
| 1:D:367:ILE:HG12 | 1:D:492:LEU:HB3   | 1.78                     | 0.66              |
| 1:D:80:SER:HB3   | 1:D:90:ILE:HG23   | 1.76                     | 0.66              |
| 1:F:49:TYR:CD1   | 1:F:57:VAL:HG12   | 2.30                     | 0.66              |
| 1:C:688:GLU:HB3  | 1:C:689:LYS:HD2   | 1.77                     | 0.66              |
| 1:C:57:VAL:HG23  | 1:C:82:SER:HB3    | 1.76                     | 0.66              |
| 1:D:442:LEU:O    | 1:D:445:ILE:HG13  | 1.95                     | 0.66              |
| 1:C:340:VAL:HG11 | 1:C:395:MET:HB3   | 1.76                     | 0.66              |
| 1:E:120:GLN:NE2  | 1:E:123:GLN:OE1   | 2.29                     | 0.66              |
| 1:E:578:LEU:HD21 | 1:E:590:VAL:HG21  | 1.77                     | 0.66              |
| 1:F:707:MET:O    | 1:F:827:ALA:N     | 2.26                     | 0.66              |
| 1:A:9:PRO:HG2    | 1:A:10:ILE:HD12   | 1.76                     | 0.66              |
| 1:D:400:LEU:HD11 | 1:D:1002:VAL:HG21 | 1.77                     | 0.66              |
| 1:D:697:LEU:HD12 | 1:D:846:LEU:HD11  | 1.77                     | 0.66              |
| 1:E:204:ILE:HG12 | 1:E:754:VAL:HG21  | 1.77                     | 0.66              |
| 1:B:683:ALA:O    | 1:B:685:LEU:N     | 2.28                     | 0.66              |
| 1:E:444:GLY:HA3  | 1:E:886:LEU:HD22  | 1.78                     | 0.66              |
| 1:E:441:ALA:O    | 1:E:445:ILE:HG23  | 1.96                     | 0.66              |
| 1:F:41:PRO:HG2   | 1:F:94:PHE:HB2    | 1.78                     | 0.66              |
| 1:F:755:ASN:O    | 1:F:766:VAL:HB    | 1.94                     | 0.66              |
| 1:B:453:PHE:O    | 1:B:471:SER:OG    | 2.11                     | 0.66              |
| 1:A:960:LEU:O    | 1:A:963:VAL:HG12  | 1.95                     | 0.66              |
| 1:E:559:LEU:HD23 | 1:E:560:PRO:HD2   | 1.78                     | 0.66              |
| 1:E:774:TYR:O    | 1:E:784:TRP:NE1   | 2.25                     | 0.65              |
| 1:F:902:LEU:HG   | 1:F:1012:LEU:HB3  | 1.78                     | 0.65              |
| 1:F:428:LYS:HG2  | 1:F:494:ALA:HB1   | 1.78                     | 0.65              |
| 1:F:939:LEU:HB3  | 1:F:966:ARG:HD2   | 1.78                     | 0.65              |
| 1:A:626:LEU:HD11 | 1:A:639:VAL:HG23  | 1.76                     | 0.65              |
| 1:C:400:LEU:HD23 | 1:C:474:ILE:HD11  | 1.78                     | 0.65              |
| 1:F:1016:PHE:HB3 | 1:F:1020:PHE:CE1  | 2.32                     | 0.65              |
| 1:F:880:PHE:HD2  | 1:F:881:LEU:HD22  | 1.62                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:32:VAL:HG22  | 1:A:390:ILE:HB    | 1.77                     | 0.65              |
| 1:D:375:VAL:HG11 | 1:D:405:LEU:HD22  | 1.78                     | 0.65              |
| 1:D:509:LYS:HG2  | 1:D:510:LYS:HG3   | 1.77                     | 0.65              |
| 1:E:101:ASP:OD1  | 1:E:131:LYS:NZ    | 2.20                     | 0.65              |
| 1:F:213:GLN:HA   | 1:F:237:GLN:O     | 1.97                     | 0.65              |
| 1:C:34:GLN:HB2   | 1:C:333:VAL:HG22  | 1.79                     | 0.65              |
| 1:C:584:GLN:HB2  | 1:C:617:GLN:HG2   | 1.79                     | 0.65              |
| 1:B:262:LEU:HG   | 1:B:268:ILE:HD11  | 1.77                     | 0.65              |
| 1:B:567:GLU:OE2  | 1:B:994:ALA:N     | 2.29                     | 0.65              |
| 1:C:146:ASP:O    | 1:C:148:THR:N     | 2.29                     | 0.65              |
| 1:F:198:LEU:HD21 | 1:F:252:LYS:HB2   | 1.77                     | 0.65              |
| 1:F:588:GLN:OE1  | 1:F:592:ASN:ND2   | 2.28                     | 0.65              |
| 1:A:940:ILE:HG12 | 1:A:966:ARG:CZ    | 2.26                     | 0.65              |
| 1:C:82:SER:HB2   | 1:C:811:LEU:HB2   | 1.79                     | 0.65              |
| 1:C:172:VAL:HG13 | 1:C:291:ILE:HG23  | 1.79                     | 0.65              |
| 1:F:527:TYR:CE1  | 1:F:1014:ILE:HD12 | 2.32                     | 0.65              |
| 1:C:188:MET:HB3  | 1:C:193:LEU:HD11  | 1.78                     | 0.65              |
| 1:D:1028:PHE:O   | 1:D:1030:ARG:N    | 2.29                     | 0.65              |
| 1:E:156:ASP:OD2  | 1:E:764:LYS:NZ    | 2.26                     | 0.65              |
| 1:F:612:VAL:HB   | 1:F:621:ILE:HG22  | 1.78                     | 0.65              |
| 1:F:197:GLN:HA   | 1:F:793:MET:SD    | 2.36                     | 0.65              |
| 1:B:573:MET:HG3  | 1:B:661:PHE:CE2   | 2.32                     | 0.65              |
| 1:D:511:GLY:HA2  | 1:D:515:TRP:CD1   | 2.31                     | 0.65              |
| 1:E:5:PHE:HA     | 1:E:8:ARG:HB2     | 1.78                     | 0.65              |
| 1:F:278:ILE:HG13 | 1:F:613:ASN:HB3   | 1.79                     | 0.65              |
| 1:F:966:ARG:HH21 | 1:F:970:ILE:HD11  | 1.60                     | 0.65              |
| 1:A:527:TYR:OH   | 1:A:1014:ILE:O    | 2.06                     | 0.65              |
| 1:D:694:ARG:NH2  | 1:D:717:GLU:OE1   | 2.29                     | 0.65              |
| 1:A:143:ILE:O    | 1:A:321:LEU:HD22  | 1.96                     | 0.64              |
| 1:A:883:LEU:HD22 | 1:A:887:TYR:CE2   | 2.32                     | 0.64              |
| 1:B:350:LEU:CD2  | 1:B:979:LEU:HB3   | 2.27                     | 0.64              |
| 1:E:326:PRO:O    | 1:E:625:SER:OG    | 2.15                     | 0.64              |
| 1:A:1037:HIS:HB3 | 1:A:1039:HIS:H    | 1.62                     | 0.64              |
| 1:A:538:THR:HG22 | 1:A:542:LEU:HD22  | 1.79                     | 0.64              |
| 1:B:61:VAL:HG13  | 1:B:118:LEU:HD22  | 1.79                     | 0.64              |
| 1:A:182:TYR:O    | 1:A:764:LYS:HD3   | 1.98                     | 0.64              |
| 1:F:664:PRO:HG3  | 1:F:670:GLY:HA3   | 1.78                     | 0.64              |
| 1:A:184:MET:HB2  | 1:A:757:PHE:CE2   | 2.32                     | 0.64              |
| 1:B:197:GLN:HA   | 1:B:793:MET:SD    | 2.37                     | 0.64              |
| 1:F:420:MET:HB3  | 1:F:500:ILE:HB    | 1.80                     | 0.64              |
| 1:A:368:PRO:HB3  | 1:A:409:ALA:HB1   | 1.79                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:236:ALA:O    | 1:E:723:LYS:NZ    | 2.30                     | 0.64              |
| 1:E:330:THR:HG22 | 1:E:334:LYS:HE2   | 1.80                     | 0.64              |
| 1:B:139:VAL:O    | 1:B:326:PRO:HD2   | 1.98                     | 0.64              |
| 1:C:249:ILE:HB   | 1:C:262:LEU:HB2   | 1.80                     | 0.64              |
| 1:C:32:VAL:HG22  | 1:C:390:ILE:HB    | 1.80                     | 0.64              |
| 1:E:213:GLN:HA   | 1:E:237:GLN:O     | 1.97                     | 0.64              |
| 1:E:687:HIS:NE2  | 1:E:808:SER:HB2   | 2.13                     | 0.64              |
| 1:F:582:ALA:HB2  | 1:F:586:ARG:HH21  | 1.63                     | 0.64              |
| 1:C:388:PHE:CZ   | 1:C:472:ILE:HG21  | 2.33                     | 0.64              |
| 1:D:200:PRO:HA   | 1:D:203:VAL:HG23  | 1.79                     | 0.64              |
| 1:E:610:PHE:N    | 1:E:623:PHE:O     | 2.26                     | 0.64              |
| 1:A:643:THR:HB   | 1:A:660:ALA:O     | 1.98                     | 0.64              |
| 1:A:827:ALA:HB3  | 1:A:830:LYS:HB2   | 1.78                     | 0.64              |
| 1:E:605:ASN:OD1  | 1:E:637:ASN:ND2   | 2.31                     | 0.64              |
| 1:F:164:ASP:HB3  | 1:F:168:ARG:NH2   | 2.13                     | 0.64              |
| 1:B:572:PHE:HA   | 1:B:663:LEU:HD21  | 1.80                     | 0.64              |
| 1:F:895:SER:HB3  | 1:F:1024:VAL:HG11 | 1.80                     | 0.64              |
| 1:F:527:TYR:CE2  | 1:F:963:VAL:HG13  | 2.33                     | 0.64              |
| 1:A:564:LEU:HB2  | 1:A:666:ILE:HD11  | 1.78                     | 0.63              |
| 1:A:966:ARG:O    | 1:A:970:ILE:HG12  | 1.98                     | 0.63              |
| 1:B:222:THR:HA   | 1:B:224:PRO:HD3   | 1.81                     | 0.63              |
| 1:D:45:ILE:HA    | 1:D:128:SER:O     | 1.97                     | 0.63              |
| 1:E:579:PRO:HD3  | 1:E:656:ALA:HB2   | 1.78                     | 0.63              |
| 1:F:240:LEU:HB2  | 1:F:246:PHE:CE1   | 2.33                     | 0.63              |
| 1:F:75:LEU:HD21  | 1:F:78:MET:HB2    | 1.81                     | 0.63              |
| 1:A:94:PHE:CE1   | 1:A:103:ALA:HB1   | 2.34                     | 0.63              |
| 1:E:94:PHE:CE1   | 1:E:103:ALA:HB1   | 2.34                     | 0.63              |
| 1:F:932:LEU:HD22 | 1:F:1006:MET:HE1  | 1.80                     | 0.63              |
| 1:F:914:ARG:O    | 1:F:916:LEU:N     | 2.28                     | 0.63              |
| 1:B:201:VAL:O    | 1:B:205:THR:OG1   | 2.11                     | 0.63              |
| 1:F:144:ASN:O    | 1:F:148:THR:OG1   | 2.11                     | 0.63              |
| 1:F:151:GLN:NE2  | 1:F:279:ALA:O     | 2.31                     | 0.63              |
| 1:F:653:ILE:HD12 | 1:F:654:LYS:HE2   | 1.79                     | 0.63              |
| 1:B:527:TYR:OH   | 1:B:1014:ILE:O    | 2.11                     | 0.63              |
| 1:B:455:PRO:HG2  | 1:B:875:SER:OG    | 1.97                     | 0.63              |
| 1:B:190:PRO:HG3  | 1:B:774:TYR:HB3   | 1.78                     | 0.63              |
| 1:E:445:ILE:HG21 | 1:E:935:LYS:HD2   | 1.80                     | 0.63              |
| 1:F:344:LEU:O    | 1:F:348:ILE:HG13  | 1.98                     | 0.63              |
| 1:F:689:LYS:H    | 1:F:689:LYS:HD2   | 1.62                     | 0.63              |
| 1:E:778:PRO:O    | 1:E:781:ILE:HG12  | 1.98                     | 0.63              |
| 1:F:135:SER:HB3  | 1:F:668:GLU:HB3   | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:45:ILE:HB    | 1:F:90:ILE:HD12  | 1.79                     | 0.63              |
| 1:C:892:ILE:HG23 | 1:C:941:VAL:HG11 | 1.80                     | 0.63              |
| 1:D:632:ARG:NH1  | 1:D:637:ASN:O    | 2.32                     | 0.63              |
| 1:D:677:PHE:HD2  | 1:D:822:ILE:HD12 | 1.61                     | 0.63              |
| 1:E:189:ASN:HB3  | 1:E:192:GLU:HB2  | 1.80                     | 0.63              |
| 1:E:840:GLU:HG2  | 1:E:852:TYR:CE1  | 2.33                     | 0.63              |
| 1:F:890:TRP:HA   | 1:F:890:TRP:CE3  | 2.33                     | 0.63              |
| 1:C:464:GLY:O    | 1:C:468:ARG:HB2  | 1.98                     | 0.63              |
| 1:D:198:LEU:HD11 | 1:D:251:LEU:O    | 1.98                     | 0.63              |
| 1:D:394:THR:HG23 | 1:D:469:GLN:HB3  | 1.79                     | 0.63              |
| 1:D:536:ARG:NH1  | 2:D:2000:LMT:O3B | 2.32                     | 0.63              |
| 1:F:54:ALA:HB2   | 1:F:809:PRO:O    | 1.99                     | 0.63              |
| 1:A:189:ASN:HB3  | 1:A:192:GLU:HB2  | 1.80                     | 0.63              |
| 1:A:241:THR:N    | 1:A:245:GLU:OE2  | 2.29                     | 0.63              |
| 1:A:883:LEU:HD22 | 1:A:887:TYR:HE2  | 1.63                     | 0.63              |
| 1:E:14:VAL:HG22  | 1:F:881:LEU:HD12 | 1.79                     | 0.63              |
| 1:F:66:GLU:OE1   | 1:F:816:GLY:HA2  | 1.99                     | 0.63              |
| 1:F:44:THR:HA    | 1:F:90:ILE:O     | 1.99                     | 0.63              |
| 1:C:99:ASP:HB3   | 1:C:102:ILE:HB   | 1.80                     | 0.62              |
| 1:E:953:LYS:HB3  | 1:E:958:ALA:HB2  | 1.81                     | 0.62              |
| 1:F:663:LEU:HD23 | 1:F:663:LEU:H    | 1.64                     | 0.62              |
| 1:B:978:ILE:HG23 | 1:B:1003:MET:HG3 | 1.81                     | 0.62              |
| 1:D:361:ASN:O    | 1:D:365:THR:HG22 | 1.99                     | 0.62              |
| 1:E:100:ALA:HB1  | 1:E:131:LYS:HE3  | 1.81                     | 0.62              |
| 1:E:165:ALA:HB3  | 1:E:313:MET:CE   | 2.29                     | 0.62              |
| 1:F:201:VAL:O    | 1:F:205:THR:OG1  | 2.14                     | 0.62              |
| 1:B:189:ASN:HB3  | 1:B:192:GLU:HB2  | 1.79                     | 0.62              |
| 1:D:871:LEU:HD23 | 1:D:874:ILE:HD12 | 1.80                     | 0.62              |
| 1:D:216:ALA:N    | 1:E:51:GLY:O     | 2.30                     | 0.62              |
| 1:C:577:GLN:HG3  | 1:C:619:THR:HG22 | 1.82                     | 0.62              |
| 1:E:525:HIS:HA   | 1:E:528:THR:HG22 | 1.81                     | 0.62              |
| 1:A:137:LEU:HD22 | 1:A:293:LEU:HD23 | 1.81                     | 0.62              |
| 1:C:757:PHE:CE1  | 1:C:759:ASP:HB2  | 2.35                     | 0.62              |
| 1:F:146:ASP:O    | 1:F:148:THR:N    | 2.30                     | 0.62              |
| 1:F:211:ASN:ND2  | 1:F:246:PHE:HZ   | 1.97                     | 0.62              |
| 1:A:462:SER:O    | 1:A:466:ILE:HG12 | 1.99                     | 0.62              |
| 1:B:24:GLY:O     | 1:B:28:LEU:HD23  | 1.99                     | 0.62              |
| 1:C:396:PHE:O    | 1:C:400:LEU:HB2  | 2.00                     | 0.62              |
| 1:D:445:ILE:O    | 1:D:449:LEU:HB2  | 2.00                     | 0.62              |
| 1:E:405:LEU:HD22 | 1:E:481:SER:HB3  | 1.82                     | 0.62              |
| 1:A:966:ARG:HB3  | 1:A:966:ARG:NH1  | 2.15                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:842:LEU:O    | 1:B:845:LYS:HB2   | 2.00                     | 0.62              |
| 1:C:453:PHE:HB3  | 1:C:471:SER:HA    | 1.82                     | 0.62              |
| 1:C:947:LEU:HD23 | 1:C:951:GLU:HG3   | 1.81                     | 0.62              |
| 1:F:74:ASN:HB3   | 1:F:95:GLU:HB2    | 1.81                     | 0.62              |
| 1:B:355:MET:HG3  | 1:B:359:LEU:HD12  | 1.81                     | 0.62              |
| 1:C:545:TYR:CE2  | 1:C:1020:PHE:HZ   | 2.17                     | 0.62              |
| 1:C:553:ALA:O    | 1:C:557:VAL:HG23  | 2.00                     | 0.62              |
| 1:D:219:LEU:HG   | 1:D:234:ILE:HD11  | 1.81                     | 0.62              |
| 1:E:679:LEU:HD22 | 1:E:822:ILE:HD11  | 1.81                     | 0.62              |
| 1:F:645:ARG:O    | 1:F:648:ARG:HB3   | 2.00                     | 0.62              |
| 1:A:326:PRO:O    | 1:A:625:SER:OG    | 2.17                     | 0.61              |
| 1:B:248:LYS:HA   | 1:B:261:LEU:HD13  | 1.82                     | 0.61              |
| 1:B:435:MET:SD   | 1:B:490:PRO:HB3   | 2.40                     | 0.61              |
| 1:D:4:PHE:HB2    | 1:D:5:PHE:CD1     | 2.35                     | 0.61              |
| 1:E:908:LEU:HD23 | 1:E:922:PHE:CZ    | 2.34                     | 0.61              |
| 1:E:691:THR:HG23 | 1:E:694:ARG:HH12  | 1.65                     | 0.61              |
| 1:F:367:ILE:HB   | 1:F:368:PRO:HD3   | 1.82                     | 0.61              |
| 1:A:901:PRO:O    | 1:A:904:VAL:N     | 2.33                     | 0.61              |
| 1:F:522:LYS:O    | 1:F:525:HIS:N     | 2.32                     | 0.61              |
| 1:B:941:VAL:HG13 | 1:B:1021:PHE:HE1  | 1.64                     | 0.61              |
| 1:A:974:SER:OG   | 1:A:1010:THR:HG21 | 2.01                     | 0.61              |
| 1:B:204:ILE:HG12 | 1:B:754:VAL:HG21  | 1.83                     | 0.61              |
| 1:D:219:LEU:HD23 | 1:E:749:TRP:CZ3   | 2.36                     | 0.61              |
| 1:F:902:LEU:HD21 | 1:F:1016:PHE:HB2  | 1.82                     | 0.61              |
| 1:A:75:LEU:HD13  | 1:A:92:LEU:HD23   | 1.81                     | 0.61              |
| 1:D:445:ILE:HG21 | 1:D:935:LYS:HD2   | 1.81                     | 0.61              |
| 1:B:1006:MET:O   | 1:B:1010:THR:HG23 | 2.00                     | 0.61              |
| 1:B:80:SER:HB3   | 1:B:90:ILE:HG23   | 1.82                     | 0.61              |
| 1:C:453:PHE:CD2  | 1:C:456:MET:HE1   | 2.34                     | 0.61              |
| 1:D:344:LEU:CD2  | 1:D:402:ILE:HD11  | 2.30                     | 0.61              |
| 1:E:280:GLU:HG3  | 1:E:285:PRO:HA    | 1.81                     | 0.61              |
| 1:E:427:PRO:HD3  | 1:E:499:PRO:HB3   | 1.83                     | 0.61              |
| 1:B:111:LEU:HD21 | 1:B:127:VAL:HG11  | 1.83                     | 0.61              |
| 1:B:172:VAL:HG13 | 1:B:291:ILE:HG23  | 1.83                     | 0.61              |
| 1:C:200:PRO:HB2  | 1:C:744:THR:HG22  | 1.83                     | 0.61              |
| 1:C:348:ILE:HG13 | 1:C:402:ILE:HD13  | 1.83                     | 0.61              |
| 1:E:531:VAL:O    | 1:E:534:ILE:HG13  | 2.01                     | 0.61              |
| 1:C:1032:ASN:H   | 1:C:1033:GLU:HB2  | 1.65                     | 0.61              |
| 1:C:254:ASN:ND2  | 1:C:258:SER:OG    | 2.22                     | 0.61              |
| 1:E:511:GLY:HA2  | 1:E:515:TRP:CD1   | 2.36                     | 0.61              |
| 1:F:57:VAL:HG23  | 1:F:82:SER:HB3    | 1.83                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:49:TYR:HD2   | 1:B:50:PRO:HD2    | 1.66                     | 0.61              |
| 1:E:694:ARG:HH11 | 1:E:694:ARG:HB3   | 1.65                     | 0.61              |
| 1:F:34:GLN:O     | 1:F:391:ASN:HB2   | 2.01                     | 0.61              |
| 1:F:340:VAL:CG1  | 1:F:395:MET:HB3   | 2.28                     | 0.61              |
| 1:F:121:GLU:O    | 1:F:124:GLN:HG2   | 2.00                     | 0.60              |
| 1:A:525:HIS:HA   | 1:A:528:THR:HG22  | 1.82                     | 0.60              |
| 1:B:395:MET:O    | 1:B:398:MET:HB2   | 2.00                     | 0.60              |
| 1:B:697:LEU:HD22 | 1:B:846:LEU:HD11  | 1.83                     | 0.60              |
| 1:C:697:LEU:HD12 | 1:C:846:LEU:HD11  | 1.82                     | 0.60              |
| 1:D:695:ASN:HA   | 1:D:698:LEU:HD12  | 1.83                     | 0.60              |
| 1:E:76:MET:HE3   | 1:E:95:GLU:HA     | 1.83                     | 0.60              |
| 1:B:1038:SER:OG  | 1:B:1039:HIS:N    | 2.31                     | 0.60              |
| 1:C:752:SER:O    | 1:C:767:TYR:HA    | 2.00                     | 0.60              |
| 1:D:26:ALA:HB1   | 1:D:384:ALA:HB2   | 1.84                     | 0.60              |
| 1:E:332:PHE:O    | 1:E:336:SER:OG    | 2.15                     | 0.60              |
| 1:E:544:LEU:O    | 1:E:548:ILE:HG13  | 2.01                     | 0.60              |
| 1:D:75:LEU:HD11  | 1:D:92:LEU:HD23   | 1.82                     | 0.60              |
| 1:F:538:THR:HG23 | 1:F:542:LEU:HD13  | 1.83                     | 0.60              |
| 1:A:448:VAL:HG22 | 1:A:882:CYS:HB3   | 1.84                     | 0.60              |
| 1:A:723:LYS:HD2  | 1:C:235:ILE:O     | 2.01                     | 0.60              |
| 1:C:925:GLY:HA2  | 1:C:1002:VAL:HG22 | 1.84                     | 0.60              |
| 1:E:1006:MET:O   | 1:E:1010:THR:HG23 | 2.00                     | 0.60              |
| 1:F:896:VAL:HG23 | 1:F:937:ALA:CB    | 2.32                     | 0.60              |
| 1:A:281:PHE:CE1  | 1:A:324:VAL:HG21  | 2.36                     | 0.60              |
| 1:A:605:ASN:OD1  | 1:A:637:ASN:ND2   | 2.34                     | 0.60              |
| 1:C:515:TRP:HD1  | 1:C:518:ARG:HH12  | 1.49                     | 0.60              |
| 1:C:689:LYS:HA   | 1:C:692:GLN:OE1   | 2.01                     | 0.60              |
| 1:C:892:ILE:O    | 1:C:896:VAL:HG12  | 2.02                     | 0.60              |
| 1:E:670:GLY:HA2  | 1:E:857:MET:SD    | 2.42                     | 0.60              |
| 1:F:576:VAL:HG13 | 1:F:658:VAL:HG22  | 1.84                     | 0.60              |
| 1:F:638:LYS:HE2  | 1:F:640:GLU:HG3   | 1.84                     | 0.60              |
| 1:F:935:LYS:HE2  | 1:F:936:ASN:OD1   | 2.01                     | 0.60              |
| 1:B:213:GLN:HA   | 1:B:237:GLN:O     | 2.02                     | 0.60              |
| 1:B:7:ASP:OD2    | 1:B:432:ARG:NH2   | 2.34                     | 0.60              |
| 1:C:676:ASP:HB3  | 1:C:823:LEU:HD23  | 1.82                     | 0.60              |
| 1:E:57:VAL:HB    | 1:E:88:VAL:HG23   | 1.84                     | 0.60              |
| 1:A:188:MET:O    | 1:A:771:GLU:HB2   | 2.02                     | 0.60              |
| 1:B:778:PRO:O    | 1:B:781:ILE:HG12  | 2.02                     | 0.60              |
| 1:D:3:ASN:O      | 1:D:6:ILE:N       | 2.35                     | 0.60              |
| 1:E:1008:THR:O   | 1:E:1012:LEU:HB2  | 2.01                     | 0.60              |
| 1:F:359:LEU:HB2  | 1:F:365:THR:HG22  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:880:PHE:HD1  | 1:A:897:MET:CE    | 2.15                     | 0.60              |
| 1:C:171:GLY:HA3  | 1:C:302:THR:OG1   | 2.01                     | 0.60              |
| 1:C:582:ALA:HA   | 1:C:586:ARG:HH21  | 1.67                     | 0.60              |
| 1:C:694:ARG:HD3  | 1:C:820:MET:SD    | 2.42                     | 0.60              |
| 1:D:30:LEU:HD12  | 1:D:31:PRO:HD2    | 1.84                     | 0.60              |
| 1:F:379:THR:HG23 | 1:F:476:SER:OG    | 2.02                     | 0.60              |
| 1:B:757:PHE:HE1  | 1:B:759:ASP:HB2   | 1.65                     | 0.59              |
| 1:C:1030:ARG:HB2 | 1:C:1030:ARG:HH21 | 1.66                     | 0.59              |
| 1:C:884:ALA:HB1  | 1:C:890:TRP:CZ3   | 2.37                     | 0.59              |
| 1:D:13:TRP:CZ2   | 1:D:492:LEU:HD21  | 2.36                     | 0.59              |
| 1:E:396:PHE:O    | 1:E:400:LEU:HB2   | 2.02                     | 0.59              |
| 1:F:239:ARG:NH1  | 1:F:756:ASP:HB2   | 2.17                     | 0.59              |
| 1:A:549:VAL:O    | 1:A:552:MET:HB3   | 2.02                     | 0.59              |
| 1:C:15:ILE:O     | 1:C:19:ILE:HG13   | 2.02                     | 0.59              |
| 1:D:95:GLU:HB2   | 1:D:98:THR:OG1    | 2.02                     | 0.59              |
| 1:F:61:VAL:HG13  | 1:F:118:LEU:HD13  | 1.83                     | 0.59              |
| 1:F:470:PHE:CD2  | 1:F:924:VAL:HG11  | 2.37                     | 0.59              |
| 1:F:892:ILE:HD12 | 1:F:1021:PHE:HE1  | 1.67                     | 0.59              |
| 1:A:216:ALA:HB1  | 1:A:234:ILE:O     | 2.02                     | 0.59              |
| 1:A:602:GLU:HG3  | 1:A:605:ASN:HB2   | 1.84                     | 0.59              |
| 1:A:771:GLU:HB3  | 1:A:774:TYR:HD1   | 1.68                     | 0.59              |
| 1:B:187:TRP:HB3  | 1:B:771:GLU:HA    | 1.85                     | 0.59              |
| 1:C:291:ILE:HG21 | 1:C:306:ILE:HD11  | 1.84                     | 0.59              |
| 1:D:1036:GLU:HB3 | 1:D:1037:HIS:CB   | 2.32                     | 0.59              |
| 1:D:414:GLU:CD   | 1:D:969:PRO:HG3   | 2.22                     | 0.59              |
| 1:D:467:TYR:HE1  | 1:D:920:VAL:HG22  | 1.66                     | 0.59              |
| 1:D:941:VAL:HG13 | 1:D:1021:PHE:HE1  | 1.68                     | 0.59              |
| 1:E:361:ASN:O    | 1:E:365:THR:HG22  | 2.01                     | 0.59              |
| 1:F:54:ALA:HB2   | 1:F:809:PRO:C     | 2.22                     | 0.59              |
| 1:A:523:SER:O    | 1:A:526:HIS:HB2   | 2.03                     | 0.59              |
| 1:A:700:GLU:HB3  | 1:A:842:LEU:HD22  | 1.84                     | 0.59              |
| 1:B:94:PHE:CE1   | 1:B:103:ALA:HB1   | 2.37                     | 0.59              |
| 1:B:327:TYR:HB2  | 1:B:623:PHE:CE2   | 2.34                     | 0.59              |
| 1:B:598:TYR:HB3  | 1:B:606:VAL:HG21  | 1.82                     | 0.59              |
| 1:F:15:ILE:O     | 1:F:19:ILE:HG13   | 2.01                     | 0.59              |
| 1:A:721:GLN:HB3  | 1:C:233:SER:O     | 2.02                     | 0.59              |
| 1:C:249:ILE:O    | 1:C:262:LEU:N     | 2.35                     | 0.59              |
| 1:C:545:TYR:OH   | 1:C:898:LEU:O     | 2.13                     | 0.59              |
| 1:E:1032:ASN:CB  | 1:E:1033:GLU:HB3  | 2.32                     | 0.59              |
| 1:A:610:PHE:O    | 1:A:622:ALA:HA    | 2.03                     | 0.59              |
| 1:B:143:ILE:HG12 | 1:B:322:LYS:O     | 2.02                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:945:LYS:HZ1  | 1:B:1025:ARG:HH21 | 1.50                     | 0.59              |
| 1:E:545:TYR:OH   | 1:E:898:LEU:O     | 2.19                     | 0.59              |
| 1:B:677:PHE:HE2  | 1:B:679:LEU:HB2   | 1.67                     | 0.59              |
| 1:E:853:ASP:OD1  | 1:E:854:TRP:N     | 2.35                     | 0.59              |
| 1:D:213:GLN:HA   | 1:D:237:GLN:O     | 2.02                     | 0.59              |
| 1:D:26:ALA:HB1   | 1:D:384:ALA:CB    | 2.33                     | 0.59              |
| 1:E:140:VAL:HG13 | 1:E:324:VAL:O     | 2.02                     | 0.59              |
| 1:B:492:LEU:O    | 1:B:496:MET:HG2   | 2.03                     | 0.59              |
| 1:B:858:SER:O    | 1:B:862:ARG:HB2   | 2.02                     | 0.59              |
| 1:D:737:SER:O    | 1:D:741:ILE:HG13  | 2.03                     | 0.59              |
| 1:D:795:PRO:HG2  | 1:D:798:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:920:VAL:O    | 1:A:924:VAL:HG23  | 2.03                     | 0.58              |
| 1:C:455:PRO:HG2  | 1:C:875:SER:HA    | 1.85                     | 0.58              |
| 1:D:694:ARG:NH1  | 1:D:820:MET:SD    | 2.76                     | 0.58              |
| 1:F:595:THR:O    | 1:F:599:LEU:HG    | 2.03                     | 0.58              |
| 1:A:593:GLU:OE2  | 1:A:654:LYS:NZ    | 2.34                     | 0.58              |
| 1:E:599:LEU:HD21 | 1:E:609:VAL:HG23  | 1.84                     | 0.58              |
| 1:E:955:LEU:HD21 | 1:E:1022:VAL:HA   | 1.85                     | 0.58              |
| 1:F:133:SER:O    | 1:F:134:SER:HB2   | 2.02                     | 0.58              |
| 1:F:689:LYS:CD   | 1:F:689:LYS:H     | 2.16                     | 0.58              |
| 1:A:582:ALA:HB2  | 1:A:586:ARG:HH21  | 1.68                     | 0.58              |
| 1:A:736:VAL:HG22 | 1:A:788:ALA:HB2   | 1.85                     | 0.58              |
| 1:D:465:ALA:O    | 1:D:469:GLN:HG2   | 2.02                     | 0.58              |
| 1:E:7:ASP:CG     | 1:E:432:ARG:HH21  | 2.07                     | 0.58              |
| 1:C:700:GLU:OE1  | 1:C:845:LYS:HE2   | 2.03                     | 0.58              |
| 1:D:549:VAL:O    | 1:D:552:MET:HB3   | 2.03                     | 0.58              |
| 1:D:887:TYR:CD2  | 1:D:892:ILE:HG22  | 2.38                     | 0.58              |
| 1:E:540:ARG:HH22 | 2:E:1101:LMT:HG'2 | 1.68                     | 0.58              |
| 1:F:184:MET:HB2  | 1:F:757:PHE:CE2   | 2.38                     | 0.58              |
| 1:F:452:VAL:O    | 1:F:455:PRO:HD2   | 2.03                     | 0.58              |
| 1:F:693:ALA:O    | 1:F:696:GLN:HB3   | 2.03                     | 0.58              |
| 1:A:400:LEU:HD12 | 1:A:928:THR:HG21  | 1.85                     | 0.58              |
| 1:A:574:THR:HG21 | 1:A:598:TYR:CE2   | 2.32                     | 0.58              |
| 1:B:908:LEU:HD23 | 1:B:922:PHE:HZ    | 1.68                     | 0.58              |
| 1:D:181:GLN:HG2  | 1:D:182:TYR:N     | 2.18                     | 0.58              |
| 1:D:773:LYS:HB3  | 1:F:225:VAL:HG11  | 1.85                     | 0.58              |
| 1:E:367:ILE:HD11 | 1:E:497:LEU:HD13  | 1.84                     | 0.58              |
| 1:E:38:ILE:HD13  | 1:E:466:ILE:HG12  | 1.85                     | 0.58              |
| 1:E:415:ASN:O    | 1:E:419:VAL:HG23  | 2.03                     | 0.58              |
| 1:E:463:THR:O    | 1:E:467:TYR:HD1   | 1.86                     | 0.58              |
| 1:F:571:VAL:HG22 | 1:F:625:SER:HA    | 1.86                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:616:GLY:O    | 1:F:618:ASN:N     | 2.37                     | 0.58              |
| 1:F:884:ALA:HB2  | 1:F:893:PRO:HG2   | 1.85                     | 0.58              |
| 1:A:530:SER:HG   | 2:A:1101:LMT:H2O2 | 1.49                     | 0.58              |
| 1:C:597:TYR:HE1  | 1:C:601:LYS:HD2   | 1.68                     | 0.58              |
| 1:E:166:ILE:HA   | 1:E:309:GLU:HG2   | 1.84                     | 0.58              |
| 1:E:526:HIS:O    | 1:E:530:SER:HB2   | 2.03                     | 0.58              |
| 1:A:770:SER:HB3  | 1:A:775:ARG:HD3   | 1.83                     | 0.58              |
| 1:B:906:GLY:HA3  | 1:B:1008:THR:OG1  | 2.04                     | 0.58              |
| 1:A:881:LEU:HB3  | 1:C:14:VAL:HG13   | 1.85                     | 0.58              |
| 1:D:388:PHE:HE1  | 1:D:472:ILE:HG21  | 1.69                     | 0.58              |
| 1:A:130:GLU:OE1  | 1:A:174:ASP:HB2   | 2.04                     | 0.58              |
| 1:B:149:MET:HB2  | 1:B:153:ASP:HB2   | 1.86                     | 0.58              |
| 1:C:140:VAL:HG11 | 1:C:310:LEU:HD21  | 1.86                     | 0.58              |
| 1:C:336:SER:O    | 1:C:340:VAL:HG23  | 2.04                     | 0.58              |
| 1:D:251:LEU:HD11 | 1:D:262:LEU:HD13  | 1.84                     | 0.58              |
| 1:E:687:HIS:CE1  | 1:E:808:SER:HB2   | 2.38                     | 0.58              |
| 1:F:563:PHE:CZ   | 1:F:564:LEU:HD13  | 2.39                     | 0.58              |
| 1:A:1032:ASN:N   | 1:A:1035:ILE:HD11 | 2.18                     | 0.58              |
| 1:A:728:GLN:HE22 | 1:A:738:ILE:HG21  | 1.69                     | 0.58              |
| 1:B:545:TYR:CE2  | 1:B:1020:PHE:HZ   | 2.21                     | 0.58              |
| 1:C:211:ASN:OD1  | 1:C:240:LEU:HG    | 2.04                     | 0.58              |
| 1:B:602:GLU:OE1  | 1:B:645:ARG:HD2   | 2.04                     | 0.58              |
| 1:C:222:THR:HA   | 1:C:224:PRO:HD3   | 1.85                     | 0.58              |
| 1:D:438:ILE:O    | 1:D:441:ALA:HB3   | 2.03                     | 0.58              |
| 1:F:185:ARG:NH2  | 1:F:273:GLU:O     | 2.28                     | 0.58              |
| 1:F:536:ARG:HD2  | 2:F:2000:LMT:O4'  | 2.04                     | 0.58              |
| 1:A:105:VAL:HG13 | 1:B:109:ASN:HD21  | 1.68                     | 0.57              |
| 1:A:749:TRP:HZ3  | 1:C:219:LEU:HD23  | 1.67                     | 0.57              |
| 1:B:559:LEU:HD22 | 1:B:560:PRO:HD2   | 1.85                     | 0.57              |
| 1:E:239:ARG:NH1  | 1:E:755:ASN:OD1   | 2.37                     | 0.57              |
| 1:E:653:ILE:HG13 | 1:E:654:LYS:HD2   | 1.86                     | 0.57              |
| 1:E:686:GLY:H    | 1:E:689:LYS:HB2   | 1.68                     | 0.57              |
| 1:C:216:ALA:HB1  | 1:C:234:ILE:O     | 2.05                     | 0.57              |
| 1:C:356:TYR:CD1  | 1:C:365:THR:HG21  | 2.39                     | 0.57              |
| 1:F:164:ASP:CG   | 1:F:762:ARG:HH22  | 2.07                     | 0.57              |
| 1:F:187:TRP:HB3  | 1:F:771:GLU:HA    | 1.85                     | 0.57              |
| 1:A:531:VAL:O    | 1:A:535:LEU:HG    | 2.05                     | 0.57              |
| 1:E:78:MET:N     | 1:E:815:ASN:OD1   | 2.33                     | 0.57              |
| 1:E:354:VAL:HG21 | 1:E:976:ALA:HB2   | 1.86                     | 0.57              |
| 1:F:982:MET:HB3  | 1:F:983:PRO:HD3   | 1.86                     | 0.57              |
| 1:A:1022:VAL:O   | 1:A:1026:ARG:HG3  | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:1035:ILE:O   | 1:D:1036:GLU:HG3 | 2.04                     | 0.57              |
| 1:D:264:ASP:N    | 1:D:264:ASP:OD1  | 2.37                     | 0.57              |
| 1:E:902:LEU:HG   | 1:E:1012:LEU:HB3 | 1.85                     | 0.57              |
| 1:E:1029:SER:OG  | 1:E:1030:ARG:N   | 2.31                     | 0.57              |
| 1:A:280:GLU:HG3  | 1:A:285:PRO:HA   | 1.85                     | 0.57              |
| 1:B:677:PHE:CE2  | 1:B:822:ILE:HD12 | 2.39                     | 0.57              |
| 1:D:525:HIS:HA   | 1:D:528:THR:HG22 | 1.86                     | 0.57              |
| 1:A:350:LEU:HD13 | 1:A:980:GLY:HA2  | 1.86                     | 0.57              |
| 1:B:415:ASN:O    | 1:B:419:VAL:HG23 | 2.05                     | 0.57              |
| 1:C:756:ASP:OD1  | 1:C:765:LYS:HA   | 2.04                     | 0.57              |
| 1:E:278:ILE:CG1  | 1:E:613:ASN:HB3  | 2.35                     | 0.57              |
| 1:E:854:TRP:CE3  | 1:E:858:SER:HB3  | 2.40                     | 0.57              |
| 1:B:676:ASP:N    | 1:B:858:SER:OG   | 2.33                     | 0.57              |
| 1:C:597:TYR:CE1  | 1:C:601:LYS:HD2  | 2.39                     | 0.57              |
| 1:C:739:ASN:O    | 1:C:743:THR:OG1  | 2.18                     | 0.57              |
| 1:C:75:LEU:HD11  | 1:C:92:LEU:HD12  | 1.86                     | 0.57              |
| 1:D:527:TYR:O    | 1:D:531:VAL:HG23 | 2.05                     | 0.57              |
| 1:E:889:SER:HB3  | 1:E:892:ILE:HG13 | 1.87                     | 0.57              |
| 1:A:259:ARG:NH1  | 1:B:729:GLU:OE2  | 2.38                     | 0.57              |
| 1:B:531:VAL:HA   | 1:B:534:ILE:HG12 | 1.87                     | 0.57              |
| 1:C:563:PHE:O    | 1:C:919:ASP:HB2  | 2.05                     | 0.57              |
| 1:C:884:ALA:HB2  | 1:C:893:PRO:HG2  | 1.85                     | 0.57              |
| 1:C:939:LEU:C    | 1:C:966:ARG:HD2  | 2.24                     | 0.57              |
| 1:D:405:LEU:HD21 | 1:D:477:ALA:HB1  | 1.87                     | 0.57              |
| 1:D:405:LEU:HD22 | 1:D:481:SER:HB3  | 1.87                     | 0.57              |
| 1:E:577:GLN:NE2  | 1:E:618:ASN:OD1  | 2.38                     | 0.57              |
| 1:E:643:THR:O    | 1:E:647:THR:OG1  | 2.23                     | 0.57              |
| 1:B:484:VAL:O    | 1:B:489:THR:HG23 | 2.05                     | 0.57              |
| 1:D:1030:ARG:HE  | 1:D:1031:LYS:HB2 | 1.69                     | 0.57              |
| 1:D:453:PHE:CE2  | 1:D:474:ILE:HG21 | 2.40                     | 0.57              |
| 1:D:677:PHE:CD2  | 1:D:822:ILE:HD12 | 2.39                     | 0.57              |
| 1:E:154:ILE:HG22 | 1:E:287:SER:HB3  | 1.86                     | 0.57              |
| 1:E:540:ARG:HH22 | 2:E:1101:LMT:C6B | 2.18                     | 0.57              |
| 1:F:393:LEU:HD12 | 1:F:469:GLN:HG3  | 1.86                     | 0.57              |
| 1:F:435:MET:HE1  | 1:F:490:PRO:HB3  | 1.85                     | 0.57              |
| 1:F:771:GLU:HB2  | 1:F:774:TYR:CD1  | 2.39                     | 0.57              |
| 1:A:916:LEU:HD13 | 1:A:917:THR:HG22 | 1.87                     | 0.57              |
| 1:A:963:VAL:HA   | 1:A:966:ARG:HH22 | 1.69                     | 0.57              |
| 1:E:697:LEU:HD11 | 1:E:842:LEU:HB3  | 1.86                     | 0.57              |
| 1:F:23:GLY:HA2   | 1:F:381:ALA:HB2  | 1.86                     | 0.57              |
| 1:A:133:SER:OG   | 1:A:134:SER:N    | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:457:ALA:HB2  | 1:A:471:SER:OG   | 2.04                     | 0.56              |
| 1:E:172:VAL:HG22 | 1:E:306:ILE:HD11 | 1.87                     | 0.56              |
| 1:D:225:VAL:H    | 1:E:776:MET:HE1  | 1.70                     | 0.56              |
| 1:A:363:ARG:O    | 1:A:366:LEU:HB2  | 2.05                     | 0.56              |
| 1:A:448:VAL:O    | 1:A:451:ALA:HB3  | 2.05                     | 0.56              |
| 1:B:560:PRO:O    | 1:B:918:ASN:HB3  | 2.04                     | 0.56              |
| 1:C:890:TRP:CE3  | 1:C:890:TRP:HA   | 2.41                     | 0.56              |
| 1:D:247:GLY:O    | 1:D:263:ARG:N    | 2.33                     | 0.56              |
| 1:D:393:LEU:HD22 | 1:D:470:PHE:HE1  | 1.69                     | 0.56              |
| 1:D:516:PHE:HA   | 1:D:519:MET:HG3  | 1.86                     | 0.56              |
| 1:D:564:LEU:HB2  | 1:D:666:ILE:HD11 | 1.87                     | 0.56              |
| 1:D:966:ARG:HH11 | 1:D:966:ARG:HB3  | 1.70                     | 0.56              |
| 1:E:597:TYR:OH   | 1:E:646:ALA:HA   | 2.05                     | 0.56              |
| 1:A:418:ARG:O    | 1:A:422:GLU:HB2  | 2.05                     | 0.56              |
| 1:C:352:PHE:HD1  | 1:C:369:THR:HG21 | 1.70                     | 0.56              |
| 1:D:124:GLN:HA   | 1:E:117:LEU:HD12 | 1.87                     | 0.56              |
| 1:E:470:PHE:O    | 1:E:474:ILE:HG13 | 2.04                     | 0.56              |
| 1:E:697:LEU:HD13 | 1:E:846:LEU:HD21 | 1.87                     | 0.56              |
| 1:F:375:VAL:O    | 1:F:379:THR:OG1  | 2.09                     | 0.56              |
| 1:C:188:MET:SD   | 1:C:200:PRO:HG3  | 2.45                     | 0.56              |
| 1:C:449:LEU:O    | 1:C:452:VAL:HG23 | 2.06                     | 0.56              |
| 1:C:185:ARG:HH12 | 1:C:769:MET:HB2  | 1.70                     | 0.56              |
| 1:E:842:LEU:O    | 1:E:845:LYS:HB2  | 2.05                     | 0.56              |
| 1:A:534:ILE:HD12 | 1:A:535:LEU:HD23 | 1.87                     | 0.56              |
| 1:A:80:SER:HB3   | 1:A:90:ILE:HG23  | 1.88                     | 0.56              |
| 1:A:399:VAL:HG11 | 1:A:984:LEU:HD11 | 1.86                     | 0.56              |
| 1:C:154:ILE:HG22 | 1:C:287:SER:HB3  | 1.87                     | 0.56              |
| 1:C:355:MET:CG   | 1:C:410:ILE:HD11 | 2.36                     | 0.56              |
| 1:A:978:ILE:HG23 | 1:A:1003:MET:HG3 | 1.88                     | 0.56              |
| 1:B:525:HIS:NE2  | 1:B:529:ASP:OD1  | 2.38                     | 0.56              |
| 1:D:393:LEU:HD11 | 1:D:466:ILE:HD13 | 1.86                     | 0.56              |
| 1:E:1022:VAL:O   | 1:E:1026:ARG:HG3 | 2.06                     | 0.56              |
| 1:E:35:TYR:HE2   | 1:E:393:LEU:HD21 | 1.71                     | 0.56              |
| 1:F:514:GLY:HA2  | 1:F:517:ASN:OD1  | 2.06                     | 0.56              |
| 1:F:945:LYS:HA   | 1:F:948:MET:HE3  | 1.88                     | 0.56              |
| 1:A:10:ILE:O     | 1:A:14:VAL:HG23  | 2.04                     | 0.56              |
| 1:A:776:MET:O    | 1:C:219:LEU:HB3  | 2.05                     | 0.56              |
| 1:D:272:GLY:N    | 1:D:275:TYR:OH   | 2.35                     | 0.56              |
| 1:E:280:GLU:O    | 1:E:610:PHE:HA   | 2.06                     | 0.56              |
| 1:F:892:ILE:HD12 | 1:F:1021:PHE:CE1 | 2.40                     | 0.56              |
| 1:A:795:PRO:HG2  | 1:A:798:ALA:HB2  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:423:GLU:O    | 1:D:502:LYS:HB3  | 2.06                     | 0.56              |
| 1:F:347:ALA:HB3  | 1:F:402:ILE:HD12 | 1.88                     | 0.56              |
| 1:F:414:GLU:HG3  | 1:F:972:MET:HE1  | 1.87                     | 0.56              |
| 1:C:602:GLU:OE2  | 1:C:645:ARG:NH1  | 2.39                     | 0.56              |
| 1:E:840:GLU:HG2  | 1:E:852:TYR:HE1  | 1.71                     | 0.56              |
| 1:B:412:VAL:O    | 1:B:416:VAL:HG23 | 2.05                     | 0.56              |
| 1:D:455:PRO:HG2  | 1:D:875:SER:CB   | 2.35                     | 0.56              |
| 1:E:380:PHE:O    | 1:E:384:ALA:N    | 2.39                     | 0.56              |
| 1:E:442:LEU:O    | 1:E:445:ILE:HG13 | 2.06                     | 0.56              |
| 1:C:149:MET:HG3  | 1:C:154:ILE:HG13 | 1.88                     | 0.56              |
| 1:C:921:TYR:HD1  | 1:C:997:ALA:HB3  | 1.69                     | 0.56              |
| 1:D:423:GLU:C    | 1:D:502:LYS:HB3  | 2.26                     | 0.56              |
| 1:F:723:LYS:HG2  | 1:F:803:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:276:ASP:HA   | 1:C:222:THR:HG21 | 1.88                     | 0.55              |
| 1:A:300:LEU:HD11 | 1:A:333:VAL:HG11 | 1.88                     | 0.55              |
| 1:A:632:ARG:HB3  | 1:A:637:ASN:HB3  | 1.88                     | 0.55              |
| 1:F:351:VAL:HG22 | 1:F:976:ALA:HB1  | 1.87                     | 0.55              |
| 1:A:273:GLU:HG2  | 1:A:765:LYS:HD2  | 1.89                     | 0.55              |
| 1:B:281:PHE:CZ   | 1:B:324:VAL:HG21 | 2.40                     | 0.55              |
| 1:B:463:THR:HA   | 1:B:466:ILE:HD12 | 1.88                     | 0.55              |
| 1:B:908:LEU:HD23 | 1:B:922:PHE:CZ   | 2.41                     | 0.55              |
| 1:C:391:ASN:O    | 1:C:394:THR:OG1  | 2.21                     | 0.55              |
| 1:D:347:ALA:O    | 1:D:351:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:701:ALA:HB1  | 1:D:711:VAL:HG11 | 1.88                     | 0.55              |
| 1:D:185:ARG:HH12 | 1:D:769:MET:HB2  | 1.70                     | 0.55              |
| 1:E:157:TYR:CZ   | 1:E:318:PRO:HD3  | 2.41                     | 0.55              |
| 1:F:578:LEU:HD12 | 1:F:587:THR:HG22 | 1.88                     | 0.55              |
| 1:A:544:LEU:O    | 1:A:548:ILE:HG13 | 2.07                     | 0.55              |
| 1:D:170:SER:HB2  | 1:E:75:LEU:H     | 1.71                     | 0.55              |
| 1:D:574:THR:HG21 | 1:D:598:TYR:HE2  | 1.71                     | 0.55              |
| 1:E:412:VAL:O    | 1:E:416:VAL:HG23 | 2.07                     | 0.55              |
| 1:F:58:GLN:OE1   | 1:F:811:LEU:HB3  | 2.07                     | 0.55              |
| 1:F:896:VAL:HG23 | 1:F:937:ALA:HB1  | 1.89                     | 0.55              |
| 1:A:222:THR:HA   | 1:A:224:PRO:HD3  | 1.88                     | 0.55              |
| 1:A:572:PHE:HB2  | 1:A:661:PHE:O    | 2.05                     | 0.55              |
| 1:B:898:LEU:HB3  | 1:B:1020:PHE:CE2 | 2.42                     | 0.55              |
| 1:C:184:MET:HB3  | 1:C:766:VAL:HG13 | 1.88                     | 0.55              |
| 1:C:896:VAL:HG23 | 1:C:937:ALA:CB   | 2.36                     | 0.55              |
| 1:D:888:GLU:OE1  | 1:F:11:PHE:HB2   | 2.07                     | 0.55              |
| 1:D:59:ASP:OD2   | 1:F:758:ILE:HD13 | 2.07                     | 0.55              |
| 1:B:1031:LYS:H   | 1:B:1033:GLU:HG3 | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:165:ALA:O    | 1:C:169:THR:OG1  | 2.09                     | 0.55              |
| 1:C:391:ASN:OD1  | 1:C:393:LEU:HB2  | 2.07                     | 0.55              |
| 1:D:470:PHE:CD2  | 1:D:924:VAL:HG21 | 2.42                     | 0.55              |
| 1:E:167:SER:HB3  | 1:E:175:VAL:HG21 | 1.88                     | 0.55              |
| 1:E:281:PHE:HB2  | 1:E:610:PHE:CE1  | 2.41                     | 0.55              |
| 1:F:1028:PHE:O   | 1:F:1030:ARG:N   | 2.40                     | 0.55              |
| 1:F:135:SER:HB2  | 1:F:667:VAL:HG12 | 1.89                     | 0.55              |
| 1:A:146:ASP:OD2  | 1:A:146:ASP:N    | 2.36                     | 0.55              |
| 1:C:68:ASN:HB3   | 1:C:110:LYS:O    | 2.07                     | 0.55              |
| 1:D:778:PRO:O    | 1:D:781:ILE:HG12 | 2.06                     | 0.55              |
| 1:D:448:VAL:HG22 | 1:D:882:CYS:CB   | 2.37                     | 0.55              |
| 1:E:613:ASN:C    | 1:E:613:ASN:HD22 | 2.10                     | 0.55              |
| 1:A:3:ASN:HA     | 1:A:6:ILE:HG23   | 1.89                     | 0.55              |
| 1:A:514:GLY:C    | 1:A:516:PHE:H    | 2.10                     | 0.55              |
| 1:B:184:MET:HB2  | 1:B:757:PHE:CD2  | 2.42                     | 0.55              |
| 1:C:508:GLY:O    | 1:C:509:LYS:HB2  | 2.06                     | 0.55              |
| 1:C:722:PHE:CE2  | 1:C:802:SER:HB2  | 2.42                     | 0.55              |
| 1:C:942:GLU:HG3  | 1:C:943:PHE:HD1  | 1.71                     | 0.55              |
| 1:D:449:LEU:HB3  | 1:D:478:MET:SD   | 2.46                     | 0.55              |
| 1:D:836:MET:HG2  | 1:D:854:TRP:CZ2  | 2.42                     | 0.55              |
| 1:E:105:VAL:HG21 | 1:F:105:VAL:HG13 | 1.89                     | 0.55              |
| 1:F:974:SER:HA   | 1:F:1006:MET:HE3 | 1.89                     | 0.55              |
| 1:F:143:ILE:O    | 1:F:321:LEU:HD22 | 2.06                     | 0.55              |
| 1:F:298:ASN:HB3  | 1:F:301:ASP:OD2  | 2.07                     | 0.55              |
| 1:F:412:VAL:O    | 1:F:416:VAL:HG23 | 2.06                     | 0.55              |
| 1:F:728:GLN:OE1  | 1:F:738:ILE:HG12 | 2.07                     | 0.55              |
| 1:D:501:ALA:O    | 1:D:504:ASP:HB2  | 2.06                     | 0.55              |
| 1:D:723:LYS:HG2  | 1:D:803:ARG:CZ   | 2.37                     | 0.55              |
| 1:E:569:GLN:NE2  | 1:E:665:ALA:HA   | 2.21                     | 0.55              |
| 1:A:105:VAL:HG13 | 1:B:109:ASN:ND2  | 2.22                     | 0.55              |
| 1:A:281:PHE:CD1  | 1:A:324:VAL:HG11 | 2.42                     | 0.55              |
| 1:A:356:TYR:HD1  | 1:A:365:THR:HG21 | 1.72                     | 0.55              |
| 1:D:143:ILE:O    | 1:D:321:LEU:HD22 | 2.07                     | 0.55              |
| 1:E:149:MET:HG3  | 1:E:154:ILE:HG13 | 1.89                     | 0.55              |
| 1:E:220:GLY:HA3  | 1:E:230:LEU:O    | 2.07                     | 0.55              |
| 1:A:1002:VAL:O   | 1:A:1006:MET:HG2 | 2.07                     | 0.55              |
| 1:A:778:PRO:O    | 1:A:781:ILE:HG12 | 2.07                     | 0.55              |
| 1:B:757:PHE:CE1  | 1:B:759:ASP:HB2  | 2.41                     | 0.55              |
| 1:C:200:PRO:HA   | 1:C:203:VAL:CG2  | 2.37                     | 0.55              |
| 1:D:175:VAL:HG11 | 1:D:289:LEU:HD13 | 1.88                     | 0.55              |
| 1:D:366:LEU:HD23 | 1:D:369:THR:HB   | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:188:MET:O    | 1:E:771:GLU:HB2   | 2.06                     | 0.55              |
| 1:E:712:ARG:HH21 | 1:E:823:LEU:HB3   | 1.71                     | 0.55              |
| 1:F:352:PHE:HA   | 1:F:355:MET:HE2   | 1.88                     | 0.55              |
| 1:F:688:GLU:HB3  | 1:F:689:LYS:HD2   | 1.89                     | 0.55              |
| 1:A:396:PHE:HZ   | 1:A:995:GLN:HG2   | 1.70                     | 0.54              |
| 1:B:425:LEU:HD12 | 1:B:430:ALA:HA    | 1.89                     | 0.54              |
| 1:C:108:GLN:O    | 1:C:112:GLN:HB2   | 2.07                     | 0.54              |
| 1:C:382:VAL:HG12 | 1:C:472:ILE:HD11  | 1.89                     | 0.54              |
| 1:C:531:VAL:HA   | 1:C:534:ILE:HG12  | 1.89                     | 0.54              |
| 1:D:166:ILE:HD12 | 1:D:306:ILE:HG23  | 1.88                     | 0.54              |
| 1:D:595:THR:O    | 1:D:599:LEU:HG    | 2.05                     | 0.54              |
| 1:E:352:PHE:HE1  | 1:E:366:LEU:HD23  | 1.72                     | 0.54              |
| 1:E:435:MET:SD   | 1:E:490:PRO:HB3   | 2.46                     | 0.54              |
| 1:A:559:LEU:HD23 | 1:A:560:PRO:HD2   | 1.89                     | 0.54              |
| 1:B:631:ASP:C    | 1:B:633:PRO:HD3   | 2.28                     | 0.54              |
| 1:B:404:LEU:HD12 | 1:B:932:LEU:HD21  | 1.89                     | 0.54              |
| 1:C:568:ASP:O    | 1:C:629:TRP:CH2   | 2.61                     | 0.54              |
| 1:C:795:PRO:HG2  | 1:C:798:ALA:HB2   | 1.90                     | 0.54              |
| 1:D:449:LEU:O    | 1:D:452:VAL:HG22  | 2.07                     | 0.54              |
| 1:E:355:MET:HB3  | 1:E:365:THR:OG1   | 2.06                     | 0.54              |
| 1:E:613:ASN:ND2  | 1:E:619:THR:O     | 2.40                     | 0.54              |
| 1:E:940:ILE:HD11 | 1:E:970:ILE:HD11  | 1.90                     | 0.54              |
| 1:F:455:PRO:HG3  | 1:F:878:VAL:HG21  | 1.89                     | 0.54              |
| 1:F:974:SER:OG   | 1:F:1010:THR:HG21 | 2.07                     | 0.54              |
| 1:A:377:LEU:O    | 1:A:380:PHE:HB2   | 2.07                     | 0.54              |
| 1:B:586:ARG:O    | 1:B:589:LYS:HB3   | 2.07                     | 0.54              |
| 1:C:355:MET:HG2  | 1:C:410:ILE:HD11  | 1.88                     | 0.54              |
| 1:D:188:MET:HB3  | 1:D:193:LEU:HD11  | 1.88                     | 0.54              |
| 1:E:887:TYR:O    | 1:E:889:SER:N     | 2.40                     | 0.54              |
| 1:A:158:VAL:HG22 | 1:A:162:MET:HE3   | 1.89                     | 0.54              |
| 1:A:202:ASP:OD1  | 1:A:787:ARG:NH2   | 2.38                     | 0.54              |
| 1:A:426:PRO:HD2  | 1:A:429:GLU:HG3   | 1.87                     | 0.54              |
| 1:B:739:ASN:O    | 1:B:743:THR:OG1   | 2.09                     | 0.54              |
| 1:C:408:ASP:O    | 1:C:412:VAL:HG23  | 2.07                     | 0.54              |
| 1:D:955:LEU:N    | 1:D:1033:GLU:O    | 2.37                     | 0.54              |
| 1:D:108:GLN:O    | 1:D:112:GLN:HG2   | 2.08                     | 0.54              |
| 1:D:135:SER:O    | 1:D:292:LYS:HG2   | 2.07                     | 0.54              |
| 1:D:242:SER:O    | 1:D:246:PHE:HD1   | 1.91                     | 0.54              |
| 1:A:420:MET:HB3  | 1:A:500:ILE:HB    | 1.90                     | 0.54              |
| 1:B:423:GLU:O    | 1:B:502:LYS:HD2   | 2.06                     | 0.54              |
| 1:D:54:ALA:HB1   | 1:D:811:LEU:HG    | 1.90                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:631:ASP:C    | 1:F:633:PRO:HD3   | 2.27                     | 0.54              |
| 1:B:171:GLY:HA3  | 1:B:302:THR:OG1   | 2.07                     | 0.54              |
| 1:C:883:LEU:HD21 | 1:C:938:ILE:HD11  | 1.89                     | 0.54              |
| 1:E:36:PRO:HD3   | 1:E:391:ASN:CG    | 2.28                     | 0.54              |
| 1:A:143:ILE:HG22 | 1:A:286:ALA:CB    | 2.38                     | 0.54              |
| 1:C:136:PHE:HB2  | 1:C:327:TYR:HE2   | 1.72                     | 0.54              |
| 1:D:947:LEU:HB2  | 1:D:958:ALA:HB1   | 1.90                     | 0.54              |
| 1:F:681:ASP:O    | 1:F:817:LEU:HD13  | 2.07                     | 0.54              |
| 1:F:936:ASN:ND2  | 1:F:1010:THR:HG22 | 2.22                     | 0.54              |
| 1:A:565:PRO:HG2  | 1:A:567:GLU:OE2   | 2.08                     | 0.54              |
| 1:B:172:VAL:HG22 | 1:B:306:ILE:HD11  | 1.89                     | 0.54              |
| 1:C:1006:MET:O   | 1:C:1010:THR:OG1  | 2.25                     | 0.54              |
| 1:C:24:GLY:HA2   | 1:C:27:ILE:HG23   | 1.89                     | 0.54              |
| 1:C:642:ILE:O    | 1:C:645:ARG:HG2   | 2.08                     | 0.54              |
| 1:D:538:THR:HG23 | 1:D:542:LEU:HD13  | 1.90                     | 0.54              |
| 1:D:904:VAL:HG22 | 1:D:926:LEU:HD21  | 1.89                     | 0.54              |
| 1:D:962:ALA:O    | 1:D:965:MET:HG2   | 2.07                     | 0.54              |
| 1:E:545:TYR:CE2  | 1:E:1020:PHE:HZ   | 2.25                     | 0.54              |
| 1:E:444:GLY:O    | 1:E:448:VAL:HG23  | 2.08                     | 0.54              |
| 1:E:44:THR:HA    | 1:E:90:ILE:O      | 2.07                     | 0.54              |
| 1:E:663:LEU:HD23 | 1:E:663:LEU:H     | 1.72                     | 0.54              |
| 1:F:677:PHE:HB2  | 1:F:854:TRP:CZ3   | 2.43                     | 0.54              |
| 1:A:936:ASN:O    | 1:A:940:ILE:HG13  | 2.08                     | 0.54              |
| 1:B:412:VAL:HG22 | 1:B:438:ILE:HD11  | 1.89                     | 0.54              |
| 1:B:771:GLU:HB3  | 1:B:774:TYR:CD1   | 2.43                     | 0.54              |
| 1:B:941:VAL:HG13 | 1:B:1021:PHE:CE1  | 2.42                     | 0.54              |
| 1:C:395:MET:O    | 1:C:398:MET:HB2   | 2.07                     | 0.54              |
| 1:D:1033:GLU:HB3 | 1:D:1034:ASP:HB2  | 1.90                     | 0.54              |
| 1:D:692:GLN:HA   | 1:D:695:ASN:HB2   | 1.89                     | 0.54              |
| 1:E:536:ARG:CZ   | 2:E:1101:LMT:O3B  | 2.55                     | 0.54              |
| 1:E:770:SER:HB3  | 1:E:775:ARG:HD3   | 1.89                     | 0.54              |
