



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:29 AM UTC

PDB ID : 1NY6 / pdb\_00001ny6  
Title : Crystal structure of sigm54 activator (AAA+ ATPase) in the active state  
Authors : Lee, S.Y.; de la Torre, A.; Kustu, S.; Nixon, B.T.; Wemmer, D.E.  
Deposited on : 2003-02-11  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

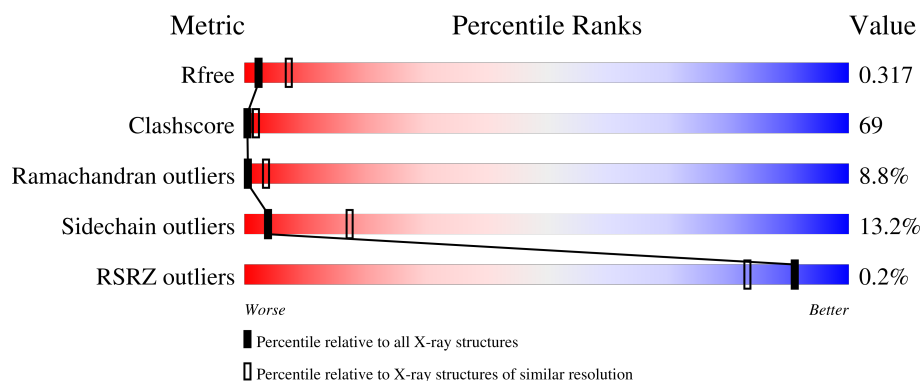
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



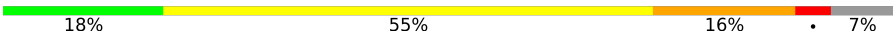
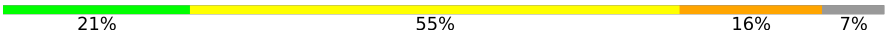
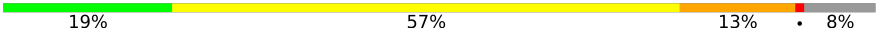
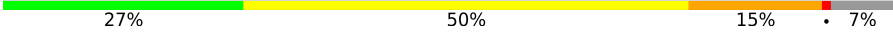
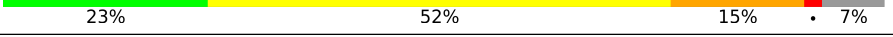
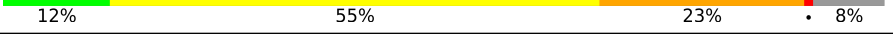
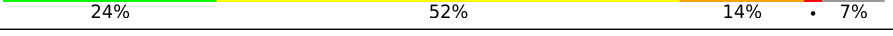
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 267    |                  |
| 1   | B     | 267    |                  |
| 1   | C     | 267    |                  |
| 1   | D     | 267    |                  |
| 1   | E     | 267    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | F     | 267    |  |
| 1   | G     | 267    |  |
| 1   | H     | 267    |  |
| 1   | I     | 267    |  |
| 1   | J     | 267    |  |
| 1   | K     | 267    |  |
| 1   | L     | 267    |  |
| 1   | M     | 267    |  |
| 1   | N     | 267    |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28041 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 transcriptional regulator (NtrC family).

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1979  | 1278 | 333 | 364 | 4 |         |         |       |
| 1   | B     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1940  | 1250 | 329 | 357 | 4 |         |         |       |
| 1   | C     | 248      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1988  | 1283 | 334 | 367 | 4 |         |         |       |
| 1   | D     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1979  | 1278 | 333 | 364 | 4 |         |         |       |
| 1   | E     | 248      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1988  | 1283 | 334 | 367 | 4 |         |         |       |
| 1   | F     | 248      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1988  | 1283 | 334 | 367 | 4 |         |         |       |
| 1   | G     | 248      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1988  | 1283 | 334 | 367 | 4 |         |         |       |
| 1   | H     | 245      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1954  | 1259 | 331 | 360 | 4 |         |         |       |
| 1   | I     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1966  | 1268 | 333 | 361 | 4 |         |         |       |
| 1   | J     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1975  | 1276 | 333 | 362 | 4 |         |         |       |
| 1   | K     | 248      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1988  | 1283 | 334 | 367 | 4 |         |         |       |
| 1   | L     | 246      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1972  | 1273 | 332 | 363 | 4 |         |         |       |
| 1   | M     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1979  | 1278 | 333 | 364 | 4 |         |         |       |
| 1   | N     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1979  | 1278 | 333 | 364 | 4 |         |         |       |

There are 14 discrepancies between the modelled and reference sequences:

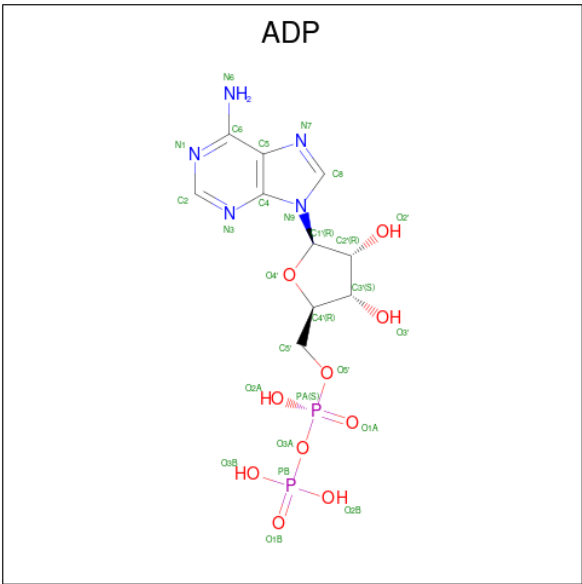
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 121     | MET      | -      | initiating methionine | UNP O67198 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| C     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| D     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| E     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| F     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| G     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| H     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| I     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| J     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| K     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| L     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| M     | 121     | MET      | -      | initiating methionine | UNP O67198 |
| N     | 121     | MET      | -      | initiating methionine | UNP O67198 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

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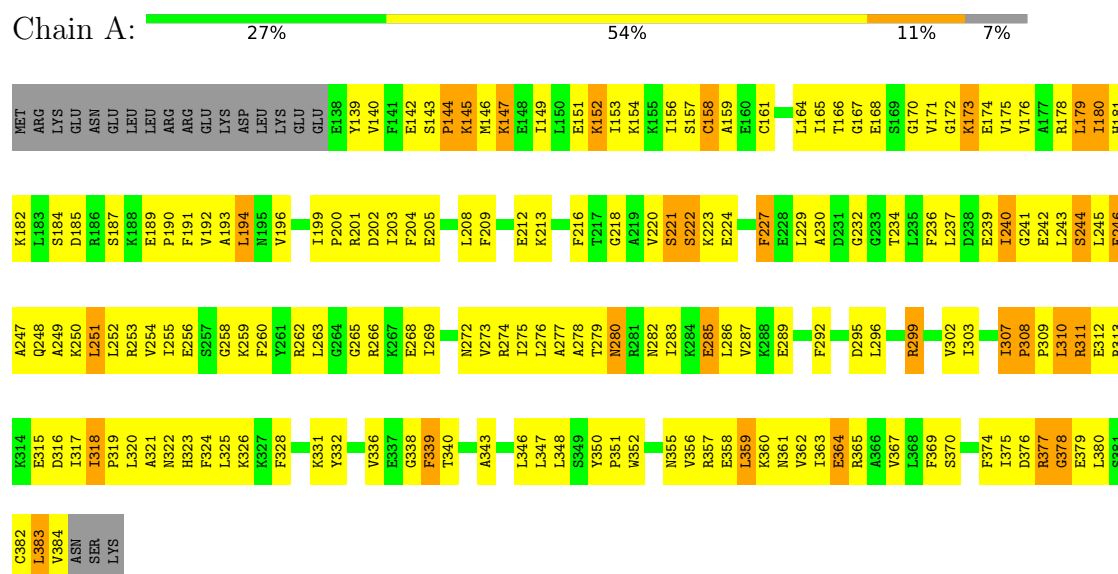
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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | I     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | J     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | K     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | L     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | M     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | N     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

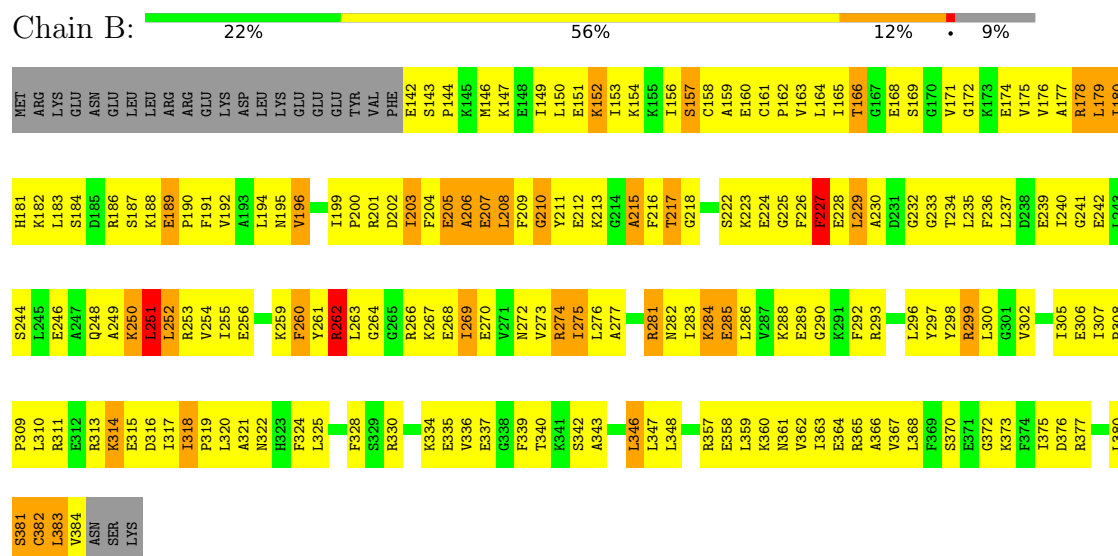
### 3 Residue-property plots

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

- Molecule 1: transcriptional regulator (NtrC family)

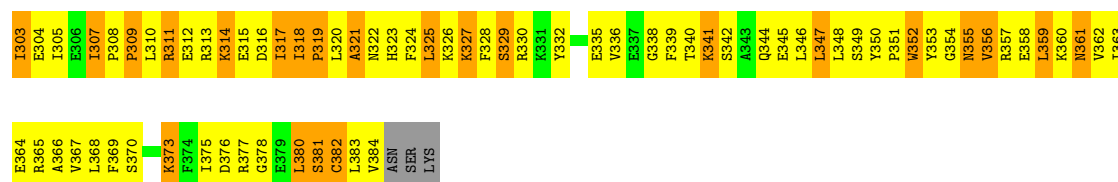


- Molecule 1: transcriptional regulator (NtrC family)



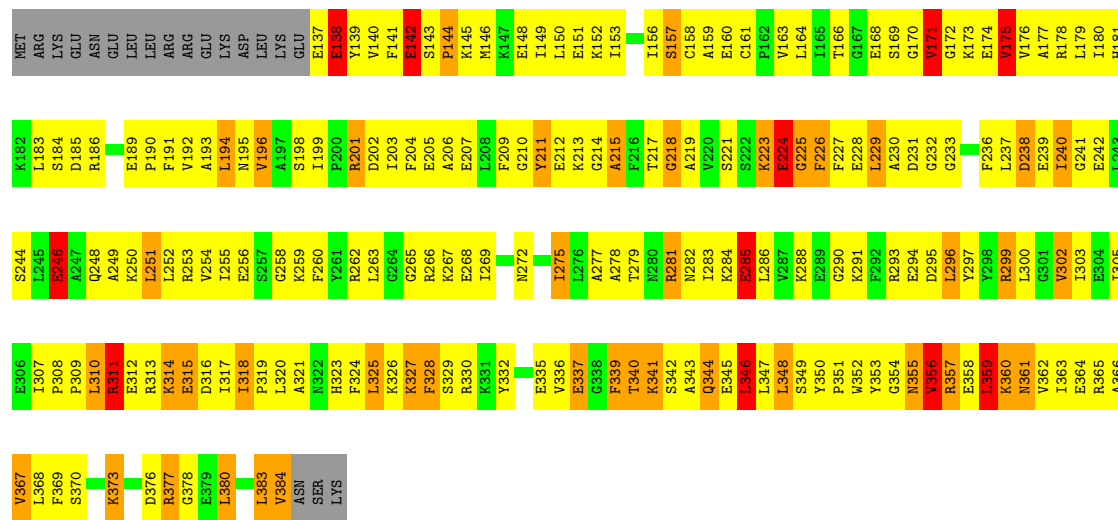
- Molecule 1: transcriptional regulator (NtrC family)





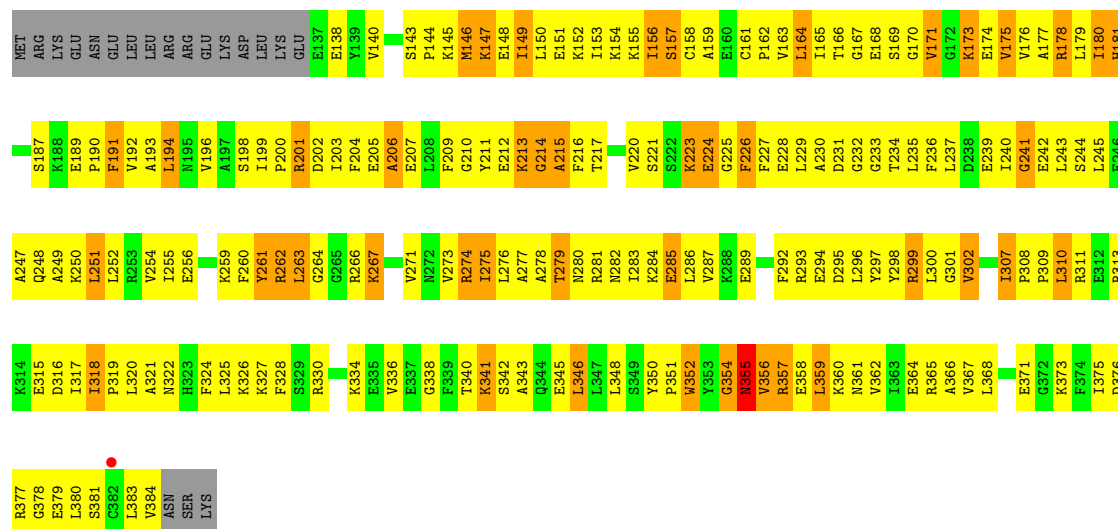
- Molecule 1: transcriptional regulator (NtrC family)

Chain F: 18% 55% 16% 7%



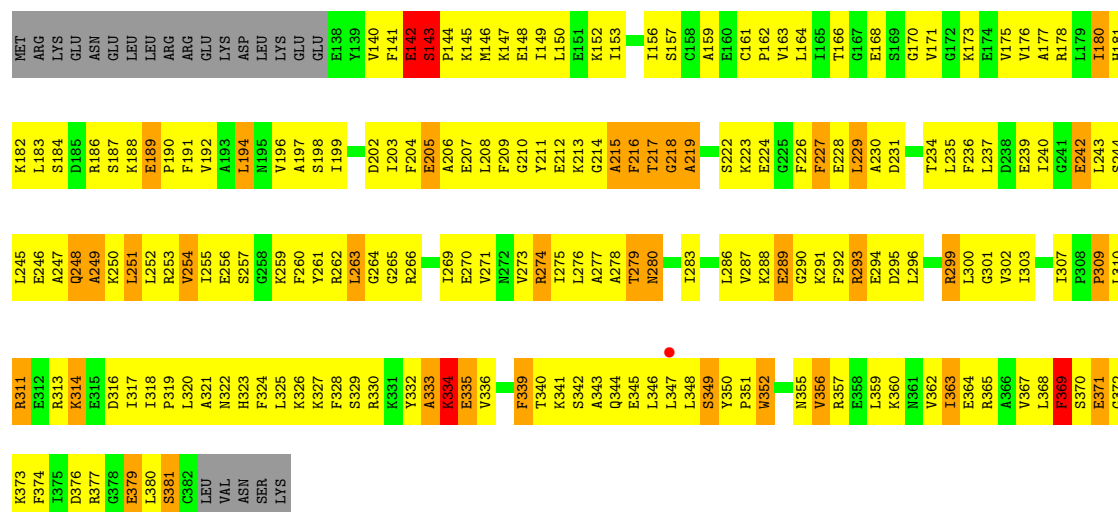
- Molecule 1: transcriptional regulator (NtrC family)

Chain G: 21% 55% 16% 7%



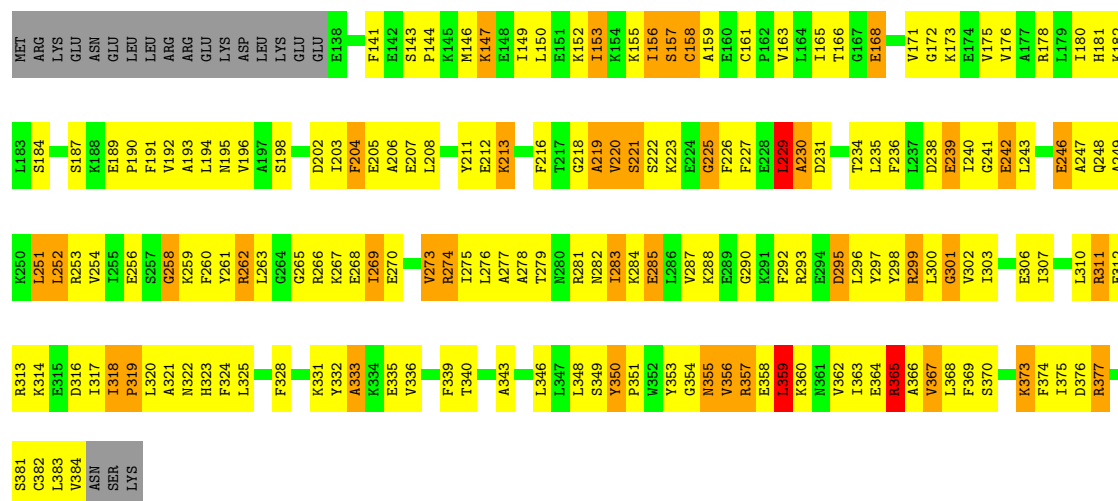
- Molecule 1: transcriptional regulator (NtrC family)

Chain H: 19% 57% 13% 8%



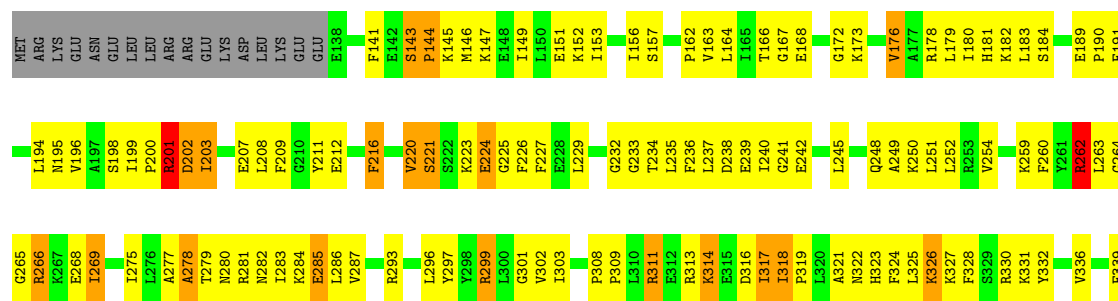
• Molecule 1: transcriptional regulator (NtrC family)

Chain I: 27% 50% 15% 7%



• Molecule 1: transcriptional regulator (NtrC family)

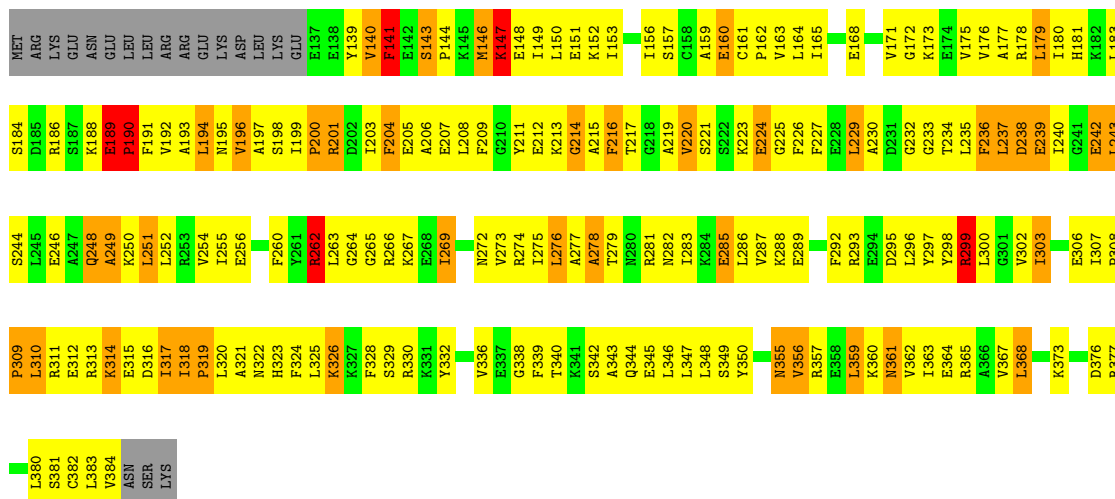
Chain J: 34% 46% 12% 7%





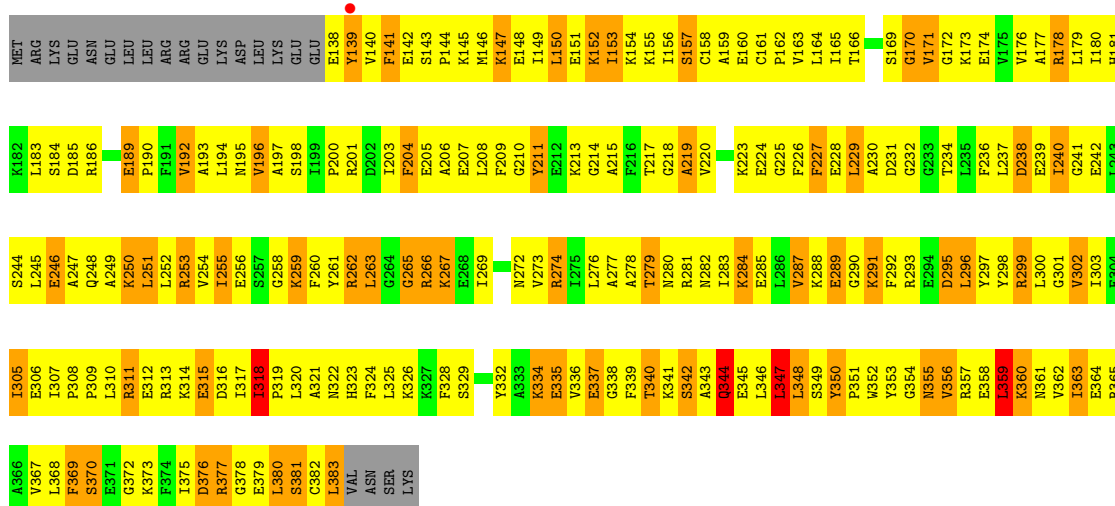
• Molecule 1: transcriptional regulator (NtrC family)

Chain K: 23% 52% 15% 7%



• Molecule 1: transcriptional regulator (NtrC family)

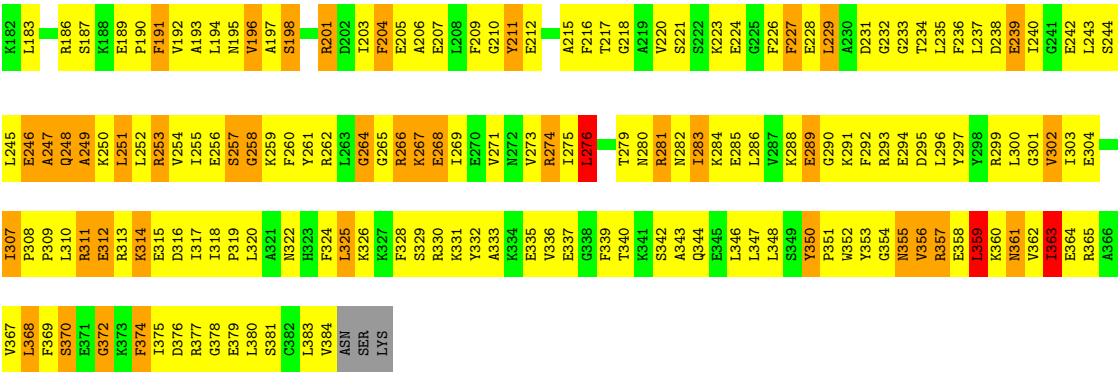
Chain L: 12% 55% 23% 8%



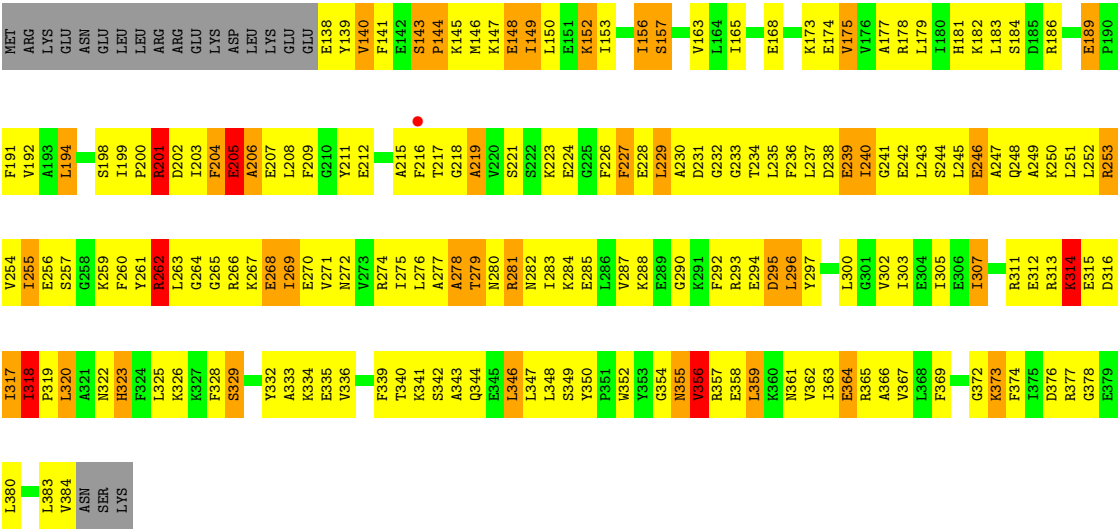
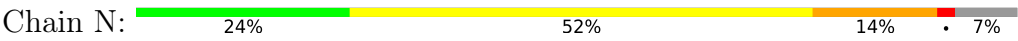
• Molecule 1: transcriptional regulator (NtrC family)

Chain M: 16% 55% 20% 7%





● Molecule 1: transcriptional regulator (NtrC family)



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 106.79Å 108.27Å 110.02Å<br>70.25° 85.90° 73.27°             | Depositor        |
| Resolution (Å)                                                          | 19.98 – 3.10<br>19.98 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.6 (19.98-3.10)<br>97.2 (19.98-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.30 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.266 , 0.329<br>0.259 , 0.317                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8701 reflections (10.04%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 94.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.079                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 73.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.006 for -l,-k,-h                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 28041                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 103.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.53         | 0/2013         | 1.01        | 9/2700 (0.3%)    |
| 1   | B     | 0.55         | 0/1972         | 1.01        | 9/2644 (0.3%)    |
| 1   | C     | 0.69         | 0/2022         | 1.14        | 12/2712 (0.4%)   |
| 1   | D     | 0.66         | 0/2013         | 1.17        | 14/2700 (0.5%)   |
| 1   | E     | 0.76         | 1/2022 (0.0%)  | 1.31        | 20/2712 (0.7%)   |
| 1   | F     | 0.62         | 1/2022 (0.0%)  | 1.11        | 14/2712 (0.5%)   |
| 1   | G     | 0.56         | 0/2022         | 1.07        | 14/2712 (0.5%)   |
| 1   | H     | 0.51         | 0/1987         | 1.12        | 11/2665 (0.4%)   |
| 1   | I     | 0.52         | 0/1999         | 1.03        | 13/2681 (0.5%)   |
| 1   | J     | 0.48         | 0/2009         | 0.94        | 5/2695 (0.2%)    |
| 1   | K     | 0.56         | 0/2022         | 1.08        | 13/2712 (0.5%)   |
| 1   | L     | 0.78         | 1/2006 (0.0%)  | 1.22        | 14/2690 (0.5%)   |
| 1   | M     | 0.60         | 0/2013         | 1.14        | 23/2700 (0.9%)   |
| 1   | N     | 0.53         | 0/2013         | 1.08        | 20/2700 (0.7%)   |
| All | All   | 0.60         | 3/28135 (0.0%) | 1.11        | 191/37735 (0.5%) |

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   | H     | 0                   | 2                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | L     | 318 | ILE  | CA-CB | 8.73  | 1.65        | 1.54     |
| 1   | F     | 356 | VAL  | CA-CB | -6.84 | 1.45        | 1.54     |
| 1   | E     | 190 | PRO  | N-CA  | 6.18  | 1.54        | 1.47     |

All (191) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | E     | 190 | PRO  | CA-N-CD | -21.16 | 82.37       | 112.00   |
| 1   | H     | 143 | SER  | C-N-CD  | -19.34 | 45.71       | 125.00   |
| 1   | C     | 190 | PRO  | CA-N-CD | -17.28 | 87.81       | 112.00   |
| 1   | D     | 358 | GLU  | N-CA-C  | -13.68 | 99.03       | 114.62   |
| 1   | H     | 142 | GLU  | O-C-N   | -11.77 | 106.93      | 122.59   |
| 1   | A     | 364 | GLU  | N-CA-C  | -11.21 | 99.08       | 111.07   |
| 1   | N     | 364 | GLU  | N-CA-C  | -11.00 | 99.26       | 111.14   |
| 1   | F     | 302 | VAL  | N-CA-C  | -10.34 | 101.33      | 110.74   |
| 1   | N     | 149 | ILE  | N-CA-C  | -10.19 | 100.78      | 111.58   |
| 1   | K     | 204 | PHE  | N-CA-C  | 9.91   | 123.11      | 111.02   |
| 1   | L     | 258 | GLY  | N-CA-C  | -9.80  | 103.09      | 113.58   |
| 1   | M     | 143 | SER  | CA-C-N  | 9.75   | 132.03      | 119.84   |
| 1   | M     | 143 | SER  | C-N-CA  | 9.75   | 132.03      | 119.84   |
| 1   | G     | 140 | VAL  | N-CA-C  | 9.53   | 123.25      | 107.24   |
| 1   | N     | 262 | ARG  | N-CA-C  | -9.49  | 96.83       | 110.59   |
| 1   | M     | 357 | ARG  | N-CA-C  | -9.21  | 99.78       | 111.02   |
| 1   | G     | 147 | LYS  | N-CA-C  | -9.02  | 101.34      | 111.71   |
| 1   | F     | 342 | SER  | N-CA-C  | -8.85  | 101.60      | 111.07   |
| 1   | M     | 220 | VAL  | N-CA-C  | 8.82   | 118.89      | 110.42   |
| 1   | K     | 220 | VAL  | N-CA-C  | 8.38   | 126.76      | 109.34   |
| 1   | I     | 258 | GLY  | N-CA-C  | -8.15  | 103.42      | 115.72   |
| 1   | L     | 302 | VAL  | N-CA-C  | -8.04  | 102.42      | 110.62   |
| 1   | N     | 329 | SER  | N-CA-C  | -7.80  | 103.72      | 113.55   |
| 1   | I     | 369 | PHE  | N-CA-C  | -7.78  | 103.85      | 112.72   |
| 1   | A     | 245 | LEU  | N-CA-C  | -7.65  | 103.04      | 112.38   |
| 1   | H     | 371 | GLU  | N-CA-C  | -7.64  | 102.88      | 111.14   |
| 1   | D     | 171 | VAL  | N-CA-C  | -7.64  | 105.32      | 112.96   |
| 1   | D     | 364 | GLU  | N-CA-C  | -7.58  | 103.01      | 111.28   |
| 1   | L     | 250 | LYS  | N-CA-C  | -7.51  | 102.79      | 110.97   |
| 1   | L     | 152 | LYS  | N-CA-C  | -7.50  | 101.39      | 111.96   |
| 1   | L     | 238 | ASP  | N-CA-C  | 7.39   | 120.21      | 111.71   |
| 1   | L     | 338 | GLY  | N-CA-C  | 7.34   | 121.36      | 110.42   |
| 1   | I     | 229 | LEU  | N-CA-C  | -7.34  | 102.89      | 111.03   |
| 1   | M     | 148 | GLU  | N-CA-C  | -7.29  | 103.03      | 110.97   |
| 1   | D     | 159 | ALA  | N-CA-C  | 7.28   | 120.28      | 108.41   |
| 1   | N     | 341 | LYS  | N-CA-C  | -7.26  | 103.30      | 111.07   |
| 1   | G     | 215 | ALA  | N-CA-C  | -7.21  | 105.67      | 114.75   |
| 1   | G     | 357 | ARG  | N-CA-C  | -7.16  | 103.56      | 111.36   |
| 1   | F     | 142 | GLU  | N-CA-C  | 7.14   | 121.59      | 113.02   |
| 1   | E     | 178 | ARG  | N-CA-C  | -7.07  | 103.65      | 111.36   |
| 1   | E     | 198 | SER  | N-CA-C  | -7.07  | 104.23      | 112.92   |
| 1   | F     | 258 | GLY  | N-CA-C  | -7.02  | 105.53      | 115.43   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 352 | TRP  | N-CA-C  | -7.02 | 104.34      | 113.12   |
| 1   | H     | 369 | PHE  | N-CA-C  | -6.99 | 105.10      | 112.93   |
| 1   | M     | 258 | GLY  | N-CA-C  | -6.96 | 105.14      | 114.95   |
| 1   | J     | 220 | VAL  | N-CA-C  | 6.95  | 119.15      | 109.29   |
| 1   | B     | 215 | ALA  | N-CA-C  | -6.90 | 104.73      | 113.01   |
| 1   | E     | 341 | LYS  | N-CA-C  | -6.87 | 103.87      | 111.36   |
| 1   | M     | 210 | GLY  | N-CA-C  | -6.79 | 103.82      | 111.63   |
| 1   | K     | 146 | MET  | N-CA-C  | -6.78 | 103.92      | 112.93   |
| 1   | D     | 234 | THR  | N-CA-C  | 6.77  | 120.34      | 107.75   |
| 1   | M     | 140 | VAL  | N-CA-C  | 6.75  | 117.58      | 107.80   |
| 1   | N     | 221 | SER  | N-CA-C  | 6.69  | 118.81      | 109.31   |
| 1   | E     | 307 | ILE  | CA-C-N  | 6.63  | 127.21      | 120.38   |
| 1   | E     | 307 | ILE  | C-N-CA  | 6.63  | 127.21      | 120.38   |
| 1   | F     | 373 | LYS  | N-CA-C  | -6.61 | 105.51      | 113.97   |
| 1   | F     | 285 | GLU  | N-CA-C  | -6.59 | 103.78      | 110.97   |
| 1   | F     | 340 | THR  | N-CA-C  | -6.59 | 101.83      | 110.33   |
| 1   | J     | 203 | ILE  | N-CA-C  | -6.59 | 107.45      | 113.71   |
| 1   | F     | 202 | ASP  | N-CA-C  | 6.58  | 118.45      | 111.28   |
| 1   | B     | 262 | ARG  | N-CA-C  | -6.51 | 101.24      | 110.35   |
| 1   | K     | 262 | ARG  | N-CA-C  | -6.51 | 101.50      | 110.35   |
| 1   | N     | 140 | VAL  | N-CA-C  | 6.50  | 117.61      | 107.28   |
| 1   | I     | 246 | GLU  | N-CA-C  | -6.49 | 104.13      | 111.14   |
| 1   | M     | 350 | TYR  | CA-C-N  | 6.46  | 125.69      | 118.97   |
| 1   | M     | 350 | TYR  | C-N-CA  | 6.46  | 125.69      | 118.97   |
| 1   | B     | 152 | LYS  | N-CA-C  | -6.44 | 104.26      | 111.28   |
| 1   | H     | 218 | GLY  | N-CA-C  | -6.42 | 105.52      | 115.73   |
| 1   | M     | 215 | ALA  | N-CA-C  | -6.41 | 106.68      | 114.75   |
| 1   | N     | 156 | ILE  | N-CA-C  | 6.40  | 116.57      | 110.74   |
| 1   | K     | 147 | LYS  | N-CA-C  | -6.40 | 104.35      | 111.71   |
| 1   | F     | 238 | ASP  | N-CA-C  | 6.40  | 118.58      | 108.67   |
| 1   | E     | 278 | ALA  | N-CA-C  | 6.39  | 118.72      | 109.71   |
| 1   | G     | 206 | ALA  | N-CA-C  | -6.37 | 106.72      | 114.75   |
| 1   | E     | 190 | PRO  | CB-CA-C | -6.33 | 101.93      | 110.85   |
| 1   | M     | 204 | PHE  | N-CA-C  | 6.31  | 118.16      | 111.28   |
| 1   | I     | 350 | TYR  | CA-C-N  | 6.25  | 125.81      | 119.19   |
| 1   | I     | 350 | TYR  | C-N-CA  | 6.25  | 125.81      | 119.19   |
| 1   | L     | 376 | ASP  | N-CA-C  | 6.23  | 116.79      | 108.38   |
| 1   | H     | 215 | ALA  | N-CA-C  | 6.22  | 120.33      | 112.87   |
| 1   | G     | 226 | PHE  | N-CA-C  | -6.21 | 104.96      | 112.54   |
| 1   | C     | 350 | TYR  | CA-C-N  | 6.18  | 125.74      | 119.19   |
| 1   | C     | 350 | TYR  | C-N-CA  | 6.18  | 125.74      | 119.19   |
| 1   | D     | 203 | ILE  | N-CA-C  | -6.15 | 107.87      | 113.71   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 258 | GLY  | N-CA-C  | -6.12 | 106.48      | 115.30   |
| 1   | L     | 259 | LYS  | N-CA-C  | 6.12  | 119.63      | 110.14   |
| 1   | D     | 140 | VAL  | N-CA-C  | 6.11  | 117.46      | 109.58   |
| 1   | B     | 199 | ILE  | CA-C-N  | 6.10  | 127.46      | 119.84   |
| 1   | B     | 199 | ILE  | C-N-CA  | 6.10  | 127.46      | 119.84   |
| 1   | D     | 235 | LEU  | N-CA-C  | -6.09 | 102.33      | 110.55   |
| 1   | B     | 147 | LYS  | N-CA-C  | -6.08 | 105.83      | 113.18   |
| 1   | A     | 280 | ASN  | N-CA-C  | -6.07 | 105.83      | 113.72   |
| 1   | N     | 206 | ALA  | N-CA-C  | -6.06 | 104.76      | 111.36   |
| 1   | C     | 273 | VAL  | N-CA-C  | 6.05  | 118.07      | 108.87   |
| 1   | F     | 246 | GLU  | N-CA-C  | -6.02 | 104.41      | 110.97   |
| 1   | C     | 203 | ILE  | N-CA-C  | 6.01  | 120.45      | 113.42   |
| 1   | D     | 212 | GLU  | N-CA-C  | -6.00 | 100.83      | 110.14   |
| 1   | K     | 143 | SER  | CA-C-N  | 5.97  | 125.94      | 120.03   |
| 1   | K     | 143 | SER  | C-N-CA  | 5.97  | 125.94      | 120.03   |
| 1   | I     | 365 | ARG  | N-CA-C  | -5.95 | 105.10      | 112.90   |
| 1   | J     | 262 | ARG  | N-CA-C  | -5.90 | 102.33      | 110.35   |
| 1   | M     | 302 | VAL  | N-CA-C  | -5.89 | 103.90      | 110.62   |
| 1   | I     | 354 | GLY  | N-CA-C  | -5.88 | 105.56      | 115.62   |
| 1   | H     | 254 | VAL  | N-CA-C  | -5.87 | 105.40      | 110.74   |
| 1   | I     | 147 | LYS  | N-CA-C  | -5.87 | 104.97      | 111.71   |
| 1   | M     | 325 | LEU  | N-CA-C  | -5.86 | 104.58      | 110.97   |
| 1   | L     | 342 | SER  | N-CA-C  | -5.84 | 105.42      | 112.54   |
| 1   | H     | 334 | LYS  | N-CA-C  | 5.82  | 123.20      | 110.80   |
| 1   | G     | 302 | VAL  | N-CA-C  | -5.82 | 104.65      | 110.30   |
| 1   | G     | 354 | GLY  | N-CA-C  | -5.81 | 99.40       | 113.18   |
| 1   | E     | 373 | LYS  | N-CA-C  | -5.80 | 106.21      | 113.28   |
| 1   | N     | 307 | ILE  | CA-C-N  | 5.78  | 123.82      | 119.66   |
| 1   | N     | 307 | ILE  | C-N-CA  | 5.78  | 123.82      | 119.66   |
| 1   | D     | 273 | VAL  | N-CA-C  | 5.75  | 116.87      | 108.53   |
| 1   | N     | 143 | SER  | CA-C-N  | 5.72  | 127.00      | 119.84   |
| 1   | N     | 143 | SER  | C-N-CA  | 5.72  | 127.00      | 119.84   |
| 1   | D     | 280 | ASN  | N-CA-C  | -5.71 | 106.94      | 114.31   |
| 1   | F     | 341 | LYS  | N-CA-C  | -5.71 | 106.32      | 113.28   |
| 1   | A     | 308 | PRO  | CA-C-N  | 5.70  | 126.02      | 119.92   |
| 1   | A     | 308 | PRO  | C-N-CA  | 5.70  | 126.02      | 119.92   |
| 1   | K     | 236 | PHE  | N-CA-C  | 5.70  | 118.55      | 108.24   |
| 1   | G     | 138 | GLU  | N-CA-C  | 5.68  | 119.16      | 108.65   |
| 1   | E     | 190 | PRO  | N-CA-CB | 5.67  | 108.58      | 103.19   |
| 1   | J     | 364 | GLU  | N-CA-C  | -5.65 | 103.95      | 111.24   |
| 1   | D     | 258 | GLY  | N-CA-C  | -5.64 | 106.97      | 115.32   |
| 1   | H     | 301 | GLY  | N-CA-C  | -5.64 | 106.86      | 115.66   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 147 | LYS  | N-CA-C  | -5.63 | 105.90      | 112.89   |
| 1   | F     | 223 | LYS  | N-CA-C  | 5.63  | 119.69      | 112.26   |
| 1   | B     | 169 | SER  | N-CA-C  | 5.61  | 117.61      | 108.63   |
| 1   | E     | 199 | ILE  | CA-C-N  | 5.61  | 125.94      | 119.93   |
| 1   | E     | 199 | ILE  | C-N-CA  | 5.61  | 125.94      | 119.93   |
| 1   | M     | 266 | ARG  | CB-CA-C | -5.58 | 109.14      | 115.79   |
| 1   | L     | 265 | GLY  | N-CA-C  | -5.58 | 103.00      | 111.14   |
| 1   | N     | 147 | LYS  | N-CA-C  | -5.57 | 105.98      | 112.89   |
| 1   | K     | 330 | ARG  | N-CA-C  | -5.56 | 104.06      | 111.24   |
| 1   | D     | 378 | GLY  | N-CA-C  | 5.55  | 119.60      | 112.83   |
| 1   | E     | 165 | ILE  | CB-CA-C | -5.55 | 102.19      | 111.29   |
| 1   | I     | 283 | ILE  | N-CA-C  | 5.54  | 115.68      | 110.30   |
| 1   | L     | 246 | GLU  | N-CA-C  | -5.54 | 104.10      | 111.24   |
| 1   | G     | 223 | LYS  | N-CA-C  | 5.53  | 118.25      | 109.96   |
| 1   | A     | 140 | VAL  | N-CA-C  | 5.49  | 116.67      | 109.21   |
| 1   | N     | 279 | THR  | N-CA-C  | 5.48  | 115.52      | 108.34   |
| 1   | K     | 153 | ILE  | N-CA-C  | -5.47 | 104.99      | 110.30   |
| 1   | N     | 205 | GLU  | N-CA-C  | -5.44 | 99.22       | 110.80   |
| 1   | G     | 371 | GLU  | N-CA-C  | -5.42 | 105.78      | 112.72   |
| 1   | E     | 353 | TYR  | N-CA-C  | -5.41 | 106.18      | 112.89   |
| 1   | E     | 300 | LEU  | N-CA-C  | -5.40 | 107.34      | 114.31   |
| 1   | A     | 147 | LYS  | N-CA-C  | -5.40 | 106.53      | 113.01   |
| 1   | N     | 354 | GLY  | N-CA-C  | -5.39 | 108.25      | 115.32   |
| 1   | F     | 256 | GLU  | N-CA-C  | 5.36  | 117.93      | 111.40   |
| 1   | J     | 176 | VAL  | N-CA-C  | -5.35 | 105.50      | 110.53   |
| 1   | I     | 225 | GLY  | N-CA-C  | -5.35 | 104.33      | 112.51   |
| 1   | M     | 276 | LEU  | N-CA-C  | -5.34 | 98.56       | 107.80   |
| 1   | C     | 287 | VAL  | N-CA-C  | -5.33 | 105.52      | 110.53   |
| 1   | C     | 258 | GLY  | N-CA-C  | -5.31 | 106.37      | 115.08   |
| 1   | N     | 323 | HIS  | N-CA-C  | -5.31 | 105.66      | 111.82   |
| 1   | M     | 307 | ILE  | CA-C-N  | 5.30  | 123.48      | 119.66   |
| 1   | M     | 307 | ILE  | C-N-CA  | 5.30  | 123.48      | 119.66   |
| 1   | L     | 289 | GLU  | N-CA-C  | -5.27 | 106.92      | 113.19   |
| 1   | M     | 331 | LYS  | N-CA-C  | -5.27 | 106.55      | 112.87   |
| 1   | C     | 147 | LYS  | N-CA-C  | -5.26 | 105.72      | 111.82   |
| 1   | C     | 341 | LYS  | N-CA-C  | -5.24 | 105.04      | 111.75   |
| 1   | D     | 275 | ILE  | CB-CA-C | -5.23 | 102.71      | 111.29   |
| 1   | K     | 193 | ALA  | N-CA-C  | 5.22  | 117.64      | 108.56   |
| 1   | G     | 180 | ILE  | N-CA-C  | -5.22 | 105.41      | 110.42   |
| 1   | M     | 220 | VAL  | CB-CA-C | -5.21 | 105.30      | 111.97   |
| 1   | L     | 302 | VAL  | CB-CA-C | -5.18 | 105.15      | 112.14   |
| 1   | C     | 354 | GLY  | N-CA-C  | -5.17 | 107.03      | 115.46   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 148 | GLU  | N-CA-C | -5.16 | 105.66      | 111.28   |
| 1   | I     | 262 | ARG  | N-CA-C | -5.16 | 102.42      | 110.10   |
| 1   | N     | 217 | THR  | N-CA-C | -5.13 | 102.05      | 109.59   |
| 1   | N     | 238 | ASP  | N-CA-C | 5.13  | 116.75      | 108.34   |
| 1   | M     | 221 | SER  | N-CA-C | 5.13  | 117.91      | 110.17   |
| 1   | K     | 317 | ILE  | N-CA-C | 5.13  | 115.56      | 110.23   |
| 1   | I     | 273 | VAL  | N-CA-C | 5.12  | 116.35      | 108.71   |
| 1   | K     | 188 | LYS  | N-CA-C | -5.12 | 107.08      | 113.38   |
| 1   | E     | 307 | ILE  | O-C-N  | 5.12  | 126.93      | 121.10   |
| 1   | E     | 187 | SER  | N-CA-C | -5.11 | 107.00      | 113.18   |
| 1   | F     | 346 | LEU  | N-CA-C | -5.10 | 103.00      | 111.37   |
| 1   | G     | 170 | GLY  | N-CA-C | 5.08  | 122.30      | 115.59   |
| 1   | B     | 163 | VAL  | N-CA-C | 5.08  | 114.80      | 106.72   |
| 1   | B     | 346 | LEU  | N-CA-C | -5.07 | 105.88      | 111.71   |
| 1   | G     | 289 | GLU  | N-CA-C | -5.06 | 107.11      | 113.28   |
| 1   | L     | 201 | ARG  | N-CA-C | 5.06  | 119.72      | 111.37   |
| 1   | A     | 374 | PHE  | N-CA-C | 5.05  | 117.09      | 109.41   |
| 1   | E     | 381 | SER  | N-CA-C | 5.05  | 117.75      | 111.24   |
| 1   | E     | 194 | LEU  | N-CA-C | 5.05  | 116.64      | 108.41   |
| 1   | C     | 286 | LEU  | N-CA-C | -5.04 | 106.31      | 112.90   |
| 1   | C     | 222 | SER  | N-CA-C | 5.02  | 117.75      | 109.76   |
| 1   | E     | 296 | LEU  | N-CA-C | -5.02 | 105.28      | 111.40   |
| 1   | M     | 268 | GLU  | N-CA-C | -5.01 | 101.70      | 109.72   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | H     | 142 | GLU  | Peptide,Mainchain |

## 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     | 1979  | 0        | 2040     | 230     | 0            |
| 1   | B     | 1940  | 0        | 2007     | 270     | 0            |
| 1   | C     | 1988  | 0        | 2046     | 293     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 1979  | 0        | 2040     | 294     | 0            |
| 1   | E     | 1988  | 0        | 2046     | 373     | 0            |
| 1   | F     | 1988  | 0        | 2046     | 305     | 0            |
| 1   | G     | 1988  | 0        | 2046     | 259     | 0            |
| 1   | H     | 1954  | 0        | 2009     | 294     | 0            |
| 1   | I     | 1966  | 0        | 2022     | 263     | 0            |
| 1   | J     | 1975  | 0        | 2036     | 210     | 0            |
| 1   | K     | 1988  | 0        | 2046     | 267     | 0            |
| 1   | L     | 1972  | 0        | 2031     | 407     | 0            |
| 1   | M     | 1979  | 0        | 2040     | 323     | 0            |
| 1   | N     | 1979  | 0        | 2040     | 285     | 0            |
| 2   | A     | 27    | 0        | 12       | 2       | 0            |
| 2   | B     | 27    | 0        | 12       | 1       | 0            |
| 2   | C     | 27    | 0        | 12       | 4       | 0            |
| 2   | D     | 27    | 0        | 12       | 6       | 0            |
| 2   | E     | 27    | 0        | 12       | 3       | 0            |
| 2   | F     | 27    | 0        | 12       | 7       | 0            |
| 2   | G     | 27    | 0        | 12       | 0       | 0            |
| 2   | H     | 27    | 0        | 12       | 3       | 0            |
| 2   | I     | 27    | 0        | 12       | 5       | 0            |
| 2   | J     | 27    | 0        | 12       | 1       | 0            |
| 2   | K     | 27    | 0        | 12       | 1       | 0            |
| 2   | L     | 27    | 0        | 12       | 6       | 0            |
| 2   | M     | 27    | 0        | 12       | 6       | 0            |
| 2   | N     | 27    | 0        | 12       | 2       | 0            |
| All | All   | 28041 | 0        | 28663    | 3938    | 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 69.