| 1:F:164:ASP:OD1  | 1:F:762:ARG:NH2   | 2.40                     | 0.54              |
| 1:A:34:GLN:HE22  | 1:A:569:GLN:NE2   | 2.06                     | 0.54              |
| 1:B:198:LEU:HD21 | 1:B:252:LYS:HB2   | 1.90                     | 0.54              |
| 1:B:272:GLY:N    | 1:B:275:TYR:OH    | 2.21                     | 0.54              |
| 1:C:520:PHE:CE2  | 1:C:968:ARG:HD2   | 2.43                     | 0.54              |
| 1:D:559:LEU:HD23 | 1:D:560:PRO:HD2   | 1.90                     | 0.54              |
| 1:E:138:MET:HG3  | 1:E:327:TYR:O     | 2.08                     | 0.54              |
| 1:E:593:GLU:OE1  | 1:E:654:LYS:NZ    | 2.34                     | 0.54              |
| 1:F:114:ALA:O    | 1:F:118:LEU:HG    | 2.08                     | 0.54              |
| 1:F:435:MET:O    | 1:F:439:GLN:HB2   | 2.08                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:488:LEU:O    | 1:F:491:ALA:HB3   | 2.07                     | 0.54              |
| 1:A:166:ILE:HD11 | 1:A:306:ILE:HG23  | 1.90                     | 0.53              |
| 1:A:220:GLY:HA3  | 1:A:230:LEU:O     | 2.08                     | 0.53              |
| 1:A:545:TYR:O    | 1:A:549:VAL:HG23  | 2.08                     | 0.53              |
| 1:A:577:GLN:OE1  | 1:A:619:THR:HG23  | 2.08                     | 0.53              |
| 1:A:769:MET:HG2  | 1:A:770:SER:H     | 1.72                     | 0.53              |
| 1:B:468:ARG:HG2  | 1:B:472:ILE:HD13  | 1.89                     | 0.53              |
| 1:D:694:ARG:HD2  | 1:D:713:PRO:HB3   | 1.90                     | 0.53              |
| 1:E:1019:VAL:O   | 1:E:1023:VAL:HG23 | 2.08                     | 0.53              |
| 1:F:38:ILE:HD13  | 1:F:466:ILE:HD13  | 1.90                     | 0.53              |
| 1:A:340:VAL:HG11 | 1:A:395:MET:HB3   | 1.90                     | 0.53              |
| 1:A:896:VAL:HG21 | 1:A:938:ILE:HG13  | 1.90                     | 0.53              |
| 1:B:945:LYS:NZ   | 1:B:1025:ARG:HH21 | 2.07                     | 0.53              |
| 1:B:1034:ASP:N   | 1:B:1035:ILE:HG22 | 2.24                     | 0.53              |
| 1:D:21:LEU:O     | 1:D:25:LEU:HB2    | 2.08                     | 0.53              |
| 1:D:185:ARG:HB2  | 1:D:271:GLY:HA3   | 1.89                     | 0.53              |
| 1:D:186:ILE:HB   | 1:D:768:VAL:HG22  | 1.91                     | 0.53              |
| 1:D:908:LEU:HD23 | 1:D:922:PHE:CZ    | 2.43                     | 0.53              |
| 1:A:492:LEU:O    | 1:A:496:MET:HG2   | 2.08                     | 0.53              |
| 1:A:728:GLN:NE2  | 1:A:738:ILE:HG21  | 2.23                     | 0.53              |
| 1:A:451:ALA:HB1  | 1:A:878:VAL:HG12  | 1.91                     | 0.53              |
| 1:A:940:ILE:HG12 | 1:A:966:ARG:NE    | 2.23                     | 0.53              |
| 1:C:893:PRO:HA   | 1:C:896:VAL:HG12  | 1.89                     | 0.53              |
| 1:C:935:LYS:NZ   | 1:C:973:THR:HG21  | 2.24                     | 0.53              |
| 1:D:17:ILE:HA    | 1:D:20:MET:HE2    | 1.89                     | 0.53              |
| 1:D:491:ALA:O    | 1:D:495:THR:OG1   | 2.24                     | 0.53              |
| 1:D:776:MET:HE1  | 1:F:225:VAL:HG22  | 1.89                     | 0.53              |
| 1:A:143:ILE:HG22 | 1:A:286:ALA:HB1   | 1.91                     | 0.53              |
| 1:A:157:TYR:CZ   | 1:A:318:PRO:HD3   | 2.44                     | 0.53              |
| 1:A:281:PHE:HB2  | 1:A:610:PHE:CE1   | 2.43                     | 0.53              |
| 1:B:902:LEU:HD11 | 1:B:1016:PHE:HD2  | 1.73                     | 0.53              |
| 1:C:23:GLY:HA2   | 1:C:381:ALA:HB2   | 1.91                     | 0.53              |
| 1:C:366:LEU:O    | 1:C:370:ILE:HG13  | 2.08                     | 0.53              |
| 1:C:525:HIS:HA   | 1:C:528:THR:HG22  | 1.91                     | 0.53              |
| 1:C:935:LYS:HE2  | 1:C:936:ASN:OD1   | 2.09                     | 0.53              |
| 1:D:873:ALA:O    | 1:D:877:ILE:HG12  | 2.08                     | 0.53              |
| 1:E:553:ALA:O    | 1:E:557:VAL:HG23  | 2.08                     | 0.53              |
| 1:F:184:MET:HB2  | 1:F:757:PHE:CD2   | 2.42                     | 0.53              |
| 1:F:446:ALA:HB3  | 1:F:482:VAL:HG22  | 1.89                     | 0.53              |
| 1:B:108:GLN:HA   | 1:B:129:VAL:HG21  | 1.90                     | 0.53              |
| 1:C:574:THR:HG21 | 1:C:598:TYR:CE2   | 2.40                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:428:LYS:O    | 1:D:431:THR:N     | 2.42                     | 0.53              |
| 1:D:559:LEU:HD12 | 1:D:908:LEU:HD22  | 1.90                     | 0.53              |
| 1:D:578:LEU:HB2  | 1:D:618:ASN:O     | 2.09                     | 0.53              |
| 1:E:482:VAL:O    | 1:E:485:ALA:HB3   | 2.09                     | 0.53              |
| 1:E:926:LEU:O    | 1:E:930:ILE:HG13  | 2.09                     | 0.53              |
| 1:E:942:GLU:O    | 1:E:945:LYS:N     | 2.42                     | 0.53              |
| 1:F:197:GLN:HG3  | 1:F:793:MET:SD    | 2.49                     | 0.53              |
| 1:A:954:GLY:HA2  | 1:A:1034:ASP:H    | 1.74                     | 0.53              |
| 1:B:952:GLY:O    | 1:B:1036:GLU:HA   | 2.08                     | 0.53              |
| 1:C:367:ILE:HB   | 1:C:368:PRO:HD3   | 1.90                     | 0.53              |
| 1:C:184:MET:HB3  | 1:C:766:VAL:HG22  | 1.91                     | 0.53              |
| 1:D:723:LYS:HG2  | 1:D:803:ARG:NH1   | 2.23                     | 0.53              |
| 1:E:26:ALA:O     | 1:E:30:LEU:HB2    | 2.09                     | 0.53              |
| 1:D:219:LEU:HD23 | 1:E:749:TRP:HZ3   | 1.73                     | 0.53              |
| 1:E:80:SER:HB3   | 1:E:90:ILE:HG23   | 1.90                     | 0.53              |
| 1:E:974:SER:OG   | 1:E:1010:THR:HG21 | 2.09                     | 0.53              |
| 1:A:953:LYS:O    | 1:A:1035:ILE:HB   | 2.09                     | 0.53              |
| 1:C:479:ALA:O    | 1:C:482:VAL:HG23  | 2.09                     | 0.53              |
| 1:D:428:LYS:HG2  | 1:D:494:ALA:HB1   | 1.91                     | 0.53              |
| 1:E:20:MET:HG3   | 1:E:374:VAL:HG22  | 1.91                     | 0.53              |
| 1:E:140:VAL:HA   | 1:E:326:PRO:HD2   | 1.91                     | 0.53              |
| 1:E:468:ARG:HG2  | 1:E:472:ILE:CD1   | 2.39                     | 0.53              |
| 1:E:670:GLY:C    | 1:E:672:ALA:H     | 2.12                     | 0.53              |
| 1:D:233:SER:HB2  | 1:E:721:GLN:HB3   | 1.91                     | 0.53              |
| 1:B:902:LEU:HD21 | 1:B:1016:PHE:HB2  | 1.90                     | 0.53              |
| 1:A:888:GLU:OE1  | 1:C:11:PHE:HB2    | 2.09                     | 0.53              |
| 1:C:544:LEU:O    | 1:C:547:ILE:HB    | 2.08                     | 0.53              |
| 1:C:770:SER:HB3  | 1:C:775:ARG:HD3   | 1.91                     | 0.53              |
| 1:D:335:ILE:O    | 1:D:339:GLU:HG2   | 2.09                     | 0.53              |
| 1:E:1005:GLY:O   | 1:E:1009:ALA:HB2  | 2.08                     | 0.53              |
| 1:F:700:GLU:HA   | 1:F:703:LYS:NZ    | 2.24                     | 0.53              |
| 1:A:21:LEU:O     | 1:A:25:LEU:HB2    | 2.09                     | 0.53              |
| 1:A:13:TRP:HE1   | 1:A:492:LEU:HD21  | 1.73                     | 0.53              |
| 1:A:626:LEU:HD11 | 1:A:639:VAL:CG2   | 2.39                     | 0.53              |
| 1:A:44:THR:HA    | 1:A:90:ILE:O      | 2.09                     | 0.53              |
| 1:B:154:ILE:O    | 1:B:158:VAL:HG23  | 2.09                     | 0.53              |
| 1:B:82:SER:HA    | 1:B:88:VAL:HG22   | 1.89                     | 0.53              |
| 1:C:65:ILE:HG23  | 1:C:111:LEU:HD23  | 1.90                     | 0.53              |
| 1:C:571:VAL:HG22 | 1:C:625:SER:HA    | 1.91                     | 0.53              |
| 1:C:899:VAL:O    | 1:C:902:LEU:HB2   | 2.09                     | 0.53              |
| 1:A:234:ILE:HD11 | 1:B:749:TRP:CE3   | 2.44                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:475:VAL:O    | 1:A:478:MET:HB3   | 2.08                     | 0.52              |
| 1:A:763:VAL:HG12 | 1:B:63:GLN:HE21   | 1.73                     | 0.52              |
| 1:C:415:ASN:O    | 1:C:419:VAL:HG23  | 2.10                     | 0.52              |
| 1:E:701:ALA:HB1  | 1:E:711:VAL:HG11  | 1.90                     | 0.52              |
| 1:F:3:ASN:ND2    | 1:F:435:MET:SD    | 2.77                     | 0.52              |
| 1:F:45:ILE:HD13  | 1:F:111:LEU:HG    | 1.89                     | 0.52              |
| 1:F:676:ASP:HB3  | 1:F:823:LEU:HD23  | 1.91                     | 0.52              |
| 1:F:75:LEU:HD11  | 1:F:92:LEU:HD12   | 1.91                     | 0.52              |
| 1:F:966:ARG:NE   | 1:F:966:ARG:O     | 2.40                     | 0.52              |
| 1:A:910:ALA:HB2  | 1:A:1004:GLY:HA3  | 1.90                     | 0.52              |
| 1:A:527:TYR:CE1  | 1:A:1014:ILE:HD12 | 2.44                     | 0.52              |
| 1:A:536:ARG:NH1  | 2:A:1101:LMT:O4'  | 2.41                     | 0.52              |
| 1:B:377:LEU:O    | 1:B:380:PHE:HB2   | 2.09                     | 0.52              |
| 1:B:841:GLN:O    | 1:B:844:SER:OG    | 2.26                     | 0.52              |
| 1:C:151:GLN:HE22 | 1:C:286:ALA:H     | 1.56                     | 0.52              |
| 1:C:663:LEU:HA   | 1:C:672:ALA:HA    | 1.91                     | 0.52              |
| 1:C:917:THR:O    | 1:C:919:ASP:N     | 2.43                     | 0.52              |
| 1:C:977:PHE:HE2  | 1:C:1002:VAL:HG12 | 1.75                     | 0.52              |
| 1:D:137:LEU:HD13 | 1:D:293:LEU:HB2   | 1.91                     | 0.52              |
| 1:D:211:ASN:OD1  | 1:D:240:LEU:HG    | 2.09                     | 0.52              |
| 1:D:991:GLY:O    | 1:D:993:GLY:N     | 2.42                     | 0.52              |
| 1:E:355:MET:SD   | 1:E:368:PRO:HG2   | 2.48                     | 0.52              |
| 1:E:15:ILE:HD12  | 1:E:487:ILE:HG21  | 1.91                     | 0.52              |
| 1:E:854:TRP:HE3  | 1:E:858:SER:HB3   | 1.72                     | 0.52              |
| 1:F:452:VAL:C    | 1:F:455:PRO:HD2   | 2.30                     | 0.52              |
| 1:A:8:ARG:O      | 1:A:11:PHE:N      | 2.42                     | 0.52              |
| 1:A:940:ILE:HD12 | 1:A:1017:VAL:HG11 | 1.90                     | 0.52              |
| 1:B:677:PHE:CD2  | 1:B:822:ILE:HD12  | 2.45                     | 0.52              |
| 1:C:371:ALA:O    | 1:C:375:VAL:HG23  | 2.10                     | 0.52              |
| 1:D:366:LEU:HA   | 1:D:369:THR:HB    | 1.90                     | 0.52              |
| 1:D:896:VAL:HG21 | 1:D:938:ILE:HG13  | 1.90                     | 0.52              |
| 1:E:445:ILE:HG22 | 1:E:938:ILE:CD1   | 2.38                     | 0.52              |
| 1:E:961:ASP:O    | 1:E:964:ARG:HB3   | 2.09                     | 0.52              |
| 1:F:47:ALA:HB2   | 1:F:127:VAL:HG13  | 1.92                     | 0.52              |
| 1:F:154:ILE:HG22 | 1:F:287:SER:HB3   | 1.90                     | 0.52              |
| 1:F:446:ALA:CB   | 1:F:482:VAL:HG22  | 2.40                     | 0.52              |
| 1:A:272:GLY:N    | 1:A:275:TYR:OH    | 2.34                     | 0.52              |
| 1:C:244:GLU:HG2  | 1:C:248:LYS:HE3   | 1.90                     | 0.52              |
| 1:C:600:THR:O    | 1:C:603:LYS:HG3   | 2.09                     | 0.52              |
| 1:D:278:ILE:CG1  | 1:D:613:ASN:HB3   | 2.40                     | 0.52              |
| 1:D:434:SER:O    | 1:D:438:ILE:HG12  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:452:VAL:HA   | 1:A:875:SER:OG    | 2.09                     | 0.52              |
| 1:B:36:PRO:HD3   | 1:B:391:ASN:CG    | 2.30                     | 0.52              |
| 1:C:190:PRO:HG3  | 1:C:774:TYR:CG    | 2.44                     | 0.52              |
| 1:C:940:ILE:HA   | 1:C:966:ARG:NH1   | 2.25                     | 0.52              |
| 1:D:121:GLU:O    | 1:D:124:GLN:HG2   | 2.10                     | 0.52              |
| 1:D:546:LEU:O    | 1:D:550:VAL:HG23  | 2.10                     | 0.52              |
| 1:D:673:THR:HA   | 1:D:832:THR:OG1   | 2.10                     | 0.52              |
| 1:E:982:MET:HB3  | 1:E:983:PRO:HD3   | 1.91                     | 0.52              |
| 1:F:329:THR:O    | 1:F:333:VAL:HG23  | 2.09                     | 0.52              |
| 1:F:456:MET:HA   | 1:F:459:PHE:CD1   | 2.45                     | 0.52              |
| 1:B:796:PHE:HA   | 1:B:799:PHE:CZ    | 2.45                     | 0.52              |
| 1:B:953:LYS:O    | 1:B:1035:ILE:HG12 | 2.09                     | 0.52              |
| 1:C:11:PHE:O     | 1:C:15:ILE:HG13   | 2.10                     | 0.52              |
| 1:C:355:MET:SD   | 1:C:368:PRO:HB2   | 2.50                     | 0.52              |
| 1:D:153:ASP:OD2  | 1:D:153:ASP:N     | 2.42                     | 0.52              |
| 1:F:184:MET:HB3  | 1:F:766:VAL:HG22  | 1.91                     | 0.52              |
| 1:A:4:PHE:HB3    | 1:A:8:ARG:CZ      | 2.39                     | 0.52              |
| 1:A:966:ARG:C    | 1:A:969:PRO:HD2   | 2.30                     | 0.52              |
| 1:B:510:LYS:HB3  | 1:B:513:PHE:HB3   | 1.92                     | 0.52              |
| 1:C:189:ASN:HB3  | 1:C:192:GLU:HB2   | 1.91                     | 0.52              |
| 1:C:662:ASN:O    | 1:C:673:THR:N     | 2.37                     | 0.52              |
| 1:D:278:ILE:HD13 | 1:D:584:GLN:OE1   | 2.09                     | 0.52              |
| 1:E:199:THR:HG21 | 1:E:787:ARG:H     | 1.73                     | 0.52              |
| 1:E:524:THR:O    | 1:E:527:TYR:HB3   | 2.09                     | 0.52              |
| 1:F:408:ASP:O    | 1:F:412:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:708:LEU:HD21 | 1:A:838:LEU:HD12  | 1.90                     | 0.52              |
| 1:C:251:LEU:HD11 | 1:C:262:LEU:HD13  | 1.92                     | 0.52              |
| 1:C:549:VAL:O    | 1:C:552:MET:HB3   | 2.10                     | 0.52              |
| 1:D:478:MET:O    | 1:D:482:VAL:HG23  | 2.09                     | 0.52              |
| 1:D:653:ILE:HG13 | 1:D:654:LYS:HE2   | 1.92                     | 0.52              |
| 1:D:771:GLU:HB3  | 1:D:774:TYR:HD1   | 1.75                     | 0.52              |
| 1:D:940:ILE:HG12 | 1:D:966:ARG:CZ    | 2.39                     | 0.52              |
| 1:E:47:ALA:O     | 1:E:87:THR:HA     | 2.10                     | 0.52              |
| 1:F:94:PHE:CE1   | 1:F:103:ALA:HB1   | 2.45                     | 0.52              |
| 1:F:314:GLU:HB2  | 1:F:315:PRO:HD3   | 1.92                     | 0.52              |
| 1:F:559:LEU:HD11 | 1:F:911:ALA:HB1   | 1.92                     | 0.52              |
| 1:A:968:ARG:HG2  | 1:A:972:MET:CE    | 2.40                     | 0.52              |
| 1:C:545:TYR:CE2  | 1:C:1020:PHE:CZ   | 2.98                     | 0.52              |
| 1:C:884:ALA:HB1  | 1:C:890:TRP:HZ3   | 1.74                     | 0.52              |
| 1:D:17:ILE:HA    | 1:D:20:MET:CE     | 2.40                     | 0.52              |
| 1:D:542:LEU:O    | 1:D:546:LEU:HG    | 2.09                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:858:SER:HA   | 1:D:861:GLU:CD    | 2.31                     | 0.52              |
| 1:F:757:PHE:HE1  | 1:F:759:ASP:HB2   | 1.74                     | 0.52              |
| 1:A:902:LEU:HD21 | 1:A:1016:PHE:CD1  | 2.44                     | 0.52              |
| 1:A:415:ASN:HD22 | 1:A:434:SER:HB2   | 1.74                     | 0.52              |
| 1:B:340:VAL:HG11 | 1:B:395:MET:HB3   | 1.91                     | 0.52              |
| 1:B:58:GLN:O     | 1:B:63:GLN:HG3    | 2.09                     | 0.52              |
| 1:D:276:ASP:O    | 1:D:614:GLY:HA2   | 2.10                     | 0.52              |
| 1:D:27:ILE:HG23  | 1:D:390:ILE:HD11  | 1.91                     | 0.52              |
| 1:D:137:LEU:HB3  | 1:D:291:ILE:O     | 2.10                     | 0.52              |
| 1:D:361:ASN:HD21 | 1:D:363:ARG:HG2   | 1.74                     | 0.52              |
| 1:D:23:GLY:HA2   | 1:D:381:ALA:HB2   | 1.90                     | 0.52              |
| 1:D:936:ASN:ND2  | 1:D:970:ILE:HG23  | 2.25                     | 0.52              |
| 1:E:695:ASN:O    | 1:E:698:LEU:HB2   | 2.10                     | 0.52              |
| 1:F:453:PHE:HB2  | 1:F:475:VAL:HG23  | 1.90                     | 0.52              |
| 1:F:778:PRO:O    | 1:F:781:ILE:HG12  | 2.10                     | 0.52              |
| 1:F:986:ILE:HG23 | 1:F:986:ILE:O     | 2.10                     | 0.52              |
| 1:A:442:LEU:O    | 1:A:445:ILE:HG13  | 2.10                     | 0.51              |
| 1:A:553:ALA:O    | 1:A:557:VAL:HG23  | 2.10                     | 0.51              |
| 1:B:30:LEU:HD12  | 1:B:31:PRO:HD2    | 1.92                     | 0.51              |
| 1:B:413:VAL:O    | 1:B:417:GLU:HG2   | 2.11                     | 0.51              |
| 1:C:493:CYS:O    | 1:C:497:LEU:HB2   | 2.11                     | 0.51              |
| 1:E:757:PHE:HD2  | 1:E:766:VAL:HG22  | 1.75                     | 0.51              |
| 1:D:225:VAL:H    | 1:E:776:MET:CE    | 2.22                     | 0.51              |
| 1:F:872:TYR:O    | 1:F:876:LEU:HD12  | 2.09                     | 0.51              |
| 1:F:905:ILE:O    | 1:F:909:LEU:HB2   | 2.10                     | 0.51              |
| 1:A:694:ARG:NH2  | 1:A:717:GLU:OE1   | 2.43                     | 0.51              |
| 1:B:549:VAL:O    | 1:B:552:MET:HB3   | 2.10                     | 0.51              |
| 1:B:578:LEU:HB2  | 1:B:618:ASN:O     | 2.10                     | 0.51              |
| 1:D:201:VAL:O    | 1:D:205:THR:OG1   | 2.26                     | 0.51              |
| 1:D:974:SER:OG   | 1:D:1010:THR:HG21 | 2.10                     | 0.51              |
| 1:E:32:VAL:HG21  | 1:E:300:LEU:HD13  | 1.90                     | 0.51              |
| 1:E:514:GLY:C    | 1:E:516:PHE:N     | 2.63                     | 0.51              |
| 1:E:76:MET:HB2   | 1:E:93:THR:O      | 2.09                     | 0.51              |
| 1:A:13:TRP:O     | 1:A:17:ILE:HG13   | 2.09                     | 0.51              |
| 1:C:906:GLY:HA3  | 1:C:1008:THR:OG1  | 2.10                     | 0.51              |
| 1:C:219:LEU:HD12 | 1:C:232:ALA:HB3   | 1.92                     | 0.51              |
| 1:D:636:GLU:HB2  | 1:D:645:ARG:NH2   | 2.25                     | 0.51              |
| 1:D:966:ARG:C    | 1:D:969:PRO:HD2   | 2.30                     | 0.51              |
| 1:E:534:ILE:HG21 | 2:E:1101:LMT:H12  | 1.92                     | 0.51              |
| 1:D:881:LEU:HD13 | 1:F:18:ILE:HG13   | 1.92                     | 0.51              |
| 1:F:382:VAL:HG21 | 1:F:476:SER:HB2   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:ILE:HG21 | 1:A:281:PHE:CD2  | 2.45                     | 0.51              |
| 1:A:58:GLN:HA    | 1:A:62:THR:HB    | 1.92                     | 0.51              |
| 1:B:52:ALA:HB1   | 1:B:56:THR:HB    | 1.93                     | 0.51              |
| 1:B:700:GLU:HB3  | 1:B:842:LEU:HD22 | 1.92                     | 0.51              |
| 1:B:950:LYS:O    | 1:B:951:GLU:HG2  | 2.10                     | 0.51              |
| 1:C:110:LYS:O    | 1:C:113:LEU:HB2  | 2.10                     | 0.51              |
| 1:C:781:ILE:O    | 1:C:796:PHE:HB2  | 2.11                     | 0.51              |
| 1:C:985:VAL:HG13 | 1:C:1000:THR:OG1 | 2.10                     | 0.51              |
| 1:D:575:MET:HG2  | 1:D:661:PHE:CE1  | 2.42                     | 0.51              |
| 1:D:56:THR:O     | 1:D:60:THR:HG22  | 2.10                     | 0.51              |
| 1:D:757:PHE:CE1  | 1:D:759:ASP:HB2  | 2.45                     | 0.51              |
| 1:E:484:VAL:HG12 | 1:E:489:THR:HG23 | 1.92                     | 0.51              |
| 1:A:417:GLU:HG2  | 1:A:497:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:632:ARG:NH1  | 1:A:637:ASN:O    | 2.44                     | 0.51              |
| 1:A:841:GLN:O    | 1:A:844:SER:OG   | 2.25                     | 0.51              |
| 1:B:515:TRP:O    | 1:B:519:MET:HG3  | 2.11                     | 0.51              |
| 1:B:673:THR:HA   | 1:B:832:THR:OG1  | 2.11                     | 0.51              |
| 1:B:560:PRO:HG2  | 1:B:917:THR:HA   | 1.93                     | 0.51              |
| 1:C:568:ASP:CG   | 1:C:632:ARG:HH22 | 2.13                     | 0.51              |
| 1:C:445:ILE:HG12 | 1:C:935:LYS:HG3  | 1.91                     | 0.51              |
| 1:D:113:LEU:HD11 | 1:F:128:SER:CB   | 2.30                     | 0.51              |
| 1:D:340:VAL:HG11 | 1:D:395:MET:HB3  | 1.92                     | 0.51              |
| 1:D:363:ARG:O    | 1:D:366:LEU:HB2  | 2.10                     | 0.51              |
| 1:F:110:LYS:O    | 1:F:113:LEU:HB2  | 2.10                     | 0.51              |
| 1:F:395:MET:O    | 1:F:398:MET:HB2  | 2.11                     | 0.51              |
| 1:F:422:GLU:HB3  | 1:F:423:GLU:HG3  | 1.93                     | 0.51              |
| 1:F:667:VAL:HB   | 1:F:668:GLU:OE2  | 2.10                     | 0.51              |
| 1:F:666:ILE:HD12 | 1:F:857:MET:SD   | 2.51                     | 0.51              |
| 1:B:375:VAL:HG11 | 1:B:405:LEU:HD22 | 1.92                     | 0.51              |
| 1:B:44:THR:HA    | 1:B:90:ILE:O     | 2.10                     | 0.51              |
| 1:C:538:THR:CG2  | 1:C:542:LEU:HD13 | 2.41                     | 0.51              |
| 1:C:568:ASP:O    | 1:C:629:TRP:HH2  | 1.94                     | 0.51              |
| 1:C:80:SER:HB3   | 1:C:90:ILE:HG23  | 1.92                     | 0.51              |
| 1:C:982:MET:O    | 1:C:985:VAL:N    | 2.44                     | 0.51              |
| 1:D:225:VAL:HG12 | 1:E:772:ALA:HB1  | 1.93                     | 0.51              |
| 1:D:457:ALA:CA   | 1:D:468:ARG:HG3  | 2.37                     | 0.51              |
| 1:D:899:VAL:HA   | 1:D:902:LEU:HD22 | 1.92                     | 0.51              |
| 1:E:1016:PHE:O   | 1:E:1019:VAL:HB  | 2.10                     | 0.51              |
| 1:E:162:MET:HA   | 1:E:313:MET:HE1  | 1.91                     | 0.51              |
| 1:F:639:VAL:HA   | 1:F:642:ILE:HD12 | 1.92                     | 0.51              |
| 1:F:892:ILE:CG2  | 1:F:941:VAL:HG11 | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:400:LEU:HD11 | 1:A:925:GLY:HA2  | 1.92                     | 0.51              |
| 1:B:393:LEU:HD22 | 1:B:470:PHE:HE1  | 1.76                     | 0.51              |
| 1:B:544:LEU:HA   | 1:B:547:ILE:HD12 | 1.92                     | 0.51              |
| 1:C:778:PRO:O    | 1:C:781:ILE:HG12 | 2.10                     | 0.51              |
| 1:E:438:ILE:O    | 1:E:441:ALA:HB3  | 2.11                     | 0.51              |
| 1:E:511:GLY:HA2  | 1:E:515:TRP:HD1  | 1.76                     | 0.51              |
| 1:F:144:ASN:O    | 1:F:284:GLN:NE2  | 2.42                     | 0.51              |
| 1:F:455:PRO:HG2  | 1:F:875:SER:HA   | 1.91                     | 0.51              |
| 1:F:375:VAL:HA   | 1:F:480:LEU:HD13 | 1.91                     | 0.51              |
| 1:F:770:SER:HB2  | 1:F:784:TRP:CZ2  | 2.46                     | 0.51              |
| 1:A:166:ILE:HG22 | 1:A:175:VAL:HG21 | 1.93                     | 0.51              |
| 1:D:573:MET:HG3  | 1:D:661:PHE:CE2  | 2.45                     | 0.51              |
| 1:E:68:ASN:HB3   | 1:E:114:ALA:HB2  | 1.92                     | 0.51              |
| 1:A:209:ALA:O    | 1:A:237:GLN:NE2  | 2.43                     | 0.51              |
| 1:A:219:LEU:HD13 | 1:A:230:LEU:HD21 | 1.93                     | 0.51              |
| 1:B:143:ILE:O    | 1:B:321:LEU:HG   | 2.11                     | 0.51              |
| 1:B:415:ASN:OD1  | 1:B:418:ARG:NH1  | 2.44                     | 0.51              |
| 1:B:678:GLU:HG2  | 1:B:814:TYR:CG   | 2.46                     | 0.51              |
| 1:C:329:THR:O    | 1:C:332:PHE:HB3  | 2.11                     | 0.51              |
| 1:C:616:GLY:N    | 1:C:619:THR:OG1  | 2.43                     | 0.51              |
| 1:C:74:ASN:HB3   | 1:C:95:GLU:HB2   | 1.93                     | 0.51              |
| 1:C:966:ARG:O    | 1:C:970:ILE:HG13 | 2.11                     | 0.51              |
| 1:C:982:MET:HB3  | 1:C:983:PRO:HD3  | 1.93                     | 0.51              |
| 1:D:562:SER:N    | 1:D:917:THR:OG1  | 2.39                     | 0.51              |
| 1:E:109:ASN:OD1  | 1:E:110:LYS:N    | 2.44                     | 0.51              |
| 1:E:7:ASP:OD1    | 1:E:432:ARG:NH2  | 2.44                     | 0.51              |
| 1:F:409:ALA:O    | 1:F:413:VAL:HG23 | 2.11                     | 0.51              |
| 1:F:542:LEU:O    | 1:F:546:LEU:HG   | 2.11                     | 0.51              |
| 1:F:687:HIS:NE2  | 1:F:718:ASP:OD1  | 2.43                     | 0.51              |
| 1:E:237:GLN:OE1  | 1:F:742:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:571:VAL:CG2  | 1:A:625:SER:HA   | 2.35                     | 0.51              |
| 1:B:372:VAL:O    | 1:B:376:LEU:HG   | 2.10                     | 0.51              |
| 1:B:501:ALA:O    | 1:B:504:ASP:HB2  | 2.10                     | 0.51              |
| 1:C:287:SER:OG   | 1:C:288:GLY:N    | 2.42                     | 0.51              |
| 1:D:216:ALA:HB1  | 1:D:234:ILE:O    | 2.10                     | 0.51              |
| 1:D:577:GLN:OE1  | 1:D:619:THR:HG22 | 2.11                     | 0.51              |
| 1:D:678:GLU:HA   | 1:D:678:GLU:OE1  | 2.11                     | 0.51              |
| 1:D:168:ARG:NH2  | 1:E:816:GLY:HA3  | 2.26                     | 0.51              |
| 1:F:406:VAL:O    | 1:F:407:ASP:C    | 2.49                     | 0.51              |
| 1:F:465:ALA:HA   | 1:F:468:ARG:NH1  | 2.25                     | 0.51              |
| 1:A:228:GLN:NE2  | 1:A:230:LEU:H    | 2.09                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:607:GLU:OE1  | 1:A:627:LYS:HA   | 2.12                     | 0.50              |
| 1:B:181:GLN:HG2  | 1:B:182:TYR:N    | 2.25                     | 0.50              |
| 1:B:574:THR:HA   | 1:B:660:ALA:HA   | 1.92                     | 0.50              |
| 1:E:281:PHE:CZ   | 1:E:324:VAL:HG21 | 2.46                     | 0.50              |
| 1:E:423:GLU:O    | 1:E:502:LYS:HB2  | 2.11                     | 0.50              |
| 1:E:953:LYS:HG3  | 1:E:957:GLU:CD   | 2.31                     | 0.50              |
| 1:F:445:ILE:HG12 | 1:F:935:LYS:HG3  | 1.93                     | 0.50              |
| 1:F:830:LYS:HG3  | 1:F:831:SER:N    | 2.26                     | 0.50              |
| 1:A:605:ASN:ND2  | 1:A:637:ASN:HA   | 2.24                     | 0.50              |
| 1:B:307:ARG:NH2  | 1:B:328:ASP:OD2  | 2.44                     | 0.50              |
| 1:B:375:VAL:HG11 | 1:B:481:SER:HB3  | 1.92                     | 0.50              |
| 1:C:393:LEU:HD11 | 1:C:466:ILE:HD13 | 1.92                     | 0.50              |
| 1:D:368:PRO:HD3  | 1:D:413:VAL:HG21 | 1.94                     | 0.50              |
| 1:F:836:MET:HG2  | 1:F:854:TRP:CH2  | 2.46                     | 0.50              |
| 1:A:511:GLY:CA   | 1:A:515:TRP:CD1  | 2.94                     | 0.50              |
| 1:A:908:LEU:O    | 1:A:911:ALA:HB3  | 2.10                     | 0.50              |
| 1:B:493:CYS:O    | 1:B:497:LEU:HB2  | 2.11                     | 0.50              |
| 1:C:129:VAL:O    | 1:C:130:GLU:HG3  | 2.10                     | 0.50              |
| 1:C:377:LEU:O    | 1:C:380:PHE:HB2  | 2.12                     | 0.50              |
| 1:C:666:ILE:HD13 | 1:C:669:LEU:HD12 | 1.94                     | 0.50              |
| 1:C:939:LEU:HB3  | 1:C:966:ARG:CD   | 2.37                     | 0.50              |
| 1:D:200:PRO:HA   | 1:D:203:VAL:CG2  | 2.41                     | 0.50              |
| 1:D:899:VAL:HG21 | 1:D:937:ALA:HB2  | 1.93                     | 0.50              |
| 1:E:583:THR:HG23 | 1:E:585:GLU:H    | 1.77                     | 0.50              |
| 1:F:262:LEU:HG   | 1:F:268:ILE:HD11 | 1.93                     | 0.50              |
| 1:F:508:GLY:O    | 1:F:509:LYS:HB2  | 2.09                     | 0.50              |
| 1:F:49:TYR:N     | 1:F:86:GLY:O     | 2.40                     | 0.50              |
| 1:F:947:LEU:HD22 | 1:F:953:LYS:CE   | 2.42                     | 0.50              |
| 1:A:372:VAL:HG13 | 1:A:405:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:567:GLU:HG2  | 1:A:665:ALA:HB2  | 1.92                     | 0.50              |
| 1:B:917:THR:O    | 1:B:919:ASP:N    | 2.45                     | 0.50              |
| 1:C:737:SER:O    | 1:C:741:ILE:HG22 | 2.10                     | 0.50              |
| 1:C:927:LEU:O    | 1:C:930:ILE:HB   | 2.11                     | 0.50              |
| 1:D:691:THR:HG23 | 1:D:694:ARG:NH2  | 2.26                     | 0.50              |
| 1:D:83:ASP:OD2   | 1:D:810:ARG:NH1  | 2.44                     | 0.50              |
| 1:E:115:MET:SD   | 1:E:123:GLN:HG2  | 2.52                     | 0.50              |
| 1:F:338:HIS:O    | 1:F:341:VAL:HB   | 2.12                     | 0.50              |
| 1:F:3:ASN:OD1    | 1:F:486:LEU:HB3  | 2.11                     | 0.50              |
| 1:F:918:ASN:ND2  | 1:F:918:ASN:O    | 2.39                     | 0.50              |
| 1:A:894:PHE:HA   | 1:A:897:MET:HE3  | 1.93                     | 0.50              |
| 1:C:11:PHE:HD2   | 1:C:11:PHE:O     | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:456:MET:HB3  | 1:C:871:LEU:HD21 | 1.94                     | 0.50              |
| 1:C:860:GLN:O    | 1:C:863:LEU:HB3  | 2.11                     | 0.50              |
| 1:C:887:TYR:O    | 1:C:889:SER:N    | 2.42                     | 0.50              |
| 1:C:927:LEU:O    | 1:C:928:THR:C    | 2.50                     | 0.50              |
| 1:C:953:LYS:HG2  | 1:C:957:GLU:OE2  | 2.11                     | 0.50              |
| 1:D:616:GLY:N    | 1:D:619:THR:OG1  | 2.44                     | 0.50              |
| 1:E:355:MET:HB3  | 1:E:365:THR:CB   | 2.41                     | 0.50              |
| 1:E:45:ILE:O     | 1:E:89:GLN:HA    | 2.12                     | 0.50              |
| 1:E:700:GLU:HB3  | 1:E:842:LEU:HD22 | 1.93                     | 0.50              |
| 1:A:375:VAL:HG13 | 1:A:480:LEU:CB   | 2.42                     | 0.50              |
| 1:A:649:ALA:O    | 1:A:653:ILE:HG12 | 2.12                     | 0.50              |
| 1:A:989:GLY:N    | 1:A:992:SER:OG   | 2.44                     | 0.50              |
| 1:B:573:MET:HG3  | 1:B:661:PHE:HE2  | 1.77                     | 0.50              |
| 1:B:80:SER:HB3   | 1:B:90:ILE:HG12  | 1.94                     | 0.50              |
| 1:C:68:ASN:O     | 1:C:110:LYS:HB3  | 2.11                     | 0.50              |
| 1:C:963:VAL:HA   | 1:C:966:ARG:HH22 | 1.77                     | 0.50              |
| 1:D:172:VAL:HG22 | 1:D:302:THR:HG23 | 1.93                     | 0.50              |
| 1:D:917:THR:O    | 1:D:919:ASP:N    | 2.45                     | 0.50              |
| 1:F:406:VAL:O    | 1:F:408:ASP:N    | 2.45                     | 0.50              |
| 1:F:773:LYS:HG3  | 1:F:774:TYR:CZ   | 2.47                     | 0.50              |
| 1:A:394:THR:HG22 | 1:A:473:THR:OG1  | 2.12                     | 0.50              |
| 1:B:27:ILE:HD13  | 1:B:380:PHE:CG   | 2.47                     | 0.50              |
| 1:C:311:ALA:O    | 1:C:314:GLU:HB2  | 2.12                     | 0.50              |
| 1:D:545:TYR:HB2  | 1:D:1016:PHE:HE2 | 1.76                     | 0.50              |
| 1:D:242:SER:OG   | 1:D:245:GLU:HG2  | 2.11                     | 0.50              |
| 1:D:747:ALA:O    | 1:D:769:MET:HA   | 2.12                     | 0.50              |
| 1:E:697:LEU:HD12 | 1:E:700:GLU:HB2  | 1.94                     | 0.50              |
| 1:F:355:MET:SD   | 1:F:368:PRO:HB2  | 2.52                     | 0.50              |
| 1:F:893:PRO:O    | 1:F:897:MET:HG2  | 2.11                     | 0.50              |
| 2:B:2000:LMT:H6E | 2:B:2000:LMT:O5B | 2.11                     | 0.50              |
| 1:B:595:THR:O    | 1:B:599:LEU:HG   | 2.12                     | 0.50              |
| 1:C:162:MET:O    | 1:C:166:ILE:N    | 2.41                     | 0.50              |
| 1:D:188:MET:HB3  | 1:D:193:LEU:CD1  | 2.42                     | 0.50              |
| 1:D:222:THR:HA   | 1:D:224:PRO:CD   | 2.38                     | 0.50              |
| 1:D:249:ILE:O    | 1:D:262:LEU:N    | 2.45                     | 0.50              |
| 1:D:525:HIS:NE2  | 1:D:529:ASP:OD1  | 2.45                     | 0.50              |
| 1:D:854:TRP:CE3  | 1:D:858:SER:HB2  | 2.46                     | 0.50              |
| 1:E:468:ARG:HG2  | 1:E:472:ILE:HD13 | 1.94                     | 0.50              |
| 1:E:632:ARG:NH1  | 1:E:637:ASN:O    | 2.45                     | 0.50              |
| 1:F:1016:PHE:HB3 | 1:F:1020:PHE:CZ  | 2.46                     | 0.50              |
| 1:B:771:GLU:HB3  | 1:B:774:TYR:HD1  | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:248:LYS:HG2  | 1:D:263:ARG:HH21 | 1.76                     | 0.50              |
| 1:D:168:ARG:HB3  | 1:E:75:LEU:HD22  | 1.93                     | 0.50              |
| 1:E:76:MET:SD    | 1:E:859:TYR:HE2  | 2.35                     | 0.50              |
| 1:F:112:GLN:HG3  | 1:F:115:MET:HG3  | 1.93                     | 0.50              |
| 1:F:219:LEU:HD12 | 1:F:219:LEU:H    | 1.76                     | 0.50              |
| 1:F:966:ARG:NH2  | 1:F:970:ILE:HD11 | 2.25                     | 0.50              |
| 1:A:408:ASP:O    | 1:A:412:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:431:THR:HG21 | 1:A:490:PRO:O    | 2.12                     | 0.49              |
| 1:B:709:THR:HB   | 1:B:827:ALA:HA   | 1.94                     | 0.49              |
| 1:B:962:ALA:O    | 1:B:965:MET:HG2  | 2.12                     | 0.49              |
| 1:C:602:GLU:OE1  | 1:C:645:ARG:HD2  | 2.12                     | 0.49              |
| 1:C:740:ASP:O    | 1:C:744:THR:OG1  | 2.22                     | 0.49              |
| 1:D:337:ILE:HA   | 1:D:340:VAL:HG23 | 1.94                     | 0.49              |
| 1:D:51:GLY:O     | 1:F:217:GLY:N    | 2.44                     | 0.49              |
| 1:D:632:ARG:NH1  | 1:D:638:LYS:HA   | 2.23                     | 0.49              |
| 1:D:889:SER:HB3  | 1:D:892:ILE:HB   | 1.92                     | 0.49              |
| 1:D:920:VAL:HA   | 1:D:923:GLN:OE1  | 2.11                     | 0.49              |
| 1:E:452:VAL:HA   | 1:E:875:SER:OG   | 2.12                     | 0.49              |
| 1:F:484:VAL:O    | 1:F:487:ILE:N    | 2.38                     | 0.49              |
| 1:F:5:PHE:O      | 1:F:7:ASP:N      | 2.42                     | 0.49              |
| 1:C:687:HIS:NE2  | 1:C:718:ASP:OD2  | 2.35                     | 0.49              |
| 1:D:154:ILE:HG22 | 1:D:287:SER:HB3  | 1.94                     | 0.49              |
| 1:E:281:PHE:HB2  | 1:E:610:PHE:HE1  | 1.77                     | 0.49              |
| 1:A:753:TYR:HB2  | 1:A:767:TYR:CE1  | 2.47                     | 0.49              |
| 1:B:412:VAL:HG22 | 1:B:438:ILE:CD1  | 2.41                     | 0.49              |
| 1:C:465:ALA:O    | 1:C:469:GLN:HG2  | 2.12                     | 0.49              |
| 1:D:1006:MET:O   | 1:D:1009:ALA:HB3 | 2.11                     | 0.49              |
| 1:E:172:VAL:HG13 | 1:E:291:ILE:HG23 | 1.95                     | 0.49              |
| 1:E:356:TYR:HD1  | 1:E:365:THR:HG21 | 1.76                     | 0.49              |
| 1:E:478:MET:O    | 1:E:482:VAL:HG12 | 2.12                     | 0.49              |
| 1:E:748:ALA:O    | 1:E:770:SER:HB3  | 2.12                     | 0.49              |
| 1:E:769:MET:HG2  | 1:E:770:SER:H    | 1.77                     | 0.49              |
| 1:F:479:ALA:O    | 1:F:483:LEU:HG   | 2.12                     | 0.49              |
| 1:F:893:PRO:HA   | 1:F:896:VAL:HG12 | 1.93                     | 0.49              |
| 1:A:212:ALA:HA   | 1:A:239:ARG:HE   | 1.78                     | 0.49              |
| 1:A:475:VAL:HA   | 1:A:478:MET:HE1  | 1.95                     | 0.49              |
| 1:B:57:VAL:HG11  | 1:B:86:GLY:O     | 2.11                     | 0.49              |
| 1:C:425:LEU:HB3  | 1:C:429:GLU:CG   | 2.42                     | 0.49              |
| 1:C:569:GLN:OE1  | 1:C:663:LEU:HD11 | 2.12                     | 0.49              |
| 1:D:695:ASN:O    | 1:D:698:LEU:HB2  | 2.12                     | 0.49              |
| 1:E:146:ASP:OD2  | 1:E:146:ASP:N    | 2.45                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:18:ILE:HG13  | 1:E:881:LEU:HD23  | 1.93                     | 0.49              |
| 1:E:987:SER:O    | 1:E:992:SER:HB2   | 2.12                     | 0.49              |
| 1:A:177:LEU:HD13 | 1:A:179:GLY:O     | 2.11                     | 0.49              |
| 1:A:475:VAL:HA   | 1:A:478:MET:CE    | 2.43                     | 0.49              |
| 1:B:770:SER:HG   | 1:B:775:ARG:HG2   | 1.76                     | 0.49              |
| 1:D:249:ILE:HB   | 1:D:262:LEU:HB2   | 1.94                     | 0.49              |
| 1:D:415:ASN:O    | 1:D:419:VAL:HG23  | 2.13                     | 0.49              |
| 1:D:393:LEU:HD12 | 1:D:469:GLN:HG3   | 1.94                     | 0.49              |
| 1:D:691:THR:HG23 | 1:D:694:ARG:HH22  | 1.77                     | 0.49              |
| 1:D:826:ALA:HB2  | 1:D:835:ALA:HB2   | 1.93                     | 0.49              |
| 1:E:484:VAL:HG13 | 1:E:488:LEU:HB3   | 1.95                     | 0.49              |
| 1:F:272:GLY:N    | 1:F:275:TYR:OH    | 2.22                     | 0.49              |
| 1:A:695:ASN:HA   | 1:A:698:LEU:HD12  | 1.94                     | 0.49              |
| 1:B:428:LYS:HG2  | 1:B:494:ALA:HB1   | 1.95                     | 0.49              |
| 1:B:574:THR:HG23 | 1:B:622:ALA:HB3   | 1.92                     | 0.49              |
| 1:B:906:GLY:HA3  | 1:B:1008:THR:HG21 | 1.95                     | 0.49              |
| 1:B:961:ASP:O    | 1:B:964:ARG:HB3   | 2.11                     | 0.49              |
| 1:E:434:SER:O    | 1:E:438:ILE:HG12  | 2.13                     | 0.49              |
| 1:E:514:GLY:C    | 1:E:516:PHE:H     | 2.15                     | 0.49              |
| 1:E:747:ALA:O    | 1:E:769:MET:HA    | 2.13                     | 0.49              |
| 1:A:952:GLY:HA2  | 1:A:1035:ILE:HG22 | 1.93                     | 0.49              |
| 1:B:174:ASP:HB3  | 1:B:292:LYS:HD2   | 1.94                     | 0.49              |
| 1:B:280:GLU:HG2  | 1:B:283:GLY:C     | 2.32                     | 0.49              |
| 1:B:362:PHE:HA   | 1:B:365:THR:CG2   | 2.42                     | 0.49              |
| 1:B:56:THR:O     | 1:B:60:THR:OG1    | 2.19                     | 0.49              |
| 1:E:527:TYR:O    | 1:E:531:VAL:HG23  | 2.13                     | 0.49              |
| 1:F:365:THR:O    | 1:F:368:PRO:HD2   | 2.13                     | 0.49              |
| 1:A:156:ASP:OD2  | 1:A:182:TYR:HB2   | 2.12                     | 0.49              |
| 1:B:896:VAL:HG23 | 1:B:937:ALA:HB3   | 1.93                     | 0.49              |
| 1:D:475:VAL:HA   | 1:D:478:MET:HE1   | 1.94                     | 0.49              |
| 1:D:278:ILE:HG13 | 1:D:613:ASN:HB3   | 1.93                     | 0.49              |
| 1:E:43:VAL:HG13  | 1:E:130:GLU:C     | 2.33                     | 0.49              |
| 1:E:356:TYR:C    | 1:E:358:PHE:H     | 2.16                     | 0.49              |
| 1:E:375:VAL:HG11 | 1:E:481:SER:HB3   | 1.95                     | 0.49              |
| 1:F:213:GLN:OE1  | 1:F:238:THR:HA    | 2.13                     | 0.49              |
| 1:F:406:VAL:O    | 1:F:409:ALA:N     | 2.45                     | 0.49              |
| 1:F:81:ASN:HB2   | 1:F:89:GLN:HB2    | 1.95                     | 0.49              |
| 1:A:636:GLU:HA   | 1:A:641:ALA:CB    | 2.42                     | 0.49              |
| 1:A:199:THR:HG21 | 1:A:786:VAL:HA    | 1.95                     | 0.49              |
| 1:B:988:THR:HA   | 1:B:992:SER:OG    | 2.13                     | 0.49              |
| 1:C:599:LEU:O    | 1:C:603:LYS:HG2   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:151:GLN:HG3  | 1:D:152:GLU:N     | 2.28                     | 0.49              |
| 1:F:144:ASN:ND2  | 1:F:319:SER:O     | 2.40                     | 0.49              |
| 1:F:75:LEU:CD1   | 1:F:92:LEU:HD12   | 2.43                     | 0.49              |
| 1:A:1016:PHE:HB3 | 1:A:1020:PHE:CE1  | 2.48                     | 0.49              |
| 1:A:330:THR:HB   | 1:A:331:PRO:HD3   | 1.95                     | 0.49              |
| 1:A:453:PHE:O    | 1:A:471:SER:OG    | 2.23                     | 0.49              |
| 1:A:574:THR:HG23 | 1:A:622:ALA:HB3   | 1.94                     | 0.49              |
| 1:C:492:LEU:O    | 1:C:496:MET:HG2   | 2.12                     | 0.49              |
| 1:C:678:GLU:HG2  | 1:C:814:TYR:CG    | 2.48                     | 0.49              |
| 1:C:708:LEU:HD21 | 1:C:839:MET:HG2   | 1.95                     | 0.49              |
| 1:D:375:VAL:HG22 | 1:D:484:VAL:HG21  | 1.95                     | 0.49              |
| 1:D:281:PHE:CZ   | 1:D:608:SER:HB2   | 2.47                     | 0.49              |
| 1:F:133:SER:OG   | 1:F:293:LEU:O     | 2.14                     | 0.49              |
| 1:F:375:VAL:HB   | 1:F:405:LEU:HD22  | 1.95                     | 0.49              |
| 1:A:225:VAL:HG11 | 1:B:773:LYS:HA    | 1.95                     | 0.48              |
| 1:A:645:ARG:HA   | 1:A:648:ARG:HB3   | 1.95                     | 0.48              |
| 1:D:527:TYR:CE1  | 1:D:1014:ILE:HD12 | 2.47                     | 0.48              |
| 1:D:462:SER:O    | 1:D:466:ILE:HG12  | 2.13                     | 0.48              |
| 1:D:860:GLN:O    | 1:D:863:LEU:HB2   | 2.13                     | 0.48              |
| 1:F:311:ALA:HA   | 1:F:314:GLU:HG3   | 1.95                     | 0.48              |
| 1:F:900:VAL:O    | 1:F:904:VAL:HG23  | 2.12                     | 0.48              |
| 1:A:697:LEU:HD21 | 1:A:839:MET:HE1   | 1.95                     | 0.48              |
| 1:B:508:GLY:O    | 1:B:510:LYS:N     | 2.42                     | 0.48              |
| 1:C:686:GLY:O    | 1:C:690:LEU:N     | 2.37                     | 0.48              |
| 1:D:155:SER:OG   | 1:D:179:GLY:HA3   | 2.13                     | 0.48              |
| 1:D:413:VAL:O    | 1:D:417:GLU:HG2   | 2.13                     | 0.48              |
| 1:D:749:TRP:HZ3  | 1:F:219:LEU:HG    | 1.78                     | 0.48              |
| 1:E:101:ASP:HA   | 1:E:131:LYS:HZ2   | 1.78                     | 0.48              |
| 1:A:948:MET:O    | 1:A:1035:ILE:HG21 | 2.13                     | 0.48              |
| 1:A:378:GLY:O    | 1:A:381:ALA:HB3   | 2.14                     | 0.48              |
| 1:A:401:ALA:O    | 1:A:405:LEU:HG    | 2.13                     | 0.48              |
| 1:B:441:ALA:HB2  | 1:B:942:GLU:OE1   | 2.13                     | 0.48              |
| 1:C:520:PHE:HE2  | 1:C:968:ARG:HD2   | 1.76                     | 0.48              |
| 1:C:538:THR:HG23 | 1:C:542:LEU:HD13  | 1.94                     | 0.48              |
| 1:D:184:MET:HB3  | 1:D:766:VAL:HG22  | 1.95                     | 0.48              |
| 1:D:966:ARG:HB3  | 1:D:966:ARG:NH1   | 2.28                     | 0.48              |
| 1:E:359:LEU:C    | 1:E:360:GLN:HG2   | 2.32                     | 0.48              |
| 1:E:187:TRP:CZ3  | 1:E:769:MET:HB3   | 2.48                     | 0.48              |
| 1:F:2:PRO:O      | 1:F:5:PHE:HB3     | 2.13                     | 0.48              |
| 1:A:573:MET:HG3  | 1:A:661:PHE:CE2   | 2.48                     | 0.48              |
| 1:A:795:PRO:O    | 1:A:798:ALA:HB3   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:47:ALA:HB3   | 1:A:88:VAL:HG13   | 1.94                     | 0.48              |
| 1:B:175:VAL:HG23 | 1:C:70:ASN:HD22   | 1.78                     | 0.48              |
| 1:C:72:ILE:HD13  | 1:C:107:VAL:HG22  | 1.95                     | 0.48              |
| 1:C:356:TYR:HD1  | 1:C:365:THR:HG21  | 1.77                     | 0.48              |
| 1:C:645:ARG:O    | 1:C:648:ARG:HB3   | 2.13                     | 0.48              |
| 1:D:391:ASN:O    | 1:D:395:MET:HG2   | 2.13                     | 0.48              |
| 1:D:375:VAL:HG11 | 1:D:481:SER:HB3   | 1.96                     | 0.48              |
| 1:D:568:ASP:OD1  | 1:D:632:ARG:NH2   | 2.43                     | 0.48              |
| 1:D:7:ASP:OD2    | 1:D:432:ARG:NH2   | 2.41                     | 0.48              |
| 1:D:354:VAL:HG22 | 1:D:975:LEU:HD23  | 1.96                     | 0.48              |
| 1:E:137:LEU:HD12 | 1:E:329:THR:HG22  | 1.94                     | 0.48              |
| 1:F:189:ASN:HB3  | 1:F:192:GLU:HB2   | 1.95                     | 0.48              |
| 1:F:36:PRO:HD3   | 1:F:391:ASN:ND2   | 2.29                     | 0.48              |
| 1:A:577:GLN:O    | 1:A:656:ALA:HB1   | 2.14                     | 0.48              |
| 1:B:277:ILE:HG13 | 1:B:277:ILE:H     | 1.44                     | 0.48              |
| 1:A:225:VAL:HG22 | 1:B:776:MET:HE2   | 1.95                     | 0.48              |
| 1:C:185:ARG:HB2  | 1:C:271:GLY:HA3   | 1.95                     | 0.48              |
| 1:D:32:VAL:HB    | 1:D:300:LEU:HD22  | 1.94                     | 0.48              |
| 1:E:43:VAL:HG22  | 1:E:131:LYS:HG3   | 1.94                     | 0.48              |
| 1:E:372:VAL:O    | 1:E:376:LEU:HG    | 2.12                     | 0.48              |
| 1:E:757:PHE:CD2  | 1:E:766:VAL:HG22  | 2.49                     | 0.48              |
| 1:F:361:ASN:ND2  | 1:F:364:ALA:HB2   | 2.28                     | 0.48              |
| 1:F:9:PRO:HB3    | 1:F:495:THR:HG21  | 1.96                     | 0.48              |
| 1:B:344:LEU:HD23 | 1:B:402:ILE:HG12  | 1.96                     | 0.48              |
| 1:B:559:LEU:HA   | 1:B:560:PRO:HD2   | 1.45                     | 0.48              |
| 1:C:6:ILE:H      | 1:C:6:ILE:HG12    | 1.43                     | 0.48              |
| 1:C:54:ALA:HB3   | 1:C:808:SER:O     | 2.14                     | 0.48              |
| 1:C:925:GLY:O    | 1:C:929:THR:OG1   | 2.24                     | 0.48              |
| 1:D:830:LYS:HG2  | 1:D:834:GLU:OE2   | 2.13                     | 0.48              |
| 1:D:836:MET:HE1  | 1:D:862:ARG:HD2   | 1.94                     | 0.48              |
| 1:D:936:ASN:O    | 1:D:940:ILE:HG13  | 2.14                     | 0.48              |
| 1:D:896:VAL:HG23 | 1:D:937:ALA:HB3   | 1.95                     | 0.48              |
| 1:E:239:ARG:HH12 | 1:E:756:ASP:H     | 1.60                     | 0.48              |
| 1:F:400:LEU:O    | 1:F:404:LEU:HD22  | 2.14                     | 0.48              |
| 1:F:587:THR:HG21 | 1:F:617:GLN:O     | 2.13                     | 0.48              |
| 1:F:940:ILE:HA   | 1:F:966:ARG:NH1   | 2.28                     | 0.48              |
| 1:A:607:GLU:HB2  | 1:A:627:LYS:N     | 2.28                     | 0.48              |
| 1:B:954:GLY:HA2  | 1:B:1035:ILE:HG23 | 1.96                     | 0.48              |
| 1:B:349:ILE:O    | 1:B:352:PHE:HB3   | 2.13                     | 0.48              |
| 1:B:872:TYR:HA   | 1:B:875:SER:HB2   | 1.95                     | 0.48              |
| 1:C:318:PRO:HG2  | 1:C:321:LEU:HB2   | 1.94                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:393:LEU:HB3  | 1:D:470:PHE:CE1   | 2.49                     | 0.48              |
| 1:D:514:GLY:C    | 1:D:516:PHE:H     | 2.16                     | 0.48              |
| 1:D:571:VAL:CG2  | 1:D:625:SER:HA    | 2.35                     | 0.48              |
| 1:E:317:PHE:CZ   | 1:E:323:ILE:HG12  | 2.49                     | 0.48              |
| 1:E:422:GLU:O    | 1:E:502:LYS:HG3   | 2.13                     | 0.48              |
| 1:D:75:LEU:HD23  | 1:F:168:ARG:HB3   | 1.96                     | 0.48              |
| 1:F:362:PHE:H    | 1:F:363:ARG:NH2   | 2.12                     | 0.48              |
| 1:F:414:GLU:OE1  | 1:F:968:ARG:NH1   | 2.43                     | 0.48              |
| 1:F:900:VAL:HG22 | 1:F:930:ILE:HG23  | 1.95                     | 0.48              |
| 1:B:535:LEU:HD21 | 1:B:1019:VAL:HA   | 1.96                     | 0.48              |
| 1:C:902:LEU:HG   | 1:C:1012:LEU:HB3  | 1.95                     | 0.48              |
| 1:C:1031:LYS:HD2 | 1:C:1033:GLU:HB2  | 1.95                     | 0.48              |
| 1:F:152:GLU:HG2  | 1:F:275:TYR:HE2   | 1.79                     | 0.48              |
| 1:F:58:GLN:OE1   | 1:F:813:ARG:HD2   | 2.14                     | 0.48              |
| 1:F:853:ASP:OD2  | 1:F:854:TRP:N     | 2.46                     | 0.48              |
| 1:A:70:ASN:OD1   | 1:A:110:LYS:HD2   | 2.14                     | 0.48              |
| 1:A:361:ASN:O    | 1:A:365:THR:HG22  | 2.14                     | 0.48              |
| 1:A:532:GLY:O    | 1:A:536:ARG:HG2   | 2.14                     | 0.48              |
| 1:A:723:LYS:HB2  | 1:A:805:GLU:OE2   | 2.14                     | 0.48              |
| 1:B:952:GLY:HA2  | 1:B:1035:ILE:HD11 | 1.95                     | 0.48              |
| 1:C:278:ILE:HD13 | 1:C:584:GLN:OE1   | 2.14                     | 0.48              |
| 1:C:654:LYS:HD3  | 1:C:654:LYS:HA    | 1.51                     | 0.48              |
| 1:C:893:PRO:O    | 1:C:897:MET:HG2   | 2.14                     | 0.48              |
| 1:D:956:ILE:HD12 | 1:D:957:GLU:H     | 1.79                     | 0.48              |
| 1:E:143:ILE:O    | 1:E:321:LEU:HG    | 2.13                     | 0.48              |
| 1:E:78:MET:O     | 1:E:815:ASN:N     | 2.35                     | 0.48              |
| 1:E:887:TYR:HB3  | 1:E:892:ILE:HD12  | 1.95                     | 0.48              |
| 1:E:906:GLY:HA3  | 1:E:1008:THR:CG2  | 2.41                     | 0.48              |
| 1:F:459:PHE:CE1  | 1:F:871:LEU:HG    | 2.48                     | 0.48              |
| 1:A:893:PRO:HB2  | 1:A:897:MET:HE2   | 1.94                     | 0.48              |
| 1:B:535:LEU:HD13 | 1:B:1022:VAL:HG21 | 1.96                     | 0.48              |
| 1:C:110:LYS:HD3  | 1:C:110:LYS:HA    | 1.68                     | 0.48              |
| 1:D:61:VAL:HG13  | 1:D:118:LEU:HD13  | 1.95                     | 0.48              |
| 1:E:401:ALA:HB2  | 1:E:474:ILE:HG23  | 1.96                     | 0.48              |
| 1:E:414:GLU:HG3  | 1:E:969:PRO:HB3   | 1.96                     | 0.48              |
| 1:F:901:PRO:O    | 1:F:904:VAL:N     | 2.47                     | 0.48              |
| 1:F:956:ILE:H    | 1:F:956:ILE:HD12  | 1.79                     | 0.48              |
| 1:A:157:TYR:OH   | 1:A:316:PHE:O     | 2.32                     | 0.47              |
| 1:B:277:ILE:HD12 | 1:B:277:ILE:O     | 2.14                     | 0.47              |
| 1:B:708:LEU:HG   | 1:B:838:LEU:HD12  | 1.95                     | 0.47              |
| 1:B:753:TYR:OH   | 1:B:756:ASP:OD1   | 2.23                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1032:ASN:OD1 | 1:C:1033:GLU:HA   | 2.14                     | 0.47              |
| 1:C:211:ASN:CG   | 1:C:240:LEU:HG    | 2.35                     | 0.47              |
| 1:D:164:ASP:HB3  | 1:D:168:ARG:NH2   | 2.28                     | 0.47              |
| 1:D:890:TRP:NE1  | 1:F:10:ILE:HG12   | 2.29                     | 0.47              |
| 1:D:908:LEU:HD23 | 1:D:922:PHE:HZ    | 1.79                     | 0.47              |
| 1:E:906:GLY:CA   | 1:E:1008:THR:HG21 | 2.44                     | 0.47              |
| 1:E:339:GLU:HA   | 1:E:342:LYS:HB2   | 1.95                     | 0.47              |
| 1:F:103:ALA:O    | 1:F:107:VAL:HG23  | 2.14                     | 0.47              |
| 1:F:120:GLN:HG3  | 1:F:123:GLN:OE1   | 2.14                     | 0.47              |
| 1:F:398:MET:HE3  | 1:F:398:MET:HB3   | 1.77                     | 0.47              |
| 1:F:692:GLN:HA   | 1:F:695:ASN:HB2   | 1.96                     | 0.47              |
| 1:F:770:SER:HB3  | 1:F:775:ARG:HD3   | 1.95                     | 0.47              |
| 1:F:54:ALA:HB3   | 1:F:808:SER:O     | 2.13                     | 0.47              |
| 1:F:983:PRO:HA   | 1:F:986:ILE:HG22  | 1.94                     | 0.47              |
| 1:A:278:ILE:CG1  | 1:A:613:ASN:HB3   | 2.44                     | 0.47              |
| 1:B:352:PHE:HZ   | 1:B:362:PHE:CE1   | 2.32                     | 0.47              |
| 1:B:422:GLU:O    | 1:B:502:LYS:NZ    | 2.47                     | 0.47              |
| 1:C:409:ALA:O    | 1:C:413:VAL:HG23  | 2.13                     | 0.47              |
| 1:C:551:GLY:O    | 1:C:555:LEU:HB2   | 2.14                     | 0.47              |
| 1:E:57:VAL:HG23  | 1:E:82:SER:HB3    | 1.96                     | 0.47              |
| 1:D:233:SER:O    | 1:E:721:GLN:HB2   | 2.14                     | 0.47              |
| 1:E:887:TYR:C    | 1:E:889:SER:H     | 2.17                     | 0.47              |
| 1:E:99:ASP:HB3   | 1:E:102:ILE:HB    | 1.96                     | 0.47              |
| 1:F:917:THR:O    | 1:F:919:ASP:N     | 2.47                     | 0.47              |
| 1:A:165:ALA:HB3  | 1:A:313:MET:CE    | 2.44                     | 0.47              |
| 1:A:241:THR:HG23 | 1:A:758:ILE:O     | 2.14                     | 0.47              |
| 1:A:669:LEU:HA   | 1:A:669:LEU:HD23  | 1.61                     | 0.47              |
| 1:B:45:ILE:HA    | 1:B:128:SER:O     | 2.14                     | 0.47              |
| 1:D:137:LEU:HD22 | 1:D:293:LEU:HB2   | 1.96                     | 0.47              |
| 1:E:20:MET:CG    | 1:E:374:VAL:HG22  | 2.44                     | 0.47              |
| 1:E:638:LYS:NZ   | 1:E:988:THR:HG23  | 2.29                     | 0.47              |
| 1:F:914:ARG:C    | 1:F:916:LEU:H     | 2.16                     | 0.47              |
| 1:F:959:THR:O    | 1:F:963:VAL:HB    | 2.14                     | 0.47              |
| 1:A:127:VAL:O    | 1:B:113:LEU:HD13  | 2.15                     | 0.47              |
| 1:A:143:ILE:HG12 | 1:A:322:LYS:O     | 2.15                     | 0.47              |
| 1:A:317:PHE:CD2  | 1:A:321:LEU:HD12  | 2.49                     | 0.47              |
| 1:A:2:PRO:HB2    | 1:A:3:ASN:H       | 1.45                     | 0.47              |
| 1:B:625:SER:O    | 1:B:626:LEU:HD23  | 2.14                     | 0.47              |
| 1:B:773:LYS:HG3  | 1:B:774:TYR:CZ    | 2.49                     | 0.47              |
| 1:C:242:SER:HB2  | 1:C:245:GLU:H     | 1.78                     | 0.47              |
| 1:C:826:ALA:HB3  | 1:C:830:LYS:HG3   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:574:THR:HG21 | 1:D:598:TYR:CE2  | 2.49                     | 0.47              |
| 1:D:872:TYR:O    | 1:D:876:LEU:HB2  | 2.14                     | 0.47              |
| 1:A:169:THR:HB   | 1:A:172:VAL:CG2  | 2.45                     | 0.47              |
| 1:C:544:LEU:HD12 | 1:C:547:ILE:HD12 | 1.97                     | 0.47              |
| 1:D:400:LEU:HA   | 1:D:400:LEU:HD12 | 1.52                     | 0.47              |
| 1:E:165:ALA:HB3  | 1:E:313:MET:HE2  | 1.97                     | 0.47              |
| 1:E:148:THR:HG21 | 1:E:319:SER:HB2  | 1.96                     | 0.47              |
| 1:E:356:TYR:O    | 1:E:358:PHE:N    | 2.47                     | 0.47              |
| 1:E:35:TYR:CE2   | 1:E:393:LEU:HD21 | 2.49                     | 0.47              |
| 1:E:543:VAL:HA   | 1:E:546:LEU:HG   | 1.95                     | 0.47              |
| 1:A:864:SER:OG   | 1:A:865:GLY:N    | 2.47                     | 0.47              |
| 1:A:880:PHE:HD1  | 1:A:897:MET:HE2  | 1.79                     | 0.47              |
| 1:B:167:SER:HB3  | 1:B:175:VAL:HG21 | 1.97                     | 0.47              |
| 1:B:364:ALA:O    | 1:B:368:PRO:HD3  | 2.14                     | 0.47              |
| 1:C:119:PRO:O    | 1:C:122:VAL:HB   | 2.15                     | 0.47              |
| 1:C:203:VAL:O    | 1:C:207:ILE:HG13 | 2.14                     | 0.47              |
| 1:C:395:MET:HA   | 1:C:398:MET:HG3  | 1.97                     | 0.47              |
| 1:C:966:ARG:HE   | 1:C:970:ILE:HD11 | 1.79                     | 0.47              |
| 1:D:235:ILE:O    | 1:E:723:LYS:HD2  | 2.14                     | 0.47              |
| 1:D:531:VAL:HG13 | 1:D:534:ILE:HD11 | 1.96                     | 0.47              |
| 1:D:282:ASN:HD21 | 1:D:608:SER:HA   | 1.78                     | 0.47              |
| 1:D:675:PHE:HB2  | 1:D:854:TRP:CZ3  | 2.49                     | 0.47              |
| 1:E:518:ARG:O    | 1:E:521:GLU:N    | 2.47                     | 0.47              |
| 1:E:749:TRP:CZ2  | 1:E:781:ILE:HD13 | 2.50                     | 0.47              |
| 1:F:144:ASN:HB3  | 1:F:148:THR:HG23 | 1.95                     | 0.47              |
| 1:F:248:LYS:O    | 1:F:261:LEU:HD22 | 2.14                     | 0.47              |
| 1:A:602:GLU:OE1  | 1:A:645:ARG:HD2  | 2.14                     | 0.47              |
| 1:A:587:THR:HB   | 1:A:613:ASN:ND2  | 2.30                     | 0.47              |
| 1:B:418:ARG:O    | 1:B:422:GLU:HB2  | 2.15                     | 0.47              |
| 1:B:513:PHE:O    | 1:B:515:TRP:N    | 2.48                     | 0.47              |
| 1:B:49:TYR:HB3   | 1:B:57:VAL:HG12  | 1.97                     | 0.47              |
| 1:B:653:ILE:O    | 1:B:654:LYS:HD2  | 2.15                     | 0.47              |
| 1:D:1030:ARG:HE  | 1:D:1031:LYS:N   | 2.13                     | 0.47              |
| 1:D:456:MET:HE2  | 1:D:471:SER:HA   | 1.97                     | 0.47              |
| 1:D:736:VAL:HG21 | 1:D:799:PHE:CE1  | 2.50                     | 0.47              |
| 1:D:776:MET:CE   | 1:F:225:VAL:HG22 | 2.45                     | 0.47              |
| 1:D:905:ILE:O    | 1:D:909:LEU:HB2  | 2.15                     | 0.47              |
| 1:E:351:VAL:O    | 1:E:354:VAL:HB   | 2.13                     | 0.47              |
| 1:E:355:MET:CE   | 1:E:410:ILE:HG12 | 2.44                     | 0.47              |
| 1:E:571:VAL:HG13 | 1:E:623:PHE:HE1  | 1.80                     | 0.47              |
| 1:E:780:ASP:O    | 1:E:783:ASP:HB2  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:836:MET:O    | 1:E:840:GLU:HG3   | 2.13                     | 0.47              |
| 1:F:1008:THR:O   | 1:F:1012:LEU:HB2  | 2.15                     | 0.47              |
| 1:A:157:TYR:HE2  | 1:A:317:PHE:CD1   | 2.33                     | 0.47              |
| 1:A:770:SER:HG   | 1:A:775:ARG:HG2   | 1.80                     | 0.47              |
| 1:B:1035:ILE:H   | 1:B:1036:GLU:HG3  | 1.79                     | 0.47              |
| 1:B:770:SER:HB2  | 1:B:784:TRP:CZ2   | 2.50                     | 0.47              |
| 1:C:203:VAL:HG12 | 1:C:207:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:351:VAL:HG11 | 1:C:406:VAL:HG21  | 1.97                     | 0.47              |
| 1:D:188:MET:SD   | 1:D:200:PRO:HG3   | 2.55                     | 0.47              |
| 1:D:582:ALA:HA   | 1:D:586:ARG:HH21  | 1.79                     | 0.47              |
| 1:E:182:TYR:O    | 1:E:764:LYS:HD3   | 2.15                     | 0.47              |
| 1:E:508:GLY:HA2  | 1:E:514:GLY:O     | 2.14                     | 0.47              |
| 1:E:578:LEU:O    | 1:E:618:ASN:ND2   | 2.38                     | 0.47              |
| 1:F:228:GLN:NE2  | 1:F:230:LEU:O     | 2.45                     | 0.47              |
| 1:F:480:LEU:O    | 1:F:484:VAL:HG23  | 2.15                     | 0.47              |
| 1:F:689:LYS:N    | 1:F:689:LYS:HD2   | 2.29                     | 0.47              |
| 1:B:1007:VAL:O   | 1:B:1011:VAL:HG23 | 2.14                     | 0.47              |
| 1:B:960:LEU:O    | 1:B:963:VAL:HG12  | 2.15                     | 0.47              |
| 1:C:204:ILE:O    | 1:C:207:ILE:HB    | 2.15                     | 0.47              |
| 1:C:402:ILE:O    | 1:C:406:VAL:HG22  | 2.15                     | 0.47              |
| 1:D:103:ALA:O    | 1:D:107:VAL:HG23  | 2.15                     | 0.47              |
| 1:D:199:THR:O    | 1:D:202:ASP:N     | 2.47                     | 0.47              |
| 1:D:770:SER:HB2  | 1:D:784:TRP:CZ2   | 2.49                     | 0.47              |
| 1:E:944:ALA:HB3  | 1:E:1021:PHE:HE1  | 1.78                     | 0.47              |
| 1:F:1006:MET:O   | 1:F:1010:THR:HG23 | 2.15                     | 0.47              |
| 1:F:356:TYR:C    | 1:F:358:PHE:H     | 2.16                     | 0.47              |
| 1:F:407:ASP:O    | 1:F:411:VAL:HG23  | 2.15                     | 0.47              |
| 1:F:516:PHE:O    | 1:F:520:PHE:N     | 2.43                     | 0.47              |
| 1:A:23:GLY:HA3   | 1:A:377:LEU:O     | 2.14                     | 0.47              |
| 1:A:300:LEU:O    | 1:A:303:ALA:HB3   | 2.15                     | 0.47              |
| 1:A:826:ALA:HB2  | 1:A:835:ALA:HB2   | 1.97                     | 0.47              |
| 1:A:41:PRO:HD3   | 1:A:97:GLY:H      | 1.79                     | 0.47              |
| 1:B:740:ASP:O    | 1:B:744:THR:OG1   | 2.23                     | 0.47              |
| 1:E:410:ILE:HD13 | 1:E:972:MET:HB3   | 1.97                     | 0.47              |
| 1:E:466:ILE:HD13 | 1:E:564:LEU:HD11  | 1.97                     | 0.47              |
| 1:F:154:ILE:O    | 1:F:158:VAL:HG23  | 2.15                     | 0.47              |
| 1:F:222:THR:HA   | 1:F:224:PRO:HD3   | 1.97                     | 0.47              |
| 1:A:1032:ASN:O   | 1:A:1033:GLU:HB2  | 2.13                     | 0.47              |
| 1:A:68:ASN:O     | 1:A:110:LYS:HB3   | 2.16                     | 0.47              |
| 1:A:190:PRO:HG3  | 1:A:784:TRP:CH2   | 2.50                     | 0.47              |
| 1:A:559:LEU:HD13 | 1:A:918:ASN:HB2   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1008:THR:O   | 1:B:1012:LEU:HB2  | 2.15                     | 0.47              |
| 1:C:413:VAL:O    | 1:C:417:GLU:HG2   | 2.15                     | 0.47              |
| 1:C:422:GLU:HB3  | 1:C:423:GLU:HG3   | 1.96                     | 0.47              |
| 1:C:669:LEU:HA   | 1:C:669:LEU:HD23  | 1.61                     | 0.47              |
| 1:D:404:LEU:HD21 | 1:D:449:LEU:HD13  | 1.96                     | 0.47              |
| 1:E:594:VAL:HG22 | 1:E:650:PHE:CE2   | 2.50                     | 0.47              |
| 1:E:61:VAL:HG22  | 1:E:118:LEU:HD22  | 1.97                     | 0.47              |
| 1:E:932:LEU:HA   | 1:E:932:LEU:HD23  | 1.72                     | 0.47              |
| 1:F:371:ALA:O    | 1:F:375:VAL:HG23  | 2.15                     | 0.47              |
| 1:F:471:SER:O    | 1:F:475:VAL:HB    | 2.14                     | 0.47              |
| 1:F:506:GLY:C    | 1:F:508:GLY:H     | 2.18                     | 0.47              |
| 1:F:53:ASP:OD1   | 1:F:56:THR:OG1    | 2.28                     | 0.47              |
| 1:F:559:LEU:HA   | 1:F:560:PRO:HD2   | 1.49                     | 0.47              |
| 1:F:69:MET:SD    | 1:F:72:ILE:HD11   | 2.55                     | 0.47              |
| 1:B:959:THR:HG21 | 1:B:1022:VAL:HG23 | 1.97                     | 0.46              |
| 1:B:480:LEU:HA   | 1:B:480:LEU:HD23  | 1.68                     | 0.46              |
| 1:B:583:THR:HG23 | 1:B:585:GLU:H     | 1.80                     | 0.46              |
| 1:C:104:GLN:HG3  | 1:C:105:VAL:N     | 2.29                     | 0.46              |
| 1:C:340:VAL:CG1  | 1:C:395:MET:HB3   | 2.43                     | 0.46              |
| 1:E:318:PRO:HG2  | 1:E:321:LEU:HB2   | 1.97                     | 0.46              |
| 1:E:356:TYR:CD1  | 1:E:365:THR:HG21  | 2.50                     | 0.46              |
| 1:E:728:GLN:NE2  | 1:E:738:ILE:HG21  | 2.30                     | 0.46              |
| 1:E:785:TYR:CZ   | 1:E:795:PRO:HB3   | 2.50                     | 0.46              |
| 1:D:742:ASN:ND2  | 1:F:214:VAL:HG21  | 2.30                     | 0.46              |
| 1:F:510:LYS:O    | 1:F:512:PHE:N     | 2.40                     | 0.46              |
| 1:F:697:LEU:HD12 | 1:F:846:LEU:HD11  | 1.97                     | 0.46              |
| 1:F:723:LYS:HG2  | 1:F:803:ARG:CZ    | 2.45                     | 0.46              |
| 1:A:166:ILE:HD13 | 1:A:166:ILE:HA    | 1.59                     | 0.46              |
| 1:A:340:VAL:O    | 1:A:343:THR:HB    | 2.15                     | 0.46              |
| 1:B:344:LEU:HD11 | 1:B:398:MET:HE2   | 1.98                     | 0.46              |
| 1:B:393:LEU:HD22 | 1:B:470:PHE:CE1   | 2.50                     | 0.46              |
| 1:B:709:THR:O    | 1:B:710:SER:OG    | 2.31                     | 0.46              |
| 1:C:527:TYR:HE2  | 1:C:963:VAL:HG13  | 1.80                     | 0.46              |
| 1:D:880:PHE:HA   | 1:D:883:LEU:HD12  | 1.97                     | 0.46              |
| 1:F:486:LEU:O    | 1:F:490:PRO:HG2   | 2.15                     | 0.46              |
| 1:F:563:PHE:CE2  | 1:F:564:LEU:HD13  | 2.50                     | 0.46              |
| 1:A:200:PRO:HB2  | 1:A:744:THR:HG22  | 1.98                     | 0.46              |
| 1:A:281:PHE:HB2  | 1:A:610:PHE:HE1   | 1.80                     | 0.46              |
| 1:A:190:PRO:HG2  | 1:A:774:TYR:CG    | 2.51                     | 0.46              |
| 1:A:932:LEU:HD23 | 1:A:932:LEU:HA    | 1.51                     | 0.46              |
| 1:B:366:LEU:O    | 1:B:369:THR:HB    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:899:VAL:CG2  | 1:C:1017:VAL:HG22 | 2.45                     | 0.46              |
| 1:A:772:ALA:HB1  | 1:C:225:VAL:HG12  | 1.97                     | 0.46              |
| 1:C:587:THR:HG21 | 1:C:617:GLN:O     | 2.15                     | 0.46              |
| 1:C:572:PHE:CE1  | 1:C:643:THR:HG22  | 2.51                     | 0.46              |
| 1:D:23:GLY:O     | 1:D:27:ILE:HG13   | 2.15                     | 0.46              |
| 1:D:544:LEU:O    | 1:D:548:ILE:HG13  | 2.16                     | 0.46              |
| 1:E:101:ASP:HA   | 1:E:131:LYS:NZ    | 2.30                     | 0.46              |
| 1:F:351:VAL:O    | 1:F:355:MET:HE2   | 2.15                     | 0.46              |
| 1:F:419:VAL:HG21 | 1:F:434:SER:HB3   | 1.96                     | 0.46              |
| 1:F:859:TYR:HD2  | 1:F:859:TYR:O     | 1.98                     | 0.46              |
| 1:A:172:VAL:HG13 | 1:A:291:ILE:HG23  | 1.96                     | 0.46              |
| 1:A:412:VAL:HG22 | 1:A:438:ILE:HD11  | 1.96                     | 0.46              |
| 1:A:574:THR:HG22 | 1:A:624:VAL:CG2   | 2.45                     | 0.46              |
| 1:A:836:MET:HG2  | 1:A:854:TRP:CH2   | 2.49                     | 0.46              |
| 1:B:293:LEU:HD22 | 1:B:297:ALA:HB3   | 1.97                     | 0.46              |
| 1:B:507:GLU:O    | 1:B:509:LYS:HG3   | 2.16                     | 0.46              |
| 1:C:1007:VAL:O   | 1:C:1011:VAL:HG23 | 2.16                     | 0.46              |
| 1:C:293:LEU:HD22 | 1:C:297:ALA:HB3   | 1.96                     | 0.46              |
| 1:C:45:ILE:HG21  | 1:C:111:LEU:HG    | 1.96                     | 0.46              |
| 1:D:55:LYS:HE2   | 1:D:55:LYS:HB3    | 1.71                     | 0.46              |
| 1:E:394:THR:HG23 | 1:E:469:GLN:HB3   | 1.98                     | 0.46              |
| 1:E:653:ILE:C    | 1:E:654:LYS:HD2   | 2.36                     | 0.46              |
| 1:E:841:GLN:O    | 1:E:844:SER:OG    | 2.33                     | 0.46              |
| 1:D:749:TRP:CZ3  | 1:F:219:LEU:HG    | 2.51                     | 0.46              |
| 1:F:288:GLY:O    | 1:F:289:LEU:HD23  | 2.16                     | 0.46              |
| 1:F:36:PRO:HD3   | 1:F:391:ASN:CG    | 2.35                     | 0.46              |
| 1:F:795:PRO:HG2  | 1:F:798:ALA:HB2   | 1.97                     | 0.46              |
| 1:A:379:THR:HG21 | 1:A:477:ALA:HB2   | 1.96                     | 0.46              |
| 1:B:527:TYR:CE1  | 1:B:1014:ILE:HD12 | 2.51                     | 0.46              |
| 1:B:462:SER:O    | 1:B:466:ILE:HG13  | 2.15                     | 0.46              |
| 1:B:525:HIS:HA   | 1:B:528:THR:HG22  | 1.97                     | 0.46              |
| 1:B:932:LEU:HD23 | 1:B:932:LEU:HA    | 1.78                     | 0.46              |
| 1:C:153:ASP:N    | 1:C:153:ASP:OD2   | 2.47                     | 0.46              |
| 1:D:621:ILE:HD12 | 1:D:622:ALA:H     | 1.79                     | 0.46              |
| 1:D:698:LEU:HD21 | 1:D:713:PRO:HD3   | 1.96                     | 0.46              |
| 1:D:796:PHE:O    | 1:D:800:SER:OG    | 2.30                     | 0.46              |
| 1:E:453:PHE:O    | 1:E:471:SER:OG    | 2.32                     | 0.46              |
| 1:E:484:VAL:O    | 1:E:489:THR:HG23  | 2.15                     | 0.46              |
| 1:E:720:PRO:HA   | 1:E:806:TYR:HA    | 1.96                     | 0.46              |
| 1:F:139:VAL:O    | 1:F:326:PRO:HD2   | 2.15                     | 0.46              |
| 1:F:293:LEU:HD13 | 1:F:294:ALA:O     | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:6:ILE:H      | 1:F:6:ILE:HG12    | 1.40                     | 0.46              |
| 1:F:96:SER:HB3   | 1:F:461:GLY:HA2   | 1.98                     | 0.46              |
| 1:A:21:LEU:HA    | 1:A:21:LEU:HD13   | 1.74                     | 0.46              |
| 1:A:359:LEU:C    | 1:A:360:GLN:HG2   | 2.34                     | 0.46              |
| 1:A:375:VAL:HG13 | 1:A:480:LEU:HB2   | 1.97                     | 0.46              |
| 1:A:211:ASN:O    | 1:A:755:ASN:ND2   | 2.46                     | 0.46              |
| 1:B:394:THR:HG23 | 1:B:469:GLN:OE1   | 2.15                     | 0.46              |
| 1:B:76:MET:HB2   | 1:B:93:THR:O      | 2.16                     | 0.46              |
| 1:B:840:GLU:HG2  | 1:B:852:TYR:CE1   | 2.51                     | 0.46              |
| 1:A:749:TRP:CZ3  | 1:C:219:LEU:HD23  | 2.49                     | 0.46              |
| 1:C:242:SER:O    | 1:C:246:PHE:HD1   | 1.99                     | 0.46              |
| 1:C:47:ALA:HB3   | 1:C:88:VAL:HG13   | 1.98                     | 0.46              |
| 1:C:855:THR:HG23 | 1:C:856:GLY:N     | 2.31                     | 0.46              |
| 1:D:21:LEU:HA    | 1:D:21:LEU:HD13   | 1.57                     | 0.46              |
| 1:D:30:LEU:CD1   | 1:D:384:ALA:HA    | 2.46                     | 0.46              |
| 1:D:420:MET:HB3  | 1:D:500:ILE:HB    | 1.98                     | 0.46              |
| 1:D:749:TRP:CE3  | 1:F:234:ILE:HD11  | 2.51                     | 0.46              |
| 1:E:222:THR:HA   | 1:E:224:PRO:HD3   | 1.98                     | 0.46              |
| 1:E:896:VAL:HG23 | 1:E:937:ALA:HB3   | 1.98                     | 0.46              |
| 1:F:664:PRO:HD3  | 1:F:672:ALA:C     | 2.36                     | 0.46              |
| 1:F:967:LEU:HA   | 1:F:970:ILE:HD12  | 1.98                     | 0.46              |
| 1:A:1006:MET:O   | 1:A:1010:THR:HG23 | 2.16                     | 0.46              |
| 1:B:352:PHE:C    | 1:B:352:PHE:CD2   | 2.88                     | 0.46              |
| 1:C:210:GLN:OE1  | 1:C:249:ILE:HG23  | 2.15                     | 0.46              |
| 1:C:135:SER:HB3  | 1:C:668:GLU:HA    | 1.98                     | 0.46              |
| 1:C:900:VAL:O    | 1:C:904:VAL:HG23  | 2.16                     | 0.46              |
| 1:D:136:PHE:CE2  | 1:D:292:LYS:HE3   | 2.50                     | 0.46              |
| 1:D:277:ILE:HG12 | 1:D:614:GLY:HA3   | 1.98                     | 0.46              |
| 1:D:787:ARG:HA   | 1:D:792:GLN:O     | 2.15                     | 0.46              |
| 1:A:100:ALA:HB1  | 1:A:131:LYS:HD2   | 1.98                     | 0.46              |
| 1:A:212:ALA:HA   | 1:A:239:ARG:NE    | 2.30                     | 0.46              |
| 1:A:249:ILE:HB   | 1:A:262:LEU:HB2   | 1.97                     | 0.46              |
| 1:A:255:GLN:H    | 1:A:255:GLN:HG3   | 1.57                     | 0.46              |
| 1:A:375:VAL:HG21 | 1:A:481:SER:HA    | 1.97                     | 0.46              |
| 1:A:636:GLU:HA   | 1:A:641:ALA:HB3   | 1.98                     | 0.46              |
| 1:B:906:GLY:HA3  | 1:B:1008:THR:CG2  | 2.46                     | 0.46              |
| 1:B:727:ASP:OD1  | 1:B:730:LYS:HG3   | 2.16                     | 0.46              |
| 1:C:144:ASN:HA   | 1:C:320:GLY:O     | 2.16                     | 0.46              |
| 1:C:250:LEU:CD1  | 1:C:259:ARG:HB3   | 2.45                     | 0.46              |
| 1:C:277:ILE:HA   | 1:C:614:GLY:HA2   | 1.98                     | 0.46              |
| 1:C:534:ILE:HD13 | 1:C:534:ILE:HG21  | 1.67                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:757:PHE:HE1  | 1:D:759:ASP:HB2  | 1.81                     | 0.46              |
| 1:E:648:ARG:O    | 1:E:651:SER:OG   | 2.34                     | 0.46              |
| 1:F:105:VAL:HA   | 1:F:108:GLN:HE21 | 1.80                     | 0.46              |
| 1:F:10:ILE:O     | 1:F:14:VAL:HG23  | 2.16                     | 0.46              |
| 1:F:421:ALA:O    | 1:F:503:GLY:N    | 2.30                     | 0.46              |
| 1:F:757:PHE:CE1  | 1:F:759:ASP:HB2  | 2.50                     | 0.46              |
| 1:A:325:TYR:HA   | 1:A:326:PRO:HD2  | 1.86                     | 0.46              |
| 1:A:438:ILE:O    | 1:A:442:LEU:HG   | 2.16                     | 0.46              |
| 1:B:667:VAL:HB   | 1:B:668:GLU:CD   | 2.36                     | 0.46              |
| 1:B:677:PHE:HB3  | 1:B:822:ILE:O    | 2.16                     | 0.46              |
| 1:B:900:VAL:HG22 | 1:B:930:ILE:HG23 | 1.98                     | 0.46              |
| 1:C:902:LEU:HD23 | 1:C:1013:ALA:HA  | 1.97                     | 0.46              |
| 1:C:731:ALA:HA   | 1:C:736:VAL:HG23 | 1.97                     | 0.46              |
| 1:D:30:LEU:HD13  | 1:D:384:ALA:HA   | 1.98                     | 0.46              |
| 1:F:425:LEU:HB3  | 1:F:429:GLU:HG2  | 1.98                     | 0.46              |
| 1:F:738:ILE:O    | 1:F:741:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:72:ILE:HD13  | 1:A:107:VAL:HG22 | 1.98                     | 0.46              |
| 1:B:457:ALA:HB2  | 1:B:471:SER:OG   | 2.16                     | 0.46              |
| 1:B:544:LEU:O    | 1:B:547:ILE:HB   | 2.16                     | 0.46              |
| 1:B:68:ASN:CB    | 1:B:114:ALA:HB2  | 2.46                     | 0.46              |
| 1:B:787:ARG:HA   | 1:B:792:GLN:O    | 2.15                     | 0.46              |
| 1:C:2:PRO:HB2    | 1:C:3:ASN:OD1    | 2.15                     | 0.46              |
| 1:C:836:MET:HA   | 1:C:854:TRP:CH2  | 2.51                     | 0.46              |
| 1:E:190:PRO:HB3  | 1:E:784:TRP:CE2  | 2.51                     | 0.46              |
| 1:E:4:PHE:O      | 1:E:8:ARG:HD2    | 2.15                     | 0.46              |
| 1:E:691:THR:HA   | 1:E:694:ARG:NH1  | 2.31                     | 0.46              |
| 1:E:748:ALA:O    | 1:E:769:MET:HG2  | 2.16                     | 0.46              |
| 1:F:30:LEU:HD23  | 1:F:390:ILE:HD11 | 1.98                     | 0.46              |
| 1:F:352:PHE:HA   | 1:F:355:MET:CE   | 2.46                     | 0.46              |
| 1:F:26:ALA:HB1   | 1:F:384:ALA:CB   | 2.45                     | 0.46              |
| 1:F:566:ASP:CG   | 1:F:673:THR:HG23 | 2.36                     | 0.46              |
| 1:F:945:LYS:O    | 1:F:948:MET:N    | 2.49                     | 0.46              |
| 1:A:488:LEU:O    | 1:A:491:ALA:HB3  | 2.15                     | 0.45              |
| 1:A:514:GLY:C    | 1:A:516:PHE:N    | 2.69                     | 0.45              |
| 1:A:516:PHE:HA   | 1:A:519:MET:HG3  | 1.98                     | 0.45              |
| 1:B:110:LYS:HA   | 1:B:110:LYS:HD3  | 1.51                     | 0.45              |
| 1:B:427:PRO:O    | 1:B:430:ALA:HB3  | 2.17                     | 0.45              |
| 1:B:455:PRO:HG2  | 1:B:875:SER:HG   | 1.81                     | 0.45              |
| 1:C:423:GLU:HB2  | 1:C:425:LEU:HG   | 1.98                     | 0.45              |
| 1:C:986:ILE:O    | 1:C:986:ILE:HD13 | 2.16                     | 0.45              |
| 1:D:136:PHE:HD2  | 1:D:292:LYS:HG3  | 1.81                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:250:LEU:CD1  | 1:D:259:ARG:HB3   | 2.44                     | 0.45              |
| 1:D:559:LEU:HD13 | 1:D:918:ASN:HB2   | 1.96                     | 0.45              |
| 1:D:332:PHE:CD1  | 1:D:569:GLN:HG2   | 2.50                     | 0.45              |
| 1:E:748:ALA:HB3  | 1:E:749:TRP:HD1   | 1.81                     | 0.45              |
| 1:F:110:LYS:HA   | 1:F:110:LYS:HD3   | 1.61                     | 0.45              |
| 1:F:344:LEU:HD13 | 1:F:402:ILE:HD11  | 1.98                     | 0.45              |
| 1:F:654:LYS:HB3  | 1:F:656:ALA:H     | 1.81                     | 0.45              |
| 1:A:681:ASP:OD1  | 1:A:684:GLY:N     | 2.47                     | 0.45              |
| 1:B:470:PHE:O    | 1:B:474:ILE:HG13  | 2.15                     | 0.45              |
| 1:C:200:PRO:HA   | 1:C:203:VAL:HG23  | 1.98                     | 0.45              |
| 1:C:33:ALA:O     | 1:C:391:ASN:HA    | 2.16                     | 0.45              |
| 1:C:343:THR:HG23 | 1:C:983:PRO:HB2   | 1.98                     | 0.45              |
| 1:C:542:LEU:O    | 1:C:546:LEU:HG    | 2.16                     | 0.45              |
| 1:C:890:TRP:HA   | 1:C:890:TRP:HE3   | 1.81                     | 0.45              |
| 1:D:184:MET:HB3  | 1:D:766:VAL:HG13  | 1.97                     | 0.45              |
| 1:D:3:ASN:O      | 1:D:5:PHE:N       | 2.49                     | 0.45              |
| 1:E:106:GLN:HA   | 1:E:109:ASN:ND2   | 2.31                     | 0.45              |
| 1:E:172:VAL:CG2  | 1:E:306:ILE:HD11  | 2.46                     | 0.45              |
| 1:E:445:ILE:HG21 | 1:E:935:LYS:CD    | 2.46                     | 0.45              |
| 1:E:955:LEU:HD13 | 1:E:1025:ARG:HG2  | 1.98                     | 0.45              |
| 1:F:101:ASP:OD1  | 1:F:131:LYS:NZ    | 2.46                     | 0.45              |
| 1:F:171:GLY:HA3  | 1:F:302:THR:OG1   | 2.15                     | 0.45              |
| 1:A:363:ARG:O    | 1:A:366:LEU:N     | 2.49                     | 0.45              |
| 1:A:278:ILE:HG13 | 1:A:613:ASN:HB3   | 1.97                     | 0.45              |
| 1:B:119:PRO:HG2  | 1:B:122:VAL:CG2   | 2.46                     | 0.45              |
| 1:B:363:ARG:HD2  | 1:B:498:LYS:HD2   | 1.97                     | 0.45              |
| 1:B:23:GLY:HA3   | 1:B:377:LEU:HB3   | 1.99                     | 0.45              |
| 1:B:469:GLN:O    | 1:B:473:THR:OG1   | 2.14                     | 0.45              |
| 1:B:510:LYS:HB2  | 1:B:514:GLY:H     | 1.82                     | 0.45              |
| 1:C:1006:MET:HA  | 1:C:1009:ALA:HB3  | 1.97                     | 0.45              |
| 1:C:514:GLY:O    | 1:C:518:ARG:HD3   | 2.16                     | 0.45              |
| 1:D:974:SER:CB   | 1:D:1010:THR:HG21 | 2.47                     | 0.45              |
| 1:D:72:ILE:HD13  | 1:D:107:VAL:HG22  | 1.99                     | 0.45              |
| 1:D:470:PHE:CE2  | 1:D:924:VAL:HG21  | 2.51                     | 0.45              |
| 1:E:186:ILE:O    | 1:E:768:VAL:HA    | 2.16                     | 0.45              |
| 1:F:1003:MET:O   | 1:F:1007:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:941:VAL:HG13 | 1:F:1021:PHE:CZ   | 2.52                     | 0.45              |
| 1:F:65:ILE:HD13  | 1:F:90:ILE:HD11   | 1.97                     | 0.45              |
| 1:F:77:TYR:CE1   | 1:F:93:THR:HG21   | 2.52                     | 0.45              |
| 1:F:676:ASP:HB3  | 1:F:823:LEU:CD2   | 2.46                     | 0.45              |
| 1:A:349:ILE:O    | 1:A:352:PHE:HB3   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:654:LYS:HA   | 1:A:654:LYS:HD3  | 1.62                     | 0.45              |
| 1:B:347:ALA:O    | 1:B:351:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:418:ARG:HD2  | 1:B:965:MET:HB2  | 1.98                     | 0.45              |
| 1:C:407:ASP:OD1  | 1:C:407:ASP:N    | 2.48                     | 0.45              |
| 1:C:662:ASN:OD1  | 1:C:663:LEU:HD23 | 2.16                     | 0.45              |
| 1:E:166:ILE:HG23 | 1:E:306:ILE:HG12 | 1.99                     | 0.45              |
| 1:E:54:ALA:N     | 1:E:84:SER:HA    | 2.31                     | 0.45              |
| 1:E:876:LEU:HD23 | 1:E:876:LEU:HA   | 1.82                     | 0.45              |
| 1:E:982:MET:O    | 1:E:985:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:459:PHE:CZ   | 1:F:871:LEU:HG   | 2.52                     | 0.45              |
| 1:A:377:LEU:HA   | 1:A:377:LEU:HD23 | 1.78                     | 0.45              |
| 1:A:981:VAL:O    | 1:A:984:LEU:N    | 2.46                     | 0.45              |
| 1:C:527:TYR:OH   | 1:C:1014:ILE:O   | 2.24                     | 0.45              |
| 1:C:527:TYR:CE2  | 1:C:963:VAL:HG13 | 2.52                     | 0.45              |
| 1:C:812:GLU:HB2  | 1:C:819:SER:O    | 2.16                     | 0.45              |
| 1:C:892:ILE:HD12 | 1:C:1021:PHE:HE1 | 1.81                     | 0.45              |
| 1:D:293:LEU:HD13 | 1:D:294:ALA:O    | 2.16                     | 0.45              |
| 1:D:414:GLU:OE2  | 1:D:969:PRO:HG3  | 2.16                     | 0.45              |
| 1:D:3:ASN:O      | 1:D:4:PHE:C      | 2.55                     | 0.45              |
| 1:D:572:PHE:CE1  | 1:D:643:THR:HG22 | 2.50                     | 0.45              |
| 1:E:331:PRO:HA   | 1:E:334:LYS:HD2  | 1.98                     | 0.45              |
| 1:E:697:LEU:HD12 | 1:E:697:LEU:HA   | 1.75                     | 0.45              |
| 1:F:694:ARG:HD3  | 1:F:820:MET:SD   | 2.57                     | 0.45              |
| 1:A:30:LEU:HD11  | 1:A:384:ALA:HA   | 1.98                     | 0.45              |
| 1:A:708:LEU:HA   | 1:A:825:GLN:O    | 2.16                     | 0.45              |
| 1:A:900:VAL:O    | 1:A:904:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:948:MET:HG3  | 1:A:954:GLY:O    | 2.17                     | 0.45              |
| 1:B:373:PRO:O    | 1:B:376:LEU:HB2  | 2.17                     | 0.45              |
| 1:B:442:LEU:O    | 1:B:445:ILE:HG13 | 2.16                     | 0.45              |
| 1:B:961:ASP:OD2  | 1:B:964:ARG:NH2  | 2.50                     | 0.45              |
| 1:C:121:GLU:O    | 1:C:124:GLN:HG2  | 2.15                     | 0.45              |
| 1:C:786:VAL:HG23 | 1:C:796:PHE:CE2  | 2.51                     | 0.45              |
| 1:D:251:LEU:HD12 | 1:D:265:VAL:HG21 | 1.99                     | 0.45              |
| 1:E:377:LEU:O    | 1:E:380:PHE:HB2  | 2.17                     | 0.45              |
| 1:E:415:ASN:HD22 | 1:E:434:SER:CB   | 2.27                     | 0.45              |
| 1:F:250:LEU:HD13 | 1:F:259:ARG:HB3  | 1.98                     | 0.45              |
| 1:F:642:ILE:O    | 1:F:645:ARG:HG2  | 2.17                     | 0.45              |
| 1:F:980:GLY:O    | 1:F:983:PRO:HD2  | 2.17                     | 0.45              |
| 1:A:941:VAL:HG22 | 1:A:1021:PHE:CD1 | 2.52                     | 0.45              |
| 1:B:580:ALA:HB1  | 1:B:719:THR:HG22 | 1.99                     | 0.45              |
| 1:B:647:THR:CG2  | 1:B:660:ALA:H    | 2.29                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:394:THR:O    | 1:C:398:MET:HG2  | 2.17                     | 0.45              |
| 1:D:977:PHE:HD2  | 1:D:1006:MET:HG3 | 1.82                     | 0.45              |
| 1:D:1016:PHE:O   | 1:D:1019:VAL:HB  | 2.17                     | 0.45              |
| 1:D:383:LEU:HD22 | 1:D:388:PHE:CD1  | 2.52                     | 0.45              |
| 1:D:383:LEU:HD22 | 1:D:388:PHE:HD1  | 1.81                     | 0.45              |
| 1:D:618:ASN:N    | 1:D:618:ASN:OD1  | 2.50                     | 0.45              |
| 1:E:278:ILE:HG13 | 1:E:613:ASN:HB3  | 1.98                     | 0.45              |
| 1:E:708:LEU:HG   | 1:E:708:LEU:H    | 1.42                     | 0.45              |
| 1:E:354:VAL:CG1  | 1:E:972:MET:HG2  | 2.46                     | 0.45              |
| 1:F:361:ASN:HD22 | 1:F:364:ALA:HB2  | 1.80                     | 0.45              |
| 1:F:5:PHE:HD2    | 1:F:6:ILE:HG12   | 1.82                     | 0.45              |
| 1:F:932:LEU:O    | 1:F:935:LYS:HB3  | 2.17                     | 0.45              |
| 1:A:184:MET:HB3  | 1:A:766:VAL:HG13 | 1.98                     | 0.45              |
| 1:A:597:TYR:CD2  | 1:A:650:PHE:CZ   | 3.05                     | 0.45              |
| 1:A:873:ALA:O    | 1:A:877:ILE:HG12 | 2.16                     | 0.45              |
| 1:A:956:ILE:HG13 | 1:A:956:ILE:H    | 1.38                     | 0.45              |
| 1:B:139:VAL:HA   | 1:B:289:LEU:O    | 2.16                     | 0.45              |
| 1:B:293:LEU:HD11 | 1:B:297:ALA:O    | 2.17                     | 0.45              |
| 1:B:428:LYS:O    | 1:B:431:THR:N    | 2.49                     | 0.45              |
| 1:C:376:LEU:HD22 | 1:C:398:MET:CE   | 2.47                     | 0.45              |
| 1:C:379:THR:HG23 | 1:C:476:SER:OG   | 2.17                     | 0.45              |
| 1:D:240:LEU:HD22 | 1:D:245:GLU:OE1  | 2.16                     | 0.45              |
| 1:D:763:VAL:HG12 | 1:E:63:GLN:OE1   | 2.17                     | 0.45              |
| 1:D:7:ASP:O      | 1:D:8:ARG:HG3    | 2.16                     | 0.45              |
| 1:D:880:PHE:O    | 1:D:883:LEU:HB2  | 2.17                     | 0.45              |
| 1:D:979:LEU:HA   | 1:D:979:LEU:HD23 | 1.34                     | 0.45              |
| 1:E:425:LEU:HD12 | 1:E:430:ALA:HA   | 1.99                     | 0.45              |
| 1:E:564:LEU:CD1  | 1:E:666:ILE:HD12 | 2.47                     | 0.45              |
| 1:E:564:LEU:HD13 | 1:E:666:ILE:HD12 | 1.98                     | 0.45              |
| 1:F:521:GLU:O    | 1:F:524:THR:HB   | 2.16                     | 0.45              |
| 1:F:700:GLU:HA   | 1:F:703:LYS:HZ2  | 1.82                     | 0.45              |
| 1:F:787:ARG:HA   | 1:F:792:GLN:O    | 2.17                     | 0.45              |
| 1:A:158:VAL:HA   | 1:A:162:MET:HE2  | 1.99                     | 0.45              |
| 1:A:882:CYS:O    | 1:A:885:ALA:HB3  | 2.16                     | 0.45              |
| 1:B:445:ILE:HG21 | 1:B:935:LYS:HD2  | 1.98                     | 0.45              |
| 1:C:181:GLN:HG2  | 1:C:182:TYR:N    | 2.31                     | 0.45              |
| 1:D:441:ALA:HB2  | 1:D:942:GLU:OE2  | 2.17                     | 0.45              |
| 1:A:444:GLY:O    | 1:A:448:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:720:PRO:HA   | 1:A:805:GLU:O    | 2.16                     | 0.45              |
| 1:A:75:LEU:CD1   | 1:A:92:LEU:HD23  | 2.47                     | 0.45              |
| 1:B:383:LEU:HD22 | 1:B:472:ILE:HG22 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:650:PHE:HB3  | 1:B:658:VAL:HB   | 1.99                     | 0.45              |
| 1:B:354:VAL:HG22 | 1:B:975:LEU:HD23 | 1.99                     | 0.45              |
| 1:C:461:GLY:HA3  | 1:C:863:LEU:HD21 | 1.99                     | 0.45              |
| 1:D:343:THR:O    | 1:D:344:LEU:C    | 2.55                     | 0.45              |
| 1:D:685:LEU:O    | 1:D:689:LYS:HD2  | 2.16                     | 0.45              |
| 1:E:427:PRO:O    | 1:E:430:ALA:HB3  | 2.16                     | 0.45              |
| 1:E:367:ILE:CD1  | 1:E:497:LEU:HD13 | 2.47                     | 0.45              |
| 1:E:108:GLN:CD   | 1:F:112:GLN:HG2  | 2.37                     | 0.45              |
| 1:F:363:ARG:CZ   | 1:F:363:ARG:H    | 2.29                     | 0.45              |
| 1:F:887:TYR:C    | 1:F:889:SER:N    | 2.70                     | 0.45              |
| 1:A:35:TYR:CE2   | 1:A:564:LEU:HD21 | 2.52                     | 0.44              |
| 1:A:388:PHE:CZ   | 1:A:472:ILE:HG21 | 2.52                     | 0.44              |
| 1:B:193:LEU:HD23 | 1:B:193:LEU:HA   | 1.83                     | 0.44              |
| 1:B:525:HIS:O    | 1:B:528:THR:HG22 | 2.17                     | 0.44              |
| 1:B:674:GLY:HA2  | 1:B:825:GLN:HA   | 1.98                     | 0.44              |
| 1:B:723:LYS:HE3  | 1:B:725:ASP:OD2  | 2.17                     | 0.44              |
| 1:B:873:ALA:O    | 1:B:877:ILE:HG13 | 2.17                     | 0.44              |
| 1:C:163:LYS:HE3  | 1:C:177:LEU:HB2  | 1.99                     | 0.44              |
| 1:C:694:ARG:HG2  | 1:C:698:LEU:HD12 | 1.98                     | 0.44              |
| 1:C:845:LYS:HD2  | 1:C:845:LYS:O    | 2.17                     | 0.44              |
| 1:D:214:VAL:HG21 | 1:E:742:ASN:ND2  | 2.32                     | 0.44              |
| 1:D:262:LEU:HG   | 1:D:268:ILE:HD11 | 1.99                     | 0.44              |
| 1:D:831:SER:OG   | 1:D:832:THR:N    | 2.49                     | 0.44              |
| 1:D:685:LEU:HD21 | 1:D:848:THR:O    | 2.18                     | 0.44              |
| 1:E:111:LEU:HD21 | 1:E:127:VAL:HG11 | 1.98                     | 0.44              |
| 1:E:108:GLN:HA   | 1:E:129:VAL:HG21 | 1.98                     | 0.44              |
| 1:E:571:VAL:HG22 | 1:E:625:SER:HA   | 1.98                     | 0.44              |
| 1:F:187:TRP:O    | 1:F:266:ALA:HB1  | 2.17                     | 0.44              |
| 1:F:614:GLY:O    | 1:F:616:GLY:HA3  | 2.16                     | 0.44              |
| 1:A:388:PHE:CE2  | 1:A:472:ILE:HD13 | 2.53                     | 0.44              |
| 1:A:722:PHE:CD1  | 1:A:804:TRP:CE2  | 3.05                     | 0.44              |
| 1:A:470:PHE:CD2  | 1:A:924:VAL:HG11 | 2.52                     | 0.44              |
| 1:A:904:VAL:HA   | 1:A:926:LEU:HD21 | 1.99                     | 0.44              |
| 1:B:329:THR:O    | 1:B:333:VAL:HG23 | 2.16                     | 0.44              |
| 1:B:576:VAL:HG22 | 1:B:658:VAL:HG22 | 1.99                     | 0.44              |
| 1:D:214:VAL:HG11 | 1:E:742:ASN:CG   | 2.38                     | 0.44              |
| 1:D:307:ARG:HA   | 1:D:307:ARG:HD3  | 1.88                     | 0.44              |
| 1:D:336:SER:O    | 1:D:340:VAL:HG23 | 2.17                     | 0.44              |
| 1:D:723:LYS:HB3  | 1:D:803:ARG:HG2  | 2.00                     | 0.44              |
| 1:E:102:ILE:O    | 1:E:106:GLN:HG3  | 2.17                     | 0.44              |
| 1:E:255:GLN:HG3  | 1:E:255:GLN:H    | 1.38                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:329:THR:O    | 1:E:332:PHE:HB3   | 2.18                     | 0.44              |
| 1:E:409:ALA:O    | 1:E:413:VAL:HG23  | 2.17                     | 0.44              |
| 1:E:568:ASP:O    | 1:E:629:TRP:CZ3   | 2.70                     | 0.44              |
| 1:E:770:SER:OG   | 1:E:775:ARG:HG2   | 2.18                     | 0.44              |
| 1:F:65:ILE:O     | 1:F:69:MET:HG2    | 2.17                     | 0.44              |
| 1:F:940:ILE:HG12 | 1:F:966:ARG:NH2   | 2.32                     | 0.44              |
| 1:A:213:GLN:HA   | 1:A:237:GLN:O     | 2.17                     | 0.44              |
| 1:A:663:LEU:HD12 | 1:A:667:VAL:HG13  | 1.98                     | 0.44              |
| 1:A:871:LEU:O    | 1:A:874:ILE:HB    | 2.17                     | 0.44              |
| 1:B:235:ILE:HD11 | 1:C:721:GLN:OE1   | 2.17                     | 0.44              |
| 1:B:330:THR:HB   | 1:B:331:PRO:HD3   | 1.98                     | 0.44              |
| 1:B:65:ILE:O     | 1:B:69:MET:HG2    | 2.17                     | 0.44              |
| 1:B:984:LEU:HB3  | 1:B:995:GLN:O     | 2.17                     | 0.44              |
| 1:C:615:GLY:HA2  | 1:C:616:GLY:HA3   | 1.69                     | 0.44              |
| 1:D:463:THR:HG22 | 1:D:467:TYR:CE2   | 2.51                     | 0.44              |
| 1:D:827:ALA:O    | 1:D:830:LYS:N     | 2.39                     | 0.44              |
| 1:D:123:GLN:HB3  | 1:E:116:PRO:HB3   | 1.99                     | 0.44              |
| 1:A:34:GLN:O     | 1:A:392:THR:OG1   | 2.16                     | 0.44              |
| 1:A:376:LEU:HD22 | 1:A:398:MET:SD    | 2.57                     | 0.44              |
| 1:A:344:LEU:CD2  | 1:A:402:ILE:HD11  | 2.45                     | 0.44              |
| 1:A:650:PHE:HD1  | 1:A:653:ILE:HD11  | 1.83                     | 0.44              |
| 1:D:531:VAL:O    | 1:D:535:LEU:HG    | 2.17                     | 0.44              |
| 1:D:833:GLY:O    | 1:D:836:MET:HB2   | 2.17                     | 0.44              |
| 1:D:871:LEU:HA   | 1:D:871:LEU:HD23  | 1.66                     | 0.44              |
| 1:D:911:ALA:HB2  | 1:D:922:PHE:CE1   | 2.53                     | 0.44              |
| 1:E:344:LEU:O    | 1:E:348:ILE:HG13  | 2.18                     | 0.44              |
| 1:E:632:ARG:HB3  | 1:E:637:ASN:HB3   | 1.99                     | 0.44              |
| 1:E:837:GLU:O    | 1:E:840:GLU:HB2   | 2.18                     | 0.44              |
| 1:F:247:GLY:O    | 1:F:261:LEU:HB3   | 2.18                     | 0.44              |
| 1:F:312:LYS:HD3  | 1:F:312:LYS:O     | 2.17                     | 0.44              |
| 1:A:892:ILE:HG12 | 1:A:1025:ARG:CD   | 2.46                     | 0.44              |
| 1:C:103:ALA:O    | 1:C:107:VAL:HG23  | 2.18                     | 0.44              |
| 1:C:343:THR:HA   | 1:C:346:GLU:OE1   | 2.17                     | 0.44              |
| 1:C:53:ASP:HA    | 1:C:84:SER:HB2    | 1.99                     | 0.44              |
| 1:D:328:ASP:O    | 1:D:331:PRO:HD2   | 2.18                     | 0.44              |
| 1:D:366:LEU:HD22 | 1:D:370:ILE:HG13  | 2.00                     | 0.44              |
| 1:D:982:MET:HB3  | 1:D:983:PRO:HD3   | 2.00                     | 0.44              |
| 1:E:568:ASP:O    | 1:E:629:TRP:HZ3   | 2.00                     | 0.44              |
| 1:E:685:LEU:HD11 | 1:E:690:LEU:HG    | 1.99                     | 0.44              |
| 1:F:400:LEU:HD11 | 1:F:1002:VAL:HG21 | 1.99                     | 0.44              |
| 1:F:728:GLN:HE22 | 1:F:738:ILE:HG21  | 1.83                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:413:VAL:HA   | 1:A:493:CYS:SG    | 2.57                     | 0.44              |
| 1:A:691:THR:HG23 | 1:A:694:ARG:NH1   | 2.25                     | 0.44              |
| 1:A:769:MET:HG2  | 1:A:770:SER:N     | 2.33                     | 0.44              |
| 1:A:959:THR:HG21 | 1:A:1022:VAL:HG23 | 1.99                     | 0.44              |
| 1:B:399:VAL:HA   | 1:B:402:ILE:HG13  | 2.00                     | 0.44              |
| 1:B:61:VAL:HG22  | 1:B:119:PRO:HD2   | 1.99                     | 0.44              |
| 1:B:707:MET:SD   | 1:B:830:LYS:HG2   | 2.58                     | 0.44              |
| 1:C:538:THR:HG21 | 1:C:1023:VAL:CG2  | 2.48                     | 0.44              |
| 1:C:6:ILE:HG22   | 1:C:8:ARG:O       | 2.17                     | 0.44              |
| 1:D:345:VAL:O    | 1:D:349:ILE:HD12  | 2.18                     | 0.44              |
| 1:D:682:GLN:HG3  | 1:D:817:LEU:HD13  | 2.00                     | 0.44              |
| 1:D:400:LEU:HG   | 1:D:928:THR:OG1   | 2.18                     | 0.44              |
| 1:E:198:LEU:HD21 | 1:E:252:LYS:HB2   | 1.99                     | 0.44              |
| 1:E:309:GLU:OE2  | 1:E:313:MET:HE3   | 2.17                     | 0.44              |
| 1:E:420:MET:SD   | 1:E:499:PRO:HA    | 2.58                     | 0.44              |
| 1:E:610:PHE:HB2  | 1:E:623:PHE:HB3   | 2.00                     | 0.44              |
| 1:E:728:GLN:HE22 | 1:E:738:ILE:HG21  | 1.82                     | 0.44              |
| 1:F:1018:PRO:O   | 1:F:1022:VAL:HG23 | 2.18                     | 0.44              |
| 1:F:484:VAL:C    | 1:F:486:LEU:N     | 2.71                     | 0.44              |
| 1:F:647:THR:HG23 | 1:F:659:PHE:CE1   | 2.53                     | 0.44              |
| 1:F:927:LEU:O    | 1:F:928:THR:C     | 2.55                     | 0.44              |
| 1:A:415:ASN:O    | 1:A:419:VAL:HG23  | 2.17                     | 0.44              |
| 1:A:424:GLY:C    | 1:A:502:LYS:HZ2   | 2.20                     | 0.44              |
| 1:B:478:MET:O    | 1:B:482:VAL:HG12  | 2.17                     | 0.44              |
| 1:C:574:THR:HG23 | 1:C:622:ALA:HB3   | 1.98                     | 0.44              |
| 1:C:65:ILE:HD11  | 1:C:118:LEU:HD11  | 1.99                     | 0.44              |
| 1:C:955:LEU:O    | 1:C:959:THR:HG23  | 2.17                     | 0.44              |
| 1:C:975:LEU:O    | 1:C:976:ALA:C     | 2.55                     | 0.44              |
| 1:D:346:GLU:O    | 1:D:350:LEU:HD12  | 2.17                     | 0.44              |
| 1:D:395:MET:O    | 1:D:399:VAL:HG23  | 2.17                     | 0.44              |
| 1:D:514:GLY:C    | 1:D:516:PHE:N     | 2.71                     | 0.44              |
| 1:D:975:LEU:HA   | 1:D:975:LEU:HD12  | 1.82                     | 0.44              |
| 1:E:21:LEU:O     | 1:E:25:LEU:HB2    | 2.18                     | 0.44              |
| 1:E:694:ARG:NH2  | 1:E:717:GLU:OE1   | 2.50                     | 0.44              |
| 1:F:101:ASP:O    | 1:F:105:VAL:HG23  | 2.17                     | 0.44              |
| 1:F:345:VAL:O    | 1:F:349:ILE:HD12  | 2.18                     | 0.44              |
| 1:F:468:ARG:HA   | 1:F:471:SER:OG    | 2.18                     | 0.44              |
| 1:B:72:ILE:HG12  | 1:B:106:GLN:HB3   | 1.99                     | 0.44              |
| 1:B:13:TRP:O     | 1:B:17:ILE:HG13   | 2.17                     | 0.44              |
| 1:D:164:ASP:HB3  | 1:D:168:ARG:HH21  | 1.82                     | 0.44              |
| 1:D:956:ILE:H    | 1:D:956:ILE:HG13  | 1.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:602:GLU:HB3  | 1:F:606:VAL:HG23 | 1.99                     | 0.44              |
| 1:F:916:LEU:HD23 | 1:F:916:LEU:HA   | 1.76                     | 0.44              |
| 1:A:895:SER:HB2  | 1:A:1021:PHE:HA  | 1.99                     | 0.44              |
| 1:A:130:GLU:HB3  | 1:A:132:SER:HB2  | 2.00                     | 0.44              |
| 1:A:324:VAL:HG22 | 1:A:325:TYR:H    | 1.82                     | 0.44              |
| 1:A:483:LEU:HD13 | 1:A:487:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:636:GLU:HB2  | 1:A:645:ARG:NH2  | 2.30                     | 0.44              |
| 1:B:399:VAL:O    | 1:B:402:ILE:HG13 | 2.18                     | 0.44              |
| 1:B:445:ILE:HD12 | 1:B:449:LEU:HD12 | 2.00                     | 0.44              |
| 1:B:721:GLN:CD   | 1:B:807:GLY:HA3  | 2.38                     | 0.44              |
| 1:B:975:LEU:O    | 1:B:979:LEU:HB2  | 2.18                     | 0.44              |
| 1:C:429:GLU:O    | 1:C:433:LYS:HB2  | 2.18                     | 0.44              |
| 1:C:663:LEU:H    | 1:C:663:LEU:HD23 | 1.83                     | 0.44              |
| 2:D:2000:LMT:H6E | 2:D:2000:LMT:O5B | 2.18                     | 0.44              |
| 1:D:563:PHE:O    | 1:D:564:LEU:HD12 | 2.18                     | 0.44              |
| 1:E:172:VAL:HG22 | 1:E:302:THR:HG23 | 2.00                     | 0.44              |
| 1:E:515:TRP:O    | 1:E:519:MET:HG3  | 2.18                     | 0.44              |
| 1:E:905:ILE:HG23 | 1:E:906:GLY:N    | 2.33                     | 0.44              |
| 1:F:669:LEU:HD22 | 1:F:856:GLY:HA2  | 1.98                     | 0.44              |
| 1:A:270:LEU:HA   | 1:A:270:LEU:HD12 | 1.85                     | 0.43              |
| 1:A:451:ALA:CB   | 1:A:878:VAL:HG12 | 2.48                     | 0.43              |
| 1:B:214:VAL:HG21 | 1:C:742:ASN:ND2  | 2.32                     | 0.43              |
| 1:B:194:ASN:HA   | 1:B:793:MET:HE2  | 2.00                     | 0.43              |
| 1:B:902:LEU:HD11 | 1:B:1016:PHE:CD2 | 2.53                     | 0.43              |
| 1:B:959:THR:HG21 | 1:B:1022:VAL:CG2 | 2.48                     | 0.43              |
| 1:C:370:ILE:C    | 1:C:373:PRO:HD2  | 2.39                     | 0.43              |
| 1:C:722:PHE:CZ   | 1:C:802:SER:HB2  | 2.53                     | 0.43              |
| 1:D:196:PHE:CG   | 1:D:260:VAL:HG11 | 2.53                     | 0.43              |
| 1:D:377:LEU:O    | 1:D:380:PHE:HB2  | 2.17                     | 0.43              |
| 1:D:712:ARG:O    | 1:D:822:ILE:HG23 | 2.17                     | 0.43              |
| 1:E:110:LYS:HD3  | 1:E:110:LYS:HA   | 1.60                     | 0.43              |
| 1:E:149:MET:HB2  | 1:E:153:ASP:CB   | 2.43                     | 0.43              |
| 1:F:146:ASP:OD2  | 1:F:147:GLY:N    | 2.49                     | 0.43              |
| 1:F:343:THR:O    | 1:F:346:GLU:N    | 2.51                     | 0.43              |
| 1:F:35:TYR:HB3   | 1:F:38:ILE:HD12  | 2.00                     | 0.43              |
| 1:F:425:LEU:HB3  | 1:F:429:GLU:HB3  | 2.00                     | 0.43              |
| 1:F:49:TYR:CD1   | 1:F:57:VAL:HA    | 2.52                     | 0.43              |
| 1:F:281:PHE:HB2  | 1:F:610:PHE:CE1  | 2.53                     | 0.43              |
| 1:F:770:SER:OG   | 1:F:775:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:1035:ILE:O   | 1:A:1036:GLU:HB2 | 2.18                     | 0.43              |
| 1:A:788:ALA:HB3  | 1:A:790:ASP:OD2  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:424:GLY:HA3  | 1:B:502:LYS:HB2  | 2.00                     | 0.43              |
| 1:B:526:HIS:O    | 1:B:529:ASP:HB2  | 2.18                     | 0.43              |
| 1:B:691:THR:HG23 | 1:B:694:ARG:NH1  | 2.33                     | 0.43              |
| 1:B:755:ASN:O    | 1:B:766:VAL:HB   | 2.18                     | 0.43              |
| 1:D:1020:PHE:O   | 1:D:1024:VAL:HB  | 2.18                     | 0.43              |
| 1:D:34:GLN:HB2   | 1:D:333:VAL:HG22 | 2.00                     | 0.43              |
| 1:D:960:LEU:HD23 | 1:D:960:LEU:HA   | 1.75                     | 0.43              |
| 1:E:370:ILE:HD12 | 1:E:492:LEU:HD13 | 2.00                     | 0.43              |
| 1:E:187:TRP:HZ3  | 1:E:769:MET:HB3  | 1.82                     | 0.43              |
| 1:E:821:GLU:HG2  | 1:E:822:ILE:N    | 2.33                     | 0.43              |
| 1:E:676:ASP:HA   | 1:E:823:LEU:HD23 | 1.99                     | 0.43              |
| 1:F:343:THR:HA   | 1:F:346:GLU:OE1  | 2.18                     | 0.43              |
| 1:F:610:PHE:O    | 1:F:622:ALA:HA   | 2.18                     | 0.43              |
| 1:A:158:VAL:HA   | 1:A:162:MET:CE   | 2.48                     | 0.43              |
| 1:A:480:LEU:HA   | 1:A:480:LEU:HD23 | 1.78                     | 0.43              |
| 1:A:527:TYR:O    | 1:A:530:SER:HB3  | 2.18                     | 0.43              |
| 1:A:667:VAL:HG12 | 1:A:668:GLU:OE1  | 2.19                     | 0.43              |
| 1:A:770:SER:OG   | 1:A:775:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:962:ALA:O    | 1:A:965:MET:HG2  | 2.18                     | 0.43              |
| 1:B:544:LEU:O    | 1:B:548:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:405:LEU:HD12 | 1:C:406:VAL:N    | 2.34                     | 0.43              |
| 1:C:679:LEU:O    | 1:C:819:SER:HB2  | 2.18                     | 0.43              |
| 1:C:905:ILE:HG13 | 1:C:909:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:911:ALA:HB2  | 1:C:922:PHE:CE1  | 2.52                     | 0.43              |
| 1:D:246:PHE:O    | 1:D:262:LEU:HD23 | 2.18                     | 0.43              |
| 1:D:415:ASN:ND2  | 1:D:943:PHE:HZ   | 2.15                     | 0.43              |
| 1:D:559:LEU:HA   | 1:D:560:PRO:HD2  | 1.68                     | 0.43              |
| 1:D:588:GLN:NE2  | 1:D:588:GLN:O    | 2.51                     | 0.43              |
| 1:D:691:THR:HA   | 1:D:694:ARG:NH1  | 2.33                     | 0.43              |
| 1:D:343:THR:HG21 | 1:D:984:LEU:HD21 | 2.00                     | 0.43              |
| 1:E:238:THR:HG22 | 1:E:239:ARG:O    | 2.17                     | 0.43              |
| 1:E:559:LEU:CD2  | 1:E:560:PRO:HD2  | 2.46                     | 0.43              |
| 1:F:143:ILE:HG12 | 1:F:322:LYS:O    | 2.19                     | 0.43              |