All (3938) 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:D:235:LEU:HD12 | 1:D:236:PHE:N    | 1.44                     | 1.30              |
| 1:L:334:LYS:NZ   | 1:L:367:VAL:HG13 | 1.51                     | 1.24              |
| 1:E:177:ALA:CA   | 1:E:180:ILE:HD12 | 1.69                     | 1.21              |
| 1:E:240:ILE:CD1  | 1:E:277:ALA:HB1  | 1.72                     | 1.18              |
| 1:F:318:ILE:HG13 | 1:F:319:PRO:HD3  | 1.23                     | 1.17              |
| 1:E:177:ALA:HA   | 1:E:180:ILE:CD1  | 1.76                     | 1.15              |
| 1:E:240:ILE:HD11 | 1:E:277:ALA:CB   | 1.77                     | 1.14              |
| 1:C:220:VAL:HG12 | 1:C:221:SER:H    | 1.11                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:262:ARG:HG2  | 1:D:262:ARG:HH11 | 1.05                     | 1.13              |
| 1:L:350:TYR:CD2  | 1:L:351:PRO:HD2  | 1.82                     | 1.13              |
| 1:F:340:THR:CG2  | 1:F:376:ASP:HB3  | 1.79                     | 1.12              |
| 1:A:343:ALA:HB2  | 1:A:376:ASP:HA   | 1.24                     | 1.12              |
| 1:E:344:GLN:O    | 1:E:348:LEU:HD12 | 1.48                     | 1.11              |
| 1:B:283:ILE:HA   | 1:B:286:LEU:HD12 | 1.22                     | 1.11              |
| 1:G:259:LYS:HB3  | 1:G:267:LYS:HG3  | 1.14                     | 1.11              |
| 1:L:140:VAL:HG11 | 1:L:320:LEU:HG   | 1.21                     | 1.10              |
| 1:L:343:ALA:HB2  | 1:L:376:ASP:HA   | 1.29                     | 1.10              |
| 1:G:320:LEU:HD22 | 1:G:359:LEU:HD13 | 1.31                     | 1.10              |
| 1:H:214:GLY:H    | 1:H:219:ALA:HB1  | 1.11                     | 1.10              |
| 1:L:224:GLU:HA   | 1:L:262:ARG:HH21 | 1.17                     | 1.10              |
| 1:D:318:ILE:HG13 | 1:D:319:PRO:HD3  | 1.31                     | 1.09              |
| 1:G:318:ILE:HG12 | 1:G:348:LEU:HD21 | 1.30                     | 1.09              |
| 1:J:189:GLU:HG3  | 1:J:190:PRO:HD2  | 1.34                     | 1.09              |
| 1:L:362:VAL:HG13 | 1:L:383:LEU:HD13 | 1.31                     | 1.09              |
| 1:M:318:ILE:HG13 | 1:M:319:PRO:HD3  | 1.15                     | 1.09              |
| 1:E:139:TYR:HB3  | 1:E:141:PHE:HE1  | 1.18                     | 1.08              |
| 1:C:181:HIS:CD2  | 1:C:191:PHE:HB2  | 1.89                     | 1.08              |
| 1:M:201:ARG:HB2  | 1:M:201:ARG:HH11 | 1.01                     | 1.07              |
| 1:D:275:ILE:H    | 1:D:275:ILE:HD12 | 1.20                     | 1.07              |
| 1:C:178:ARG:HH11 | 1:C:178:ARG:HG3  | 1.16                     | 1.06              |
| 1:M:194:LEU:HD21 | 1:M:237:LEU:HD23 | 1.34                     | 1.06              |
| 1:C:318:ILE:HG13 | 1:C:319:PRO:HD3  | 1.33                     | 1.06              |
| 1:N:240:ILE:HD11 | 1:N:277:ALA:HB1  | 1.09                     | 1.06              |
| 1:B:275:ILE:HD12 | 1:B:275:ILE:H    | 1.18                     | 1.05              |
| 1:G:189:GLU:HG3  | 1:G:190:PRO:HD2  | 1.38                     | 1.05              |
| 1:F:240:ILE:HD11 | 1:F:277:ALA:HB1  | 1.07                     | 1.04              |
| 1:F:340:THR:HG21 | 1:F:376:ASP:HB3  | 1.34                     | 1.04              |
| 1:A:318:ILE:HG12 | 1:A:348:LEU:HD21 | 1.40                     | 1.04              |
| 1:H:343:ALA:HB2  | 1:H:376:ASP:HA   | 1.34                     | 1.03              |
| 1:E:176:VAL:HG12 | 1:E:180:ILE:HD11 | 1.32                     | 1.03              |
| 1:H:293:ARG:HG2  | 1:H:293:ARG:HH11 | 1.21                     | 1.03              |
| 1:L:143:SER:HB2  | 1:L:144:PRO:HD2  | 1.37                     | 1.02              |
| 1:L:329:SER:HA   | 1:L:334:LYS:HE2  | 1.38                     | 1.02              |
| 1:N:146:MET:HE1  | 1:N:307:ILE:HG23 | 1.40                     | 1.02              |
| 1:M:211:TYR:HE1  | 1:M:223:LYS:HB2  | 1.18                     | 1.01              |
| 1:E:325:LEU:O    | 1:E:329:SER:HB2  | 1.59                     | 1.01              |
| 1:D:164:LEU:HD12 | 1:D:165:ILE:H    | 1.20                     | 1.01              |
| 1:E:282:ASN:ND2  | 1:E:285:GLU:HB2  | 1.76                     | 1.01              |
| 1:L:334:LYS:NZ   | 1:L:367:VAL:CG1  | 2.24                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:139:TYR:HB3  | 1:L:141:PHE:CE2  | 1.95                     | 1.01              |
| 1:C:150:LEU:HG   | 1:C:154:LYS:HZ1  | 1.26                     | 1.00              |
| 1:D:240:ILE:HG13 | 1:D:277:ALA:HB1  | 1.44                     | 1.00              |
| 1:E:309:PRO:HG2  | 1:E:312:GLU:HG3  | 1.40                     | 1.00              |
| 1:H:318:ILE:HD11 | 1:H:348:LEU:HD11 | 1.43                     | 1.00              |
| 1:I:318:ILE:HG13 | 1:I:319:PRO:HD3  | 1.44                     | 1.00              |
| 1:N:282:ASN:HD22 | 1:N:285:GLU:HG2  | 1.26                     | 0.99              |
| 1:K:198:SER:O    | 1:K:199:ILE:HG13 | 1.61                     | 0.99              |
| 1:J:282:ASN:HD22 | 1:J:285:GLU:HB2  | 1.27                     | 0.98              |
| 1:M:243:LEU:HD22 | 1:M:247:ALA:HB1  | 1.45                     | 0.98              |
| 1:M:180:ILE:HG21 | 1:M:276:LEU:HD11 | 1.43                     | 0.98              |
| 1:I:194:LEU:HD23 | 1:I:194:LEU:H    | 1.28                     | 0.98              |
| 1:D:207:GLU:HB3  | 1:D:226:PHE:HE1  | 1.25                     | 0.98              |
| 1:M:253:ARG:HG3  | 1:N:198:SER:HB2  | 1.47                     | 0.97              |
| 1:A:325:LEU:O    | 1:A:325:LEU:HD23 | 1.63                     | 0.97              |
| 1:G:168:GLU:O    | 1:G:171:VAL:HG23 | 1.63                     | 0.97              |
| 1:J:224:GLU:HG2  | 1:J:225:GLY:H    | 1.28                     | 0.97              |
| 1:E:363:ILE:O    | 1:E:367:VAL:HG23 | 1.63                     | 0.97              |
| 1:J:201:ARG:HB2  | 1:J:201:ARG:HH11 | 1.27                     | 0.97              |
| 1:C:235:LEU:HD12 | 1:C:236:PHE:N    | 1.79                     | 0.97              |
| 1:I:220:VAL:HG12 | 1:I:221:SER:H    | 1.28                     | 0.96              |
| 1:H:357:ARG:HH12 | 1:N:252:LEU:HD21 | 1.29                     | 0.96              |
| 1:F:240:ILE:CD1  | 1:F:277:ALA:HB1  | 1.96                     | 0.95              |
| 1:L:138:GLU:HG3  | 1:L:139:TYR:N    | 1.77                     | 0.95              |
| 1:B:217:THR:HG23 | 1:B:218:GLY:H    | 1.30                     | 0.95              |
| 1:E:201:ARG:HB2  | 1:E:201:ARG:HH11 | 1.32                     | 0.95              |
| 1:L:334:LYS:HZ2  | 1:L:367:VAL:HG13 | 1.13                     | 0.95              |
| 1:F:189:GLU:HG3  | 1:F:190:PRO:HD2  | 1.46                     | 0.95              |
| 1:H:189:GLU:HG3  | 1:H:190:PRO:HD2  | 1.47                     | 0.95              |
| 1:C:235:LEU:HD12 | 1:C:236:PHE:H    | 1.32                     | 0.95              |
| 1:I:261:TYR:HE1  | 1:J:199:ILE:HG12 | 1.30                     | 0.95              |
| 1:J:216:PHE:H    | 1:J:216:PHE:HD2  | 1.09                     | 0.95              |
| 1:L:143:SER:HB2  | 1:L:144:PRO:CD   | 1.95                     | 0.95              |
| 1:E:325:LEU:HD21 | 1:E:336:VAL:HG12 | 1.49                     | 0.94              |
| 1:K:164:LEU:HD12 | 1:K:165:ILE:H    | 1.33                     | 0.94              |
| 1:F:326:LYS:HE2  | 1:F:330:ARG:NH2  | 1.83                     | 0.94              |
| 1:F:309:PRO:HG3  | 1:F:311:ARG:NH1  | 1.82                     | 0.94              |
| 1:M:201:ARG:HB2  | 1:M:201:ARG:NH1  | 1.83                     | 0.93              |
| 1:N:228:GLU:OE2  | 1:N:262:ARG:NE   | 2.01                     | 0.93              |
| 1:H:214:GLY:N    | 1:H:219:ALA:HB1  | 1.81                     | 0.93              |
| 1:N:281:ARG:H    | 1:N:281:ARG:HD3  | 1.31                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:228:GLU:OE2  | 1:D:262:ARG:NE   | 2.02                     | 0.93              |
| 1:M:143:SER:HB2  | 1:M:144:PRO:HD2  | 1.51                     | 0.93              |
| 1:H:302:VAL:HG12 | 1:H:303:ILE:HG13 | 1.49                     | 0.93              |
| 1:B:314:LYS:H    | 1:B:314:LYS:HD2  | 1.33                     | 0.93              |
| 1:M:308:PRO:HG2  | 1:M:313:ARG:HD2  | 1.51                     | 0.93              |
| 1:N:240:ILE:HD11 | 1:N:277:ALA:CB   | 1.99                     | 0.92              |
| 1:C:150:LEU:HG   | 1:C:154:LYS:NZ   | 1.83                     | 0.92              |
| 1:N:201:ARG:HH11 | 1:N:201:ARG:HB2  | 1.33                     | 0.92              |
| 1:H:176:VAL:HG21 | 1:H:307:ILE:HD11 | 1.50                     | 0.92              |
| 1:N:146:MET:HE2  | 1:N:149:ILE:HD12 | 1.50                     | 0.92              |
| 1:E:214:GLY:HA2  | 1:E:219:ALA:HB3  | 1.52                     | 0.92              |
| 1:I:343:ALA:HB2  | 1:I:376:ASP:HA   | 1.52                     | 0.92              |
| 1:D:164:LEU:HD12 | 1:D:165:ILE:N    | 1.83                     | 0.91              |
| 1:B:317:ILE:HB   | 1:B:348:LEU:HD23 | 1.53                     | 0.91              |
| 1:E:302:VAL:HG12 | 1:E:303:ILE:HG12 | 1.52                     | 0.91              |
| 1:H:362:VAL:HG22 | 1:H:365:ARG:NH2  | 1.85                     | 0.91              |
| 1:H:362:VAL:HG22 | 1:H:365:ARG:HH21 | 1.34                     | 0.91              |
| 1:M:211:TYR:CE1  | 1:M:223:LYS:HB2  | 2.05                     | 0.91              |
| 1:D:262:ARG:HG2  | 1:D:262:ARG:NH1  | 1.80                     | 0.91              |
| 1:L:362:VAL:HG13 | 1:L:383:LEU:CD1  | 1.99                     | 0.91              |
| 1:B:362:VAL:HG13 | 1:B:384:VAL:HG21 | 1.51                     | 0.91              |
| 1:G:149:ILE:O    | 1:G:153:ILE:HG12 | 1.69                     | 0.91              |
| 1:G:212:GLU:HB2  | 1:G:262:ARG:O    | 1.69                     | 0.91              |
| 1:E:152:LYS:HG2  | 1:F:369:PHE:CE1  | 2.05                     | 0.91              |
| 1:H:194:LEU:HD21 | 1:H:237:LEU:HD23 | 1.53                     | 0.91              |
| 1:D:235:LEU:HD12 | 1:D:236:PHE:H    | 1.16                     | 0.91              |
| 1:K:264:GLY:HA2  | 1:L:207:GLU:OE2  | 1.71                     | 0.91              |
| 1:E:177:ALA:HA   | 1:E:180:ILE:HD12 | 0.92                     | 0.90              |
| 1:K:201:ARG:HH11 | 1:K:201:ARG:HB2  | 1.37                     | 0.90              |
| 1:E:139:TYR:HB3  | 1:E:141:PHE:CE1  | 2.07                     | 0.90              |
| 1:K:213:LYS:HD2  | 1:K:220:VAL:O    | 1.71                     | 0.90              |
| 1:C:140:VAL:HG11 | 1:C:320:LEU:HD23 | 1.54                     | 0.90              |
| 1:F:240:ILE:HD11 | 1:F:277:ALA:CB   | 1.98                     | 0.90              |
| 1:H:214:GLY:H    | 1:H:219:ALA:CB   | 1.83                     | 0.90              |
| 1:L:329:SER:CA   | 1:L:334:LYS:HE2  | 2.00                     | 0.90              |
| 1:M:164:LEU:HD21 | 1:M:283:ILE:HG13 | 1.53                     | 0.90              |
| 1:B:318:ILE:HG12 | 1:B:348:LEU:HD21 | 1.53                     | 0.90              |
| 1:G:240:ILE:HG13 | 1:G:277:ALA:HB1  | 1.52                     | 0.90              |
| 1:L:227:PHE:CE2  | 1:L:254:VAL:HG11 | 2.06                     | 0.90              |
| 1:E:165:ILE:HD11 | 1:E:177:ALA:HB2  | 1.52                     | 0.89              |
| 1:C:220:VAL:HG12 | 1:C:221:SER:N    | 1.86                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:171:VAL:HG12 | 1:E:355:ASN:OD1  | 1.71                     | 0.89              |
| 1:H:255:ILE:HG12 | 1:H:275:ILE:CD1  | 2.03                     | 0.89              |
| 1:L:165:ILE:H    | 1:L:278:ALA:HB2  | 1.35                     | 0.89              |
| 1:E:354:GLY:HA3  | 1:E:358:GLU:HB2  | 1.54                     | 0.88              |
| 1:E:365:ARG:HH11 | 1:E:383:LEU:HD22 | 1.38                     | 0.88              |
| 1:H:156:ILE:HD12 | 1:H:303:ILE:HD13 | 1.54                     | 0.88              |
| 1:H:234:THR:HG21 | 1:H:276:LEU:HD12 | 1.55                     | 0.88              |
| 1:N:145:LYS:HA   | 1:N:148:GLU:HG2  | 1.55                     | 0.88              |
| 1:C:251:LEU:HD22 | 1:C:255:ILE:HD11 | 1.55                     | 0.88              |
| 1:H:255:ILE:HG12 | 1:H:275:ILE:HD13 | 1.55                     | 0.88              |
| 1:H:198:SER:HB2  | 1:N:250:LYS:HB2  | 1.55                     | 0.88              |
| 1:M:318:ILE:HG23 | 1:M:348:LEU:HD21 | 1.55                     | 0.88              |
| 1:I:240:ILE:HD11 | 1:I:277:ALA:HB1  | 1.55                     | 0.88              |
| 1:G:224:GLU:HG2  | 1:G:225:GLY:H    | 1.39                     | 0.88              |
| 1:L:140:VAL:CG1  | 1:L:320:LEU:HG   | 2.03                     | 0.88              |
| 1:N:251:LEU:HD22 | 1:N:296:LEU:HD21 | 1.54                     | 0.88              |
| 1:A:275:ILE:H    | 1:A:275:ILE:HD12 | 1.38                     | 0.88              |
| 1:E:227:PHE:CE2  | 1:E:254:VAL:HG11 | 2.09                     | 0.88              |
| 1:E:240:ILE:HD11 | 1:E:277:ALA:HB1  | 0.91                     | 0.88              |
| 1:J:343:ALA:HB2  | 1:J:376:ASP:HA   | 1.56                     | 0.88              |
| 1:F:201:ARG:HH11 | 1:F:201:ARG:HB2  | 1.37                     | 0.88              |
| 1:L:229:LEU:HD13 | 1:L:229:LEU:C    | 1.98                     | 0.88              |
| 1:H:143:SER:HA   | 1:H:147:LYS:HE3  | 1.56                     | 0.87              |
| 1:L:163:VAL:HG22 | 1:L:303:ILE:HG21 | 1.54                     | 0.87              |
| 1:E:267:LYS:H    | 1:E:267:LYS:HD2  | 1.38                     | 0.87              |
| 1:J:318:ILE:HG13 | 1:J:319:PRO:HD3  | 1.54                     | 0.87              |
| 1:F:347:LEU:HD21 | 1:F:380:LEU:HD12 | 1.57                     | 0.87              |
| 1:I:189:GLU:HB3  | 1:I:190:PRO:HD2  | 1.56                     | 0.87              |
| 1:B:240:ILE:HG13 | 1:B:277:ALA:HB1  | 1.55                     | 0.87              |
| 1:F:153:ILE:HG23 | 1:F:180:ILE:HG12 | 1.57                     | 0.87              |
| 1:L:189:GLU:HG3  | 1:L:190:PRO:HD2  | 1.57                     | 0.87              |
| 1:F:223:LYS:O    | 1:F:225:GLY:N    | 2.07                     | 0.86              |
| 1:M:318:ILE:CG1  | 1:M:319:PRO:HD3  | 2.03                     | 0.86              |
| 1:L:347:LEU:O    | 1:L:349:SER:N    | 2.08                     | 0.86              |
| 1:D:282:ASN:HD22 | 1:D:285:GLU:HB2  | 1.39                     | 0.86              |
| 1:L:165:ILE:O    | 1:L:278:ALA:HB1  | 1.75                     | 0.86              |
| 1:B:189:GLU:HG3  | 1:B:190:PRO:HD2  | 1.57                     | 0.86              |
| 1:M:181:HIS:CE1  | 1:M:187:SER:HA   | 2.11                     | 0.86              |
| 1:C:143:SER:O    | 1:C:147:LYS:HB2  | 1.75                     | 0.86              |
| 1:I:284:LYS:HE2  | 1:I:297:TYR:OH   | 1.75                     | 0.86              |
| 1:M:143:SER:O    | 1:M:147:LYS:HB2  | 1.76                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:141:PHE:CB   | 1:I:150:LEU:HD11 | 2.06                     | 0.86              |
| 1:M:146:MET:HE3  | 1:M:149:ILE:HD12 | 1.55                     | 0.86              |
| 1:E:292:PHE:CZ   | 1:E:296:LEU:HD12 | 2.11                     | 0.86              |
| 1:L:239:GLU:O    | 1:L:241:GLY:N    | 2.07                     | 0.86              |
| 1:N:325:LEU:O    | 1:N:325:LEU:HD23 | 1.76                     | 0.85              |
| 1:H:192:VAL:HG21 | 1:H:230:ALA:HB2  | 1.58                     | 0.85              |
| 1:M:318:ILE:HG13 | 1:M:319:PRO:CD   | 2.03                     | 0.85              |
| 1:N:259:LYS:HG2  | 1:N:270:GLU:HB2  | 1.58                     | 0.85              |
| 1:B:275:ILE:HD12 | 1:B:275:ILE:N    | 1.91                     | 0.85              |
| 1:F:143:SER:HB2  | 1:F:144:PRO:HD2  | 1.59                     | 0.85              |
| 1:N:318:ILE:HG13 | 1:N:319:PRO:HD3  | 1.58                     | 0.85              |
| 1:B:146:MET:HG3  | 1:B:313:ARG:HH21 | 1.41                     | 0.85              |
| 1:A:362:VAL:HG13 | 1:A:383:LEU:HD12 | 1.59                     | 0.85              |
| 1:D:143:SER:HB2  | 1:D:315:GLU:HB2  | 1.55                     | 0.85              |
| 1:E:354:GLY:N    | 1:E:358:GLU:OE1  | 2.10                     | 0.85              |
| 1:K:318:ILE:HG12 | 1:K:348:LEU:HD21 | 1.58                     | 0.84              |
| 1:I:141:PHE:CD2  | 1:I:150:LEU:HD21 | 2.11                     | 0.84              |
| 1:M:256:GLU:HG2  | 1:M:257:SER:H    | 1.41                     | 0.84              |
| 1:E:150:LEU:HD12 | 1:E:150:LEU:O    | 1.76                     | 0.84              |
| 1:F:153:ILE:HG21 | 1:F:179:LEU:HD22 | 1.60                     | 0.84              |
| 1:N:200:PRO:HG2  | 1:N:203:ILE:HD12 | 1.59                     | 0.84              |
| 1:C:365:ARG:NH1  | 1:C:383:LEU:HD22 | 1.93                     | 0.84              |
| 1:D:284:LYS:HG2  | 1:D:297:TYR:OH   | 1.78                     | 0.84              |
| 1:H:146:MET:HG2  | 1:H:313:ARG:CZ   | 2.08                     | 0.84              |
| 1:N:139:TYR:CE2  | 1:N:175:VAL:HG13 | 2.12                     | 0.84              |
| 1:K:209:PHE:CD2  | 1:K:250:LYS:HD3  | 2.12                     | 0.84              |
| 1:L:376:ASP:O    | 1:L:378:GLY:N    | 2.10                     | 0.84              |
| 1:D:357:ARG:HD3  | 2:D:2:ADP:H5'2   | 1.59                     | 0.84              |
| 1:L:141:PHE:CE1  | 1:L:150:LEU:HG   | 2.12                     | 0.84              |
| 1:L:334:LYS:CE   | 1:L:367:VAL:HG13 | 2.08                     | 0.84              |
| 1:K:139:TYR:O    | 1:K:140:VAL:HG23 | 1.75                     | 0.84              |
| 1:K:279:THR:HG21 | 1:K:283:ILE:HD11 | 1.59                     | 0.84              |
| 1:D:235:LEU:CD1  | 1:D:236:PHE:N    | 2.38                     | 0.83              |
| 1:J:365:ARG:HD2  | 1:J:383:LEU:HD22 | 1.60                     | 0.83              |
| 1:C:178:ARG:HH11 | 1:C:178:ARG:CG   | 1.90                     | 0.83              |
| 1:I:220:VAL:HG12 | 1:I:221:SER:N    | 1.90                     | 0.83              |
| 1:C:300:LEU:O    | 1:C:302:VAL:N    | 2.10                     | 0.83              |
| 1:D:207:GLU:HB3  | 1:D:226:PHE:CE1  | 2.14                     | 0.83              |
| 1:I:194:LEU:HD13 | 1:I:226:PHE:HD1  | 1.44                     | 0.83              |
| 1:J:318:ILE:HG12 | 1:J:348:LEU:HD21 | 1.58                     | 0.83              |
| 1:L:141:PHE:CD1  | 1:L:150:LEU:HG   | 2.14                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:283:ILE:HA   | 1:M:286:LEU:HD12 | 1.58                     | 0.83              |
| 1:A:358:GLU:O    | 1:A:362:VAL:HG23 | 1.78                     | 0.83              |
| 1:H:194:LEU:HD23 | 1:H:194:LEU:H    | 1.44                     | 0.83              |
| 1:A:143:SER:HB2  | 1:A:144:PRO:HD2  | 1.61                     | 0.82              |
| 1:L:240:ILE:O    | 1:L:240:ILE:HG22 | 1.78                     | 0.82              |
| 1:F:238:ASP:O    | 1:F:239:GLU:HG2  | 1.79                     | 0.82              |
| 1:L:140:VAL:HG11 | 1:L:320:LEU:CG   | 2.07                     | 0.82              |
| 1:L:240:ILE:HD11 | 1:L:277:ALA:HB3  | 1.59                     | 0.82              |
| 1:L:163:VAL:HG22 | 1:L:303:ILE:CG2  | 2.09                     | 0.82              |
| 1:F:240:ILE:O    | 1:F:242:GLU:N    | 2.13                     | 0.82              |
| 1:G:263:LEU:CG   | 1:G:264:GLY:H    | 1.92                     | 0.82              |
| 1:I:172:GLY:O    | 1:I:176:VAL:HG23 | 1.80                     | 0.82              |
| 1:C:146:MET:HE2  | 1:C:313:ARG:NH2  | 1.94                     | 0.82              |
| 1:J:200:PRO:HG2  | 1:J:203:ILE:HD12 | 1.59                     | 0.82              |
| 1:N:245:LEU:HD22 | 1:N:293:ARG:HG3  | 1.60                     | 0.82              |
| 1:K:207:GLU:OE1  | 1:K:207:GLU:HA   | 1.78                     | 0.82              |
| 1:C:181:HIS:HD2  | 1:C:191:PHE:CD1  | 1.98                     | 0.82              |
| 1:F:343:ALA:O    | 1:F:345:GLU:N    | 2.12                     | 0.82              |
| 1:H:168:GLU:HG3  | 1:H:311:ARG:HH22 | 1.44                     | 0.82              |
| 1:K:186:ARG:HH22 | 1:K:272:ASN:ND2  | 1.78                     | 0.82              |
| 1:D:211:TYR:CE1  | 1:D:223:LYS:HB3  | 2.14                     | 0.82              |
| 1:F:194:LEU:HD23 | 1:F:194:LEU:H    | 1.42                     | 0.82              |
| 1:B:324:PHE:HD1  | 1:B:363:ILE:HD12 | 1.44                     | 0.81              |
| 1:E:354:GLY:CA   | 1:E:358:GLU:HB2  | 2.09                     | 0.81              |
| 1:L:334:LYS:HE3  | 1:L:336:VAL:HB   | 1.60                     | 0.81              |
| 1:C:240:ILE:HG12 | 1:C:277:ALA:HB1  | 1.60                     | 0.81              |
| 1:D:309:PRO:HB2  | 1:D:311:ARG:HG2  | 1.61                     | 0.81              |
| 1:E:309:PRO:HB2  | 1:E:311:ARG:HD3  | 1.61                     | 0.81              |
| 1:H:197:ALA:O    | 1:N:246:GLU:HA   | 1.79                     | 0.81              |
| 1:K:235:LEU:HB2  | 1:K:273:VAL:HG11 | 1.61                     | 0.81              |
| 1:N:146:MET:CE   | 1:N:307:ILE:HG23 | 2.10                     | 0.81              |
| 1:C:181:HIS:HD2  | 1:C:191:PHE:HB2  | 1.38                     | 0.81              |
| 1:E:310:LEU:O    | 1:E:317:ILE:HD11 | 1.80                     | 0.81              |
| 1:I:220:VAL:CG1  | 1:I:221:SER:H    | 1.93                     | 0.81              |
| 1:F:172:GLY:HA2  | 2:F:4:ADP:PA     | 2.21                     | 0.81              |
| 1:I:301:GLY:O    | 1:J:365:ARG:NH2  | 2.14                     | 0.81              |
| 1:M:207:GLU:O    | 1:M:226:PHE:HD1  | 1.64                     | 0.81              |
| 1:E:137:GLU:HG2  | 1:E:138:GLU:H    | 1.45                     | 0.81              |
| 1:E:358:GLU:O    | 1:E:362:VAL:HG23 | 1.81                     | 0.81              |
| 1:H:265:GLY:O    | 1:H:266:ARG:HD3  | 1.80                     | 0.81              |
| 1:I:143:SER:HB3  | 1:I:316:ASP:OD2  | 1.81                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:138:GLU:HG3  | 1:L:139:TYR:H    | 1.44                     | 0.81              |
| 1:I:240:ILE:CD1  | 1:I:277:ALA:HB1  | 2.10                     | 0.81              |
| 1:K:216:PHE:CD1  | 1:K:219:ALA:HB2  | 2.16                     | 0.81              |
| 1:C:227:PHE:CE2  | 1:C:254:VAL:HG11 | 2.15                     | 0.81              |
| 1:A:240:ILE:HG13 | 1:A:277:ALA:HB1  | 1.61                     | 0.81              |
| 1:E:138:GLU:HB2  | 1:E:323:HIS:NE2  | 1.95                     | 0.81              |
| 1:G:231:ASP:OD1  | 1:G:271:VAL:HA   | 1.81                     | 0.81              |
| 1:I:252:LEU:HD13 | 1:I:296:LEU:HA   | 1.60                     | 0.81              |
| 1:K:204:PHE:HE2  | 1:K:208:LEU:HD12 | 1.47                     | 0.80              |
| 1:B:321:ALA:HA   | 1:B:363:ILE:HD11 | 1.63                     | 0.80              |
| 1:N:165:ILE:O    | 1:N:278:ALA:HA   | 1.81                     | 0.80              |
| 1:K:216:PHE:HD1  | 1:K:219:ALA:HB2  | 1.46                     | 0.80              |
| 1:I:267:LYS:H    | 1:I:267:LYS:HD2  | 1.46                     | 0.80              |
| 1:M:249:ALA:HA   | 1:M:293:ARG:HH12 | 1.46                     | 0.80              |
| 1:B:178:ARG:HD2  | 1:B:191:PHE:CE2  | 2.16                     | 0.80              |
| 1:E:316:ASP:O    | 1:E:319:PRO:HD2  | 1.81                     | 0.80              |
| 1:K:161:CYS:HB2  | 1:K:162:PRO:HD2  | 1.61                     | 0.80              |
| 1:K:215:ALA:H    | 1:K:219:ALA:CB   | 1.95                     | 0.80              |
| 1:L:350:TYR:CD2  | 1:L:351:PRO:CD   | 2.62                     | 0.80              |
| 1:E:279:THR:HG21 | 1:E:283:ILE:HD11 | 1.64                     | 0.79              |
| 1:G:209:PHE:O    | 1:G:225:GLY:HA3  | 1.82                     | 0.79              |
| 1:L:141:PHE:HD2  | 1:L:141:PHE:N    | 1.79                     | 0.79              |
| 1:H:189:GLU:CG   | 1:H:190:PRO:HD2  | 2.13                     | 0.79              |
| 1:D:350:TYR:CD1  | 1:D:351:PRO:HD2  | 2.17                     | 0.79              |
| 1:J:200:PRO:CG   | 1:J:203:ILE:HD12 | 2.11                     | 0.79              |
| 1:L:281:ARG:HD2  | 1:L:282:ASN:H    | 1.46                     | 0.79              |
| 1:L:334:LYS:HZ2  | 1:L:367:VAL:CG1  | 1.88                     | 0.79              |
| 1:N:328:PHE:O    | 1:N:367:VAL:HG11 | 1.82                     | 0.79              |
| 1:C:181:HIS:CD2  | 1:C:191:PHE:HD1  | 2.01                     | 0.79              |
| 1:L:339:PHE:CE2  | 1:L:375:ILE:HD11 | 2.18                     | 0.79              |
| 1:N:359:LEU:O    | 1:N:363:ILE:HG13 | 1.83                     | 0.79              |
| 1:M:191:PHE:HE2  | 1:M:193:ALA:HB2  | 1.46                     | 0.79              |
| 1:D:235:LEU:HD11 | 1:D:237:LEU:HD23 | 1.63                     | 0.79              |
| 1:H:145:LYS:HB2  | 1:H:313:ARG:HH21 | 1.45                     | 0.79              |
| 1:J:316:ASP:O    | 1:J:319:PRO:HD2  | 1.80                     | 0.79              |
| 1:K:143:SER:HB2  | 1:K:144:PRO:HD2  | 1.62                     | 0.79              |
| 1:M:363:ILE:H    | 1:M:363:ILE:CD1  | 1.96                     | 0.79              |
| 1:B:318:ILE:HG13 | 1:B:319:PRO:HD3  | 1.63                     | 0.79              |
| 1:D:235:LEU:CD1  | 1:D:236:PHE:H    | 1.96                     | 0.79              |
| 1:E:234:THR:HG23 | 1:E:274:ARG:HB3  | 1.65                     | 0.79              |
| 1:M:167:GLY:O    | 1:M:280:ASN:HA   | 1.83                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:203:ILE:HG22 | 1:D:207:GLU:HG2  | 1.65                     | 0.79              |
| 1:I:314:LYS:HA   | 1:I:317:ILE:CD1  | 2.13                     | 0.79              |
| 1:M:246:GLU:O    | 1:M:249:ALA:HB3  | 1.83                     | 0.79              |
| 1:C:153:ILE:HG21 | 1:C:179:LEU:HD22 | 1.64                     | 0.79              |
| 1:F:309:PRO:HG3  | 1:F:311:ARG:HH12 | 1.47                     | 0.79              |
| 1:E:196:VAL:O    | 1:E:196:VAL:HG12 | 1.83                     | 0.78              |
| 1:H:350:TYR:HB3  | 1:H:351:PRO:HA   | 1.65                     | 0.78              |
| 1:K:282:ASN:HD22 | 1:K:285:GLU:HB2  | 1.47                     | 0.78              |
| 1:H:196:VAL:HA   | 1:H:204:PHE:CE1  | 2.19                     | 0.78              |
| 1:C:172:GLY:O    | 1:C:176:VAL:HG23 | 1.83                     | 0.78              |
| 1:L:195:ASN:HB3  | 1:L:198:SER:OG   | 1.84                     | 0.78              |
| 1:E:269:ILE:H    | 1:E:269:ILE:HD12 | 1.49                     | 0.78              |
| 1:F:178:ARG:HH11 | 1:F:178:ARG:HG3  | 1.46                     | 0.78              |
| 1:G:340:THR:OG1  | 1:G:342:SER:HB3  | 1.82                     | 0.78              |
| 1:K:205:GLU:OE1  | 1:K:246:GLU:HB2  | 1.83                     | 0.78              |
| 1:K:249:ALA:HB2  | 1:K:293:ARG:HH11 | 1.49                     | 0.78              |
| 1:L:138:GLU:CG   | 1:L:139:TYR:H    | 1.93                     | 0.78              |
| 1:M:146:MET:HG3  | 1:M:313:ARG:HE   | 1.47                     | 0.78              |
| 1:E:192:VAL:CG2  | 1:E:230:ALA:HB2  | 2.13                     | 0.78              |
| 1:E:216:PHE:CD2  | 1:E:219:ALA:HB2  | 2.18                     | 0.78              |
| 1:K:143:SER:HB2  | 1:K:315:GLU:HB2  | 1.64                     | 0.78              |
| 1:M:281:ARG:HG2  | 1:M:286:LEU:HD21 | 1.66                     | 0.78              |
| 1:A:189:GLU:HG3  | 1:A:190:PRO:HD2  | 1.66                     | 0.78              |
| 1:N:200:PRO:CG   | 1:N:203:ILE:HD12 | 2.14                     | 0.78              |
| 1:N:357:ARG:HH12 | 1:N:361:ASN:CG   | 1.92                     | 0.78              |
| 1:A:139:TYR:CD2  | 1:A:175:VAL:HG13 | 2.19                     | 0.78              |
| 1:D:192:VAL:O    | 1:D:192:VAL:HG12 | 1.84                     | 0.78              |
| 1:C:253:ARG:HG2  | 1:C:253:ARG:HH11 | 1.49                     | 0.77              |
| 1:E:167:GLY:O    | 1:E:173:LYS:HE3  | 1.84                     | 0.77              |
| 1:H:356:VAL:HG11 | 2:H:14:ADP:C8    | 2.20                     | 0.77              |
| 1:E:165:ILE:CD1  | 1:E:177:ALA:HB2  | 2.14                     | 0.77              |
| 1:F:325:LEU:HD21 | 1:F:336:VAL:HG12 | 1.66                     | 0.77              |
| 1:C:314:LYS:HA   | 1:C:317:ILE:HG13 | 1.66                     | 0.77              |
| 1:D:210:GLY:HA3  | 1:D:225:GLY:H    | 1.48                     | 0.77              |
| 1:L:311:ARG:HG2  | 1:L:351:PRO:O    | 1.83                     | 0.77              |
| 1:E:325:LEU:O    | 1:E:325:LEU:HD23 | 1.85                     | 0.77              |
| 1:F:357:ARG:HH11 | 1:F:357:ARG:HG3  | 1.49                     | 0.77              |
| 1:B:275:ILE:H    | 1:B:275:ILE:CD1  | 1.93                     | 0.77              |
| 1:M:143:SER:CB   | 1:M:144:PRO:HD2  | 2.11                     | 0.77              |
| 1:E:203:ILE:O    | 1:E:206:ALA:HB3  | 1.85                     | 0.77              |
| 1:F:176:VAL:O    | 1:F:180:ILE:HG13 | 1.84                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:350:TYR:HD2  | 1:L:352:TRP:H    | 1.33                     | 0.77              |
| 1:G:252:LEU:HB2  | 1:G:296:LEU:HD23 | 1.66                     | 0.77              |
| 1:J:332:TYR:CE1  | 1:J:368:LEU:HD21 | 2.19                     | 0.77              |
| 1:L:194:LEU:HD21 | 1:L:237:LEU:HD23 | 1.67                     | 0.77              |
| 1:M:189:GLU:HG3  | 1:M:190:PRO:HD2  | 1.67                     | 0.77              |
| 1:A:325:LEU:HD13 | 1:A:338:GLY:HA2  | 1.67                     | 0.76              |
| 1:L:334:LYS:HZ3  | 1:L:367:VAL:CG1  | 1.95                     | 0.76              |
| 1:N:245:LEU:HA   | 1:N:248:GLN:HE21 | 1.48                     | 0.76              |
| 1:G:263:LEU:CD2  | 1:G:264:GLY:H    | 1.97                     | 0.76              |
| 1:E:192:VAL:HG21 | 1:E:230:ALA:HB2  | 1.67                     | 0.76              |
| 1:F:347:LEU:HD21 | 1:F:380:LEU:CD1  | 2.15                     | 0.76              |
| 1:I:377:ARG:HD2  | 1:I:381:SER:HB3  | 1.68                     | 0.76              |
| 1:L:140:VAL:O    | 1:L:140:VAL:HG12 | 1.84                     | 0.76              |
| 1:N:208:LEU:HA   | 1:N:226:PHE:HB2  | 1.68                     | 0.76              |
| 1:H:240:ILE:HG13 | 1:H:277:ALA:HB1  | 1.67                     | 0.76              |
| 1:I:283:ILE:O    | 1:I:287:VAL:HG23 | 1.84                     | 0.76              |
| 1:K:325:LEU:HD13 | 1:K:338:GLY:HA2  | 1.68                     | 0.76              |
| 1:L:314:LYS:HA   | 1:L:317:ILE:CD1  | 2.15                     | 0.76              |
| 1:A:252:LEU:HD13 | 1:A:296:LEU:HA   | 1.67                     | 0.76              |
| 1:C:150:LEU:CG   | 1:C:154:LYS:HZ1  | 1.96                     | 0.76              |
| 1:C:176:VAL:O    | 1:C:180:ILE:HG13 | 1.86                     | 0.76              |
| 1:H:161:CYS:HB2  | 1:H:162:PRO:HD2  | 1.68                     | 0.76              |
| 1:M:256:GLU:HG2  | 1:M:257:SER:N    | 2.01                     | 0.76              |
| 1:H:250:LYS:HG3  | 1:I:198:SER:HB2  | 1.66                     | 0.76              |
| 1:F:157:SER:OG   | 1:F:183:LEU:HB2  | 1.86                     | 0.75              |
| 1:H:254:VAL:HG22 | 1:H:260:PHE:HB3  | 1.67                     | 0.75              |
| 1:L:248:GLN:HE22 | 1:L:292:PHE:HA   | 1.49                     | 0.75              |
| 1:N:209:PHE:CD1  | 1:N:250:LYS:HD3  | 2.20                     | 0.75              |
| 1:N:281:ARG:HD3  | 1:N:281:ARG:N    | 1.99                     | 0.75              |
| 1:I:173:LYS:HE3  | 2:I:8:ADP:O1B    | 1.87                     | 0.75              |
| 1:J:350:TYR:CD1  | 1:J:351:PRO:HD2  | 2.22                     | 0.75              |
| 1:D:158:CYS:HA   | 1:D:185:ASP:OD1  | 1.87                     | 0.75              |
| 1:E:355:ASN:H    | 1:E:355:ASN:HD22 | 1.34                     | 0.75              |
| 1:G:263:LEU:HD23 | 1:G:264:GLY:H    | 1.51                     | 0.75              |
| 1:I:208:LEU:HD21 | 1:I:227:PHE:CD1  | 2.21                     | 0.75              |
| 1:L:250:LYS:O    | 1:L:253:ARG:HB3  | 1.87                     | 0.75              |
| 1:M:139:TYR:HB3  | 2:M:12:ADP:N1    | 2.02                     | 0.75              |
| 1:N:325:LEU:HD23 | 1:N:325:LEU:C    | 2.11                     | 0.75              |
| 1:D:237:LEU:HD12 | 1:D:243:LEU:HD11 | 1.68                     | 0.75              |
| 1:E:292:PHE:HE2  | 1:E:296:LEU:HB3  | 1.50                     | 0.75              |
| 1:F:355:ASN:OD1  | 1:F:355:ASN:N    | 2.17                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:141:PHE:N    | 1:L:141:PHE:CD2  | 2.49                     | 0.75              |
| 1:L:340:THR:CG2  | 1:L:376:ASP:HB3  | 2.15                     | 0.75              |
| 1:M:227:PHE:CE2  | 1:M:273:VAL:HG21 | 2.22                     | 0.75              |
| 1:I:253:ARG:NE   | 1:J:198:SER:HB2  | 2.02                     | 0.75              |
| 1:K:252:LEU:HB2  | 1:K:296:LEU:HD23 | 1.68                     | 0.75              |
| 1:M:201:ARG:HH11 | 1:M:201:ARG:CB   | 1.91                     | 0.75              |
| 1:N:153:ILE:HG21 | 1:N:179:LEU:HD22 | 1.67                     | 0.75              |
| 1:B:192:VAL:HG21 | 1:B:230:ALA:HB2  | 1.69                     | 0.75              |
| 1:B:201:ARG:HB2  | 1:B:201:ARG:NH1  | 2.00                     | 0.75              |
| 1:F:275:ILE:H    | 1:F:275:ILE:HD12 | 1.52                     | 0.75              |
| 1:G:245:LEU:HD22 | 1:G:248:GLN:NE2  | 2.01                     | 0.75              |
| 1:I:297:TYR:HD2  | 1:I:298:TYR:CD1  | 2.04                     | 0.75              |
| 1:J:282:ASN:ND2  | 1:J:285:GLU:HB2  | 2.00                     | 0.75              |
| 1:J:365:ARG:HD2  | 1:J:383:LEU:CD2  | 2.16                     | 0.75              |
| 1:K:302:VAL:HG21 | 1:L:361:ASN:HB3  | 1.68                     | 0.75              |
| 1:N:240:ILE:CD1  | 1:N:277:ALA:HB1  | 2.05                     | 0.75              |
| 1:B:176:VAL:O    | 1:B:180:ILE:HG13 | 1.86                     | 0.75              |
| 1:D:235:LEU:HD11 | 1:D:237:LEU:CD2  | 2.17                     | 0.75              |
| 1:L:281:ARG:HD2  | 1:L:282:ASN:N    | 2.01                     | 0.75              |
| 1:N:143:SER:HB2  | 1:N:144:PRO:HD2  | 1.68                     | 0.75              |
| 1:A:340:THR:OG1  | 1:A:376:ASP:HB3  | 1.87                     | 0.74              |
| 1:E:292:PHE:CE2  | 1:E:296:LEU:HD12 | 2.22                     | 0.74              |
| 1:H:320:LEU:HB3  | 1:H:324:PHE:HE1  | 1.52                     | 0.74              |
| 1:M:347:LEU:HD21 | 1:M:380:LEU:HG   | 1.69                     | 0.74              |
| 1:N:246:GLU:CD   | 1:N:246:GLU:H    | 1.89                     | 0.74              |
| 1:F:311:ARG:HH11 | 1:F:311:ARG:HG2  | 1.52                     | 0.74              |
| 1:I:176:VAL:O    | 1:I:180:ILE:HG13 | 1.87                     | 0.74              |
| 1:F:163:VAL:HG13 | 1:F:303:ILE:HG22 | 1.69                     | 0.74              |
| 1:L:314:LYS:HA   | 1:L:317:ILE:HD11 | 1.67                     | 0.74              |
| 1:C:194:LEU:H    | 1:C:194:LEU:CD2  | 2.00                     | 0.74              |
| 1:M:171:VAL:HB   | 1:M:307:ILE:HG22 | 1.68                     | 0.74              |
| 1:G:189:GLU:HG2  | 1:G:232:GLY:O    | 1.87                     | 0.74              |
| 1:M:168:GLU:OE1  | 1:M:309:PRO:HB3  | 1.87                     | 0.74              |
| 1:E:157:SER:HB3  | 1:E:183:LEU:O    | 1.88                     | 0.74              |
| 1:F:213:LYS:HD3  | 1:G:220:VAL:HG11 | 1.69                     | 0.74              |
| 1:I:204:PHE:HE2  | 1:I:208:LEU:HD12 | 1.51                     | 0.74              |
| 1:H:377:ARG:HG2  | 1:H:381:SER:HB3  | 1.70                     | 0.74              |
| 1:I:256:GLU:HG2  | 1:I:299:ARG:HE   | 1.51                     | 0.74              |
| 1:L:315:GLU:N    | 1:L:315:GLU:OE1  | 2.20                     | 0.74              |
| 1:B:194:LEU:HD21 | 1:B:237:LEU:HD23 | 1.69                     | 0.74              |
| 1:D:337:GLU:OE1  | 1:D:373:LYS:HD3  | 1.87                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:380:LEU:O    | 1:B:384:VAL:HB   | 1.88                     | 0.74              |
| 1:C:165:ILE:HB   | 1:C:278:ALA:HB2  | 1.67                     | 0.74              |
| 1:F:340:THR:HG23 | 1:F:376:ASP:HB3  | 1.69                     | 0.74              |
| 1:J:208:LEU:HA   | 1:J:226:PHE:HB2  | 1.69                     | 0.74              |
| 1:K:314:LYS:HA   | 1:K:317:ILE:HG13 | 1.70                     | 0.74              |
| 1:E:205:GLU:OE2  | 1:E:246:GLU:HB2  | 1.87                     | 0.73              |
| 1:I:194:LEU:HD23 | 1:I:194:LEU:N    | 2.02                     | 0.73              |
| 1:J:172:GLY:O    | 1:J:176:VAL:HG23 | 1.88                     | 0.73              |
| 1:M:192:VAL:O    | 1:M:235:LEU:HD12 | 1.87                     | 0.73              |
| 1:L:176:VAL:O    | 1:L:180:ILE:HG13 | 1.88                     | 0.73              |
| 1:L:224:GLU:HA   | 1:L:262:ARG:NH2  | 1.99                     | 0.73              |
| 1:B:192:VAL:CG2  | 1:B:230:ALA:HB2  | 2.18                     | 0.73              |
| 1:C:181:HIS:CE1  | 1:C:187:SER:HA   | 2.24                     | 0.73              |
| 1:D:143:SER:HB2  | 1:D:144:PRO:HD2  | 1.70                     | 0.73              |
| 1:D:266:ARG:HH22 | 1:E:207:GLU:HG2  | 1.54                     | 0.73              |
| 1:L:298:TYR:CE1  | 1:M:354:GLY:HA3  | 2.23                     | 0.73              |
| 1:B:227:PHE:CE2  | 1:B:254:VAL:HG11 | 2.23                     | 0.73              |
| 1:E:365:ARG:NH1  | 1:E:383:LEU:HD22 | 2.02                     | 0.73              |
| 1:H:311:ARG:HG2  | 1:H:352:TRP:HA   | 1.70                     | 0.73              |
| 1:I:165:ILE:HB   | 1:I:278:ALA:HB2  | 1.70                     | 0.73              |
| 1:M:265:GLY:HA2  | 1:N:203:ILE:HD13 | 1.70                     | 0.73              |
| 1:E:201:ARG:HB2  | 1:E:201:ARG:NH1  | 2.03                     | 0.73              |
| 1:F:321:ALA:HA   | 1:F:363:ILE:CD1  | 2.18                     | 0.73              |
| 1:K:164:LEU:HD12 | 1:K:165:ILE:N    | 2.03                     | 0.73              |
| 1:L:352:TRP:CH2  | 1:L:362:VAL:HG21 | 2.23                     | 0.73              |
| 1:M:363:ILE:N    | 1:M:363:ILE:HD12 | 2.03                     | 0.73              |
| 1:G:275:ILE:HD12 | 1:G:275:ILE:N    | 2.04                     | 0.73              |
| 1:L:343:ALA:HB2  | 1:L:376:ASP:CA   | 2.15                     | 0.73              |
| 1:N:363:ILE:O    | 1:N:367:VAL:HG23 | 1.88                     | 0.73              |
| 1:B:201:ARG:HB2  | 1:B:201:ARG:HH11 | 1.53                     | 0.73              |
| 1:K:342:SER:OG   | 1:K:377:ARG:HB2  | 1.88                     | 0.73              |
| 1:B:365:ARG:HH11 | 1:B:383:LEU:HB3  | 1.52                     | 0.73              |
| 1:D:248:GLN:HE22 | 1:D:292:PHE:HA   | 1.54                     | 0.73              |
| 1:E:236:PHE:HD1  | 1:E:276:LEU:O    | 1.71                     | 0.73              |
| 1:B:260:PHE:C    | 1:B:260:PHE:HD1  | 1.97                     | 0.73              |
| 1:C:283:ILE:HG21 | 1:C:297:TYR:CD1  | 2.23                     | 0.73              |
| 1:I:165:ILE:HG22 | 1:I:173:LYS:HG2  | 1.70                     | 0.73              |
| 1:L:283:ILE:HB   | 1:L:297:TYR:CZ   | 2.24                     | 0.73              |
| 1:D:244:SER:O    | 1:D:248:GLN:HG3  | 1.88                     | 0.72              |
| 1:A:309:PRO:HG3  | 1:A:311:ARG:NH1  | 2.04                     | 0.72              |
| 1:C:140:VAL:O    | 1:C:140:VAL:HG12 | 1.89                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:162:PRO:HG2  | 1:C:302:VAL:HG23 | 1.70                     | 0.72              |
| 1:D:189:GLU:HG3  | 1:D:190:PRO:HD2  | 1.71                     | 0.72              |
| 1:D:194:LEU:O    | 1:D:194:LEU:HD23 | 1.89                     | 0.72              |
| 1:H:321:ALA:HA   | 1:H:363:ILE:CD1  | 2.18                     | 0.72              |
| 1:N:239:GLU:O    | 1:N:241:GLY:N    | 2.23                     | 0.72              |
| 1:F:309:PRO:HA   | 1:F:355:ASN:HD22 | 1.51                     | 0.72              |
| 1:L:240:ILE:HB   | 1:L:279:THR:HG22 | 1.71                     | 0.72              |
| 1:B:161:CYS:HB2  | 1:B:162:PRO:HD2  | 1.71                     | 0.72              |
| 1:E:176:VAL:HG21 | 1:E:307:ILE:HD11 | 1.71                     | 0.72              |
| 1:G:299:ARG:HA   | 1:G:299:ARG:HE   | 1.54                     | 0.72              |
| 1:J:189:GLU:CG   | 1:J:190:PRO:HD2  | 2.18                     | 0.72              |
| 1:K:157:SER:OG   | 1:K:183:LEU:HB2  | 1.90                     | 0.72              |
| 1:M:282:ASN:ND2  | 1:M:285:GLU:HB2  | 2.04                     | 0.72              |
| 1:E:236:PHE:HE1  | 1:E:278:ALA:HB2  | 1.52                     | 0.72              |
| 1:J:269:ILE:HD12 | 1:J:269:ILE:N    | 2.05                     | 0.72              |
| 1:K:216:PHE:HD1  | 1:K:216:PHE:N    | 1.88                     | 0.72              |
| 1:B:186:ARG:HD3  | 1:B:232:GLY:O    | 1.88                     | 0.72              |
| 1:C:181:HIS:HD2  | 1:C:191:PHE:HD1  | 1.33                     | 0.72              |
| 1:D:263:LEU:HD23 | 1:D:264:GLY:N    | 2.04                     | 0.72              |
| 1:F:357:ARG:HG2  | 2:F:4:ADP:H5'2   | 1.70                     | 0.72              |
| 1:G:194:LEU:HD21 | 1:G:237:LEU:HD22 | 1.71                     | 0.72              |
| 1:I:143:SER:N    | 1:I:316:ASP:OD1  | 2.23                     | 0.72              |
| 1:I:318:ILE:HG12 | 1:I:348:LEU:HD21 | 1.69                     | 0.72              |
| 1:B:153:ILE:HG21 | 1:B:179:LEU:HD22 | 1.71                     | 0.72              |
| 1:E:146:MET:CE   | 1:E:149:ILE:HD12 | 2.20                     | 0.72              |
| 1:G:310:LEU:HB2  | 1:G:355:ASN:CB   | 2.19                     | 0.72              |
| 1:H:170:GLY:C    | 1:H:355:ASN:HB2  | 2.14                     | 0.72              |
| 1:H:208:LEU:HD23 | 1:H:209:PHE:CE1  | 2.25                     | 0.72              |
| 1:I:261:TYR:CE1  | 1:J:199:ILE:HG12 | 2.20                     | 0.72              |
| 1:M:265:GLY:HA2  | 1:N:203:ILE:CD1  | 2.20                     | 0.72              |
| 1:N:357:ARG:HH12 | 1:N:361:ASN:ND2  | 1.88                     | 0.72              |
| 1:F:279:THR:HG21 | 1:F:283:ILE:HD11 | 1.72                     | 0.72              |
| 1:H:357:ARG:HG3  | 2:H:14:ADP:H5'2  | 1.72                     | 0.72              |
| 1:J:201:ARG:HH11 | 1:J:201:ARG:CB   | 2.02                     | 0.72              |
| 1:F:362:VAL:HG13 | 1:F:383:LEU:HD12 | 1.71                     | 0.71              |
| 1:J:168:GLU:OE1  | 1:J:309:PRO:HB3  | 1.90                     | 0.71              |
| 1:M:253:ARG:HG3  | 1:N:198:SER:CB   | 2.19                     | 0.71              |
| 1:D:341:LYS:O    | 1:D:345:GLU:HG3  | 1.90                     | 0.71              |
| 1:E:347:LEU:HD21 | 1:E:380:LEU:CD1  | 2.19                     | 0.71              |
| 1:F:173:LYS:H    | 2:F:4:ADP:PB     | 2.14                     | 0.71              |
| 1:G:313:ARG:HB3  | 1:G:316:ASP:OD2  | 1.89                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:149:ILE:O    | 1:E:152:LYS:N    | 2.23                     | 0.71              |
| 1:G:189:GLU:CG   | 1:G:190:PRO:HD2  | 2.19                     | 0.71              |
| 1:K:146:MET:HE2  | 1:K:313:ARG:NH2  | 2.05                     | 0.71              |
| 1:E:186:ARG:NH2  | 1:E:272:ASN:HD21 | 1.87                     | 0.71              |
| 1:E:328:PHE:CE1  | 1:E:364:GLU:HB2  | 2.25                     | 0.71              |
| 1:E:346:LEU:C    | 1:E:348:LEU:H    | 1.96                     | 0.71              |
| 1:F:194:LEU:HD23 | 1:F:194:LEU:N    | 2.04                     | 0.71              |
| 1:F:321:ALA:HA   | 1:F:363:ILE:HD11 | 1.72                     | 0.71              |
| 1:I:254:VAL:HG22 | 1:I:260:PHE:HB3  | 1.71                     | 0.71              |
| 1:I:335:GLU:O    | 1:I:373:LYS:HG2  | 1.89                     | 0.71              |
| 1:J:194:LEU:HD21 | 1:J:237:LEU:HD23 | 1.73                     | 0.71              |
| 1:J:340:THR:OG1  | 1:J:376:ASP:HB2  | 1.90                     | 0.71              |
| 1:L:239:GLU:C    | 1:L:241:GLY:H    | 1.97                     | 0.71              |
| 1:L:334:LYS:HD3  | 1:L:367:VAL:HG13 | 1.70                     | 0.71              |
| 1:B:174:GLU:HB3  | 2:B:7:ADP:O1A    | 1.90                     | 0.71              |