| 1:F:348:ILE:HG12 | 1:F:402:ILE:HD13 | 2.00                     | 0.43              |
| 1:F:650:PHE:HB2  | 1:F:658:VAL:O    | 2.18                     | 0.43              |
| 1:F:707:MET:HB2  | 1:F:708:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:154:ILE:HG22 | 1:A:287:SER:HB3  | 2.01                     | 0.43              |
| 1:A:615:GLY:HA2  | 1:A:617:GLN:H    | 1.82                     | 0.43              |
| 1:A:695:ASN:O    | 1:A:698:LEU:HB2  | 2.18                     | 0.43              |
| 1:A:722:PHE:HD1  | 1:A:804:TRP:CE2  | 2.37                     | 0.43              |
| 1:A:932:LEU:O    | 1:A:935:LYS:HB3  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1031:LYS:HA  | 1:B:1032:ASN:HA   | 1.68                     | 0.43              |
| 1:B:452:VAL:HG23 | 1:B:453:PHE:CD2   | 2.53                     | 0.43              |
| 1:B:594:VAL:HG22 | 1:B:650:PHE:CZ    | 2.53                     | 0.43              |
| 1:B:574:THR:HG21 | 1:B:598:TYR:HE2   | 1.83                     | 0.43              |
| 1:C:1031:LYS:HD2 | 1:C:1033:GLU:CB   | 2.49                     | 0.43              |
| 1:C:143:ILE:HG22 | 1:C:286:ALA:CB    | 2.48                     | 0.43              |
| 1:C:146:ASP:O    | 1:C:148:THR:OG1   | 2.36                     | 0.43              |
| 1:C:363:ARG:NH2  | 1:C:498:LYS:HD2   | 2.33                     | 0.43              |
| 1:D:1007:VAL:O   | 1:D:1011:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:124:GLN:NE2  | 1:D:753:TYR:HD2   | 2.16                     | 0.43              |
| 1:D:454:VAL:O    | 1:D:457:ALA:HB3   | 2.19                     | 0.43              |
| 1:D:771:GLU:HB3  | 1:D:774:TYR:CD1   | 2.53                     | 0.43              |
| 1:D:786:VAL:HG23 | 1:D:796:PHE:CE2   | 2.53                     | 0.43              |
| 1:D:81:ASN:O     | 1:D:88:VAL:HG23   | 2.19                     | 0.43              |
| 1:E:173:GLY:O    | 1:F:71:GLY:HA3    | 2.18                     | 0.43              |
| 1:F:144:ASN:OD1  | 1:F:148:THR:HA    | 2.18                     | 0.43              |
| 1:F:54:ALA:HB1   | 1:F:811:LEU:HG    | 2.00                     | 0.43              |
| 1:F:84:SER:HB3   | 1:F:809:PRO:O     | 2.17                     | 0.43              |
| 1:A:137:LEU:HD13 | 1:A:293:LEU:HG    | 1.99                     | 0.43              |
| 1:A:189:ASN:HA   | 1:A:190:PRO:HD3   | 1.74                     | 0.43              |
| 1:B:681:ASP:HA   | 1:B:849:GLY:O     | 2.18                     | 0.43              |
| 1:C:546:LEU:O    | 1:C:550:VAL:HG23  | 2.18                     | 0.43              |
| 1:D:959:THR:HG21 | 1:D:1022:VAL:CG2  | 2.49                     | 0.43              |
| 1:D:199:THR:HG21 | 1:D:787:ARG:H     | 1.82                     | 0.43              |
| 1:E:30:LEU:HA    | 1:E:30:LEU:HD12   | 1.78                     | 0.43              |
| 1:E:597:TYR:O    | 1:E:601:LYS:HB2   | 2.18                     | 0.43              |
| 1:F:196:PHE:CD2  | 1:F:260:VAL:HG21  | 2.54                     | 0.43              |
| 1:F:544:LEU:O    | 1:F:547:ILE:HB    | 2.18                     | 0.43              |
| 1:F:771:GLU:HB2  | 1:F:774:TYR:HD1   | 1.82                     | 0.43              |
| 1:A:3:ASN:O      | 1:A:4:PHE:C       | 2.57                     | 0.43              |
| 1:A:530:SER:O    | 1:A:533:GLY:N     | 2.51                     | 0.43              |
| 1:A:639:VAL:CG1  | 1:A:662:ASN:HB2   | 2.42                     | 0.43              |
| 1:A:79:SER:HA    | 1:A:813:ARG:O     | 2.19                     | 0.43              |
| 1:A:814:TYR:OH   | 1:A:854:TRP:O     | 2.29                     | 0.43              |
| 1:B:1033:GLU:OE2 | 1:B:1034:ASP:HB2  | 2.18                     | 0.43              |
| 1:B:407:ASP:OD1  | 1:B:973:THR:HG21  | 2.19                     | 0.43              |
| 1:B:281:PHE:HB2  | 1:B:610:PHE:CE1   | 2.53                     | 0.43              |
| 1:B:949:ASP:O    | 1:B:951:GLU:N     | 2.52                     | 0.43              |
| 1:B:981:VAL:O    | 1:B:982:MET:C     | 2.57                     | 0.43              |
| 1:C:531:VAL:O    | 1:C:535:LEU:HG    | 2.19                     | 0.43              |
| 1:C:836:MET:HG2  | 1:C:854:TRP:CZ3   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:927:LEU:O    | 1:C:930:ILE:N     | 2.51                     | 0.43              |
| 1:C:963:VAL:HA   | 1:C:966:ARG:HH12  | 1.82                     | 0.43              |
| 1:D:852:TYR:CD2  | 1:D:852:TYR:N     | 2.86                     | 0.43              |
| 1:D:966:ARG:O    | 1:D:970:ILE:HG12  | 2.18                     | 0.43              |
| 1:E:250:LEU:HD21 | 1:E:253:VAL:HG22  | 2.00                     | 0.43              |
| 1:F:38:ILE:HD13  | 1:F:466:ILE:CD1   | 2.49                     | 0.43              |
| 1:F:462:SER:O    | 1:F:466:ILE:HG12  | 2.19                     | 0.43              |
| 1:F:602:GLU:HG3  | 1:F:605:ASN:HB2   | 2.01                     | 0.43              |
| 1:A:1013:ALA:C   | 1:A:1015:PHE:H    | 2.21                     | 0.43              |
| 1:A:142:VAL:O    | 1:A:286:ALA:HB1   | 2.18                     | 0.43              |
| 1:A:497:LEU:HD12 | 1:A:497:LEU:HA    | 1.79                     | 0.43              |
| 1:A:540:ARG:HH22 | 2:A:1101:LMT:HG'2 | 1.84                     | 0.43              |
| 1:A:728:GLN:OE1  | 1:A:738:ILE:HG12  | 2.19                     | 0.43              |
| 1:A:946:ASP:OD1  | 1:A:946:ASP:C     | 2.56                     | 0.43              |
| 1:B:535:LEU:CD2  | 1:B:1019:VAL:HA   | 2.49                     | 0.43              |
| 1:B:26:ALA:HB1   | 1:B:384:ALA:CB    | 2.49                     | 0.43              |
| 1:C:188:MET:HB3  | 1:C:193:LEU:CD1   | 2.46                     | 0.43              |
| 1:C:677:PHE:CE1  | 1:C:852:TYR:HB2   | 2.53                     | 0.43              |
| 1:C:966:ARG:HG2  | 1:C:966:ARG:O     | 2.19                     | 0.43              |
| 1:D:102:ILE:HD12 | 1:F:101:ASP:HB3   | 2.01                     | 0.43              |
| 1:E:324:VAL:O    | 1:E:326:PRO:HD3   | 2.19                     | 0.43              |
| 1:E:602:GLU:O    | 1:E:602:GLU:HG3   | 2.19                     | 0.43              |
| 1:F:376:LEU:HD22 | 1:F:398:MET:CE    | 2.49                     | 0.43              |
| 1:F:344:LEU:CD2  | 1:F:402:ILE:HD11  | 2.48                     | 0.43              |
| 1:F:49:TYR:CE1   | 1:F:57:VAL:HA     | 2.53                     | 0.43              |
| 1:F:49:TYR:CG    | 1:F:57:VAL:HG12   | 2.54                     | 0.43              |
| 1:F:706:ASP:OD1  | 1:F:706:ASP:N     | 2.49                     | 0.43              |
| 1:A:242:SER:OG   | 1:A:245:GLU:HG2   | 2.19                     | 0.43              |
| 1:A:722:PHE:HB2  | 1:A:804:TRP:CZ3   | 2.52                     | 0.43              |
| 1:A:893:PRO:O    | 1:A:896:VAL:HG13  | 2.18                     | 0.43              |
| 1:C:166:ILE:HG23 | 1:C:172:VAL:HG11  | 2.01                     | 0.43              |
| 1:C:211:ASN:OD1  | 1:C:239:ARG:HA    | 2.18                     | 0.43              |
| 1:C:139:VAL:HG22 | 1:C:290:GLY:HA2   | 1.99                     | 0.43              |
| 1:C:66:GLU:HG2   | 1:C:78:MET:SD     | 2.59                     | 0.43              |
| 1:C:979:LEU:HA   | 1:C:979:LEU:HD23  | 1.51                     | 0.43              |
| 1:D:14:VAL:HG13  | 1:E:881:LEU:HB3   | 2.01                     | 0.43              |
| 1:D:339:GLU:HA   | 1:D:342:LYS:HB2   | 2.00                     | 0.43              |
| 1:D:464:GLY:O    | 1:D:468:ARG:HB2   | 2.18                     | 0.43              |
| 1:D:470:PHE:HD2  | 1:D:924:VAL:HG11  | 1.84                     | 0.43              |
| 1:D:507:GLU:O    | 1:D:509:LYS:N     | 2.52                     | 0.43              |
| 1:D:531:VAL:HA   | 1:D:534:ILE:CG1   | 2.49                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:553:ALA:O     | 1:D:557:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:663:LEU:H     | 1:D:663:LEU:HD23 | 1.83                     | 0.43              |
| 1:E:45:ILE:HA     | 1:E:128:SER:O    | 2.19                     | 0.43              |
| 1:E:248:LYS:HG2   | 1:E:263:ARG:NH2  | 2.33                     | 0.43              |
| 1:E:350:LEU:O     | 1:E:353:LEU:HB2  | 2.19                     | 0.43              |
| 1:F:180:SER:CB    | 1:F:274:ASN:H    | 2.31                     | 0.43              |
| 1:F:681:ASP:CG    | 1:F:682:GLN:N    | 2.71                     | 0.43              |
| 1:A:545:TYR:HA    | 1:A:548:ILE:HD12 | 1.99                     | 0.43              |
| 1:A:748:ALA:HB3   | 1:A:749:TRP:HD1  | 1.83                     | 0.43              |
| 1:A:966:ARG:NE    | 1:A:970:ILE:HD11 | 2.25                     | 0.43              |
| 1:B:352:PHE:HD2   | 1:B:353:LEU:HD23 | 1.84                     | 0.43              |
| 1:C:548:ILE:CD1   | 1:C:1016:PHE:HE1 | 2.32                     | 0.43              |
| 1:C:393:LEU:HD13  | 1:C:466:ILE:HA   | 2.00                     | 0.43              |
| 1:C:992:SER:HA    | 1:C:995:GLN:HG3  | 2.00                     | 0.43              |
| 1:D:1035:ILE:HG22 | 1:D:1036:GLU:O   | 2.19                     | 0.43              |
| 1:D:293:LEU:HD22  | 1:D:294:ALA:H    | 1.83                     | 0.43              |
| 1:D:485:ALA:O     | 1:D:490:PRO:HD3  | 2.18                     | 0.43              |
| 1:D:83:ASP:OD1    | 1:D:810:ARG:HD3  | 2.18                     | 0.43              |
| 1:D:867:GLN:HB3   | 1:D:871:LEU:HD12 | 2.00                     | 0.43              |
| 1:E:32:VAL:HA     | 1:E:390:ILE:O    | 2.19                     | 0.43              |
| 1:E:899:VAL:CG1   | 1:E:933:SER:HB2  | 2.48                     | 0.43              |
| 1:F:344:LEU:CD1   | 1:F:402:ILE:HD11 | 2.48                     | 0.43              |
| 1:F:871:LEU:HD22  | 1:F:927:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:763:VAL:HG12  | 1:B:63:GLN:NE2   | 2.33                     | 0.43              |
| 1:A:969:PRO:HA    | 1:A:972:MET:CE   | 2.49                     | 0.43              |
| 1:C:291:ILE:HD13  | 1:C:306:ILE:HD13 | 2.01                     | 0.43              |
| 1:C:544:LEU:O     | 1:C:548:ILE:HG13 | 2.19                     | 0.43              |
| 1:C:559:LEU:HA    | 1:C:560:PRO:HD2  | 1.77                     | 0.43              |
| 1:D:402:ILE:HD13  | 1:D:402:ILE:HG21 | 1.81                     | 0.43              |
| 1:D:5:PHE:CD2     | 1:D:487:ILE:HG23 | 2.53                     | 0.43              |
| 1:D:992:SER:HA    | 1:D:995:GLN:HG3  | 2.00                     | 0.43              |
| 1:E:219:LEU:HD23  | 1:F:749:TRP:CZ3  | 2.53                     | 0.43              |
| 1:E:685:LEU:HD12  | 1:E:686:GLY:O    | 2.18                     | 0.43              |
| 1:E:580:ALA:HB1   | 1:E:719:THR:HG21 | 2.00                     | 0.43              |
| 1:E:723:LYS:HE3   | 1:E:725:ASP:HB2  | 2.01                     | 0.43              |
| 1:F:355:MET:CG    | 1:F:410:ILE:HD11 | 2.49                     | 0.43              |
| 1:F:53:ASP:O      | 1:F:57:VAL:HG13  | 2.19                     | 0.43              |
| 1:A:26:ALA:O      | 1:A:30:LEU:HB2   | 2.19                     | 0.42              |
| 1:A:726:ILE:H     | 1:A:726:ILE:HG12 | 1.13                     | 0.42              |
| 1:B:612:VAL:HB    | 1:B:621:ILE:HG23 | 2.01                     | 0.42              |
| 1:B:695:ASN:O     | 1:B:698:LEU:HB2  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:969:PRO:HA   | 1:B:972:MET:HE3   | 2.00                     | 0.42              |
| 1:B:982:MET:HB3  | 1:B:983:PRO:CD    | 2.48                     | 0.42              |
| 1:C:1034:ASP:O   | 1:C:1035:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:356:TYR:HA   | 1:C:365:THR:HG21  | 2.01                     | 0.42              |
| 1:C:415:ASN:ND2  | 1:C:438:ILE:HG21  | 2.34                     | 0.42              |
| 1:C:447:MET:SD   | 1:C:886:LEU:HD22  | 2.59                     | 0.42              |
| 1:D:157:TYR:O    | 1:D:161:ASN:ND2   | 2.46                     | 0.42              |
| 1:D:25:LEU:HD12  | 1:D:25:LEU:HA     | 1.64                     | 0.42              |
| 1:D:82:SER:HB2   | 1:D:811:LEU:HB2   | 2.00                     | 0.42              |
| 1:E:164:ASP:O    | 1:E:168:ARG:HG3   | 2.19                     | 0.42              |
| 1:E:190:PRO:HG3  | 1:E:774:TYR:CG    | 2.54                     | 0.42              |
| 1:E:191:ASN:O    | 1:E:195:LYS:HB2   | 2.19                     | 0.42              |
| 1:E:597:TYR:HH   | 1:E:646:ALA:HA    | 1.84                     | 0.42              |
| 1:F:114:ALA:HA   | 1:F:117:LEU:HD12  | 2.00                     | 0.42              |
| 1:F:344:LEU:HD11 | 1:F:376:LEU:HD11  | 2.01                     | 0.42              |
| 1:F:356:TYR:C    | 1:F:358:PHE:N     | 2.73                     | 0.42              |
| 1:A:1008:THR:O   | 1:A:1012:LEU:HB2  | 2.20                     | 0.42              |
| 1:B:9:PRO:O      | 1:B:12:ALA:HB3    | 2.18                     | 0.42              |
| 1:C:184:MET:HE3  | 1:C:185:ARG:N     | 2.34                     | 0.42              |
| 1:C:649:ALA:O    | 1:C:653:ILE:HG12  | 2.19                     | 0.42              |
| 1:D:564:LEU:HA   | 1:D:565:PRO:HD2   | 1.84                     | 0.42              |
| 1:D:959:THR:HG21 | 1:D:1022:VAL:HG22 | 2.01                     | 0.42              |
| 1:E:459:PHE:HE1  | 1:E:872:TYR:HH    | 1.65                     | 0.42              |
| 1:F:686:GLY:CA   | 1:F:689:LYS:HD3   | 2.40                     | 0.42              |
| 1:F:920:VAL:HA   | 1:F:923:GLN:OE1   | 2.19                     | 0.42              |
| 1:B:5:PHE:CE1    | 1:B:487:ILE:HG12  | 2.53                     | 0.42              |
| 1:B:984:LEU:HA   | 1:B:984:LEU:HD23  | 1.77                     | 0.42              |
| 1:A:776:MET:HE2  | 1:C:225:VAL:HG22  | 2.02                     | 0.42              |
| 1:C:352:PHE:CD2  | 1:C:352:PHE:C     | 2.93                     | 0.42              |
| 1:B:219:LEU:HD23 | 1:C:749:TRP:HZ3   | 1.84                     | 0.42              |
| 1:D:1012:LEU:O   | 1:D:1016:PHE:HB2  | 2.19                     | 0.42              |
| 1:D:576:VAL:HG21 | 1:D:591:LEU:HD21  | 2.00                     | 0.42              |
| 1:E:430:ALA:O    | 1:E:433:LYS:HB3   | 2.19                     | 0.42              |
| 1:D:13:TRP:HB3   | 1:E:890:TRP:HZ2   | 1.84                     | 0.42              |
| 1:F:464:GLY:HA2  | 1:F:467:TYR:CD1   | 2.53                     | 0.42              |
| 1:F:483:LEU:O    | 1:F:486:LEU:HB2   | 2.19                     | 0.42              |
| 1:A:34:GLN:HB2   | 1:A:333:VAL:HG22  | 2.00                     | 0.42              |
| 1:A:80:SER:HA    | 1:A:89:GLN:O      | 2.18                     | 0.42              |
| 1:B:2:PRO:HB2    | 1:B:439:GLN:OE1   | 2.19                     | 0.42              |
| 1:B:667:VAL:HB   | 1:B:668:GLU:OE2   | 2.20                     | 0.42              |
| 1:B:847:PRO:O    | 1:B:850:VAL:HB    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:GLU:O    | 1:C:195:LYS:HB3  | 2.19                     | 0.42              |
| 1:C:347:ALA:HB3  | 1:C:402:ILE:HD12 | 2.01                     | 0.42              |
| 1:C:42:ALA:HA    | 1:C:92:LEU:O     | 2.19                     | 0.42              |
| 1:C:836:MET:HG2  | 1:C:854:TRP:CH2  | 2.54                     | 0.42              |
| 1:D:39:ALA:HA    | 1:D:40:PRO:HD2   | 1.76                     | 0.42              |
| 1:D:626:LEU:HB3  | 1:D:632:ARG:HD3  | 2.01                     | 0.42              |
| 1:D:883:LEU:CB   | 1:D:893:PRO:HB3  | 2.49                     | 0.42              |
| 1:D:976:ALA:O    | 1:D:980:GLY:N    | 2.52                     | 0.42              |
| 1:E:310:LEU:CD2  | 1:E:323:ILE:HG21 | 2.49                     | 0.42              |
| 1:E:356:TYR:C    | 1:E:358:PHE:N    | 2.71                     | 0.42              |
| 1:E:404:LEU:HD12 | 1:E:404:LEU:HA   | 1.84                     | 0.42              |
| 1:E:588:GLN:NE2  | 1:E:588:GLN:O    | 2.52                     | 0.42              |
| 1:E:898:LEU:O    | 1:E:901:PRO:HD2  | 2.19                     | 0.42              |
| 1:F:32:VAL:HG22  | 1:F:390:ILE:HB   | 2.01                     | 0.42              |
| 1:F:603:LYS:HB3  | 1:F:603:LYS:HE2  | 1.65                     | 0.42              |
| 1:A:1030:ARG:O   | 1:A:1031:LYS:HG2 | 2.20                     | 0.42              |
| 1:A:368:PRO:HB3  | 1:A:409:ALA:CB   | 2.47                     | 0.42              |
| 1:A:677:PHE:CZ   | 1:A:852:TYR:HB2  | 2.54                     | 0.42              |
| 1:A:916:LEU:HB3  | 1:A:917:THR:H    | 1.66                     | 0.42              |
| 1:B:525:HIS:O    | 1:B:526:HIS:C    | 2.58                     | 0.42              |
| 1:B:574:THR:HG21 | 1:B:598:TYR:CE2  | 2.55                     | 0.42              |
| 1:A:219:LEU:HD11 | 1:B:722:PHE:HB2  | 2.01                     | 0.42              |
| 1:C:1008:THR:C   | 1:C:1010:THR:H   | 2.23                     | 0.42              |
| 1:C:249:ILE:HB   | 1:C:262:LEU:CB   | 2.49                     | 0.42              |
| 1:C:423:GLU:OE1  | 1:C:425:LEU:HD11 | 2.19                     | 0.42              |
| 1:D:1021:PHE:O   | 1:D:1025:ARG:HG2 | 2.19                     | 0.42              |
| 1:D:30:LEU:HD12  | 1:D:31:PRO:CD    | 2.48                     | 0.42              |
| 1:D:586:ARG:O    | 1:D:589:LYS:HB3  | 2.19                     | 0.42              |
| 1:D:182:TYR:O    | 1:D:764:LYS:HD3  | 2.20                     | 0.42              |
| 1:D:813:ARG:NH2  | 1:D:816:GLY:O    | 2.53                     | 0.42              |
| 1:E:69:MET:HE1   | 1:E:107:VAL:HG13 | 2.01                     | 0.42              |
| 1:E:692:GLN:O    | 1:E:695:ASN:HB2  | 2.20                     | 0.42              |
| 1:E:695:ASN:HA   | 1:E:698:LEU:HD12 | 2.01                     | 0.42              |
| 1:F:307:ARG:NH2  | 1:F:311:ALA:HB2  | 2.35                     | 0.42              |
| 1:F:638:LYS:HE2  | 1:F:640:GLU:CG   | 2.48                     | 0.42              |
| 1:F:723:LYS:HG3  | 1:F:725:ASP:OD1  | 2.20                     | 0.42              |
| 1:A:895:SER:HB3  | 1:A:1024:VAL:HB  | 2.02                     | 0.42              |
| 1:A:142:VAL:O    | 1:A:287:SER:N    | 2.51                     | 0.42              |
| 1:A:679:LEU:HD12 | 1:A:679:LEU:HA   | 1.76                     | 0.42              |
| 1:B:281:PHE:CE1  | 1:B:608:SER:HB2  | 2.54                     | 0.42              |
| 1:B:5:PHE:C      | 1:B:8:ARG:H      | 2.22                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:300:LEU:HD11 | 1:C:333:VAL:HG11  | 2.02                     | 0.42              |
| 1:C:353:LEU:HA   | 1:C:353:LEU:HD23  | 1.79                     | 0.42              |
| 1:C:360:GLN:HE21 | 1:C:360:GLN:HB3   | 1.66                     | 0.42              |
| 1:C:425:LEU:HB3  | 1:C:429:GLU:HG3   | 1.99                     | 0.42              |
| 1:C:506:GLY:O    | 1:C:508:GLY:N     | 2.48                     | 0.42              |
| 1:C:541:TYR:OH   | 2:C:1101:LMT:O6'  | 2.34                     | 0.42              |
| 1:D:251:LEU:CD1  | 1:D:265:VAL:HG21  | 2.50                     | 0.42              |
| 1:D:538:THR:HG22 | 1:D:539:GLY:N     | 2.34                     | 0.42              |
| 1:D:562:SER:H    | 1:D:917:THR:HG1   | 1.61                     | 0.42              |
| 1:E:443:VAL:O    | 1:E:447:MET:HG2   | 2.20                     | 0.42              |
| 1:E:534:ILE:CG2  | 2:E:1101:LMT:H12  | 2.49                     | 0.42              |
| 1:E:633:PRO:HD2  | 1:E:637:ASN:OD1   | 2.19                     | 0.42              |
| 1:E:690:LEU:HB3  | 1:E:820:MET:SD    | 2.59                     | 0.42              |
| 1:E:883:LEU:HA   | 1:E:883:LEU:HD23  | 1.85                     | 0.42              |
| 1:E:944:ALA:HB3  | 1:E:1021:PHE:CE1  | 2.54                     | 0.42              |
| 1:F:1010:THR:O   | 1:F:1014:ILE:HG23 | 2.20                     | 0.42              |
| 1:F:152:GLU:HG2  | 1:F:275:TYR:CE2   | 2.55                     | 0.42              |
| 1:F:831:SER:HB3  | 1:F:834:GLU:HG3   | 2.01                     | 0.42              |
| 1:A:409:ALA:O    | 1:A:413:VAL:HG23  | 2.20                     | 0.42              |
| 1:A:855:THR:OG1  | 1:A:856:GLY:N     | 2.52                     | 0.42              |
| 1:A:81:ASN:O     | 1:A:88:VAL:HA     | 2.20                     | 0.42              |
| 1:A:982:MET:HB3  | 1:A:983:PRO:HD3   | 2.01                     | 0.42              |
| 1:B:1022:VAL:O   | 1:B:1026:ARG:HG3  | 2.19                     | 0.42              |
| 1:B:345:VAL:O    | 1:B:348:ILE:HB    | 2.20                     | 0.42              |
| 1:B:375:VAL:HG22 | 1:B:484:VAL:HG21  | 2.01                     | 0.42              |
| 1:B:553:ALA:O    | 1:B:557:VAL:HG23  | 2.20                     | 0.42              |
| 1:C:102:ILE:HD13 | 1:C:102:ILE:HA    | 1.78                     | 0.42              |
| 1:C:186:ILE:O    | 1:C:768:VAL:HG23  | 2.19                     | 0.42              |
| 1:C:488:LEU:O    | 1:C:491:ALA:HB3   | 2.20                     | 0.42              |
| 1:C:571:VAL:HG22 | 1:C:624:VAL:O     | 2.19                     | 0.42              |
| 1:D:146:ASP:OD2  | 1:D:146:ASP:N     | 2.52                     | 0.42              |
| 1:D:200:PRO:HB2  | 1:D:744:THR:HG22  | 2.02                     | 0.42              |
| 1:D:435:MET:O    | 1:D:439:GLN:HB2   | 2.20                     | 0.42              |
| 1:D:578:LEU:HD11 | 1:D:587:THR:N     | 2.35                     | 0.42              |
| 1:D:914:ARG:HD2  | 1:D:1000:THR:HG21 | 2.02                     | 0.42              |
| 1:E:463:THR:O    | 1:E:467:TYR:CD1   | 2.69                     | 0.42              |
| 1:F:211:ASN:OD1  | 1:F:240:LEU:HG    | 2.19                     | 0.42              |
| 1:F:304:ALA:O    | 1:F:307:ARG:HB3   | 2.19                     | 0.42              |
| 1:F:932:LEU:HD11 | 1:F:977:PHE:CE2   | 2.55                     | 0.42              |
| 1:A:166:ILE:HG23 | 1:A:166:ILE:HD12  | 1.74                     | 0.42              |
| 1:A:13:TRP:NE1   | 1:A:492:LEU:HD21  | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:948:MET:SD   | 1:A:955:LEU:HA   | 2.58                     | 0.42              |
| 1:B:26:ALA:O     | 1:B:30:LEU:HB2   | 2.20                     | 0.42              |
| 1:B:409:ALA:O    | 1:B:413:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:607:GLU:OE1  | 1:B:627:LYS:HG2  | 2.20                     | 0.42              |
| 1:B:701:ALA:HB3  | 1:B:711:VAL:HG11 | 2.01                     | 0.42              |
| 1:D:475:VAL:O    | 1:D:478:MET:HB3  | 2.20                     | 0.42              |
| 1:D:886:LEU:HA   | 1:D:886:LEU:HD12 | 1.76                     | 0.42              |
| 1:F:509:LYS:HA   | 1:F:509:LYS:HD2  | 1.83                     | 0.42              |
| 1:F:399:VAL:HG11 | 1:F:984:LEU:HD21 | 2.02                     | 0.42              |
| 1:A:199:THR:HG21 | 1:A:787:ARG:H    | 1.85                     | 0.42              |
| 1:B:3:ASN:O      | 1:B:6:ILE:HB     | 2.20                     | 0.42              |
| 1:B:671:THR:O    | 1:B:671:THR:OG1  | 2.35                     | 0.42              |
| 1:B:898:LEU:HB3  | 1:B:1020:PHE:CZ  | 2.54                     | 0.42              |
| 1:C:55:LYS:HE2   | 1:C:55:LYS:HB3   | 1.72                     | 0.42              |
| 1:C:926:LEU:HA   | 1:C:926:LEU:HD23 | 1.82                     | 0.42              |
| 1:C:343:THR:HG21 | 1:C:984:LEU:HD23 | 2.02                     | 0.42              |
| 1:D:852:TYR:HD2  | 1:D:852:TYR:N    | 2.18                     | 0.42              |
| 1:E:113:LEU:HA   | 1:E:113:LEU:HD23 | 1.80                     | 0.42              |
| 1:E:235:ILE:HD11 | 1:F:721:GLN:OE1  | 2.20                     | 0.42              |
| 1:E:294:ALA:HB3  | 1:E:297:ALA:HB2  | 2.01                     | 0.42              |
| 1:E:30:LEU:HA    | 1:E:31:PRO:HD3   | 1.82                     | 0.42              |
| 1:E:544:LEU:O    | 1:E:547:ILE:HB   | 2.19                     | 0.42              |
| 1:E:843:ALA:O    | 1:E:846:LEU:HG   | 2.20                     | 0.42              |
| 1:E:921:TYR:HB3  | 1:E:998:VAL:HG23 | 2.02                     | 0.42              |
| 1:F:974:SER:HA   | 1:F:1006:MET:CE  | 2.49                     | 0.42              |
| 1:F:25:LEU:HD12  | 1:F:25:LEU:HA    | 1.62                     | 0.42              |
| 1:F:41:PRO:O     | 1:F:94:PHE:HB2   | 2.20                     | 0.42              |
| 1:F:883:LEU:HD11 | 1:F:938:ILE:HD11 | 2.00                     | 0.42              |
| 1:A:282:ASN:HD21 | 1:A:608:SER:CB   | 2.33                     | 0.42              |
| 1:A:442:LEU:HA   | 1:A:442:LEU:HD23 | 1.84                     | 0.42              |
| 1:A:563:PHE:O    | 1:A:564:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:694:ARG:HH11 | 1:A:694:ARG:HB3  | 1.85                     | 0.42              |
| 1:B:955:LEU:O    | 1:B:959:THR:HG23 | 2.20                     | 0.42              |
| 1:C:159:ALA:HB2  | 1:C:177:LEU:HD11 | 2.02                     | 0.42              |
| 1:C:335:ILE:HG12 | 1:C:990:ALA:HB2  | 2.02                     | 0.42              |
| 1:C:753:TYR:HD1  | 1:C:767:TYR:HE2  | 1.66                     | 0.42              |
| 1:D:193:LEU:CD2  | 1:D:265:VAL:HB   | 2.50                     | 0.42              |
| 1:D:836:MET:CE   | 1:D:862:ARG:HD2  | 2.49                     | 0.42              |
| 1:D:941:VAL:HG22 | 1:D:1021:PHE:CD1 | 2.55                     | 0.42              |
| 1:E:1029:SER:HG  | 1:E:1030:ARG:H   | 1.61                     | 0.42              |
| 1:E:43:VAL:HG13  | 1:E:130:GLU:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:722:PHE:CZ   | 1:E:802:SER:HB2  | 2.55                     | 0.42              |
| 1:E:722:PHE:CD1  | 1:E:804:TRP:CE2  | 3.08                     | 0.42              |
| 1:E:960:LEU:O    | 1:E:963:VAL:HG12 | 2.20                     | 0.42              |
| 1:F:364:ALA:O    | 1:F:368:PRO:HD3  | 2.19                     | 0.42              |
| 1:F:786:VAL:HG23 | 1:F:796:PHE:CE2  | 2.55                     | 0.42              |
| 1:F:960:LEU:HD23 | 1:F:960:LEU:HA   | 1.89                     | 0.42              |
| 1:A:585:GLU:O    | 1:A:588:GLN:HB3  | 2.20                     | 0.41              |
| 1:B:15:ILE:HD13  | 1:B:15:ILE:HG21  | 1.86                     | 0.41              |
| 1:C:148:THR:HG22 | 1:C:149:MET:O    | 2.20                     | 0.41              |
| 1:C:24:GLY:CA    | 1:C:27:ILE:HG23  | 2.50                     | 0.41              |
| 1:C:453:PHE:CD2  | 1:C:456:MET:CE   | 2.95                     | 0.41              |
| 1:C:278:ILE:CG1  | 1:C:613:ASN:HB3  | 2.48                     | 0.41              |
| 1:C:855:THR:CA   | 1:C:859:TYR:HB2  | 2.47                     | 0.41              |
| 1:C:899:VAL:HG12 | 1:C:933:SER:HB2  | 2.02                     | 0.41              |
| 1:C:977:PHE:HE2  | 1:C:1002:VAL:CG1 | 2.32                     | 0.41              |
| 1:D:152:GLU:CD   | 1:D:152:GLU:H    | 2.24                     | 0.41              |
| 1:D:235:ILE:HG23 | 1:D:235:ILE:HD12 | 1.74                     | 0.41              |
| 1:D:393:LEU:HD13 | 1:D:466:ILE:HA   | 2.02                     | 0.41              |
| 1:D:470:PHE:CD2  | 1:D:924:VAL:HG11 | 2.54                     | 0.41              |
| 1:E:579:PRO:HD3  | 1:E:656:ALA:CB   | 2.48                     | 0.41              |
| 1:E:727:ASP:OD1  | 1:E:730:LYS:HG3  | 2.20                     | 0.41              |
| 1:E:741:ILE:O    | 1:E:744:THR:OG1  | 2.34                     | 0.41              |
| 1:F:355:MET:HG2  | 1:F:410:ILE:HD11 | 2.01                     | 0.41              |
| 1:F:3:ASN:HD21   | 1:F:486:LEU:HA   | 1.85                     | 0.41              |
| 1:F:587:THR:HG21 | 1:F:618:ASN:HA   | 2.02                     | 0.41              |
| 1:A:149:MET:HG3  | 1:A:154:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:427:PRO:O    | 1:A:430:ALA:HB3  | 2.19                     | 0.41              |
| 1:A:55:LYS:HB3   | 1:A:55:LYS:HE2   | 1.76                     | 0.41              |
| 1:A:901:PRO:HA   | 1:A:904:VAL:HB   | 2.02                     | 0.41              |
| 1:B:1015:PHE:CZ  | 2:B:2000:LMT:H52 | 2.55                     | 0.41              |
| 1:B:248:LYS:O    | 1:B:261:LEU:HD22 | 2.20                     | 0.41              |
| 1:B:368:PRO:HG3  | 1:B:413:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:486:LEU:HA   | 1:B:486:LEU:HD23 | 1.77                     | 0.41              |
| 1:B:4:PHE:CZ     | 1:B:8:ARG:HD3    | 2.55                     | 0.41              |
| 1:B:914:ARG:NH1  | 1:B:985:VAL:HG12 | 2.35                     | 0.41              |
| 1:C:443:VAL:O    | 1:C:447:MET:HB3  | 2.20                     | 0.41              |
| 1:C:584:GLN:N    | 1:C:617:GLN:HB3  | 2.34                     | 0.41              |
| 1:C:187:TRP:HB3  | 1:C:771:GLU:HA   | 2.02                     | 0.41              |
| 1:E:363:ARG:CZ   | 1:E:498:LYS:HE3  | 2.49                     | 0.41              |
| 1:E:493:CYS:O    | 1:E:497:LEU:HB2  | 2.19                     | 0.41              |
| 1:F:344:LEU:HD22 | 1:F:402:ILE:HD11 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:504:ASP:C    | 1:F:506:GLY:N     | 2.72                     | 0.41              |
| 1:A:169:THR:HB   | 1:A:172:VAL:HG23  | 2.02                     | 0.41              |
| 1:B:363:ARG:NH1  | 1:B:498:LYS:HG3   | 2.35                     | 0.41              |
| 1:B:463:THR:O    | 1:B:466:ILE:HB    | 2.20                     | 0.41              |
| 1:B:480:LEU:O    | 1:B:484:VAL:HG23  | 2.20                     | 0.41              |
| 1:B:482:VAL:O    | 1:B:485:ALA:HB3   | 2.20                     | 0.41              |
| 1:B:527:TYR:O    | 1:B:531:VAL:HG23  | 2.20                     | 0.41              |
| 1:B:701:ALA:CB   | 1:B:711:VAL:HG11  | 2.50                     | 0.41              |
| 1:C:443:VAL:HG12 | 1:C:886:LEU:HD21  | 2.01                     | 0.41              |
| 1:C:753:TYR:HD1  | 1:C:767:TYR:CE2   | 2.38                     | 0.41              |
| 1:C:966:ARG:HH21 | 1:C:970:ILE:HD11  | 1.85                     | 0.41              |
| 1:D:459:PHE:O    | 1:D:468:ARG:NH2   | 2.54                     | 0.41              |
| 1:D:482:VAL:O    | 1:D:486:LEU:HG    | 2.20                     | 0.41              |
| 1:E:158:VAL:HG11 | 1:E:289:LEU:HG    | 2.01                     | 0.41              |
| 1:E:202:ASP:OD2  | 1:E:787:ARG:NH2   | 2.46                     | 0.41              |
| 1:E:306:ILE:O    | 1:E:309:GLU:HB3   | 2.20                     | 0.41              |
| 1:E:62:THR:O     | 1:E:66:GLU:HG3    | 2.21                     | 0.41              |
| 1:E:927:LEU:HA   | 1:E:930:ILE:HD12  | 2.02                     | 0.41              |
| 1:F:356:TYR:HD1  | 1:F:365:THR:HG21  | 1.84                     | 0.41              |
| 1:F:578:LEU:HA   | 1:F:656:ALA:HB1   | 2.02                     | 0.41              |
| 1:A:1017:VAL:HB  | 1:A:1018:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:54:ALA:HB2   | 1:A:809:PRO:O     | 2.20                     | 0.41              |
| 1:A:273:GLU:CG   | 1:A:765:LYS:HD2   | 2.50                     | 0.41              |
| 1:B:27:ILE:HD12  | 1:B:27:ILE:HA     | 1.86                     | 0.41              |
| 1:B:576:VAL:HG13 | 1:B:658:VAL:HG22  | 2.01                     | 0.41              |
| 1:B:676:ASP:H    | 1:B:858:SER:HG    | 1.62                     | 0.41              |
| 1:B:968:ARG:O    | 1:B:972:MET:HE2   | 2.20                     | 0.41              |
| 1:C:614:GLY:O    | 1:C:616:GLY:HA3   | 2.20                     | 0.41              |
| 1:C:664:PRO:HG2  | 1:C:666:ILE:O     | 2.20                     | 0.41              |
| 1:D:432:ARG:HH11 | 1:D:432:ARG:HD2   | 1.68                     | 0.41              |
| 1:D:531:VAL:O    | 1:D:534:ILE:HG13  | 2.20                     | 0.41              |
| 1:D:544:LEU:O    | 1:D:547:ILE:HB    | 2.20                     | 0.41              |
| 1:D:5:PHE:CE1    | 1:D:487:ILE:HG12  | 2.55                     | 0.41              |
| 1:D:726:ILE:H    | 1:D:726:ILE:HG12  | 1.24                     | 0.41              |
| 1:D:679:LEU:HD11 | 1:D:850:VAL:HG12  | 2.02                     | 0.41              |
| 1:D:898:LEU:O    | 1:D:901:PRO:HD2   | 2.20                     | 0.41              |
| 1:D:941:VAL:HG13 | 1:D:1021:PHE:CD1  | 2.56                     | 0.41              |
| 1:E:1015:PHE:O   | 1:E:1019:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:448:VAL:HG13 | 1:E:879:VAL:CG1   | 2.47                     | 0.41              |
| 1:D:234:ILE:HA   | 1:E:722:PHE:O     | 2.20                     | 0.41              |
| 1:E:7:ASP:O      | 1:E:8:ARG:HG3     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:578:LEU:CD1  | 1:F:587:THR:HG22 | 2.50                     | 0.41              |
| 1:A:165:ALA:HA   | 1:A:168:ARG:NH1  | 2.35                     | 0.41              |
| 1:A:446:ALA:CB   | 1:A:482:VAL:HG21 | 2.51                     | 0.41              |
| 1:B:572:PHE:CE1  | 1:B:643:THR:HG22 | 2.56                     | 0.41              |
| 1:D:473:THR:O    | 1:D:476:SER:OG   | 2.38                     | 0.41              |
| 1:D:531:VAL:HA   | 1:D:534:ILE:HD11 | 2.01                     | 0.41              |
| 1:D:634:GLY:O    | 1:D:638:LYS:HG3  | 2.20                     | 0.41              |
| 1:D:9:PRO:O      | 1:D:13:TRP:CD1   | 2.74                     | 0.41              |
| 1:E:697:LEU:HA   | 1:E:700:GLU:HB2  | 2.02                     | 0.41              |
| 1:F:149:MET:HB2  | 1:F:153:ASP:HB3  | 2.03                     | 0.41              |
| 1:F:620:GLY:O    | 1:F:621:ILE:HD12 | 2.20                     | 0.41              |
| 1:F:666:ILE:HD13 | 1:F:669:LEU:HD12 | 2.03                     | 0.41              |
| 1:F:694:ARG:HE   | 1:F:713:PRO:HB3  | 1.85                     | 0.41              |
| 1:F:720:PRO:HA   | 1:F:805:GLU:O    | 2.20                     | 0.41              |
| 1:F:199:THR:HG22 | 1:F:785:TYR:O    | 2.20                     | 0.41              |
| 1:A:118:LEU:HA   | 1:A:119:PRO:HD3  | 1.77                     | 0.41              |
| 1:A:578:LEU:HB2  | 1:A:618:ASN:HA   | 2.02                     | 0.41              |
| 1:A:650:PHE:HB3  | 1:A:658:VAL:HB   | 2.02                     | 0.41              |
| 1:A:204:ILE:HG12 | 1:A:754:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:121:GLU:O    | 1:B:125:GLN:HB2  | 2.21                     | 0.41              |
| 1:B:149:MET:H    | 1:B:149:MET:HG2  | 1.75                     | 0.41              |
| 1:B:167:SER:HB2  | 1:C:70:ASN:HB3   | 2.02                     | 0.41              |
| 1:C:376:LEU:HD22 | 1:C:398:MET:HE3  | 2.02                     | 0.41              |
| 1:C:836:MET:O    | 1:C:854:TRP:HZ2  | 2.03                     | 0.41              |
| 1:D:138:MET:CG   | 1:D:291:ILE:HB   | 2.51                     | 0.41              |
| 1:D:355:MET:HE2  | 1:D:368:PRO:HG2  | 2.03                     | 0.41              |
| 1:D:58:GLN:HA    | 1:D:62:THR:HB    | 2.03                     | 0.41              |
| 1:D:44:THR:HA    | 1:D:90:ILE:O     | 2.20                     | 0.41              |
| 1:D:418:ARG:HH21 | 1:D:943:PHE:HE2  | 1.69                     | 0.41              |
| 1:E:175:VAL:HG11 | 1:E:289:LEU:HD13 | 2.02                     | 0.41              |
| 1:E:189:ASN:O    | 1:E:192:GLU:HB2  | 2.21                     | 0.41              |
| 1:E:262:LEU:HG   | 1:E:268:ILE:HD11 | 2.02                     | 0.41              |
| 1:E:559:LEU:HA   | 1:E:560:PRO:HD2  | 1.55                     | 0.41              |
| 1:E:585:GLU:O    | 1:E:588:GLN:HB3  | 2.20                     | 0.41              |
| 1:E:914:ARG:NH1  | 1:E:985:VAL:HG12 | 2.36                     | 0.41              |
| 1:E:927:LEU:O    | 1:E:930:ILE:HB   | 2.21                     | 0.41              |
| 1:F:540:ARG:O    | 1:F:543:VAL:HB   | 2.20                     | 0.41              |
| 1:F:679:LEU:HD23 | 1:F:820:MET:HB2  | 2.03                     | 0.41              |
| 1:F:970:ILE:H    | 1:F:970:ILE:HG13 | 1.64                     | 0.41              |
| 1:A:367:ILE:HD13 | 1:A:367:ILE:HG21 | 1.84                     | 0.41              |
| 1:A:66:GLU:OE1   | 1:A:816:GLY:HA2  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:144:ASN:HA    | 1:B:321:LEU:HA   | 2.02                     | 0.41              |
| 1:C:1012:LEU:HD12 | 1:C:1012:LEU:HA  | 1.85                     | 0.41              |
| 1:C:370:ILE:O     | 1:C:373:PRO:HD2  | 2.20                     | 0.41              |
| 1:C:591:LEU:HD11  | 1:C:620:GLY:HA3  | 2.01                     | 0.41              |
| 1:C:689:LYS:CD    | 1:C:689:LYS:H    | 2.33                     | 0.41              |
| 1:D:366:LEU:HD23  | 1:D:366:LEU:HA   | 1.74                     | 0.41              |
| 1:D:572:PHE:CD1   | 1:D:643:THR:HG22 | 2.56                     | 0.41              |
| 1:D:667:VAL:HG12  | 1:D:668:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:788:ALA:HB3   | 1:D:790:ASP:OD2  | 2.20                     | 0.41              |
| 1:E:250:LEU:HD13  | 1:E:259:ARG:HB2  | 2.02                     | 0.41              |
| 1:F:510:LYS:HA    | 1:F:518:ARG:HH12 | 1.86                     | 0.41              |
| 1:F:914:ARG:NH1   | 1:F:996:ASN:HB3  | 2.36                     | 0.41              |
| 2:A:1101:LMT:H51  | 2:A:1101:LMT:H81 | 1.51                     | 0.41              |
| 1:A:11:PHE:CE1    | 1:A:15:ILE:HD11  | 2.56                     | 0.41              |
| 1:A:355:MET:HE1   | 1:A:368:PRO:HG2  | 2.02                     | 0.41              |
| 1:A:57:VAL:CG1    | 1:A:88:VAL:HB    | 2.50                     | 0.41              |
| 1:A:574:THR:OG1   | 1:A:659:PHE:O    | 2.22                     | 0.41              |
| 1:A:694:ARG:HD2   | 1:A:713:PRO:HB3  | 2.03                     | 0.41              |
| 1:A:82:SER:HB2    | 1:A:811:LEU:HB2  | 2.02                     | 0.41              |
| 1:A:979:LEU:HD23  | 1:A:979:LEU:HA   | 1.80                     | 0.41              |
| 1:A:343:THR:HG21  | 1:A:984:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:82:SER:HB2    | 1:B:811:LEU:HB2  | 2.03                     | 0.41              |
| 1:B:883:LEU:HA    | 1:B:883:LEU:HD23 | 1.88                     | 0.41              |
| 1:B:923:GLN:O     | 1:B:926:LEU:HB2  | 2.21                     | 0.41              |
| 1:C:153:ASP:HA    | 1:C:182:TYR:OH   | 2.20                     | 0.41              |
| 1:E:186:ILE:HG12  | 1:E:268:ILE:HG12 | 2.02                     | 0.41              |
| 1:E:224:PRO:HD2   | 1:F:584:GLN:NE2  | 2.35                     | 0.41              |
| 1:E:555:LEU:HB3   | 1:E:908:LEU:HD13 | 2.03                     | 0.41              |
| 1:E:916:LEU:HD11  | 1:E:997:ALA:HA   | 2.03                     | 0.41              |
| 1:F:120:GLN:O     | 1:F:123:GLN:HB2  | 2.21                     | 0.41              |
| 1:F:345:VAL:HA    | 1:F:348:ILE:HD12 | 2.03                     | 0.41              |
| 1:F:356:TYR:O     | 1:F:358:PHE:N    | 2.53                     | 0.41              |
| 1:F:407:ASP:HB3   | 1:F:445:ILE:HD13 | 2.03                     | 0.41              |
| 1:F:600:THR:C     | 1:F:602:GLU:H    | 2.22                     | 0.41              |
| 1:F:61:VAL:O      | 1:F:65:ILE:HG13  | 2.19                     | 0.41              |
| 1:F:649:ALA:O     | 1:F:653:ILE:HG12 | 2.20                     | 0.41              |
| 1:E:219:LEU:HD23  | 1:F:749:TRP:HZ3  | 1.85                     | 0.41              |
| 1:F:741:ILE:HG22  | 1:F:786:VAL:HG11 | 2.03                     | 0.41              |
| 1:F:803:ARG:NH1   | 1:F:805:GLU:OE2  | 2.54                     | 0.41              |
| 1:A:189:ASN:O     | 1:A:192:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:261:LEU:O     | 1:A:265:VAL:HG22 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:492:LEU:HD22 | 1:A:496:MET:SD    | 2.61                     | 0.41              |
| 1:A:645:ARG:C    | 1:A:648:ARG:HB3   | 2.41                     | 0.41              |
| 1:B:105:VAL:HG21 | 1:C:105:VAL:HG13  | 2.03                     | 0.41              |
| 1:B:40:PRO:HA    | 1:B:41:PRO:HD3    | 1.82                     | 0.41              |
| 1:A:223:PRO:HD2  | 1:B:775:ARG:NH2   | 2.36                     | 0.41              |
| 1:C:1029:SER:OG  | 1:C:1030:ARG:N    | 2.48                     | 0.41              |
| 1:C:64:VAL:HG11  | 1:C:117:LEU:HB2   | 2.01                     | 0.41              |
| 1:D:11:PHE:HB2   | 1:E:888:GLU:OE2   | 2.21                     | 0.41              |
| 1:D:293:LEU:HD22 | 1:D:294:ALA:N     | 2.36                     | 0.41              |
| 1:D:770:SER:OG   | 1:D:775:ARG:HG2   | 2.20                     | 0.41              |
| 1:D:963:VAL:HA   | 1:D:966:ARG:HH12  | 1.85                     | 0.41              |
| 1:E:535:LEU:HD13 | 1:E:1022:VAL:HG21 | 2.02                     | 0.41              |
| 1:E:685:LEU:HD13 | 1:E:689:LYS:HB3   | 2.02                     | 0.41              |
| 1:E:527:TYR:CE2  | 1:E:967:LEU:HG    | 2.56                     | 0.41              |
| 1:F:33:ALA:HB2   | 1:F:298:ASN:OD1   | 2.21                     | 0.41              |
| 1:F:510:LYS:HA   | 1:F:518:ARG:NH1   | 2.35                     | 0.41              |
| 1:F:545:TYR:O    | 1:F:549:VAL:HG23  | 2.21                     | 0.41              |
| 1:F:932:LEU:HD11 | 1:F:977:PHE:HE2   | 1.85                     | 0.41              |
| 1:B:361:ASN:O    | 1:B:365:THR:HG22  | 2.21                     | 0.41              |
| 1:B:80:SER:CB    | 1:B:90:ILE:HG12   | 2.51                     | 0.41              |
| 1:A:75:LEU:HD23  | 1:C:168:ARG:HB3   | 2.03                     | 0.41              |
| 1:C:605:ASN:HD21 | 1:C:637:ASN:HA    | 1.85                     | 0.41              |
| 1:C:930:ILE:HG21 | 1:C:930:ILE:HD13  | 1.87                     | 0.41              |
| 1:D:166:ILE:HA   | 1:D:166:ILE:HD13  | 1.91                     | 0.41              |
| 1:E:103:ALA:O    | 1:E:107:VAL:HG23  | 2.21                     | 0.41              |
| 1:E:313:MET:HA   | 1:E:316:PHE:HD2   | 1.86                     | 0.41              |
| 1:E:559:LEU:HD22 | 1:E:917:THR:HA    | 2.03                     | 0.41              |
| 1:F:379:THR:N    | 1:F:480:LEU:HD11  | 2.35                     | 0.41              |
| 1:F:553:ALA:O    | 1:F:557:VAL:HG23  | 2.20                     | 0.41              |
| 1:A:757:PHE:CE1  | 1:A:759:ASP:HB2   | 2.55                     | 0.41              |
| 1:A:903:GLY:HA2  | 1:A:1009:ALA:HB2  | 2.03                     | 0.41              |
| 1:B:407:ASP:O    | 1:B:411:VAL:HG23  | 2.21                     | 0.41              |
| 1:B:914:ARG:HH12 | 1:B:985:VAL:HG12  | 1.86                     | 0.41              |
| 1:B:926:LEU:HD23 | 1:B:926:LEU:HA    | 1.69                     | 0.41              |
| 1:B:914:ARG:NH2  | 1:B:996:ASN:HB3   | 2.36                     | 0.41              |
| 1:C:199:THR:HG21 | 1:C:787:ARG:H     | 1.86                     | 0.41              |
| 1:C:404:LEU:HB3  | 1:C:478:MET:SD    | 2.61                     | 0.41              |
| 1:C:509:LYS:HA   | 1:C:509:LYS:HD2   | 1.83                     | 0.41              |
| 1:C:65:ILE:HG21  | 1:C:90:ILE:HD13   | 2.03                     | 0.41              |
| 1:D:317:PHE:CD1  | 1:D:321:LEU:HD12  | 2.56                     | 0.41              |
| 1:D:339:GLU:OE1  | 1:D:342:LYS:HD3   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:780:ASP:O    | 1:D:783:ASP:HB2   | 2.20                     | 0.41              |
| 1:E:142:VAL:O    | 1:E:154:ILE:HD13  | 2.21                     | 0.41              |
| 1:E:235:ILE:HB   | 1:F:723:LYS:HA    | 2.01                     | 0.41              |
| 1:E:567:GLU:O    | 1:E:569:GLN:HG3   | 2.21                     | 0.41              |
| 1:E:838:LEU:HD22 | 1:E:841:GLN:HB2   | 2.02                     | 0.41              |
| 1:F:726:ILE:H    | 1:F:726:ILE:HG13  | 1.65                     | 0.41              |
| 1:F:979:LEU:HD23 | 1:F:979:LEU:HA    | 1.75                     | 0.41              |
| 1:A:678:GLU:HG2  | 1:A:814:TYR:CG    | 2.56                     | 0.40              |
| 1:B:138:MET:HE2  | 1:B:138:MET:HB2   | 1.94                     | 0.40              |
| 1:B:773:LYS:HG3  | 1:B:774:TYR:CE2   | 2.56                     | 0.40              |
| 1:C:1010:THR:O   | 1:C:1014:ILE:HG23 | 2.21                     | 0.40              |
| 1:C:497:LEU:HA   | 1:C:497:LEU:HD12  | 1.82                     | 0.40              |
| 1:C:632:ARG:HH12 | 1:C:638:LYS:HA    | 1.86                     | 0.40              |
| 1:D:143:ILE:HG22 | 1:D:286:ALA:HB2   | 2.02                     | 0.40              |
| 1:D:442:LEU:HA   | 1:D:442:LEU:HD23  | 1.70                     | 0.40              |
| 1:D:591:LEU:HD23 | 1:D:591:LEU:HA    | 1.71                     | 0.40              |
| 1:D:654:LYS:HD3  | 1:D:654:LYS:HA    | 1.77                     | 0.40              |
| 1:D:940:ILE:HG12 | 1:D:966:ARG:NH2   | 2.36                     | 0.40              |
| 1:E:343:THR:HG21 | 1:E:399:VAL:CG1   | 2.43                     | 0.40              |
| 1:E:56:THR:O     | 1:E:60:THR:OG1    | 2.25                     | 0.40              |
| 1:E:723:LYS:HG2  | 1:E:803:ARG:NH1   | 2.36                     | 0.40              |
| 1:E:736:VAL:HB   | 1:E:741:ILE:HD11  | 2.03                     | 0.40              |
| 1:F:104:GLN:OE1  | 1:F:108:GLN:NE2   | 2.54                     | 0.40              |
| 1:F:217:GLY:O    | 1:F:234:ILE:HB    | 2.22                     | 0.40              |
| 1:C:527:TYR:O    | 1:C:531:VAL:HG23  | 2.21                     | 0.40              |
| 1:C:963:VAL:HA   | 1:C:966:ARG:NH2   | 2.37                     | 0.40              |
| 1:C:984:LEU:HB3  | 1:C:995:GLN:O     | 2.21                     | 0.40              |
| 1:D:540:ARG:NH2  | 2:D:2000:LMT:H6'2 | 2.36                     | 0.40              |
| 1:D:162:MET:HA   | 1:D:313:MET:SD    | 2.62                     | 0.40              |
| 1:D:404:LEU:HD21 | 1:D:449:LEU:HD22  | 2.02                     | 0.40              |
| 1:D:564:LEU:HD22 | 1:D:666:ILE:HG12  | 2.04                     | 0.40              |
| 1:D:564:LEU:CD2  | 1:D:666:ILE:HG12  | 2.51                     | 0.40              |
| 1:E:541:TYR:HH   | 2:E:1101:LMT:H6'  | 1.54                     | 0.40              |
| 1:E:330:THR:HB   | 1:E:331:PRO:HD3   | 2.03                     | 0.40              |
| 1:E:516:PHE:HA   | 1:E:519:MET:CG    | 2.45                     | 0.40              |
| 1:E:956:ILE:HG13 | 1:E:956:ILE:H     | 1.27                     | 0.40              |
| 1:F:941:VAL:HG13 | 1:F:1021:PHE:CE1  | 2.56                     | 0.40              |
| 1:F:489:THR:HA   | 1:F:492:LEU:HB2   | 2.03                     | 0.40              |
| 1:F:868:ALA:HB2  | 1:F:923:GLN:NE2   | 2.36                     | 0.40              |
| 1:A:676:ASP:HB2  | 1:A:857:MET:HE3   | 2.04                     | 0.40              |
| 1:A:697:LEU:HA   | 1:A:700:GLU:HB2   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:722:PHE:HB2  | 1:A:804:TRP:CH2  | 2.56                     | 0.40              |
| 1:A:969:PRO:HA   | 1:A:972:MET:HE2  | 2.03                     | 0.40              |
| 1:B:786:VAL:HG23 | 1:B:796:PHE:CE2  | 2.55                     | 0.40              |
| 1:B:983:PRO:O    | 1:B:987:SER:HB2  | 2.22                     | 0.40              |
| 1:C:152:GLU:H    | 1:C:152:GLU:CD   | 2.24                     | 0.40              |
| 1:C:364:ALA:O    | 1:C:368:PRO:HD3  | 2.21                     | 0.40              |
| 1:C:584:GLN:N    | 1:C:617:GLN:OE1  | 2.31                     | 0.40              |
| 1:B:233:SER:HB2  | 1:C:721:GLN:HG2  | 2.03                     | 0.40              |
| 1:D:231:ASN:ND2  | 1:E:617:GLN:HE22 | 2.20                     | 0.40              |
| 1:D:511:GLY:CA   | 1:D:515:TRP:CD1  | 3.01                     | 0.40              |
| 1:E:667:VAL:H    | 1:E:667:VAL:HG23 | 1.58                     | 0.40              |
| 1:A:19:ILE:HD13  | 1:A:19:ILE:HG21  | 1.83                     | 0.40              |
| 1:A:351:VAL:O    | 1:A:355:MET:HG2  | 2.22                     | 0.40              |
| 1:A:340:VAL:HB   | 1:A:395:MET:HE2  | 2.02                     | 0.40              |
| 1:A:467:TYR:CE2  | 1:A:920:VAL:HG22 | 2.55                     | 0.40              |
| 1:C:137:LEU:HB2  | 1:C:293:LEU:HB2  | 2.03                     | 0.40              |
| 1:C:188:MET:O    | 1:C:771:GLU:HG3  | 2.20                     | 0.40              |
| 1:C:252:LYS:HE2  | 1:C:253:VAL:O    | 2.21                     | 0.40              |
| 1:C:431:THR:HG21 | 1:C:490:PRO:O    | 2.22                     | 0.40              |
| 1:C:55:LYS:HA    | 1:C:811:LEU:HD11 | 2.03                     | 0.40              |
| 1:D:188:MET:HE3  | 1:D:188:MET:HB2  | 1.78                     | 0.40              |
| 1:D:281:PHE:C    | 1:D:281:PHE:CD2  | 2.95                     | 0.40              |
| 1:E:587:THR:HB   | 1:E:613:ASN:OD1  | 2.21                     | 0.40              |
| 1:E:681:ASP:HB2  | 1:E:690:LEU:HG   | 2.04                     | 0.40              |
| 1:E:722:PHE:HD1  | 1:E:804:TRP:CE2  | 2.40                     | 0.40              |
| 1:F:180:SER:HB3  | 1:F:273:GLU:CB   | 2.51                     | 0.40              |
| 1:F:525:HIS:O    | 1:F:526:HIS:C    | 2.60                     | 0.40              |
| 1:F:546:LEU:O    | 1:F:550:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:142:VAL:N    | 1:A:287:SER:O    | 2.44                     | 0.40              |
| 1:A:615:GLY:HA2  | 1:A:616:GLY:HA2  | 1.75                     | 0.40              |
| 1:A:778:PRO:HG3  | 1:A:804:TRP:HZ2  | 1.87                     | 0.40              |
| 1:B:534:ILE:HD13 | 1:B:534:ILE:HG21 | 1.91                     | 0.40              |
| 1:B:58:GLN:OE1   | 1:B:811:LEU:HB3  | 2.21                     | 0.40              |
| 1:C:1031:LYS:HD3 | 1:C:1031:LYS:HA  | 1.86                     | 0.40              |
| 1:C:359:LEU:HB2  | 1:C:365:THR:HG22 | 2.03                     | 0.40              |
| 1:C:44:THR:HA    | 1:C:90:ILE:O     | 2.21                     | 0.40              |
| 1:D:407:ASP:O    | 1:D:411:VAL:HG23 | 2.22                     | 0.40              |
| 1:D:554:TYR:CE2  | 1:D:558:ARG:HG3  | 2.56                     | 0.40              |
| 1:D:704:HIS:CE1  | 1:D:842:LEU:HD21 | 2.56                     | 0.40              |
| 1:D:916:LEU:HB3  | 1:D:917:THR:H    | 1.68                     | 0.40              |
| 1:D:984:LEU:HB3  | 1:D:995:GLN:O    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:936:ASN:ND2  | 1:E:970:ILE:HG23 | 2.36                     | 0.40              |
| 1:F:337:ILE:HD11 | 1:F:391:ASN:HA   | 2.04                     | 0.40              |
| 1:F:348:ILE:HG13 | 1:F:348:ILE:H    | 1.68                     | 0.40              |
| 1:F:478:MET:O    | 1:F:482:VAL:HG23 | 2.21                     | 0.40              |
| 1:F:497:LEU:HD12 | 1:F:497:LEU:HA   | 1.75                     | 0.40              |
| 1:F:527:TYR:O    | 1:F:531:VAL:HG23 | 2.21                     | 0.40              |
| 1:F:887:TYR:C    | 1:F:889:SER:H    | 2.13                     | 0.40              |
| 1:F:343:THR:HG21 | 1:F:984:LEU:HD23 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 1036/1044 (99%) | 942 (91%)  | 79 (8%)  | 15 (1%)  | 11          | 37 |
| 1   | B     | 1037/1044 (99%) | 942 (91%)  | 85 (8%)  | 10 (1%)  | 15          | 46 |
| 1   | C     | 1033/1044 (99%) | 931 (90%)  | 84 (8%)  | 18 (2%)  | 9           | 34 |
| 1   | D     | 1036/1044 (99%) | 934 (90%)  | 83 (8%)  | 19 (2%)  | 8           | 32 |
| 1   | E     | 1035/1044 (99%) | 937 (90%)  | 87 (8%)  | 11 (1%)  | 14          | 44 |
| 1   | F     | 1035/1044 (99%) | 926 (90%)  | 84 (8%)  | 25 (2%)  | 6           | 28 |
| All | All   | 6212/6264 (99%) | 5612 (90%) | 502 (8%) | 98 (2%)  | 9           | 34 |

All (98) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 672  | ALA  |
| 1   | A     | 986  | ILE  |
| 1   | A     | 1029 | SER  |
| 1   | A     | 1033 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 617  | GLN  |
| 1   | B     | 1029 | SER  |
| 1   | B     | 1038 | SER  |
| 1   | C     | 509  | LYS  |
| 1   | C     | 915  | GLY  |
| 1   | C     | 1009 | ALA  |
| 1   | C     | 1029 | SER  |
| 1   | C     | 1035 | ILE  |
| 1   | D     | 508  | GLY  |
| 1   | D     | 511  | GLY  |
| 1   | D     | 668  | GLU  |
| 1   | D     | 915  | GLY  |
| 1   | D     | 1029 | SER  |
| 1   | D     | 1034 | ASP  |
| 1   | D     | 1035 | ILE  |
| 1   | D     | 1036 | GLU  |
| 1   | D     | 1038 | SER  |
| 1   | E     | 667  | VAL  |
| 1   | E     | 1029 | SER  |
| 1   | E     | 1033 | GLU  |
| 1   | E     | 1036 | GLU  |
| 1   | F     | 134  | SER  |
| 1   | F     | 145  | THR  |
| 1   | F     | 509  | LYS  |
| 1   | F     | 617  | GLN  |
| 1   | F     | 888  | GLU  |
| 1   | F     | 1029 | SER  |
| 1   | F     | 1032 | ASN  |
| 1   | F     | 1035 | ILE  |
| 1   | A     | 915  | GLY  |
| 1   | A     | 987  | SER  |
| 1   | A     | 1032 | ASN  |
| 1   | B     | 514  | GLY  |
| 1   | B     | 684  | GLY  |
| 1   | B     | 1035 | ILE  |
| 1   | C     | 147  | GLY  |
| 1   | C     | 831  | SER  |
| 1   | D     | 4    | PHE  |
| 1   | D     | 987  | SER  |
| 1   | D     | 1028 | PHE  |
| 1   | D     | 1031 | LYS  |
| 1   | E     | 668  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 6    | ILE  |
| 1   | F     | 146  | ASP  |
| 1   | F     | 147  | GLY  |
| 1   | F     | 511  | GLY  |
| 1   | F     | 684  | GLY  |
| 1   | F     | 918  | ASN  |
| 1   | F     | 1028 | PHE  |
| 1   | A     | 615  | GLY  |
| 1   | A     | 1031 | LYS  |
| 1   | B     | 918  | ASN  |
| 1   | C     | 134  | SER  |
| 1   | C     | 146  | ASP  |
| 1   | C     | 360  | GLN  |
| 1   | C     | 888  | GLU  |
| 1   | F     | 407  | ASP  |
| 1   | F     | 507  | GLU  |
| 1   | F     | 831  | SER  |
| 1   | F     | 1034 | ASP  |
| 1   | A     | 215  | ALA  |
| 1   | B     | 215  | ALA  |
| 1   | C     | 6    | ILE  |
| 1   | C     | 1033 | GLU  |
| 1   | D     | 614  | GLY  |
| 1   | D     | 653  | ILE  |
| 1   | D     | 909  | LEU  |
| 1   | F     | 360  | GLN  |
| 1   | A     | 918  | ASN  |
| 1   | A     | 1036 | GLU  |
| 1   | B     | 1039 | HIS  |
| 1   | C     | 215  | ALA  |
| 1   | C     | 918  | ASN  |
| 1   | D     | 215  | ALA  |
| 1   | E     | 216  | ALA  |
| 1   | F     | 150  | THR  |
| 1   | F     | 215  | ALA  |
| 1   | A     | 509  | LYS  |
| 1   | E     | 778  | PRO  |
| 1   | F     | 773  | LYS  |
| 1   | F     | 915  | GLY  |
| 1   | A     | 666  | ILE  |
| 1   | A     | 778  | PRO  |
| 1   | C     | 998  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 511  | GLY  |
| 1   | E     | 1035 | ILE  |
| 1   | D     | 616  | GLY  |
| 1   | C     | 828  | PRO  |
| 1   | E     | 508  | GLY  |
| 1   | E     | 539  | GLY  |
| 1   | F     | 778  | PRO  |
| 1   | B     | 318  | PRO  |
| 1   | C     | 653  | ILE  |
| 1   | D     | 200  | PRO  |