| 1:E:216:PHE:CE2  | 1:E:219:ALA:HB2  | 2.26                     | 0.71              |
| 1:I:156:ILE:O    | 1:I:158:CYS:N    | 2.22                     | 0.71              |
| 1:K:266:ARG:HH22 | 1:L:207:GLU:CD   | 1.97                     | 0.71              |
| 1:L:211:TYR:HE1  | 1:L:223:LYS:HD3  | 1.55                     | 0.71              |
| 1:M:363:ILE:H    | 1:M:363:ILE:HD12 | 1.55                     | 0.71              |
| 1:L:138:GLU:OE1  | 1:L:323:HIS:NE2  | 2.24                     | 0.71              |
| 1:M:180:ILE:CG2  | 1:M:276:LEU:HD11 | 2.18                     | 0.71              |
| 1:D:316:ASP:C    | 1:D:319:PRO:HD2  | 2.16                     | 0.71              |
| 1:F:314:LYS:HA   | 1:F:317:ILE:HG13 | 1.72                     | 0.71              |
| 1:K:269:ILE:HD12 | 1:K:269:ILE:H    | 1.56                     | 0.71              |
| 1:N:201:ARG:HB2  | 1:N:201:ARG:NH1  | 2.06                     | 0.71              |
| 1:B:234:THR:HG23 | 1:B:274:ARG:O    | 1.90                     | 0.71              |
| 1:C:194:LEU:H    | 1:C:194:LEU:HD23 | 1.55                     | 0.71              |
| 1:C:244:SER:O    | 1:C:248:GLN:HG3  | 1.89                     | 0.71              |
| 1:D:316:ASP:O    | 1:D:319:PRO:HD2  | 1.90                     | 0.71              |
| 1:N:145:LYS:CA   | 1:N:148:GLU:HG2  | 2.19                     | 0.71              |
| 1:N:339:PHE:CE2  | 1:N:347:LEU:HD11 | 2.25                     | 0.71              |
| 1:E:355:ASN:HD22 | 1:E:355:ASN:N    | 1.86                     | 0.71              |
| 1:A:139:TYR:CE2  | 1:A:175:VAL:HG22 | 2.26                     | 0.71              |
| 1:B:208:LEU:HG   | 1:B:209:PHE:CD1  | 2.26                     | 0.71              |
| 1:E:181:HIS:CD2  | 1:E:234:THR:OG1  | 2.43                     | 0.71              |
| 1:F:201:ARG:HB2  | 1:F:201:ARG:NH1  | 2.06                     | 0.71              |
| 1:G:178:ARG:HA   | 1:G:191:PHE:HE1  | 1.56                     | 0.71              |
| 1:L:146:MET:HE2  | 1:L:313:ARG:HH21 | 1.55                     | 0.71              |
| 1:D:308:PRO:HG2  | 1:D:313:ARG:HD2  | 1.72                     | 0.70              |
| 1:E:236:PHE:HE1  | 1:E:278:ALA:CB   | 2.03                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:282:ASN:ND2  | 1:K:285:GLU:HB2  | 2.06                     | 0.70              |
| 1:E:231:ASP:OD2  | 1:E:271:VAL:HG12 | 1.90                     | 0.70              |
| 1:F:153:ILE:HD12 | 1:F:180:ILE:HG12 | 1.73                     | 0.70              |
| 1:I:239:GLU:HG2  | 1:I:281:ARG:HH21 | 1.56                     | 0.70              |
| 1:A:254:VAL:HG22 | 1:A:260:PHE:HB3  | 1.73                     | 0.70              |
| 1:C:220:VAL:CG1  | 1:C:221:SER:H    | 1.90                     | 0.70              |
| 1:E:267:LYS:HD2  | 1:E:267:LYS:N    | 2.06                     | 0.70              |
| 1:H:146:MET:HG2  | 1:H:313:ARG:NH1  | 2.05                     | 0.70              |
| 1:M:211:TYR:HE1  | 1:M:223:LYS:CB   | 2.02                     | 0.70              |
| 1:E:214:GLY:HA2  | 1:E:219:ALA:CB   | 2.20                     | 0.70              |
| 1:B:204:PHE:HE2  | 1:B:208:LEU:HD22 | 1.55                     | 0.70              |
| 1:D:235:LEU:HD12 | 1:D:235:LEU:C    | 2.16                     | 0.70              |
| 1:E:173:LYS:NZ   | 2:E:3:ADP:O1B    | 2.23                     | 0.70              |
| 1:B:194:LEU:HD21 | 1:B:237:LEU:CD2  | 2.22                     | 0.70              |
| 1:B:337:GLU:HG2  | 1:B:373:LYS:HB3  | 1.73                     | 0.70              |
| 1:C:252:LEU:HD13 | 1:C:296:LEU:HA   | 1.73                     | 0.70              |
| 1:E:137:GLU:HG2  | 1:E:138:GLU:HG2  | 1.74                     | 0.70              |
| 1:E:310:LEU:HG   | 1:E:317:ILE:HG12 | 1.72                     | 0.70              |
| 1:E:313:ARG:HB3  | 1:E:316:ASP:OD2  | 1.91                     | 0.70              |
| 1:I:143:SER:HB3  | 1:I:316:ASP:CG   | 2.15                     | 0.70              |
| 1:L:211:TYR:CE1  | 1:L:223:LYS:HD3  | 2.27                     | 0.70              |
| 1:M:249:ALA:HA   | 1:M:293:ARG:NH1  | 2.07                     | 0.70              |
| 1:E:354:GLY:C    | 1:E:358:GLU:HB2  | 2.17                     | 0.70              |
| 1:F:146:MET:HE2  | 1:F:313:ARG:NH2  | 2.07                     | 0.70              |
| 1:H:215:ALA:HA   | 1:I:211:TYR:OH   | 1.92                     | 0.70              |
| 1:K:302:VAL:HG13 | 1:L:365:ARG:HB2  | 1.73                     | 0.70              |
| 1:G:198:SER:O    | 1:G:199:ILE:HG13 | 1.91                     | 0.70              |
| 1:L:343:ALA:O    | 1:L:345:GLU:N    | 2.25                     | 0.70              |
| 1:M:314:LYS:HA   | 1:M:317:ILE:CD1  | 2.22                     | 0.70              |
| 1:E:277:ALA:CB   | 1:E:300:LEU:HD13 | 2.22                     | 0.70              |
| 1:J:284:LYS:HE2  | 1:J:297:TYR:OH   | 1.92                     | 0.70              |
| 1:K:361:ASN:HD22 | 1:K:361:ASN:N    | 1.90                     | 0.70              |
| 1:L:265:GLY:C    | 1:L:266:ARG:HG2  | 2.17                     | 0.70              |
| 1:N:251:LEU:HD23 | 1:N:251:LEU:C    | 2.16                     | 0.70              |
| 1:C:162:PRO:HG2  | 1:C:302:VAL:CG2  | 2.22                     | 0.70              |
| 1:G:320:LEU:HD11 | 1:G:356:VAL:HG13 | 1.74                     | 0.70              |
| 1:K:216:PHE:CD1  | 1:K:216:PHE:N    | 2.58                     | 0.70              |
| 1:N:235:LEU:HD12 | 1:N:236:PHE:N    | 2.06                     | 0.70              |
| 1:H:198:SER:HB2  | 1:N:250:LYS:CB   | 2.22                     | 0.69              |
| 1:B:244:SER:O    | 1:B:248:GLN:HG3  | 1.92                     | 0.69              |
| 1:E:316:ASP:C    | 1:E:319:PRO:HD2  | 2.17                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:207:GLU:OE1  | 1:L:207:GLU:HA   | 1.90                     | 0.69              |
| 1:M:299:ARG:HD3  | 1:N:357:ARG:NH2  | 2.08                     | 0.69              |
| 1:J:254:VAL:HG22 | 1:J:260:PHE:HB3  | 1.74                     | 0.69              |
| 1:A:189:GLU:CG   | 1:A:190:PRO:HD2  | 2.22                     | 0.69              |
| 1:J:383:LEU:HD23 | 1:J:383:LEU:N    | 2.07                     | 0.69              |
| 1:B:208:LEU:HG   | 1:B:209:PHE:CE1  | 2.26                     | 0.69              |
| 1:B:266:ARG:HB3  | 1:C:229:LEU:CD2  | 2.22                     | 0.69              |
| 1:B:317:ILE:HB   | 1:B:348:LEU:CD2  | 2.22                     | 0.69              |
| 1:F:149:ILE:HD13 | 1:F:307:ILE:HD13 | 1.73                     | 0.69              |
| 1:H:215:ALA:HB2  | 1:I:223:LYS:NZ   | 2.07                     | 0.69              |
| 1:E:303:ILE:HG22 | 1:E:303:ILE:O    | 1.92                     | 0.69              |
| 1:H:234:THR:HG21 | 1:H:276:LEU:CD1  | 2.21                     | 0.69              |
| 1:I:240:ILE:HD11 | 1:I:277:ALA:CB   | 2.22                     | 0.69              |
| 1:L:322:ASN:HA   | 1:L:339:PHE:HE1  | 1.55                     | 0.69              |
| 1:L:340:THR:HG23 | 1:L:376:ASP:HB3  | 1.72                     | 0.69              |
| 1:N:165:ILE:HB   | 1:N:278:ALA:HB2  | 1.73                     | 0.69              |
| 1:N:283:ILE:O    | 1:N:287:VAL:HG23 | 1.91                     | 0.69              |
| 1:C:161:CYS:HB2  | 1:C:302:VAL:HG11 | 1.74                     | 0.69              |
| 1:C:300:LEU:O    | 1:C:302:VAL:HG23 | 1.93                     | 0.69              |
| 1:E:308:PRO:HG2  | 1:E:313:ARG:HD2  | 1.75                     | 0.69              |
| 1:F:157:SER:HB3  | 1:F:183:LEU:C    | 2.17                     | 0.69              |
| 1:F:267:LYS:HD2  | 1:F:267:LYS:N    | 2.08                     | 0.69              |
| 1:I:172:GLY:HA2  | 2:I:8:ADP:O1A    | 1.93                     | 0.69              |
| 1:J:240:ILE:O    | 1:J:242:GLU:N    | 2.25                     | 0.69              |
| 1:B:189:GLU:CG   | 1:B:190:PRO:HD2  | 2.23                     | 0.69              |
| 1:B:260:PHE:C    | 1:B:260:PHE:CD1  | 2.68                     | 0.69              |
| 1:D:210:GLY:CA   | 1:D:225:GLY:H    | 2.04                     | 0.69              |
| 1:E:171:VAL:HB   | 1:E:307:ILE:HG22 | 1.75                     | 0.69              |
| 1:F:346:LEU:HG   | 1:F:377:ARG:HH11 | 1.56                     | 0.69              |
| 1:G:310:LEU:HD22 | 1:G:317:ILE:HG12 | 1.74                     | 0.69              |
| 1:I:207:GLU:OE1  | 1:I:207:GLU:HA   | 1.92                     | 0.69              |
| 1:I:208:LEU:HD23 | 1:I:208:LEU:C    | 2.18                     | 0.69              |
| 1:L:160:GLU:C    | 1:L:274:ARG:HE   | 2.00                     | 0.69              |
| 1:M:350:TYR:CG   | 1:M:351:PRO:HD2  | 2.27                     | 0.69              |
| 1:A:369:PHE:HA   | 1:G:155:LYS:HD3  | 1.75                     | 0.69              |
| 1:D:227:PHE:HD2  | 1:D:273:VAL:HG21 | 1.58                     | 0.69              |
| 1:J:144:PRO:HG2  | 1:J:145:LYS:H    | 1.58                     | 0.69              |
| 1:C:266:ARG:NH1  | 1:D:216:PHE:CZ   | 2.58                     | 0.69              |
| 1:F:172:GLY:O    | 1:F:176:VAL:HG23 | 1.92                     | 0.69              |
| 1:I:365:ARG:NE   | 1:I:383:LEU:HD22 | 2.08                     | 0.69              |
| 1:L:302:VAL:O    | 1:M:365:ARG:HD3  | 1.93                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:236:PHE:CE2  | 1:C:238:ASP:HB2  | 2.28                     | 0.68              |
| 1:C:325:LEU:C    | 1:C:325:LEU:HD23 | 2.18                     | 0.68              |
| 1:I:256:GLU:HG2  | 1:I:299:ARG:NE   | 2.08                     | 0.68              |
| 1:K:208:LEU:HD22 | 1:K:209:PHE:CD1  | 2.28                     | 0.68              |
| 1:A:237:LEU:HB2  | 1:A:240:ILE:CD1  | 2.23                     | 0.68              |
| 1:A:325:LEU:CD1  | 1:A:338:GLY:HA2  | 2.23                     | 0.68              |
| 1:B:178:ARG:HD2  | 1:B:191:PHE:HE2  | 1.59                     | 0.68              |
| 1:D:246:GLU:CD   | 1:D:246:GLU:H    | 2.00                     | 0.68              |
| 1:E:186:ARG:HB2  | 1:E:189:GLU:HB2  | 1.75                     | 0.68              |
| 1:E:313:ARG:O    | 1:E:315:GLU:N    | 2.26                     | 0.68              |
| 1:G:308:PRO:HG2  | 1:G:313:ARG:HD2  | 1.75                     | 0.68              |
| 1:H:227:PHE:CE2  | 1:H:254:VAL:HG11 | 2.28                     | 0.68              |
| 1:H:359:LEU:O    | 1:H:359:LEU:HD23 | 1.94                     | 0.68              |
| 1:M:244:SER:O    | 1:M:247:ALA:HB3  | 1.92                     | 0.68              |
| 1:A:161:CYS:O    | 1:A:274:ARG:NH1  | 2.25                     | 0.68              |
| 1:D:302:VAL:HG12 | 1:D:303:ILE:HD13 | 1.75                     | 0.68              |
| 1:E:350:TYR:CD1  | 1:E:384:VAL:HG13 | 2.28                     | 0.68              |
| 1:F:242:GLU:HG2  | 1:F:281:ARG:HH22 | 1.58                     | 0.68              |
| 1:M:216:PHE:O    | 1:M:218:GLY:N    | 2.26                     | 0.68              |
| 1:M:240:ILE:HG23 | 1:M:243:LEU:HD12 | 1.75                     | 0.68              |
| 1:N:240:ILE:HG23 | 1:N:243:LEU:HD12 | 1.74                     | 0.68              |
| 1:B:246:GLU:HG3  | 1:C:197:ALA:O    | 1.93                     | 0.68              |
| 1:G:350:TYR:CD1  | 1:G:351:PRO:HD2  | 2.28                     | 0.68              |
| 1:H:296:LEU:HD23 | 1:H:296:LEU:O    | 1.92                     | 0.68              |
| 1:H:318:ILE:HG13 | 1:H:348:LEU:HD21 | 1.75                     | 0.68              |
| 1:I:350:TYR:CD1  | 1:I:351:PRO:HD2  | 2.28                     | 0.68              |
| 1:B:321:ALA:HA   | 1:B:363:ILE:CD1  | 2.23                     | 0.68              |
| 1:D:240:ILE:CG1  | 1:D:277:ALA:HB1  | 2.22                     | 0.68              |
| 1:E:365:ARG:NH1  | 1:E:383:LEU:HB3  | 2.08                     | 0.68              |
| 1:M:175:VAL:HG23 | 2:M:12:ADP:O1A   | 1.94                     | 0.68              |
| 1:G:245:LEU:HD22 | 1:G:248:GLN:HE22 | 1.56                     | 0.68              |
| 1:H:192:VAL:CG2  | 1:H:230:ALA:HB2  | 2.24                     | 0.68              |
| 1:L:334:LYS:CD   | 1:L:367:VAL:HG13 | 2.23                     | 0.68              |
| 1:J:325:LEU:HD23 | 1:J:326:LYS:N    | 2.09                     | 0.68              |
| 1:M:261:TYR:HE2  | 1:N:199:ILE:HG12 | 1.58                     | 0.68              |
| 1:N:140:VAL:HG11 | 1:N:320:LEU:HD23 | 1.75                     | 0.68              |
| 1:E:186:ARG:HH22 | 1:E:272:ASN:ND2  | 1.91                     | 0.68              |
| 1:G:320:LEU:O    | 1:G:320:LEU:HD23 | 1.93                     | 0.68              |
| 1:B:204:PHE:O    | 1:B:205:GLU:C    | 2.37                     | 0.68              |
| 1:D:161:CYS:O    | 1:D:274:ARG:NH1  | 2.26                     | 0.68              |
| 1:F:299:ARG:HA   | 1:F:299:ARG:HE   | 1.59                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:318:ILE:HD13 | 1:H:344:GLN:HE21 | 1.59                     | 0.68              |
| 1:C:181:HIS:CD2  | 1:C:191:PHE:CD1  | 2.78                     | 0.68              |
| 1:L:149:ILE:HD11 | 1:L:306:GLU:O    | 1.93                     | 0.68              |
| 1:L:285:GLU:OE2  | 1:L:289:GLU:HB2  | 1.94                     | 0.68              |
| 1:N:139:TYR:CD2  | 1:N:175:VAL:HG13 | 2.29                     | 0.68              |
| 1:A:170:GLY:O    | 1:A:355:ASN:HB2  | 1.93                     | 0.67              |
| 1:C:318:ILE:CG1  | 1:C:319:PRO:HD3  | 2.19                     | 0.67              |
| 1:F:317:ILE:HG21 | 1:F:347:LEU:O    | 1.94                     | 0.67              |
| 1:K:196:VAL:HG22 | 1:K:204:PHE:CZ   | 2.29                     | 0.67              |
| 1:M:253:ARG:HD2  | 1:M:259:LYS:O    | 1.93                     | 0.67              |
| 1:A:292:PHE:CZ   | 1:A:296:LEU:HD12 | 2.30                     | 0.67              |
| 1:D:310:LEU:HD22 | 1:D:317:ILE:HG12 | 1.76                     | 0.67              |
| 1:H:140:VAL:HG12 | 1:H:141:PHE:H    | 1.60                     | 0.67              |
| 1:I:208:LEU:HD21 | 1:I:227:PHE:HD1  | 1.57                     | 0.67              |
| 1:M:267:LYS:H    | 1:M:267:LYS:HD2  | 1.58                     | 0.67              |
| 1:B:210:GLY:O    | 1:B:263:LEU:N    | 2.23                     | 0.67              |
| 1:F:282:ASN:HD22 | 1:F:285:GLU:HB2  | 1.58                     | 0.67              |
| 1:G:191:PHE:HE2  | 1:G:236:PHE:HB3  | 1.60                     | 0.67              |
| 1:G:259:LYS:HB3  | 1:G:267:LYS:CG   | 2.08                     | 0.67              |
| 1:H:143:SER:HB2  | 1:H:316:ASP:OD1  | 1.95                     | 0.67              |
| 1:I:314:LYS:HA   | 1:I:317:ILE:HG13 | 1.76                     | 0.67              |
| 1:L:350:TYR:CG   | 1:L:351:PRO:HD2  | 2.29                     | 0.67              |
| 1:L:365:ARG:CZ   | 1:L:383:LEU:HD21 | 2.24                     | 0.67              |
| 1:C:140:VAL:CG1  | 1:C:320:LEU:HD23 | 2.24                     | 0.67              |
| 1:D:207:GLU:O    | 1:D:225:GLY:HA2  | 1.94                     | 0.67              |
| 1:E:320:LEU:O    | 1:E:322:ASN:N    | 2.27                     | 0.67              |
| 1:G:320:LEU:HD23 | 1:G:320:LEU:C    | 2.20                     | 0.67              |
| 1:H:216:PHE:CG   | 1:H:216:PHE:O    | 2.47                     | 0.67              |
| 1:M:141:PHE:HD2  | 1:M:150:LEU:HB2  | 1.57                     | 0.67              |
| 1:E:319:PRO:O    | 1:E:322:ASN:HB2  | 1.94                     | 0.67              |
| 1:L:240:ILE:O    | 1:L:240:ILE:CG2  | 2.42                     | 0.67              |
| 1:L:324:PHE:O    | 1:L:328:PHE:HD1  | 1.77                     | 0.67              |
| 1:B:164:LEU:HD12 | 1:B:165:ILE:H    | 1.59                     | 0.67              |
| 1:C:178:ARG:HG3  | 1:C:178:ARG:NH1  | 1.97                     | 0.67              |
| 1:D:282:ASN:ND2  | 1:D:285:GLU:HB2  | 2.09                     | 0.67              |
| 1:E:314:LYS:HA   | 1:E:317:ILE:HD12 | 1.77                     | 0.67              |
| 1:H:215:ALA:N    | 1:I:223:LYS:NZ   | 2.42                     | 0.67              |
| 1:H:253:ARG:HH22 | 1:H:261:TYR:HE1  | 1.41                     | 0.67              |
| 1:L:291:LYS:O    | 1:L:291:LYS:HD3  | 1.94                     | 0.67              |
| 1:A:316:ASP:C    | 1:A:319:PRO:HD2  | 2.20                     | 0.67              |
| 1:D:362:VAL:HG12 | 1:D:362:VAL:O    | 1.93                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:220:VAL:HG12 | 1:J:221:SER:N    | 2.09                     | 0.67              |
| 1:M:172:GLY:HA2  | 2:M:12:ADP:O1A   | 1.94                     | 0.67              |
| 1:I:141:PHE:CG   | 1:I:150:LEU:HD11 | 2.29                     | 0.67              |
| 1:N:152:LYS:HA   | 1:N:152:LYS:HE3  | 1.77                     | 0.67              |
| 1:N:363:ILE:HA   | 1:N:366:ALA:HB3  | 1.76                     | 0.67              |
| 1:E:212:GLU:O    | 1:E:222:SER:HA   | 1.95                     | 0.67              |
| 1:F:138:GLU:CG   | 1:F:139:TYR:H    | 2.08                     | 0.67              |
| 1:F:194:LEU:HD21 | 1:F:237:LEU:HD23 | 1.76                     | 0.67              |
| 1:F:376:ASP:O    | 1:F:378:GLY:N    | 2.28                     | 0.67              |
| 1:K:209:PHE:CE2  | 1:K:250:LYS:HD3  | 2.30                     | 0.67              |
| 1:M:146:MET:HA   | 1:M:146:MET:HE2  | 1.77                     | 0.67              |
| 1:M:191:PHE:CE2  | 1:M:193:ALA:HB2  | 2.30                     | 0.67              |
| 1:N:318:ILE:HG12 | 1:N:348:LEU:HD21 | 1.77                     | 0.67              |
| 1:E:282:ASN:HD22 | 1:E:285:GLU:HB2  | 1.56                     | 0.67              |
| 1:F:316:ASP:C    | 1:F:319:PRO:HD2  | 2.19                     | 0.67              |
| 1:K:208:LEU:HD22 | 1:K:209:PHE:CE1  | 2.30                     | 0.67              |
| 1:N:342:SER:OG   | 1:N:377:ARG:HB2  | 1.94                     | 0.67              |
| 1:F:308:PRO:HG2  | 1:F:313:ARG:HD2  | 1.77                     | 0.66              |
| 1:J:324:PHE:CD1  | 1:J:360:LYS:HA   | 2.30                     | 0.66              |
| 1:K:206:ALA:HB1  | 1:K:211:TYR:HB3  | 1.76                     | 0.66              |
| 1:K:240:ILE:HG13 | 1:K:277:ALA:HB1  | 1.77                     | 0.66              |
| 1:L:229:LEU:O    | 1:L:229:LEU:HD22 | 1.94                     | 0.66              |
| 1:M:157:SER:C    | 1:M:159:ALA:H    | 2.03                     | 0.66              |
| 1:B:314:LYS:H    | 1:B:314:LYS:CD   | 2.03                     | 0.66              |
| 1:J:157:SER:HB3  | 1:J:183:LEU:C    | 2.19                     | 0.66              |
| 1:N:228:GLU:O    | 1:N:231:ASP:N    | 2.27                     | 0.66              |
| 1:N:262:ARG:HG2  | 1:N:262:ARG:HH11 | 1.60                     | 0.66              |
| 1:A:320:LEU:O    | 1:A:323:HIS:N    | 2.27                     | 0.66              |
| 1:B:204:PHE:CE2  | 1:B:208:LEU:HD22 | 2.30                     | 0.66              |
| 1:D:170:GLY:O    | 1:D:355:ASN:HB2  | 1.96                     | 0.66              |
| 1:D:236:PHE:CD1  | 1:D:236:PHE:C    | 2.74                     | 0.66              |
| 1:D:296:LEU:O    | 1:D:300:LEU:HG   | 1.96                     | 0.66              |
| 1:L:161:CYS:HB3  | 1:M:364:GLU:OE1  | 1.94                     | 0.66              |
| 1:D:156:ILE:HD11 | 1:D:303:ILE:HG21 | 1.76                     | 0.66              |
| 1:G:263:LEU:HG   | 1:G:264:GLY:H    | 1.58                     | 0.66              |
| 1:G:315:GLU:OE1  | 1:G:315:GLU:N    | 2.27                     | 0.66              |
| 1:H:176:VAL:HG21 | 1:H:307:ILE:CD1  | 2.23                     | 0.66              |
| 1:M:149:ILE:O    | 1:M:153:ILE:HG12 | 1.95                     | 0.66              |
| 1:M:171:VAL:HB   | 1:M:307:ILE:CG2  | 2.24                     | 0.66              |
| 1:C:292:PHE:CZ   | 1:C:296:LEU:HD12 | 2.30                     | 0.66              |
| 1:F:178:ARG:HG3  | 1:F:178:ARG:NH1  | 2.09                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:196:VAL:HG13 | 1:F:204:PHE:HE1  | 1.61                     | 0.66              |
| 1:I:141:PHE:CE2  | 1:I:150:LEU:HD21 | 2.30                     | 0.66              |
| 1:I:153:ILE:HD11 | 1:I:176:VAL:HG13 | 1.78                     | 0.66              |
| 1:H:215:ALA:HB2  | 1:I:223:LYS:HZ1  | 1.60                     | 0.66              |
| 1:I:269:ILE:N    | 1:I:269:ILE:HD12 | 2.10                     | 0.66              |
| 1:K:269:ILE:HD12 | 1:K:269:ILE:N    | 2.10                     | 0.66              |
| 1:L:153:ILE:HD11 | 1:L:176:VAL:HG13 | 1.78                     | 0.66              |
| 1:L:318:ILE:HD12 | 1:L:319:PRO:HD3  | 1.76                     | 0.66              |
| 1:M:254:VAL:HG22 | 1:M:260:PHE:HB3  | 1.77                     | 0.66              |
| 1:F:223:LYS:C    | 1:F:225:GLY:H    | 2.03                     | 0.66              |
| 1:J:212:GLU:HG3  | 1:J:265:GLY:HA2  | 1.78                     | 0.66              |
| 1:N:346:LEU:HD12 | 1:N:377:ARG:HD2  | 1.76                     | 0.66              |
| 1:C:236:PHE:HA   | 1:C:276:LEU:O    | 1.95                     | 0.66              |
| 1:E:345:GLU:O    | 1:E:348:LEU:HB2  | 1.94                     | 0.66              |
| 1:G:252:LEU:HD22 | 1:G:293:ARG:HH12 | 1.61                     | 0.66              |
| 1:H:215:ALA:H    | 1:I:223:LYS:NZ   | 1.94                     | 0.66              |
| 1:K:309:PRO:O    | 1:K:313:ARG:HD3  | 1.96                     | 0.66              |
| 1:M:352:TRP:HA   | 1:M:352:TRP:CE3  | 2.30                     | 0.66              |
| 1:A:149:ILE:O    | 1:A:153:ILE:HG12 | 1.96                     | 0.66              |
| 1:H:309:PRO:O    | 1:H:313:ARG:HG3  | 1.96                     | 0.66              |
| 1:M:299:ARG:HD3  | 1:N:357:ARG:HH21 | 1.59                     | 0.66              |
| 1:N:157:SER:HB3  | 1:N:184:SER:HA   | 1.76                     | 0.66              |
| 1:N:259:LYS:HD2  | 1:N:268:GLU:HG2  | 1.78                     | 0.66              |
| 1:G:318:ILE:HG13 | 1:G:319:PRO:HD3  | 1.76                     | 0.65              |
| 1:H:227:PHE:HE2  | 1:H:254:VAL:HG21 | 1.61                     | 0.65              |
| 1:H:321:ALA:HA   | 1:H:363:ILE:HD11 | 1.76                     | 0.65              |
| 1:I:318:ILE:HG13 | 1:I:319:PRO:CD   | 2.24                     | 0.65              |
| 1:K:201:ARG:HB2  | 1:K:201:ARG:NH1  | 2.07                     | 0.65              |
| 1:L:163:VAL:HB   | 1:L:276:LEU:CD2  | 2.26                     | 0.65              |
| 1:L:350:TYR:HD2  | 1:L:352:TRP:N    | 1.95                     | 0.65              |
| 1:L:352:TRP:HH2  | 1:L:362:VAL:HG21 | 1.60                     | 0.65              |
| 1:B:204:PHE:O    | 1:B:206:ALA:N    | 2.29                     | 0.65              |
| 1:B:330:ARG:HH11 | 1:B:330:ARG:HG3  | 1.61                     | 0.65              |
| 1:H:328:PHE:CD1  | 1:H:364:GLU:HG2  | 2.32                     | 0.65              |
| 1:L:283:ILE:HG22 | 1:L:287:VAL:HG23 | 1.78                     | 0.65              |
| 1:L:314:LYS:HA   | 1:L:317:ILE:HG13 | 1.79                     | 0.65              |
| 1:N:267:LYS:HD2  | 1:N:267:LYS:N    | 2.12                     | 0.65              |
| 1:A:282:ASN:ND2  | 1:A:285:GLU:HB2  | 2.11                     | 0.65              |
| 1:C:308:PRO:HG2  | 1:C:313:ARG:HD2  | 1.78                     | 0.65              |
| 1:D:236:PHE:O    | 1:D:236:PHE:CG   | 2.48                     | 0.65              |
| 1:K:204:PHE:CE2  | 1:K:208:LEU:HD12 | 2.29                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:178:ARG:HH11 | 1:M:178:ARG:HG3  | 1.61                     | 0.65              |
| 1:N:206:ALA:HB2  | 1:N:216:PHE:CZ   | 2.31                     | 0.65              |
| 1:A:363:ILE:O    | 1:A:367:VAL:HG23 | 1.95                     | 0.65              |
| 1:B:143:SER:HB2  | 1:B:144:PRO:HD2  | 1.78                     | 0.65              |
| 1:E:177:ALA:N    | 1:E:180:ILE:HD12 | 2.12                     | 0.65              |
| 1:M:363:ILE:CD1  | 1:M:363:ILE:N    | 2.59                     | 0.65              |
| 1:H:270:GLU:O    | 1:H:271:VAL:HG23 | 1.95                     | 0.65              |
| 1:H:334:LYS:HG2  | 1:H:335:GLU:N    | 2.11                     | 0.65              |
| 1:I:141:PHE:HB3  | 1:I:150:LEU:HD11 | 1.77                     | 0.65              |
| 1:K:186:ARG:NH2  | 1:K:272:ASN:ND2  | 2.44                     | 0.65              |
| 1:K:249:ALA:CB   | 1:K:293:ARG:HH11 | 2.09                     | 0.65              |
| 1:L:247:ALA:O    | 1:L:251:LEU:HB2  | 1.97                     | 0.65              |
| 1:C:160:GLU:HA   | 1:C:274:ARG:NH1  | 2.12                     | 0.65              |
| 1:J:352:TRP:CZ2  | 1:J:359:LEU:HD23 | 2.32                     | 0.65              |
| 1:L:146:MET:HE2  | 1:L:313:ARG:HE   | 1.61                     | 0.65              |
| 1:A:139:TYR:HD2  | 1:A:175:VAL:HG13 | 1.60                     | 0.65              |
| 1:C:318:ILE:HG13 | 1:C:319:PRO:CD   | 2.20                     | 0.65              |
| 1:E:176:VAL:O    | 1:E:180:ILE:CD1  | 2.45                     | 0.65              |
| 1:E:186:ARG:HH22 | 1:E:272:ASN:HD21 | 1.42                     | 0.65              |
| 1:F:311:ARG:HB3  | 1:F:351:PRO:O    | 1.97                     | 0.65              |
| 1:A:244:SER:HB2  | 1:A:247:ALA:H    | 1.61                     | 0.65              |
| 1:J:153:ILE:HG21 | 1:J:179:LEU:HD22 | 1.76                     | 0.65              |
| 1:K:143:SER:CB   | 1:K:315:GLU:HB2  | 2.27                     | 0.65              |
| 1:L:314:LYS:HA   | 1:L:317:ILE:CG1  | 2.27                     | 0.65              |
| 1:A:145:LYS:O    | 1:A:149:ILE:HG13 | 1.96                     | 0.65              |
| 1:E:309:PRO:CG   | 1:E:312:GLU:HG3  | 2.22                     | 0.65              |
| 1:H:339:PHE:N    | 1:H:339:PHE:CD1  | 2.65                     | 0.65              |
| 1:H:360:LYS:O    | 1:H:364:GLU:HG3  | 1.96                     | 0.65              |
| 1:C:143:SER:OG   | 1:C:144:PRO:HD2  | 1.97                     | 0.65              |
| 1:C:181:HIS:HD2  | 1:C:191:PHE:CB   | 2.09                     | 0.65              |
| 1:D:181:HIS:HD2  | 1:D:234:THR:CB   | 2.10                     | 0.65              |
| 1:F:206:ALA:O    | 1:F:210:GLY:N    | 2.28                     | 0.65              |
| 1:F:326:LYS:HE2  | 1:F:330:ARG:HH22 | 1.61                     | 0.65              |
| 1:G:310:LEU:HD12 | 1:G:356:VAL:H    | 1.61                     | 0.65              |
| 1:H:196:VAL:HA   | 1:H:204:PHE:HE1  | 1.62                     | 0.65              |
| 1:K:310:LEU:CD2  | 1:K:317:ILE:HG12 | 2.27                     | 0.65              |
| 1:N:358:GLU:O    | 1:N:362:VAL:HG23 | 1.97                     | 0.65              |
| 1:D:181:HIS:HD2  | 1:D:234:THR:HB   | 1.61                     | 0.64              |
| 1:E:143:SER:O    | 1:E:147:LYS:HB2  | 1.97                     | 0.64              |
| 1:G:209:PHE:CE1  | 1:G:250:LYS:HD3  | 2.32                     | 0.64              |
| 1:G:340:THR:HG21 | 1:G:376:ASP:HB3  | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:267:LYS:HD2  | 1:I:267:LYS:N    | 2.11                     | 0.64              |
| 1:K:240:ILE:HG22 | 1:K:292:PHE:HE1  | 1.62                     | 0.64              |
| 1:L:178:ARG:HG3  | 1:L:178:ARG:HH11 | 1.62                     | 0.64              |
| 1:L:194:LEU:HD23 | 1:L:194:LEU:H    | 1.62                     | 0.64              |
| 1:M:316:ASP:O    | 1:M:320:LEU:HG   | 1.97                     | 0.64              |
| 1:A:259:LYS:HD3  | 1:A:268:GLU:OE1  | 1.96                     | 0.64              |
| 1:A:377:ARG:HH21 | 1:L:285:GLU:HG2  | 1.62                     | 0.64              |
| 1:B:283:ILE:CA   | 1:B:286:LEU:HD12 | 2.14                     | 0.64              |
| 1:C:191:PHE:CE2  | 1:C:193:ALA:HB2  | 2.31                     | 0.64              |
| 1:E:137:GLU:HG2  | 1:E:138:GLU:N    | 2.11                     | 0.64              |
| 1:E:292:PHE:HZ   | 1:E:296:LEU:HD12 | 1.58                     | 0.64              |
| 1:G:178:ARG:HG2  | 1:G:191:PHE:CE1  | 2.33                     | 0.64              |
| 1:A:180:ILE:O    | 1:A:180:ILE:HG22 | 1.98                     | 0.64              |
| 1:D:302:VAL:HG12 | 1:D:303:ILE:CD1  | 2.27                     | 0.64              |
| 1:E:346:LEU:C    | 1:E:348:LEU:N    | 2.54                     | 0.64              |
| 1:E:346:LEU:O    | 1:E:348:LEU:N    | 2.29                     | 0.64              |
| 1:H:283:ILE:O    | 1:H:287:VAL:HG23 | 1.96                     | 0.64              |
| 1:H:288:LYS:C    | 1:H:290:GLY:H    | 2.05                     | 0.64              |
| 1:J:308:PRO:HG2  | 1:J:313:ARG:HD2  | 1.78                     | 0.64              |
| 1:K:275:ILE:N    | 1:K:275:ILE:HD12 | 2.11                     | 0.64              |
| 1:L:153:ILE:HG21 | 1:L:179:LEU:HD22 | 1.80                     | 0.64              |
| 1:M:228:GLU:CD   | 1:M:262:ARG:HH21 | 2.05                     | 0.64              |
| 1:D:200:PRO:HG2  | 1:D:203:ILE:HB   | 1.79                     | 0.64              |
| 1:E:181:HIS:HD2  | 1:E:234:THR:OG1  | 1.80                     | 0.64              |
| 1:F:163:VAL:HG13 | 1:F:303:ILE:CG2  | 2.27                     | 0.64              |
| 1:F:356:VAL:HG11 | 2:F:4:ADP:C8     | 2.33                     | 0.64              |
| 1:I:168:GLU:O    | 1:I:171:VAL:HG23 | 1.97                     | 0.64              |
| 1:M:228:GLU:OE2  | 1:M:262:ARG:NH2  | 2.22                     | 0.64              |
| 1:N:311:ARG:HH11 | 1:N:311:ARG:HG3  | 1.61                     | 0.64              |
| 1:A:266:ARG:NH1  | 1:B:224:GLU:O    | 2.30                     | 0.64              |
| 1:B:176:VAL:O    | 1:B:179:LEU:HB3  | 1.96                     | 0.64              |
| 1:B:254:VAL:HG22 | 1:B:260:PHE:HB3  | 1.78                     | 0.64              |
| 1:D:262:ARG:O    | 1:D:265:GLY:N    | 2.31                     | 0.64              |
| 1:F:194:LEU:HD13 | 1:F:226:PHE:CD1  | 2.32                     | 0.64              |
| 1:G:355:ASN:N    | 1:G:355:ASN:ND2  | 2.45                     | 0.64              |
| 1:I:317:ILE:HB   | 1:I:348:LEU:HD23 | 1.80                     | 0.64              |
| 1:J:201:ARG:HB2  | 1:J:201:ARG:NH1  | 2.06                     | 0.64              |
| 1:L:343:ALA:O    | 1:L:344:GLN:C    | 2.40                     | 0.64              |
| 1:M:259:LYS:HA   | 1:M:269:ILE:O    | 1.98                     | 0.64              |
| 1:A:292:PHE:CE2  | 1:A:296:LEU:HD12 | 2.32                     | 0.64              |
| 1:B:210:GLY:C    | 1:B:262:ARG:HG3  | 2.23                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:284:LYS:H    | 1:B:284:LYS:HD3  | 1.62                     | 0.64              |
| 1:D:361:ASN:O    | 1:D:363:ILE:N    | 2.30                     | 0.64              |
| 1:H:248:GLN:O    | 1:H:249:ALA:C    | 2.37                     | 0.64              |
| 1:K:328:PHE:HB2  | 1:K:367:VAL:HG21 | 1.78                     | 0.64              |
| 1:L:334:LYS:NZ   | 1:L:367:VAL:HG22 | 2.12                     | 0.64              |
| 1:N:282:ASN:O    | 1:N:285:GLU:HB2  | 1.96                     | 0.64              |
| 1:N:316:ASP:C    | 1:N:319:PRO:HD2  | 2.23                     | 0.64              |
| 1:E:310:LEU:HD23 | 1:E:352:TRP:CD1  | 2.33                     | 0.64              |
| 1:G:325:LEU:HD23 | 1:G:325:LEU:C    | 2.22                     | 0.64              |
| 1:L:172:GLY:O    | 1:L:176:VAL:HG23 | 1.98                     | 0.64              |
| 1:L:310:LEU:O    | 1:L:313:ARG:N    | 2.20                     | 0.64              |
| 1:M:339:PHE:HB3  | 1:M:343:ALA:HB3  | 1.78                     | 0.64              |
| 1:C:207:GLU:HG3  | 1:C:226:PHE:HE1  | 1.63                     | 0.64              |
| 1:E:279:THR:OG1  | 1:E:280:ASN:N    | 2.29                     | 0.64              |
| 1:H:162:PRO:HB2  | 1:H:300:LEU:HD22 | 1.80                     | 0.64              |
| 1:A:296:LEU:HD13 | 1:A:296:LEU:C    | 2.23                     | 0.64              |
| 1:F:326:LYS:HE2  | 1:F:330:ARG:HH21 | 1.58                     | 0.64              |
| 1:H:293:ARG:HH11 | 1:H:293:ARG:CG   | 2.02                     | 0.64              |
| 1:I:168:GLU:O    | 1:I:173:LYS:HE2  | 1.98                     | 0.64              |
| 1:I:299:ARG:O    | 1:I:302:VAL:HG23 | 1.98                     | 0.64              |
| 1:I:314:LYS:HA   | 1:I:317:ILE:HD11 | 1.79                     | 0.64              |
| 1:J:163:VAL:HG13 | 1:J:303:ILE:O    | 1.98                     | 0.64              |
| 1:K:303:ILE:HD11 | 1:L:368:LEU:HD13 | 1.79                     | 0.64              |
| 1:M:353:TYR:C    | 1:M:355:ASN:H    | 2.05                     | 0.64              |
| 1:N:245:LEU:HD23 | 1:N:248:GLN:NE2  | 2.13                     | 0.64              |
| 1:B:236:PHE:HD1  | 1:B:276:LEU:O    | 1.80                     | 0.63              |
| 1:B:337:GLU:OE1  | 1:B:373:LYS:HD3  | 1.98                     | 0.63              |
| 1:J:346:LEU:HD23 | 1:J:346:LEU:O    | 1.97                     | 0.63              |
| 1:F:335:GLU:O    | 1:F:373:LYS:HA   | 1.99                     | 0.63              |
| 1:H:334:LYS:CG   | 1:H:335:GLU:N    | 2.62                     | 0.63              |
| 1:I:153:ILE:HG23 | 1:I:180:ILE:HG12 | 1.79                     | 0.63              |
| 1:L:171:VAL:HB   | 1:L:307:ILE:HG22 | 1.81                     | 0.63              |
| 1:N:194:LEU:O    | 1:N:194:LEU:HD23 | 1.98                     | 0.63              |
| 1:A:143:SER:HB3  | 1:A:316:ASP:OD1  | 1.98                     | 0.63              |
| 1:J:189:GLU:HG2  | 1:J:232:GLY:O    | 1.98                     | 0.63              |
| 1:B:359:LEU:C    | 1:B:361:ASN:H    | 2.06                     | 0.63              |
| 1:D:284:LYS:HG2  | 1:D:297:TYR:CZ   | 2.33                     | 0.63              |
| 1:F:337:GLU:OE1  | 1:F:373:LYS:HD3  | 1.99                     | 0.63              |
| 1:G:280:ASN:OD1  | 1:G:281:ARG:HD3  | 1.97                     | 0.63              |
| 1:H:293:ARG:HG2  | 1:H:293:ARG:NH1  | 2.01                     | 0.63              |
| 1:H:309:PRO:HB3  | 1:H:311:ARG:CZ   | 2.28                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:208:LEU:HD21 | 1:L:227:PHE:CD1  | 2.33                     | 0.63              |
| 1:M:166:THR:O    | 1:M:307:ILE:N    | 2.29                     | 0.63              |
| 1:A:172:GLY:O    | 1:A:173:LYS:C    | 2.40                     | 0.63              |
| 1:A:204:PHE:HE2  | 1:A:243:LEU:HD21 | 1.63                     | 0.63              |
| 1:B:143:SER:OG   | 1:B:146:MET:HB2  | 1.97                     | 0.63              |
| 1:C:365:ARG:HH11 | 1:C:383:LEU:HD22 | 1.63                     | 0.63              |
| 1:D:163:VAL:HB   | 1:D:276:LEU:HD22 | 1.80                     | 0.63              |
| 1:D:365:ARG:HD2  | 1:D:383:LEU:CD2  | 2.29                     | 0.63              |
| 1:E:259:LYS:HG2  | 1:E:270:GLU:HB2  | 1.81                     | 0.63              |
| 1:F:196:VAL:HG13 | 1:F:204:PHE:CE1  | 2.34                     | 0.63              |
| 1:K:157:SER:HB3  | 1:K:183:LEU:O    | 1.98                     | 0.63              |
| 1:K:316:ASP:C    | 1:K:319:PRO:HD2  | 2.22                     | 0.63              |
| 1:M:181:HIS:HD2  | 1:M:234:THR:HB   | 1.64                     | 0.63              |
| 1:N:282:ASN:HD21 | 1:N:284:LYS:HB2  | 1.62                     | 0.63              |
| 1:A:165:ILE:O    | 1:A:278:ALA:HA   | 1.99                     | 0.63              |
| 1:A:377:ARG:HH21 | 1:L:285:GLU:CG   | 2.11                     | 0.63              |
| 1:B:150:LEU:HD11 | 1:B:154:LYS:HZ2  | 1.64                     | 0.63              |
| 1:B:250:LYS:HG3  | 1:C:198:SER:HB2  | 1.81                     | 0.63              |
| 1:B:324:PHE:CD1  | 1:B:363:ILE:HD12 | 2.29                     | 0.63              |
| 1:E:176:VAL:HG21 | 1:E:307:ILE:CD1  | 2.27                     | 0.63              |
| 1:F:170:GLY:O    | 1:F:172:GLY:N    | 2.32                     | 0.63              |
| 1:K:303:ILE:O    | 1:K:303:ILE:HG22 | 1.98                     | 0.63              |
| 1:L:165:ILE:N    | 1:L:278:ALA:HB2  | 2.13                     | 0.63              |
| 1:N:251:LEU:HD23 | 1:N:251:LEU:O    | 1.98                     | 0.63              |
| 1:F:170:GLY:C    | 1:F:172:GLY:H    | 2.06                     | 0.63              |
| 1:F:313:ARG:O    | 1:F:315:GLU:N    | 2.32                     | 0.63              |
| 1:I:211:TYR:CE1  | 1:I:223:LYS:HB2  | 2.33                     | 0.63              |
| 1:K:201:ARG:HH11 | 1:K:201:ARG:CB   | 2.09                     | 0.63              |
| 1:L:315:GLU:CD   | 1:L:315:GLU:H    | 2.06                     | 0.63              |
| 1:B:237:LEU:HB2  | 1:B:240:ILE:HD11 | 1.79                     | 0.63              |
| 1:B:264:GLY:HA2  | 1:C:207:GLU:OE2  | 1.98                     | 0.63              |
| 1:C:275:ILE:HD12 | 1:C:275:ILE:N    | 2.13                     | 0.63              |
| 1:F:343:ALA:HB2  | 1:F:376:ASP:HA   | 1.79                     | 0.63              |
| 1:K:161:CYS:O    | 1:K:274:ARG:NH1  | 2.32                     | 0.63              |
| 1:K:279:THR:HG21 | 1:K:283:ILE:CD1  | 2.27                     | 0.63              |
| 1:M:354:GLY:O    | 1:M:357:ARG:HB3  | 1.99                     | 0.63              |
| 1:A:144:PRO:HG2  | 1:A:145:LYS:H    | 1.63                     | 0.63              |
| 1:D:161:CYS:HB2  | 1:D:162:PRO:HD2  | 1.81                     | 0.63              |
| 1:D:301:GLY:O    | 1:D:302:VAL:C    | 2.41                     | 0.63              |
| 1:E:269:ILE:HD12 | 1:E:269:ILE:N    | 2.13                     | 0.63              |
| 1:G:340:THR:C    | 1:G:342:SER:N    | 2.54                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:336:VAL:HG21 | 1:L:370:SER:OG   | 1.99                     | 0.63              |
| 1:N:311:ARG:O    | 1:N:312:GLU:HG2  | 1.99                     | 0.63              |
| 1:A:299:ARG:HH21 | 1:A:302:VAL:HG21 | 1.63                     | 0.62              |
| 1:E:173:LYS:NZ   | 1:E:173:LYS:HB2  | 2.14                     | 0.62              |
| 1:F:309:PRO:CG   | 1:F:311:ARG:NH1  | 2.60                     | 0.62              |
| 1:L:200:PRO:HG2  | 1:L:203:ILE:HD12 | 1.81                     | 0.62              |
| 1:M:243:LEU:HD22 | 1:M:247:ALA:CB   | 2.26                     | 0.62              |
| 1:M:357:ARG:O    | 1:M:361:ASN:HB2  | 2.00                     | 0.62              |
| 1:C:160:GLU:OE2  | 1:C:186:ARG:NH2  | 2.32                     | 0.62              |
| 1:E:344:GLN:O    | 1:E:348:LEU:CD1  | 2.36                     | 0.62              |
| 1:H:216:PHE:O    | 1:H:218:GLY:N    | 2.26                     | 0.62              |
| 1:J:262:ARG:HG2  | 1:J:262:ARG:HH11 | 1.64                     | 0.62              |
| 1:K:266:ARG:NH1  | 1:L:224:GLU:O    | 2.32                     | 0.62              |
| 1:M:140:VAL:C    | 1:M:141:PHE:HD1  | 2.07                     | 0.62              |
| 1:M:186:ARG:HD3  | 1:M:233:GLY:HA2  | 1.80                     | 0.62              |
| 1:M:246:GLU:H    | 1:M:246:GLU:CD   | 2.07                     | 0.62              |
| 1:M:281:ARG:CG   | 1:M:286:LEU:HD21 | 2.29                     | 0.62              |
| 1:D:325:LEU:HD23 | 1:D:325:LEU:C    | 2.23                     | 0.62              |
| 1:M:191:PHE:CD2  | 1:M:191:PHE:C    | 2.77                     | 0.62              |
| 1:N:234:THR:HG23 | 1:N:274:ARG:O    | 1.99                     | 0.62              |
| 1:A:179:LEU:C    | 1:A:181:HIS:H    | 2.07                     | 0.62              |
| 1:A:234:THR:HG23 | 1:A:274:ARG:O    | 1.99                     | 0.62              |
| 1:B:207:GLU:O    | 1:B:225:GLY:HA2  | 1.99                     | 0.62              |
| 1:B:217:THR:HG23 | 1:B:218:GLY:N    | 2.10                     | 0.62              |
| 1:C:347:LEU:HD21 | 1:C:380:LEU:CD1  | 2.28                     | 0.62              |
| 1:E:156:ILE:CD1  | 1:F:368:LEU:HD13 | 2.30                     | 0.62              |
| 1:I:314:LYS:HA   | 1:I:317:ILE:CG1  | 2.29                     | 0.62              |
| 1:K:310:LEU:HD22 | 1:K:317:ILE:HG12 | 1.80                     | 0.62              |
| 1:L:248:GLN:NE2  | 1:L:292:PHE:HA   | 2.15                     | 0.62              |
| 1:L:350:TYR:CD2  | 1:L:352:TRP:N    | 2.66                     | 0.62              |
| 1:N:282:ASN:HD22 | 1:N:285:GLU:CG   | 2.08                     | 0.62              |
| 1:A:157:SER:HB3  | 1:A:184:SER:HA   | 1.81                     | 0.62              |
| 1:D:157:SER:C    | 1:D:159:ALA:H    | 2.07                     | 0.62              |
| 1:E:196:VAL:HG11 | 1:E:243:LEU:HD23 | 1.82                     | 0.62              |
| 1:F:365:ARG:HG2  | 1:F:369:PHE:CE2  | 2.34                     | 0.62              |
| 1:H:142:GLU:HB3  | 1:H:146:MET:HB2  | 1.81                     | 0.62              |
| 1:I:367:VAL:O    | 1:I:367:VAL:HG12 | 1.98                     | 0.62              |
| 1:J:302:VAL:O    | 1:J:303:ILE:HD13 | 2.00                     | 0.62              |
| 1:C:228:GLU:O    | 1:C:231:ASP:HB2  | 1.99                     | 0.62              |
| 1:L:240:ILE:HD13 | 1:L:300:LEU:CD1  | 2.30                     | 0.62              |
| 1:L:376:ASP:C    | 1:L:378:GLY:N    | 2.58                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:253:ARG:HH21 | 1:M:259:LYS:HE3  | 1.63                     | 0.62              |
| 1:N:227:PHE:O    | 1:N:228:GLU:C    | 2.42                     | 0.62              |
| 1:N:251:LEU:CD2  | 1:N:296:LEU:HD21 | 2.29                     | 0.62              |
| 1:D:156:ILE:CD1  | 1:D:303:ILE:HG21 | 2.29                     | 0.62              |
| 1:D:275:ILE:H    | 1:D:275:ILE:CD1  | 2.00                     | 0.62              |
| 1:I:189:GLU:OE1  | 1:I:189:GLU:HA   | 1.99                     | 0.62              |
| 1:J:341:LYS:O    | 1:J:345:GLU:HG3  | 1.99                     | 0.62              |
| 1:M:146:MET:HA   | 1:M:146:MET:CE   | 2.29                     | 0.62              |
| 1:N:181:HIS:CD2  | 1:N:234:THR:HB   | 2.35                     | 0.62              |
| 1:B:250:LYS:O    | 1:B:253:ARG:HG2  | 2.00                     | 0.62              |
| 1:F:343:ALA:C    | 1:F:345:GLU:N    | 2.58                     | 0.62              |
| 1:G:240:ILE:CG1  | 1:G:277:ALA:HB1  | 2.25                     | 0.62              |
| 1:I:171:VAL:HG11 | 1:I:307:ILE:O    | 1.99                     | 0.62              |
| 1:D:352:TRP:O    | 1:D:355:ASN:N    | 2.33                     | 0.62              |
| 1:E:201:ARG:HH11 | 1:E:201:ARG:CB   | 2.11                     | 0.62              |
| 1:B:194:LEU:HD23 | 1:B:194:LEU:H    | 1.64                     | 0.62              |
| 1:C:178:ARG:CG   | 1:C:178:ARG:NH1  | 2.53                     | 0.62              |
| 1:E:189:GLU:HG2  | 1:E:232:GLY:O    | 1.99                     | 0.62              |
| 1:E:238:ASP:O    | 1:E:239:GLU:HG2  | 1.99                     | 0.62              |
| 1:K:316:ASP:O    | 1:K:319:PRO:HD2  | 1.99                     | 0.62              |
| 1:A:174:GLU:HG3  | 1:A:236:PHE:HE2  | 1.65                     | 0.61              |
| 1:B:251:LEU:HD22 | 1:B:255:ILE:HD11 | 1.82                     | 0.61              |
| 1:E:354:GLY:C    | 1:E:358:GLU:CB   | 2.72                     | 0.61              |
| 1:F:326:LYS:O    | 1:F:329:SER:HB3  | 2.00                     | 0.61              |
| 1:H:309:PRO:HB2  | 1:H:311:ARG:HD2  | 1.82                     | 0.61              |
| 1:I:171:VAL:HG12 | 1:I:307:ILE:CG2  | 2.30                     | 0.61              |
| 1:L:266:ARG:NH2  | 1:M:207:GLU:OE2  | 2.33                     | 0.61              |
| 1:A:316:ASP:O    | 1:A:319:PRO:HD2  | 2.00                     | 0.61              |
| 1:D:143:SER:CB   | 1:D:144:PRO:HD2  | 2.30                     | 0.61              |
| 1:E:352:TRP:HE3  | 1:E:358:GLU:HG2  | 1.65                     | 0.61              |
| 1:F:172:GLY:HA2  | 2:F:4:ADP:O3A    | 1.99                     | 0.61              |
| 1:G:320:LEU:HD21 | 1:G:324:PHE:CE1  | 2.36                     | 0.61              |
| 1:I:263:LEU:HD23 | 1:I:263:LEU:C    | 2.25                     | 0.61              |
| 1:L:146:MET:HE2  | 1:L:313:ARG:NH2  | 2.15                     | 0.61              |
| 1:A:240:ILE:HG12 | 1:A:278:ALA:O    | 2.01                     | 0.61              |
| 1:A:323:HIS:O    | 1:A:326:LYS:HB3  | 2.00                     | 0.61              |
| 1:C:266:ARG:NE   | 1:D:203:ILE:HD12 | 2.15                     | 0.61              |
| 1:D:296:LEU:CD1  | 1:D:300:LEU:HD11 | 2.30                     | 0.61              |
| 1:G:169:SER:O    | 1:G:355:ASN:ND2  | 2.32                     | 0.61              |
| 1:H:168:GLU:HG3  | 1:H:311:ARG:NH2  | 2.15                     | 0.61              |
| 1:K:163:VAL:HB   | 1:K:276:LEU:HD22 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:275:ILE:HD12 | 1:K:275:ILE:H    | 1.63                     | 0.61              |
| 1:K:340:THR:HG21 | 1:K:376:ASP:HB3  | 1.82                     | 0.61              |
| 1:E:236:PHE:CE1  | 1:E:278:ALA:CB   | 2.83                     | 0.61              |
| 1:H:236:PHE:HD1  | 1:H:276:LEU:O    | 1.83                     | 0.61              |
| 1:I:157:SER:HB2  | 1:I:184:SER:HA   | 1.82                     | 0.61              |
| 1:I:259:LYS:HD3  | 1:I:268:GLU:OE1  | 2.00                     | 0.61              |
| 1:K:340:THR:O    | 1:K:344:GLN:HG3  | 2.00                     | 0.61              |
| 1:N:322:ASN:O    | 1:N:326:LYS:HB2  | 2.00                     | 0.61              |
| 1:A:318:ILE:CG1  | 1:A:348:LEU:HD21 | 2.25                     | 0.61              |
| 1:D:318:ILE:CG1  | 1:D:319:PRO:HD3  | 2.19                     | 0.61              |
| 1:E:266:ARG:HA   | 1:E:266:ARG:HE   | 1.66                     | 0.61              |
| 1:L:195:ASN:O    | 1:L:197:ALA:N    | 2.33                     | 0.61              |
| 1:M:140:VAL:HB   | 1:M:320:LEU:CD2  | 2.30                     | 0.61              |
| 1:A:194:LEU:HD23 | 1:A:194:LEU:H    | 1.64                     | 0.61              |
| 1:C:139:TYR:HB2  | 1:C:141:PHE:CE1  | 2.36                     | 0.61              |
| 1:E:155:LYS:HD3  | 1:F:369:PHE:HA   | 1.83                     | 0.61              |
| 1:E:216:PHE:H    | 1:E:216:PHE:HD2  | 1.47                     | 0.61              |
| 1:I:358:GLU:O    | 1:I:362:VAL:HG23 | 2.00                     | 0.61              |
| 1:K:163:VAL:HB   | 1:K:276:LEU:CD2  | 2.31                     | 0.61              |
| 1:M:248:GLN:HG3  | 1:M:293:ARG:HB2  | 1.81                     | 0.61              |
| 1:N:200:PRO:HB2  | 1:N:202:ASP:OD1  | 2.01                     | 0.61              |
| 1:N:260:PHE:CD1  | 1:N:260:PHE:C    | 2.78                     | 0.61              |
| 1:N:303:ILE:O    | 1:N:305:ILE:HG13 | 2.01                     | 0.61              |
| 1:B:325:LEU:HD21 | 1:B:336:VAL:CG1  | 2.31                     | 0.61              |
| 1:C:231:ASP:C    | 1:C:233:GLY:H    | 2.09                     | 0.61              |
| 1:D:178:ARG:HG3  | 1:D:178:ARG:HH11 | 1.66                     | 0.61              |
| 1:E:226:PHE:O    | 1:E:227:PHE:C    | 2.44                     | 0.61              |
| 1:F:269:ILE:H    | 1:F:269:ILE:HD12 | 1.66                     | 0.61              |
| 1:F:314:LYS:O    | 1:F:317:ILE:HG13 | 2.00                     | 0.61              |
| 1:L:152:LYS:O    | 1:L:155:LYS:N    | 2.30                     | 0.61              |
| 1:L:322:ASN:O    | 1:L:325:LEU:N    | 2.33                     | 0.61              |
| 1:N:274:ARG:HG2  | 1:N:274:ARG:HH11 | 1.64                     | 0.61              |
| 1:C:172:GLY:HA2  | 2:C:1:ADP:O1A    | 2.00                     | 0.61              |
| 1:C:266:ARG:HH21 | 1:D:203:ILE:HD11 | 1.66                     | 0.61              |
| 1:D:146:MET:HA   | 1:D:146:MET:HE3  | 1.83                     | 0.61              |
| 1:E:316:ASP:O    | 1:E:319:PRO:CD   | 2.47                     | 0.61              |
| 1:G:164:LEU:HD12 | 1:G:165:ILE:N    | 2.16                     | 0.61              |
| 1:G:261:TYR:CD1  | 1:G:261:TYR:N    | 2.68                     | 0.61              |
| 1:G:294:GLU:O    | 1:G:297:TYR:HB3  | 2.00                     | 0.61              |
| 1:L:251:LEU:O    | 1:L:252:LEU:C    | 2.42                     | 0.61              |
| 1:N:383:LEU:O    | 1:N:384:VAL:HG23 | 2.01                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:282:ASN:HD22 | 1:A:285:GLU:HB2  | 1.66                     | 0.61              |
| 1:A:324:PHE:CE2  | 1:A:360:LYS:HG3  | 2.36                     | 0.61              |
| 1:C:156:ILE:HD13 | 1:C:303:ILE:HG21 | 1.81                     | 0.61              |
| 1:G:252:LEU:HD13 | 1:G:296:LEU:HA   | 1.83                     | 0.61              |
| 1:G:263:LEU:HD23 | 1:G:264:GLY:N    | 2.16                     | 0.61              |
| 1:F:284:LYS:HE2  | 1:F:297:TYR:OH   | 2.00                     | 0.61              |
| 1:I:181:HIS:CE1  | 1:I:191:PHE:HB2  | 2.36                     | 0.61              |
| 1:J:216:PHE:CD2  | 1:J:216:PHE:N    | 2.63                     | 0.61              |
| 1:L:143:SER:HB3  | 1:L:316:ASP:OD2  | 2.01                     | 0.61              |
| 1:L:146:MET:CE   | 1:L:313:ARG:HE   | 2.13                     | 0.61              |
| 1:L:334:LYS:CE   | 1:L:336:VAL:HB   | 2.29                     | 0.61              |
| 1:H:323:HIS:O    | 1:H:327:LYS:HB2  | 2.00                     | 0.60              |
| 1:I:159:ALA:HB1  | 1:J:332:TYR:OH   | 2.01                     | 0.60              |
| 1:I:204:PHE:O    | 1:I:207:GLU:N    | 2.32                     | 0.60              |
| 1:K:181:HIS:HD2  | 1:K:234:THR:OG1  | 1.84                     | 0.60              |
| 1:K:316:ASP:O    | 1:K:320:LEU:HG   | 2.01                     | 0.60              |
| 1:K:340:THR:CG2  | 1:K:376:ASP:HB3  | 2.31                     | 0.60              |
| 1:L:365:ARG:HG3  | 1:L:369:PHE:HE2  | 1.66                     | 0.60              |
| 1:N:178:ARG:HH11 | 1:N:178:ARG:HG3  | 1.65                     | 0.60              |
| 1:F:209:PHE:HE2  | 1:F:254:VAL:HG21 | 1.67                     | 0.60              |
| 1:G:318:ILE:O    | 1:G:321:ALA:HB3  | 2.00                     | 0.60              |
| 1:I:204:PHE:CE2  | 1:I:208:LEU:HD12 | 2.36                     | 0.60              |
| 1:K:157:SER:HB3  | 1:K:183:LEU:C    | 2.26                     | 0.60              |
| 1:M:195:ASN:HB3  | 1:M:198:SER:OG   | 2.01                     | 0.60              |
| 1:D:314:LYS:HA   | 1:D:317:ILE:HG13 | 1.83                     | 0.60              |
| 1:D:324:PHE:CD1  | 1:D:359:LEU:HD22 | 2.36                     | 0.60              |
| 1:E:195:ASN:O    | 1:E:197:ALA:N    | 2.33                     | 0.60              |
| 1:H:234:THR:CG2  | 1:H:276:LEU:HD12 | 2.29                     | 0.60              |
| 1:I:203:ILE:O    | 1:I:206:ALA:HB3  | 2.01                     | 0.60              |
| 1:K:302:VAL:O    | 1:K:302:VAL:HG12 | 2.01                     | 0.60              |
| 1:M:176:VAL:O    | 1:M:177:ALA:C    | 2.44                     | 0.60              |
| 1:B:314:LYS:HD2  | 1:B:314:LYS:N    | 2.12                     | 0.60              |
| 1:C:163:VAL:HB   | 1:C:276:LEU:CD2  | 2.31                     | 0.60              |
| 1:C:303:ILE:HD13 | 1:D:365:ARG:HG3  | 1.84                     | 0.60              |
| 1:D:189:GLU:CG   | 1:D:190:PRO:HD2  | 2.30                     | 0.60              |
| 1:I:171:VAL:HG12 | 1:I:307:ILE:HG22 | 1.81                     | 0.60              |
| 1:J:313:ARG:HB3  | 1:J:316:ASP:OD2  | 2.02                     | 0.60              |
| 1:J:365:ARG:CD   | 1:J:383:LEU:HD22 | 2.30                     | 0.60              |
| 1:B:204:PHE:C    | 1:B:206:ALA:N    | 2.55                     | 0.60              |
| 1:B:235:LEU:HG   | 1:B:237:LEU:HD21 | 1.82                     | 0.60              |
| 1:B:256:GLU:OE2  | 1:C:357:ARG:HD3  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:328:PHE:HB2  | 1:B:367:VAL:HG21 | 1.83                     | 0.60              |
| 1:C:311:ARG:HH21 | 1:C:353:TYR:HD2  | 1.46                     | 0.60              |
| 1:J:262:ARG:HG2  | 1:J:262:ARG:NH1  | 2.16                     | 0.60              |
| 1:K:302:VAL:CG2  | 1:L:361:ASN:HB3  | 2.31                     | 0.60              |
| 1:L:140:VAL:HG21 | 1:L:320:LEU:HD23 | 1.84                     | 0.60              |
| 1:L:314:LYS:O    | 1:L:317:ILE:HG13 | 2.01                     | 0.60              |
| 1:M:252:LEU:HD11 | 1:M:299:ARG:HG3  | 1.83                     | 0.60              |
| 1:B:142:GLU:HG3  | 1:B:142:GLU:O    | 2.01                     | 0.60              |
| 1:E:189:GLU:CG   | 1:E:232:GLY:O    | 2.49                     | 0.60              |
| 1:F:201:ARG:HH11 | 1:F:201:ARG:CB   | 2.11                     | 0.60              |
| 1:F:213:LYS:HB3  | 1:G:220:VAL:HG11 | 1.82                     | 0.60              |
| 1:F:229:LEU:HD13 | 1:F:229:LEU:O    | 2.02                     | 0.60              |
| 1:G:310:LEU:HB2  | 1:G:355:ASN:HB2  | 1.83                     | 0.60              |
| 1:K:176:VAL:HG21 | 1:K:307:ILE:HD11 | 1.84                     | 0.60              |
| 1:K:248:GLN:O    | 1:K:250:LYS:N    | 2.35                     | 0.60              |
| 1:C:194:LEU:CD2  | 1:C:235:LEU:HD11 | 2.32                     | 0.60              |
| 1:C:207:GLU:HG3  | 1:C:226:PHE:CE1  | 2.36                     | 0.60              |
| 1:G:263:LEU:CG   | 1:G:264:GLY:N    | 2.64                     | 0.60              |
| 1:H:176:VAL:CG2  | 1:H:307:ILE:HD11 | 2.30                     | 0.60              |
| 1:H:334:LYS:HE3  | 1:H:336:VAL:O    | 2.00                     | 0.60              |
| 1:L:138:GLU:O    | 1:L:139:TYR:CG   | 2.54                     | 0.60              |
| 1:L:329:SER:CB   | 1:L:334:LYS:HE2  | 2.30                     | 0.60              |
| 1:N:283:ILE:HG23 | 1:N:292:PHE:CD1  | 2.37                     | 0.60              |
| 1:A:339:PHE:CD1  | 1:A:339:PHE:N    | 2.68                     | 0.60              |
| 1:B:269:ILE:CG2  | 1:B:270:GLU:N    | 2.64                     | 0.60              |
| 1:B:296:LEU:C    | 1:B:296:LEU:HD13 | 2.26                     | 0.60              |
| 1:C:172:GLY:HA2  | 2:C:1:ADP:PA     | 2.41                     | 0.60              |
| 1:E:168:GLU:HB2  | 1:E:171:VAL:CG1  | 2.32                     | 0.60              |
| 1:F:350:TYR:HD2  | 1:F:352:TRP:CD2  | 2.19                     | 0.60              |
| 1:N:282:ASN:ND2  | 1:N:285:GLU:HG2  | 2.09                     | 0.60              |
| 1:A:237:LEU:HB2  | 1:A:240:ILE:HD13 | 1.84                     | 0.60              |
| 1:B:261:TYR:O    | 1:B:262:ARG:C    | 2.43                     | 0.60              |
| 1:E:239:GLU:HA   | 1:E:279:THR:HA   | 1.83                     | 0.60              |
| 1:F:309:PRO:HA   | 1:F:355:ASN:ND2  | 2.17                     | 0.60              |
| 1:K:322:ASN:O    | 1:K:326:LYS:HB2  | 2.02                     | 0.60              |
| 1:L:225:GLY:O    | 1:L:226:PHE:C    | 2.44                     | 0.60              |
| 1:M:339:PHE:HA   | 1:M:375:ILE:O    | 2.02                     | 0.60              |
| 1:N:339:PHE:CD2  | 1:N:347:LEU:HD11 | 2.37                     | 0.60              |
| 1:A:143:SER:HB3  | 1:A:316:ASP:CG   | 2.26                     | 0.60              |
| 1:A:220:VAL:O    | 1:A:221:SER:HB3  | 2.02                     | 0.60              |
| 1:G:252:LEU:HD11 | 1:G:299:ARG:HG3  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:347:LEU:HD21 | 1:L:380:LEU:HD11 | 1.84                     | 0.60              |
| 1:N:194:LEU:H    | 1:N:194:LEU:CD2  | 2.15                     | 0.60              |
| 1:N:313:ARG:O    | 1:N:315:GLU:N    | 2.35                     | 0.60              |
| 1:N:357:ARG:NH1  | 1:N:361:ASN:OD1  | 2.35                     | 0.60              |
| 1:A:325:LEU:HD23 | 1:A:325:LEU:C    | 2.25                     | 0.59              |
| 1:B:224:GLU:HG2  | 1:B:228:GLU:HB2  | 1.83                     | 0.59              |
| 1:F:164:LEU:HD12 | 1:F:277:ALA:O    | 2.02                     | 0.59              |
| 1:F:341:LYS:O    | 1:F:345:GLU:HG3  | 2.02                     | 0.59              |
| 1:I:194:LEU:CD2  | 1:I:235:LEU:HD11 | 2.31                     | 0.59              |
| 1:I:249:ALA:HB2  | 1:I:293:ARG:NH1  | 2.17                     | 0.59              |
| 1:M:164:LEU:CD2  | 1:M:283:ILE:HG13 | 2.31                     | 0.59              |
| 1:C:318:ILE:O    | 1:C:321:ALA:HB3  | 2.02                     | 0.59              |
| 1:D:283:ILE:HD12 | 1:D:292:PHE:CE1  | 2.37                     | 0.59              |
| 1:D:341:LYS:HD2  | 1:D:345:GLU:OE2  | 2.01                     | 0.59              |
| 1:G:163:VAL:HB   | 1:G:276:LEU:CD2  | 2.32                     | 0.59              |
| 1:G:341:LYS:O    | 1:G:345:GLU:HG3  | 2.01                     | 0.59              |
| 1:I:318:ILE:CG1  | 1:I:319:PRO:HD3  | 2.28                     | 0.59              |
| 1:K:325:LEU:HD21 | 1:K:336:VAL:HG12 | 1.83                     | 0.59              |
| 1:L:240:ILE:HD13 | 1:L:300:LEU:HD13 | 1.84                     | 0.59              |
| 1:L:252:LEU:HD11 | 1:L:256:GLU:OE1  | 2.01                     | 0.59              |
| 1:M:191:PHE:C    | 1:M:191:PHE:HD2  | 2.10                     | 0.59              |
| 1:A:328:PHE:HA   | 1:A:331:LYS:HB3  | 1.83                     | 0.59              |
| 1:C:146:MET:HE2  | 1:C:313:ARG:HH21 | 1.67                     | 0.59              |
| 1:G:146:MET:CE   | 1:G:149:ILE:HD12 | 2.31                     | 0.59              |
| 1:G:210:GLY:HA2  | 1:G:224:GLU:O    | 2.02                     | 0.59              |
| 1:G:249:ALA:HA   | 1:G:293:ARG:NH1  | 2.16                     | 0.59              |
| 1:J:352:TRP:CZ3  | 1:J:358:GLU:HG2  | 2.37                     | 0.59              |
| 1:K:165:ILE:O    | 1:K:165:ILE:HG22 | 2.01                     | 0.59              |
| 1:M:140:VAL:O    | 1:M:141:PHE:HD1  | 1.85                     | 0.59              |
| 1:M:145:LYS:O    | 1:M:148:GLU:HB3  | 2.02                     | 0.59              |
| 1:C:173:LYS:H    | 2:C:1:ADP:PB     | 2.25                     | 0.59              |
| 1:C:322:ASN:O    | 1:C:325:LEU:N    | 2.35                     | 0.59              |
| 1:C:365:ARG:O    | 1:C:368:LEU:HB2  | 2.02                     | 0.59              |
| 1:D:227:PHE:CD2  | 1:D:273:VAL:HG21 | 2.36                     | 0.59              |
| 1:E:171:VAL:O    | 1:E:307:ILE:HG21 | 2.02                     | 0.59              |
| 1:E:283:ILE:O    | 1:E:287:VAL:HG23 | 2.01                     | 0.59              |
| 1:E:325:LEU:HD21 | 1:E:336:VAL:CG1  | 2.29                     | 0.59              |
| 1:G:261:TYR:HB3  | 1:G:266:ARG:C    | 2.26                     | 0.59              |
| 1:H:247:ALA:O    | 1:H:248:GLN:C    | 2.45                     | 0.59              |
| 1:L:209:PHE:HE2  | 1:L:254:VAL:HG21 | 1.67                     | 0.59              |
| 1:L:342:SER:OG   | 1:L:376:ASP:HB2  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:139:TYR:HB3  | 1:N:141:PHE:HE1  | 1.67                     | 0.59              |
| 1:N:267:LYS:O    | 1:N:269:ILE:N    | 2.35                     | 0.59              |
| 1:N:335:GLU:O    | 1:N:373:LYS:HA   | 2.01                     | 0.59              |
| 1:D:252:LEU:O    | 1:D:255:ILE:HG13 | 2.01                     | 0.59              |
| 1:F:346:LEU:HG   | 1:F:377:ARG:NH1  | 2.17                     | 0.59              |
| 1:H:145:LYS:HB2  | 1:H:313:ARG:NH2  | 2.17                     | 0.59              |
| 1:H:328:PHE:C    | 1:H:367:VAL:HG11 | 2.27                     | 0.59              |
| 1:I:310:LEU:HD22 | 1:I:317:ILE:HG12 | 1.83                     | 0.59              |
| 1:N:320:LEU:O    | 1:N:323:HIS:N    | 2.35                     | 0.59              |
| 1:A:191:PHE:CE2  | 1:A:193:ALA:HB2  | 2.36                     | 0.59              |
| 1:D:281:ARG:HH11 | 1:D:281:ARG:HG2  | 1.66                     | 0.59              |
| 1:E:176:VAL:O    | 1:E:180:ILE:HD12 | 2.03                     | 0.59              |
| 1:E:176:VAL:CG1  | 1:E:180:ILE:HD11 | 2.21                     | 0.59              |
| 1:K:141:PHE:CE1  | 1:K:150:LEU:HD13 | 2.38                     | 0.59              |
| 1:B:330:ARG:HG3  | 1:B:330:ARG:NH1  | 2.17                     | 0.59              |
| 1:C:322:ASN:O    | 1:C:323:HIS:C    | 2.46                     | 0.59              |
| 1:E:139:TYR:CD2  | 1:E:179:LEU:HD11 | 2.37                     | 0.59              |
| 1:E:320:LEU:C    | 1:E:322:ASN:N    | 2.60                     | 0.59              |
| 1:H:266:ARG:HB3  | 1:I:229:LEU:HD23 | 1.84                     | 0.59              |
| 1:I:302:VAL:HG12 | 1:I:303:ILE:HG12 | 1.83                     | 0.59              |
| 1:I:366:ALA:C    | 1:I:368:LEU:H    | 2.09                     | 0.59              |
| 1:N:178:ARG:NE   | 1:N:191:PHE:CE2  | 2.70                     | 0.59              |
| 1:D:275:ILE:HD12 | 1:D:275:ILE:N    | 2.04                     | 0.59              |
| 1:F:318:ILE:HG13 | 1:F:319:PRO:CD   | 2.16                     | 0.59              |
| 1:H:194:LEU:HD23 | 1:H:194:LEU:N    | 2.15                     | 0.59              |
| 1:I:146:MET:SD   | 1:I:313:ARG:CZ   | 2.91                     | 0.59              |
| 1:K:143:SER:O    | 1:K:147:LYS:HB2  | 2.02                     | 0.59              |
| 1:L:337:GLU:OE1  | 1:L:373:LYS:HD3  | 2.01                     | 0.59              |
| 1:E:176:VAL:C    | 1:E:180:ILE:HD12 | 2.28                     | 0.59              |
| 1:E:347:LEU:HD21 | 1:E:380:LEU:HD13 | 1.84                     | 0.59              |
| 1:H:339:PHE:HD1  | 1:H:339:PHE:H    | 1.51                     | 0.59              |
| 1:I:318:ILE:O    | 1:I:321:ALA:HB3  | 2.02                     | 0.59              |
| 1:J:202:ASP:O    | 1:J:202:ASP:CG   | 2.45                     | 0.59              |
| 1:A:164:LEU:HD12 | 1:A:165:ILE:N    | 2.16                     | 0.59              |
| 1:C:163:VAL:HB   | 1:C:276:LEU:HD23 | 1.85                     | 0.59              |
| 1:D:252:LEU:HA   | 1:D:255:ILE:CD1  | 2.33                     | 0.59              |
| 1:J:269:ILE:HD12 | 1:J:269:ILE:H    | 1.68                     | 0.59              |
| 1:M:161:CYS:HB2  | 1:M:302:VAL:HG11 | 1.83                     | 0.59              |
| 1:B:317:ILE:CB   | 1:B:348:LEU:HD23 | 2.32                     | 0.58              |
| 1:C:336:VAL:HG21 | 1:C:370:SER:CB   | 2.33                     | 0.58              |
| 1:H:214:GLY:N    | 1:H:219:ALA:CB   | 2.55                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:239:GLU:N    | 1:J:278:ALA:O    | 2.35                     | 0.58              |
| 1:L:315:GLU:O    | 1:L:319:PRO:HG2  | 2.03                     | 0.58              |
| 1:L:343:ALA:O    | 1:L:346:LEU:N    | 2.36                     | 0.58              |
| 1:N:325:LEU:HD12 | 1:N:339:PHE:CE1  | 2.38                     | 0.58              |
| 1:A:194:LEU:HD21 | 1:A:237:LEU:HD22 | 1.86                     | 0.58              |
| 1:E:166:THR:HG22 | 1:E:167:GLY:N    | 2.18                     | 0.58              |
| 1:E:209:PHE:HD1  | 1:E:209:PHE:H    | 1.51                     | 0.58              |
| 1:F:341:LYS:HA   | 1:F:344:GLN:HB2  | 1.84                     | 0.58              |
| 1:G:320:LEU:CD2  | 1:G:359:LEU:HD13 | 2.22                     | 0.58              |
| 1:I:208:LEU:CD2  | 1:I:227:PHE:HD1  | 2.16                     | 0.58              |
| 1:J:157:SER:HB3  | 1:J:184:SER:N    | 2.18                     | 0.58              |
| 1:L:145:LYS:O    | 1:L:148:GLU:HB3  | 2.03                     | 0.58              |
| 1:L:213:LYS:O    | 1:L:219:ALA:HB1  | 2.03                     | 0.58              |
| 1:B:171:VAL:HG21 | 1:B:307:ILE:HB   | 1.84                     | 0.58              |
| 1:C:215:ALA:C    | 1:C:217:THR:H    | 2.12                     | 0.58              |
| 1:C:249:ALA:O    | 1:C:252:LEU:HB3  | 2.02                     | 0.58              |
| 1:E:170:GLY:O    | 1:E:356:VAL:HG23 | 2.03                     | 0.58              |
| 1:E:253:ARG:HH11 | 1:E:253:ARG:HG3  | 1.68                     | 0.58              |
| 1:E:351:PRO:O    | 1:E:352:TRP:C    | 2.46                     | 0.58              |
| 1:F:252:LEU:HD13 | 1:F:296:LEU:HA   | 1.84                     | 0.58              |
| 1:F:359:LEU:O    | 1:F:361:ASN:N    | 2.35                     | 0.58              |
| 1:N:192:VAL:CG2  | 1:N:230:ALA:HB2  | 2.34                     | 0.58              |
| 1:B:208:LEU:CD2  | 1:B:209:PHE:HE1  | 2.16                     | 0.58              |
| 1:B:292:PHE:CE2  | 1:B:296:LEU:HD12 | 2.37                     | 0.58              |
| 1:D:266:ARG:HH22 | 1:E:207:GLU:CG   | 2.16                     | 0.58              |
| 1:E:342:SER:OG   | 1:E:377:ARG:HB2  | 2.04                     | 0.58              |
| 1:F:343:ALA:O    | 1:F:344:GLN:C    | 2.46                     | 0.58              |
| 1:M:248:GLN:O    | 1:M:252:LEU:N    | 2.31                     | 0.58              |
| 1:M:266:ARG:HH21 | 1:M:267:LYS:NZ   | 2.01                     | 0.58              |
| 1:D:324:PHE:HD1  | 1:D:359:LEU:HD22 | 1.68                     | 0.58              |
| 1:E:365:ARG:HD2  | 1:E:383:LEU:HD13 | 1.85                     | 0.58              |
| 1:H:350:TYR:HB3  | 1:H:351:PRO:CA   | 2.33                     | 0.58              |
| 1:J:352:TRP:CE3  | 1:J:358:GLU:HG2  | 2.39                     | 0.58              |
| 1:K:215:ALA:H    | 1:K:219:ALA:HB1  | 1.66                     | 0.58              |
| 1:M:164:LEU:HD21 | 1:M:283:ILE:CG1  | 2.31                     | 0.58              |
| 1:N:313:ARG:C    | 1:N:315:GLU:H    | 2.12                     | 0.58              |
| 1:A:143:SER:CB   | 1:A:144:PRO:HD2  | 2.32                     | 0.58              |
| 1:B:318:ILE:HD13 | 1:B:348:LEU:HD11 | 1.84                     | 0.58              |
| 1:C:261:TYR:O    | 1:C:262:ARG:C    | 2.46                     | 0.58              |
| 1:G:176:VAL:O    | 1:G:177:ALA:C    | 2.46                     | 0.58              |
| 1:I:189:GLU:HB3  | 1:I:190:PRO:CD   | 2.27                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:216:PHE:H    | 1:K:219:ALA:CB   | 2.17                     | 0.58              |
| 1:K:314:LYS:HA   | 1:K:317:ILE:CD1  | 2.34                     | 0.58              |
| 1:L:146:MET:SD   | 1:L:313:ARG:NE   | 2.77                     | 0.58              |
| 1:L:240:ILE:HB   | 1:L:279:THR:CG2  | 2.33                     | 0.58              |
| 1:A:365:ARG:HD2  | 1:A:383:LEU:CD1  | 2.34                     | 0.58              |
| 1:B:156:ILE:O    | 1:B:158:CYS:N    | 2.36                     | 0.58              |
| 1:C:328:PHE:CE1  | 1:C:364:GLU:HB2  | 2.38                     | 0.58              |
| 1:D:181:HIS:CD2  | 1:D:234:THR:OG1  | 2.57                     | 0.58              |
| 1:E:173:LYS:HB2  | 1:E:173:LYS:HZ3  | 1.69                     | 0.58              |
| 1:G:242:GLU:HG2  | 1:G:281:ARG:NH2  | 2.19                     | 0.58              |
| 1:K:237:LEU:HB2  | 1:K:240:ILE:HD11 | 1.85                     | 0.58              |
| 1:L:376:ASP:C    | 1:L:378:GLY:H    | 2.11                     | 0.58              |
| 1:N:186:ARG:HD3  | 1:N:232:GLY:O    | 2.04                     | 0.58              |
| 1:E:259:LYS:HE2  | 1:E:270:GLU:OE2  | 2.03                     | 0.58              |
| 1:F:149:ILE:CD1  | 1:F:307:ILE:HD13 | 2.32                     | 0.58              |
| 1:G:231:ASP:HA   | 1:G:273:VAL:HG22 | 1.85                     | 0.58              |
| 1:H:311:ARG:O    | 1:H:314:LYS:HE2  | 2.03                     | 0.58              |
| 1:I:350:TYR:CG   | 1:I:351:PRO:HD2  | 2.39                     | 0.58              |
| 1:I:355:ASN:O    | 1:I:358:GLU:N    | 2.27                     | 0.58              |
| 1:J:200:PRO:HG3  | 1:J:203:ILE:HD12 | 1.86                     | 0.58              |
| 1:K:314:LYS:HA   | 1:K:317:ILE:CG1  | 2.33                     | 0.58              |
| 1:L:156:ILE:O    | 1:L:158:CYS:N    | 2.36                     | 0.58              |
| 1:L:208:LEU:HD22 | 1:L:209:PHE:CD1  | 2.39                     | 0.58              |
| 1:M:350:TYR:CD1  | 1:M:351:PRO:HD2  | 2.39                     | 0.58              |
| 1:B:251:LEU:O    | 1:B:252:LEU:C    | 2.47                     | 0.58              |
| 1:H:332:TYR:O    | 1:H:333:ALA:HB3  | 2.02                     | 0.58              |
| 1:I:325:LEU:HD23 | 1:I:325:LEU:C    | 2.28                     | 0.58              |
| 1:J:167:GLY:O    | 1:J:280:ASN:HA   | 2.04                     | 0.58              |
| 1:M:172:GLY:O    | 1:M:176:VAL:HG23 | 2.04                     | 0.58              |
| 1:M:324:PHE:CD1  | 1:M:359:LEU:HD23 | 2.38                     | 0.58              |
| 1:M:352:TRP:HA   | 1:M:352:TRP:HE3  | 1.69                     | 0.58              |
| 1:E:335:GLU:HG3  | 1:E:335:GLU:O    | 2.04                     | 0.58              |
| 1:F:343:ALA:C    | 1:F:345:GLU:H    | 2.12                     | 0.58              |
| 1:K:265:GLY:O    | 1:K:266:ARG:NE   | 2.36                     | 0.58              |
| 1:N:211:TYR:OH   | 1:N:223:LYS:HG3  | 2.04                     | 0.58              |
| 1:B:142:GLU:HG2  | 1:B:319:PRO:HG2  | 1.85                     | 0.57              |
| 1:C:244:SER:O    | 1:C:247:ALA:HB3  | 2.04                     | 0.57              |
| 1:E:214:GLY:CA   | 1:E:219:ALA:HB3  | 2.29                     | 0.57              |
| 1:F:194:LEU:HD13 | 1:F:226:PHE:HD1  | 1.67                     | 0.57              |
| 1:G:211:TYR:HE1  | 1:G:263:LEU:HD13 | 1.69                     | 0.57              |
| 1:G:318:ILE:CG1  | 1:G:319:PRO:HD3  | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:211:TYR:CE2  | 1:J:223:LYS:HB3  | 2.39                     | 0.57              |
| 1:K:349:SER:OG   | 1:K:350:TYR:N    | 2.36                     | 0.57              |
| 1:M:358:GLU:O    | 1:M:359:LEU:C    | 2.46                     | 0.57              |
| 1:D:296:LEU:HD11 | 1:D:300:LEU:HD11 | 1.86                     | 0.57              |
| 1:E:239:GLU:C    | 1:E:241:GLY:H    | 2.11                     | 0.57              |
| 1:D:351:PRO:HB2  | 1:D:353:TYR:CE2  | 2.39                     | 0.57              |
| 1:E:294:GLU:OE2  | 1:F:169:SER:HB3  | 2.05                     | 0.57              |
| 1:F:160:GLU:OE2  | 1:F:186:ARG:NH2  | 2.37                     | 0.57              |
| 1:F:275:ILE:HD12 | 1:F:275:ILE:N    | 2.19                     | 0.57              |
| 1:F:300:LEU:C    | 1:F:302:VAL:H    | 2.12                     | 0.57              |
| 1:G:211:TYR:CE1  | 1:G:263:LEU:HD13 | 2.39                     | 0.57              |
| 1:G:279:THR:HG21 | 1:G:283:ILE:HD11 | 1.86                     | 0.57              |
| 1:I:196:VAL:HG13 | 1:I:204:PHE:CE1  | 2.39                     | 0.57              |
| 1:M:340:THR:OG1  | 1:M:376:ASP:HA   | 2.04                     | 0.57              |
| 1:N:314:LYS:HB2  | 1:N:314:LYS:NZ   | 2.19                     | 0.57              |
| 1:A:158:CYS:HA   | 1:A:185:ASP:OD2  | 2.04                     | 0.57              |
| 1:A:275:ILE:H    | 1:A:275:ILE:CD1  | 2.15                     | 0.57              |
| 1:B:230:ALA:O    | 1:B:273:VAL:HG22 | 2.05                     | 0.57              |
| 1:B:266:ARG:NH2  | 1:C:207:GLU:OE2  | 2.34                     | 0.57              |
| 1:G:340:THR:C    | 1:G:342:SER:H    | 2.12                     | 0.57              |
| 1:H:140:VAL:HG12 | 1:H:141:PHE:N    | 2.19                     | 0.57              |
| 1:H:226:PHE:O    | 1:H:227:PHE:C    | 2.46                     | 0.57              |
| 1:H:334:LYS:CG   | 1:H:335:GLU:H    | 2.18                     | 0.57              |
| 1:K:192:VAL:HB   | 1:K:230:ALA:HB2  | 1.87                     | 0.57              |
| 1:L:152:LYS:C    | 1:L:154:LYS:N    | 2.60                     | 0.57              |
| 1:L:334:LYS:NZ   | 1:L:367:VAL:CG2  | 2.67                     | 0.57              |
| 1:M:141:PHE:O    | 1:M:142:GLU:C    | 2.47                     | 0.57              |
| 1:M:314:LYS:HA   | 1:M:317:ILE:HD11 | 1.86                     | 0.57              |
| 1:M:336:VAL:HG11 | 1:M:375:ILE:HG13 | 1.86                     | 0.57              |
| 1:A:194:LEU:HD21 | 1:A:237:LEU:CD2  | 2.34                     | 0.57              |
| 1:C:251:LEU:CD2  | 1:C:255:ILE:HD11 | 2.32                     | 0.57              |
| 1:G:282:ASN:ND2  | 1:G:285:GLU:HB2  | 2.20                     | 0.57              |
| 1:G:355:ASN:O    | 1:G:357:ARG:N    | 2.35                     | 0.57              |
| 1:H:215:ALA:CB   | 1:I:223:LYS:HZ1  | 2.18                     | 0.57              |
| 1:K:194:LEU:HD22 | 1:K:226:PHE:CD1  | 2.38                     | 0.57              |
| 1:M:206:ALA:HB2  | 1:M:216:PHE:CZ   | 2.39                     | 0.57              |
| 1:N:201:ARG:HH11 | 1:N:201:ARG:CB   | 2.11                     | 0.57              |
| 1:N:254:VAL:C    | 1:N:256:GLU:H    | 2.12                     | 0.57              |
| 1:E:176:VAL:O    | 1:E:180:ILE:HG13 | 2.04                     | 0.57              |
| 1:E:324:PHE:O    | 1:E:326:LYS:N    | 2.38                     | 0.57              |
| 1:F:145:LYS:O    | 1:F:148:GLU:HB3  | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:359:LEU:O    | 1:F:362:VAL:N    | 2.38                     | 0.57              |
| 1:H:250:LYS:O    | 1:H:251:LEU:C    | 2.47                     | 0.57              |
| 1:H:324:PHE:HB2  | 1:H:363:ILE:HG21 | 1.86                     | 0.57              |
| 1:I:340:THR:OG1  | 1:I:376:ASP:HB3  | 2.04                     | 0.57              |
| 1:J:224:GLU:HG2  | 1:J:225:GLY:N    | 2.10                     | 0.57              |
| 1:A:240:ILE:C    | 1:A:242:GLU:H    | 2.13                     | 0.57              |
| 1:C:181:HIS:ND1  | 1:C:181:HIS:C    | 2.63                     | 0.57              |
| 1:H:146:MET:CG   | 1:H:313:ARG:CZ   | 2.82                     | 0.57              |
| 1:H:161:CYS:SG   | 1:H:303:ILE:CD1  | 2.93                     | 0.57              |
| 1:H:161:CYS:SG   | 1:H:303:ILE:HD12 | 2.45                     | 0.57              |
| 1:H:235:LEU:HD23 | 1:H:236:PHE:N    | 2.19                     | 0.57              |
| 1:J:201:ARG:NH2  | 1:J:242:GLU:O    | 2.38                     | 0.57              |
| 1:M:155:LYS:O    | 1:M:156:ILE:C    | 2.48                     | 0.57              |
| 1:B:315:GLU:OE1  | 1:B:315:GLU:N    | 2.35                     | 0.57              |
| 1:B:321:ALA:HB1  | 1:B:339:PHE:CZ   | 2.40                     | 0.57              |
| 1:E:381:SER:C    | 1:E:383:LEU:H    | 2.13                     | 0.57              |
| 1:F:143:SER:HB2  | 1:F:144:PRO:CD   | 2.33                     | 0.57              |
| 1:F:365:ARG:HD2  | 1:F:383:LEU:CD2  | 2.35                     | 0.57              |
| 1:H:363:ILE:O    | 1:H:367:VAL:HG23 | 2.04                     | 0.57              |
| 1:J:181:HIS:CD2  | 1:J:191:PHE:HD1  | 2.23                     | 0.57              |
| 1:N:194:LEU:HD23 | 1:N:194:LEU:H    | 1.70                     | 0.57              |
| 1:B:288:LYS:C    | 1:B:290:GLY:H    | 2.13                     | 0.57              |
| 1:C:310:LEU:HD22 | 1:C:317:ILE:HG12 | 1.86                     | 0.57              |
| 1:D:181:HIS:HD2  | 1:D:234:THR:OG1  | 1.88                     | 0.57              |
| 1:E:195:ASN:C    | 1:E:197:ALA:H    | 2.13                     | 0.57              |
| 1:F:157:SER:O    | 1:F:184:SER:HA   | 2.05                     | 0.57              |
| 1:F:240:ILE:C    | 1:F:242:GLU:H    | 2.12                     | 0.57              |
| 1:F:313:ARG:O    | 1:F:314:LYS:C    | 2.46                     | 0.57              |
| 1:J:352:TRP:CH2  | 1:J:359:LEU:HD23 | 2.39                     | 0.57              |
| 1:L:138:GLU:O    | 1:L:139:TYR:CD1  | 2.58                     | 0.57              |
| 1:L:218:GLY:O    | 1:L:220:VAL:HG23 | 2.05                     | 0.57              |
| 1:L:237:LEU:HB2  | 1:L:277:ALA:HB2  | 1.86                     | 0.57              |
| 1:N:174:GLU:O    | 1:N:177:ALA:N    | 2.38                     | 0.57              |
| 1:A:212:GLU:O    | 1:A:213:LYS:C    | 2.48                     | 0.57              |
| 1:B:359:LEU:O    | 1:B:361:ASN:N    | 2.38                     | 0.57              |
| 1:C:299:ARG:HG2  | 1:C:299:ARG:HH11 | 1.70                     | 0.57              |
| 1:C:347:LEU:HD21 | 1:C:380:LEU:HD11 | 1.87                     | 0.57              |
| 1:E:211:TYR:HD1  | 1:E:223:LYS:HE2  | 1.70                     | 0.57              |
| 1:F:242:GLU:CG   | 1:F:281:ARG:HH22 | 2.18                     | 0.57              |
| 1:G:224:GLU:HG2  | 1:G:225:GLY:N    | 2.16                     | 0.57              |
| 1:I:182:LYS:O    | 1:I:187:SER:HB3  | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:363:ILE:O    | 1:J:367:VAL:HG23 | 2.05                     | 0.57              |
| 1:K:275:ILE:H    | 1:K:275:ILE:CD1  | 2.18                     | 0.57              |
| 1:L:146:MET:HE2  | 1:L:313:ARG:NE   | 2.20                     | 0.57              |
| 1:M:244:SER:O    | 1:M:248:GLN:NE2  | 2.38                     | 0.57              |
| 1:N:352:TRP:HZ3  | 1:N:362:VAL:HG21 | 1.70                     | 0.57              |
| 1:A:179:LEU:C    | 1:A:181:HIS:N    | 2.61                     | 0.56              |
| 1:B:250:LYS:HZ3  | 1:B:253:ARG:NH2  | 2.02                     | 0.56              |
| 1:B:325:LEU:HD23 | 1:B:325:LEU:O    | 2.03                     | 0.56              |
| 1:C:293:ARG:NH2  | 1:C:295:ASP:OD2  | 2.37                     | 0.56              |
| 1:E:320:LEU:O    | 1:E:321:ALA:C    | 2.47                     | 0.56              |
| 1:H:266:ARG:HB3  | 1:I:229:LEU:CD2  | 2.35                     | 0.56              |
| 1:H:346:LEU:O    | 1:H:346:LEU:HD23 | 2.04                     | 0.56              |
| 1:I:351:PRO:HB2  | 1:I:353:TYR:CE2  | 2.40                     | 0.56              |
| 1:K:143:SER:CB   | 1:K:144:PRO:HD2  | 2.34                     | 0.56              |
| 1:B:359:LEU:C    | 1:B:361:ASN:N    | 2.61                     | 0.56              |
| 1:D:209:PHE:CD1  | 1:D:250:LYS:HD3  | 2.40                     | 0.56              |
| 1:I:328:PHE:CZ   | 1:I:364:GLU:HB2  | 2.40                     | 0.56              |
| 1:A:139:TYR:CE2  | 1:A:175:VAL:HG13 | 2.41                     | 0.56              |
| 1:A:232:GLY:HA2  | 1:A:272:ASN:HD22 | 1.69                     | 0.56              |
| 1:B:285:GLU:OE2  | 1:K:349:SER:HB3  | 2.04                     | 0.56              |
| 1:B:343:ALA:HB2  | 1:B:376:ASP:HA   | 1.87                     | 0.56              |
| 1:B:358:GLU:O    | 1:B:362:VAL:HG23 | 2.05                     | 0.56              |
| 1:C:324:PHE:CD1  | 1:C:360:LYS:HA   | 2.41                     | 0.56              |
| 1:E:152:LYS:HG2  | 1:F:369:PHE:HE1  | 1.66                     | 0.56              |
| 1:E:254:VAL:HG22 | 1:E:260:PHE:HB3  | 1.88                     | 0.56              |
| 1:G:207:GLU:HG2  | 1:G:226:PHE:CE1  | 2.41                     | 0.56              |
| 1:H:347:LEU:HD21 | 1:H:380:LEU:HD13 | 1.87                     | 0.56              |
| 1:K:190:PRO:HD2  | 1:K:233:GLY:HA3  | 1.86                     | 0.56              |
| 1:L:287:VAL:HG12 | 1:L:288:LYS:N    | 2.19                     | 0.56              |
| 1:L:359:LEU:O    | 1:L:362:VAL:N    | 2.38                     | 0.56              |
| 1:M:308:PRO:HG2  | 1:M:313:ARG:CD   | 2.28                     | 0.56              |
| 1:N:296:LEU:HD13 | 1:N:300:LEU:HG   | 1.88                     | 0.56              |
| 1:N:302:VAL:O    | 1:N:303:ILE:HD13 | 2.05                     | 0.56              |
| 1:A:172:GLY:O    | 1:A:175:VAL:N    | 2.38                     | 0.56              |
| 1:A:275:ILE:O    | 1:A:276:LEU:HD23 | 2.05                     | 0.56              |
| 1:A:285:GLU:O    | 1:A:289:GLU:HG3  | 2.06                     | 0.56              |
| 1:C:382:CYS:O    | 1:C:383:LEU:HD23 | 2.06                     | 0.56              |
| 1:D:163:VAL:HB   | 1:D:276:LEU:CD2  | 2.36                     | 0.56              |
| 1:D:368:LEU:C    | 1:D:370:SER:H    | 2.13                     | 0.56              |
| 1:E:171:VAL:CG1  | 1:E:355:ASN:OD1  | 2.51                     | 0.56              |
| 1:I:152:LYS:O    | 1:I:155:LYS:N    | 2.37                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:178:ARG:HE   | 1:K:191:PHE:HD2  | 1.51                     | 0.56              |
| 1:L:288:LYS:C    | 1:L:290:GLY:H    | 2.12                     | 0.56              |
| 1:M:194:LEU:HD21 | 1:M:237:LEU:CD2  | 2.23                     | 0.56              |
| 1:M:261:TYR:CE2  | 1:N:199:ILE:HG12 | 2.39                     | 0.56              |
| 1:M:280:ASN:OD1  | 1:M:281:ARG:N    | 2.38                     | 0.56              |
| 1:B:146:MET:HE2  | 1:B:313:ARG:NH2  | 2.21                     | 0.56              |
| 1:D:303:ILE:CD1  | 1:E:365:ARG:HG3  | 2.35                     | 0.56              |
| 1:E:365:ARG:HG2  | 1:E:369:PHE:CE2  | 2.41                     | 0.56              |
| 1:E:378:GLY:O    | 1:E:381:SER:OG   | 2.15                     | 0.56              |
| 1:G:310:LEU:HB2  | 1:G:355:ASN:HB3  | 1.87                     | 0.56              |
| 1:L:173:LYS:HB2  | 1:L:173:LYS:NZ   | 2.21                     | 0.56              |
| 1:M:244:SER:O    | 1:M:247:ALA:CB   | 2.53                     | 0.56              |
| 1:B:366:ALA:O    | 1:B:370:SER:HB3  | 2.06                     | 0.56              |
| 1:E:186:ARG:NH2  | 1:E:272:ASN:ND2  | 2.50                     | 0.56              |
| 1:F:366:ALA:O    | 1:F:368:LEU:N    | 2.39                     | 0.56              |
| 1:G:275:ILE:N    | 1:G:275:ILE:CD1  | 2.67                     | 0.56              |
| 1:H:271:VAL:CG1  | 1:H:273:VAL:HG23 | 2.35                     | 0.56              |
| 1:I:266:ARG:HH11 | 1:J:216:PHE:HE1  | 1.54                     | 0.56              |
| 1:N:174:GLU:O    | 1:N:175:VAL:C    | 2.49                     | 0.56              |
| 1:N:228:GLU:O    | 1:N:230:ALA:N    | 2.39                     | 0.56              |
| 1:N:255:ILE:O    | 1:N:255:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:376:ASP:O    | 1:A:378:GLY:N    | 2.38                     | 0.56              |
| 1:B:365:ARG:NH1  | 1:B:383:LEU:O    | 2.39                     | 0.56              |
| 1:J:143:SER:O    | 1:J:147:LYS:HB2  | 2.06                     | 0.56              |
| 1:N:277:ALA:O    | 1:N:278:ALA:HB2  | 2.05                     | 0.56              |
| 1:N:303:ILE:O    | 1:N:303:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:299:ARG:HE   | 1:A:299:ARG:CA   | 2.19                     | 0.56              |
| 1:G:324:PHE:CD1  | 1:G:360:LYS:HA   | 2.41                     | 0.56              |
| 1:H:152:LYS:O    | 1:H:156:ILE:HG12 | 2.05                     | 0.56              |
| 1:H:194:LEU:HD13 | 1:H:226:PHE:CD2  | 2.40                     | 0.56              |
| 1:H:231:ASP:CG   | 1:H:271:VAL:HG13 | 2.31                     | 0.56              |
| 1:H:324:PHE:CB   | 1:H:363:ILE:HG21 | 2.36                     | 0.56              |
| 1:H:357:ARG:NH1  | 1:N:252:LEU:HD21 | 2.10                     | 0.56              |
| 1:K:178:ARG:NE   | 1:K:191:PHE:CE2  | 2.74                     | 0.56              |
| 1:K:200:PRO:HG2  | 1:K:203:ILE:CG1  | 2.35                     | 0.56              |
| 1:B:203:ILE:HG22 | 1:B:203:ILE:O    | 2.06                     | 0.56              |
| 1:B:251:LEU:HD22 | 1:B:255:ILE:CD1  | 2.36                     | 0.56              |
| 1:C:208:LEU:HD11 | 1:C:227:PHE:CD1  | 2.41                     | 0.56              |
| 1:H:157:SER:OG   | 1:H:183:LEU:HB2  | 2.06                     | 0.56              |
| 1:H:177:ALA:O    | 1:H:178:ARG:C    | 2.49                     | 0.56              |
| 1:H:254:VAL:CG2  | 1:H:260:PHE:HB3  | 2.34                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:209:PHE:C    | 1:K:225:GLY:HA3  | 2.31                     | 0.56              |
| 1:N:316:ASP:O    | 1:N:319:PRO:HD2  | 2.06                     | 0.56              |
| 1:B:152:LYS:O    | 1:B:156:ILE:HG12 | 2.06                     | 0.56              |
| 1:C:252:LEU:HB2  | 1:C:296:LEU:HD23 | 1.88                     | 0.56              |
| 1:D:186:ARG:O    | 1:D:189:GLU:HB2  | 2.06                     | 0.56              |
| 1:F:174:GLU:HG2  | 1:F:178:ARG:NH1  | 2.21                     | 0.56              |
| 1:F:321:ALA:HB1  | 1:F:339:PHE:CZ   | 2.41                     | 0.56              |
| 1:F:357:ARG:HH11 | 1:F:357:ARG:CG   | 2.17                     | 0.56              |
| 1:F:376:ASP:O    | 1:F:377:ARG:C    | 2.49                     | 0.56              |
| 1:G:173:LYS:O    | 1:G:175:VAL:N    | 2.38                     | 0.56              |
| 1:J:152:LYS:O    | 1:J:156:ILE:HG12 | 2.05                     | 0.56              |
| 1:L:170:GLY:C    | 1:L:172:GLY:H    | 2.14                     | 0.56              |
| 1:L:240:ILE:HD11 | 1:L:277:ALA:CB   | 2.31                     | 0.56              |
| 1:M:310:LEU:HD22 | 1:M:317:ILE:HG12 | 1.88                     | 0.56              |
| 1:B:248:GLN:OE1  | 1:B:293:ARG:HG3  | 2.05                     | 0.55              |
| 1:B:266:ARG:HB3  | 1:C:229:LEU:HD21 | 1.87                     | 0.55              |
| 1:C:299:ARG:HH12 | 1:D:357:ARG:NH1  | 2.03                     | 0.55              |
| 1:D:292:PHE:CE2  | 1:D:296:LEU:HD12 | 2.40                     | 0.55              |
| 1:F:323:HIS:HD1  | 1:F:323:HIS:C    | 2.15                     | 0.55              |
| 1:G:168:GLU:OE1  | 1:G:309:PRO:HB3  | 2.05                     | 0.55              |
| 1:I:252:LEU:HD21 | 1:I:295:ASP:HB2  | 1.88                     | 0.55              |
| 1:L:184:SER:O    | 1:L:186:ARG:N    | 2.39                     | 0.55              |
| 1:M:253:ARG:CG   | 1:N:198:SER:CB   | 2.84                     | 0.55              |
| 1:B:269:ILE:HG22 | 1:B:270:GLU:N    | 2.19                     | 0.55              |
| 1:G:203:ILE:O    | 1:G:203:ILE:HG22 | 2.06                     | 0.55              |
| 1:I:196:VAL:HA   | 1:I:204:PHE:HE1  | 1.72                     | 0.55              |
| 1:I:205:GLU:HG2  | 1:I:247:ALA:HB2  | 1.86                     | 0.55              |
| 1:L:149:ILE:HD13 | 1:L:307:ILE:CD1  | 2.36                     | 0.55              |
| 1:N:143:SER:CB   | 1:N:144:PRO:HD2  | 2.31                     | 0.55              |
| 1:C:253:ARG:HH11 | 1:C:253:ARG:CG   | 2.19                     | 0.55              |
| 1:D:171:VAL:HG21 | 1:D:307:ILE:HB   | 1.89                     | 0.55              |
| 1:F:209:PHE:C    | 1:F:225:GLY:HA3  | 2.31                     | 0.55              |
| 1:F:223:LYS:C    | 1:F:225:GLY:N    | 2.63                     | 0.55              |
| 1:F:310:LEU:C    | 1:F:312:GLU:H    | 2.14                     | 0.55              |
| 1:F:347:LEU:CD2  | 1:F:380:LEU:HD12 | 2.34                     | 0.55              |
| 1:G:198:SER:C    | 1:G:199:ILE:HG13 | 2.31                     | 0.55              |
| 1:H:299:ARG:O    | 1:H:302:VAL:HG23 | 2.06                     | 0.55              |
| 1:I:172:GLY:HA2  | 2:I:8:ADP:PA     | 2.46                     | 0.55              |
| 1:I:350:TYR:CE1  | 1:I:384:VAL:HB   | 2.42                     | 0.55              |
| 1:J:339:PHE:HB3  | 1:J:343:ALA:HB3  | 1.88                     | 0.55              |
| 1:J:346:LEU:HD23 | 1:J:346:LEU:C    | 2.31                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:139:TYR:CE1  | 1:K:175:VAL:HG13 | 2.41                     | 0.55              |
| 1:K:321:ALA:HA   | 1:K:363:ILE:CD1  | 2.36                     | 0.55              |
| 1:M:340:THR:C    | 1:M:342:SER:H    | 2.13                     | 0.55              |
| 1:N:245:LEU:HD23 | 1:N:248:GLN:HE21 | 1.70                     | 0.55              |
| 1:A:192:VAL:CG2  | 1:A:230:ALA:HB2  | 2.37                     | 0.55              |
| 1:E:357:ARG:O    | 1:E:358:GLU:C    | 2.46                     | 0.55              |
| 1:F:355:ASN:O    | 1:F:357:ARG:N    | 2.34                     | 0.55              |
| 1:F:365:ARG:HD2  | 1:F:383:LEU:HD21 | 1.88                     | 0.55              |
| 1:I:300:LEU:C    | 1:I:302:VAL:H    | 2.13                     | 0.55              |
| 1:J:216:PHE:HD2  | 1:J:216:PHE:N    | 1.90                     | 0.55              |
| 1:J:281:ARG:HG2  | 1:J:281:ARG:HH11 | 1.71                     | 0.55              |
| 1:K:189:GLU:HA   | 1:K:189:GLU:OE1  | 2.04                     | 0.55              |
| 1:L:173:LYS:H    | 2:L:11:ADP:PB    | 2.29                     | 0.55              |
| 1:M:211:TYR:N    | 1:M:211:TYR:CD1  | 2.74                     | 0.55              |
| 1:M:294:GLU:HG2  | 1:M:295:ASP:N    | 2.22                     | 0.55              |
| 1:E:168:GLU:HB2  | 1:E:171:VAL:HG11 | 1.88                     | 0.55              |
| 1:E:236:PHE:CE1  | 1:E:278:ALA:HB2  | 2.38                     | 0.55              |
| 1:E:326:LYS:HE2  | 1:E:330:ARG:HH21 | 1.71                     | 0.55              |
| 1:I:249:ALA:HB2  | 1:I:293:ARG:HH11 | 1.71                     | 0.55              |
| 1:I:311:ARG:HG3  | 1:I:312:GLU:HG3  | 1.88                     | 0.55              |
| 1:I:313:ARG:HB3  | 1:I:316:ASP:OD2  | 2.06                     | 0.55              |
| 1:K:240:ILE:HG22 | 1:K:292:PHE:CE1  | 2.41                     | 0.55              |
| 1:L:157:SER:HB2  | 1:L:183:LEU:O    | 2.06                     | 0.55              |
| 1:B:362:VAL:HG11 | 1:B:384:VAL:HG11 | 1.88                     | 0.55              |