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

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 846/852 (99%)   | 781 (92%)  | 65 (8%)  | 13          | 40 |
| 1   | B     | 847/852 (99%)   | 789 (93%)  | 58 (7%)  | 16          | 45 |
| 1   | C     | 843/852 (99%)   | 774 (92%)  | 69 (8%)  | 11          | 37 |
| 1   | D     | 846/852 (99%)   | 789 (93%)  | 57 (7%)  | 16          | 46 |
| 1   | E     | 845/852 (99%)   | 775 (92%)  | 70 (8%)  | 11          | 36 |
| 1   | F     | 845/852 (99%)   | 789 (93%)  | 56 (7%)  | 16          | 46 |
| All | All   | 5072/5112 (99%) | 4697 (93%) | 375 (7%) | 13          | 42 |

All (375) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ILE  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 44  | THR  |
| 1   | A     | 49  | TYR  |
| 1   | A     | 70  | ASN  |
| 1   | A     | 101 | ASP  |
| 1   | A     | 146 | ASP  |
| 1   | A     | 148 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 152 | GLU  |
| 1   | A     | 166 | ILE  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 243 | THR  |
| 1   | A     | 255 | GLN  |
| 1   | A     | 281 | PHE  |
| 1   | A     | 293 | LEU  |
| 1   | A     | 295 | THR  |
| 1   | A     | 337 | ILE  |
| 1   | A     | 342 | LYS  |
| 1   | A     | 349 | ILE  |
| 1   | A     | 350 | LEU  |
| 1   | A     | 360 | GLN  |
| 1   | A     | 362 | PHE  |
| 1   | A     | 400 | LEU  |
| 1   | A     | 429 | GLU  |
| 1   | A     | 434 | SER  |
| 1   | A     | 437 | GLN  |
| 1   | A     | 463 | THR  |
| 1   | A     | 483 | LEU  |
| 1   | A     | 489 | THR  |
| 1   | A     | 502 | LYS  |
| 1   | A     | 512 | PHE  |
| 1   | A     | 519 | MET  |
| 1   | A     | 524 | THR  |
| 1   | A     | 536 | ARG  |
| 1   | A     | 538 | THR  |
| 1   | A     | 542 | LEU  |
| 1   | A     | 558 | ARG  |
| 1   | A     | 566 | ASP  |
| 1   | A     | 575 | MET  |
| 1   | A     | 603 | LYS  |
| 1   | A     | 610 | PHE  |
| 1   | A     | 669 | LEU  |
| 1   | A     | 682 | GLN  |
| 1   | A     | 690 | LEU  |
| 1   | A     | 694 | ARG  |
| 1   | A     | 708 | LEU  |
| 1   | A     | 711 | VAL  |
| 1   | A     | 726 | ILE  |
| 1   | A     | 736 | VAL  |
| 1   | A     | 830 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 896  | VAL  |
| 1   | A     | 916  | LEU  |
| 1   | A     | 917  | THR  |
| 1   | A     | 926  | LEU  |
| 1   | A     | 942  | GLU  |
| 1   | A     | 946  | ASP  |
| 1   | A     | 956  | ILE  |
| 1   | A     | 959  | THR  |
| 1   | A     | 966  | ARG  |
| 1   | A     | 977  | PHE  |
| 1   | A     | 985  | VAL  |
| 1   | A     | 1012 | LEU  |
| 1   | A     | 1014 | ILE  |
| 1   | A     | 1024 | VAL  |
| 1   | A     | 1035 | ILE  |
| 1   | B     | 6    | ILE  |
| 1   | B     | 10   | ILE  |
| 1   | B     | 11   | PHE  |
| 1   | B     | 29   | LYS  |
| 1   | B     | 34   | GLN  |
| 1   | B     | 49   | TYR  |
| 1   | B     | 96   | SER  |
| 1   | B     | 117  | LEU  |
| 1   | B     | 131  | LYS  |
| 1   | B     | 177  | LEU  |
| 1   | B     | 185  | ARG  |
| 1   | B     | 229  | GLN  |
| 1   | B     | 243  | THR  |
| 1   | B     | 255  | GLN  |
| 1   | B     | 259  | ARG  |
| 1   | B     | 293  | LEU  |
| 1   | B     | 295  | THR  |
| 1   | B     | 323  | ILE  |
| 1   | B     | 350  | LEU  |
| 1   | B     | 355  | MET  |
| 1   | B     | 358  | PHE  |
| 1   | B     | 360  | GLN  |
| 1   | B     | 365  | THR  |
| 1   | B     | 372  | VAL  |
| 1   | B     | 389  | SER  |
| 1   | B     | 400  | LEU  |
| 1   | B     | 422  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 482  | VAL  |
| 1   | B     | 489  | THR  |
| 1   | B     | 538  | THR  |
| 1   | B     | 542  | LEU  |
| 1   | B     | 559  | LEU  |
| 1   | B     | 563  | PHE  |
| 1   | B     | 571  | VAL  |
| 1   | B     | 575  | MET  |
| 1   | B     | 578  | LEU  |
| 1   | B     | 583  | THR  |
| 1   | B     | 610  | PHE  |
| 1   | B     | 663  | LEU  |
| 1   | B     | 668  | GLU  |
| 1   | B     | 673  | THR  |
| 1   | B     | 682  | GLN  |
| 1   | B     | 690  | LEU  |
| 1   | B     | 694  | ARG  |
| 1   | B     | 830  | LYS  |
| 1   | B     | 839  | MET  |
| 1   | B     | 860  | GLN  |
| 1   | B     | 916  | LEU  |
| 1   | B     | 946  | ASP  |
| 1   | B     | 961  | ASP  |
| 1   | B     | 966  | ARG  |
| 1   | B     | 968  | ARG  |
| 1   | B     | 1012 | LEU  |
| 1   | B     | 1029 | SER  |
| 1   | B     | 1032 | ASN  |
| 1   | B     | 1033 | GLU  |
| 1   | B     | 1035 | ILE  |
| 1   | B     | 1039 | HIS  |
| 1   | C     | 3    | ASN  |
| 1   | C     | 6    | ILE  |
| 1   | C     | 11   | PHE  |
| 1   | C     | 25   | LEU  |
| 1   | C     | 27   | ILE  |
| 1   | C     | 28   | LEU  |
| 1   | C     | 49   | TYR  |
| 1   | C     | 55   | LYS  |
| 1   | C     | 88   | VAL  |
| 1   | C     | 90   | ILE  |
| 1   | C     | 102  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 104 | GLN  |
| 1   | C     | 112 | GLN  |
| 1   | C     | 120 | GLN  |
| 1   | C     | 145 | THR  |
| 1   | C     | 153 | ASP  |
| 1   | C     | 177 | LEU  |
| 1   | C     | 219 | LEU  |
| 1   | C     | 243 | THR  |
| 1   | C     | 264 | ASP  |
| 1   | C     | 293 | LEU  |
| 1   | C     | 337 | ILE  |
| 1   | C     | 342 | LYS  |
| 1   | C     | 358 | PHE  |
| 1   | C     | 360 | GLN  |
| 1   | C     | 407 | ASP  |
| 1   | C     | 429 | GLU  |
| 1   | C     | 439 | GLN  |
| 1   | C     | 447 | MET  |
| 1   | C     | 452 | VAL  |
| 1   | C     | 463 | THR  |
| 1   | C     | 470 | PHE  |
| 1   | C     | 472 | ILE  |
| 1   | C     | 482 | VAL  |
| 1   | C     | 510 | LYS  |
| 1   | C     | 512 | PHE  |
| 1   | C     | 540 | ARG  |
| 1   | C     | 564 | LEU  |
| 1   | C     | 571 | VAL  |
| 1   | C     | 575 | MET  |
| 1   | C     | 587 | THR  |
| 1   | C     | 596 | HIS  |
| 1   | C     | 610 | PHE  |
| 1   | C     | 644 | MET  |
| 1   | C     | 652 | GLN  |
| 1   | C     | 661 | PHE  |
| 1   | C     | 689 | LYS  |
| 1   | C     | 711 | VAL  |
| 1   | C     | 736 | VAL  |
| 1   | C     | 741 | ILE  |
| 1   | C     | 838 | LEU  |
| 1   | C     | 842 | LEU  |
| 1   | C     | 855 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 860  | GLN  |
| 1   | C     | 881  | LEU  |
| 1   | C     | 890  | TRP  |
| 1   | C     | 909  | LEU  |
| 1   | C     | 942  | GLU  |
| 1   | C     | 956  | ILE  |
| 1   | C     | 963  | VAL  |
| 1   | C     | 966  | ARG  |
| 1   | C     | 986  | ILE  |
| 1   | C     | 1008 | THR  |
| 1   | C     | 1010 | THR  |
| 1   | C     | 1012 | LEU  |
| 1   | C     | 1030 | ARG  |
| 1   | C     | 1033 | GLU  |
| 1   | C     | 1035 | ILE  |
| 1   | C     | 1036 | GLU  |
| 1   | D     | 6    | ILE  |
| 1   | D     | 11   | PHE  |
| 1   | D     | 25   | LEU  |
| 1   | D     | 70   | ASN  |
| 1   | D     | 102  | ILE  |
| 1   | D     | 146  | ASP  |
| 1   | D     | 148  | THR  |
| 1   | D     | 152  | GLU  |
| 1   | D     | 153  | ASP  |
| 1   | D     | 177  | LEU  |
| 1   | D     | 205  | THR  |
| 1   | D     | 229  | GLN  |
| 1   | D     | 264  | ASP  |
| 1   | D     | 280  | GLU  |
| 1   | D     | 281  | PHE  |
| 1   | D     | 295  | THR  |
| 1   | D     | 350  | LEU  |
| 1   | D     | 358  | PHE  |
| 1   | D     | 362  | PHE  |
| 1   | D     | 365  | THR  |
| 1   | D     | 404  | LEU  |
| 1   | D     | 429  | GLU  |
| 1   | D     | 437  | GLN  |
| 1   | D     | 489  | THR  |
| 1   | D     | 519  | MET  |
| 1   | D     | 534  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 538  | THR  |
| 1   | D     | 559  | LEU  |
| 1   | D     | 561  | SER  |
| 1   | D     | 571  | VAL  |
| 1   | D     | 575  | MET  |
| 1   | D     | 603  | LYS  |
| 1   | D     | 610  | PHE  |
| 1   | D     | 628  | ASP  |
| 1   | D     | 629  | TRP  |
| 1   | D     | 637  | ASN  |
| 1   | D     | 690  | LEU  |
| 1   | D     | 708  | LEU  |
| 1   | D     | 726  | ILE  |
| 1   | D     | 738  | ILE  |
| 1   | D     | 852  | TYR  |
| 1   | D     | 862  | ARG  |
| 1   | D     | 909  | LEU  |
| 1   | D     | 913  | PHE  |
| 1   | D     | 916  | LEU  |
| 1   | D     | 917  | THR  |
| 1   | D     | 926  | LEU  |
| 1   | D     | 930  | ILE  |
| 1   | D     | 942  | GLU  |
| 1   | D     | 946  | ASP  |
| 1   | D     | 956  | ILE  |
| 1   | D     | 961  | ASP  |
| 1   | D     | 966  | ARG  |
| 1   | D     | 1012 | LEU  |
| 1   | D     | 1024 | VAL  |
| 1   | D     | 1030 | ARG  |
| 1   | D     | 1035 | ILE  |
| 1   | E     | 6    | ILE  |
| 1   | E     | 11   | PHE  |
| 1   | E     | 25   | LEU  |
| 1   | E     | 28   | LEU  |
| 1   | E     | 49   | TYR  |
| 1   | E     | 96   | SER  |
| 1   | E     | 105  | VAL  |
| 1   | E     | 117  | LEU  |
| 1   | E     | 131  | LYS  |
| 1   | E     | 146  | ASP  |
| 1   | E     | 153  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 177 | LEU  |
| 1   | E     | 249 | ILE  |
| 1   | E     | 255 | GLN  |
| 1   | E     | 259 | ARG  |
| 1   | E     | 270 | LEU  |
| 1   | E     | 280 | GLU  |
| 1   | E     | 310 | LEU  |
| 1   | E     | 312 | LYS  |
| 1   | E     | 323 | ILE  |
| 1   | E     | 336 | SER  |
| 1   | E     | 355 | MET  |
| 1   | E     | 356 | TYR  |
| 1   | E     | 358 | PHE  |
| 1   | E     | 372 | VAL  |
| 1   | E     | 398 | MET  |
| 1   | E     | 404 | LEU  |
| 1   | E     | 459 | PHE  |
| 1   | E     | 482 | VAL  |
| 1   | E     | 512 | PHE  |
| 1   | E     | 526 | HIS  |
| 1   | E     | 538 | THR  |
| 1   | E     | 555 | LEU  |
| 1   | E     | 564 | LEU  |
| 1   | E     | 566 | ASP  |
| 1   | E     | 571 | VAL  |
| 1   | E     | 574 | THR  |
| 1   | E     | 575 | MET  |
| 1   | E     | 583 | THR  |
| 1   | E     | 610 | PHE  |
| 1   | E     | 613 | ASN  |
| 1   | E     | 619 | THR  |
| 1   | E     | 629 | TRP  |
| 1   | E     | 647 | THR  |
| 1   | E     | 648 | ARG  |
| 1   | E     | 654 | LYS  |
| 1   | E     | 667 | VAL  |
| 1   | E     | 668 | GLU  |
| 1   | E     | 669 | LEU  |
| 1   | E     | 685 | LEU  |
| 1   | E     | 689 | LYS  |
| 1   | E     | 690 | LEU  |
| 1   | E     | 694 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 706  | ASP  |
| 1   | E     | 707  | MET  |
| 1   | E     | 708  | LEU  |
| 1   | E     | 712  | ARG  |
| 1   | E     | 726  | ILE  |
| 1   | E     | 736  | VAL  |
| 1   | E     | 799  | PHE  |
| 1   | E     | 830  | LYS  |
| 1   | E     | 852  | TYR  |
| 1   | E     | 896  | VAL  |
| 1   | E     | 909  | LEU  |
| 1   | E     | 917  | THR  |
| 1   | E     | 953  | LYS  |
| 1   | E     | 956  | ILE  |
| 1   | E     | 961  | ASP  |
| 1   | E     | 1012 | LEU  |
| 1   | E     | 1021 | PHE  |
| 1   | F     | 6    | ILE  |
| 1   | F     | 25   | LEU  |
| 1   | F     | 27   | ILE  |
| 1   | F     | 28   | LEU  |
| 1   | F     | 49   | TYR  |
| 1   | F     | 70   | ASN  |
| 1   | F     | 88   | VAL  |
| 1   | F     | 102  | ILE  |
| 1   | F     | 104  | GLN  |
| 1   | F     | 112  | GLN  |
| 1   | F     | 153  | ASP  |
| 1   | F     | 197  | GLN  |
| 1   | F     | 205  | THR  |
| 1   | F     | 243  | THR  |
| 1   | F     | 280  | GLU  |
| 1   | F     | 293  | LEU  |
| 1   | F     | 312  | LYS  |
| 1   | F     | 327  | TYR  |
| 1   | F     | 350  | LEU  |
| 1   | F     | 358  | PHE  |
| 1   | F     | 360  | GLN  |
| 1   | F     | 363  | ARG  |
| 1   | F     | 407  | ASP  |
| 1   | F     | 431  | THR  |
| 1   | F     | 447  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 448  | VAL  |
| 1   | F     | 515  | TRP  |
| 1   | F     | 538  | THR  |
| 1   | F     | 542  | LEU  |
| 1   | F     | 575  | MET  |
| 1   | F     | 587  | THR  |
| 1   | F     | 610  | PHE  |
| 1   | F     | 621  | ILE  |
| 1   | F     | 644  | MET  |
| 1   | F     | 657  | MET  |
| 1   | F     | 663  | LEU  |
| 1   | F     | 689  | LYS  |
| 1   | F     | 694  | ARG  |
| 1   | F     | 711  | VAL  |
| 1   | F     | 714  | ASN  |
| 1   | F     | 726  | ILE  |
| 1   | F     | 779  | ASP  |
| 1   | F     | 838  | LEU  |
| 1   | F     | 842  | LEU  |
| 1   | F     | 845  | LYS  |
| 1   | F     | 859  | TYR  |
| 1   | F     | 860  | GLN  |
| 1   | F     | 881  | LEU  |
| 1   | F     | 918  | ASN  |
| 1   | F     | 961  | ASP  |
| 1   | F     | 963  | VAL  |
| 1   | F     | 966  | ARG  |
| 1   | F     | 986  | ILE  |
| 1   | F     | 1021 | PHE  |
| 1   | F     | 1030 | ARG  |
| 1   | F     | 1034 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 231 | ASN  |
| 1   | A     | 237 | GLN  |
| 1   | A     | 569 | GLN  |
| 1   | B     | 63  | GLN  |
| 1   | B     | 109 | ASN  |
| 1   | B     | 742 | ASN  |
| 1   | C     | 151 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 613 | ASN  |
| 1   | C     | 755 | ASN  |
| 1   | D     | 109 | ASN  |
| 1   | D     | 231 | ASN  |
| 1   | D     | 437 | GLN  |
| 1   | D     | 742 | ASN  |
| 1   | E     | 34  | GLN  |
| 1   | E     | 67  | GLN  |
| 1   | E     | 231 | ASN  |
| 1   | E     | 569 | GLN  |
| 1   | E     | 605 | ASN  |
| 1   | E     | 613 | ASN  |
| 1   | E     | 637 | ASN  |
| 1   | E     | 732 | GLN  |
| 1   | F     | 108 | GLN  |
| 1   | F     | 584 | GLN  |
| 1   | F     | 613 | ASN  |
| 1   | F     | 682 | GLN  |
| 1   | F     | 704 | HIS  |
| 1   | F     | 732 | GLN  |
| 1   | F     | 755 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | LMT  | D     | 2000 | -    | 36,36,36     | 1.87 | 9 (25%)  | 47,47,47    | 1.70 | 8 (17%)  |
| 2   | LMT  | F     | 2000 | -    | 36,36,36     | 1.85 | 8 (22%)  | 47,47,47    | 1.14 | 4 (8%)   |
| 2   | LMT  | B     | 2000 | -    | 36,36,36     | 1.81 | 12 (33%) | 47,47,47    | 1.50 | 8 (17%)  |
| 2   | LMT  | A     | 1101 | -    | 36,36,36     | 1.80 | 11 (30%) | 47,47,47    | 1.37 | 6 (12%)  |
| 2   | LMT  | C     | 1101 | -    | 36,36,36     | 1.85 | 10 (27%) | 47,47,47    | 1.40 | 6 (12%)  |
| 2   | LMT  | E     | 1101 | -    | 36,36,36     | 1.83 | 10 (27%) | 47,47,47    | 1.92 | 9 (19%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|------|------|-----------|-------------|---------|
| 2   | LMT  | D     | 2000 | -    | 1/1/10/10 | 12/21/61/61 | 0/2/2/2 |
| 2   | LMT  | F     | 2000 | -    | -         | 15/21/61/61 | 0/2/2/2 |
| 2   | LMT  | B     | 2000 | -    | -         | 13/21/61/61 | 0/2/2/2 |
| 2   | LMT  | A     | 1101 | -    | -         | 8/21/61/61  | 0/2/2/2 |
| 2   | LMT  | C     | 1101 | -    | -         | 12/21/61/61 | 0/2/2/2 |
| 2   | LMT  | E     | 1101 | -    | 1/1/10/10 | 12/21/61/61 | 0/2/2/2 |

All (60) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | E     | 1101 | LMT  | O1'-C1' | 4.20 | 1.47        | 1.40     |
| 2   | C     | 1101 | LMT  | O5'-C5' | 4.10 | 1.54        | 1.44     |
| 2   | F     | 2000 | LMT  | O5'-C1' | 4.07 | 1.52        | 1.41     |
| 2   | F     | 2000 | LMT  | O5'-C5' | 3.97 | 1.54        | 1.44     |
| 2   | B     | 2000 | LMT  | O5'-C5' | 3.97 | 1.54        | 1.44     |
| 2   | F     | 2000 | LMT  | O1'-C1' | 3.95 | 1.46        | 1.40     |
| 2   | D     | 2000 | LMT  | O1'-C1' | 3.94 | 1.46        | 1.40     |
| 2   | A     | 1101 | LMT  | O5'-C5' | 3.91 | 1.53        | 1.44     |
| 2   | D     | 2000 | LMT  | O5'-C5' | 3.85 | 1.53        | 1.44     |
| 2   | C     | 1101 | LMT  | O1'-C1' | 3.65 | 1.46        | 1.40     |
| 2   | E     | 1101 | LMT  | O5'-C5' | 3.60 | 1.53        | 1.44     |
| 2   | D     | 2000 | LMT  | O5B-C1B | 3.52 | 1.50        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | E     | 1101 | LMT  | O5'-C1' | 3.47  | 1.50        | 1.41     |
| 2   | C     | 1101 | LMT  | C6'-C5' | -3.46 | 1.40        | 1.51     |
| 2   | F     | 2000 | LMT  | C6'-C5' | -3.42 | 1.40        | 1.51     |
| 2   | F     | 2000 | LMT  | O5B-C1B | 3.40  | 1.50        | 1.41     |
| 2   | A     | 1101 | LMT  | O5B-C1B | 3.36  | 1.50        | 1.41     |
| 2   | E     | 1101 | LMT  | C6'-C5' | -3.35 | 1.40        | 1.51     |
| 2   | A     | 1101 | LMT  | O1'-C1' | 3.34  | 1.45        | 1.40     |
| 2   | C     | 1101 | LMT  | O5'-C1' | 3.33  | 1.50        | 1.41     |
| 2   | B     | 2000 | LMT  | C6'-C5' | -3.25 | 1.40        | 1.51     |
| 2   | C     | 1101 | LMT  | O5B-C1B | 3.21  | 1.50        | 1.41     |
| 2   | A     | 1101 | LMT  | C6'-C5' | -3.20 | 1.41        | 1.51     |
| 2   | B     | 2000 | LMT  | O5B-C1B | 3.19  | 1.50        | 1.41     |
| 2   | D     | 2000 | LMT  | C3'-C2' | -3.14 | 1.44        | 1.52     |
| 2   | E     | 1101 | LMT  | O5B-C1B | 3.12  | 1.49        | 1.41     |
| 2   | B     | 2000 | LMT  | O1'-C1' | 3.07  | 1.45        | 1.40     |
| 2   | D     | 2000 | LMT  | C6'-C5' | -3.05 | 1.41        | 1.51     |
| 2   | C     | 1101 | LMT  | O3B-C3B | 3.05  | 1.50        | 1.43     |
| 2   | B     | 2000 | LMT  | O5'-C1' | 2.96  | 1.49        | 1.41     |
| 2   | B     | 2000 | LMT  | C3'-C2' | -2.94 | 1.44        | 1.52     |
| 2   | B     | 2000 | LMT  | C3B-C2B | -2.87 | 1.45        | 1.52     |
| 2   | D     | 2000 | LMT  | O5'-C1' | 2.86  | 1.49        | 1.41     |
| 2   | D     | 2000 | LMT  | O3B-C3B | 2.86  | 1.49        | 1.43     |
| 2   | E     | 1101 | LMT  | C3'-C2' | -2.83 | 1.45        | 1.52     |
| 2   | F     | 2000 | LMT  | C3'-C2' | -2.80 | 1.45        | 1.52     |
| 2   | E     | 1101 | LMT  | O3B-C3B | 2.68  | 1.49        | 1.43     |
| 2   | D     | 2000 | LMT  | C3B-C2B | -2.66 | 1.45        | 1.52     |
| 2   | E     | 1101 | LMT  | O1B-C1B | -2.65 | 1.34        | 1.41     |
| 2   | A     | 1101 | LMT  | O5'-C1' | 2.65  | 1.48        | 1.41     |
| 2   | A     | 1101 | LMT  | C3'-C2' | -2.63 | 1.45        | 1.52     |
| 2   | D     | 2000 | LMT  | O2'-C2' | 2.51  | 1.48        | 1.43     |
| 2   | F     | 2000 | LMT  | O3B-C3B | 2.38  | 1.48        | 1.43     |
| 2   | A     | 1101 | LMT  | O2'-C2' | 2.35  | 1.48        | 1.43     |
| 2   | C     | 1101 | LMT  | C3'-C2' | -2.33 | 1.46        | 1.52     |
| 2   | C     | 1101 | LMT  | O2'-C2' | 2.32  | 1.48        | 1.43     |
| 2   | A     | 1101 | LMT  | C1'-C2' | -2.28 | 1.45        | 1.52     |
| 2   | A     | 1101 | LMT  | O3B-C3B | 2.26  | 1.48        | 1.43     |
| 2   | A     | 1101 | LMT  | C3B-C2B | -2.23 | 1.46        | 1.52     |
| 2   | B     | 2000 | LMT  | O3B-C3B | 2.23  | 1.48        | 1.43     |
| 2   | E     | 1101 | LMT  | O1B-C4' | -2.16 | 1.38        | 1.43     |
| 2   | B     | 2000 | LMT  | C5-C4   | 2.09  | 1.63        | 1.51     |
| 2   | E     | 1101 | LMT  | O3'-C3' | 2.07  | 1.47        | 1.43     |
| 2   | C     | 1101 | LMT  | O3'-C3' | 2.07  | 1.47        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 2000 | LMT  | O2'-C2' | 2.06  | 1.47        | 1.43     |
| 2   | F     | 2000 | LMT  | C5-C4   | 2.05  | 1.63        | 1.51     |
| 2   | B     | 2000 | LMT  | O3'-C3' | 2.03  | 1.47        | 1.43     |
| 2   | A     | 1101 | LMT  | O1B-C1B | -2.03 | 1.36        | 1.41     |
| 2   | C     | 1101 | LMT  | C5-C4   | 2.01  | 1.62        | 1.51     |
| 2   | B     | 2000 | LMT  | C4'-C5' | 2.00  | 1.58        | 1.52     |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | E     | 1101 | LMT  | O1B-C4'-C5' | -5.21 | 95.18       | 109.45   |
| 2   | D     | 2000 | LMT  | O1'-C1'-C2' | 5.11  | 116.28      | 108.30   |
| 2   | C     | 1101 | LMT  | O1'-C1'-C2' | 4.87  | 115.91      | 108.30   |
| 2   | E     | 1101 | LMT  | C4B-C3B-C2B | 4.82  | 119.23      | 110.82   |
| 2   | E     | 1101 | LMT  | C3B-C4B-C5B | 4.70  | 118.63      | 110.24   |
| 2   | D     | 2000 | LMT  | C1-O1'-C1'  | 4.70  | 121.63      | 113.84   |
| 2   | A     | 1101 | LMT  | C1B-O5B-C5B | 4.43  | 122.37      | 113.69   |
| 2   | E     | 1101 | LMT  | O1'-C1'-C2' | 4.15  | 114.78      | 108.30   |
| 2   | A     | 1101 | LMT  | O5B-C5B-C4B | 4.02  | 116.99      | 109.69   |
| 2   | B     | 2000 | LMT  | C1B-O1B-C4' | -3.87 | 108.39      | 117.96   |
| 2   | B     | 2000 | LMT  | O5B-C5B-C4B | 3.72  | 116.44      | 109.69   |
| 2   | E     | 1101 | LMT  | O4'-C4B-C3B | -3.67 | 101.86      | 110.35   |
| 2   | D     | 2000 | LMT  | O2'-C2'-C1' | 3.62  | 118.84      | 110.05   |
| 2   | B     | 2000 | LMT  | C1'-C2'-C3' | -3.57 | 102.57      | 110.00   |
| 2   | D     | 2000 | LMT  | C1B-O1B-C4' | -3.33 | 109.73      | 117.96   |
| 2   | E     | 1101 | LMT  | O5'-C5'-C6' | 3.06  | 114.03      | 106.44   |
| 2   | B     | 2000 | LMT  | O3B-C3B-C2B | -3.03 | 103.34      | 110.35   |
| 2   | D     | 2000 | LMT  | C1'-O5'-C5' | 2.96  | 119.49      | 113.69   |
| 2   | D     | 2000 | LMT  | C1'-C2'-C3' | -2.82 | 104.11      | 110.00   |
| 2   | F     | 2000 | LMT  | C1B-O5B-C5B | -2.81 | 108.17      | 113.69   |
| 2   | E     | 1101 | LMT  | O5B-C5B-C4B | 2.76  | 114.70      | 109.69   |
| 2   | E     | 1101 | LMT  | O1B-C1B-C2B | -2.70 | 101.11      | 108.10   |
| 2   | C     | 1101 | LMT  | C1'-C2'-C3' | -2.69 | 104.40      | 110.00   |
| 2   | B     | 2000 | LMT  | O1'-C1'-C2' | 2.61  | 112.38      | 108.30   |
| 2   | C     | 1101 | LMT  | C3'-C4'-C5' | -2.55 | 105.07      | 110.93   |
| 2   | C     | 1101 | LMT  | O3'-C3'-C4' | 2.49  | 116.54      | 109.94   |
| 2   | B     | 2000 | LMT  | C1B-O5B-C5B | 2.46  | 118.51      | 113.69   |
| 2   | B     | 2000 | LMT  | O1B-C1B-C2B | 2.46  | 114.46      | 108.10   |
| 2   | C     | 1101 | LMT  | C1B-O1B-C4' | -2.43 | 111.94      | 117.96   |
| 2   | D     | 2000 | LMT  | O3'-C3'-C4' | 2.42  | 116.37      | 109.94   |
| 2   | A     | 1101 | LMT  | C1B-C2B-C3B | 2.38  | 114.96      | 110.00   |
| 2   | F     | 2000 | LMT  | O5B-C5B-C4B | 2.37  | 114.00      | 109.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | F     | 2000 | LMT  | C1'-O5'-C5' | 2.32  | 118.23      | 113.69   |
| 2   | A     | 1101 | LMT  | O3B-C3B-C4B | -2.29 | 105.06      | 110.35   |
| 2   | D     | 2000 | LMT  | C4B-C3B-C2B | 2.29  | 114.81      | 110.82   |
| 2   | B     | 2000 | LMT  | C1'-O5'-C5' | -2.28 | 109.21      | 113.69   |
| 2   | E     | 1101 | LMT  | O2'-C2'-C1' | 2.22  | 115.44      | 110.05   |
| 2   | F     | 2000 | LMT  | O5B-C5B-C6B | 2.17  | 111.82      | 106.44   |
| 2   | C     | 1101 | LMT  | C1B-C2B-C3B | 2.14  | 114.46      | 110.00   |
| 2   | A     | 1101 | LMT  | O5B-C1B-C2B | 2.13  | 114.86      | 110.35   |
| 2   | A     | 1101 | LMT  | C6B-C5B-C4B | -2.10 | 108.09      | 113.00   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 2   | D     | 2000 | LMT  | C3B  |
| 2   | E     | 1101 | LMT  | C2B  |

All (72) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | F     | 2000 | LMT  | C2'-C1'-O1'-C1  |
| 2   | C     | 1101 | LMT  | C2'-C1'-O1'-C1  |
| 2   | C     | 1101 | LMT  | O5'-C1'-O1'-C1  |
| 2   | E     | 1101 | LMT  | C2-C1-O1'-C1'   |
| 2   | E     | 1101 | LMT  | C4B-C5B-C6B-O6B |
| 2   | F     | 2000 | LMT  | O5'-C5'-C6'-O6' |
| 2   | A     | 1101 | LMT  | O5'-C5'-C6'-O6' |
| 2   | E     | 1101 | LMT  | O5B-C5B-C6B-O6B |
| 2   | C     | 1101 | LMT  | O5B-C5B-C6B-O6B |
| 2   | E     | 1101 | LMT  | O5'-C5'-C6'-O6' |
| 2   | D     | 2000 | LMT  | O5'-C5'-C6'-O6' |
| 2   | E     | 1101 | LMT  | C4'-C5'-C6'-O6' |
| 2   | D     | 2000 | LMT  | C4'-C5'-C6'-O6' |
| 2   | A     | 1101 | LMT  | C4'-C5'-C6'-O6' |
| 2   | B     | 2000 | LMT  | C2-C3-C4-C5     |
| 2   | C     | 1101 | LMT  | C4-C5-C6-C7     |
| 2   | A     | 1101 | LMT  | C3-C4-C5-C6     |
| 2   | C     | 1101 | LMT  | O5'-C5'-C6'-O6' |
| 2   | F     | 2000 | LMT  | C4'-C5'-C6'-O6' |
| 2   | F     | 2000 | LMT  | O5B-C5B-C6B-O6B |
| 2   | B     | 2000 | LMT  | C4'-C5'-C6'-O6' |
| 2   | F     | 2000 | LMT  | C4B-C5B-C6B-O6B |
| 2   | C     | 1101 | LMT  | C4'-C5'-C6'-O6' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1101 | LMT  | C5-C6-C7-C8     |
| 2   | C     | 1101 | LMT  | C4B-C5B-C6B-O6B |
| 2   | A     | 1101 | LMT  | O5B-C5B-C6B-O6B |
| 2   | C     | 1101 | LMT  | C6-C7-C8-C9     |
| 2   | A     | 1101 | LMT  | O1'-C1-C2-C3    |
| 2   | D     | 2000 | LMT  | O5'-C1'-O1'-C1  |
| 2   | B     | 2000 | LMT  | O5'-C5'-C6'-O6' |
| 2   | B     | 2000 | LMT  | O1'-C1-C2-C3    |
| 2   | E     | 1101 | LMT  | C5-C6-C7-C8     |
| 2   | E     | 1101 | LMT  | C11-C10-C9-C8   |
| 2   | C     | 1101 | LMT  | C2-C3-C4-C5     |
| 2   | F     | 2000 | LMT  | C11-C10-C9-C8   |
| 2   | D     | 2000 | LMT  | C2'-C1'-O1'-C1  |
| 2   | A     | 1101 | LMT  | C4-C5-C6-C7     |
| 2   | F     | 2000 | LMT  | C6-C7-C8-C9     |
| 2   | B     | 2000 | LMT  | C5-C6-C7-C8     |
| 2   | B     | 2000 | LMT  | C11-C10-C9-C8   |
| 2   | F     | 2000 | LMT  | O5'-C1'-O1'-C1  |
| 2   | B     | 2000 | LMT  | C1-C2-C3-C4     |
| 2   | E     | 1101 | LMT  | C3-C4-C5-C6     |
| 2   | C     | 1101 | LMT  | C5-C6-C7-C8     |
| 2   | D     | 2000 | LMT  | O5B-C5B-C6B-O6B |
| 2   | F     | 2000 | LMT  | C7-C8-C9-C10    |
| 2   | F     | 2000 | LMT  | C1-C2-C3-C4     |
| 2   | C     | 1101 | LMT  | C1-C2-C3-C4     |
| 2   | E     | 1101 | LMT  | C2-C3-C4-C5     |
| 2   | F     | 2000 | LMT  | C2-C3-C4-C5     |
| 2   | B     | 2000 | LMT  | C9-C10-C11-C12  |
| 2   | B     | 2000 | LMT  | O5'-C1'-O1'-C1  |
| 2   | B     | 2000 | LMT  | C7-C8-C9-C10    |
| 2   | D     | 2000 | LMT  | C1-C2-C3-C4     |
| 2   | D     | 2000 | LMT  | C6-C7-C8-C9     |
| 2   | F     | 2000 | LMT  | C9-C10-C11-C12  |
| 2   | E     | 1101 | LMT  | C5'-C4'-O1B-C1B |
| 2   | B     | 2000 | LMT  | C2-C1-O1'-C1'   |
| 2   | B     | 2000 | LMT  | O5B-C5B-C6B-O6B |
| 2   | F     | 2000 | LMT  | C4-C5-C6-C7     |
| 2   | E     | 1101 | LMT  | C3'-C4'-O1B-C1B |
| 2   | D     | 2000 | LMT  | C5-C6-C7-C8     |
| 2   | D     | 2000 | LMT  | C11-C10-C9-C8   |
| 2   | B     | 2000 | LMT  | C4-C5-C6-C7     |
| 2   | D     | 2000 | LMT  | C7-C8-C9-C10    |

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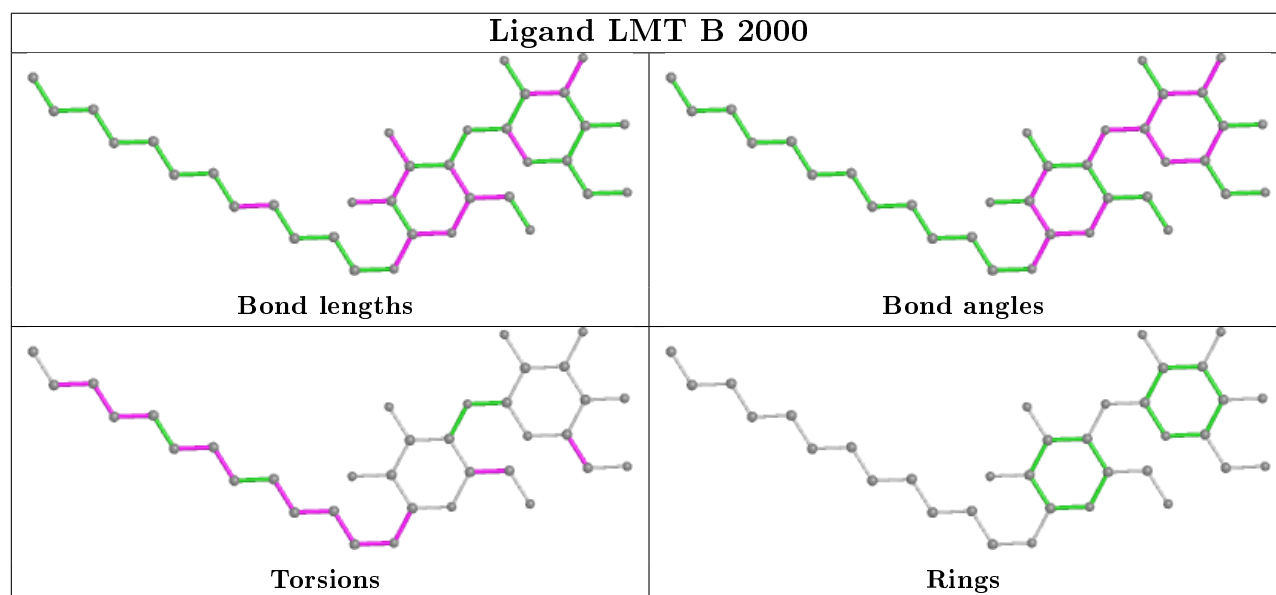
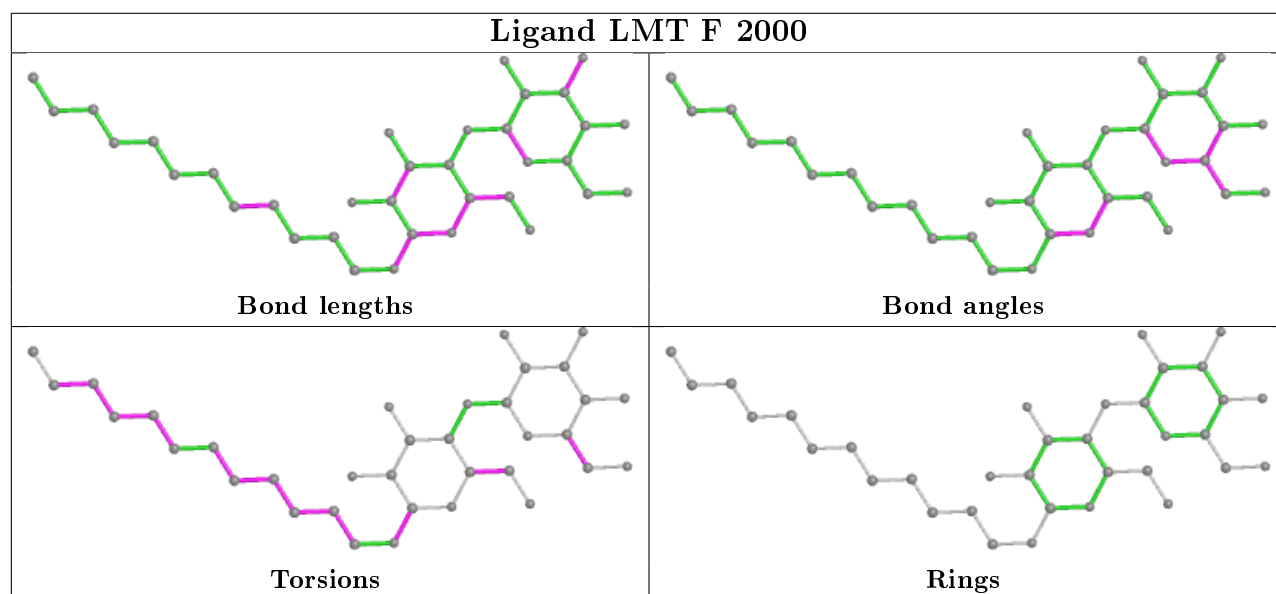
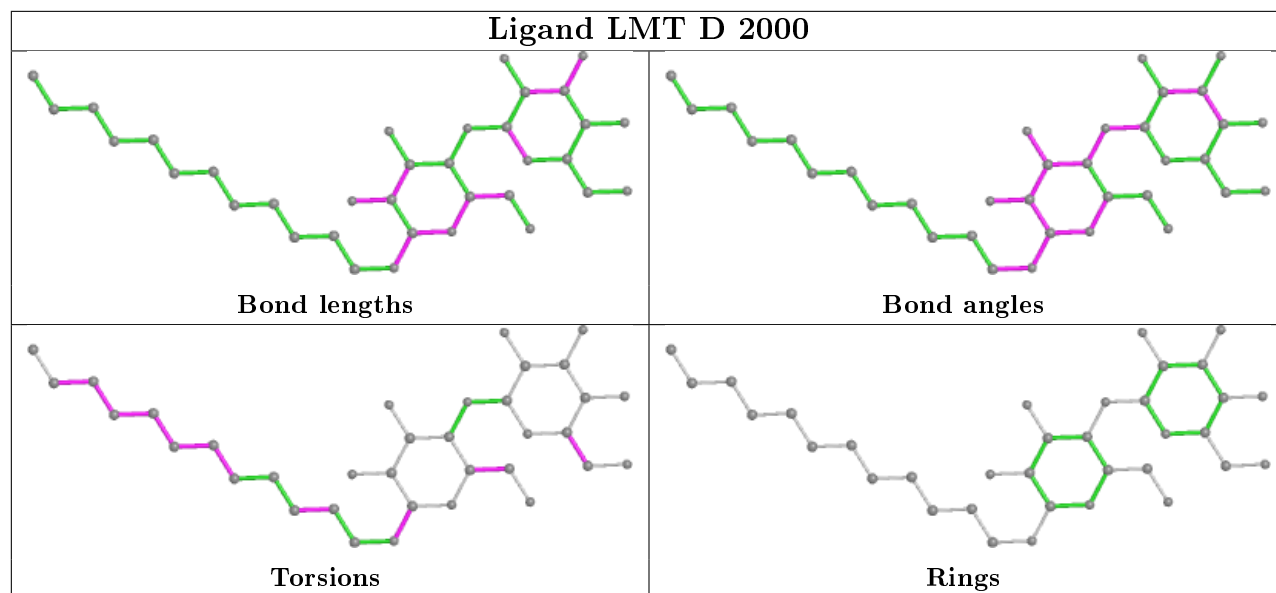
| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 2   | D     | 2000 | LMT  | C4-C5-C6-C7    |
| 2   | F     | 2000 | LMT  | C3-C4-C5-C6    |
| 2   | F     | 2000 | LMT  | O1'-C1-C2-C3   |
| 2   | D     | 2000 | LMT  | C9-C10-C11-C12 |
| 2   | A     | 1101 | LMT  | C6-C7-C8-C9    |
| 2   | E     | 1101 | LMT  | C9-C10-C11-C12 |
| 2   | C     | 1101 | LMT  | O1'-C1-C2-C3   |

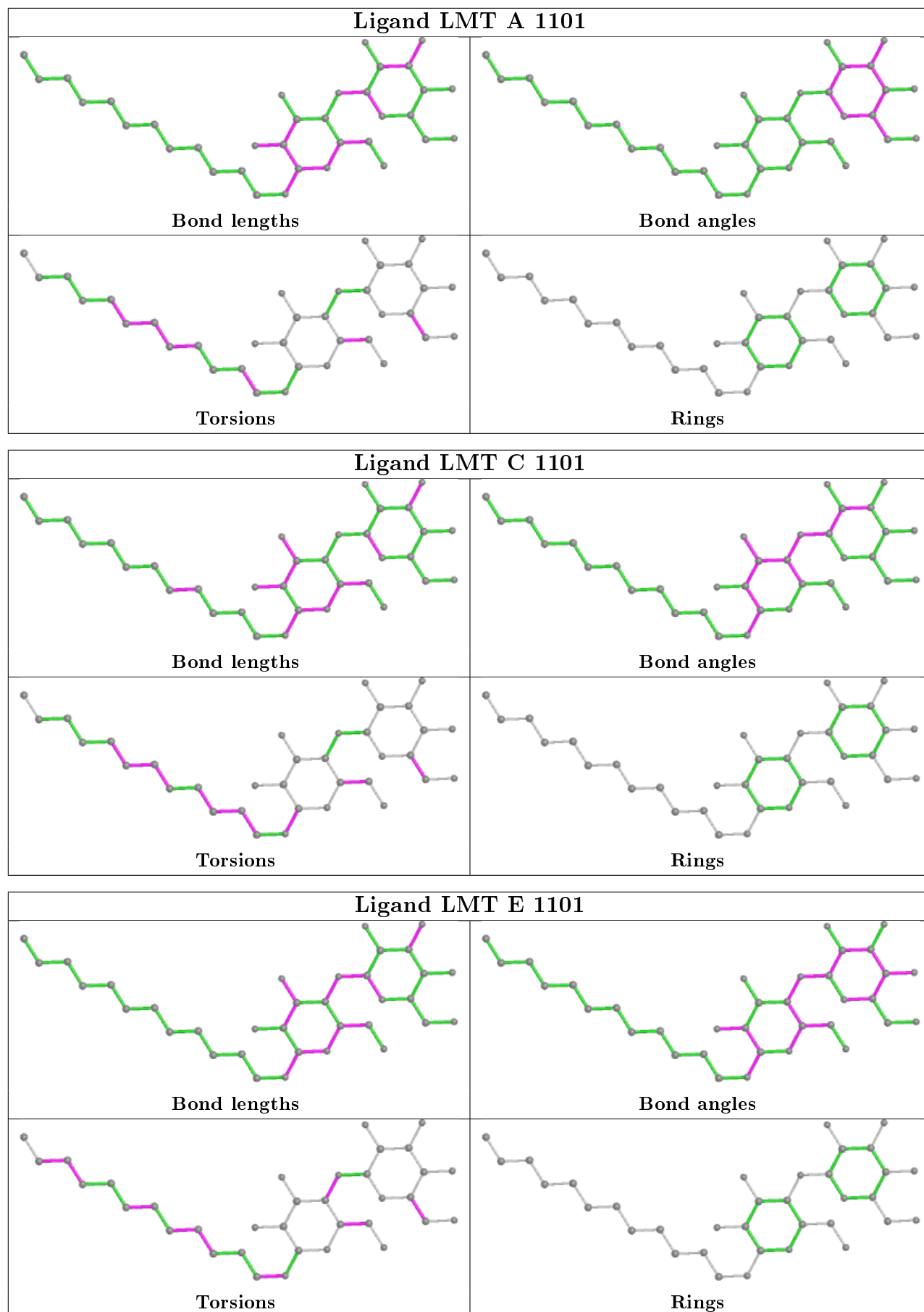
There are no ring outliers.

6 monomers are involved in 20 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | D     | 2000 | LMT  | 3       | 0            |
| 2   | F     | 2000 | LMT  | 1       | 0            |
| 2   | B     | 2000 | LMT  | 3       | 0            |
| 2   | A     | 1101 | LMT  | 4       | 0            |
| 2   | C     | 1101 | LMT  | 1       | 0            |
| 2   | E     | 1101 | LMT  | 8       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------|-----------------------|-------|
| 1   | A     | 1038/1044 (99%) | 0.42   | 127 (12%) <b>4</b> <b>5</b> | 27, 75, 109, 132      | 0     |
| 1   | B     | 1039/1044 (99%) | 0.37   | 102 (9%) <b>7</b> <b>9</b>  | 18, 68, 104, 130      | 0     |
| 1   | C     | 1035/1044 (99%) | 0.49   | 125 (12%) <b>4</b> <b>5</b> | 17, 69, 104, 126      | 0     |
| 1   | D     | 1038/1044 (99%) | 0.59   | 162 (15%) <b>2</b> <b>2</b> | 16, 90, 130, 173      | 0     |
| 1   | E     | 1037/1044 (99%) | 0.69   | 180 (17%) <b>1</b> <b>1</b> | 40, 91, 115, 134      | 0     |
| 1   | F     | 1037/1044 (99%) | 0.73   | 177 (17%) <b>1</b> <b>2</b> | 24, 84, 118, 142      | 0     |
| All | All   | 6224/6264 (99%) | 0.55   | 873 (14%) <b>2</b> <b>3</b> | 16, 80, 115, 173      | 0     |