| 1:E:162:PRO:HG3  | 1:E:299:ARG:O    | 2.06                     | 0.55              |
| 1:F:194:LEU:HD23 | 1:F:236:PHE:O    | 2.06                     | 0.55              |
| 1:F:283:ILE:O    | 1:F:286:LEU:N    | 2.40                     | 0.55              |
| 1:G:150:LEU:O    | 1:G:153:ILE:HB   | 2.06                     | 0.55              |
| 1:H:346:LEU:HD12 | 1:H:377:ARG:HE   | 1.71                     | 0.55              |
| 1:I:161:CYS:O    | 1:I:274:ARG:NH1  | 2.40                     | 0.55              |
| 1:I:195:ASN:ND2  | 1:I:238:ASP:OD2  | 2.38                     | 0.55              |
| 1:L:267:LYS:O    | 1:L:269:ILE:HD12 | 2.05                     | 0.55              |
| 1:L:328:PHE:CE2  | 1:L:364:GLU:HB2  | 2.41                     | 0.55              |
| 1:L:342:SER:O    | 1:L:377:ARG:HD2  | 2.07                     | 0.55              |
| 1:C:292:PHE:CE2  | 1:C:296:LEU:HD12 | 2.41                     | 0.55              |
| 1:D:203:ILE:CG2  | 1:D:207:GLU:HG2  | 2.37                     | 0.55              |
| 1:D:332:TYR:CD1  | 1:D:368:LEU:HD21 | 2.41                     | 0.55              |
| 1:E:176:VAL:C    | 1:E:180:ILE:CD1  | 2.80                     | 0.55              |
| 1:F:142:GLU:OE1  | 1:F:142:GLU:HA   | 2.06                     | 0.55              |
| 1:J:220:VAL:CG1  | 1:J:221:SER:N    | 2.68                     | 0.55              |
| 1:L:339:PHE:CD2  | 1:L:375:ILE:HD11 | 2.41                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:141:PHE:CD2  | 1:M:150:LEU:HB2  | 2.41                     | 0.55              |
| 1:B:164:LEU:HD12 | 1:B:165:ILE:N    | 2.22                     | 0.55              |
| 1:D:141:PHE:HE1  | 1:D:179:LEU:HD12 | 1.70                     | 0.55              |
| 1:E:209:PHE:N    | 1:E:209:PHE:CD1  | 2.74                     | 0.55              |
| 1:E:244:SER:O    | 1:E:246:GLU:N    | 2.39                     | 0.55              |
| 1:E:298:TYR:CE1  | 1:F:354:GLY:CA   | 2.90                     | 0.55              |
| 1:H:215:ALA:HB3  | 1:H:264:GLY:HA3  | 1.88                     | 0.55              |
| 1:K:346:LEU:O    | 1:K:346:LEU:HD23 | 2.07                     | 0.55              |
| 1:L:311:ARG:HH11 | 1:L:353:TYR:HE2  | 1.53                     | 0.55              |
| 1:N:192:VAL:HB   | 1:N:230:ALA:HB2  | 1.87                     | 0.55              |
| 1:B:381:SER:O    | 1:B:382:CYS:C    | 2.49                     | 0.55              |
| 1:D:149:ILE:O    | 1:D:153:ILE:HG12 | 2.06                     | 0.55              |
| 1:E:177:ALA:HB1  | 1:E:276:LEU:HD12 | 1.88                     | 0.55              |
| 1:E:341:LYS:O    | 1:E:341:LYS:HD3  | 2.07                     | 0.55              |
| 1:F:156:ILE:O    | 1:F:158:CYS:N    | 2.39                     | 0.55              |
| 1:G:153:ILE:HG23 | 1:G:180:ILE:HG12 | 1.89                     | 0.55              |
| 1:G:191:PHE:HD2  | 1:G:191:PHE:C    | 2.15                     | 0.55              |
| 1:G:252:LEU:CD1  | 1:G:299:ARG:HG3  | 2.37                     | 0.55              |
| 1:H:271:VAL:HG12 | 1:H:273:VAL:HG23 | 1.88                     | 0.55              |
| 1:C:240:ILE:HD12 | 1:C:243:LEU:HD12 | 1.88                     | 0.55              |
| 1:E:267:LYS:H    | 1:E:267:LYS:CD   | 2.15                     | 0.55              |
| 1:G:310:LEU:CD2  | 1:G:317:ILE:HG12 | 2.37                     | 0.55              |
| 1:I:143:SER:HB2  | 1:I:144:PRO:HD2  | 1.89                     | 0.55              |
| 1:I:292:PHE:HE2  | 1:I:296:LEU:HB3  | 1.71                     | 0.55              |
| 1:I:336:VAL:HA   | 1:I:373:LYS:O    | 2.07                     | 0.55              |
| 1:J:349:SER:OG   | 1:J:350:TYR:N    | 2.40                     | 0.55              |
| 1:M:211:TYR:N    | 1:M:211:TYR:HD1  | 2.05                     | 0.55              |
| 1:M:256:GLU:O    | 1:M:258:GLY:N    | 2.40                     | 0.55              |
| 1:D:271:VAL:HG23 | 1:D:273:VAL:HG23 | 1.88                     | 0.54              |
| 1:E:203:ILE:O    | 1:E:203:ILE:HG22 | 2.05                     | 0.54              |
| 1:G:191:PHE:CE2  | 1:G:193:ALA:HB2  | 2.42                     | 0.54              |
| 1:L:165:ILE:HG22 | 1:L:173:LYS:HG2  | 1.89                     | 0.54              |
| 1:N:152:LYS:O    | 1:N:156:ILE:HG12 | 2.08                     | 0.54              |
| 1:B:192:VAL:CG2  | 1:B:229:LEU:HD12 | 2.37                     | 0.54              |
| 1:C:376:ASP:O    | 1:C:378:GLY:N    | 2.41                     | 0.54              |
| 1:F:311:ARG:HH11 | 1:F:311:ARG:CG   | 2.18                     | 0.54              |
| 1:G:235:LEU:HD21 | 1:G:237:LEU:HD21 | 1.89                     | 0.54              |
| 1:J:318:ILE:CG1  | 1:J:348:LEU:HD21 | 2.34                     | 0.54              |
| 1:K:234:THR:HG23 | 1:K:274:ARG:O    | 2.07                     | 0.54              |
| 1:K:325:LEU:CD1  | 1:K:338:GLY:HA2  | 2.35                     | 0.54              |
| 1:L:152:LYS:O    | 1:L:154:LYS:N    | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:208:LEU:HD22 | 1:A:209:PHE:CE1  | 2.43                     | 0.54              |
| 1:B:253:ARG:HG3  | 1:B:254:VAL:N    | 2.21                     | 0.54              |
| 1:C:258:GLY:O    | 1:C:270:GLU:HA   | 2.07                     | 0.54              |
| 1:E:161:CYS:HB2  | 1:E:302:VAL:HG11 | 1.88                     | 0.54              |
| 1:E:249:ALA:HA   | 1:E:293:ARG:HH11 | 1.73                     | 0.54              |
| 1:F:171:VAL:HG21 | 1:F:307:ILE:HB   | 1.88                     | 0.54              |
| 1:F:171:VAL:HG22 | 1:F:173:LYS:HG3  | 1.89                     | 0.54              |
| 1:H:343:ALA:HB2  | 1:H:376:ASP:CA   | 2.23                     | 0.54              |
| 1:B:157:SER:HB3  | 1:B:183:LEU:C    | 2.32                     | 0.54              |
| 1:C:326:LYS:HE2  | 1:C:330:ARG:HH22 | 1.72                     | 0.54              |
| 1:F:239:GLU:N    | 1:F:278:ALA:O    | 2.39                     | 0.54              |
| 1:F:316:ASP:O    | 1:F:319:PRO:HD2  | 2.07                     | 0.54              |
| 1:G:260:PHE:HE2  | 1:G:271:VAL:HG11 | 1.73                     | 0.54              |
| 1:H:226:PHE:O    | 1:H:229:LEU:N    | 2.41                     | 0.54              |
| 1:H:287:VAL:CG1  | 1:H:294:GLU:HG2  | 2.38                     | 0.54              |
| 1:H:316:ASP:HB3  | 1:H:320:LEU:HD11 | 1.90                     | 0.54              |
| 1:I:251:LEU:O    | 1:I:253:ARG:N    | 2.40                     | 0.54              |
| 1:I:279:THR:HG21 | 1:I:283:ILE:HD11 | 1.89                     | 0.54              |
| 1:L:337:GLU:N    | 1:L:373:LYS:O    | 2.40                     | 0.54              |
| 1:A:194:LEU:H    | 1:A:194:LEU:CD2  | 2.21                     | 0.54              |
| 1:B:235:LEU:CG   | 1:B:237:LEU:HD21 | 2.38                     | 0.54              |
| 1:C:324:PHE:CZ   | 1:C:360:LYS:HB2  | 2.42                     | 0.54              |
| 1:C:340:THR:HG21 | 1:C:376:ASP:HB3  | 1.89                     | 0.54              |
| 1:D:157:SER:HB3  | 1:D:184:SER:HA   | 1.89                     | 0.54              |
| 1:E:196:VAL:O    | 1:E:196:VAL:CG1  | 2.55                     | 0.54              |
| 1:E:346:LEU:HB2  | 1:E:377:ARG:NH1  | 2.22                     | 0.54              |
| 1:F:153:ILE:HD12 | 1:F:180:ILE:CG1  | 2.37                     | 0.54              |
| 1:I:163:VAL:HB   | 1:I:276:LEU:HD23 | 1.89                     | 0.54              |
| 1:I:355:ASN:O    | 1:I:357:ARG:N    | 2.40                     | 0.54              |
| 1:K:144:PRO:C    | 1:K:146:MET:H    | 2.16                     | 0.54              |
| 1:K:216:PHE:H    | 1:K:219:ALA:HB2  | 1.73                     | 0.54              |
| 1:L:296:LEU:O    | 1:L:299:ARG:N    | 2.36                     | 0.54              |
| 1:M:359:LEU:O    | 1:M:360:LYS:C    | 2.50                     | 0.54              |
| 1:D:343:ALA:HB2  | 1:D:376:ASP:HA   | 1.90                     | 0.54              |
| 1:K:355:ASN:O    | 1:K:356:VAL:C    | 2.50                     | 0.54              |
| 1:M:293:ARG:O    | 1:M:296:LEU:HB3  | 2.07                     | 0.54              |
| 1:M:347:LEU:HD21 | 1:M:380:LEU:CG   | 2.36                     | 0.54              |
| 1:N:204:PHE:CD2  | 1:N:204:PHE:O    | 2.61                     | 0.54              |
| 1:A:310:LEU:HD13 | 1:A:317:ILE:HG12 | 1.90                     | 0.54              |
| 1:B:160:GLU:CA   | 1:B:274:ARG:HH12 | 2.21                     | 0.54              |
| 1:C:251:LEU:O    | 1:C:255:ILE:HG13 | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:324:PHE:O    | 1:E:325:LEU:C    | 2.51                     | 0.54              |
| 1:F:194:LEU:N    | 1:F:194:LEU:CD2  | 2.71                     | 0.54              |
| 1:F:195:ASN:HA   | 1:F:238:ASP:HB3  | 1.88                     | 0.54              |
| 1:F:199:ILE:HD13 | 1:F:207:GLU:HG2  | 1.89                     | 0.54              |
| 1:F:325:LEU:CD2  | 1:F:336:VAL:HG12 | 2.36                     | 0.54              |
| 1:G:296:LEU:O    | 1:G:296:LEU:HD13 | 2.08                     | 0.54              |
| 1:G:381:SER:C    | 1:G:383:LEU:H    | 2.15                     | 0.54              |
| 1:L:174:GLU:O    | 1:L:177:ALA:HB3  | 2.07                     | 0.54              |
| 1:N:186:ARG:NH1  | 1:N:232:GLY:O    | 2.40                     | 0.54              |
| 1:B:216:PHE:O    | 1:B:217:THR:C    | 2.50                     | 0.54              |
| 1:B:227:PHE:O    | 1:B:230:ALA:N    | 2.40                     | 0.54              |
| 1:B:365:ARG:NH1  | 1:B:383:LEU:HB3  | 2.22                     | 0.54              |
| 1:C:262:ARG:O    | 1:C:263:LEU:C    | 2.48                     | 0.54              |
| 1:D:262:ARG:O    | 1:D:263:LEU:C    | 2.51                     | 0.54              |
| 1:E:311:ARG:CG   | 1:E:351:PRO:O    | 2.56                     | 0.54              |
| 1:F:225:GLY:O    | 1:F:226:PHE:C    | 2.51                     | 0.54              |
| 1:G:144:PRO:HG2  | 1:G:145:LYS:H    | 1.73                     | 0.54              |
| 1:G:211:TYR:HE1  | 1:G:215:ALA:HB3  | 1.71                     | 0.54              |
| 1:H:339:PHE:N    | 1:H:339:PHE:HD1  | 2.04                     | 0.54              |
| 1:K:162:PRO:HG3  | 1:K:299:ARG:O    | 2.08                     | 0.54              |
| 1:K:192:VAL:O    | 1:K:192:VAL:HG12 | 2.06                     | 0.54              |
| 1:K:361:ASN:N    | 1:K:361:ASN:ND2  | 2.54                     | 0.54              |
| 1:L:208:LEU:HD23 | 1:L:208:LEU:C    | 2.33                     | 0.54              |
| 1:L:339:PHE:HE2  | 1:L:375:ILE:HD11 | 1.70                     | 0.54              |
| 1:N:239:GLU:O    | 1:N:240:ILE:C    | 2.51                     | 0.54              |
| 1:A:234:THR:HG21 | 1:A:276:LEU:CD1  | 2.38                     | 0.54              |
| 1:A:244:SER:O    | 1:A:248:GLN:HG3  | 2.07                     | 0.54              |
| 1:A:309:PRO:HG3  | 1:A:311:ARG:HH11 | 1.70                     | 0.54              |
| 1:B:249:ALA:HB2  | 1:B:293:ARG:HH11 | 1.73                     | 0.54              |
| 1:D:294:GLU:OE1  | 1:D:298:TYR:HE1  | 1.90                     | 0.54              |
| 1:E:157:SER:HB3  | 1:E:183:LEU:C    | 2.32                     | 0.54              |
| 1:F:315:GLU:N    | 1:F:315:GLU:OE1  | 2.31                     | 0.54              |
| 1:G:181:HIS:HE1  | 1:G:187:SER:O    | 1.91                     | 0.54              |
| 1:I:253:ARG:NE   | 1:J:198:SER:CB   | 2.71                     | 0.54              |
| 1:L:165:ILE:HB   | 1:L:278:ALA:CB   | 2.38                     | 0.54              |
| 1:L:379:GLU:C    | 1:L:381:SER:H    | 2.14                     | 0.54              |
| 1:N:325:LEU:C    | 1:N:325:LEU:CD2  | 2.80                     | 0.54              |
| 1:B:292:PHE:CZ   | 1:B:296:LEU:HD12 | 2.43                     | 0.54              |
| 1:E:146:MET:HE1  | 1:E:149:ILE:HD12 | 1.90                     | 0.54              |
| 1:G:191:PHE:C    | 1:G:191:PHE:CD2  | 2.86                     | 0.54              |
| 1:G:252:LEU:CD2  | 1:G:293:ARG:HH12 | 2.21                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:208:LEU:C    | 1:I:208:LEU:CD2  | 2.81                     | 0.54              |
| 1:I:321:ALA:HA   | 1:I:363:ILE:CD1  | 2.38                     | 0.54              |
| 1:I:336:VAL:HG11 | 1:I:375:ILE:HD11 | 1.90                     | 0.54              |
| 1:K:275:ILE:O    | 1:K:276:LEU:HD23 | 2.07                     | 0.54              |
| 1:L:329:SER:HA   | 1:L:334:LYS:HG3  | 1.88                     | 0.54              |
| 1:M:274:ARG:HD3  | 1:M:276:LEU:HD21 | 1.90                     | 0.54              |
| 1:M:281:ARG:HG2  | 1:M:281:ARG:HH11 | 1.72                     | 0.54              |
| 1:A:377:ARG:HH21 | 1:L:285:GLU:CD   | 2.15                     | 0.53              |
| 1:C:150:LEU:O    | 1:C:154:LYS:HG3  | 2.07                     | 0.53              |
| 1:C:298:TYR:HE2  | 1:D:358:GLU:OE2  | 1.90                     | 0.53              |
| 1:L:305:ILE:HG23 | 1:L:307:ILE:HD11 | 1.90                     | 0.53              |
| 1:L:320:LEU:O    | 1:L:321:ALA:C    | 2.50                     | 0.53              |
| 1:L:329:SER:HA   | 1:L:334:LYS:CG   | 2.38                     | 0.53              |
| 1:A:244:SER:C    | 1:A:246:GLU:N    | 2.62                     | 0.53              |
| 1:A:275:ILE:HD12 | 1:A:275:ILE:N    | 2.16                     | 0.53              |
| 1:C:243:LEU:O    | 1:C:248:GLN:NE2  | 2.37                     | 0.53              |
| 1:D:230:ALA:O    | 1:D:231:ASP:C    | 2.51                     | 0.53              |
| 1:E:211:TYR:CD2  | 1:E:263:LEU:HB2  | 2.43                     | 0.53              |
| 1:G:152:LYS:O    | 1:G:156:ILE:HG12 | 2.08                     | 0.53              |
| 1:I:230:ALA:O    | 1:I:273:VAL:HG22 | 2.08                     | 0.53              |
| 1:L:204:PHE:CE2  | 1:L:208:LEU:HD12 | 2.43                     | 0.53              |
| 1:L:272:ASN:HD22 | 1:L:272:ASN:C    | 2.16                     | 0.53              |
| 1:L:342:SER:O    | 1:L:377:ARG:HB2  | 2.09                     | 0.53              |
| 1:M:176:VAL:O    | 1:M:179:LEU:N    | 2.39                     | 0.53              |
| 1:M:195:ASN:ND2  | 1:M:238:ASP:OD2  | 2.41                     | 0.53              |
| 1:D:159:ALA:CB   | 1:E:332:TYR:HE2  | 2.21                     | 0.53              |
| 1:D:209:PHE:HE2  | 1:D:227:PHE:CE1  | 2.27                     | 0.53              |
| 1:E:269:ILE:H    | 1:E:269:ILE:CD1  | 2.19                     | 0.53              |
| 1:F:153:ILE:HG21 | 1:F:179:LEU:CD2  | 2.36                     | 0.53              |
| 1:H:244:SER:C    | 1:H:246:GLU:H    | 2.15                     | 0.53              |
| 1:I:211:TYR:CZ   | 1:I:223:LYS:HB2  | 2.43                     | 0.53              |
| 1:I:266:ARG:HD2  | 1:J:216:PHE:HE1  | 1.74                     | 0.53              |
| 1:L:139:TYR:HB3  | 1:L:141:PHE:CD2  | 2.41                     | 0.53              |
| 1:L:326:LYS:O    | 1:L:329:SER:HB3  | 2.08                     | 0.53              |
| 1:M:286:LEU:HA   | 1:M:289:GLU:OE1  | 2.07                     | 0.53              |
| 1:N:209:PHE:CE1  | 1:N:250:LYS:HB3  | 2.43                     | 0.53              |
| 1:A:252:LEU:HD22 | 1:A:295:ASP:OD1  | 2.09                     | 0.53              |
| 1:A:325:LEU:HD12 | 1:A:339:PHE:CE1  | 2.43                     | 0.53              |
| 1:D:259:LYS:HE2  | 1:D:270:GLU:OE2  | 2.07                     | 0.53              |
| 1:D:308:PRO:O    | 1:D:313:ARG:HD2  | 2.08                     | 0.53              |
| 1:F:365:ARG:NH1  | 1:F:383:LEU:HD22 | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:194:LEU:HD13 | 1:I:226:PHE:CD1  | 2.32                     | 0.53              |
| 1:J:262:ARG:HD3  | 1:J:269:ILE:HD11 | 1.90                     | 0.53              |
| 1:K:384:VAL:O    | 1:K:384:VAL:HG12 | 2.07                     | 0.53              |
| 1:L:159:ALA:CB   | 1:M:368:LEU:HD21 | 2.38                     | 0.53              |
| 1:N:157:SER:HB3  | 1:N:183:LEU:C    | 2.32                     | 0.53              |
| 1:A:237:LEU:HB2  | 1:A:240:ILE:HD11 | 1.91                     | 0.53              |
| 1:A:313:ARG:HB3  | 1:A:316:ASP:OD2  | 2.08                     | 0.53              |
| 1:A:347:LEU:HD21 | 1:A:380:LEU:HD11 | 1.91                     | 0.53              |
| 1:B:160:GLU:HA   | 1:B:274:ARG:NH1  | 2.23                     | 0.53              |
| 1:B:201:ARG:HH11 | 1:B:201:ARG:CB   | 2.20                     | 0.53              |
| 1:C:236:PHE:HE2  | 1:C:238:ASP:HB2  | 1.71                     | 0.53              |
| 1:G:261:TYR:HD2  | 1:G:263:LEU:O    | 1.91                     | 0.53              |
| 1:H:240:ILE:HG23 | 1:H:243:LEU:HD12 | 1.90                     | 0.53              |
| 1:J:224:GLU:CG   | 1:J:225:GLY:H    | 2.06                     | 0.53              |
| 1:J:309:PRO:CB   | 1:J:311:ARG:NH1  | 2.72                     | 0.53              |
| 1:K:269:ILE:H    | 1:K:269:ILE:CD1  | 2.20                     | 0.53              |
| 1:L:266:ARG:C    | 1:L:267:LYS:HG2  | 2.34                     | 0.53              |
| 1:B:240:ILE:HG13 | 1:B:277:ALA:CB   | 2.32                     | 0.53              |
| 1:C:309:PRO:CB   | 1:C:311:ARG:NH1  | 2.72                     | 0.53              |
| 1:F:215:ALA:HB3  | 1:F:219:ALA:HB3  | 1.91                     | 0.53              |
| 1:I:194:LEU:N    | 1:I:194:LEU:CD2  | 2.72                     | 0.53              |
| 1:K:148:GLU:O    | 1:K:151:GLU:HB2  | 2.08                     | 0.53              |
| 1:L:173:LYS:NZ   | 2:L:11:ADP:PB    | 2.81                     | 0.53              |
| 1:L:228:GLU:O    | 1:L:231:ASP:N    | 2.40                     | 0.53              |
| 1:L:267:LYS:O    | 1:L:269:ILE:CD1  | 2.57                     | 0.53              |
| 1:M:252:LEU:HA   | 1:M:255:ILE:HD12 | 1.90                     | 0.53              |
| 1:N:279:THR:HG23 | 1:N:280:ASN:N    | 2.22                     | 0.53              |
| 1:C:140:VAL:CB   | 1:C:320:LEU:HD23 | 2.39                     | 0.53              |
| 1:E:156:ILE:HD11 | 1:E:303:ILE:HD12 | 1.91                     | 0.53              |
| 1:E:179:LEU:C    | 1:E:181:HIS:H    | 2.16                     | 0.53              |
| 1:H:340:THR:HG22 | 1:H:341:LYS:N    | 2.23                     | 0.53              |
| 1:I:216:PHE:CZ   | 1:I:218:GLY:HA3  | 2.44                     | 0.53              |
| 1:J:195:ASN:HB3  | 1:J:198:SER:OG   | 2.08                     | 0.53              |
| 1:L:354:GLY:HA3  | 1:L:358:GLU:HB2  | 1.91                     | 0.53              |
| 1:A:142:GLU:HA   | 1:A:147:LYS:HE2  | 1.91                     | 0.53              |
| 1:A:223:LYS:NZ   | 1:G:266:ARG:HD2  | 2.24                     | 0.53              |
| 1:A:346:LEU:HD21 | 1:A:384:VAL:O    | 2.08                     | 0.53              |
| 1:C:259:LYS:HA   | 1:C:269:ILE:O    | 2.08                     | 0.53              |
| 1:E:292:PHE:CE2  | 1:E:296:LEU:HB3  | 2.37                     | 0.53              |
| 1:H:355:ASN:O    | 1:H:357:ARG:N    | 2.42                     | 0.53              |
| 1:I:300:LEU:O    | 1:I:302:VAL:N    | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:173:LYS:NZ   | 2:L:11:ADP:O1B   | 2.41                     | 0.53              |
| 1:L:318:ILE:CD1  | 1:L:319:PRO:HD3  | 2.39                     | 0.53              |
| 1:N:292:PHE:CZ   | 1:N:296:LEU:HD12 | 2.43                     | 0.53              |
| 1:B:191:PHE:HE1  | 1:B:276:LEU:HD12 | 1.74                     | 0.53              |
| 1:C:314:LYS:HA   | 1:C:317:ILE:CG1  | 2.37                     | 0.53              |
| 1:C:336:VAL:HG21 | 1:C:370:SER:HB2  | 1.91                     | 0.53              |
| 1:D:335:GLU:O    | 1:D:373:LYS:HA   | 2.09                     | 0.53              |
| 1:E:166:THR:HG22 | 1:E:167:GLY:H    | 1.74                     | 0.53              |
| 1:E:279:THR:CG2  | 1:E:283:ILE:HD11 | 2.36                     | 0.53              |
| 1:E:282:ASN:ND2  | 1:E:285:GLU:CB   | 2.64                     | 0.53              |
| 1:E:305:ILE:HG22 | 1:E:305:ILE:O    | 2.08                     | 0.53              |
| 1:F:282:ASN:ND2  | 1:F:285:GLU:HB2  | 2.24                     | 0.53              |
| 1:F:354:GLY:O    | 1:F:358:GLU:N    | 2.36                     | 0.53              |
| 1:G:181:HIS:C    | 1:G:181:HIS:ND1  | 2.66                     | 0.53              |
| 1:G:340:THR:O    | 1:G:342:SER:N    | 2.41                     | 0.53              |
| 1:I:213:LYS:O    | 1:I:220:VAL:O    | 2.26                     | 0.53              |
| 1:M:181:HIS:ND1  | 1:M:187:SER:HA   | 2.24                     | 0.53              |
| 1:A:325:LEU:HD21 | 1:A:336:VAL:HG12 | 1.90                     | 0.53              |
| 1:D:284:LYS:HE2  | 1:D:297:TYR:OH   | 2.09                     | 0.53              |
| 1:D:299:ARG:NH2  | 1:D:302:VAL:HG21 | 2.24                     | 0.53              |
| 1:H:309:PRO:HB2  | 1:H:311:ARG:CD   | 2.39                     | 0.53              |
| 1:J:200:PRO:HG2  | 1:J:203:ILE:CD1  | 2.36                     | 0.53              |
| 1:J:245:LEU:HD23 | 1:J:248:GLN:NE2  | 2.24                     | 0.53              |
| 1:J:266:ARG:NH1  | 1:K:224:GLU:O    | 2.41                     | 0.53              |
| 1:L:248:GLN:OE1  | 1:L:293:ARG:N    | 2.34                     | 0.53              |
| 1:L:318:ILE:CG1  | 1:L:319:PRO:HD3  | 2.39                     | 0.53              |
| 1:L:318:ILE:O    | 1:L:321:ALA:HB3  | 2.09                     | 0.53              |
| 1:A:283:ILE:O    | 1:A:287:VAL:HG23 | 2.09                     | 0.52              |
| 1:A:376:ASP:O    | 1:A:377:ARG:C    | 2.51                     | 0.52              |
| 1:B:284:LYS:H    | 1:B:284:LYS:CD   | 2.18                     | 0.52              |
| 1:C:254:VAL:CG2  | 1:C:260:PHE:HB3  | 2.38                     | 0.52              |
| 1:E:174:GLU:O    | 1:E:175:VAL:C    | 2.51                     | 0.52              |
| 1:G:322:ASN:O    | 1:G:326:LYS:HB2  | 2.09                     | 0.52              |
| 1:H:286:LEU:HD22 | 1:H:291:LYS:HD3  | 1.91                     | 0.52              |
| 1:I:319:PRO:O    | 1:I:320:LEU:C    | 2.51                     | 0.52              |
| 1:L:250:LYS:NZ   | 1:L:263:LEU:HG   | 2.23                     | 0.52              |
| 1:M:195:ASN:O    | 1:M:197:ALA:N    | 2.42                     | 0.52              |
| 1:M:204:PHE:HE2  | 1:M:243:LEU:HD21 | 1.74                     | 0.52              |
| 1:M:234:THR:HG23 | 1:M:276:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:365:ARG:NE   | 1:C:383:LEU:HD13 | 2.24                     | 0.52              |
| 1:E:227:PHE:O    | 1:E:228:GLU:C    | 2.52                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:273:VAL:O    | 1:E:275:ILE:HD12 | 2.09                     | 0.52              |
| 1:F:171:VAL:O    | 1:F:171:VAL:HG23 | 2.07                     | 0.52              |
| 1:I:171:VAL:CG1  | 1:I:307:ILE:HG22 | 2.39                     | 0.52              |
| 1:J:145:LYS:O    | 1:J:149:ILE:HG13 | 2.10                     | 0.52              |
| 1:J:178:ARG:HH11 | 1:J:178:ARG:HG3  | 1.74                     | 0.52              |
| 1:J:336:VAL:HG21 | 1:J:367:VAL:HG13 | 1.90                     | 0.52              |
| 1:K:296:LEU:O    | 1:K:296:LEU:HD13 | 2.09                     | 0.52              |
| 1:L:181:HIS:O    | 1:L:184:SER:OG   | 2.27                     | 0.52              |
| 1:M:238:ASP:O    | 1:M:239:GLU:HB3  | 2.10                     | 0.52              |
| 1:N:283:ILE:O    | 1:N:284:LYS:C    | 2.52                     | 0.52              |
| 1:B:150:LEU:HD11 | 1:B:154:LYS:NZ   | 2.24                     | 0.52              |
| 1:C:145:LYS:O    | 1:C:148:GLU:HB3  | 2.08                     | 0.52              |
| 1:E:318:ILE:O    | 1:E:322:ASN:ND2  | 2.42                     | 0.52              |
| 1:F:203:ILE:O    | 1:F:206:ALA:HB3  | 2.09                     | 0.52              |
| 1:G:229:LEU:O    | 1:G:229:LEU:HD13 | 2.09                     | 0.52              |
| 1:G:343:ALA:O    | 1:G:346:LEU:HB3  | 2.09                     | 0.52              |
| 1:C:139:TYR:O    | 1:C:139:TYR:HD1  | 1.92                     | 0.52              |
| 1:F:140:VAL:HG11 | 1:F:320:LEU:HG   | 1.90                     | 0.52              |
| 1:F:242:GLU:CD   | 1:F:281:ARG:HH22 | 2.18                     | 0.52              |
| 1:I:296:LEU:C    | 1:I:296:LEU:HD23 | 2.34                     | 0.52              |
| 1:J:194:LEU:HD23 | 1:J:236:PHE:O    | 2.09                     | 0.52              |
| 1:J:350:TYR:HD2  | 1:J:352:TRP:CD2  | 2.27                     | 0.52              |
| 1:L:172:GLY:HA2  | 2:L:11:ADP:O1A   | 2.09                     | 0.52              |
| 1:M:316:ASP:C    | 1:M:319:PRO:HD2  | 2.34                     | 0.52              |
| 1:A:379:GLU:CD   | 1:A:379:GLU:H    | 2.17                     | 0.52              |
| 1:G:263:LEU:HG   | 1:G:264:GLY:N    | 2.23                     | 0.52              |
| 1:I:163:VAL:HB   | 1:I:276:LEU:CD2  | 2.40                     | 0.52              |
| 1:J:352:TRP:HZ3  | 1:J:362:VAL:HG21 | 1.74                     | 0.52              |
| 1:K:208:LEU:HD21 | 1:K:227:PHE:CE1  | 2.45                     | 0.52              |
| 1:L:143:SER:CB   | 1:L:316:ASP:OD2  | 2.57                     | 0.52              |
| 1:L:252:LEU:HD12 | 1:L:252:LEU:O    | 2.10                     | 0.52              |
| 1:M:236:PHE:HA   | 1:M:276:LEU:O    | 2.10                     | 0.52              |
| 1:M:351:PRO:O    | 1:M:352:TRP:HB2  | 2.09                     | 0.52              |
| 1:N:163:VAL:HB   | 1:N:276:LEU:CD2  | 2.39                     | 0.52              |
| 1:A:251:LEU:O    | 1:A:255:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:299:ARG:HE   | 1:A:299:ARG:HA   | 1.74                     | 0.52              |
| 1:B:215:ALA:HB1  | 1:B:264:GLY:HA3  | 1.92                     | 0.52              |
| 1:E:139:TYR:HE2  | 1:E:179:LEU:HD21 | 1.74                     | 0.52              |
| 1:F:175:VAL:HG12 | 1:F:176:VAL:N    | 2.23                     | 0.52              |
| 1:F:354:GLY:O    | 1:F:355:ASN:C    | 2.53                     | 0.52              |
| 1:G:173:LYS:O    | 1:G:176:VAL:N    | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:228:GLU:HG3  | 1:G:260:PHE:HZ   | 1.74                     | 0.52              |
| 1:G:346:LEU:HD21 | 1:G:384:VAL:HG21 | 1.91                     | 0.52              |
| 1:I:252:LEU:HD13 | 1:I:296:LEU:CA   | 2.37                     | 0.52              |
| 1:J:194:LEU:HD23 | 1:J:194:LEU:H    | 1.75                     | 0.52              |
| 1:K:208:LEU:HD11 | 1:K:237:LEU:HD11 | 1.91                     | 0.52              |
| 1:L:171:VAL:HG12 | 1:L:309:PRO:HA   | 1.90                     | 0.52              |
| 1:L:194:LEU:HD13 | 1:L:226:PHE:CD1  | 2.45                     | 0.52              |
| 1:L:308:PRO:O    | 1:L:313:ARG:HD3  | 2.10                     | 0.52              |
| 1:M:248:GLN:HG3  | 1:M:293:ARG:CB   | 2.39                     | 0.52              |
| 1:N:355:ASN:O    | 1:N:358:GLU:N    | 2.41                     | 0.52              |
| 1:C:202:ASP:C    | 1:C:203:ILE:HD13 | 2.35                     | 0.52              |
| 1:E:332:TYR:OH   | 1:E:364:GLU:OE1  | 2.21                     | 0.52              |
| 1:E:359:LEU:HD22 | 1:E:363:ILE:CG1  | 2.39                     | 0.52              |
| 1:F:186:ARG:HD3  | 1:F:232:GLY:O    | 2.09                     | 0.52              |
| 1:F:223:LYS:O    | 1:F:223:LYS:HG3  | 2.10                     | 0.52              |
| 1:H:194:LEU:N    | 1:H:194:LEU:CD2  | 2.72                     | 0.52              |
| 1:I:204:PHE:O    | 1:I:207:GLU:HB2  | 2.10                     | 0.52              |
| 1:I:366:ALA:O    | 1:I:370:SER:HB3  | 2.09                     | 0.52              |
| 1:L:171:VAL:HG23 | 1:L:307:ILE:HG21 | 1.92                     | 0.52              |
| 1:L:237:LEU:HB2  | 1:L:277:ALA:CB   | 2.39                     | 0.52              |
| 1:L:325:LEU:O    | 1:L:329:SER:HB2  | 2.10                     | 0.52              |
| 1:A:310:LEU:HD11 | 1:A:359:LEU:HD12 | 1.92                     | 0.52              |
| 1:B:179:LEU:O    | 1:B:181:HIS:N    | 2.43                     | 0.52              |
| 1:D:209:PHE:O    | 1:D:262:ARG:HD2  | 2.10                     | 0.52              |
| 1:E:303:ILE:HD13 | 1:F:365:ARG:HG3  | 1.91                     | 0.52              |
| 1:F:383:LEU:N    | 1:F:383:LEU:HD23 | 2.23                     | 0.52              |
| 1:H:362:VAL:CG2  | 1:H:365:ARG:HH21 | 2.14                     | 0.52              |
| 1:K:146:MET:HE2  | 1:K:313:ARG:CZ   | 2.39                     | 0.52              |
| 1:K:149:ILE:HA   | 1:K:152:LYS:HE3  | 1.90                     | 0.52              |
| 1:K:299:ARG:HA   | 1:L:361:ASN:ND2  | 2.25                     | 0.52              |
| 1:K:323:HIS:O    | 1:K:326:LYS:HB3  | 2.10                     | 0.52              |
| 1:A:144:PRO:HD3  | 1:A:315:GLU:OE2  | 2.09                     | 0.52              |
| 1:E:236:PHE:CE1  | 1:E:278:ALA:HB3  | 2.44                     | 0.52              |
| 1:F:174:GLU:CD   | 1:F:178:ARG:HH12 | 2.18                     | 0.52              |
| 1:H:223:LYS:NZ   | 1:N:264:GLY:HA3  | 2.25                     | 0.52              |
| 1:I:152:LYS:O    | 1:I:153:ILE:C    | 2.53                     | 0.52              |
| 1:I:302:VAL:O    | 1:J:365:ARG:NE   | 2.43                     | 0.52              |
| 1:J:296:LEU:C    | 1:J:296:LEU:HD13 | 2.35                     | 0.52              |
| 1:K:324:PHE:CD1  | 1:K:360:LYS:HA   | 2.45                     | 0.52              |
| 1:L:218:GLY:O    | 1:L:220:VAL:N    | 2.35                     | 0.52              |
| 1:L:382:CYS:HB2  | 1:L:383:LEU:HG   | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:141:PHE:CE2  | 1:M:150:LEU:HD13 | 2.45                     | 0.52              |
| 1:M:294:GLU:HG2  | 1:M:295:ASP:H    | 1.75                     | 0.52              |
| 1:N:262:ARG:HG2  | 1:N:262:ARG:NH1  | 2.22                     | 0.52              |
| 1:N:305:ILE:HG22 | 1:N:307:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:139:TYR:CD2  | 1:A:175:VAL:CG1  | 2.92                     | 0.52              |
| 1:E:213:LYS:HB2  | 1:E:213:LYS:NZ   | 2.25                     | 0.52              |
| 1:E:326:LYS:HE2  | 1:E:330:ARG:NH2  | 2.25                     | 0.52              |
| 1:G:166:THR:HG22 | 1:G:279:THR:HG22 | 1.92                     | 0.52              |
| 1:H:207:GLU:CD   | 1:N:266:ARG:HH22 | 2.17                     | 0.52              |
| 1:H:356:VAL:O    | 1:H:357:ARG:C    | 2.52                     | 0.52              |
| 1:J:173:LYS:O    | 1:J:176:VAL:HB   | 2.10                     | 0.52              |
| 1:J:176:VAL:O    | 1:J:180:ILE:HG13 | 2.10                     | 0.52              |
| 1:K:347:LEU:HD21 | 1:K:380:LEU:HD11 | 1.91                     | 0.52              |
| 1:L:310:LEU:O    | 1:L:312:GLU:N    | 2.43                     | 0.52              |
| 1:M:273:VAL:O    | 1:M:273:VAL:HG23 | 2.10                     | 0.52              |
| 1:N:350:TYR:HD2  | 1:N:352:TRP:H    | 1.58                     | 0.52              |
| 1:A:166:THR:HG22 | 1:A:279:THR:HG22 | 1.92                     | 0.51              |
| 1:B:146:MET:HG3  | 1:B:313:ARG:NH2  | 2.20                     | 0.51              |
| 1:B:192:VAL:HG21 | 1:B:229:LEU:HD12 | 1.92                     | 0.51              |
| 1:B:229:LEU:CD1  | 1:B:229:LEU:C    | 2.83                     | 0.51              |
| 1:C:296:LEU:O    | 1:C:297:TYR:C    | 2.53                     | 0.51              |
| 1:C:321:ALA:HA   | 1:C:363:ILE:CD1  | 2.40                     | 0.51              |
| 1:D:350:TYR:CD1  | 1:D:384:VAL:HG13 | 2.45                     | 0.51              |
| 1:H:342:SER:OG   | 1:H:376:ASP:HB2  | 2.09                     | 0.51              |
| 1:J:340:THR:HG1  | 1:J:376:ASP:HB2  | 1.76                     | 0.51              |
| 1:K:152:LYS:O    | 1:K:156:ILE:HG12 | 2.10                     | 0.51              |
| 1:K:198:SER:O    | 1:K:199:ILE:CG1  | 2.47                     | 0.51              |
| 1:K:227:PHE:CZ   | 1:K:254:VAL:HG11 | 2.44                     | 0.51              |
| 1:K:279:THR:CG2  | 1:K:283:ILE:HD11 | 2.36                     | 0.51              |
| 1:L:355:ASN:O    | 1:L:358:GLU:N    | 2.43                     | 0.51              |
| 1:M:139:TYR:N    | 1:M:139:TYR:CD1  | 2.77                     | 0.51              |
| 1:N:244:SER:O    | 1:N:245:LEU:C    | 2.51                     | 0.51              |
| 1:N:365:ARG:HG3  | 1:N:369:PHE:CE2  | 2.45                     | 0.51              |
| 1:B:144:PRO:HD3  | 1:B:315:GLU:CD   | 2.35                     | 0.51              |
| 1:C:211:TYR:HD1  | 1:C:211:TYR:C    | 2.18                     | 0.51              |
| 1:D:157:SER:C    | 1:D:159:ALA:N    | 2.68                     | 0.51              |
| 1:D:159:ALA:CB   | 1:E:332:TYR:CE2  | 2.93                     | 0.51              |
| 1:D:292:PHE:C    | 1:D:292:PHE:CD2  | 2.88                     | 0.51              |
| 1:D:350:TYR:CG   | 1:D:384:VAL:HG13 | 2.46                     | 0.51              |
| 1:E:316:ASP:O    | 1:E:317:ILE:C    | 2.53                     | 0.51              |
| 1:E:361:ASN:ND2  | 1:E:361:ASN:N    | 2.57                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:239:GLU:HA   | 1:F:279:THR:HA   | 1.93                     | 0.51              |
| 1:F:351:PRO:HB2  | 1:F:353:TYR:CE2  | 2.45                     | 0.51              |
| 1:H:255:ILE:HD13 | 1:H:300:LEU:HD21 | 1.93                     | 0.51              |
| 1:I:275:ILE:HD12 | 1:I:275:ILE:N    | 2.26                     | 0.51              |
| 1:J:209:PHE:HE2  | 1:J:254:VAL:HG21 | 1.74                     | 0.51              |
| 1:N:272:ASN:CG   | 1:N:272:ASN:O    | 2.51                     | 0.51              |
| 1:A:365:ARG:HH11 | 1:A:383:LEU:HD22 | 1.76                     | 0.51              |
| 1:B:168:GLU:OE2  | 1:B:311:ARG:NH2  | 2.44                     | 0.51              |
| 1:D:226:PHE:HA   | 1:D:229:LEU:HB2  | 1.92                     | 0.51              |
| 1:D:281:ARG:HG2  | 1:D:281:ARG:NH1  | 2.23                     | 0.51              |
| 1:F:283:ILE:HG21 | 1:F:297:TYR:HD1  | 1.76                     | 0.51              |
| 1:G:164:LEU:HD12 | 1:G:164:LEU:C    | 2.35                     | 0.51              |
| 1:H:244:SER:C    | 1:H:246:GLU:N    | 2.67                     | 0.51              |
| 1:J:299:ARG:HA   | 1:J:299:ARG:HE   | 1.76                     | 0.51              |
| 1:K:143:SER:HB2  | 1:K:315:GLU:CB   | 2.37                     | 0.51              |
| 1:L:229:LEU:HD13 | 1:L:229:LEU:O    | 2.08                     | 0.51              |
| 1:M:252:LEU:O    | 1:M:253:ARG:C    | 2.53                     | 0.51              |
| 1:M:324:PHE:HD1  | 1:M:359:LEU:HD23 | 1.75                     | 0.51              |
| 1:M:324:PHE:CE1  | 1:M:360:LYS:HB2  | 2.45                     | 0.51              |
| 1:M:325:LEU:HD23 | 1:M:325:LEU:C    | 2.36                     | 0.51              |
| 1:N:204:PHE:O    | 1:N:204:PHE:CG   | 2.60                     | 0.51              |
| 1:N:218:GLY:O    | 1:N:219:ALA:C    | 2.52                     | 0.51              |
| 1:A:192:VAL:HG21 | 1:A:230:ALA:HB2  | 1.91                     | 0.51              |
| 1:B:178:ARG:NH1  | 1:B:191:PHE:CD2  | 2.79                     | 0.51              |
| 1:B:285:GLU:O    | 1:B:288:LYS:N    | 2.42                     | 0.51              |
| 1:C:181:HIS:HE1  | 1:C:187:SER:HA   | 1.69                     | 0.51              |
| 1:C:288:LYS:C    | 1:C:290:GLY:H    | 2.18                     | 0.51              |
| 1:C:381:SER:C    | 1:C:383:LEU:H    | 2.18                     | 0.51              |
| 1:D:240:ILE:O    | 1:D:242:GLU:N    | 2.43                     | 0.51              |
| 1:E:156:ILE:O    | 1:E:158:CYS:N    | 2.40                     | 0.51              |
| 1:E:241:GLY:HA3  | 1:E:281:ARG:NH2  | 2.24                     | 0.51              |
| 1:E:302:VAL:HG23 | 1:F:361:ASN:OD1  | 2.09                     | 0.51              |
| 1:E:355:ASN:N    | 1:E:355:ASN:ND2  | 2.53                     | 0.51              |
| 1:F:171:VAL:HG12 | 1:F:355:ASN:HD22 | 1.75                     | 0.51              |
| 1:G:352:TRP:HA   | 1:G:358:GLU:OE1  | 2.11                     | 0.51              |
| 1:H:194:LEU:H    | 1:H:194:LEU:CD2  | 2.18                     | 0.51              |
| 1:H:227:PHE:CD1  | 1:H:235:LEU:CD1  | 2.93                     | 0.51              |
| 1:H:360:LYS:HG2  | 1:H:364:GLU:OE2  | 2.10                     | 0.51              |
| 1:J:269:ILE:N    | 1:J:269:ILE:CD1  | 2.74                     | 0.51              |
| 1:L:174:GLU:O    | 1:L:177:ALA:N    | 2.43                     | 0.51              |
| 1:L:204:PHE:O    | 1:L:207:GLU:N    | 2.42                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:251:LEU:O    | 1:M:252:LEU:C    | 2.54                     | 0.51              |
| 1:A:365:ARG:HD2  | 1:A:383:LEU:HD11 | 1.92                     | 0.51              |
| 1:D:240:ILE:C    | 1:D:242:GLU:H    | 2.18                     | 0.51              |
| 1:D:292:PHE:C    | 1:D:292:PHE:HD2  | 2.18                     | 0.51              |
| 1:E:325:LEU:HD23 | 1:E:325:LEU:C    | 2.35                     | 0.51              |
| 1:H:255:ILE:HG12 | 1:H:275:ILE:HD11 | 1.89                     | 0.51              |
| 1:H:346:LEU:HD12 | 1:H:377:ARG:HG2  | 1.93                     | 0.51              |
| 1:I:321:ALA:HA   | 1:I:363:ILE:HD11 | 1.91                     | 0.51              |
| 1:L:181:HIS:HD2  | 1:L:234:THR:HB   | 1.73                     | 0.51              |
| 1:A:143:SER:HB2  | 1:A:144:PRO:CD   | 2.37                     | 0.51              |
| 1:D:356:VAL:HG11 | 2:D:2:ADP:C8     | 2.45                     | 0.51              |
| 1:E:182:LYS:C    | 1:E:183:LEU:HD23 | 2.36                     | 0.51              |
| 1:F:170:GLY:C    | 1:F:172:GLY:N    | 2.67                     | 0.51              |
| 1:F:174:GLU:O    | 1:F:177:ALA:N    | 2.44                     | 0.51              |
| 1:F:239:GLU:HG3  | 1:F:239:GLU:O    | 2.11                     | 0.51              |
| 1:H:227:PHE:HD1  | 1:H:235:LEU:HD12 | 1.74                     | 0.51              |
| 1:H:256:GLU:OE2  | 1:I:357:ARG:HD3  | 2.11                     | 0.51              |
| 1:H:332:TYR:CZ   | 1:H:370:SER:HB2  | 2.44                     | 0.51              |
| 1:L:322:ASN:HA   | 1:L:339:PHE:CE1  | 2.40                     | 0.51              |
| 1:M:368:LEU:O    | 1:M:368:LEU:HD13 | 2.10                     | 0.51              |
| 1:A:260:PHE:CD1  | 1:A:260:PHE:C    | 2.88                     | 0.51              |
| 1:B:189:GLU:HB3  | 1:B:233:GLY:HA2  | 1.92                     | 0.51              |
| 1:D:324:PHE:O    | 1:D:325:LEU:C    | 2.54                     | 0.51              |
| 1:F:192:VAL:CG2  | 1:F:230:ALA:HB2  | 2.40                     | 0.51              |
| 1:H:260:PHE:C    | 1:H:260:PHE:CD1  | 2.88                     | 0.51              |
| 1:J:365:ARG:HD2  | 1:J:383:LEU:CD1  | 2.41                     | 0.51              |
| 1:K:147:LYS:HD3  | 1:K:150:LEU:HD23 | 1.93                     | 0.51              |
| 1:L:300:LEU:C    | 1:L:302:VAL:H    | 2.18                     | 0.51              |
| 1:M:157:SER:O    | 1:M:159:ALA:N    | 2.43                     | 0.51              |
| 1:N:240:ILE:HG23 | 1:N:243:LEU:CD1  | 2.40                     | 0.51              |
| 1:N:334:LYS:HB3  | 1:N:336:VAL:HG23 | 1.92                     | 0.51              |
| 1:C:230:ALA:O    | 1:C:233:GLY:N    | 2.41                     | 0.51              |
| 1:E:249:ALA:HB2  | 1:E:293:ARG:HD2  | 1.92                     | 0.51              |
| 1:E:262:ARG:HG3  | 1:E:269:ILE:CD1  | 2.41                     | 0.51              |
| 1:E:298:TYR:CE1  | 1:F:354:GLY:HA3  | 2.46                     | 0.51              |
| 1:I:256:GLU:CG   | 1:I:299:ARG:HE   | 2.23                     | 0.51              |
| 1:K:349:SER:O    | 1:K:350:TYR:C    | 2.54                     | 0.51              |
| 1:M:247:ALA:O    | 1:M:248:GLN:C    | 2.52                     | 0.51              |
| 1:B:225:GLY:O    | 1:B:226:PHE:C    | 2.54                     | 0.51              |
| 1:C:146:MET:CE   | 1:C:313:ARG:NH2  | 2.72                     | 0.51              |
| 1:C:211:TYR:C    | 1:C:211:TYR:CD1  | 2.89                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:265:GLY:O    | 1:D:266:ARG:NE   | 2.27                     | 0.51              |
| 1:E:178:ARG:O    | 1:E:181:HIS:HB3  | 2.11                     | 0.51              |
| 1:E:279:THR:HG21 | 1:E:283:ILE:CD1  | 2.38                     | 0.51              |
| 1:F:315:GLU:O    | 1:F:319:PRO:HG2  | 2.11                     | 0.51              |
| 1:H:150:LEU:HD12 | 1:H:150:LEU:O    | 2.10                     | 0.51              |
| 1:I:192:VAL:CG2  | 1:I:230:ALA:HB2  | 2.41                     | 0.51              |
| 1:I:203:ILE:HG22 | 1:I:207:GLU:HG2  | 1.92                     | 0.51              |
| 1:J:309:PRO:HB2  | 1:J:311:ARG:NH1  | 2.26                     | 0.51              |
| 1:J:340:THR:CG2  | 1:J:376:ASP:HB3  | 2.41                     | 0.51              |
| 1:K:273:VAL:O    | 1:K:275:ILE:HD12 | 2.11                     | 0.51              |
| 1:N:243:LEU:HB3  | 1:N:248:GLN:HG2  | 1.92                     | 0.51              |
| 1:B:236:PHE:CD1  | 1:B:276:LEU:O    | 2.62                     | 0.51              |
| 1:C:360:LYS:HG2  | 1:C:361:ASN:ND2  | 2.25                     | 0.51              |
| 1:D:318:ILE:HG12 | 1:D:348:LEU:HD21 | 1.92                     | 0.51              |
| 1:G:340:THR:HG23 | 1:G:375:ILE:O    | 2.11                     | 0.51              |
| 1:G:359:LEU:HD23 | 1:G:359:LEU:O    | 2.11                     | 0.51              |
| 1:H:182:LYS:HA   | 1:H:187:SER:HB2  | 1.93                     | 0.51              |
| 1:L:226:PHE:O    | 1:L:227:PHE:C    | 2.52                     | 0.51              |
| 1:M:248:GLN:HA   | 1:M:251:LEU:HB3  | 1.93                     | 0.51              |
| 1:N:325:LEU:HD11 | 1:N:336:VAL:HG12 | 1.93                     | 0.51              |
| 1:A:212:GLU:OE2  | 1:A:222:SER:OG   | 2.29                     | 0.50              |
| 1:A:339:PHE:CZ   | 1:A:363:ILE:HD13 | 2.46                     | 0.50              |
| 1:B:176:VAL:HG12 | 1:B:180:ILE:HD11 | 1.93                     | 0.50              |
| 1:B:181:HIS:O    | 1:B:184:SER:N    | 2.39                     | 0.50              |
| 1:E:156:ILE:C    | 1:E:158:CYS:H    | 2.19                     | 0.50              |
| 1:E:340:THR:O    | 1:E:344:GLN:HG3  | 2.11                     | 0.50              |
| 1:F:209:PHE:CE2  | 1:F:254:VAL:HG21 | 2.46                     | 0.50              |
| 1:G:256:GLU:HG2  | 1:G:299:ARG:HH11 | 1.76                     | 0.50              |
| 1:G:336:VAL:HA   | 1:G:373:LYS:O    | 2.11                     | 0.50              |
| 1:J:157:SER:OG   | 1:J:183:LEU:HB2  | 2.11                     | 0.50              |
| 1:J:220:VAL:CG1  | 1:J:221:SER:H    | 2.25                     | 0.50              |
| 1:K:209:PHE:CD1  | 1:K:209:PHE:N    | 2.79                     | 0.50              |
| 1:L:181:HIS:HA   | 1:L:184:SER:OG   | 2.11                     | 0.50              |
| 1:L:352:TRP:CZ3  | 1:L:358:GLU:HG2  | 2.46                     | 0.50              |
| 1:N:145:LYS:HA   | 1:N:148:GLU:CG   | 2.36                     | 0.50              |
| 1:N:292:PHE:HZ   | 1:N:296:LEU:HD12 | 1.76                     | 0.50              |
| 1:B:177:ALA:O    | 1:B:178:ARG:C    | 2.54                     | 0.50              |
| 1:D:328:PHE:C    | 1:D:330:ARG:N    | 2.69                     | 0.50              |
| 1:E:146:MET:HA   | 1:E:146:MET:HE3  | 1.93                     | 0.50              |
| 1:F:214:GLY:O    | 1:F:215:ALA:HB2  | 2.11                     | 0.50              |
| 1:F:363:ILE:O    | 1:F:366:ALA:N    | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:204:PHE:C    | 1:G:206:ALA:H    | 2.17                     | 0.50              |
| 1:H:149:ILE:O    | 1:H:153:ILE:HG12 | 2.11                     | 0.50              |
| 1:H:170:GLY:O    | 1:H:355:ASN:HB2  | 2.12                     | 0.50              |
| 1:J:143:SER:CB   | 1:J:144:PRO:HD2  | 2.40                     | 0.50              |
| 1:J:157:SER:O    | 1:J:184:SER:HA   | 2.12                     | 0.50              |
| 1:L:283:ILE:HG21 | 1:L:297:TYR:CD1  | 2.46                     | 0.50              |
| 1:L:328:PHE:O    | 1:L:332:TYR:HD1  | 1.94                     | 0.50              |
| 1:L:358:GLU:O    | 1:L:362:VAL:HG23 | 2.11                     | 0.50              |
| 1:M:143:SER:CB   | 1:M:144:PRO:CD   | 2.85                     | 0.50              |
| 1:M:209:PHE:HE2  | 1:M:227:PHE:HE1  | 1.59                     | 0.50              |
| 1:M:251:LEU:HD22 | 1:M:255:ILE:HG13 | 1.93                     | 0.50              |
| 1:M:312:GLU:C    | 1:M:314:LYS:H    | 2.20                     | 0.50              |
| 1:M:346:LEU:HD12 | 1:M:380:LEU:HB3  | 1.93                     | 0.50              |
| 1:N:294:GLU:O    | 1:N:295:ASP:C    | 2.53                     | 0.50              |
| 1:N:311:ARG:HG3  | 1:N:311:ARG:NH1  | 2.25                     | 0.50              |
| 1:B:249:ALA:CB   | 1:B:293:ARG:HH11 | 2.25                     | 0.50              |
| 1:B:310:LEU:CD1  | 1:B:359:LEU:HD12 | 2.41                     | 0.50              |
| 1:D:186:ARG:HD3  | 1:D:233:GLY:HA2  | 1.93                     | 0.50              |
| 1:D:315:GLU:N    | 1:D:315:GLU:OE1  | 2.41                     | 0.50              |
| 1:E:179:LEU:C    | 1:E:181:HIS:N    | 2.67                     | 0.50              |
| 1:G:167:GLY:H    | 1:G:173:LYS:HD3  | 1.76                     | 0.50              |
| 1:G:178:ARG:HA   | 1:G:191:PHE:CE1  | 2.42                     | 0.50              |
| 1:H:230:ALA:O    | 1:H:273:VAL:HG22 | 2.11                     | 0.50              |
| 1:K:186:ARG:HB2  | 1:K:189:GLU:HB2  | 1.94                     | 0.50              |
| 1:K:244:SER:C    | 1:K:246:GLU:N    | 2.70                     | 0.50              |
| 1:M:145:LYS:HD2  | 1:M:308:PRO:HG3  | 1.92                     | 0.50              |
| 1:N:211:TYR:CZ   | 1:N:223:LYS:HB2  | 2.46                     | 0.50              |
| 1:B:166:THR:HB   | 1:B:306:GLU:OE2  | 2.11                     | 0.50              |
| 1:C:309:PRO:HB2  | 1:C:311:ARG:NH1  | 2.26                     | 0.50              |
| 1:C:347:LEU:HD21 | 1:C:380:LEU:HD12 | 1.92                     | 0.50              |
| 1:E:191:PHE:HD1  | 1:E:234:THR:HB   | 1.75                     | 0.50              |
| 1:E:257:SER:C    | 1:E:259:LYS:H    | 2.19                     | 0.50              |
| 1:E:280:ASN:CG   | 1:E:280:ASN:O    | 2.53                     | 0.50              |
| 1:F:310:LEU:O    | 1:F:312:GLU:N    | 2.41                     | 0.50              |
| 1:G:154:LYS:O    | 1:G:157:SER:OG   | 2.18                     | 0.50              |
| 1:H:255:ILE:CG1  | 1:H:275:ILE:HD13 | 2.34                     | 0.50              |
| 1:J:301:GLY:O    | 1:J:302:VAL:C    | 2.54                     | 0.50              |
| 1:K:227:PHE:CE2  | 1:K:254:VAL:HG11 | 2.47                     | 0.50              |
| 1:M:254:VAL:CG2  | 1:M:260:PHE:HB3  | 2.42                     | 0.50              |
| 1:N:181:HIS:HD2  | 1:N:234:THR:CB   | 2.24                     | 0.50              |
| 1:F:179:LEU:O    | 1:F:183:LEU:HG   | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:171:VAL:HB   | 1:H:307:ILE:CG2  | 2.41                     | 0.50              |
| 1:H:302:VAL:O    | 1:I:365:ARG:HG3  | 2.11                     | 0.50              |
| 1:I:194:LEU:HD22 | 1:I:235:LEU:HD11 | 1.93                     | 0.50              |
| 1:K:267:LYS:O    | 1:K:269:ILE:HD12 | 2.12                     | 0.50              |
| 1:N:274:ARG:HG2  | 1:N:274:ARG:NH1  | 2.24                     | 0.50              |
| 1:A:213:LYS:HG2  | 1:A:221:SER:N    | 2.27                     | 0.50              |
| 1:D:189:GLU:CB   | 1:D:190:PRO:HD2  | 2.42                     | 0.50              |
| 1:D:342:SER:OG   | 1:D:377:ARG:HB2  | 2.11                     | 0.50              |
| 1:G:224:GLU:CG   | 1:G:225:GLY:H    | 2.18                     | 0.50              |
| 1:H:349:SER:HB2  | 1:H:350:TYR:CD1  | 2.46                     | 0.50              |
| 1:H:368:LEU:C    | 1:H:370:SER:H    | 2.17                     | 0.50              |
| 1:I:189:GLU:OE1  | 1:I:190:PRO:HD3  | 2.11                     | 0.50              |
| 1:I:311:ARG:HG2  | 1:I:311:ARG:HH11 | 1.77                     | 0.50              |
| 1:I:365:ARG:CD   | 1:I:383:LEU:HD22 | 2.42                     | 0.50              |
| 1:K:237:LEU:CB   | 1:K:240:ILE:HD11 | 2.41                     | 0.50              |
| 1:L:211:TYR:N    | 1:L:211:TYR:CD1  | 2.78                     | 0.50              |
| 1:L:303:ILE:O    | 1:L:303:ILE:HG22 | 2.12                     | 0.50              |
| 1:L:334:LYS:HD2  | 1:L:336:VAL:CG2  | 2.42                     | 0.50              |
| 1:M:299:ARG:CD   | 1:N:357:ARG:HH21 | 2.24                     | 0.50              |
| 1:N:149:ILE:O    | 1:N:153:ILE:HG12 | 2.11                     | 0.50              |
| 1:B:186:ARG:HH22 | 1:B:272:ASN:CG   | 2.20                     | 0.50              |
| 1:C:194:LEU:CD2  | 1:C:194:LEU:N    | 2.68                     | 0.50              |
| 1:D:216:PHE:CD1  | 1:D:216:PHE:C    | 2.90                     | 0.50              |
| 1:E:280:ASN:O    | 1:E:280:ASN:OD1  | 2.30                     | 0.50              |
| 1:E:363:ILE:C    | 1:E:367:VAL:HG23 | 2.35                     | 0.50              |
| 1:H:164:LEU:HD21 | 1:H:283:ILE:CD1  | 2.41                     | 0.50              |
| 1:H:204:PHE:O    | 1:H:205:GLU:C    | 2.55                     | 0.50              |
| 1:H:292:PHE:HE2  | 1:H:296:LEU:HB3  | 1.76                     | 0.50              |
| 1:J:153:ILE:HD12 | 1:J:180:ILE:HG12 | 1.93                     | 0.50              |
| 1:L:152:LYS:O    | 1:L:153:ILE:C    | 2.55                     | 0.50              |
| 1:L:362:VAL:O    | 1:L:365:ARG:HB3  | 2.12                     | 0.50              |
| 1:N:325:LEU:O    | 1:N:329:SER:HB2  | 2.12                     | 0.50              |
| 1:A:189:GLU:HG2  | 1:A:232:GLY:O    | 2.12                     | 0.50              |
| 1:C:243:LEU:CD1  | 1:C:251:LEU:HD12 | 2.41                     | 0.50              |
| 1:D:250:LYS:O    | 1:D:254:VAL:HG23 | 2.12                     | 0.50              |
| 1:F:309:PRO:O    | 1:F:313:ARG:HD3  | 2.12                     | 0.50              |
| 1:I:296:LEU:HD21 | 1:I:300:LEU:HD12 | 1.94                     | 0.50              |
| 1:L:319:PRO:O    | 1:L:322:ASN:HB2  | 2.11                     | 0.50              |
| 1:L:324:PHE:CE2  | 1:L:360:LYS:HE2  | 2.47                     | 0.50              |
| 1:M:266:ARG:HH21 | 1:M:267:LYS:HZ3  | 1.59                     | 0.50              |
| 1:N:194:LEU:HD21 | 1:N:237:LEU:HD23 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:245:LEU:HB2  | 1:N:246:GLU:OE2  | 2.12                     | 0.50              |
| 1:A:339:PHE:H    | 1:A:339:PHE:HD1  | 1.55                     | 0.50              |
| 1:A:375:ILE:HG22 | 1:A:380:LEU:HD23 | 1.93                     | 0.50              |
| 1:C:284:LYS:HG3  | 1:C:285:GLU:N    | 2.26                     | 0.50              |
| 1:C:325:LEU:HD23 | 1:C:326:LYS:N    | 2.26                     | 0.50              |
| 1:D:146:MET:HE3  | 1:D:146:MET:CA   | 2.42                     | 0.50              |
| 1:D:166:THR:HG22 | 1:D:279:THR:HG22 | 1.94                     | 0.50              |
| 1:D:240:ILE:HG13 | 1:D:277:ALA:CB   | 2.29                     | 0.50              |
| 1:D:381:SER:HA   | 1:D:384:VAL:O    | 2.12                     | 0.50              |
| 1:E:239:GLU:C    | 1:E:241:GLY:N    | 2.69                     | 0.50              |
| 1:F:195:ASN:HB3  | 1:F:198:SER:OG   | 2.11                     | 0.50              |
| 1:H:156:ILE:HG22 | 1:H:274:ARG:HH22 | 1.76                     | 0.50              |
| 1:K:161:CYS:N    | 1:K:274:ARG:HH12 | 2.10                     | 0.50              |
| 1:L:164:LEU:CD1  | 1:L:278:ALA:HA   | 2.41                     | 0.50              |
| 1:L:350:TYR:CD2  | 1:L:350:TYR:C    | 2.90                     | 0.50              |
| 1:L:376:ASP:O    | 1:L:377:ARG:C    | 2.54                     | 0.50              |
| 1:N:157:SER:HB3  | 1:N:184:SER:CA   | 2.41                     | 0.50              |
| 1:N:349:SER:O    | 1:N:350:TYR:C    | 2.55                     | 0.50              |
| 1:C:179:LEU:O    | 1:C:179:LEU:HD23 | 2.12                     | 0.49              |
| 1:E:150:LEU:O    | 1:E:154:LYS:HG3  | 2.12                     | 0.49              |
| 1:G:148:GLU:O    | 1:G:150:LEU:N    | 2.45                     | 0.49              |
| 1:G:233:GLY:O    | 1:G:273:VAL:HG13 | 2.11                     | 0.49              |
| 1:I:253:ARG:CD   | 1:J:198:SER:HB2  | 2.42                     | 0.49              |
| 1:I:322:ASN:O    | 1:I:323:HIS:C    | 2.55                     | 0.49              |
| 1:K:230:ALA:O    | 1:K:273:VAL:HG22 | 2.12                     | 0.49              |
| 1:K:267:LYS:HD2  | 1:K:267:LYS:N    | 2.26                     | 0.49              |
| 1:M:347:LEU:HD21 | 1:M:380:LEU:CD1  | 2.42                     | 0.49              |
| 1:N:340:THR:O    | 1:N:344:GLN:N    | 2.34                     | 0.49              |
| 1:B:206:ALA:O    | 1:B:210:GLY:N    | 2.44                     | 0.49              |
| 1:C:288:LYS:C    | 1:C:290:GLY:N    | 2.71                     | 0.49              |
| 1:D:239:GLU:HA   | 1:D:279:THR:HA   | 1.94                     | 0.49              |
| 1:D:275:ILE:O    | 1:D:276:LEU:HD23 | 2.12                     | 0.49              |
| 1:D:365:ARG:HD2  | 1:D:383:LEU:HD22 | 1.94                     | 0.49              |
| 1:D:380:LEU:O    | 1:D:384:VAL:N    | 2.43                     | 0.49              |
| 1:E:149:ILE:C    | 1:E:151:GLU:N    | 2.69                     | 0.49              |
| 1:E:159:ALA:O    | 1:E:274:ARG:NH1  | 2.45                     | 0.49              |
| 1:F:138:GLU:HG3  | 1:F:139:TYR:H    | 1.76                     | 0.49              |
| 1:G:146:MET:HE1  | 1:G:307:ILE:HG23 | 1.94                     | 0.49              |
| 1:H:171:VAL:HB   | 1:H:307:ILE:HG22 | 1.94                     | 0.49              |
| 1:H:322:ASN:O    | 1:H:326:LYS:HG3  | 2.12                     | 0.49              |
| 1:K:156:ILE:O    | 1:K:159:ALA:N    | 2.41                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:359:LEU:HD23 | 1:K:363:ILE:HG13 | 1.94                     | 0.49              |
| 1:L:140:VAL:CG1  | 1:L:140:VAL:O    | 2.56                     | 0.49              |
| 1:L:210:GLY:C    | 1:L:262:ARG:HG2  | 2.37                     | 0.49              |
| 1:M:195:ASN:C    | 1:M:197:ALA:N    | 2.68                     | 0.49              |
| 1:M:212:GLU:CB   | 1:M:264:GLY:HA3  | 2.42                     | 0.49              |
| 1:M:342:SER:O    | 1:M:377:ARG:HD2  | 2.12                     | 0.49              |
| 1:D:171:VAL:HG23 | 1:D:172:GLY:N    | 2.27                     | 0.49              |
| 1:F:314:LYS:HA   | 1:F:317:ILE:CG1  | 2.41                     | 0.49              |
| 1:F:327:LYS:O    | 1:F:330:ARG:N    | 2.46                     | 0.49              |
| 1:G:299:ARG:O    | 1:G:302:VAL:HG23 | 2.12                     | 0.49              |
| 1:G:365:ARG:HH11 | 1:G:383:LEU:HD22 | 1.77                     | 0.49              |
| 1:H:178:ARG:HH11 | 1:H:178:ARG:HG3  | 1.77                     | 0.49              |
| 1:H:328:PHE:HB3  | 1:H:367:VAL:HG21 | 1.93                     | 0.49              |
| 1:L:236:PHE:HA   | 1:L:276:LEU:O    | 2.12                     | 0.49              |
| 1:L:288:LYS:C    | 1:L:290:GLY:N    | 2.71                     | 0.49              |
| 1:M:356:VAL:O    | 1:M:357:ARG:C    | 2.54                     | 0.49              |
| 1:A:365:ARG:NH2  | 1:G:302:VAL:O    | 2.44                     | 0.49              |
| 1:B:157:SER:C    | 1:B:159:ALA:H    | 2.21                     | 0.49              |
| 1:C:366:ALA:C    | 1:C:368:LEU:N    | 2.70                     | 0.49              |
| 1:D:317:ILE:O    | 1:D:318:ILE:C    | 2.54                     | 0.49              |
| 1:F:172:GLY:HA2  | 2:F:4:ADP:O1A    | 2.11                     | 0.49              |
| 1:G:153:ILE:HG23 | 1:G:180:ILE:CG1  | 2.42                     | 0.49              |
| 1:G:194:LEU:CD2  | 1:G:237:LEU:HD22 | 2.42                     | 0.49              |
| 1:H:142:GLU:HB3  | 1:H:146:MET:CB   | 2.43                     | 0.49              |
| 1:H:237:LEU:HB2  | 1:H:240:ILE:HD11 | 1.93                     | 0.49              |
| 1:H:320:LEU:O    | 1:H:324:PHE:CD1  | 2.65                     | 0.49              |
| 1:H:355:ASN:O    | 1:H:356:VAL:C    | 2.56                     | 0.49              |
| 1:I:156:ILE:HG22 | 1:I:157:SER:N    | 2.28                     | 0.49              |
| 1:K:255:ILE:HD11 | 1:K:300:LEU:HD21 | 1.93                     | 0.49              |
| 1:L:164:LEU:HA   | 1:L:277:ALA:O    | 2.12                     | 0.49              |
| 1:M:212:GLU:HB3  | 1:M:264:GLY:HA3  | 1.94                     | 0.49              |
| 1:M:227:PHE:HE2  | 1:M:273:VAL:HG21 | 1.71                     | 0.49              |
| 1:M:234:THR:HG22 | 1:M:235:LEU:N    | 2.28                     | 0.49              |
| 1:M:252:LEU:CD1  | 1:M:299:ARG:HG3  | 2.42                     | 0.49              |
| 1:N:181:HIS:HD2  | 1:N:234:THR:HB   | 1.76                     | 0.49              |
| 1:B:142:GLU:O    | 1:B:143:SER:HB3  | 2.12                     | 0.49              |
| 1:B:177:ALA:HB1  | 1:B:276:LEU:HD13 | 1.93                     | 0.49              |
| 1:B:266:ARG:HB3  | 1:C:229:LEU:HD23 | 1.95                     | 0.49              |
| 1:C:175:VAL:HG23 | 2:C:1:ADP:O1A    | 2.13                     | 0.49              |
| 1:E:363:ILE:O    | 1:E:366:ALA:HB3  | 2.12                     | 0.49              |
| 1:F:366:ALA:O    | 1:F:369:PHE:N    | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:324:PHE:CE1  | 1:G:360:LYS:HA   | 2.48                     | 0.49              |
| 1:H:320:LEU:O    | 1:H:324:PHE:HD1  | 1.94                     | 0.49              |
| 1:I:249:ALA:CB   | 1:I:293:ARG:NH1  | 2.75                     | 0.49              |
| 1:I:251:LEU:O    | 1:I:254:VAL:N    | 2.45                     | 0.49              |
| 1:I:300:LEU:C    | 1:I:302:VAL:N    | 2.69                     | 0.49              |
| 1:L:158:CYS:O    | 1:L:158:CYS:SG   | 2.71                     | 0.49              |
| 1:L:161:CYS:O    | 1:L:274:ARG:NE   | 2.45                     | 0.49              |
| 1:N:316:ASP:O    | 1:N:320:LEU:HG   | 2.12                     | 0.49              |
| 1:A:192:VAL:HG21 | 1:A:229:LEU:HD12 | 1.94                     | 0.49              |
| 1:C:341:LYS:O    | 1:C:345:GLU:HG3  | 2.12                     | 0.49              |
| 1:F:223:LYS:O    | 1:F:223:LYS:CG   | 2.59                     | 0.49              |
| 1:F:240:ILE:C    | 1:F:242:GLU:N    | 2.69                     | 0.49              |
| 1:G:151:GLU:O    | 1:G:152:LYS:C    | 2.52                     | 0.49              |
| 1:G:328:PHE:C    | 1:G:330:ARG:N    | 2.70                     | 0.49              |
| 1:J:324:PHE:O    | 1:J:327:LYS:HB3  | 2.13                     | 0.49              |
| 1:L:347:LEU:HD23 | 1:L:347:LEU:N    | 2.28                     | 0.49              |
| 1:M:173:LYS:HB2  | 2:M:12:ADP:O2B   | 2.12                     | 0.49              |
| 1:M:207:GLU:O    | 1:M:226:PHE:CD1  | 2.56                     | 0.49              |
| 1:M:265:GLY:HA2  | 1:N:203:ILE:HD11 | 1.94                     | 0.49              |
| 1:M:353:TYR:C    | 1:M:355:ASN:N    | 2.71                     | 0.49              |
| 1:M:359:LEU:O    | 1:M:363:ILE:HD13 | 2.12                     | 0.49              |
| 1:N:200:PRO:O    | 1:N:202:ASP:N    | 2.46                     | 0.49              |
| 1:A:143:SER:HA   | 1:A:315:GLU:HB2  | 1.93                     | 0.49              |
| 1:A:168:GLU:O    | 1:A:171:VAL:HG22 | 2.13                     | 0.49              |
| 1:B:177:ALA:HA   | 1:B:180:ILE:HD12 | 1.93                     | 0.49              |
| 1:B:328:PHE:CE1  | 1:B:364:GLU:HB2  | 2.47                     | 0.49              |
| 1:C:171:VAL:HG21 | 1:C:307:ILE:HB   | 1.94                     | 0.49              |
| 1:E:138:GLU:HB2  | 1:E:323:HIS:CD2  | 2.48                     | 0.49              |
| 1:F:345:GLU:O    | 1:F:346:LEU:C    | 2.56                     | 0.49              |
| 1:F:357:ARG:CG   | 1:F:357:ARG:NH1  | 2.75                     | 0.49              |
| 1:G:192:VAL:O    | 1:G:235:LEU:HD12 | 2.13                     | 0.49              |
| 1:G:248:GLN:OE1  | 1:G:292:PHE:HA   | 2.12                     | 0.49              |
| 1:G:327:LYS:O    | 1:G:330:ARG:HB3  | 2.12                     | 0.49              |
| 1:H:227:PHE:CE2  | 1:H:254:VAL:HG21 | 2.45                     | 0.49              |
| 1:J:313:ARG:O    | 1:J:314:LYS:C    | 2.55                     | 0.49              |
| 1:L:352:TRP:CZ3  | 1:L:362:VAL:HG21 | 2.47                     | 0.49              |
| 1:M:171:VAL:HG12 | 1:M:309:PRO:HA   | 1.93                     | 0.49              |
| 1:M:252:LEU:HD22 | 1:M:295:ASP:OD1  | 2.12                     | 0.49              |
| 1:C:321:ALA:HA   | 1:C:363:ILE:HD12 | 1.95                     | 0.49              |
| 1:E:176:VAL:O    | 1:E:180:ILE:CG1  | 2.61                     | 0.49              |
| 1:E:250:LYS:HG3  | 1:F:198:SER:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:144:PRO:HG2  | 1:F:145:LYS:H    | 1.78                     | 0.49              |
| 1:F:310:LEU:HB2  | 1:F:355:ASN:HB3  | 1.94                     | 0.49              |
| 1:H:143:SER:CA   | 1:H:147:LYS:HE3  | 2.38                     | 0.49              |
| 1:H:198:SER:HB2  | 1:N:250:LYS:CG   | 2.43                     | 0.49              |
| 1:J:149:ILE:O    | 1:J:153:ILE:HG12 | 2.13                     | 0.49              |
| 1:J:157:SER:HB3  | 1:J:184:SER:HA   | 1.95                     | 0.49              |
| 1:J:382:CYS:HB2  | 1:J:383:LEU:HD23 | 1.94                     | 0.49              |
| 1:K:283:ILE:HG21 | 1:K:297:TYR:CD1  | 2.48                     | 0.49              |
| 1:K:298:TYR:C    | 1:K:300:LEU:N    | 2.69                     | 0.49              |
| 1:A:176:VAL:O    | 1:A:180:ILE:HG13 | 2.13                     | 0.49              |
| 1:A:265:GLY:O    | 1:A:266:ARG:NE   | 2.43                     | 0.49              |
| 1:D:145:LYS:O    | 1:D:149:ILE:HG13 | 2.13                     | 0.49              |
| 1:D:209:PHE:HE2  | 1:D:227:PHE:HE1  | 1.60                     | 0.49              |
| 1:D:343:ALA:O    | 1:D:344:GLN:C    | 2.56                     | 0.49              |
| 1:E:141:PHE:CG   | 1:E:150:LEU:HD22 | 2.48                     | 0.49              |
| 1:E:156:ILE:HG13 | 1:E:303:ILE:HG21 | 1.95                     | 0.49              |
| 1:G:155:LYS:C    | 1:G:157:SER:N    | 2.70                     | 0.49              |
| 1:G:267:LYS:O    | 1:G:267:LYS:HD3  | 2.12                     | 0.49              |
| 1:H:163:VAL:HB   | 1:H:276:LEU:HD23 | 1.94                     | 0.49              |
| 1:I:194:LEU:HD21 | 1:I:235:LEU:HD11 | 1.94                     | 0.49              |
| 1:I:310:LEU:O    | 1:I:312:GLU:N    | 2.46                     | 0.49              |
| 1:K:298:TYR:O    | 1:K:300:LEU:N    | 2.45                     | 0.49              |
| 1:L:194:LEU:HD21 | 1:L:237:LEU:CD2  | 2.40                     | 0.49              |
| 1:L:225:GLY:O    | 1:L:228:GLU:N    | 2.30                     | 0.49              |
| 1:L:240:ILE:CG2  | 1:L:292:PHE:HE1  | 2.26                     | 0.49              |
| 1:L:283:ILE:HB   | 1:L:297:TYR:CE1  | 2.47                     | 0.49              |
| 1:L:380:LEU:O    | 1:L:381:SER:C    | 2.56                     | 0.49              |
| 1:N:257:SER:C    | 1:N:259:LYS:H    | 2.20                     | 0.49              |
| 1:A:220:VAL:O    | 1:A:221:SER:CB   | 2.60                     | 0.49              |
| 1:B:285:GLU:O    | 1:B:286:LEU:C    | 2.56                     | 0.49              |
| 1:C:181:HIS:NE2  | 1:C:191:PHE:HB2  | 2.26                     | 0.49              |
| 1:C:350:TYR:CG   | 1:C:351:PRO:HD2  | 2.47                     | 0.49              |
| 1:D:361:ASN:C    | 1:D:363:ILE:H    | 2.21                     | 0.49              |
| 1:E:282:ASN:O    | 1:E:283:ILE:C    | 2.56                     | 0.49              |
| 1:E:309:PRO:HD2  | 1:E:312:GLU:OE1  | 2.13                     | 0.49              |
| 1:F:363:ILE:O    | 1:F:364:GLU:C    | 2.55                     | 0.49              |
| 1:G:161:CYS:HB2  | 1:G:302:VAL:HG11 | 1.95                     | 0.49              |
| 1:G:163:VAL:HB   | 1:G:276:LEU:HD22 | 1.94                     | 0.49              |
| 1:G:282:ASN:HD22 | 1:G:285:GLU:HB2  | 1.75                     | 0.49              |
| 1:J:157:SER:C    | 1:J:184:SER:HA   | 2.38                     | 0.49              |
| 1:K:213:LYS:NZ   | 1:K:220:VAL:HG13 | 2.28                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:365:ARG:HD2  | 1:K:383:LEU:CD2  | 2.42                     | 0.49              |
| 1:L:144:PRO:HD3  | 1:L:315:GLU:OE2  | 2.13                     | 0.49              |
| 1:L:164:LEU:HD12 | 1:L:165:ILE:H    | 1.77                     | 0.49              |
| 1:L:379:GLU:C    | 1:L:381:SER:N    | 2.70                     | 0.49              |
| 1:A:178:ARG:HE   | 1:A:191:PHE:HE2  | 1.58                     | 0.48              |
| 1:B:157:SER:OG   | 1:B:183:LEU:HB2  | 2.13                     | 0.48              |
| 1:B:362:VAL:HG13 | 1:B:384:VAL:CG2  | 2.32                     | 0.48              |
| 1:C:256:GLU:HG2  | 1:C:299:ARG:NH2  | 2.28                     | 0.48              |
| 1:C:311:ARG:NH2  | 1:C:353:TYR:HD2  | 2.11                     | 0.48              |
| 1:H:240:ILE:HG22 | 1:H:292:PHE:HE1  | 1.78                     | 0.48              |
| 1:I:269:ILE:HD12 | 1:I:269:ILE:H    | 1.77                     | 0.48              |
| 1:L:192:VAL:HG21 | 1:L:230:ALA:HB2  | 1.95                     | 0.48              |
| 1:L:254:VAL:HG22 | 1:L:260:PHE:HB3  | 1.95                     | 0.48              |
| 1:M:162:PRO:HG2  | 1:M:302:VAL:CG2  | 2.42                     | 0.48              |
| 1:N:168:GLU:OE1  | 1:N:311:ARG:NH2  | 2.45                     | 0.48              |
| 1:N:352:TRP:CZ3  | 1:N:358:GLU:HG2  | 2.48                     | 0.48              |
| 1:N:357:ARG:HH12 | 1:N:361:ASN:HD21 | 1.60                     | 0.48              |
| 1:B:235:LEU:HG   | 1:B:237:LEU:CD2  | 2.43                     | 0.48              |
| 1:B:256:GLU:HG2  | 1:B:299:ARG:HD3  | 1.95                     | 0.48              |
| 1:C:179:LEU:HD23 | 1:C:183:LEU:HG   | 1.95                     | 0.48              |
| 1:C:186:ARG:NH1  | 1:C:232:GLY:O    | 2.46                     | 0.48              |
| 1:E:204:PHE:O    | 1:E:205:GLU:C    | 2.55                     | 0.48              |
| 1:E:313:ARG:C    | 1:E:315:GLU:N    | 2.70                     | 0.48              |
| 1:E:324:PHE:C    | 1:E:326:LYS:N    | 2.70                     | 0.48              |
| 1:F:217:THR:HG22 | 1:F:218:GLY:N    | 2.28                     | 0.48              |
| 1:F:253:ARG:HG3  | 1:F:253:ARG:HH11 | 1.78                     | 0.48              |
| 1:F:299:ARG:HE   | 1:F:299:ARG:CA   | 2.25                     | 0.48              |
| 1:F:324:PHE:HB2  | 1:F:363:ILE:HD12 | 1.95                     | 0.48              |
| 1:G:355:ASN:C    | 1:G:357:ARG:H    | 2.21                     | 0.48              |
| 1:J:328:PHE:CD2  | 1:J:364:GLU:HG3  | 2.48                     | 0.48              |
| 1:L:171:VAL:CG2  | 1:L:307:ILE:CG2  | 2.90                     | 0.48              |
| 1:M:304:GLU:HA   | 1:M:304:GLU:OE2  | 2.13                     | 0.48              |
| 1:M:310:LEU:HD12 | 1:M:355:ASN:HA   | 1.96                     | 0.48              |
| 1:N:140:VAL:HG11 | 1:N:320:LEU:CD2  | 2.41                     | 0.48              |
| 1:N:359:LEU:HD23 | 1:N:363:ILE:CD1  | 2.43                     | 0.48              |
| 1:A:382:CYS:C    | 1:A:383:LEU:HD23 | 2.38                     | 0.48              |
| 1:C:177:ALA:O    | 1:C:180:ILE:HB   | 2.13                     | 0.48              |
| 1:D:262:ARG:HH11 | 1:D:262:ARG:CG   | 1.98                     | 0.48              |
| 1:E:149:ILE:O    | 1:E:151:GLU:N    | 2.46                     | 0.48              |
| 1:E:153:ILE:HD11 | 1:E:176:VAL:HG13 | 1.96                     | 0.48              |
| 1:E:346:LEU:HA   | 1:E:349:SER:OG   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:376:ASP:O    | 1:G:378:GLY:N    | 2.46                     | 0.48              |
| 1:H:181:HIS:O    | 1:H:187:SER:HB3  | 2.13                     | 0.48              |
| 1:H:239:GLU:N    | 1:H:278:ALA:O    | 2.46                     | 0.48              |
| 1:H:262:ARG:HG3  | 1:H:269:ILE:HD12 | 1.95                     | 0.48              |
| 1:K:206:ALA:HB1  | 1:K:211:TYR:HD1  | 1.78                     | 0.48              |
| 1:A:158:CYS:HA   | 1:A:185:ASP:CG   | 2.39                     | 0.48              |
| 1:A:240:ILE:O    | 1:A:242:GLU:N    | 2.46                     | 0.48              |
| 1:A:331:LYS:HD3  | 1:A:332:TYR:CZ   | 2.48                     | 0.48              |
| 1:B:216:PHE:CD1  | 1:B:217:THR:HG22 | 2.49                     | 0.48              |
| 1:B:334:LYS:HG3  | 1:B:367:VAL:O    | 2.13                     | 0.48              |
| 1:C:149:ILE:O    | 1:C:153:ILE:HG12 | 2.12                     | 0.48              |
| 1:C:244:SER:O    | 1:C:248:GLN:CG   | 2.60                     | 0.48              |
| 1:C:326:LYS:HE2  | 1:C:330:ARG:NH2  | 2.28                     | 0.48              |
| 1:E:234:THR:HG23 | 1:E:274:ARG:O    | 2.13                     | 0.48              |
| 1:E:253:ARG:HG3  | 1:E:253:ARG:NH1  | 2.27                     | 0.48              |
| 1:F:174:GLU:O    | 1:F:175:VAL:C    | 2.55                     | 0.48              |
| 1:G:310:LEU:HD11 | 1:G:359:LEU:HD12 | 1.96                     | 0.48              |
| 1:H:209:PHE:O    | 1:H:262:ARG:HG2  | 2.13                     | 0.48              |
| 1:I:146:MET:SD   | 1:I:313:ARG:NE   | 2.86                     | 0.48              |
| 1:J:281:ARG:HG2  | 1:J:281:ARG:NH1  | 2.28                     | 0.48              |
| 1:K:302:VAL:C    | 1:K:303:ILE:HG12 | 2.38                     | 0.48              |
| 1:L:261:TYR:C    | 1:L:262:ARG:O    | 2.56                     | 0.48              |
| 1:M:283:ILE:HG22 | 1:M:284:LYS:N    | 2.28                     | 0.48              |
| 1:M:324:PHE:CE2  | 1:M:360:LYS:HG3  | 2.47                     | 0.48              |
| 1:N:296:LEU:O    | 1:N:300:LEU:HG   | 2.13                     | 0.48              |
| 1:A:204:PHE:CE2  | 1:A:243:LEU:HD21 | 2.45                     | 0.48              |
| 1:B:156:ILE:O    | 1:B:157:SER:C    | 2.57                     | 0.48              |
| 1:D:294:GLU:O    | 1:D:297:TYR:HB3  | 2.12                     | 0.48              |
| 1:E:173:LYS:HB2  | 2:E:3:ADP:O1B    | 2.13                     | 0.48              |
| 1:E:230:ALA:O    | 1:E:273:VAL:HG22 | 2.12                     | 0.48              |
| 1:E:313:ARG:C    | 1:E:315:GLU:H    | 2.20                     | 0.48              |
| 1:F:149:ILE:O    | 1:F:153:ILE:HG12 | 2.13                     | 0.48              |
| 1:F:359:LEU:O    | 1:F:360:LYS:C    | 2.56                     | 0.48              |
| 1:G:145:LYS:O    | 1:G:149:ILE:HG13 | 2.13                     | 0.48              |
| 1:I:328:PHE:HZ   | 1:I:360:LYS:HG3  | 1.78                     | 0.48              |
| 1:K:240:ILE:HG13 | 1:K:277:ALA:CB   | 2.42                     | 0.48              |
| 1:K:244:SER:C    | 1:K:246:GLU:H    | 2.19                     | 0.48              |
| 1:N:209:PHE:CE1  | 1:N:250:LYS:HD3  | 2.48                     | 0.48              |
| 1:B:318:ILE:O    | 1:B:322:ASN:ND2  | 2.46                     | 0.48              |
| 1:C:349:SER:O    | 1:C:350:TYR:C    | 2.56                     | 0.48              |
| 1:D:212:GLU:HA   | 1:D:222:SER:HB2  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:252:LEU:HD11 | 1:D:299:ARG:HG3  | 1.96                     | 0.48              |
| 1:E:380:LEU:O    | 1:E:384:VAL:HB   | 2.13                     | 0.48              |
| 1:F:156:ILE:O    | 1:F:159:ALA:N    | 2.46                     | 0.48              |
| 1:F:254:VAL:HG22 | 1:F:260:PHE:HB3  | 1.96                     | 0.48              |
| 1:F:380:LEU:N    | 1:F:380:LEU:CD2  | 2.77                     | 0.48              |
| 1:G:148:GLU:O    | 1:G:151:GLU:N    | 2.46                     | 0.48              |
| 1:G:234:THR:HG21 | 1:G:276:LEU:HD12 | 1.95                     | 0.48              |
| 1:G:235:LEU:HB2  | 1:G:273:VAL:HG11 | 1.96                     | 0.48              |
| 1:G:310:LEU:HG   | 1:G:356:VAL:CG2  | 2.44                     | 0.48              |
| 1:H:168:GLU:CG   | 1:H:311:ARG:HH22 | 2.20                     | 0.48              |
| 1:J:200:PRO:C    | 1:J:202:ASP:N    | 2.71                     | 0.48              |
| 1:K:177:ALA:HB1  | 1:K:276:LEU:CD1  | 2.44                     | 0.48              |
| 1:L:143:SER:O    | 1:L:147:LYS:HB2  | 2.13                     | 0.48              |
| 1:L:210:GLY:O    | 1:L:263:LEU:HB2  | 2.13                     | 0.48              |
| 1:N:157:SER:OG   | 1:N:183:LEU:HB2  | 2.13                     | 0.48              |
| 1:N:245:LEU:CD2  | 1:N:293:ARG:HG3  | 2.38                     | 0.48              |
| 1:A:171:VAL:HB   | 1:A:307:ILE:CG2  | 2.43                     | 0.48              |
| 1:A:311:ARG:HB3  | 1:A:351:PRO:O    | 2.13                     | 0.48              |
| 1:B:162:PRO:HB2  | 1:B:300:LEU:HD23 | 1.96                     | 0.48              |
| 1:D:236:PHE:CD1  | 1:D:236:PHE:O    | 2.67                     | 0.48              |
| 1:F:179:LEU:O    | 1:F:179:LEU:HD23 | 2.14                     | 0.48              |
| 1:F:193:ALA:HB1  | 1:F:236:PHE:HD2  | 1.78                     | 0.48              |
| 1:F:206:ALA:O    | 1:F:210:GLY:CA   | 2.62                     | 0.48              |
| 1:F:283:ILE:HG21 | 1:F:297:TYR:CD1  | 2.49                     | 0.48              |
| 1:G:240:ILE:HG13 | 1:G:277:ALA:CB   | 2.33                     | 0.48              |
| 1:G:376:ASP:C    | 1:G:378:GLY:N    | 2.72                     | 0.48              |
| 1:K:252:LEU:HD11 | 1:K:299:ARG:HG3  | 1.96                     | 0.48              |
| 1:K:313:ARG:O    | 1:K:315:GLU:N    | 2.47                     | 0.48              |
| 1:L:211:TYR:N    | 1:L:211:TYR:HD1  | 2.12                     | 0.48              |
| 1:L:289:GLU:HG2  | 1:L:289:GLU:O    | 2.14                     | 0.48              |
| 1:L:324:PHE:HE2  | 1:L:360:LYS:HE2  | 1.79                     | 0.48              |
| 1:L:329:SER:HA   | 1:L:334:LYS:CE   | 2.26                     | 0.48              |
| 1:M:194:LEU:HD23 | 1:M:194:LEU:H    | 1.78                     | 0.48              |
| 1:M:209:PHE:HE2  | 1:M:227:PHE:CE1  | 2.32                     | 0.48              |
| 1:M:248:GLN:NE2  | 1:M:248:GLN:H    | 2.11                     | 0.48              |
| 1:N:173:LYS:HB2  | 2:N:13:ADP:O2B   | 2.14                     | 0.48              |
| 1:A:256:GLU:OE2  | 1:B:357:ARG:NH1  | 2.47                     | 0.48              |
| 1:B:179:LEU:HD23 | 1:B:179:LEU:C    | 2.39                     | 0.48              |
| 1:B:314:LYS:CD   | 1:B:314:LYS:N    | 2.74                     | 0.48              |
| 1:B:335:GLU:O    | 1:B:373:LYS:HA   | 2.13                     | 0.48              |
| 1:C:282:ASN:O    | 1:C:284:LYS:N    | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:308:PRO:O    | 1:D:313:ARG:CD   | 2.62                     | 0.48              |
| 1:D:328:PHE:CD2  | 1:D:364:GLU:HG3  | 2.48                     | 0.48              |
| 1:D:362:VAL:O    | 1:D:362:VAL:CG1  | 2.59                     | 0.48              |
| 1:E:170:GLY:O    | 1:E:355:ASN:HB2  | 2.14                     | 0.48              |
| 1:E:299:ARG:HE   | 1:E:299:ARG:HA   | 1.79                     | 0.48              |
| 1:F:244:SER:O    | 1:F:248:GLN:HG3  | 2.14                     | 0.48              |
| 1:G:167:GLY:N    | 1:G:173:LYS:HD3  | 2.29                     | 0.48              |
| 1:G:173:LYS:C    | 1:G:175:VAL:N    | 2.72                     | 0.48              |
| 1:G:191:PHE:CE2  | 1:G:236:PHE:HB3  | 2.45                     | 0.48              |
| 1:G:251:LEU:HD22 | 1:G:255:ILE:HD11 | 1.95                     | 0.48              |
| 1:G:261:TYR:CD2  | 1:G:263:LEU:O    | 2.67                     | 0.48              |
| 1:I:365:ARG:HD2  | 1:I:383:LEU:HD22 | 1.96                     | 0.48              |
| 1:K:325:LEU:O    | 1:K:325:LEU:HD23 | 2.12                     | 0.48              |
| 1:L:165:ILE:O    | 1:L:165:ILE:HG22 | 2.13                     | 0.48              |
| 1:M:259:LYS:HD2  | 1:M:268:GLU:OE2  | 2.12                     | 0.48              |
| 1:N:294:GLU:O    | 1:N:297:TYR:N    | 2.47                     | 0.48              |
| 1:D:275:ILE:HG22 | 1:D:276:LEU:N    | 2.29                     | 0.48              |
| 1:I:143:SER:O    | 1:I:147:LYS:HG3  | 2.13                     | 0.48              |
| 1:I:288:LYS:C    | 1:I:290:GLY:H    | 2.21                     | 0.48              |
| 1:K:283:ILE:O    | 1:K:287:VAL:HG23 | 2.13                     | 0.48              |
| 1:L:269:ILE:HD12 | 1:L:269:ILE:N    | 2.28                     | 0.48              |
| 1:L:310:LEU:O    | 1:L:311:ARG:C    | 2.56                     | 0.48              |
| 1:M:302:VAL:O    | 1:M:303:ILE:HD13 | 2.13                     | 0.48              |
| 1:N:227:PHE:CE2  | 1:N:235:LEU:HD23 | 2.47                     | 0.48              |
| 1:N:231:ASP:OD1  | 1:N:271:VAL:HB   | 2.14                     | 0.48              |
| 1:N:292:PHE:C    | 1:N:292:PHE:CD2  | 2.91                     | 0.48              |
| 1:N:296:LEU:HD13 | 1:N:296:LEU:O    | 2.14                     | 0.48              |
| 1:A:176:VAL:HG21 | 1:A:307:ILE:CD1  | 2.44                     | 0.48              |
| 1:A:194:LEU:CD2  | 1:A:194:LEU:N    | 2.76                     | 0.48              |
| 1:A:377:ARG:NH2  | 1:L:285:GLU:HG2  | 2.26                     | 0.48              |
| 1:E:177:ALA:HB1  | 1:E:276:LEU:CD1  | 2.43                     | 0.48              |
| 1:E:336:VAL:HG21 | 1:E:370:SER:CB   | 2.44                     | 0.48              |
| 1:F:224:GLU:O    | 1:F:225:GLY:O    | 2.31                     | 0.48              |
| 1:F:249:ALA:HB2  | 1:F:293:ARG:HH11 | 1.79                     | 0.48              |
| 1:F:366:ALA:C    | 1:F:368:LEU:N    | 2.71                     | 0.48              |
| 1:H:329:SER:N    | 1:H:367:VAL:HG11 | 2.29                     | 0.48              |
| 1:L:164:LEU:HD12 | 1:L:165:ILE:N    | 2.29                     | 0.48              |
| 1:M:247:ALA:C    | 1:M:249:ALA:N    | 2.69                     | 0.48              |
| 1:N:240:ILE:HA   | 1:N:243:LEU:HD12 | 1.96                     | 0.48              |
| 1:N:352:TRP:HZ3  | 1:N:358:GLU:HG2  | 1.78                     | 0.48              |
| 1:A:199:ILE:HG22 | 1:A:200:PRO:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:227:PHE:HD2  | 1:A:273:VAL:HG21 | 1.79                     | 0.47              |
| 1:B:328:PHE:C    | 1:B:367:VAL:HG11 | 2.39                     | 0.47              |
| 1:C:283:ILE:O    | 1:C:286:LEU:N    | 2.34                     | 0.47              |
| 1:C:297:TYR:C    | 1:C:299:ARG:H    | 2.22                     | 0.47              |
| 1:C:309:PRO:HG3  | 1:C:311:ARG:HH11 | 1.79                     | 0.47              |
| 1:C:330:ARG:O    | 1:C:333:ALA:N    | 2.43                     | 0.47              |
| 1:D:292:PHE:HD2  | 1:D:293:ARG:O    | 1.97                     | 0.47              |
| 1:D:321:ALA:HA   | 1:D:363:ILE:HD12 | 1.96                     | 0.47              |
| 1:D:344:GLN:O    | 1:D:347:LEU:HB2  | 2.14                     | 0.47              |
| 1:F:156:ILE:O    | 1:F:157:SER:C    | 2.56                     | 0.47              |
| 1:F:224:GLU:O    | 1:F:228:GLU:HB2  | 2.13                     | 0.47              |
| 1:F:358:GLU:O    | 1:F:362:VAL:HG23 | 2.14                     | 0.47              |
| 1:H:141:PHE:O    | 1:H:142:GLU:HG3  | 2.14                     | 0.47              |
| 1:H:346:LEU:HD12 | 1:H:377:ARG:NE   | 2.29                     | 0.47              |
| 1:I:165:ILE:HB   | 1:I:278:ALA:CB   | 2.42                     | 0.47              |
| 1:J:322:ASN:O    | 1:J:323:HIS:C    | 2.56                     | 0.47              |
| 1:J:364:GLU:O    | 1:J:365:ARG:C    | 2.57                     | 0.47              |
| 1:K:149:ILE:HD13 | 1:K:307:ILE:HD13 | 1.96                     | 0.47              |
| 1:K:325:LEU:HD23 | 1:K:325:LEU:C    | 2.39                     | 0.47              |
| 1:L:165:ILE:H    | 1:L:278:ALA:CB   | 2.19                     | 0.47              |
| 1:M:146:MET:HE2  | 1:M:146:MET:CA   | 2.41                     | 0.47              |
| 1:M:316:ASP:O    | 1:M:319:PRO:HD2  | 2.14                     | 0.47              |
| 1:N:252:LEU:O    | 1:N:253:ARG:C    | 2.57                     | 0.47              |
| 1:N:282:ASN:ND2  | 1:N:284:LYS:HB2  | 2.29                     | 0.47              |
| 1:A:208:LEU:HD22 | 1:A:209:PHE:CZ   | 2.49                     | 0.47              |
| 1:B:179:LEU:O    | 1:B:180:ILE:C    | 2.57                     | 0.47              |
| 1:B:181:HIS:CE1  | 1:B:191:PHE:HB2  | 2.49                     | 0.47              |
| 1:B:186:ARG:O    | 1:B:188:LYS:N    | 2.47                     | 0.47              |
| 1:B:235:LEU:CD2  | 1:B:237:LEU:HD21 | 2.43                     | 0.47              |
| 1:E:350:TYR:CE2  | 1:E:352:TRP:HA   | 2.49                     | 0.47              |
| 1:G:155:LYS:O    | 1:G:157:SER:N    | 2.47                     | 0.47              |
| 1:G:234:THR:HG22 | 1:G:235:LEU:N    | 2.28                     | 0.47              |
| 1:H:332:TYR:O    | 1:H:332:TYR:CG   | 2.68                     | 0.47              |
| 1:I:165:ILE:CG2  | 1:I:173:LYS:HG2  | 2.41                     | 0.47              |
| 1:I:208:LEU:O    | 1:I:226:PHE:N    | 2.47                     | 0.47              |
| 1:J:263:LEU:HD23 | 1:J:264:GLY:N    | 2.29                     | 0.47              |
| 1:J:325:LEU:HD23 | 1:J:325:LEU:C    | 2.39                     | 0.47              |
| 1:J:325:LEU:O    | 1:J:327:LYS:N    | 2.47                     | 0.47              |
| 1:L:150:LEU:O    | 1:L:150:LEU:HD22 | 2.14                     | 0.47              |
| 1:L:300:LEU:O    | 1:L:302:VAL:N    | 2.47                     | 0.47              |
| 1:N:179:LEU:HD23 | 1:N:183:LEU:HG   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:376:ASP:C    | 1:C:378:GLY:N    | 2.72                     | 0.47              |
| 1:E:244:SER:C    | 1:E:246:GLU:N    | 2.71                     | 0.47              |
| 1:F:193:ALA:CB   | 1:F:236:PHE:HB3  | 2.44                     | 0.47              |
| 1:F:211:TYR:C    | 1:F:212:GLU:HG2  | 2.39                     | 0.47              |
| 1:G:181:HIS:HD2  | 1:G:234:THR:OG1  | 1.97                     | 0.47              |
| 1:H:157:SER:HB3  | 1:H:183:LEU:C    | 2.39                     | 0.47              |
| 1:H:316:ASP:O    | 1:H:320:LEU:HG   | 2.14                     | 0.47              |
| 1:L:318:ILE:O    | 1:L:319:PRO:C    | 2.56                     | 0.47              |
| 1:N:254:VAL:C    | 1:N:256:GLU:N    | 2.70                     | 0.47              |
| 1:D:271:VAL:CG2  | 1:D:273:VAL:HG23 | 2.43                     | 0.47              |
| 1:F:196:VAL:HG22 | 1:F:204:PHE:HZ   | 1.79                     | 0.47              |
| 1:G:155:LYS:C    | 1:G:157:SER:H    | 2.22                     | 0.47              |
| 1:L:362:VAL:HA   | 1:L:365:ARG:HH21 | 1.79                     | 0.47              |
| 1:M:157:SER:C    | 1:M:159:ALA:N    | 2.69                     | 0.47              |
| 1:N:192:VAL:O    | 1:N:235:LEU:HD12 | 2.15                     | 0.47              |
| 1:A:236:PHE:HE1  | 1:A:278:ALA:HB3  | 1.78                     | 0.47              |
| 1:B:174:GLU:HG2  | 1:B:178:ARG:HD3  | 1.96                     | 0.47              |
| 1:C:150:LEU:HG   | 1:C:154:LYS:HZ2  | 1.78                     | 0.47              |
| 1:C:156:ILE:CD1  | 1:C:303:ILE:HG21 | 2.45                     | 0.47              |
| 1:D:263:LEU:HD23 | 1:D:263:LEU:C    | 2.39                     | 0.47              |
| 1:E:227:PHE:O    | 1:E:230:ALA:N    | 2.47                     | 0.47              |
| 1:E:311:ARG:HG2  | 1:E:351:PRO:O    | 2.14                     | 0.47              |
| 1:F:149:ILE:HD13 | 1:F:307:ILE:CD1  | 2.42                     | 0.47              |
| 1:F:323:HIS:C    | 1:F:323:HIS:ND1  | 2.72                     | 0.47              |
| 1:G:209:PHE:CZ   | 1:G:250:LYS:HB3  | 2.50                     | 0.47              |
| 1:H:369:PHE:CD1  | 1:H:369:PHE:N    | 2.82                     | 0.47              |
| 1:I:316:ASP:C    | 1:I:319:PRO:HD2  | 2.39                     | 0.47              |
| 1:J:346:LEU:C    | 1:J:346:LEU:CD2  | 2.88                     | 0.47              |
| 1:K:160:GLU:OE1  | 1:K:160:GLU:O    | 2.32                     | 0.47              |
| 1:K:260:PHE:CD1  | 1:K:260:PHE:C    | 2.93                     | 0.47              |
| 1:K:343:ALA:O    | 1:K:347:LEU:HG   | 2.14                     | 0.47              |
| 1:L:203:ILE:O    | 1:L:206:ALA:HB3  | 2.15                     | 0.47              |
| 1:L:305:ILE:O    | 1:L:305:ILE:HG22 | 2.15                     | 0.47              |
| 1:M:234:THR:CG2  | 1:M:276:LEU:HD23 | 2.45                     | 0.47              |
| 1:C:240:ILE:CD1  | 1:C:243:LEU:HD12 | 2.44                     | 0.47              |
| 1:C:314:LYS:HA   | 1:C:317:ILE:CD1  | 2.45                     | 0.47              |
| 1:C:318:ILE:H    | 1:C:318:ILE:HG12 | 1.43                     | 0.47              |
| 1:F:239:GLU:HA   | 1:F:278:ALA:O    | 2.14                     | 0.47              |
| 1:F:328:PHE:CE1  | 1:F:364:GLU:HB2  | 2.50                     | 0.47              |
| 1:H:248:GLN:O    | 1:H:250:LYS:N    | 2.47                     | 0.47              |
| 1:H:325:LEU:HD23 | 1:H:363:ILE:HG23 | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:324:PHE:O    | 1:K:325:LEU:C    | 2.57                     | 0.47              |
| 1:N:372:GLY:O    | 1:N:374:PHE:N    | 2.47                     | 0.47              |
| 1:A:172:GLY:O    | 1:A:174:GLU:N    | 2.47                     | 0.47              |
| 1:A:350:TYR:HD2  | 1:A:352:TRP:CD2  | 2.33                     | 0.47              |
| 1:B:181:HIS:ND1  | 1:B:191:PHE:HB2  | 2.30                     | 0.47              |
| 1:B:336:VAL:HG13 | 1:B:373:LYS:O    | 2.15                     | 0.47              |
| 1:B:384:VAL:O    | 1:B:384:VAL:HG12 | 2.14                     | 0.47              |
| 1:C:177:ALA:O    | 1:C:180:ILE:N    | 2.47                     | 0.47              |
| 1:C:212:GLU:O    | 1:C:215:ALA:HB2  | 2.13                     | 0.47              |
| 1:C:213:LYS:HG2  | 1:C:214:GLY:N    | 2.29                     | 0.47              |
| 1:C:300:LEU:N    | 1:C:300:LEU:HD23 | 2.30                     | 0.47              |
| 1:D:251:LEU:HD13 | 1:D:296:LEU:HD21 | 1.96                     | 0.47              |
| 1:E:205:GLU:CB   | 1:E:263:LEU:HD11 | 2.45                     | 0.47              |
| 1:E:298:TYR:CE1  | 1:F:354:GLY:HA2  | 2.50                     | 0.47              |
| 1:G:262:ARG:O    | 1:G:263:LEU:HB3  | 2.15                     | 0.47              |
| 1:H:196:VAL:HG22 | 1:H:204:PHE:CZ   | 2.50                     | 0.47              |
| 1:H:204:PHE:O    | 1:H:206:ALA:N    | 2.48                     | 0.47              |
| 1:H:359:LEU:HD23 | 1:H:359:LEU:C    | 2.40                     | 0.47              |
| 1:I:251:LEU:O    | 1:I:252:LEU:C    | 2.58                     | 0.47              |
| 1:I:258:GLY:O    | 1:I:270:GLU:HG3  | 2.14                     | 0.47              |
| 1:K:214:GLY:HA2  | 1:K:219:ALA:O    | 2.15                     | 0.47              |
| 1:K:306:GLU:O    | 1:K:308:PRO:HD3  | 2.15                     | 0.47              |
| 1:K:321:ALA:HA   | 1:K:363:ILE:HD12 | 1.95                     | 0.47              |
| 1:K:321:ALA:HB1  | 1:K:339:PHE:CZ   | 2.49                     | 0.47              |
| 1:L:145:LYS:O    | 1:L:146:MET:C    | 2.58                     | 0.47              |
| 1:L:149:ILE:HG22 | 1:L:150:LEU:N    | 2.28                     | 0.47              |
| 1:L:204:PHE:O    | 1:L:205:GLU:C    | 2.56                     | 0.47              |
| 1:L:299:ARG:O    | 1:L:302:VAL:HG23 | 2.15                     | 0.47              |
| 1:M:209:PHE:CE1  | 1:M:250:LYS:HB3  | 2.50                     | 0.47              |
| 1:M:227:PHE:C    | 1:M:229:LEU:N    | 2.69                     | 0.47              |
| 1:N:251:LEU:HD21 | 1:N:255:ILE:HD11 | 1.95                     | 0.47              |
| 1:N:313:ARG:C    | 1:N:315:GLU:N    | 2.70                     | 0.47              |
| 1:N:378:GLY:C    | 1:N:380:LEU:H    | 2.22                     | 0.47              |
| 1:A:328:PHE:HB2  | 1:A:367:VAL:HG21 | 1.97                     | 0.47              |
| 1:B:229:LEU:C    | 1:B:229:LEU:HD13 | 2.40                     | 0.47              |
| 1:B:339:PHE:CE2  | 1:B:347:LEU:HD11 | 2.50                     | 0.47              |