All (873) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 128 | SER  | 16.7 |
| 1   | E     | 314 | GLU  | 14.0 |
| 1   | E     | 315 | PRO  | 12.2 |
| 1   | F     | 714 | ASN  | 11.8 |
| 1   | F     | 442 | LEU  | 11.2 |
| 1   | F     | 128 | SER  | 11.2 |
| 1   | E     | 311 | ALA  | 10.4 |
| 1   | F     | 832 | THR  | 10.4 |
| 1   | F     | 481 | SER  | 10.4 |
| 1   | F     | 830 | LYS  | 10.1 |
| 1   | F     | 831 | SER  | 10.0 |
| 1   | C     | 403 | GLY  | 9.3  |
| 1   | C     | 402 | ILE  | 9.2  |
| 1   | E     | 406 | VAL  | 9.1  |
| 1   | C     | 714 | ASN  | 8.7  |
| 1   | E     | 405 | LEU  | 8.5  |
| 1   | C     | 715 | GLY  | 8.5  |
| 1   | B     | 315 | PRO  | 8.5  |
| 1   | D     | 459 | PHE  | 8.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 129 | VAL  | 8.4  |
| 1   | F     | 936 | ASN  | 8.0  |
| 1   | A     | 371 | ALA  | 7.9  |
| 1   | F     | 127 | VAL  | 7.8  |
| 1   | D     | 685 | LEU  | 7.7  |
| 1   | B     | 314 | GLU  | 7.7  |
| 1   | F     | 823 | LEU  | 7.5  |
| 1   | C     | 831 | SER  | 7.5  |
| 1   | E     | 973 | THR  | 7.3  |
| 1   | D     | 461 | GLY  | 7.2  |
| 1   | D     | 322 | LYS  | 7.2  |
| 1   | D     | 683 | ALA  | 7.2  |
| 1   | D     | 864 | SER  | 7.1  |
| 1   | F     | 410 | ILE  | 7.1  |
| 1   | F     | 715 | GLY  | 6.9  |
| 1   | E     | 409 | ALA  | 6.9  |
| 1   | C     | 832 | THR  | 6.8  |
| 1   | E     | 407 | ASP  | 6.8  |
| 1   | A     | 369 | THR  | 6.7  |
| 1   | F     | 406 | VAL  | 6.7  |
| 1   | E     | 488 | LEU  | 6.7  |
| 1   | F     | 695 | ASN  | 6.7  |
| 1   | F     | 448 | VAL  | 6.6  |
| 1   | D     | 407 | ASP  | 6.5  |
| 1   | D     | 389 | SER  | 6.5  |
| 1   | F     | 407 | ASP  | 6.5  |
| 1   | F     | 694 | ARG  | 6.5  |
| 1   | D     | 462 | SER  | 6.5  |
| 1   | E     | 928 | THR  | 6.4  |
| 1   | B     | 164 | ASP  | 6.4  |
| 1   | E     | 976 | ALA  | 6.4  |
| 1   | D     | 35  | TYR  | 6.3  |
| 1   | C     | 670 | GLY  | 6.3  |
| 1   | E     | 864 | SER  | 6.2  |
| 1   | F     | 405 | LEU  | 6.2  |
| 1   | B     | 128 | SER  | 6.2  |
| 1   | F     | 46  | SER  | 6.1  |
| 1   | D     | 282 | ASN  | 6.1  |
| 1   | E     | 127 | VAL  | 6.1  |
| 1   | C     | 671 | THR  | 6.1  |
| 1   | F     | 107 | VAL  | 6.1  |
| 1   | A     | 396 | PHE  | 6.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 487 | ILE  | 6.0  |
| 1   | A     | 372 | VAL  | 6.0  |
| 1   | D     | 67  | GLN  | 5.9  |
| 1   | E     | 307 | ARG  | 5.9  |
| 1   | A     | 404 | LEU  | 5.9  |
| 1   | E     | 408 | ASP  | 5.9  |
| 1   | A     | 656 | ALA  | 5.9  |
| 1   | A     | 400 | LEU  | 5.9  |
| 1   | F     | 441 | ALA  | 5.9  |
| 1   | F     | 315 | PRO  | 5.9  |
| 1   | F     | 111 | LEU  | 5.9  |
| 1   | D     | 108 | GLN  | 5.9  |
| 1   | F     | 109 | ASN  | 5.8  |
| 1   | F     | 500 | ILE  | 5.8  |
| 1   | A     | 445 | ILE  | 5.8  |
| 1   | E     | 972 | MET  | 5.7  |
| 1   | F     | 671 | THR  | 5.7  |
| 1   | D     | 70  | ASN  | 5.7  |
| 1   | A     | 35  | TYR  | 5.7  |
| 1   | F     | 449 | LEU  | 5.7  |
| 1   | E     | 310 | LEU  | 5.7  |
| 1   | C     | 716 | LEU  | 5.6  |
| 1   | C     | 406 | VAL  | 5.6  |
| 1   | E     | 932 | LEU  | 5.6  |
| 1   | F     | 193 | LEU  | 5.6  |
| 1   | F     | 178 | PHE  | 5.6  |
| 1   | D     | 486 | LEU  | 5.6  |
| 1   | F     | 821 | GLU  | 5.6  |
| 1   | D     | 834 | GLU  | 5.5  |
| 1   | D     | 460 | GLY  | 5.5  |
| 1   | C     | 401 | ALA  | 5.5  |
| 1   | F     | 47  | ALA  | 5.5  |
| 1   | D     | 111 | LEU  | 5.4  |
| 1   | B     | 111 | LEU  | 5.4  |
| 1   | E     | 578 | LEU  | 5.4  |
| 1   | E     | 410 | ILE  | 5.4  |
| 1   | E     | 312 | LYS  | 5.4  |
| 1   | B     | 129 | VAL  | 5.4  |
| 1   | D     | 658 | VAL  | 5.4  |
| 1   | A     | 48  | SER  | 5.4  |
| 1   | A     | 894 | PHE  | 5.4  |
| 1   | F     | 372 | VAL  | 5.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 487  | ILE  | 5.3  |
| 1   | C     | 830  | LYS  | 5.3  |
| 1   | D     | 847  | PRO  | 5.3  |
| 1   | C     | 821  | GLU  | 5.3  |
| 1   | E     | 67   | GLN  | 5.3  |
| 1   | F     | 482  | VAL  | 5.3  |
| 1   | A     | 16   | ALA  | 5.3  |
| 1   | C     | 404  | LEU  | 5.3  |
| 1   | F     | 872  | TYR  | 5.3  |
| 1   | D     | 404  | LEU  | 5.3  |
| 1   | C     | 405  | LEU  | 5.2  |
| 1   | C     | 398  | MET  | 5.2  |
| 1   | E     | 1014 | ILE  | 5.2  |
| 1   | F     | 501  | ALA  | 5.2  |
| 1   | E     | 355  | MET  | 5.2  |
| 1   | E     | 351  | VAL  | 5.2  |
| 1   | B     | 109  | ASN  | 5.2  |
| 1   | B     | 831  | SER  | 5.2  |
| 1   | D     | 846  | LEU  | 5.2  |
| 1   | E     | 352  | PHE  | 5.2  |
| 1   | E     | 834  | GLU  | 5.2  |
| 1   | E     | 442  | LEU  | 5.2  |
| 1   | A     | 482  | VAL  | 5.2  |
| 1   | F     | 474  | ILE  | 5.1  |
| 1   | A     | 635  | GLU  | 5.1  |
| 1   | C     | 445  | ILE  | 5.0  |
| 1   | F     | 463  | THR  | 5.0  |
| 1   | C     | 707  | MET  | 5.0  |
| 1   | E     | 330  | THR  | 5.0  |
| 1   | E     | 403  | GLY  | 5.0  |
| 1   | E     | 466  | ILE  | 5.0  |
| 1   | F     | 833  | GLY  | 4.9  |
| 1   | F     | 502  | LYS  | 4.9  |
| 1   | C     | 481  | SER  | 4.9  |
| 1   | F     | 60   | THR  | 4.9  |
| 1   | D     | 32   | VAL  | 4.9  |
| 1   | B     | 697  | LEU  | 4.9  |
| 1   | E     | 362  | PHE  | 4.9  |
| 1   | D     | 141  | GLY  | 4.9  |
| 1   | E     | 590  | VAL  | 4.8  |
| 1   | F     | 129  | VAL  | 4.8  |
| 1   | E     | 366  | LEU  | 4.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 939  | LEU  | 4.8  |
| 1   | F     | 443  | VAL  | 4.8  |
| 1   | D     | 68   | ASN  | 4.8  |
| 1   | D     | 330  | THR  | 4.8  |
| 1   | D     | 112  | GLN  | 4.8  |
| 1   | F     | 473  | THR  | 4.8  |
| 1   | B     | 830  | LYS  | 4.7  |
| 1   | E     | 198  | LEU  | 4.7  |
| 1   | C     | 833  | GLY  | 4.7  |
| 1   | F     | 879  | VAL  | 4.7  |
| 1   | B     | 108  | GLN  | 4.7  |
| 1   | D     | 411  | VAL  | 4.7  |
| 1   | E     | 484  | VAL  | 4.7  |
| 1   | D     | 487  | ILE  | 4.6  |
| 1   | E     | 483  | LEU  | 4.6  |
| 1   | A     | 407  | ASP  | 4.6  |
| 1   | C     | 713  | PRO  | 4.6  |
| 1   | E     | 291  | ILE  | 4.6  |
| 1   | A     | 1008 | THR  | 4.6  |
| 1   | C     | 79   | SER  | 4.6  |
| 1   | C     | 936  | ASN  | 4.6  |
| 1   | D     | 323  | ILE  | 4.6  |
| 1   | F     | 467  | TYR  | 4.6  |
| 1   | B     | 656  | ALA  | 4.6  |
| 1   | F     | 362  | PHE  | 4.6  |
| 1   | F     | 408  | ASP  | 4.6  |
| 1   | C     | 706  | ASP  | 4.6  |
| 1   | C     | 473  | THR  | 4.5  |
| 1   | F     | 883  | LEU  | 4.5  |
| 1   | F     | 670  | GLY  | 4.5  |
| 1   | E     | 107  | VAL  | 4.5  |
| 1   | E     | 1010 | THR  | 4.5  |
| 1   | E     | 369  | THR  | 4.5  |
| 1   | D     | 684  | GLY  | 4.5  |
| 1   | A     | 974  | SER  | 4.5  |
| 1   | A     | 368  | PRO  | 4.5  |
| 1   | A     | 401  | ALA  | 4.4  |
| 1   | A     | 578  | LEU  | 4.4  |
| 1   | B     | 700  | GLU  | 4.4  |
| 1   | F     | 713  | PRO  | 4.4  |
| 1   | D     | 714  | ASN  | 4.4  |
| 1   | C     | 863  | LEU  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 128  | SER  | 4.4  |
| 1   | A     | 376  | LEU  | 4.4  |
| 1   | E     | 443  | VAL  | 4.4  |
| 1   | F     | 116  | PRO  | 4.4  |
| 1   | F     | 706  | ASP  | 4.4  |
| 1   | B     | 864  | SER  | 4.3  |
| 1   | F     | 485  | ALA  | 4.3  |
| 1   | D     | 849  | GLY  | 4.3  |
| 1   | B     | 282  | ASN  | 4.3  |
| 1   | F     | 48   | SER  | 4.3  |
| 1   | E     | 313  | MET  | 4.3  |
| 1   | A     | 486  | LEU  | 4.3  |
| 1   | B     | 696  | GLN  | 4.3  |
| 1   | C     | 323  | ILE  | 4.3  |
| 1   | F     | 824  | GLY  | 4.3  |
| 1   | C     | 314  | GLU  | 4.3  |
| 1   | E     | 348  | ILE  | 4.3  |
| 1   | A     | 127  | VAL  | 4.2  |
| 1   | E     | 669  | LEU  | 4.2  |
| 1   | D     | 575  | MET  | 4.2  |
| 1   | D     | 874  | ILE  | 4.2  |
| 1   | C     | 127  | VAL  | 4.2  |
| 1   | F     | 282  | ASN  | 4.2  |
| 1   | C     | 444  | GLY  | 4.2  |
| 1   | D     | 610  | PHE  | 4.2  |
| 1   | E     | 1006 | MET  | 4.2  |
| 1   | A     | 15   | ILE  | 4.1  |
| 1   | E     | 621  | ILE  | 4.1  |
| 1   | F     | 402  | ILE  | 4.1  |
| 1   | B     | 710  | SER  | 4.1  |
| 1   | A     | 397  | GLY  | 4.1  |
| 1   | D     | 682  | GLN  | 4.1  |
| 1   | F     | 868  | ALA  | 4.1  |
| 1   | E     | 402  | ILE  | 4.1  |
| 1   | C     | 64   | VAL  | 4.1  |
| 1   | E     | 46   | SER  | 4.1  |
| 1   | F     | 829  | GLY  | 4.1  |
| 1   | E     | 404  | LEU  | 4.1  |
| 1   | E     | 924  | VAL  | 4.1  |
| 1   | C     | 442  | LEU  | 4.1  |
| 1   | D     | 110  | LYS  | 4.1  |
| 1   | F     | 357  | LEU  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 848  | THR  | 4.1  |
| 1   | C     | 16   | ALA  | 4.1  |
| 1   | F     | 864  | SER  | 4.1  |
| 1   | D     | 784  | TRP  | 4.0  |
| 1   | E     | 282  | ASN  | 4.0  |
| 1   | E     | 463  | THR  | 4.0  |
| 1   | D     | 178  | PHE  | 4.0  |
| 1   | B     | 447  | MET  | 4.0  |
| 1   | E     | 1013 | ALA  | 4.0  |
| 1   | A     | 405  | LEU  | 4.0  |
| 1   | D     | 681  | ASP  | 4.0  |
| 1   | C     | 474  | ILE  | 4.0  |
| 1   | B     | 67   | GLN  | 4.0  |
| 1   | F     | 589  | LYS  | 4.0  |
| 1   | E     | 990  | ALA  | 4.0  |
| 1   | D     | 408  | ASP  | 4.0  |
| 1   | C     | 68   | ASN  | 4.0  |
| 1   | D     | 870  | SER  | 3.9  |
| 1   | D     | 371  | ALA  | 3.9  |
| 1   | D     | 400  | LEU  | 3.9  |
| 1   | A     | 410  | ILE  | 3.9  |
| 1   | A     | 339  | GLU  | 3.9  |
| 1   | E     | 308  | ALA  | 3.9  |
| 1   | E     | 353  | LEU  | 3.9  |
| 1   | E     | 400  | LEU  | 3.9  |
| 1   | F     | 68   | ASN  | 3.9  |
| 1   | F     | 369  | THR  | 3.9  |
| 1   | F     | 503  | GLY  | 3.9  |
| 1   | B     | 701  | ALA  | 3.9  |
| 1   | D     | 656  | ALA  | 3.9  |
| 1   | B     | 848  | THR  | 3.8  |
| 1   | C     | 784  | TRP  | 3.8  |
| 1   | C     | 65   | ILE  | 3.8  |
| 1   | F     | 112  | GLN  | 3.8  |
| 1   | E     | 975  | LEU  | 3.8  |
| 1   | E     | 1009 | ALA  | 3.8  |
| 1   | D     | 621  | ILE  | 3.8  |
| 1   | E     | 462  | SER  | 3.8  |
| 1   | F     | 445  | ILE  | 3.8  |
| 1   | C     | 866  | ASN  | 3.8  |
| 1   | D     | 136  | PHE  | 3.8  |
| 1   | F     | 396  | PHE  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 18   | ILE  | 3.8  |
| 1   | B     | 113  | LEU  | 3.8  |
| 1   | F     | 712  | ARG  | 3.7  |
| 1   | E     | 370  | ILE  | 3.7  |
| 1   | C     | 394  | THR  | 3.7  |
| 1   | F     | 707  | MET  | 3.7  |
| 1   | A     | 463  | THR  | 3.7  |
| 1   | D     | 128  | SER  | 3.7  |
| 1   | E     | 65   | ILE  | 3.7  |
| 1   | C     | 502  | LYS  | 3.7  |
| 1   | A     | 403  | GLY  | 3.7  |
| 1   | F     | 446  | ALA  | 3.7  |
| 1   | B     | 400  | LEU  | 3.7  |
| 1   | F     | 826  | ALA  | 3.7  |
| 1   | F     | 65   | ILE  | 3.7  |
| 1   | B     | 406  | VAL  | 3.7  |
| 1   | D     | 113  | LEU  | 3.6  |
| 1   | F     | 356  | TYR  | 3.6  |
| 1   | E     | 333  | VAL  | 3.6  |
| 1   | E     | 1011 | VAL  | 3.6  |
| 1   | F     | 373  | PRO  | 3.6  |
| 1   | E     | 111  | LEU  | 3.6  |
| 1   | F     | 118  | LEU  | 3.6  |
| 1   | E     | 935  | LYS  | 3.6  |
| 1   | B     | 107  | VAL  | 3.6  |
| 1   | C     | 939  | LEU  | 3.6  |
| 1   | B     | 575  | MET  | 3.6  |
| 1   | F     | 850  | VAL  | 3.6  |
| 1   | A     | 327  | TYR  | 3.6  |
| 1   | C     | 400  | LEU  | 3.6  |
| 1   | C     | 829  | GLY  | 3.6  |
| 1   | F     | 45   | ILE  | 3.6  |
| 1   | E     | 989  | GLY  | 3.6  |
| 1   | C     | 67   | GLN  | 3.5  |
| 1   | D     | 406  | VAL  | 3.5  |
| 1   | E     | 936  | ASN  | 3.5  |
| 1   | E     | 920  | VAL  | 3.5  |
| 1   | D     | 458  | PHE  | 3.5  |
| 1   | C     | 390  | ILE  | 3.5  |
| 1   | E     | 105  | VAL  | 3.5  |
| 1   | B     | 316  | PHE  | 3.5  |
| 1   | C     | 823  | LEU  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 929  | THR  | 3.5  |
| 1   | E     | 317  | PHE  | 3.5  |
| 1   | F     | 1012 | LEU  | 3.5  |
| 1   | B     | 311  | ALA  | 3.5  |
| 1   | C     | 935  | LYS  | 3.5  |
| 1   | C     | 129  | VAL  | 3.5  |
| 1   | E     | 322  | LYS  | 3.5  |
| 1   | C     | 69   | MET  | 3.5  |
| 1   | A     | 593  | GLU  | 3.5  |
| 1   | B     | 410  | ILE  | 3.5  |
| 1   | F     | 871  | LEU  | 3.5  |
| 1   | D     | 78   | MET  | 3.5  |
| 1   | B     | 145  | THR  | 3.5  |
| 1   | E     | 882  | CYS  | 3.4  |
| 1   | E     | 283  | GLY  | 3.4  |
| 1   | D     | 401  | ALA  | 3.4  |
| 1   | C     | 867  | GLN  | 3.4  |
| 1   | E     | 108  | GLN  | 3.4  |
| 1   | E     | 194  | ASN  | 3.4  |
| 1   | B     | 683  | ALA  | 3.4  |
| 1   | F     | 834  | GLU  | 3.4  |
| 1   | C     | 388  | PHE  | 3.4  |
| 1   | E     | 712  | ARG  | 3.4  |
| 1   | A     | 574  | THR  | 3.4  |
| 1   | C     | 860  | GLN  | 3.4  |
| 1   | E     | 398  | MET  | 3.4  |
| 1   | E     | 357  | LEU  | 3.4  |
| 1   | C     | 480  | LEU  | 3.4  |
| 1   | E     | 977  | PHE  | 3.4  |
| 1   | F     | 198  | LEU  | 3.4  |
| 1   | C     | 656  | ALA  | 3.4  |
| 1   | A     | 933  | SER  | 3.4  |
| 1   | D     | 576  | VAL  | 3.3  |
| 1   | D     | 15   | ILE  | 3.3  |
| 1   | D     | 92   | LEU  | 3.3  |
| 1   | C     | 116  | PRO  | 3.3  |
| 1   | F     | 939  | LEU  | 3.3  |
| 1   | E     | 673  | THR  | 3.3  |
| 1   | F     | 444  | GLY  | 3.3  |
| 1   | F     | 197  | GLN  | 3.3  |
| 1   | F     | 867  | GLN  | 3.3  |
| 1   | C     | 374  | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 390  | ILE  | 3.3  |
| 1   | A     | 467  | TYR  | 3.3  |
| 1   | F     | 179  | GLY  | 3.3  |
| 1   | D     | 405  | LEU  | 3.3  |
| 1   | D     | 623  | PHE  | 3.3  |
| 1   | F     | 575  | MET  | 3.3  |
| 1   | D     | 479  | ALA  | 3.3  |
| 1   | A     | 406  | VAL  | 3.3  |
| 1   | B     | 322  | LYS  | 3.3  |
| 1   | F     | 708  | LEU  | 3.3  |
| 1   | D     | 210  | GLN  | 3.3  |
| 1   | C     | 322  | LYS  | 3.3  |
| 1   | F     | 176  | GLN  | 3.3  |
| 1   | E     | 48   | SER  | 3.3  |
| 1   | C     | 38   | ILE  | 3.3  |
| 1   | B     | 881  | LEU  | 3.2  |
| 1   | A     | 411  | VAL  | 3.2  |
| 1   | A     | 365  | THR  | 3.2  |
| 1   | D     | 369  | THR  | 3.2  |
| 1   | C     | 448  | VAL  | 3.2  |
| 1   | A     | 1012 | LEU  | 3.2  |
| 1   | D     | 317  | PHE  | 3.2  |
| 1   | D     | 482  | VAL  | 3.2  |
| 1   | C     | 395  | MET  | 3.2  |
| 1   | F     | 466  | ILE  | 3.2  |
| 1   | C     | 407  | ASP  | 3.2  |
| 1   | F     | 462  | SER  | 3.2  |
| 1   | E     | 931  | GLY  | 3.2  |
| 1   | F     | 478  | MET  | 3.2  |
| 1   | A     | 13   | TRP  | 3.2  |
| 1   | A     | 398  | MET  | 3.2  |
| 1   | B     | 44   | THR  | 3.2  |
| 1   | D     | 783  | ASP  | 3.2  |
| 1   | D     | 609  | VAL  | 3.2  |
| 1   | A     | 390  | ILE  | 3.2  |
| 1   | B     | 488  | LEU  | 3.2  |
| 1   | E     | 33   | ALA  | 3.2  |
| 1   | A     | 353  | LEU  | 3.2  |
| 1   | C     | 449  | LEU  | 3.2  |
| 1   | D     | 972  | MET  | 3.2  |
| 1   | B     | 408  | ASP  | 3.2  |
| 1   | D     | 483  | LEU  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 404 | LEU  | 3.1  |
| 1   | A     | 69  | MET  | 3.1  |
| 1   | D     | 281 | PHE  | 3.1  |
| 1   | D     | 66  | GLU  | 3.1  |
| 1   | E     | 109 | ASN  | 3.1  |
| 1   | D     | 657 | MET  | 3.1  |
| 1   | F     | 281 | PHE  | 3.1  |
| 1   | C     | 834 | GLU  | 3.1  |
| 1   | F     | 484 | VAL  | 3.1  |
| 1   | C     | 330 | THR  | 3.1  |
| 1   | D     | 36  | PRO  | 3.1  |
| 1   | E     | 126 | GLY  | 3.1  |
| 1   | B     | 198 | LEU  | 3.1  |
| 1   | B     | 443 | VAL  | 3.1  |
| 1   | D     | 866 | ASN  | 3.1  |
| 1   | C     | 307 | ARG  | 3.1  |
| 1   | F     | 869 | PRO  | 3.1  |
| 1   | F     | 453 | PHE  | 3.1  |
| 1   | D     | 109 | ASN  | 3.1  |
| 1   | B     | 65  | ILE  | 3.1  |
| 1   | D     | 130 | GLU  | 3.1  |
| 1   | E     | 465 | ALA  | 3.1  |
| 1   | E     | 969 | PRO  | 3.1  |
| 1   | A     | 573 | MET  | 3.1  |
| 1   | A     | 902 | LEU  | 3.1  |
| 1   | E     | 316 | PHE  | 3.1  |
| 1   | F     | 801 | SER  | 3.1  |
| 1   | E     | 896 | VAL  | 3.1  |
| 1   | E     | 78  | MET  | 3.1  |
| 1   | A     | 408 | ASP  | 3.0  |
| 1   | E     | 59  | ASP  | 3.0  |
| 1   | E     | 112 | GLN  | 3.0  |
| 1   | E     | 593 | GLU  | 3.0  |
| 1   | D     | 321 | LEU  | 3.0  |
| 1   | E     | 674 | GLY  | 3.0  |
| 1   | B     | 46  | SER  | 3.0  |
| 1   | C     | 109 | ASN  | 3.0  |
| 1   | B     | 308 | ALA  | 3.0  |
| 1   | E     | 899 | VAL  | 3.0  |
| 1   | D     | 114 | ALA  | 3.0  |
| 1   | E     | 323 | ILE  | 3.0  |
| 1   | F     | 64  | VAL  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 355  | MET  | 3.0  |
| 1   | F     | 355  | MET  | 3.0  |
| 1   | B     | 127  | VAL  | 3.0  |
| 1   | E     | 104  | GLN  | 3.0  |
| 1   | B     | 11   | PHE  | 3.0  |
| 1   | D     | 403  | GLY  | 3.0  |
| 1   | D     | 865  | GLY  | 3.0  |
| 1   | A     | 481  | SER  | 3.0  |
| 1   | B     | 45   | ILE  | 3.0  |
| 1   | F     | 400  | LEU  | 3.0  |
| 1   | D     | 12   | ALA  | 3.0  |
| 1   | C     | 885  | ALA  | 3.0  |
| 1   | B     | 112  | GLN  | 3.0  |
| 1   | B     | 834  | GLU  | 3.0  |
| 1   | D     | 715  | GLY  | 2.9  |
| 1   | D     | 59   | ASP  | 2.9  |
| 1   | A     | 579  | PRO  | 2.9  |
| 1   | F     | 656  | ALA  | 2.9  |
| 1   | D     | 463  | THR  | 2.9  |
| 1   | F     | 110  | LYS  | 2.9  |
| 1   | C     | 712  | ARG  | 2.9  |
| 1   | C     | 883  | LEU  | 2.9  |
| 1   | F     | 117  | LEU  | 2.9  |
| 1   | B     | 177  | LEU  | 2.9  |
| 1   | E     | 473  | THR  | 2.9  |
| 1   | F     | 594  | VAL  | 2.9  |
| 1   | E     | 579  | PRO  | 2.9  |
| 1   | E     | 44   | THR  | 2.9  |
| 1   | A     | 354  | VAL  | 2.9  |
| 1   | C     | 494  | ALA  | 2.9  |
| 1   | A     | 661  | PHE  | 2.9  |
| 1   | C     | 96   | SER  | 2.9  |
| 1   | C     | 397  | GLY  | 2.9  |
| 1   | C     | 310  | LEU  | 2.9  |
| 1   | C     | 399  | VAL  | 2.9  |
| 1   | F     | 1011 | VAL  | 2.9  |
| 1   | F     | 470  | PHE  | 2.9  |
| 1   | C     | 1006 | MET  | 2.9  |
| 1   | E     | 938  | ILE  | 2.9  |
| 1   | D     | 796  | PHE  | 2.9  |
| 1   | F     | 9    | PRO  | 2.9  |
| 1   | B     | 251  | LEU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 393  | LEU  | 2.9  |
| 1   | D     | 797  | SER  | 2.9  |
| 1   | F     | 13   | TRP  | 2.9  |
| 1   | F     | 784  | TRP  | 2.9  |
| 1   | F     | 1016 | PHE  | 2.9  |
| 1   | B     | 1013 | ALA  | 2.9  |
| 1   | D     | 292  | LYS  | 2.9  |
| 1   | D     | 33   | ALA  | 2.8  |
| 1   | E     | 798  | ALA  | 2.8  |
| 1   | C     | 113  | LEU  | 2.8  |
| 1   | A     | 1007 | VAL  | 2.8  |
| 1   | F     | 399  | VAL  | 2.8  |
| 1   | A     | 145  | THR  | 2.8  |
| 1   | E     | 541  | TYR  | 2.8  |
| 1   | F     | 932  | LEU  | 2.8  |
| 1   | D     | 372  | VAL  | 2.8  |
| 1   | A     | 195  | LYS  | 2.8  |
| 1   | F     | 935  | LYS  | 2.8  |
| 1   | B     | 801  | SER  | 2.8  |
| 1   | F     | 67   | GLN  | 2.8  |
| 1   | E     | 14   | VAL  | 2.8  |
| 1   | E     | 325  | TYR  | 2.8  |
| 1   | C     | 111  | LEU  | 2.8  |
| 1   | D     | 351  | VAL  | 2.8  |
| 1   | E     | 1016 | PHE  | 2.8  |
| 1   | B     | 573  | MET  | 2.8  |
| 1   | D     | 854  | TRP  | 2.8  |
| 1   | C     | 799  | PHE  | 2.8  |
| 1   | C     | 373  | PRO  | 2.8  |
| 1   | E     | 676  | ASP  | 2.8  |
| 1   | F     | 827  | ALA  | 2.8  |
| 1   | E     | 803  | ARG  | 2.8  |
| 1   | F     | 861  | GLU  | 2.8  |
| 1   | F     | 409  | ALA  | 2.8  |
| 1   | F     | 591  | LEU  | 2.8  |
| 1   | A     | 977  | PHE  | 2.8  |
| 1   | C     | 462  | SER  | 2.8  |
| 1   | C     | 478  | MET  | 2.8  |
| 1   | C     | 786  | VAL  | 2.8  |
| 1   | C     | 300  | LEU  | 2.8  |
| 1   | A     | 386  | PHE  | 2.8  |
| 1   | D     | 324  | VAL  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 828  | PRO  | 2.8  |
| 1   | A     | 383  | LEU  | 2.7  |
| 1   | C     | 372  | VAL  | 2.7  |
| 1   | E     | 1015 | PHE  | 2.7  |
| 1   | B     | 394  | THR  | 2.7  |
| 1   | D     | 200  | PRO  | 2.7  |
| 1   | E     | 395  | MET  | 2.7  |
| 1   | D     | 622  | ALA  | 2.7  |
| 1   | F     | 246  | PHE  | 2.7  |
| 1   | A     | 577  | GLN  | 2.7  |
| 1   | A     | 971  | LEU  | 2.7  |
| 1   | D     | 14   | VAL  | 2.7  |
| 1   | F     | 108  | GLN  | 2.7  |
| 1   | D     | 396  | PHE  | 2.7  |
| 1   | C     | 376  | LEU  | 2.7  |
| 1   | E     | 591  | LEU  | 2.7  |
| 1   | A     | 487  | ILE  | 2.7  |
| 1   | A     | 874  | ILE  | 2.7  |
| 1   | F     | 726  | ILE  | 2.7  |
| 1   | D     | 11   | PHE  | 2.7  |
| 1   | E     | 145  | THR  | 2.7  |
| 1   | F     | 675  | PHE  | 2.7  |
| 1   | A     | 658  | VAL  | 2.7  |
| 1   | B     | 369  | THR  | 2.7  |
| 1   | B     | 854  | TRP  | 2.7  |
| 1   | A     | 970  | ILE  | 2.7  |
| 1   | F     | 863  | LEU  | 2.7  |
| 1   | A     | 281  | PHE  | 2.7  |
| 1   | A     | 1011 | VAL  | 2.7  |
| 1   | F     | 576  | VAL  | 2.7  |
| 1   | A     | 322  | LYS  | 2.7  |
| 1   | E     | 1007 | VAL  | 2.7  |
| 1   | B     | 934  | ALA  | 2.7  |
| 1   | B     | 110  | LYS  | 2.7  |
| 1   | E     | 45   | ILE  | 2.7  |
| 1   | E     | 401  | ALA  | 2.7  |
| 1   | B     | 407  | ASP  | 2.7  |
| 1   | B     | 711  | VAL  | 2.7  |
| 1   | E     | 280  | GLU  | 2.7  |
| 1   | A     | 630  | ALA  | 2.7  |
| 1   | B     | 798  | ALA  | 2.7  |
| 1   | C     | 17   | ILE  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 92  | LEU  | 2.6  |
| 1   | D     | 391 | ASN  | 2.6  |
| 1   | F     | 188 | MET  | 2.6  |
| 1   | C     | 446 | ALA  | 2.6  |
| 1   | D     | 973 | THR  | 2.6  |
| 1   | A     | 336 | SER  | 2.6  |
| 1   | D     | 831 | SER  | 2.6  |
| 1   | C     | 210 | GLN  | 2.6  |
| 1   | F     | 590 | VAL  | 2.6  |
| 1   | F     | 786 | VAL  | 2.6  |
| 1   | A     | 785 | TYR  | 2.6  |
| 1   | B     | 699 | ALA  | 2.6  |
| 1   | A     | 107 | VAL  | 2.6  |
| 1   | A     | 70  | ASN  | 2.6  |
| 1   | E     | 47  | ALA  | 2.6  |
| 1   | D     | 368 | PRO  | 2.6  |
| 1   | A     | 590 | VAL  | 2.6  |
| 1   | E     | 66  | GLU  | 2.6  |
| 1   | E     | 447 | MET  | 2.6  |
| 1   | F     | 657 | MET  | 2.6  |
| 1   | A     | 666 | ILE  | 2.6  |
| 1   | A     | 714 | ASN  | 2.6  |
| 1   | B     | 785 | TYR  | 2.6  |
| 1   | D     | 579 | PRO  | 2.6  |
| 1   | A     | 357 | LEU  | 2.6  |
| 1   | F     | 976 | ALA  | 2.6  |
| 1   | A     | 374 | VAL  | 2.6  |
| 1   | D     | 173 | GLY  | 2.6  |
| 1   | C     | 932 | LEU  | 2.6  |
| 1   | E     | 290 | GLY  | 2.6  |
| 1   | A     | 449 | LEU  | 2.6  |
| 1   | A     | 876 | LEU  | 2.6  |
| 1   | E     | 577 | GLN  | 2.6  |
| 1   | A     | 315 | PRO  | 2.6  |
| 1   | C     | 828 | PRO  | 2.6  |
| 1   | D     | 69  | MET  | 2.6  |
| 1   | D     | 445 | ILE  | 2.6  |
| 1   | E     | 697 | LEU  | 2.6  |
| 1   | E     | 246 | PHE  | 2.6  |
| 1   | E     | 164 | ASP  | 2.6  |
| 1   | D     | 786 | VAL  | 2.6  |
| 1   | F     | 674 | GLY  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 851  | GLY  | 2.6  |
| 1   | E     | 113  | LEU  | 2.6  |
| 1   | E     | 599  | LEU  | 2.6  |
| 1   | F     | 1010 | THR  | 2.6  |
| 1   | D     | 713  | PRO  | 2.6  |
| 1   | A     | 834  | GLU  | 2.5  |
| 1   | C     | 97   | GLY  | 2.5  |
| 1   | F     | 403  | GLY  | 2.5  |
| 1   | C     | 369  | THR  | 2.5  |
| 1   | F     | 352  | PHE  | 2.5  |
| 1   | D     | 43   | VAL  | 2.5  |
| 1   | F     | 370  | ILE  | 2.5  |
| 1   | B     | 786  | VAL  | 2.5  |
| 1   | B     | 12   | ALA  | 2.5  |
| 1   | B     | 91   | THR  | 2.5  |
| 1   | D     | 37   | THR  | 2.5  |
| 1   | E     | 587  | THR  | 2.5  |
| 1   | B     | 882  | CYS  | 2.5  |
| 1   | A     | 33   | ALA  | 2.5  |
| 1   | E     | 793  | MET  | 2.5  |
| 1   | A     | 12   | ALA  | 2.5  |
| 1   | B     | 188  | MET  | 2.5  |
| 1   | E     | 130  | GLU  | 2.5  |
| 1   | A     | 129  | VAL  | 2.5  |
| 1   | D     | 290  | GLY  | 2.5  |
| 1   | F     | 488  | LEU  | 2.5  |
| 1   | E     | 331  | PRO  | 2.5  |
| 1   | A     | 877  | ILE  | 2.5  |
| 1   | B     | 666  | ILE  | 2.5  |
| 1   | C     | 575  | MET  | 2.5  |
| 1   | D     | 447  | MET  | 2.5  |
| 1   | E     | 711  | VAL  | 2.5  |
| 1   | E     | 988  | THR  | 2.5  |
| 1   | A     | 485  | ALA  | 2.5  |
| 1   | F     | 376  | LEU  | 2.5  |
| 1   | D     | 412  | VAL  | 2.4  |
| 1   | F     | 899  | VAL  | 2.4  |
| 1   | D     | 50   | PRO  | 2.4  |
| 1   | E     | 197  | GLN  | 2.4  |
| 1   | F     | 164  | ASP  | 2.4  |
| 1   | D     | 46   | SER  | 2.4  |
| 1   | A     | 198  | LEU  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 290  | GLY  | 2.4  |
| 1   | C     | 441  | ALA  | 2.4  |
| 1   | D     | 877  | ILE  | 2.4  |
| 1   | E     | 63   | GLN  | 2.4  |
| 1   | D     | 376  | LEU  | 2.4  |
| 1   | B     | 409  | ALA  | 2.4  |
| 1   | D     | 815  | ASN  | 2.4  |
| 1   | D     | 778  | PRO  | 2.4  |
| 1   | F     | 676  | ASP  | 2.4  |
| 1   | D     | 34   | GLN  | 2.4  |
| 1   | A     | 196  | PHE  | 2.4  |
| 1   | A     | 321  | LEU  | 2.4  |
| 1   | E     | 489  | THR  | 2.4  |
| 1   | A     | 761  | GLY  | 2.4  |
| 1   | F     | 162  | MET  | 2.4  |
| 1   | D     | 409  | ALA  | 2.4  |
| 1   | B     | 355  | MET  | 2.4  |
| 1   | F     | 711  | VAL  | 2.4  |
| 1   | A     | 334  | LYS  | 2.4  |
| 1   | E     | 367  | ILE  | 2.4  |
| 1   | E     | 881  | LEU  | 2.4  |
| 1   | A     | 67   | GLN  | 2.4  |
| 1   | B     | 450  | SER  | 2.4  |
| 1   | D     | 845  | LYS  | 2.4  |
| 1   | F     | 860  | GLN  | 2.4  |
| 1   | D     | 611  | ALA  | 2.4  |
| 1   | F     | 3    | ASN  | 2.4  |
| 1   | F     | 16   | ALA  | 2.4  |
| 1   | B     | 411  | VAL  | 2.4  |
| 1   | D     | 763  | VAL  | 2.4  |
| 1   | E     | 43   | VAL  | 2.4  |
| 1   | F     | 69   | MET  | 2.4  |
| 1   | F     | 395  | MET  | 2.4  |
| 1   | A     | 19   | ILE  | 2.4  |
| 1   | B     | 591  | LEU  | 2.4  |
| 1   | D     | 392  | THR  | 2.4  |
| 1   | B     | 43   | VAL  | 2.3  |
| 1   | C     | 14   | VAL  | 2.3  |
| 1   | C     | 782  | GLY  | 2.3  |
| 1   | E     | 966  | ARG  | 2.3  |
| 1   | E     | 1017 | VAL  | 2.3  |
| 1   | E     | 281  | PHE  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 348 | ILE  | 2.3  |
| 1   | B     | 371 | ALA  | 2.3  |
| 1   | C     | 797 | SER  | 2.3  |
| 1   | C     | 350 | LEU  | 2.3  |
| 1   | D     | 72  | ILE  | 2.3  |
| 1   | E     | 796 | PHE  | 2.3  |
| 1   | A     | 164 | ASP  | 2.3  |
| 1   | D     | 19  | ILE  | 2.3  |
| 1   | D     | 383 | LEU  | 2.3  |
| 1   | B     | 802 | SER  | 2.3  |
| 1   | D     | 977 | PHE  | 2.3  |
| 1   | E     | 713 | PRO  | 2.3  |
| 1   | F     | 563 | PHE  | 2.3  |
| 1   | B     | 542 | LEU  | 2.3  |
| 1   | B     | 975 | LEU  | 2.3  |
| 1   | E     | 328 | ASP  | 2.3  |
| 1   | C     | 973 | THR  | 2.3  |
| 1   | E     | 303 | ALA  | 2.3  |
| 1   | F     | 61  | VAL  | 2.3  |
| 1   | F     | 458 | PHE  | 2.3  |
| 1   | D     | 932 | LEU  | 2.3  |
| 1   | E     | 92  | LEU  | 2.3  |
| 1   | E     | 795 | PRO  | 2.3  |
| 1   | A     | 14  | VAL  | 2.3  |
| 1   | D     | 833 | GLY  | 2.3  |
| 1   | F     | 170 | SER  | 2.3  |
| 1   | C     | 970 | ILE  | 2.3  |
| 1   | A     | 399 | VAL  | 2.3  |
| 1   | E     | 737 | SER  | 2.3  |
| 1   | E     | 801 | SER  | 2.3  |
| 1   | D     | 107 | VAL  | 2.3  |
| 1   | D     | 129 | VAL  | 2.3  |
| 1   | E     | 878 | VAL  | 2.3  |
| 1   | D     | 832 | THR  | 2.3  |
| 1   | B     | 404 | LEU  | 2.3  |
| 1   | D     | 573 | MET  | 2.3  |
| 1   | E     | 486 | LEU  | 2.3  |
| 1   | C     | 128 | SER  | 2.3  |
| 1   | F     | 477 | ALA  | 2.3  |
| 1   | B     | 486 | LEU  | 2.2  |
| 1   | E     | 714 | ASN  | 2.2  |
| 1   | A     | 36  | PRO  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 470  | PHE  | 2.2  |
| 1   | E     | 630  | ALA  | 2.2  |
| 1   | C     | 685  | LEU  | 2.2  |
| 1   | D     | 398  | MET  | 2.2  |
| 1   | A     | 370  | ILE  | 2.2  |
| 1   | D     | 1014 | ILE  | 2.2  |
| 1   | E     | 728  | GLN  | 2.2  |
| 1   | F     | 251  | LEU  | 2.2  |
| 1   | F     | 480  | LEU  | 2.2  |
| 1   | A     | 351  | VAL  | 2.2  |
| 1   | B     | 865  | GLY  | 2.2  |
| 1   | D     | 696  | GLN  | 2.2  |
| 1   | F     | 280  | GLU  | 2.2  |
| 1   | A     | 591  | LEU  | 2.2  |
| 1   | A     | 975  | LEU  | 2.2  |
| 1   | B     | 405  | LEU  | 2.2  |
| 1   | F     | 902  | LEU  | 2.2  |
| 1   | D     | 334  | LYS  | 2.2  |
| 1   | F     | 577  | GLN  | 2.2  |
| 1   | C     | 389  | SER  | 2.2  |
| 1   | F     | 797  | SER  | 2.2  |
| 1   | F     | 802  | SER  | 2.2  |
| 1   | C     | 611  | ALA  | 2.2  |
| 1   | A     | 657  | MET  | 2.2  |
| 1   | A     | 762  | ARG  | 2.2  |
| 1   | A     | 797  | SER  | 2.2  |
| 1   | D     | 315  | PRO  | 2.2  |
| 1   | A     | 898  | LEU  | 2.2  |
| 1   | D     | 817  | LEU  | 2.2  |
| 1   | E     | 971  | LEU  | 2.2  |
| 1   | C     | 610  | PHE  | 2.2  |
| 1   | B     | 72   | ILE  | 2.2  |
| 1   | E     | 397  | GLY  | 2.2  |
| 1   | D     | 823  | LEU  | 2.2  |
| 1   | B     | 970  | ILE  | 2.2  |
| 1   | D     | 134  | SER  | 2.2  |
| 1   | A     | 483  | LEU  | 2.2  |
| 1   | C     | 33   | ALA  | 2.2  |
| 1   | E     | 611  | ALA  | 2.2  |
| 1   | F     | 366  | LEU  | 2.2  |
| 1   | B     | 847  | PRO  | 2.2  |
| 1   | A     | 382  | VAL  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 18  | ILE  | 2.2  |
| 1   | B     | 392 | THR  | 2.2  |
| 1   | D     | 127 | VAL  | 2.2  |
| 1   | D     | 574 | THR  | 2.2  |
| 1   | B     | 784 | TRP  | 2.2  |
| 1   | B     | 846 | LEU  | 2.2  |
| 1   | B     | 939 | LEU  | 2.2  |
| 1   | F     | 163 | LYS  | 2.2  |
| 1   | C     | 349 | ILE  | 2.2  |
| 1   | E     | 438 | ILE  | 2.2  |
| 1   | E     | 609 | VAL  | 2.2  |
| 1   | D     | 485 | ALA  | 2.1  |
| 1   | E     | 347 | ALA  | 2.1  |
| 1   | C     | 623 | PHE  | 2.1  |
| 1   | C     | 977 | PHE  | 2.1  |
| 1   | F     | 933 | SER  | 2.1  |
| 1   | E     | 589 | LYS  | 2.1  |
| 1   | A     | 194 | ASN  | 2.1  |
| 1   | D     | 388 | PHE  | 2.1  |
| 1   | B     | 658 | VAL  | 2.1  |
| 1   | E     | 831 | SER  | 2.1  |
| 1   | C     | 669 | LEU  | 2.1  |
| 1   | D     | 442 | LEU  | 2.1  |
| 1   | E     | 193 | LEU  | 2.1  |
| 1   | A     | 934 | ALA  | 2.1  |
| 1   | C     | 796 | PHE  | 2.1  |
| 1   | D     | 762 | ARG  | 2.1  |
| 1   | A     | 43  | VAL  | 2.1  |
| 1   | D     | 738 | ILE  | 2.1  |
| 1   | F     | 565 | PRO  | 2.1  |
| 1   | C     | 501 | ALA  | 2.1  |
| 1   | D     | 348 | ILE  | 2.1  |
| 1   | B     | 79  | SER  | 2.1  |
| 1   | C     | 315 | PRO  | 2.1  |
| 1   | A     | 32  | VAL  | 2.1  |
| 1   | C     | 658 | VAL  | 2.1  |
| 1   | C     | 974 | SER  | 2.1  |
| 1   | F     | 322 | LYS  | 2.1  |
| 1   | A     | 623 | PHE  | 2.1  |
| 1   | B     | 246 | PHE  | 2.1  |
| 1   | D     | 785 | TYR  | 2.1  |
| 1   | E     | 374 | VAL  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 678  | GLU  | 2.1  |
| 1   | A     | 472  | ILE  | 2.1  |
| 1   | F     | 940  | ILE  | 2.1  |
| 1   | C     | 634  | GLY  | 2.1  |
| 1   | E     | 492  | LEU  | 2.1  |
| 1   | D     | 795  | PRO  | 2.1  |
| 1   | A     | 611  | ALA  | 2.1  |
| 1   | A     | 45   | ILE  | 2.1  |
| 1   | C     | 291  | ILE  | 2.1  |
| 1   | C     | 35   | TYR  | 2.1  |
| 1   | F     | 621  | ILE  | 2.1  |
| 1   | B     | 657  | MET  | 2.1  |
| 1   | C     | 577  | GLN  | 2.1  |
| 1   | E     | 11   | PHE  | 2.1  |
| 1   | A     | 622  | ALA  | 2.1  |
| 1   | A     | 831  | SER  | 2.1  |
| 1   | D     | 724  | ILE  | 2.1  |
| 1   | E     | 653  | ILE  | 2.1  |
| 1   | D     | 194  | ASN  | 2.1  |
| 1   | E     | 933  | SER  | 2.1  |
| 1   | E     | 575  | MET  | 2.1  |
| 1   | F     | 796  | PHE  | 2.1  |
| 1   | B     | 578  | LEU  | 2.1  |
| 1   | D     | 402  | ILE  | 2.1  |
| 1   | A     | 792  | GLN  | 2.0  |
| 1   | B     | 825  | GLN  | 2.0  |
| 1   | D     | 728  | GLN  | 2.0  |
| 1   | A     | 489  | THR  | 2.0  |
| 1   | D     | 1010 | THR  | 2.0  |
| 1   | C     | 353  | LEU  | 2.0  |
| 1   | B     | 281  | PHE  | 2.0  |
| 1   | C     | 20   | MET  | 2.0  |
| 1   | C     | 396  | PHE  | 2.0  |
| 1   | D     | 386  | PHE  | 2.0  |
| 1   | C     | 282  | ASN  | 2.0  |
| 1   | E     | 62   | THR  | 2.0  |
| 1   | F     | 1014 | ILE  | 2.0  |
| 1   | A     | 136  | PHE  | 2.0  |
| 1   | C     | 655  | ASP  | 2.0  |
| 1   | C     | 500  | ILE  | 2.0  |
| 1   | F     | 143  | ILE  | 2.0  |
| 1   | A     | 461  | GLY  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 71   | GLY  | 2.0  |
| 1   | F     | 573  | MET  | 2.0  |
| 1   | A     | 108  | GLN  | 2.0  |
| 1   | A     | 711  | VAL  | 2.0  |
| 1   | E     | 61   | VAL  | 2.0  |
| 1   | A     | 881  | LEU  | 2.0  |
| 1   | E     | 441  | ALA  | 2.0  |
| 1   | F     | 691  | THR  | 2.0  |
| 1   | B     | 197  | GLN  | 2.0  |
| 1   | D     | 974  | SER  | 2.0  |
| 1   | F     | 578  | LEU  | 2.0  |
| 1   | F     | 126  | GLY  | 2.0  |
| 1   | E     | 199  | THR  | 2.0  |
| 1   | B     | 1011 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

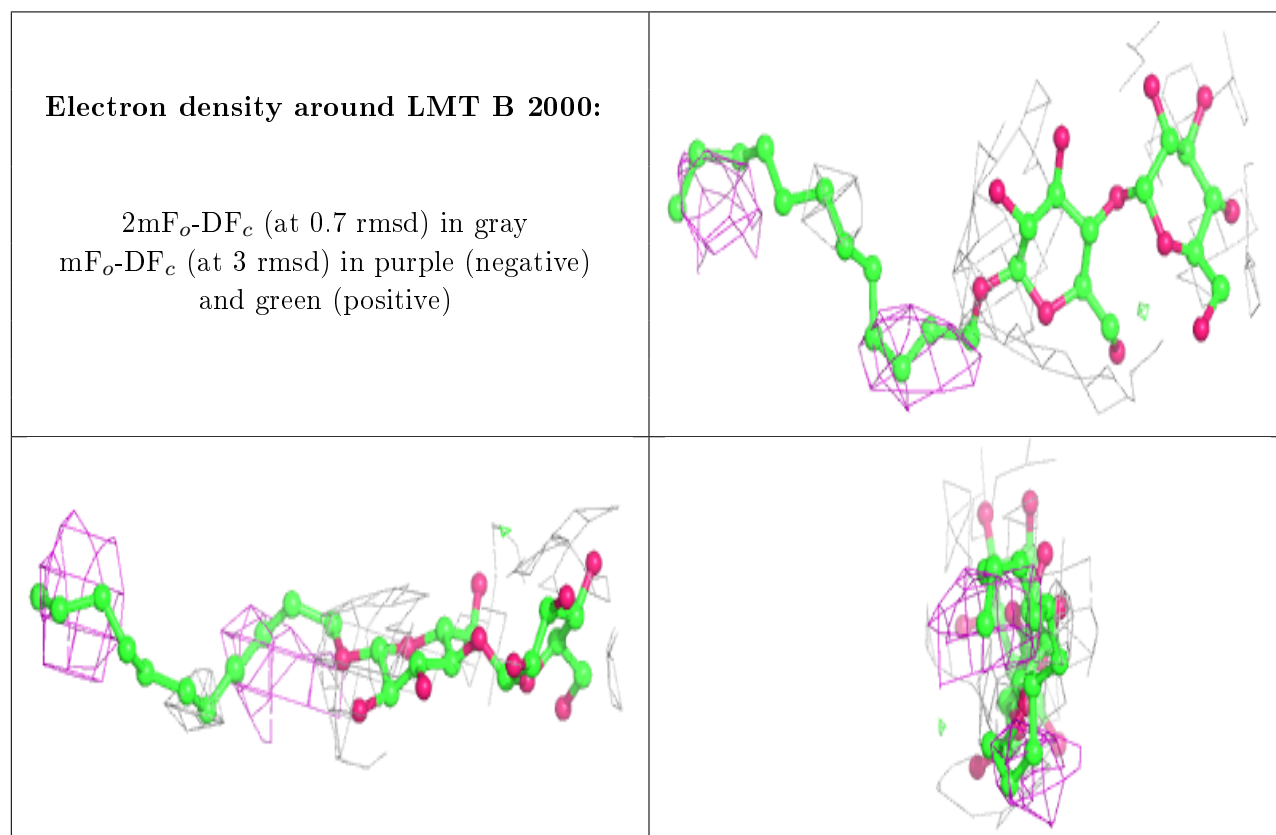
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | LMT  | B     | 2000 | 35/35 | 0.73 | 0.43 | 31,50,60,69                 | 0     |
| 2   | LMT  | E     | 1101 | 35/35 | 0.78 | 0.42 | 41,74,104,107               | 0     |
| 2   | LMT  | D     | 2000 | 35/35 | 0.82 | 0.34 | 21,41,56,63                 | 0     |
| 2   | LMT  | C     | 1101 | 35/35 | 0.82 | 0.33 | 12,41,56,72                 | 0     |
| 2   | LMT  | F     | 2000 | 35/35 | 0.82 | 0.39 | 40,64,89,94                 | 0     |
| 2   | LMT  | A     | 1101 | 35/35 | 0.86 | 0.32 | 31,41,90,99                 | 0     |
| 3   | NI   | E     | 1102 | 1/1   | 0.96 | 0.15 | 170,170,170,170             | 0     |
| 3   | NI   | A     | 1102 | 1/1   | 0.97 | 0.19 | 154,154,154,154             | 0     |
| 3   | NI   | C     | 1102 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |

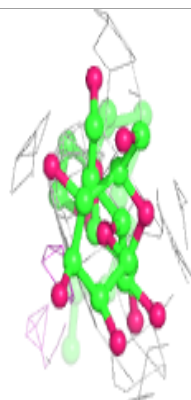
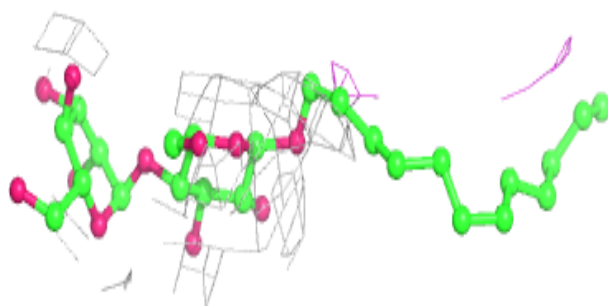
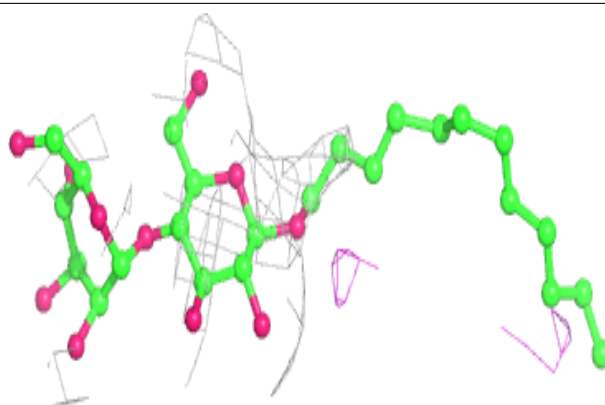
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



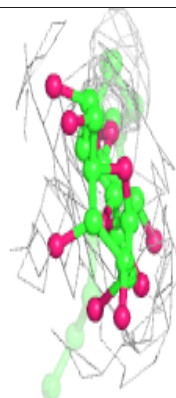
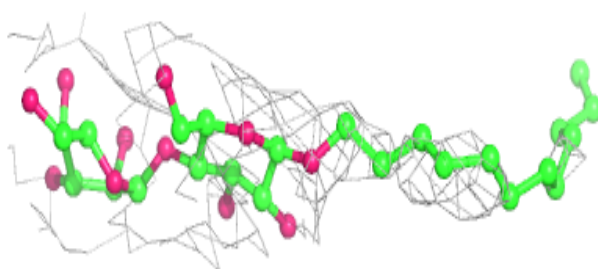
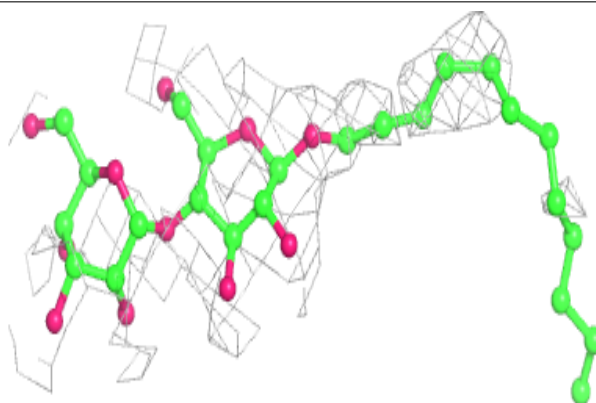


**Electron density around LMT E 1101:**

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

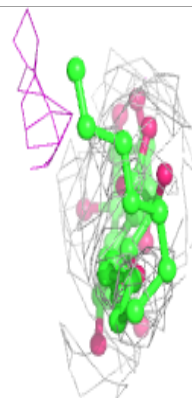
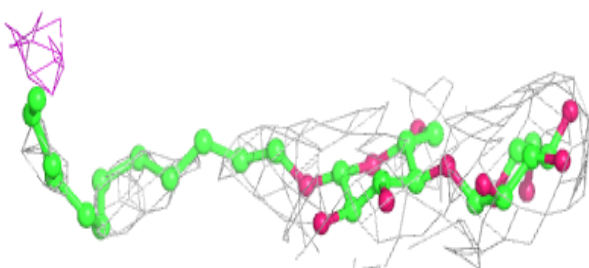
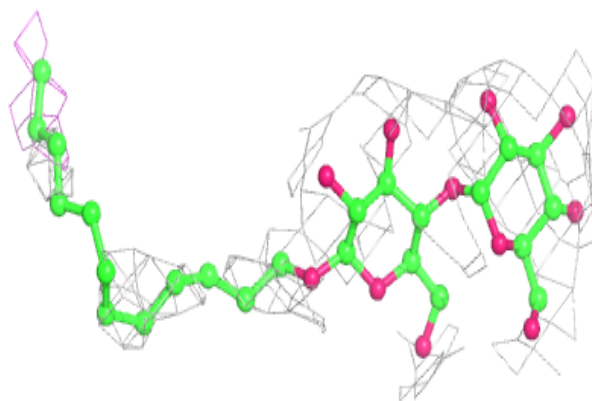
**Electron density around LMT D 2000:**

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

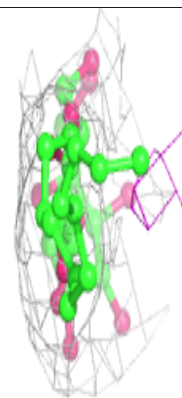
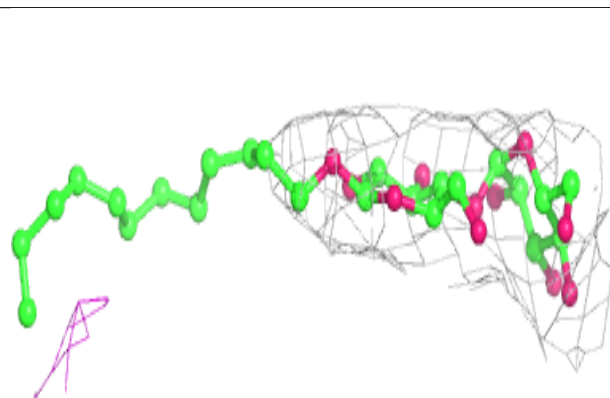
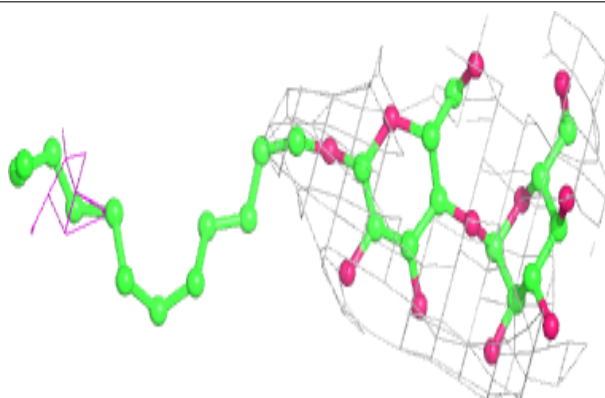


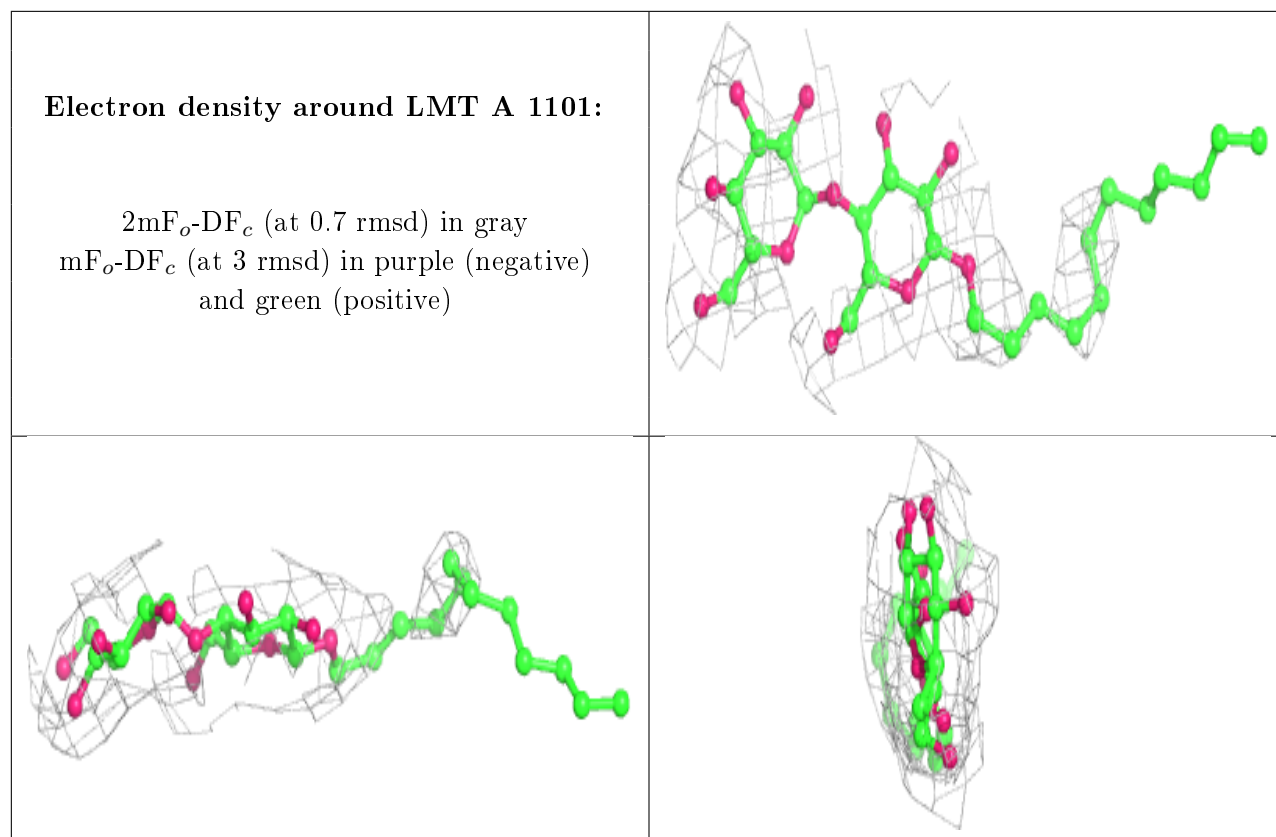
**Electron density around LMT C 1101:**

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

**Electron density around LMT F 2000:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.