| 1:D:168:GLU:CD   | 1:D:311:ARG:HH12 | 2.23                     | 0.47              |
| 1:D:368:LEU:C    | 1:D:370:SER:N    | 2.70                     | 0.47              |
| 1:E:157:SER:OG   | 1:E:183:LEU:HB2  | 2.15                     | 0.47              |
| 1:E:262:ARG:O    | 1:E:263:LEU:C    | 2.58                     | 0.47              |
| 1:E:301:GLY:HA2  | 1:E:304:GLU:HG2  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:320:LEU:O    | 1:E:323:HIS:N    | 2.48                     | 0.47              |
| 1:F:179:LEU:HD23 | 1:F:179:LEU:C    | 2.40                     | 0.47              |
| 1:G:173:LYS:C    | 1:G:175:VAL:H    | 2.23                     | 0.47              |
| 1:H:194:LEU:HD21 | 1:H:237:LEU:CD2  | 2.34                     | 0.47              |
| 1:H:328:PHE:HB3  | 1:H:367:VAL:HG11 | 1.96                     | 0.47              |
| 1:J:211:TYR:OH   | 1:J:223:LYS:HD3  | 2.14                     | 0.47              |
| 1:J:280:ASN:OD1  | 1:J:281:ARG:HD3  | 2.15                     | 0.47              |
| 1:K:178:ARG:NE   | 1:K:191:PHE:HE2  | 2.13                     | 0.47              |
| 1:K:213:LYS:CD   | 1:K:220:VAL:O    | 2.52                     | 0.47              |
| 1:C:181:HIS:HD2  | 1:C:191:PHE:CG   | 2.31                     | 0.47              |
| 1:D:157:SER:O    | 1:D:159:ALA:N    | 2.47                     | 0.47              |
| 1:E:251:LEU:O    | 1:E:255:ILE:HG13 | 2.14                     | 0.47              |
| 1:E:325:LEU:HD13 | 1:E:338:GLY:HA2  | 1.96                     | 0.47              |
| 1:F:383:LEU:HB2  | 1:F:384:VAL:H    | 1.59                     | 0.47              |
| 1:G:211:TYR:HB2  | 1:G:223:LYS:HB2  | 1.96                     | 0.47              |
| 1:H:224:GLU:HG3  | 1:H:262:ARG:NH2  | 2.30                     | 0.47              |
| 1:H:246:GLU:O    | 1:H:247:ALA:C    | 2.57                     | 0.47              |
| 1:H:328:PHE:O    | 1:H:332:TYR:HB3  | 2.15                     | 0.47              |
| 1:I:166:THR:HB   | 1:I:306:GLU:OE2  | 2.15                     | 0.47              |
| 1:J:227:PHE:CE2  | 1:J:254:VAL:HG11 | 2.50                     | 0.47              |
| 1:K:200:PRO:HG2  | 1:K:203:ILE:HG13 | 1.97                     | 0.47              |
| 1:M:246:GLU:C    | 1:M:249:ALA:HB3  | 2.38                     | 0.47              |
| 1:M:275:ILE:H    | 1:M:275:ILE:HD12 | 1.80                     | 0.47              |
| 1:N:245:LEU:O    | 1:N:246:GLU:C    | 2.58                     | 0.47              |
| 1:A:180:ILE:O    | 1:A:180:ILE:CG2  | 2.63                     | 0.47              |
| 1:B:149:ILE:O    | 1:B:153:ILE:HG12 | 2.15                     | 0.47              |
| 1:C:303:ILE:CD1  | 1:D:365:ARG:HG3  | 2.45                     | 0.47              |
| 1:D:213:LYS:C    | 1:D:215:ALA:H    | 2.23                     | 0.47              |
| 1:D:237:LEU:HD23 | 1:D:237:LEU:N    | 2.30                     | 0.47              |
| 1:E:164:LEU:C    | 1:E:164:LEU:HD12 | 2.40                     | 0.47              |
| 1:E:243:LEU:HB3  | 1:E:248:GLN:HG3  | 1.97                     | 0.47              |
| 1:F:174:GLU:OE2  | 1:F:178:ARG:NH1  | 2.35                     | 0.47              |
| 1:F:380:LEU:HD23 | 1:F:380:LEU:H    | 1.79                     | 0.47              |
| 1:G:224:GLU:HA   | 1:G:262:ARG:NH1  | 2.30                     | 0.47              |
| 1:G:240:ILE:O    | 1:G:242:GLU:N    | 2.48                     | 0.47              |
| 1:G:244:SER:O    | 1:G:248:GLN:HG3  | 2.15                     | 0.47              |
| 1:H:196:VAL:HG12 | 1:H:242:GLU:HB3  | 1.97                     | 0.47              |
| 1:I:192:VAL:HG21 | 1:I:230:ALA:HB2  | 1.96                     | 0.47              |
| 1:I:229:LEU:C    | 1:I:231:ASP:H    | 2.23                     | 0.47              |
| 1:I:283:ILE:HG21 | 1:I:297:TYR:HD1  | 1.80                     | 0.47              |
| 1:J:365:ARG:HD2  | 1:J:383:LEU:HD13 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:176:VAL:HG21 | 1:K:307:ILE:CD1  | 2.45                     | 0.47              |
| 1:K:209:PHE:CZ   | 1:K:250:LYS:HB3  | 2.50                     | 0.47              |
| 1:M:206:ALA:HB2  | 1:M:216:PHE:HZ   | 1.80                     | 0.47              |
| 1:A:377:ARG:NE   | 1:L:285:GLU:OE1  | 2.48                     | 0.46              |
| 1:B:150:LEU:O    | 1:B:154:LYS:HG3  | 2.15                     | 0.46              |
| 1:B:204:PHE:O    | 1:B:207:GLU:N    | 2.47                     | 0.46              |
| 1:B:283:ILE:HG21 | 1:B:297:TYR:CD1  | 2.50                     | 0.46              |
| 1:B:328:PHE:HD1  | 1:B:363:ILE:HG22 | 1.81                     | 0.46              |
| 1:C:165:ILE:O    | 1:C:278:ALA:HB1  | 2.16                     | 0.46              |
| 1:C:194:LEU:HD22 | 1:C:235:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:284:LYS:HG3  | 1:C:285:GLU:H    | 1.80                     | 0.46              |
| 1:D:235:LEU:CD1  | 1:D:237:LEU:HD23 | 2.38                     | 0.46              |
| 1:D:252:LEU:HA   | 1:D:255:ILE:HD12 | 1.96                     | 0.46              |
| 1:E:320:LEU:C    | 1:E:322:ASN:H    | 2.22                     | 0.46              |
| 1:F:376:ASP:C    | 1:F:378:GLY:N    | 2.73                     | 0.46              |
| 1:G:181:HIS:ND1  | 1:G:181:HIS:O    | 2.47                     | 0.46              |
| 1:G:251:LEU:HD22 | 1:G:255:ILE:HG13 | 1.96                     | 0.46              |
| 1:G:318:ILE:CB   | 1:G:319:PRO:HD3  | 2.44                     | 0.46              |
| 1:G:352:TRP:CZ3  | 1:G:359:LEU:HA   | 2.49                     | 0.46              |
| 1:H:216:PHE:O    | 1:H:216:PHE:CD2  | 2.68                     | 0.46              |
| 1:L:156:ILE:O    | 1:L:157:SER:C    | 2.58                     | 0.46              |
| 1:L:334:LYS:HZ3  | 1:L:367:VAL:HG11 | 1.76                     | 0.46              |
| 1:M:353:TYR:O    | 1:M:355:ASN:ND2  | 2.48                     | 0.46              |
| 1:N:194:LEU:HD22 | 1:N:235:LEU:HD11 | 1.97                     | 0.46              |
| 1:N:265:GLY:C    | 1:N:266:ARG:HE   | 2.23                     | 0.46              |
| 1:D:184:SER:C    | 1:D:186:ARG:H    | 2.23                     | 0.46              |
| 1:E:226:PHE:O    | 1:E:229:LEU:HB3  | 2.16                     | 0.46              |
| 1:H:309:PRO:CB   | 1:H:311:ARG:HD2  | 2.45                     | 0.46              |
| 1:H:377:ARG:O    | 1:H:381:SER:OG   | 2.30                     | 0.46              |
| 1:I:288:LYS:C    | 1:I:290:GLY:N    | 2.71                     | 0.46              |
| 1:K:226:PHE:O    | 1:K:227:PHE:C    | 2.58                     | 0.46              |
| 1:K:288:LYS:O    | 1:K:289:GLU:C    | 2.59                     | 0.46              |
| 1:K:303:ILE:HD11 | 1:L:368:LEU:CD1  | 2.44                     | 0.46              |
| 1:L:161:CYS:HB2  | 1:L:162:PRO:HD2  | 1.97                     | 0.46              |
| 1:L:244:SER:O    | 1:L:246:GLU:N    | 2.48                     | 0.46              |
| 1:L:340:THR:O    | 1:L:344:GLN:HB2  | 2.16                     | 0.46              |
| 1:L:355:ASN:O    | 1:L:356:VAL:C    | 2.58                     | 0.46              |
| 1:M:156:ILE:HD11 | 1:M:303:ILE:HD12 | 1.96                     | 0.46              |
| 1:M:314:LYS:HA   | 1:M:317:ILE:HG13 | 1.98                     | 0.46              |
| 1:N:283:ILE:HG21 | 1:N:297:TYR:CD1  | 2.51                     | 0.46              |
| 1:N:292:PHE:O    | 1:N:293:ARG:C    | 2.58                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:372:GLY:O    | 1:N:373:LYS:C    | 2.58                     | 0.46              |
| 1:A:152:LYS:O    | 1:A:156:ILE:HG12 | 2.15                     | 0.46              |
| 1:B:267:LYS:N    | 1:B:267:LYS:HD2  | 2.31                     | 0.46              |
| 1:C:163:VAL:HG22 | 1:C:303:ILE:HB   | 1.97                     | 0.46              |
| 1:C:293:ARG:HE   | 1:C:293:ARG:HB3  | 1.39                     | 0.46              |
| 1:C:376:ASP:C    | 1:C:376:ASP:OD2  | 2.58                     | 0.46              |
| 1:D:299:ARG:HE   | 1:D:299:ARG:C    | 2.23                     | 0.46              |
| 1:F:138:GLU:CG   | 1:F:139:TYR:N    | 2.78                     | 0.46              |
| 1:G:381:SER:C    | 1:G:383:LEU:N    | 2.73                     | 0.46              |
| 1:H:227:PHE:HD1  | 1:H:235:LEU:CD1  | 2.28                     | 0.46              |
| 1:I:208:LEU:HD23 | 1:I:208:LEU:O    | 2.15                     | 0.46              |
| 1:I:252:LEU:CD2  | 1:I:295:ASP:HB2  | 2.45                     | 0.46              |
| 1:J:269:ILE:H    | 1:J:269:ILE:CD1  | 2.28                     | 0.46              |
| 1:J:279:THR:HG21 | 1:J:283:ILE:HD11 | 1.97                     | 0.46              |
| 1:J:318:ILE:CG1  | 1:J:319:PRO:HD3  | 2.36                     | 0.46              |
| 1:L:195:ASN:C    | 1:L:197:ALA:N    | 2.73                     | 0.46              |
| 1:L:240:ILE:CD1  | 1:L:300:LEU:HD13 | 2.45                     | 0.46              |
| 1:L:302:VAL:O    | 1:L:303:ILE:HD12 | 2.16                     | 0.46              |
| 1:M:140:VAL:C    | 1:M:141:PHE:CD1  | 2.90                     | 0.46              |
| 1:M:324:PHE:CD1  | 1:M:360:LYS:HA   | 2.50                     | 0.46              |
| 1:N:189:GLU:HB3  | 1:N:233:GLY:HA2  | 1.97                     | 0.46              |
| 1:A:325:LEU:CD1  | 1:A:339:PHE:CE1  | 2.99                     | 0.46              |
| 1:B:239:GLU:C    | 1:B:241:GLY:N    | 2.74                     | 0.46              |
| 1:C:204:PHE:O    | 1:C:207:GLU:N    | 2.49                     | 0.46              |
| 1:C:256:GLU:HG2  | 1:C:299:ARG:CZ   | 2.45                     | 0.46              |
| 1:C:273:VAL:O    | 1:C:275:ILE:HD12 | 2.16                     | 0.46              |
| 1:D:156:ILE:O    | 1:D:157:SER:C    | 2.59                     | 0.46              |
| 1:E:150:LEU:HD12 | 1:E:150:LEU:C    | 2.37                     | 0.46              |
| 1:E:213:LYS:HE3  | 1:E:221:SER:HA   | 1.98                     | 0.46              |
| 1:F:225:GLY:O    | 1:F:227:PHE:N    | 2.49                     | 0.46              |
| 1:F:250:LYS:O    | 1:F:254:VAL:HG23 | 2.14                     | 0.46              |
| 1:G:171:VAL:HG12 | 1:G:313:ARG:NH1  | 2.31                     | 0.46              |
| 1:G:242:GLU:HG2  | 1:G:281:ARG:HH21 | 1.80                     | 0.46              |
| 1:J:143:SER:HB3  | 1:J:316:ASP:OD2  | 2.15                     | 0.46              |
| 1:J:302:VAL:C    | 1:J:303:ILE:HD13 | 2.40                     | 0.46              |
| 1:K:248:GLN:O    | 1:K:251:LEU:N    | 2.49                     | 0.46              |
| 1:K:298:TYR:C    | 1:K:300:LEU:H    | 2.23                     | 0.46              |
| 1:K:336:VAL:HA   | 1:K:373:LYS:O    | 2.15                     | 0.46              |
| 1:A:313:ARG:O    | 1:A:316:ASP:N    | 2.39                     | 0.46              |
| 1:B:229:LEU:HD13 | 1:B:229:LEU:O    | 2.15                     | 0.46              |
| 1:C:184:SER:O    | 1:C:186:ARG:N    | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:342:SER:OG   | 1:C:377:ARG:HB2  | 2.16                     | 0.46              |
| 1:C:358:GLU:O    | 1:C:362:VAL:HG23 | 2.16                     | 0.46              |
| 1:E:153:ILE:HD12 | 1:E:180:ILE:HG13 | 1.97                     | 0.46              |
| 1:F:159:ALA:C    | 1:F:160:GLU:HG3  | 2.40                     | 0.46              |
| 1:I:266:ARG:NH2  | 1:J:203:ILE:HD11 | 2.31                     | 0.46              |
| 1:K:199:ILE:O    | 1:K:200:PRO:C    | 2.57                     | 0.46              |
| 1:K:209:PHE:CE2  | 1:K:250:LYS:HB3  | 2.51                     | 0.46              |
| 1:K:238:ASP:OD1  | 1:K:238:ASP:C    | 2.59                     | 0.46              |
| 1:L:281:ARG:HH21 | 1:L:285:GLU:HG2  | 1.80                     | 0.46              |
| 1:L:318:ILE:HG13 | 1:L:319:PRO:CD   | 2.46                     | 0.46              |
| 1:L:346:LEU:O    | 1:L:347:LEU:O    | 2.33                     | 0.46              |
| 1:L:352:TRP:HZ3  | 1:L:358:GLU:HG2  | 1.79                     | 0.46              |
| 1:M:359:LEU:HG   | 1:M:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:M:365:ARG:HG2  | 1:M:383:LEU:HD22 | 1.98                     | 0.46              |
| 1:M:369:PHE:O    | 1:M:370:SER:C    | 2.59                     | 0.46              |
| 1:N:145:LYS:O    | 1:N:149:ILE:HG13 | 2.16                     | 0.46              |
| 1:N:235:LEU:HD12 | 1:N:236:PHE:H    | 1.81                     | 0.46              |
| 1:A:299:ARG:NH2  | 1:A:302:VAL:HG21 | 2.29                     | 0.46              |
| 1:A:356:VAL:HG11 | 2:A:6:ADP:C8     | 2.50                     | 0.46              |
| 1:B:382:CYS:HB3  | 1:B:383:LEU:HD22 | 1.98                     | 0.46              |
| 1:C:165:ILE:HB   | 1:C:278:ALA:CB   | 2.44                     | 0.46              |
| 1:D:226:PHE:O    | 1:D:230:ALA:N    | 2.38                     | 0.46              |
| 1:D:361:ASN:O    | 1:D:364:GLU:N    | 2.49                     | 0.46              |
| 1:E:171:VAL:HG23 | 1:E:307:ILE:HG21 | 1.97                     | 0.46              |
| 1:F:310:LEU:HD23 | 1:F:310:LEU:HA   | 1.64                     | 0.46              |
| 1:G:205:GLU:HG2  | 1:G:247:ALA:HB2  | 1.97                     | 0.46              |
| 1:K:139:TYR:HB3  | 1:K:140:VAL:H    | 1.44                     | 0.46              |
| 1:L:246:GLU:O    | 1:L:249:ALA:N    | 2.49                     | 0.46              |
| 1:M:189:GLU:CG   | 1:M:190:PRO:HD2  | 2.42                     | 0.46              |
| 1:N:235:LEU:HD12 | 1:N:235:LEU:C    | 2.40                     | 0.46              |
| 1:N:254:VAL:HG22 | 1:N:260:PHE:HB3  | 1.97                     | 0.46              |
| 1:A:178:ARG:NE   | 1:A:191:PHE:CE2  | 2.82                     | 0.46              |
| 1:A:248:GLN:O    | 1:A:249:ALA:C    | 2.58                     | 0.46              |
| 1:A:308:PRO:HG2  | 1:A:313:ARG:HD2  | 1.98                     | 0.46              |
| 1:B:244:SER:C    | 1:B:246:GLU:H    | 2.24                     | 0.46              |
| 1:D:365:ARG:HD2  | 1:D:383:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:171:VAL:CG2  | 1:E:307:ILE:CG2  | 2.94                     | 0.46              |
| 1:E:259:LYS:HD3  | 1:E:268:GLU:OE1  | 2.15                     | 0.46              |
| 1:E:336:VAL:HG21 | 1:E:370:SER:HB2  | 1.98                     | 0.46              |
| 1:G:251:LEU:HD22 | 1:G:255:ILE:CG1  | 2.45                     | 0.46              |
| 1:G:334:LYS:HB3  | 1:G:336:VAL:HG23 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:198:SER:CB   | 1:N:250:LYS:HB2  | 2.37                     | 0.46              |
| 1:I:212:GLU:HG3  | 1:I:265:GLY:HA3  | 1.98                     | 0.46              |
| 1:K:223:LYS:HA   | 1:K:223:LYS:HD3  | 1.82                     | 0.46              |
| 1:K:381:SER:C    | 1:K:383:LEU:H    | 2.22                     | 0.46              |
| 1:L:208:LEU:HD22 | 1:L:209:PHE:CG   | 2.51                     | 0.46              |
| 1:L:293:ARG:HH21 | 1:L:295:ASP:CG   | 2.23                     | 0.46              |
| 1:M:149:ILE:HD13 | 1:M:307:ILE:HD13 | 1.97                     | 0.46              |
| 1:M:288:LYS:C    | 1:M:290:GLY:H    | 2.24                     | 0.46              |
| 1:N:152:LYS:HE3  | 1:N:152:LYS:CA   | 2.44                     | 0.46              |
| 1:N:311:ARG:C    | 1:N:312:GLU:HG2  | 2.41                     | 0.46              |
| 1:A:156:ILE:O    | 1:A:157:SER:C    | 2.59                     | 0.46              |
| 1:A:320:LEU:O    | 1:A:321:ALA:C    | 2.59                     | 0.46              |
| 1:C:244:SER:OG   | 1:C:247:ALA:HB2  | 2.16                     | 0.46              |
| 1:E:302:VAL:O    | 1:E:303:ILE:HD13 | 2.16                     | 0.46              |
| 1:E:380:LEU:N    | 1:E:380:LEU:HD23 | 2.29                     | 0.46              |
| 1:F:350:TYR:CD1  | 1:F:351:PRO:HD2  | 2.50                     | 0.46              |
| 1:F:367:VAL:O    | 1:F:367:VAL:HG12 | 2.14                     | 0.46              |
| 1:G:250:LYS:O    | 1:G:254:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:352:TRP:HB3  | 1:G:355:ASN:HA   | 1.97                     | 0.46              |
| 1:H:299:ARG:HH11 | 1:H:302:VAL:HG21 | 1.81                     | 0.46              |
| 1:K:179:LEU:C    | 1:K:181:HIS:N    | 2.73                     | 0.46              |
| 1:K:325:LEU:HD21 | 1:K:336:VAL:CG1  | 2.46                     | 0.46              |
| 1:K:325:LEU:HD12 | 1:K:339:PHE:CZ   | 2.50                     | 0.46              |
| 1:K:365:ARG:HD2  | 1:K:383:LEU:HG   | 1.97                     | 0.46              |
| 1:K:365:ARG:HH11 | 1:K:383:LEU:HG   | 1.81                     | 0.46              |
| 1:L:359:LEU:HD23 | 1:L:359:LEU:C    | 2.41                     | 0.46              |
| 1:M:231:ASP:OD1  | 1:M:271:VAL:HG23 | 2.16                     | 0.46              |
| 1:M:340:THR:C    | 1:M:342:SER:N    | 2.71                     | 0.46              |
| 1:A:165:ILE:HG21 | 1:A:173:LYS:HA   | 1.97                     | 0.46              |
| 1:A:224:GLU:H    | 1:A:224:GLU:CD   | 2.24                     | 0.46              |
| 1:C:325:LEU:C    | 1:C:325:LEU:CD2  | 2.89                     | 0.46              |
| 1:E:145:LYS:O    | 1:E:149:ILE:HG13 | 2.16                     | 0.46              |
| 1:E:177:ALA:CA   | 1:E:180:ILE:CD1  | 2.60                     | 0.46              |
| 1:E:350:TYR:CE1  | 1:E:384:VAL:HG13 | 2.51                     | 0.46              |
| 1:F:153:ILE:HG22 | 1:F:183:LEU:HD12 | 1.96                     | 0.46              |
| 1:F:205:GLU:OE1  | 1:F:250:LYS:HD2  | 2.16                     | 0.46              |
| 1:F:363:ILE:O    | 1:F:366:ALA:HB3  | 2.16                     | 0.46              |
| 1:G:192:VAL:HB   | 1:G:230:ALA:HB2  | 1.98                     | 0.46              |
| 1:G:196:VAL:HG12 | 1:G:196:VAL:O    | 2.14                     | 0.46              |
| 1:G:213:LYS:O    | 1:G:214:GLY:C    | 2.59                     | 0.46              |
| 1:G:275:ILE:CD1  | 1:G:275:ILE:H    | 2.29                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:284:LYS:O    | 1:G:285:GLU:C    | 2.57                     | 0.46              |
| 1:G:307:ILE:H    | 1:G:307:ILE:HG12 | 1.62                     | 0.46              |
| 1:H:317:ILE:HG21 | 1:H:348:LEU:HD23 | 1.97                     | 0.46              |
| 1:H:318:ILE:HG23 | 1:H:339:PHE:CZ   | 2.51                     | 0.46              |
| 1:I:331:LYS:HE2  | 1:I:332:TYR:HE2  | 1.81                     | 0.46              |
| 1:J:322:ASN:O    | 1:J:325:LEU:N    | 2.49                     | 0.46              |
| 1:K:302:VAL:O    | 1:K:302:VAL:CG1  | 2.64                     | 0.46              |
| 1:M:181:HIS:C    | 1:M:183:LEU:N    | 2.72                     | 0.46              |
| 1:D:260:PHE:CD1  | 1:D:260:PHE:C    | 2.94                     | 0.46              |
| 1:E:205:GLU:C    | 1:E:263:LEU:HD11 | 2.41                     | 0.46              |
| 1:E:252:LEU:O    | 1:E:255:ILE:HB   | 2.16                     | 0.46              |
| 1:H:270:GLU:O    | 1:H:271:VAL:CG2  | 2.62                     | 0.46              |
| 1:I:325:LEU:HB2  | 1:I:339:PHE:CZ   | 2.51                     | 0.46              |
| 1:J:162:PRO:HA   | 1:J:275:ILE:O    | 2.16                     | 0.46              |
| 1:J:316:ASP:O    | 1:J:317:ILE:C    | 2.59                     | 0.46              |
| 1:K:249:ALA:HB2  | 1:K:293:ARG:HD2  | 1.96                     | 0.46              |
| 1:K:275:ILE:N    | 1:K:275:ILE:CD1  | 2.76                     | 0.46              |
| 1:L:274:ARG:NH1  | 1:L:276:LEU:HD21 | 2.31                     | 0.46              |
| 1:M:227:PHE:CD2  | 1:M:273:VAL:HG21 | 2.50                     | 0.46              |
| 1:N:181:HIS:CD2  | 1:N:234:THR:CB   | 2.98                     | 0.46              |
| 1:B:178:ARG:NH1  | 1:B:191:PHE:HD2  | 2.14                     | 0.45              |
| 1:C:310:LEU:C    | 1:C:312:GLU:H    | 2.24                     | 0.45              |
| 1:D:249:ALA:O    | 1:D:252:LEU:N    | 2.49                     | 0.45              |
| 1:E:325:LEU:HD11 | 1:E:375:ILE:HD12 | 1.97                     | 0.45              |
| 1:F:196:VAL:HG22 | 1:F:204:PHE:CZ   | 2.52                     | 0.45              |
| 1:G:340:THR:OG1  | 1:G:376:ASP:HA   | 2.16                     | 0.45              |
| 1:H:223:LYS:HZ2  | 1:N:264:GLY:HA3  | 1.82                     | 0.45              |
| 1:H:299:ARG:NH1  | 1:H:302:VAL:HG21 | 2.31                     | 0.45              |
| 1:I:192:VAL:O    | 1:I:235:LEU:HD12 | 2.16                     | 0.45              |
| 1:J:384:VAL:HG23 | 1:J:384:VAL:O    | 2.16                     | 0.45              |
| 1:K:149:ILE:HA   | 1:K:152:LYS:CE   | 2.46                     | 0.45              |
| 1:K:295:ASP:OD1  | 1:K:296:LEU:N    | 2.50                     | 0.45              |
| 1:K:310:LEU:HD21 | 1:K:317:ILE:HG12 | 1.97                     | 0.45              |
| 1:K:356:VAL:O    | 1:K:357:ARG:C    | 2.57                     | 0.45              |
| 1:L:211:TYR:HB3  | 1:L:263:LEU:HB3  | 1.98                     | 0.45              |
| 1:M:343:ALA:O    | 1:M:346:LEU:N    | 2.49                     | 0.45              |
| 1:A:239:GLU:HA   | 1:A:279:THR:HA   | 1.98                     | 0.45              |
| 1:A:250:LYS:O    | 1:A:254:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:312:GLU:O    | 1:A:313:ARG:HG3  | 2.16                     | 0.45              |
| 1:C:153:ILE:CG2  | 1:C:179:LEU:HD22 | 2.42                     | 0.45              |
| 1:E:194:LEU:HD23 | 1:E:194:LEU:H    | 1.80                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:309:PRO:CB   | 1:E:311:ARG:HD3  | 2.40                     | 0.45              |
| 1:E:340:THR:HG21 | 1:E:376:ASP:HB3  | 1.98                     | 0.45              |
| 1:F:140:VAL:HG23 | 1:F:323:HIS:HD2  | 1.82                     | 0.45              |
| 1:F:149:ILE:C    | 1:F:151:GLU:N    | 2.74                     | 0.45              |
| 1:F:191:PHE:CZ   | 1:F:236:PHE:HB2  | 2.51                     | 0.45              |
| 1:G:156:ILE:HG22 | 1:G:156:ILE:O    | 2.16                     | 0.45              |
| 1:G:276:LEU:HA   | 1:G:276:LEU:HD23 | 1.66                     | 0.45              |
| 1:I:282:ASN:HD22 | 1:I:285:GLU:HB2  | 1.81                     | 0.45              |
| 1:I:293:ARG:NH2  | 1:I:295:ASP:OD2  | 2.43                     | 0.45              |
| 1:J:163:VAL:HG22 | 1:J:303:ILE:HB   | 1.98                     | 0.45              |
| 1:J:196:VAL:HB   | 1:J:239:GLU:O    | 2.15                     | 0.45              |
| 1:K:172:GLY:HA2  | 2:K:10:ADP:O1A   | 2.15                     | 0.45              |
| 1:K:248:GLN:C    | 1:K:250:LYS:N    | 2.73                     | 0.45              |
| 1:K:346:LEU:C    | 1:K:349:SER:HG   | 2.23                     | 0.45              |
| 1:L:209:PHE:CE1  | 1:L:250:LYS:HB3  | 2.50                     | 0.45              |
| 1:L:211:TYR:HE1  | 1:L:223:LYS:HB2  | 1.81                     | 0.45              |
| 1:L:296:LEU:O    | 1:L:297:TYR:C    | 2.59                     | 0.45              |
| 1:L:341:LYS:HA   | 1:L:344:GLN:HB2  | 1.97                     | 0.45              |
| 1:M:167:GLY:HA3  | 1:M:171:VAL:HG21 | 1.97                     | 0.45              |
| 1:M:335:GLU:O    | 1:M:336:VAL:CG2  | 2.65                     | 0.45              |
| 1:N:165:ILE:HB   | 1:N:278:ALA:CB   | 2.41                     | 0.45              |
| 1:B:179:LEU:O    | 1:B:182:LYS:N    | 2.50                     | 0.45              |
| 1:D:181:HIS:CE1  | 1:D:187:SER:HA   | 2.52                     | 0.45              |
| 1:D:376:ASP:O    | 1:D:377:ARG:C    | 2.60                     | 0.45              |
| 1:E:164:LEU:CG   | 1:E:164:LEU:O    | 2.64                     | 0.45              |
| 1:E:204:PHE:C    | 1:E:206:ALA:N    | 2.73                     | 0.45              |
| 1:F:230:ALA:O    | 1:F:231:ASP:C    | 2.59                     | 0.45              |
| 1:F:328:PHE:CE2  | 1:F:364:GLU:OE2  | 2.70                     | 0.45              |
| 1:F:349:SER:HB2  | 1:I:351:PRO:HG3  | 1.98                     | 0.45              |
| 1:G:328:PHE:CD2  | 1:G:364:GLU:HG3  | 2.52                     | 0.45              |
| 1:H:208:LEU:HD23 | 1:H:209:PHE:HE1  | 1.76                     | 0.45              |
| 1:H:229:LEU:O    | 1:H:229:LEU:HD22 | 2.15                     | 0.45              |
| 1:I:219:ALA:O    | 1:I:220:VAL:HB   | 2.16                     | 0.45              |
| 1:J:283:ILE:O    | 1:J:287:VAL:HG23 | 2.16                     | 0.45              |
| 1:L:143:SER:HB3  | 1:L:316:ASP:CG   | 2.41                     | 0.45              |
| 1:M:245:LEU:C    | 1:M:247:ALA:N    | 2.72                     | 0.45              |
| 1:N:242:GLU:OE2  | 1:N:281:ARG:NH2  | 2.49                     | 0.45              |
| 1:N:282:ASN:ND2  | 1:N:285:GLU:H    | 2.13                     | 0.45              |
| 1:N:332:TYR:O    | 1:N:333:ALA:C    | 2.58                     | 0.45              |
| 1:A:151:GLU:O    | 1:A:153:ILE:N    | 2.49                     | 0.45              |
| 1:A:325:LEU:C    | 1:A:325:LEU:CD2  | 2.90                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:228:GLU:O    | 1:B:229:LEU:C    | 2.59                     | 0.45              |
| 1:C:266:ARG:NH2  | 1:D:203:ILE:HD11 | 2.32                     | 0.45              |
| 1:D:138:GLU:O    | 1:D:139:TYR:C    | 2.60                     | 0.45              |
| 1:D:200:PRO:O    | 1:D:201:ARG:C    | 2.59                     | 0.45              |
| 1:D:354:GLY:HA3  | 1:D:358:GLU:HB2  | 1.99                     | 0.45              |
| 1:E:213:LYS:HB2  | 1:E:213:LYS:HZ3  | 1.81                     | 0.45              |
| 1:E:363:ILE:O    | 1:E:367:VAL:CG2  | 2.51                     | 0.45              |
| 1:F:332:TYR:CE1  | 1:F:368:LEU:HD11 | 2.52                     | 0.45              |
| 1:F:359:LEU:C    | 1:F:361:ASN:N    | 2.74                     | 0.45              |
| 1:G:324:PHE:O    | 1:G:325:LEU:C    | 2.59                     | 0.45              |
| 1:H:309:PRO:HG3  | 1:H:311:ARG:NH1  | 2.31                     | 0.45              |
| 1:I:194:LEU:HD23 | 1:I:236:PHE:O    | 2.15                     | 0.45              |
| 1:J:325:LEU:C    | 1:J:327:LYS:N    | 2.72                     | 0.45              |
| 1:K:208:LEU:HD13 | 1:K:209:PHE:HE1  | 1.81                     | 0.45              |
| 1:L:165:ILE:C    | 1:L:278:ALA:HB1  | 2.41                     | 0.45              |
| 1:A:157:SER:C    | 1:A:159:ALA:H    | 2.24                     | 0.45              |
| 1:A:167:GLY:O    | 1:A:280:ASN:HA   | 2.16                     | 0.45              |
| 1:C:195:ASN:O    | 1:C:196:VAL:C    | 2.58                     | 0.45              |
| 1:D:194:LEU:HD23 | 1:D:194:LEU:C    | 2.42                     | 0.45              |
| 1:D:211:TYR:CE2  | 1:D:216:PHE:CZ   | 3.04                     | 0.45              |
| 1:E:234:THR:CG2  | 1:E:274:ARG:O    | 2.65                     | 0.45              |
| 1:E:317:ILE:HG21 | 1:E:347:LEU:O    | 2.16                     | 0.45              |
| 1:F:205:GLU:OE2  | 1:F:246:GLU:HB2  | 2.17                     | 0.45              |
| 1:F:366:ALA:C    | 1:F:368:LEU:H    | 2.24                     | 0.45              |
| 1:G:361:ASN:O    | 1:G:362:VAL:C    | 2.60                     | 0.45              |
| 1:H:157:SER:C    | 1:H:159:ALA:H    | 2.24                     | 0.45              |
| 1:H:162:PRO:HB2  | 1:H:300:LEU:CD2  | 2.46                     | 0.45              |
| 1:H:310:LEU:CD1  | 1:H:356:VAL:H    | 2.29                     | 0.45              |
| 1:I:175:VAL:O    | 1:I:176:VAL:C    | 2.59                     | 0.45              |
| 1:I:324:PHE:HB2  | 1:I:363:ILE:HD12 | 1.99                     | 0.45              |
| 1:I:331:LYS:HE2  | 1:I:332:TYR:CE2  | 2.51                     | 0.45              |
| 1:K:189:GLU:CG   | 1:K:232:GLY:O    | 2.64                     | 0.45              |
| 1:L:320:LEU:HB3  | 1:L:324:PHE:HE1  | 1.81                     | 0.45              |
| 1:L:350:TYR:HD2  | 1:L:350:TYR:C    | 2.25                     | 0.45              |
| 1:M:253:ARG:CZ   | 1:M:257:SER:OG   | 2.64                     | 0.45              |
| 1:M:324:PHE:CD2  | 1:M:360:LYS:HG3  | 2.52                     | 0.45              |
| 1:N:227:PHE:HE2  | 1:N:275:ILE:HD11 | 1.82                     | 0.45              |
| 1:N:350:TYR:O    | 1:N:352:TRP:CD1  | 2.69                     | 0.45              |
| 1:N:355:ASN:O    | 1:N:356:VAL:C    | 2.60                     | 0.45              |
| 1:A:144:PRO:C    | 1:A:146:MET:H    | 2.25                     | 0.45              |
| 1:B:368:LEU:C    | 1:B:370:SER:H    | 2.25                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:149:ILE:O    | 1:C:152:LYS:HB2  | 2.16                     | 0.45              |
| 1:C:349:SER:OG   | 1:C:350:TYR:N    | 2.49                     | 0.45              |
| 1:D:211:TYR:CE2  | 1:D:216:PHE:HZ   | 2.34                     | 0.45              |
| 1:E:146:MET:CE   | 1:E:146:MET:HA   | 2.47                     | 0.45              |
| 1:E:236:PHE:CD1  | 1:E:276:LEU:O    | 2.60                     | 0.45              |
| 1:E:252:LEU:O    | 1:E:253:ARG:C    | 2.60                     | 0.45              |
| 1:E:317:ILE:CG2  | 1:E:347:LEU:O    | 2.65                     | 0.45              |
| 1:G:365:ARG:O    | 1:G:367:VAL:N    | 2.50                     | 0.45              |
| 1:H:156:ILE:CG2  | 1:H:274:ARG:HH22 | 2.30                     | 0.45              |
| 1:H:215:ALA:CB   | 1:I:223:LYS:NZ   | 2.76                     | 0.45              |
| 1:H:227:PHE:CE1  | 1:H:235:LEU:HD13 | 2.52                     | 0.45              |
| 1:H:247:ALA:O    | 1:H:250:LYS:N    | 2.49                     | 0.45              |
| 1:H:318:ILE:N    | 1:H:319:PRO:HD2  | 2.32                     | 0.45              |
| 1:H:341:LYS:O    | 1:H:345:GLU:HG3  | 2.17                     | 0.45              |
| 1:I:241:GLY:O    | 1:I:243:LEU:N    | 2.50                     | 0.45              |
| 1:I:382:CYS:O    | 1:I:383:LEU:HD23 | 2.17                     | 0.45              |
| 1:J:361:ASN:O    | 1:J:362:VAL:C    | 2.59                     | 0.45              |
| 1:K:346:LEU:HD13 | 1:K:380:LEU:HB3  | 1.99                     | 0.45              |
| 1:M:281:ARG:HD3  | 1:M:282:ASN:H    | 1.81                     | 0.45              |
| 1:M:332:TYR:CE1  | 1:M:368:LEU:HD23 | 2.52                     | 0.45              |
| 1:B:195:ASN:O    | 1:B:196:VAL:C    | 2.60                     | 0.45              |
| 1:B:235:LEU:HD21 | 1:B:237:LEU:HD21 | 1.99                     | 0.45              |
| 1:B:274:ARG:HG2  | 1:B:274:ARG:HH11 | 1.82                     | 0.45              |
| 1:D:365:ARG:NH1  | 1:D:383:LEU:HD22 | 2.31                     | 0.45              |
| 1:E:146:MET:SD   | 1:E:149:ILE:HD12 | 2.57                     | 0.45              |
| 1:E:244:SER:O    | 1:E:247:ALA:N    | 2.49                     | 0.45              |
| 1:E:325:LEU:CD1  | 1:E:375:ILE:HD12 | 2.46                     | 0.45              |
| 1:F:327:LYS:O    | 1:F:329:SER:N    | 2.49                     | 0.45              |
| 1:F:380:LEU:HB3  | 1:F:384:VAL:CG2  | 2.46                     | 0.45              |
| 1:G:156:ILE:O    | 1:G:157:SER:C    | 2.59                     | 0.45              |
| 1:G:259:LYS:HD3  | 1:G:267:LYS:HD2  | 1.98                     | 0.45              |
| 1:G:352:TRP:CZ2  | 1:G:359:LEU:HG   | 2.51                     | 0.45              |
| 1:H:330:ARG:C    | 1:H:332:TYR:H    | 2.25                     | 0.45              |
| 1:J:146:MET:O    | 1:J:149:ILE:N    | 2.50                     | 0.45              |
| 1:J:344:GLN:O    | 1:J:347:LEU:N    | 2.50                     | 0.45              |
| 1:K:199:ILE:HD13 | 1:K:207:GLU:HG2  | 1.98                     | 0.45              |
| 1:K:309:PRO:HB2  | 1:K:311:ARG:HG2  | 1.99                     | 0.45              |
| 1:L:189:GLU:CG   | 1:L:190:PRO:HD2  | 2.37                     | 0.45              |
| 1:M:164:LEU:HD12 | 1:M:165:ILE:H    | 1.82                     | 0.45              |
| 1:M:275:ILE:O    | 1:M:276:LEU:HD22 | 2.17                     | 0.45              |
| 1:N:179:LEU:C    | 1:N:181:HIS:N    | 2.73                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:ARG:C    | 1:A:315:GLU:N    | 2.72                     | 0.45              |
| 1:A:380:LEU:HD12 | 1:A:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:B:302:VAL:HG22 | 1:C:361:ASN:HB3  | 1.99                     | 0.45              |
| 1:B:325:LEU:HD21 | 1:B:336:VAL:HG12 | 1.99                     | 0.45              |
| 1:B:330:ARG:NH1  | 1:B:330:ARG:O    | 2.50                     | 0.45              |
| 1:C:301:GLY:O    | 1:C:302:VAL:C    | 2.59                     | 0.45              |
| 1:D:159:ALA:HB2  | 1:E:368:LEU:HD21 | 1.99                     | 0.45              |
| 1:D:234:THR:HG21 | 1:D:276:LEU:HD12 | 1.99                     | 0.45              |
| 1:D:287:VAL:HG13 | 1:D:292:PHE:O    | 2.17                     | 0.45              |
| 1:D:296:LEU:C    | 1:D:296:LEU:HD13 | 2.41                     | 0.45              |
| 1:E:171:VAL:HG23 | 1:E:307:ILE:CG2  | 2.47                     | 0.45              |
| 1:F:204:PHE:O    | 1:F:205:GLU:C    | 2.60                     | 0.45              |
| 1:F:215:ALA:O    | 1:G:216:PHE:HE1  | 2.00                     | 0.45              |
| 1:F:267:LYS:O    | 1:F:269:ILE:HD12 | 2.17                     | 0.45              |
| 1:H:239:GLU:HA   | 1:H:279:THR:HA   | 1.98                     | 0.45              |
| 1:H:280:ASN:O    | 1:H:280:ASN:CG   | 2.60                     | 0.45              |
| 1:I:240:ILE:O    | 1:I:241:GLY:C    | 2.58                     | 0.45              |
| 1:L:143:SER:N    | 1:L:316:ASP:OD1  | 2.49                     | 0.45              |
| 1:M:139:TYR:HB3  | 2:M:12:ADP:C2    | 2.50                     | 0.45              |
| 1:M:152:LYS:O    | 1:M:153:ILE:C    | 2.60                     | 0.45              |
| 1:M:309:PRO:HG2  | 1:M:311:ARG:HD2  | 1.98                     | 0.45              |
| 1:M:329:SER:O    | 1:M:330:ARG:HD3  | 2.16                     | 0.45              |
| 1:N:260:PHE:C    | 1:N:260:PHE:HD1  | 2.25                     | 0.45              |
| 1:A:239:GLU:O    | 1:A:240:ILE:C    | 2.60                     | 0.45              |
| 1:A:339:PHE:HZ   | 1:A:363:ILE:HD13 | 1.81                     | 0.45              |
| 1:B:375:ILE:HG22 | 1:B:380:LEU:HD23 | 1.99                     | 0.45              |
| 1:C:152:LYS:C    | 1:C:154:LYS:N    | 2.75                     | 0.45              |
| 1:C:240:ILE:O    | 1:C:243:LEU:HB2  | 2.16                     | 0.45              |
| 1:C:373:LYS:C    | 1:C:374:PHE:CD1  | 2.95                     | 0.45              |
| 1:D:141:PHE:CE1  | 1:D:179:LEU:HD12 | 2.50                     | 0.45              |
| 1:E:204:PHE:O    | 1:E:206:ALA:N    | 2.49                     | 0.45              |
| 1:G:204:PHE:CE2  | 1:G:243:LEU:HD21 | 2.52                     | 0.45              |
| 1:G:352:TRP:HE3  | 1:G:358:GLU:HB3  | 1.82                     | 0.45              |
| 1:I:251:LEU:C    | 1:I:253:ARG:N    | 2.75                     | 0.45              |
| 1:J:321:ALA:O    | 1:J:322:ASN:C    | 2.60                     | 0.45              |
| 1:L:227:PHE:CD2  | 1:L:254:VAL:HG11 | 2.48                     | 0.45              |
| 1:M:206:ALA:CB   | 1:M:216:PHE:CE1  | 3.00                     | 0.45              |
| 1:M:248:GLN:O    | 1:M:249:ALA:C    | 2.59                     | 0.45              |
| 1:N:181:HIS:HD2  | 1:N:234:THR:OG1  | 2.00                     | 0.45              |
| 1:A:376:ASP:C    | 1:A:378:GLY:N    | 2.73                     | 0.45              |
| 1:D:143:SER:O    | 1:D:147:LYS:HB2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:267:LYS:HD2  | 1:D:267:LYS:N    | 2.31                     | 0.45              |
| 1:D:325:LEU:O    | 1:D:326:LYS:C    | 2.60                     | 0.45              |
| 1:F:314:LYS:O    | 1:F:316:ASP:N    | 2.50                     | 0.45              |
| 1:H:176:VAL:O    | 1:H:180:ILE:HG13 | 2.17                     | 0.45              |
| 1:H:231:ASP:HA   | 1:H:273:VAL:CG2  | 2.46                     | 0.45              |
| 1:H:236:PHE:CD1  | 1:H:276:LEU:O    | 2.68                     | 0.45              |
| 1:H:244:SER:O    | 1:H:248:GLN:HG3  | 2.17                     | 0.45              |
| 1:I:153:ILE:CD1  | 1:I:176:VAL:HG13 | 2.45                     | 0.45              |
| 1:J:182:LYS:O    | 1:J:183:LEU:HD23 | 2.16                     | 0.45              |
| 1:J:259:LYS:HD3  | 1:J:268:GLU:OE1  | 2.17                     | 0.45              |
| 1:K:345:GLU:O    | 1:K:348:LEU:N    | 2.50                     | 0.45              |
| 1:L:244:SER:C    | 1:L:246:GLU:N    | 2.72                     | 0.45              |
| 1:N:224:GLU:HA   | 1:N:262:ARG:NH2  | 2.32                     | 0.45              |
| 1:B:159:ALA:O    | 1:B:160:GLU:HG2  | 2.17                     | 0.44              |
| 1:C:140:VAL:HG21 | 1:C:320:LEU:HD23 | 1.99                     | 0.44              |
| 1:D:168:GLU:OE1  | 1:D:311:ARG:NH1  | 2.50                     | 0.44              |
| 1:D:189:GLU:HG2  | 1:D:232:GLY:O    | 2.17                     | 0.44              |
| 1:D:318:ILE:HG23 | 1:D:348:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:352:TRP:CZ3  | 1:D:359:LEU:HA   | 2.52                     | 0.44              |
| 1:E:182:LYS:O    | 1:E:183:LEU:HD23 | 2.17                     | 0.44              |
| 1:E:361:ASN:ND2  | 1:E:361:ASN:H    | 2.14                     | 0.44              |
| 1:F:232:GLY:N    | 1:F:272:ASN:O    | 2.46                     | 0.44              |
| 1:F:365:ARG:HB3  | 1:F:383:LEU:HD11 | 2.00                     | 0.44              |
| 1:G:146:MET:C    | 1:G:148:GLU:N    | 2.68                     | 0.44              |
| 1:H:303:ILE:HG22 | 1:H:303:ILE:O    | 2.16                     | 0.44              |
| 1:I:325:LEU:HD12 | 1:I:339:PHE:CZ   | 2.53                     | 0.44              |
| 1:J:332:TYR:CD1  | 1:J:368:LEU:HD21 | 2.52                     | 0.44              |
| 1:K:345:GLU:O    | 1:K:346:LEU:C    | 2.59                     | 0.44              |
| 1:L:146:MET:HE2  | 1:L:313:ARG:CZ   | 2.47                     | 0.44              |
| 1:L:281:ARG:HH21 | 1:L:285:GLU:CG   | 2.30                     | 0.44              |
| 1:M:140:VAL:O    | 2:M:12:ADP:N6    | 2.48                     | 0.44              |
| 1:M:308:PRO:O    | 1:M:313:ARG:HD2  | 2.16                     | 0.44              |
| 1:N:192:VAL:CB   | 1:N:230:ALA:HB2  | 2.46                     | 0.44              |
| 1:B:179:LEU:C    | 1:B:181:HIS:N    | 2.74                     | 0.44              |
| 1:B:227:PHE:O    | 1:B:228:GLU:C    | 2.60                     | 0.44              |
| 1:B:296:LEU:HD13 | 1:B:296:LEU:O    | 2.17                     | 0.44              |
| 1:D:223:LYS:HG3  | 1:D:224:GLU:N    | 2.31                     | 0.44              |
| 1:F:249:ALA:CB   | 1:F:293:ARG:HH11 | 2.30                     | 0.44              |
| 1:G:207:GLU:HG2  | 1:G:226:PHE:HE1  | 1.80                     | 0.44              |
| 1:H:175:VAL:HG21 | 2:H:14:ADP:C8    | 2.52                     | 0.44              |
| 1:I:173:LYS:H    | 2:I:8:ADP:PB     | 2.40                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:191:PHE:CE2  | 1:I:193:ALA:HB2  | 2.52                     | 0.44              |
| 1:K:242:GLU:OE2  | 1:K:281:ARG:NH2  | 2.50                     | 0.44              |
| 1:K:269:ILE:N    | 1:K:269:ILE:CD1  | 2.78                     | 0.44              |
| 1:K:342:SER:OG   | 1:K:377:ARG:HD3  | 2.17                     | 0.44              |
| 1:L:152:LYS:C    | 1:L:154:LYS:H    | 2.24                     | 0.44              |
| 1:L:306:GLU:O    | 1:L:307:ILE:HD13 | 2.17                     | 0.44              |
| 1:L:328:PHE:CE2  | 1:L:364:GLU:CD   | 2.96                     | 0.44              |
| 1:N:288:LYS:C    | 1:N:290:GLY:H    | 2.26                     | 0.44              |
| 1:A:143:SER:CB   | 1:A:144:PRO:CD   | 2.93                     | 0.44              |
| 1:A:170:GLY:O    | 1:A:356:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:179:LEU:O    | 1:A:181:HIS:N    | 2.50                     | 0.44              |
| 1:A:182:LYS:O    | 1:A:187:SER:HB3  | 2.17                     | 0.44              |
| 1:A:352:TRP:HZ3  | 1:A:362:VAL:HG21 | 1.82                     | 0.44              |
| 1:B:242:GLU:OE1  | 1:B:242:GLU:HA   | 2.18                     | 0.44              |
| 1:B:260:PHE:HD1  | 1:B:261:TYR:N    | 2.15                     | 0.44              |
| 1:C:254:VAL:O    | 1:C:258:GLY:HA2  | 2.17                     | 0.44              |
| 1:F:311:ARG:NH1  | 1:F:311:ARG:CG   | 2.78                     | 0.44              |
| 1:G:239:GLU:N    | 1:G:278:ALA:O    | 2.50                     | 0.44              |
| 1:H:217:THR:C    | 1:H:219:ALA:H    | 2.25                     | 0.44              |
| 1:H:257:SER:O    | 1:H:259:LYS:HG3  | 2.17                     | 0.44              |
| 1:I:253:ARG:CZ   | 1:J:198:SER:CB   | 2.95                     | 0.44              |
| 1:I:284:LYS:HE2  | 1:I:297:TYR:CZ   | 2.53                     | 0.44              |
| 1:J:239:GLU:CD   | 1:J:281:ARG:HH21 | 2.24                     | 0.44              |
| 1:J:325:LEU:O    | 1:J:326:LYS:C    | 2.60                     | 0.44              |
| 1:J:326:LYS:O    | 1:J:326:LYS:HG2  | 2.16                     | 0.44              |
| 1:K:292:PHE:C    | 1:K:292:PHE:CD2  | 2.95                     | 0.44              |
| 1:L:143:SER:CB   | 1:L:144:PRO:CD   | 2.75                     | 0.44              |
| 1:L:340:THR:OG1  | 1:L:376:ASP:HB3  | 2.16                     | 0.44              |
| 1:M:141:PHE:O    | 1:M:143:SER:N    | 2.51                     | 0.44              |
| 1:A:296:LEU:HD13 | 1:A:296:LEU:O    | 2.17                     | 0.44              |
| 1:A:365:ARG:NH2  | 1:G:301:GLY:O    | 2.50                     | 0.44              |
| 1:B:244:SER:C    | 1:B:246:GLU:N    | 2.74                     | 0.44              |
| 1:B:284:LYS:O    | 1:B:288:LYS:HG2  | 2.18                     | 0.44              |
| 1:C:191:PHE:HE2  | 1:C:193:ALA:HB2  | 1.78                     | 0.44              |
| 1:C:341:LYS:HA   | 1:C:344:GLN:HB2  | 2.00                     | 0.44              |
| 1:D:153:ILE:HG23 | 1:D:180:ILE:HG12 | 2.00                     | 0.44              |
| 1:E:302:VAL:C    | 1:E:303:ILE:HG12 | 2.42                     | 0.44              |
| 1:E:335:GLU:O    | 1:E:373:LYS:HA   | 2.17                     | 0.44              |
| 1:F:211:TYR:O    | 1:F:212:GLU:HG2  | 2.18                     | 0.44              |
| 1:G:340:THR:HG1  | 1:G:376:ASP:HA   | 1.82                     | 0.44              |
| 1:H:211:TYR:O    | 1:H:222:SER:HA   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:146:MET:HG3  | 1:J:313:ARG:NH2  | 2.33                     | 0.44              |
| 1:J:181:HIS:HD2  | 1:J:234:THR:HB   | 1.83                     | 0.44              |
| 1:J:346:LEU:HD21 | 1:J:384:VAL:HG23 | 1.98                     | 0.44              |
| 1:K:277:ALA:O    | 1:K:278:ALA:HB2  | 2.18                     | 0.44              |
| 1:M:201:ARG:NH2  | 1:M:242:GLU:O    | 2.51                     | 0.44              |
| 1:M:206:ALA:HB2  | 1:M:216:PHE:CE1  | 2.53                     | 0.44              |
| 1:M:238:ASP:O    | 1:M:239:GLU:CB   | 2.65                     | 0.44              |
| 1:B:240:ILE:CG1  | 1:B:277:ALA:HB1  | 2.39                     | 0.44              |
| 1:C:215:ALA:C    | 1:C:217:THR:N    | 2.76                     | 0.44              |
| 1:C:295:ASP:O    | 1:C:296:LEU:C    | 2.60                     | 0.44              |
| 1:D:365:ARG:HH11 | 1:D:383:LEU:HD22 | 1.82                     | 0.44              |
| 1:E:178:ARG:HE   | 1:E:191:PHE:HD2  | 1.66                     | 0.44              |
| 1:E:321:ALA:O    | 1:E:339:PHE:CE1  | 2.71                     | 0.44              |
| 1:F:214:GLY:O    | 1:F:215:ALA:CB   | 2.65                     | 0.44              |
| 1:F:283:ILE:O    | 1:F:284:LYS:C    | 2.60                     | 0.44              |
| 1:F:343:ALA:HB2  | 1:F:377:ARG:N    | 2.33                     | 0.44              |
| 1:G:358:GLU:O    | 1:G:359:LEU:C    | 2.60                     | 0.44              |
| 1:H:223:LYS:NZ   | 1:N:215:ALA:HB2  | 2.32                     | 0.44              |
| 1:H:244:SER:O    | 1:H:246:GLU:N    | 2.50                     | 0.44              |
| 1:H:346:LEU:HD12 | 1:H:377:ARG:CG   | 2.48                     | 0.44              |
| 1:I:216:PHE:O    | 1:I:218:GLY:N    | 2.49                     | 0.44              |
| 1:I:234:THR:HG21 | 1:I:276:LEU:HD12 | 1.99                     | 0.44              |
| 1:I:248:GLN:O    | 1:I:251:LEU:HB3  | 2.18                     | 0.44              |
| 1:I:349:SER:O    | 1:I:350:TYR:C    | 2.60                     | 0.44              |
| 1:J:157:SER:HB3  | 1:J:184:SER:CA   | 2.47                     | 0.44              |
| 1:J:190:PRO:O    | 1:J:233:GLY:HA3  | 2.17                     | 0.44              |
| 1:J:249:ALA:CB   | 1:J:293:ARG:HH11 | 2.31                     | 0.44              |
| 1:J:259:LYS:HA   | 1:J:269:ILE:O    | 2.18                     | 0.44              |
| 1:J:359:LEU:O    | 1:J:362:VAL:HB   | 2.18                     | 0.44              |
| 1:K:140:VAL:HG11 | 1:K:320:LEU:HD23 | 1.99                     | 0.44              |
| 1:L:310:LEU:HD12 | 1:L:352:TRP:HB3  | 1.99                     | 0.44              |
| 1:M:139:TYR:HD1  | 1:M:139:TYR:H    | 1.64                     | 0.44              |
| 1:M:195:ASN:C    | 1:M:197:ALA:H    | 2.25                     | 0.44              |
| 1:M:236:PHE:CE2  | 1:M:238:ASP:HB2  | 2.53                     | 0.44              |
| 1:B:283:ILE:HD13 | 1:B:286:LEU:CD1  | 2.47                     | 0.44              |
| 1:B:328:PHE:CB   | 1:B:367:VAL:HG21 | 2.47                     | 0.44              |
| 1:C:275:ILE:N    | 1:C:275:ILE:CD1  | 2.81                     | 0.44              |
| 1:C:311:ARG:NH2  | 1:C:353:TYR:CD2  | 2.79                     | 0.44              |
| 1:D:156:ILE:O    | 1:D:159:ALA:N    | 2.50                     | 0.44              |
| 1:E:350:TYR:HE2  | 1:E:352:TRP:HA   | 1.82                     | 0.44              |
| 1:F:380:LEU:O    | 1:F:383:LEU:N    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:181:HIS:CD2  | 1:G:234:THR:OG1  | 2.70                     | 0.44              |
| 1:G:236:PHE:HE1  | 1:G:278:ALA:HB2  | 1.82                     | 0.44              |
| 1:H:349:SER:HB2  | 1:H:350:TYR:HD1  | 1.83                     | 0.44              |
| 1:H:373:LYS:O    | 1:H:374:PHE:HB2  | 2.17                     | 0.44              |
| 1:L:193:ALA:CB   | 1:L:236:PHE:HB3  | 2.48                     | 0.44              |
| 1:L:229:LEU:C    | 1:L:229:LEU:CD1  | 2.74                     | 0.44              |
| 1:L:334:LYS:HZ2  | 1:L:367:VAL:CB   | 2.30                     | 0.44              |
| 1:L:355:ASN:O    | 1:L:357:ARG:N    | 2.50                     | 0.44              |
| 1:L:379:GLU:O    | 1:L:381:SER:N    | 2.50                     | 0.44              |
| 1:M:245:LEU:HA   | 1:M:248:GLN:NE2  | 2.32                     | 0.44              |
| 1:M:253:ARG:O    | 1:M:256:GLU:N    | 2.39                     | 0.44              |
| 1:C:165:ILE:O    | 1:C:278:ALA:HA   | 2.17                     | 0.44              |
| 1:C:177:ALA:HA   | 1:C:180:ILE:HD12 | 2.00                     | 0.44              |
| 1:C:191:PHE:HD2  | 1:C:191:PHE:O    | 2.00                     | 0.44              |
| 1:C:340:THR:OG1  | 1:C:342:SER:HB3  | 2.18                     | 0.44              |
| 1:G:310:LEU:HD12 | 1:G:356:VAL:N    | 2.30                     | 0.44              |
| 1:G:355:ASN:N    | 1:G:355:ASN:HD22 | 2.15                     | 0.44              |
| 1:G:380:LEU:O    | 1:G:384:VAL:HG22 | 2.18                     | 0.44              |
| 1:H:332:TYR:O    | 1:H:333:ALA:CB   | 2.66                     | 0.44              |
| 1:H:372:GLY:O    | 1:H:373:LYS:C    | 2.59                     | 0.44              |
| 1:J:220:VAL:O    | 1:J:221:SER:OG   | 2.29                     | 0.44              |
| 1:J:282:ASN:O    | 1:J:286:LEU:HG   | 2.16                     | 0.44              |
| 1:K:313:ARG:C    | 1:K:315:GLU:N    | 2.75                     | 0.44              |
| 1:M:335:GLU:C    | 1:M:336:VAL:HG23 | 2.43                     | 0.44              |
| 1:N:186:ARG:O    | 1:N:189:GLU:N    | 2.51                     | 0.44              |
| 1:A:196:VAL:O    | 1:A:196:VAL:HG12 | 2.17                     | 0.44              |
| 1:A:356:VAL:HG11 | 2:A:6:ADP:C5     | 2.52                     | 0.44              |
| 1:B:149:ILE:C    | 1:B:151:GLU:N    | 2.76                     | 0.44              |
| 1:B:299:ARG:O    | 1:B:302:VAL:HG23 | 2.17                     | 0.44              |
| 1:C:240:ILE:HD13 | 1:C:240:ILE:HA   | 1.77                     | 0.44              |
| 1:C:296:LEU:O    | 1:C:299:ARG:HB2  | 2.17                     | 0.44              |
| 1:C:300:LEU:C    | 1:C:302:VAL:H    | 2.16                     | 0.44              |
| 1:C:316:ASP:O    | 1:C:317:ILE:C    | 2.60                     | 0.44              |
| 1:C:376:ASP:O    | 1:C:377:ARG:C    | 2.60                     | 0.44              |
| 1:F:354:GLY:HA3  | 1:F:358:GLU:HB2  | 2.00                     | 0.44              |
| 1:I:366:ALA:C    | 1:I:368:LEU:N    | 2.75                     | 0.44              |
| 1:K:236:PHE:HD1  | 1:K:276:LEU:O    | 2.00                     | 0.44              |
| 1:K:329:SER:N    | 1:K:367:VAL:HG11 | 2.32                     | 0.44              |
| 1:L:171:VAL:HG21 | 1:L:307:ILE:HB   | 2.00                     | 0.44              |
| 1:L:211:TYR:CE1  | 1:L:223:LYS:HB2  | 2.53                     | 0.44              |
| 1:L:324:PHE:O    | 1:L:328:PHE:CD1  | 2.64                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:253:ARG:O    | 1:M:256:GLU:O    | 2.35                     | 0.44              |
| 1:M:296:LEU:HD11 | 1:M:300:LEU:CD1  | 2.47                     | 0.44              |
| 1:N:139:TYR:HB3  | 1:N:141:PHE:CE1  | 2.52                     | 0.44              |
| 1:N:178:ARG:HG3  | 1:N:178:ARG:NH1  | 2.33                     | 0.44              |
| 1:N:244:SER:O    | 1:N:247:ALA:HB3  | 2.17                     | 0.44              |
| 1:B:184:SER:C    | 1:B:186:ARG:H    | 2.25                     | 0.44              |
| 1:C:318:ILE:HG12 | 1:C:348:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:172:GLY:O    | 1:D:173:LYS:C    | 2.61                     | 0.44              |
| 1:D:178:ARG:HH11 | 1:D:178:ARG:CG   | 2.31                     | 0.44              |
| 1:D:299:ARG:O    | 1:D:302:VAL:HG23 | 2.18                     | 0.44              |
| 1:D:361:ASN:C    | 1:D:363:ILE:N    | 2.76                     | 0.44              |
| 1:E:313:ARG:O    | 1:E:314:LYS:C    | 2.61                     | 0.44              |
| 1:E:341:LYS:HD3  | 1:E:341:LYS:C    | 2.42                     | 0.44              |
| 1:H:203:ILE:O    | 1:H:206:ALA:HB3  | 2.18                     | 0.44              |
| 1:H:293:ARG:CG   | 1:H:293:ARG:NH1  | 2.69                     | 0.44              |
| 1:I:252:LEU:CD1  | 1:I:296:LEU:HA   | 2.40                     | 0.44              |
| 1:L:172:GLY:HA2  | 2:L:11:ADP:PA    | 2.57                     | 0.44              |
| 1:L:208:LEU:HD21 | 1:L:227:PHE:HD1  | 1.82                     | 0.44              |
| 1:N:340:THR:H    | 1:N:343:ALA:HB3  | 1.83                     | 0.44              |
| 1:A:240:ILE:HD11 | 1:A:277:ALA:HA   | 2.00                     | 0.43              |
| 1:C:239:GLU:N    | 1:C:278:ALA:O    | 2.42                     | 0.43              |
| 1:C:325:LEU:HD13 | 1:C:339:PHE:CE1  | 2.53                     | 0.43              |
| 1:D:168:GLU:O    | 1:D:171:VAL:HG13 | 2.18                     | 0.43              |
| 1:D:224:GLU:HG3  | 1:D:224:GLU:O    | 2.18                     | 0.43              |
| 1:D:246:GLU:N    | 1:D:246:GLU:OE2  | 2.50                     | 0.43              |
| 1:D:252:LEU:HD13 | 1:D:296:LEU:HA   | 1.99                     | 0.43              |
| 1:E:326:LYS:O    | 1:E:327:LYS:C    | 2.61                     | 0.43              |
| 1:H:286:LEU:HD22 | 1:H:291:LYS:CD   | 2.48                     | 0.43              |
| 1:I:180:ILE:O    | 1:I:184:SER:HB3  | 2.18                     | 0.43              |
| 1:I:301:GLY:O    | 1:I:302:VAL:C    | 2.60                     | 0.43              |
| 1:J:181:HIS:C    | 1:J:183:LEU:H    | 2.26                     | 0.43              |
| 1:J:324:PHE:CE1  | 1:J:359:LEU:HD12 | 2.53                     | 0.43              |
| 1:K:363:ILE:O    | 1:K:367:VAL:HG23 | 2.18                     | 0.43              |
| 1:L:277:ALA:O    | 1:L:278:ALA:HB2  | 2.17                     | 0.43              |
| 1:M:335:GLU:O    | 1:M:336:VAL:HG23 | 2.18                     | 0.43              |
| 1:N:143:SER:O    | 1:N:144:PRO:C    | 2.61                     | 0.43              |
| 1:N:203:ILE:O    | 1:N:205:GLU:N    | 2.45                     | 0.43              |
| 1:N:259:LYS:HA   | 1:N:269:ILE:O    | 2.18                     | 0.43              |
| 1:A:204:PHE:CZ   | 1:A:208:LEU:HD12 | 2.53                     | 0.43              |
| 1:C:328:PHE:CZ   | 1:C:364:GLU:HB2  | 2.53                     | 0.43              |
| 1:D:297:TYR:CD1  | 1:D:297:TYR:C    | 2.92                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:149:ILE:O    | 1:E:150:LEU:C    | 2.61                     | 0.43              |
| 1:F:314:LYS:HA   | 1:F:317:ILE:CD1  | 2.49                     | 0.43              |
| 1:G:252:LEU:HD22 | 1:G:295:ASP:OD1  | 2.18                     | 0.43              |
| 1:J:352:TRP:CZ3  | 1:J:362:VAL:HG21 | 2.52                     | 0.43              |
| 1:K:283:ILE:O    | 1:K:286:LEU:N    | 2.52                     | 0.43              |
| 1:K:311:ARG:HG3  | 1:K:312:GLU:HG3  | 2.00                     | 0.43              |
| 1:K:343:ALA:HB2  | 1:K:376:ASP:HA   | 2.00                     | 0.43              |
| 1:L:204:PHE:CZ   | 1:L:208:LEU:HD12 | 2.53                     | 0.43              |
| 1:L:220:VAL:O    | 1:L:220:VAL:HG12 | 2.18                     | 0.43              |
| 1:L:228:GLU:OE2  | 1:L:262:ARG:NH2  | 2.51                     | 0.43              |
| 1:L:279:THR:OG1  | 1:L:280:ASN:N    | 2.51                     | 0.43              |
| 1:L:363:ILE:O    | 1:L:364:GLU:C    | 2.60                     | 0.43              |
| 1:M:275:ILE:HD12 | 1:M:275:ILE:N    | 2.33                     | 0.43              |
| 1:M:328:PHE:CD2  | 1:M:364:GLU:HG3  | 2.53                     | 0.43              |
| 1:M:343:ALA:O    | 1:M:344:GLN:C    | 2.61                     | 0.43              |
| 1:M:362:VAL:O    | 1:M:363:ILE:C    | 2.61                     | 0.43              |
| 1:N:259:LYS:HA   | 1:N:270:GLU:HA   | 2.00                     | 0.43              |
| 1:N:305:ILE:HG22 | 1:N:307:ILE:CD1  | 2.47                     | 0.43              |
| 1:C:170:GLY:C    | 1:C:172:GLY:H    | 2.25                     | 0.43              |
| 1:C:266:ARG:CZ   | 1:D:203:ILE:HD12 | 2.48                     | 0.43              |
| 1:C:328:PHE:CD2  | 1:C:364:GLU:HG3  | 2.54                     | 0.43              |
| 1:D:176:VAL:O    | 1:D:177:ALA:C    | 2.61                     | 0.43              |
| 1:D:296:LEU:O    | 1:D:296:LEU:HD13 | 2.19                     | 0.43              |
| 1:F:320:LEU:O    | 1:F:321:ALA:C    | 2.59                     | 0.43              |
| 1:G:216:PHE:O    | 1:G:216:PHE:CG   | 2.71                     | 0.43              |
| 1:G:252:LEU:HD22 | 1:G:293:ARG:NH1  | 2.29                     | 0.43              |
| 1:G:325:LEU:HD21 | 1:G:336:VAL:HG12 | 2.00                     | 0.43              |
| 1:H:204:PHE:C    | 1:H:206:ALA:N    | 2.75                     | 0.43              |
| 1:K:254:VAL:HG22 | 1:K:260:PHE:HB3  | 2.01                     | 0.43              |
| 1:K:313:ARG:O    | 1:K:314:LYS:C    | 2.62                     | 0.43              |
| 1:L:178:ARG:HH11 | 1:L:178:ARG:CG   | 2.28                     | 0.43              |
| 1:L:283:ILE:HG22 | 1:L:287:VAL:CG2  | 2.47                     | 0.43              |
| 1:M:144:PRO:HG3  | 1:M:315:GLU:OE2  | 2.18                     | 0.43              |
| 1:N:227:PHE:CE2  | 1:N:275:ILE:HD11 | 2.53                     | 0.43              |
| 1:A:310:LEU:O    | 1:A:312:GLU:N    | 2.52                     | 0.43              |
| 1:A:361:ASN:O    | 1:A:362:VAL:C    | 2.61                     | 0.43              |
| 1:C:196:VAL:HG13 | 1:C:204:PHE:CE1  | 2.54                     | 0.43              |
| 1:C:319:PRO:O    | 1:C:320:LEU:C    | 2.61                     | 0.43              |
| 1:D:201:ARG:NH2  | 1:D:242:GLU:O    | 2.51                     | 0.43              |
| 1:E:161:CYS:O    | 1:E:274:ARG:NH1  | 2.51                     | 0.43              |
| 1:G:237:LEU:HB2  | 1:G:240:ILE:HD11 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:146:MET:O    | 1:H:149:ILE:HB   | 2.18                     | 0.43              |
| 1:H:166:THR:O    | 1:H:173:LYS:HD3  | 2.19                     | 0.43              |
| 1:H:192:VAL:HG21 | 1:H:230:ALA:CB   | 2.39                     | 0.43              |
| 1:L:165:ILE:O    | 1:L:173:LYS:HD2  | 2.18                     | 0.43              |
| 1:L:184:SER:C    | 1:L:186:ARG:N    | 2.77                     | 0.43              |
| 1:L:314:LYS:C    | 1:L:317:ILE:HG13 | 2.42                     | 0.43              |
| 1:L:335:GLU:HG3  | 1:L:335:GLU:O    | 2.17                     | 0.43              |
| 1:M:178:ARG:HH11 | 1:M:178:ARG:CG   | 2.27                     | 0.43              |
| 1:M:235:LEU:HD12 | 1:M:236:PHE:H    | 1.83                     | 0.43              |
| 1:M:369:PHE:O    | 1:M:370:SER:O    | 2.37                     | 0.43              |
| 1:N:145:LYS:CB   | 1:N:148:GLU:HG2  | 2.48                     | 0.43              |
| 1:N:292:PHE:C    | 1:N:292:PHE:HD2  | 2.26                     | 0.43              |
| 1:N:339:PHE:N    | 1:N:339:PHE:CD1  | 2.86                     | 0.43              |
| 1:A:139:TYR:HD2  | 1:A:175:VAL:CG1  | 2.29                     | 0.43              |
| 1:A:236:PHE:HE1  | 1:A:278:ALA:CB   | 2.31                     | 0.43              |
| 1:A:243:LEU:HD22 | 1:A:247:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:153:ILE:HG23 | 1:B:180:ILE:HG12 | 1.99                     | 0.43              |
| 1:B:346:LEU:O    | 1:B:346:LEU:HD23 | 2.19                     | 0.43              |
| 1:C:366:ALA:O    | 1:C:367:VAL:C    | 2.62                     | 0.43              |
| 1:D:141:PHE:CE2  | 1:D:146:MET:HE2  | 2.53                     | 0.43              |
| 1:E:174:GLU:O    | 1:E:177:ALA:N    | 2.51                     | 0.43              |
| 1:E:208:LEU:HB3  | 1:E:209:PHE:HD1  | 1.84                     | 0.43              |
| 1:F:161:CYS:SG   | 1:F:303:ILE:HG12 | 2.58                     | 0.43              |
| 1:H:213:LYS:HA   | 1:H:219:ALA:HB1  | 2.01                     | 0.43              |
| 1:I:149:ILE:O    | 1:I:153:ILE:HG13 | 2.19                     | 0.43              |
| 1:I:332:TYR:O    | 1:I:333:ALA:C    | 2.61                     | 0.43              |
| 1:L:145:LYS:O    | 1:L:148:GLU:N    | 2.47                     | 0.43              |
| 1:L:193:ALA:HB2  | 1:L:236:PHE:HB3  | 1.99                     | 0.43              |
| 1:L:283:ILE:O    | 1:L:284:LYS:C    | 2.61                     | 0.43              |
| 1:L:325:LEU:HD13 | 1:L:339:PHE:CZ   | 2.54                     | 0.43              |
| 1:M:206:ALA:CB   | 1:M:216:PHE:HE1  | 2.31                     | 0.43              |
| 1:M:234:THR:HG23 | 1:M:274:ARG:O    | 2.18                     | 0.43              |
| 1:M:253:ARG:HG2  | 1:N:198:SER:HB3  | 2.01                     | 0.43              |
| 1:M:284:LYS:HE3  | 1:M:297:TYR:HE2  | 1.83                     | 0.43              |
| 1:M:376:ASP:C    | 1:M:378:GLY:H    | 2.26                     | 0.43              |
| 1:N:146:MET:HG3  | 1:N:313:ARG:NE   | 2.33                     | 0.43              |
| 1:A:151:GLU:C    | 1:A:153:ILE:N    | 2.76                     | 0.43              |
| 1:B:207:GLU:O    | 1:B:208:LEU:C    | 2.61                     | 0.43              |
| 1:B:275:ILE:N    | 1:B:275:ILE:CD1  | 2.61                     | 0.43              |
| 1:B:337:GLU:CG   | 1:B:373:LYS:HB3  | 2.46                     | 0.43              |
| 1:B:358:GLU:O    | 1:B:361:ASN:HB2  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:146:MET:HG3  | 1:C:313:ARG:HH21 | 1.83                     | 0.43              |
| 1:C:343:ALA:O    | 1:C:344:GLN:C    | 2.62                     | 0.43              |
| 1:D:259:LYS:HB3  | 1:D:268:GLU:HG2  | 2.00                     | 0.43              |
| 1:E:171:VAL:CB   | 1:E:307:ILE:HG22 | 2.46                     | 0.43              |
| 1:E:292:PHE:HD2  | 1:E:293:ARG:O    | 2.01                     | 0.43              |
| 1:F:242:GLU:HG2  | 1:F:281:ARG:NH2  | 2.28                     | 0.43              |
| 1:H:141:PHE:CB   | 1:H:320:LEU:HD23 | 2.48                     | 0.43              |
| 1:H:309:PRO:HG3  | 1:H:311:ARG:HH11 | 1.84                     | 0.43              |
| 1:J:344:GLN:O    | 1:J:345:GLU:C    | 2.62                     | 0.43              |
| 1:K:181:HIS:O    | 1:K:184:SER:OG   | 2.34                     | 0.43              |
| 1:L:169:SER:O    | 1:L:169:SER:OG   | 2.32                     | 0.43              |
| 1:L:299:ARG:HH21 | 1:L:302:VAL:HG21 | 1.84                     | 0.43              |
| 1:N:365:ARG:CD   | 1:N:383:LEU:HD13 | 2.49                     | 0.43              |
| 1:A:367:VAL:O    | 1:A:370:SER:OG   | 2.29                     | 0.43              |
| 1:C:208:LEU:HD23 | 1:C:209:PHE:CZ   | 2.53                     | 0.43              |
| 1:D:292:PHE:CD2  | 1:D:293:ARG:O    | 2.71                     | 0.43              |
| 1:D:347:LEU:C    | 1:D:349:SER:H    | 2.27                     | 0.43              |
| 1:E:161:CYS:SG   | 1:E:303:ILE:HG13 | 2.59                     | 0.43              |
| 1:E:196:VAL:HG11 | 1:E:243:LEU:CD2  | 2.48                     | 0.43              |
| 1:E:206:ALA:CB   | 1:E:211:TYR:CE1  | 3.02                     | 0.43              |
| 1:E:241:GLY:HA3  | 1:E:281:ARG:HH21 | 1.82                     | 0.43              |
| 1:E:367:VAL:O    | 1:E:370:SER:OG   | 2.33                     | 0.43              |
| 1:H:142:GLU:HG2  | 1:H:146:MET:SD   | 2.59                     | 0.43              |
| 1:H:145:LYS:O    | 1:H:149:ILE:HG13 | 2.17                     | 0.43              |
| 1:I:310:LEU:C    | 1:I:312:GLU:N    | 2.75                     | 0.43              |
| 1:J:249:ALA:O    | 1:J:252:LEU:HB3  | 2.19                     | 0.43              |
| 1:K:332:TYR:CD1  | 1:K:368:LEU:HG   | 2.53                     | 0.43              |
| 1:L:203:ILE:O    | 1:L:204:PHE:C    | 2.59                     | 0.43              |
| 1:L:244:SER:O    | 1:L:247:ALA:N    | 2.52                     | 0.43              |
| 1:M:379:GLU:C    | 1:M:381:SER:H    | 2.27                     | 0.43              |
| 1:N:317:ILE:O    | 1:N:319:PRO:N    | 2.51                     | 0.43              |
| 1:A:325:LEU:HB2  | 1:A:339:PHE:CZ   | 2.54                     | 0.43              |
| 1:B:144:PRO:HD3  | 1:B:315:GLU:OE2  | 2.18                     | 0.43              |
| 1:B:160:GLU:HA   | 1:B:274:ARG:HH12 | 1.83                     | 0.43              |
| 1:B:320:LEU:O    | 1:B:321:ALA:C    | 2.61                     | 0.43              |
| 1:C:146:MET:HG3  | 1:C:313:ARG:HE   | 1.83                     | 0.43              |
| 1:C:340:THR:C    | 1:C:342:SER:N    | 2.73                     | 0.43              |
| 1:D:252:LEU:O    | 1:D:255:ILE:N    | 2.52                     | 0.43              |
| 1:D:267:LYS:HD2  | 1:D:267:LYS:H    | 1.83                     | 0.43              |
| 1:D:292:PHE:CZ   | 1:D:296:LEU:HD12 | 2.54                     | 0.43              |
| 1:D:339:PHE:N    | 1:D:339:PHE:CD1  | 2.86                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:242:GLU:HA   | 1:E:242:GLU:OE1  | 2.19                     | 0.43              |
| 1:E:247:ALA:O    | 1:E:251:LEU:N    | 2.50                     | 0.43              |
| 1:G:350:TYR:HD2  | 1:G:352:TRP:CD2  | 2.37                     | 0.43              |
| 1:I:149:ILE:HD13 | 1:I:307:ILE:HD13 | 2.00                     | 0.43              |
| 1:J:330:ARG:O    | 1:J:331:LYS:C    | 2.61                     | 0.43              |
| 1:J:352:TRP:HH2  | 1:J:362:VAL:HG11 | 1.83                     | 0.43              |
| 1:J:358:GLU:O    | 1:J:359:LEU:C    | 2.61                     | 0.43              |
| 1:K:244:SER:O    | 1:K:248:GLN:HG3  | 2.18                     | 0.43              |
| 1:K:248:GLN:OE1  | 1:K:292:PHE:CD2  | 2.72                     | 0.43              |
| 1:L:138:GLU:O    | 1:L:139:TYR:CB   | 2.66                     | 0.43              |
| 1:L:146:MET:CG   | 1:L:313:ARG:HE   | 2.31                     | 0.43              |
| 1:L:181:HIS:CD2  | 1:L:234:THR:HB   | 2.52                     | 0.43              |
| 1:M:149:ILE:CD1  | 1:M:307:ILE:HD13 | 2.48                     | 0.43              |
| 1:M:162:PRO:HG3  | 1:M:299:ARG:O    | 2.18                     | 0.43              |
| 1:M:231:ASP:CG   | 1:M:271:VAL:HG23 | 2.44                     | 0.43              |
| 1:M:355:ASN:O    | 1:M:358:GLU:N    | 2.51                     | 0.43              |
| 1:A:232:GLY:N    | 1:A:272:ASN:O    | 2.51                     | 0.43              |
| 1:B:297:TYR:O    | 1:B:298:TYR:C    | 2.62                     | 0.43              |
| 1:C:283:ILE:HG22 | 1:C:284:LYS:N    | 2.33                     | 0.43              |
| 1:D:175:VAL:HG21 | 2:D:2:ADP:C8     | 2.54                     | 0.43              |
| 1:D:262:ARG:HB2  | 1:D:269:ILE:HD13 | 2.01                     | 0.43              |
| 1:E:181:HIS:O    | 1:E:184:SER:OG   | 2.35                     | 0.43              |
| 1:E:194:LEU:HD23 | 1:E:194:LEU:O    | 2.19                     | 0.43              |
| 1:E:356:VAL:HG11 | 2:E:3:ADP:C4     | 2.54                     | 0.43              |
| 1:F:300:LEU:C    | 1:F:302:VAL:N    | 2.76                     | 0.43              |
| 1:G:284:LYS:O    | 1:G:287:VAL:HB   | 2.19                     | 0.43              |
| 1:H:178:ARG:HH11 | 1:H:178:ARG:CG   | 2.31                     | 0.43              |
| 1:H:322:ASN:HB3  | 1:H:326:LYS:HE3  | 2.01                     | 0.43              |
| 1:I:318:ILE:O    | 1:I:319:PRO:C    | 2.59                     | 0.43              |
| 1:J:376:ASP:OD2  | 1:J:376:ASP:C    | 2.61                     | 0.43              |
| 1:K:179:LEU:O    | 1:K:181:HIS:N    | 2.52                     | 0.43              |
| 1:M:299:ARG:NH1  | 1:N:357:ARG:HH21 | 2.17                     | 0.43              |
| 1:M:336:VAL:C    | 1:M:337:GLU:OE2  | 2.61                     | 0.43              |
| 1:M:354:GLY:O    | 1:M:355:ASN:C    | 2.61                     | 0.43              |
| 1:N:376:ASP:O    | 1:N:377:ARG:C    | 2.61                     | 0.43              |
| 1:A:236:PHE:CD1  | 1:A:236:PHE:C    | 2.94                     | 0.43              |
| 1:A:240:ILE:C    | 1:A:242:GLU:N    | 2.76                     | 0.43              |
| 1:A:244:SER:C    | 1:A:246:GLU:H    | 2.26                     | 0.43              |
| 1:B:250:LYS:O    | 1:B:251:LEU:C    | 2.62                     | 0.43              |
| 1:C:240:ILE:CG1  | 1:C:277:ALA:HB1  | 2.38                     | 0.43              |
| 1:C:253:ARG:CG   | 1:C:253:ARG:NH1  | 2.81                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:263:LEU:HD22 | 1:C:264:GLY:N    | 2.33                     | 0.43              |
| 1:C:299:ARG:HD3  | 1:C:299:ARG:HA   | 1.95                     | 0.43              |
| 1:C:330:ARG:O    | 1:C:331:LYS:C    | 2.62                     | 0.43              |
| 1:C:346:LEU:O    | 1:C:346:LEU:HD23 | 2.19                     | 0.43              |
| 1:D:310:LEU:HD11 | 1:D:320:LEU:HD13 | 2.01                     | 0.43              |
| 1:E:144:PRO:HD2  | 1:E:315:GLU:OE2  | 2.19                     | 0.43              |
| 1:F:157:SER:HB3  | 1:F:183:LEU:O    | 2.19                     | 0.43              |
| 1:F:325:LEU:HD11 | 1:F:336:VAL:CG1  | 2.49                     | 0.43              |
| 1:F:352:TRP:C    | 1:F:354:GLY:H    | 2.27                     | 0.43              |
| 1:H:215:ALA:CB   | 1:H:264:GLY:HA3  | 2.48                     | 0.43              |
| 1:H:317:ILE:CG2  | 1:H:348:LEU:HD23 | 2.49                     | 0.43              |
| 1:I:297:TYR:CD2  | 1:I:298:TYR:CD1  | 2.96                     | 0.43              |
| 1:J:250:LYS:O    | 1:J:254:VAL:HG23 | 2.18                     | 0.43              |
| 1:J:336:VAL:HG11 | 1:J:375:ILE:HD11 | 1.99                     | 0.43              |
| 1:K:168:GLU:O    | 1:K:171:VAL:HG13 | 2.18                     | 0.43              |
| 1:K:229:LEU:C    | 1:K:229:LEU:CD1  | 2.92                     | 0.43              |
| 1:L:173:LYS:HZ3  | 2:L:11:ADP:PB    | 2.42                     | 0.43              |
| 1:L:283:ILE:O    | 1:L:285:GLU:N    | 2.52                     | 0.43              |
| 1:N:244:SER:O    | 1:N:247:ALA:N    | 2.52                     | 0.43              |
| 1:N:343:ALA:O    | 1:N:344:GLN:C    | 2.62                     | 0.43              |
| 1:C:184:SER:C    | 1:C:186:ARG:N    | 2.77                     | 0.42              |
| 1:C:194:LEU:HD21 | 1:C:235:LEU:HD11 | 2.00                     | 0.42              |
| 1:C:283:ILE:O    | 1:C:284:LYS:C    | 2.62                     | 0.42              |
| 1:F:267:LYS:N    | 1:F:267:LYS:CD   | 2.79                     | 0.42              |
| 1:G:243:LEU:HD23 | 1:G:243:LEU:HA   | 1.79                     | 0.42              |
| 1:H:270:GLU:C    | 1:H:271:VAL:HG23 | 2.44                     | 0.42              |
| 1:J:324:PHE:CE1  | 1:J:360:LYS:HA   | 2.53                     | 0.42              |
| 1:J:376:ASP:O    | 1:J:377:ARG:C    | 2.62                     | 0.42              |
| 1:J:376:ASP:O    | 1:J:378:GLY:N    | 2.51                     | 0.42              |
| 1:K:195:ASN:O    | 1:K:197:ALA:N    | 2.52                     | 0.42              |
| 1:K:212:GLU:O    | 1:K:213:LYS:C    | 2.61                     | 0.42              |
| 1:L:157:SER:HB2  | 1:L:183:LEU:C    | 2.44                     | 0.42              |
| 1:M:325:LEU:HD12 | 1:M:339:PHE:CE1  | 2.54                     | 0.42              |
| 1:N:148:GLU:O    | 1:N:152:LYS:HD2  | 2.19                     | 0.42              |
| 1:N:350:TYR:CE1  | 1:N:384:VAL:HG21 | 2.54                     | 0.42              |
| 1:A:332:TYR:OH   | 1:A:364:GLU:OE1  | 2.37                     | 0.42              |
| 1:B:162:PRO:HD2  | 1:B:299:ARG:NH2  | 2.34                     | 0.42              |
| 1:B:282:ASN:O    | 1:B:283:ILE:C    | 2.61                     | 0.42              |
| 1:C:162:PRO:HG2  | 1:C:302:VAL:HG21 | 1.99                     | 0.42              |
| 1:C:296:LEU:O    | 1:C:299:ARG:N    | 2.38                     | 0.42              |
| 1:D:170:GLY:N    | 2:D:2:ADP:O3B    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:240:ILE:HD13 | 1:D:243:LEU:HD11 | 2.01                     | 0.42              |
| 1:D:325:LEU:HD11 | 1:D:336:VAL:HG12 | 2.01                     | 0.42              |
| 1:D:343:ALA:O    | 1:D:346:LEU:N    | 2.51                     | 0.42              |
| 1:E:350:TYR:CD1  | 1:E:384:VAL:CG1  | 3.00                     | 0.42              |
| 1:F:348:LEU:N    | 1:F:348:LEU:HD23 | 2.33                     | 0.42              |
| 1:G:340:THR:O    | 1:G:341:LYS:C    | 2.61                     | 0.42              |
| 1:H:289:GLU:O    | 1:H:289:GLU:HG2  | 2.19                     | 0.42              |
| 1:I:292:PHE:CE2  | 1:I:296:LEU:HD22 | 2.54                     | 0.42              |
| 1:L:309:PRO:HB2  | 1:L:355:ASN:OD1  | 2.20                     | 0.42              |
| 1:L:316:ASP:O    | 1:L:320:LEU:HB2  | 2.19                     | 0.42              |
| 1:L:342:SER:HB2  | 1:L:377:ARG:HB2  | 2.00                     | 0.42              |
| 1:M:283:ILE:CA   | 1:M:286:LEU:HD12 | 2.40                     | 0.42              |
| 1:M:359:LEU:O    | 1:M:362:VAL:N    | 2.52                     | 0.42              |
| 1:M:365:ARG:HH22 | 1:M:384:VAL:HA   | 1.84                     | 0.42              |
| 1:N:254:VAL:O    | 1:N:256:GLU:N    | 2.52                     | 0.42              |
| 1:B:259:LYS:HB3  | 1:B:268:GLU:HG2  | 2.00                     | 0.42              |
| 1:B:263:LEU:HD23 | 1:B:264:GLY:N    | 2.34                     | 0.42              |
| 1:D:263:LEU:C    | 1:D:263:LEU:CD2  | 2.92                     | 0.42              |
| 1:D:294:GLU:O    | 1:D:297:TYR:N    | 2.53                     | 0.42              |
| 1:E:189:GLU:OE1  | 1:E:189:GLU:HA   | 2.14                     | 0.42              |
| 1:E:257:SER:C    | 1:E:259:LYS:N    | 2.76                     | 0.42              |
| 1:E:303:ILE:O    | 1:E:304:GLU:C    | 2.60                     | 0.42              |
| 1:F:164:LEU:HA   | 1:F:277:ALA:O    | 2.19                     | 0.42              |
| 1:F:314:LYS:O    | 1:F:317:ILE:N    | 2.50                     | 0.42              |
| 1:F:328:PHE:HZ   | 1:F:360:LYS:HG3  | 1.83                     | 0.42              |
| 1:G:162:PRO:HB3  | 1:G:275:ILE:HB   | 2.00                     | 0.42              |
| 1:H:228:GLU:OE2  | 1:H:269:ILE:HD13 | 2.19                     | 0.42              |
| 1:I:156:ILE:HG22 | 1:I:274:ARG:HH22 | 1.84                     | 0.42              |
| 1:I:240:ILE:CG1  | 1:I:277:ALA:HB1  | 2.48                     | 0.42              |
| 1:I:259:LYS:HA   | 1:I:269:ILE:O    | 2.19                     | 0.42              |
| 1:J:200:PRO:O    | 1:J:202:ASP:N    | 2.53                     | 0.42              |
| 1:K:140:VAL:HG11 | 1:K:320:LEU:CD2  | 2.49                     | 0.42              |
| 1:K:199:ILE:O    | 1:K:199:ILE:HG22 | 2.19                     | 0.42              |
| 1:K:208:LEU:HB3  | 1:K:209:PHE:HD1  | 1.83                     | 0.42              |
| 1:K:319:PRO:O    | 1:K:320:LEU:C    | 2.61                     | 0.42              |
| 1:L:165:ILE:HG22 | 1:L:173:LYS:CG   | 2.48                     | 0.42              |
| 1:L:318:ILE:HG13 | 1:L:319:PRO:HD2  | 2.02                     | 0.42              |
| 1:M:245:LEU:HA   | 1:M:245:LEU:HD23 | 1.91                     | 0.42              |
| 1:N:199:ILE:HA   | 1:N:200:PRO:HD2  | 1.75                     | 0.42              |
| 1:N:257:SER:C    | 1:N:259:LYS:N    | 2.76                     | 0.42              |
| 1:A:178:ARG:O    | 1:A:181:HIS:HB3  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:LYS:HE2  | 1:A:220:VAL:HG12 | 2.00                     | 0.42              |
| 1:C:191:PHE:O    | 1:C:191:PHE:CD2  | 2.72                     | 0.42              |
| 1:C:340:THR:CG2  | 1:C:376:ASP:HB3  | 2.50                     | 0.42              |
| 1:D:212:GLU:HA   | 1:D:222:SER:CB   | 2.49                     | 0.42              |
| 1:D:359:LEU:HD23 | 1:D:359:LEU:O    | 2.19                     | 0.42              |
| 1:E:195:ASN:HB3  | 1:E:198:SER:OG   | 2.19                     | 0.42              |
| 1:E:208:LEU:O    | 1:E:226:PHE:N    | 2.52                     | 0.42              |
| 1:E:244:SER:HB2  | 1:E:246:GLU:HG2  | 2.02                     | 0.42              |
| 1:E:324:PHE:CD1  | 1:E:360:LYS:HA   | 2.55                     | 0.42              |
| 1:F:181:HIS:CD2  | 1:F:191:PHE:HB2  | 2.55                     | 0.42              |
| 1:F:259:LYS:HD3  | 1:F:268:GLU:OE2  | 2.20                     | 0.42              |
| 1:G:200:PRO:O    | 1:G:202:ASP:N    | 2.53                     | 0.42              |
| 1:G:259:LYS:HD3  | 1:G:267:LYS:HE3  | 2.01                     | 0.42              |
| 1:G:294:GLU:OE1  | 1:G:298:TYR:HE1  | 2.01                     | 0.42              |
| 1:H:212:GLU:HA   | 1:H:212:GLU:OE2  | 2.19                     | 0.42              |
| 1:H:369:PHE:N    | 1:H:369:PHE:HD1  | 2.18                     | 0.42              |
| 1:I:204:PHE:CE2  | 1:I:208:LEU:HB2  | 2.54                     | 0.42              |
| 1:I:296:LEU:HD21 | 1:I:300:LEU:CD1  | 2.49                     | 0.42              |
| 1:I:373:LYS:HB3  | 1:I:374:PHE:CD1  | 2.54                     | 0.42              |
| 1:K:178:ARG:NE   | 1:K:191:PHE:CD2  | 2.83                     | 0.42              |
| 1:M:140:VAL:HB   | 1:M:320:LEU:HD23 | 2.00                     | 0.42              |
| 1:A:153:ILE:HG23 | 1:A:180:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:253:ARG:NH2  | 1:A:268:GLU:OE2  | 2.53                     | 0.42              |
| 1:B:211:TYR:CE1  | 1:B:223:LYS:HB2  | 2.54                     | 0.42              |
| 1:C:184:SER:C    | 1:C:186:ARG:H    | 2.27                     | 0.42              |
| 1:C:217:THR:O    | 1:C:217:THR:CG2  | 2.66                     | 0.42              |
| 1:C:309:PRO:CG   | 1:C:311:ARG:HH11 | 2.32                     | 0.42              |
| 1:C:332:TYR:N    | 1:C:332:TYR:CD2  | 2.87                     | 0.42              |
| 1:C:354:GLY:O    | 1:C:355:ASN:O    | 2.38                     | 0.42              |
| 1:E:321:ALA:HB1  | 1:E:339:PHE:CE1  | 2.54                     | 0.42              |
| 1:E:328:PHE:CD1  | 1:E:364:GLU:HA   | 2.55                     | 0.42              |
| 1:F:352:TRP:C    | 1:F:354:GLY:N    | 2.77                     | 0.42              |
| 1:G:148:GLU:O    | 1:G:149:ILE:C    | 2.62                     | 0.42              |
| 1:H:223:LYS:HZ3  | 1:N:264:GLY:C    | 2.26                     | 0.42              |
| 1:I:311:ARG:HG2  | 1:I:311:ARG:NH1  | 2.35                     | 0.42              |
| 1:I:328:PHE:CE2  | 1:I:364:GLU:HB2  | 2.55                     | 0.42              |
| 1:K:250:LYS:HG3  | 1:L:198:SER:HB2  | 2.01                     | 0.42              |
| 1:K:256:GLU:HG2  | 1:K:299:ARG:HD3  | 2.00                     | 0.42              |
| 1:K:302:VAL:O    | 1:K:303:ILE:HD13 | 2.19                     | 0.42              |
| 1:K:382:CYS:C    | 1:K:383:LEU:HD12 | 2.45                     | 0.42              |
| 1:L:359:LEU:O    | 1:L:360:LYS:C    | 2.63                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:141:PHE:O    | 1:M:316:ASP:OD1  | 2.38                     | 0.42              |
| 1:N:317:ILE:O    | 1:N:318:ILE:C    | 2.61                     | 0.42              |
| 1:A:151:GLU:O    | 1:A:154:LYS:N    | 2.53                     | 0.42              |
| 1:A:158:CYS:SG   | 1:A:158:CYS:O    | 2.76                     | 0.42              |
| 1:A:179:LEU:HA   | 1:A:179:LEU:HD23 | 1.81                     | 0.42              |
| 1:D:240:ILE:C    | 1:D:242:GLU:N    | 2.77                     | 0.42              |
| 1:E:138:GLU:H    | 1:E:138:GLU:HG2  | 1.63                     | 0.42              |
| 1:E:213:LYS:O    | 1:E:215:ALA:N    | 2.53                     | 0.42              |
| 1:I:253:ARG:CZ   | 1:J:198:SER:HB3  | 2.49                     | 0.42              |
| 1:I:319:PRO:O    | 1:I:322:ASN:N    | 2.52                     | 0.42              |
| 1:K:204:PHE:O    | 1:K:205:GLU:C    | 2.58                     | 0.42              |
| 1:K:252:LEU:HD13 | 1:K:296:LEU:HA   | 2.00                     | 0.42              |
| 1:L:211:TYR:C    | 1:L:262:ARG:HD3  | 2.44                     | 0.42              |
| 1:M:177:ALA:O    | 1:M:180:ILE:HB   | 2.19                     | 0.42              |
| 1:M:292:PHE:CZ   | 1:M:296:LEU:HD12 | 2.54                     | 0.42              |
| 1:M:353:TYR:O    | 1:M:355:ASN:N    | 2.53                     | 0.42              |
| 1:N:240:ILE:O    | 1:N:241:GLY:C    | 2.62                     | 0.42              |
| 1:N:249:ALA:O    | 1:N:252:LEU:HB3  | 2.19                     | 0.42              |
| 1:N:318:ILE:CG1  | 1:N:348:LEU:HD21 | 2.48                     | 0.42              |
| 1:A:256:GLU:HG2  | 1:A:299:ARG:HD3  | 2.02                     | 0.42              |
| 1:B:160:GLU:CA   | 1:B:274:ARG:NH1  | 2.82                     | 0.42              |
| 1:B:206:ALA:O    | 1:B:207:GLU:C    | 2.61                     | 0.42              |
| 1:B:208:LEU:CD2  | 1:B:209:PHE:CE1  | 3.01                     | 0.42              |
| 1:B:211:TYR:HA   | 1:B:263:LEU:O    | 2.19                     | 0.42              |
| 1:C:310:LEU:O    | 1:C:312:GLU:N    | 2.53                     | 0.42              |
| 1:D:170:GLY:HA2  | 2:D:2:ADP:PB     | 2.60                     | 0.42              |
| 1:D:314:LYS:HE3  | 1:D:348:LEU:O    | 2.19                     | 0.42              |
| 1:D:328:PHE:C    | 1:D:330:ARG:H    | 2.25                     | 0.42              |
| 1:E:208:LEU:HD23 | 1:E:209:PHE:CE1  | 2.55                     | 0.42              |
| 1:E:307:ILE:HA   | 1:E:308:PRO:HD3  | 1.61                     | 0.42              |
| 1:F:285:GLU:O    | 1:F:288:LYS:HB2  | 2.20                     | 0.42              |
| 1:G:143:SER:HB2  | 1:G:144:PRO:HD2  | 2.00                     | 0.42              |
| 1:G:161:CYS:O    | 1:G:274:ARG:NH1  | 2.53                     | 0.42              |
| 1:G:283:ILE:O    | 1:G:284:LYS:C    | 2.62                     | 0.42              |
| 1:H:199:ILE:HD13 | 1:H:207:GLU:HG3  | 2.02                     | 0.42              |
| 1:H:210:GLY:O    | 1:H:263:LEU:N    | 2.47                     | 0.42              |
| 1:I:376:ASP:O    | 1:I:377:ARG:C    | 2.63                     | 0.42              |
| 1:J:172:GLY:O    | 1:J:173:LYS:C    | 2.60                     | 0.42              |
| 1:K:206:ALA:HB1  | 1:K:211:TYR:CD1  | 2.54                     | 0.42              |
| 1:L:214:GLY:HA3  | 1:M:223:LYS:HE2  | 2.01                     | 0.42              |
| 1:M:271:VAL:HG22 | 1:M:273:VAL:HG13 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:301:GLY:O    | 1:M:302:VAL:C    | 2.60                     | 0.42              |
| 1:M:313:ARG:O    | 1:M:315:GLU:N    | 2.52                     | 0.42              |
| 1:M:339:PHE:HE2  | 1:M:380:LEU:HD21 | 1.84                     | 0.42              |
| 1:N:239:GLU:C    | 1:N:241:GLY:N    | 2.77                     | 0.42              |
| 1:N:378:GLY:C    | 1:N:380:LEU:N    | 2.78                     | 0.42              |
| 1:B:171:VAL:HG23 | 1:B:172:GLY:N    | 2.35                     | 0.42              |
| 1:B:184:SER:C    | 1:B:186:ARG:N    | 2.76                     | 0.42              |
| 1:B:324:PHE:HB2  | 1:B:363:ILE:HD13 | 2.01                     | 0.42              |
| 1:E:240:ILE:HD11 | 1:E:277:ALA:CA   | 2.45                     | 0.42              |
| 1:E:288:LYS:C    | 1:E:290:GLY:N    | 2.76                     | 0.42              |
| 1:F:140:VAL:HG21 | 1:F:320:LEU:HD23 | 2.01                     | 0.42              |
| 1:G:240:ILE:C    | 1:G:242:GLU:N    | 2.77                     | 0.42              |
| 1:G:325:LEU:C    | 1:G:325:LEU:CD2  | 2.91                     | 0.42              |
| 1:G:365:ARG:O    | 1:G:368:LEU:N    | 2.53                     | 0.42              |
| 1:H:231:ASP:OD2  | 1:H:271:VAL:HG22 | 2.20                     | 0.42              |
| 1:J:149:ILE:C    | 1:J:151:GLU:N    | 2.77                     | 0.42              |
| 1:J:194:LEU:HD23 | 1:J:194:LEU:N    | 2.33                     | 0.42              |
| 1:J:211:TYR:CZ   | 1:J:223:LYS:HB3  | 2.55                     | 0.42              |
| 1:L:143:SER:OG   | 1:L:316:ASP:OD2  | 2.37                     | 0.42              |
| 1:L:159:ALA:HB2  | 1:M:368:LEU:HD21 | 2.01                     | 0.42              |
| 1:L:214:GLY:H    | 1:M:223:LYS:HE2  | 1.85                     | 0.42              |
| 1:L:254:VAL:O    | 1:L:255:ILE:C    | 2.63                     | 0.42              |
| 1:L:266:ARG:HH22 | 1:M:207:GLU:CD   | 2.28                     | 0.42              |
| 1:M:372:GLY:C    | 1:M:374:PHE:H    | 2.27                     | 0.42              |
| 1:A:275:ILE:HG22 | 1:A:276:LEU:N    | 2.35                     | 0.42              |
| 1:B:208:LEU:HD23 | 1:B:209:PHE:HE1  | 1.84                     | 0.42              |
| 1:B:310:LEU:HD11 | 1:B:359:LEU:HD12 | 2.02                     | 0.42              |
| 1:C:173:LYS:HB2  | 1:C:173:LYS:HE2  | 1.94                     | 0.42              |
| 1:C:235:LEU:HD12 | 1:C:235:LEU:C    | 2.39                     | 0.42              |
| 1:C:283:ILE:HG21 | 1:C:297:TYR:HD1  | 1.82                     | 0.42              |
| 1:C:375:ILE:HG22 | 1:C:380:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:142:GLU:HA   | 1:D:147:LYS:HE2  | 2.01                     | 0.42              |
| 1:D:175:VAL:HG23 | 2:D:2:ADP:O1A    | 2.20                     | 0.42              |
| 1:D:198:SER:O    | 1:D:199:ILE:HG13 | 2.20                     | 0.42              |
| 1:D:332:TYR:CE1  | 1:D:368:LEU:HD21 | 2.54                     | 0.42              |
| 1:F:230:ALA:O    | 1:F:233:GLY:N    | 2.49                     | 0.42              |
| 1:F:327:LYS:O    | 1:F:328:PHE:C    | 2.62                     | 0.42              |
| 1:G:177:ALA:O    | 1:G:178:ARG:C    | 2.61                     | 0.42              |
| 1:H:292:PHE:CE2  | 1:H:296:LEU:HB3  | 2.55                     | 0.42              |
| 1:I:204:PHE:O    | 1:I:205:GLU:C    | 2.61                     | 0.42              |
| 1:I:263:LEU:C    | 1:I:263:LEU:CD2  | 2.90                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:203:ILE:HG22 | 1:J:207:GLU:HG2  | 2.00                     | 0.42              |
| 1:J:236:PHE:CE2  | 1:J:238:ASP:HB2  | 2.55                     | 0.42              |
| 1:K:292:PHE:O    | 1:K:293:ARG:C    | 2.63                     | 0.42              |
| 1:L:208:LEU:HD22 | 1:L:209:PHE:CE1  | 2.54                     | 0.42              |
| 1:L:347:LEU:HD21 | 1:L:380:LEU:CD1  | 2.48                     | 0.42              |
| 1:M:181:HIS:ND1  | 1:M:181:HIS:C    | 2.78                     | 0.42              |
| 1:N:292:PHE:HE2  | 1:N:296:LEU:HB3  | 1.85                     | 0.42              |
| 1:N:356:VAL:O    | 1:N:357:ARG:C    | 2.63                     | 0.42              |
| 1:A:194:LEU:HD23 | 1:A:236:PHE:O    | 2.20                     | 0.42              |
| 1:A:324:PHE:O    | 1:A:325:LEU:C    | 2.62                     | 0.42              |
| 1:B:179:LEU:C    | 1:B:179:LEU:CD2  | 2.93                     | 0.42              |
| 1:B:239:GLU:C    | 1:B:241:GLY:H    | 2.27                     | 0.42              |
| 1:C:160:GLU:CA   | 1:C:274:ARG:NH1  | 2.80                     | 0.42              |
| 1:D:209:PHE:CE2  | 1:D:227:PHE:CE1  | 3.08                     | 0.42              |
| 1:D:354:GLY:O    | 1:D:355:ASN:C    | 2.63                     | 0.42              |
| 1:E:244:SER:C    | 1:E:246:GLU:H    | 2.28                     | 0.42              |
| 1:F:174:GLU:HG2  | 1:F:178:ARG:HH12 | 1.83                     | 0.42              |
| 1:H:178:ARG:NE   | 1:H:191:PHE:CE2  | 2.88                     | 0.42              |
| 1:H:235:LEU:HD23 | 1:H:235:LEU:C    | 2.45                     | 0.42              |
| 1:H:265:GLY:C    | 1:H:266:ARG:HD3  | 2.42                     | 0.42              |
| 1:H:293:ARG:NH1  | 1:H:295:ASP:OD1  | 2.53                     | 0.42              |
| 1:I:141:PHE:CG   | 1:I:150:LEU:HD21 | 2.53                     | 0.42              |
| 1:J:164:LEU:HA   | 1:J:277:ALA:HB3  | 2.01                     | 0.42              |
| 1:K:236:PHE:O    | 1:K:236:PHE:CG   | 2.73                     | 0.42              |
| 1:L:343:ALA:C    | 1:L:345:GLU:N    | 2.74                     | 0.42              |
| 1:N:149:ILE:O    | 1:N:150:LEU:C    | 2.63                     | 0.42              |
| 1:N:194:LEU:HD23 | 1:N:194:LEU:N    | 2.34                     | 0.42              |
| 1:B:248:GLN:O    | 1:B:249:ALA:C    | 2.62                     | 0.41              |
| 1:B:283:ILE:HA   | 1:B:286:LEU:CD1  | 2.17                     | 0.41              |
| 1:C:186:ARG:CD   | 1:C:233:GLY:O    | 2.67                     | 0.41              |
| 1:C:292:PHE:O    | 1:C:293:ARG:C    | 2.63                     | 0.41              |
| 1:C:320:LEU:CD1  | 1:C:356:VAL:HG13 | 2.50                     | 0.41              |
| 1:C:322:ASN:O    | 1:C:324:PHE:N    | 2.53                     | 0.41              |
| 1:C:350:TYR:CD1  | 1:C:351:PRO:HD2  | 2.55                     | 0.41              |
| 1:D:245:LEU:HA   | 1:D:248:GLN:HE21 | 1.85                     | 0.41              |
| 1:D:339:PHE:HZ   | 1:D:363:ILE:HD13 | 1.85                     | 0.41              |
| 1:F:328:PHE:CZ   | 1:F:364:GLU:HB2  | 2.55                     | 0.41              |
| 1:G:216:PHE:O    | 1:G:217:THR:C    | 2.62                     | 0.41              |
| 1:G:310:LEU:H    | 1:G:355:ASN:CB   | 2.33                     | 0.41              |
| 1:H:161:CYS:SG   | 1:H:303:ILE:HD11 | 2.60                     | 0.41              |
| 1:H:318:ILE:CD1  | 1:H:344:GLN:HE21 | 2.31                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:357:ARG:O    | 1:H:360:LYS:N    | 2.53                     | 0.41              |
| 1:I:207:GLU:O    | 1:I:225:GLY:HA2  | 2.20                     | 0.41              |
| 1:I:314:LYS:HG2  | 1:I:317:ILE:HD11 | 2.02                     | 0.41              |
| 1:J:208:LEU:HD11 | 1:J:235:LEU:HD21 | 2.01                     | 0.41              |
| 1:J:249:ALA:HB2  | 1:J:293:ARG:HH11 | 1.84                     | 0.41              |
| 1:J:343:ALA:O    | 1:J:344:GLN:C    | 2.63                     | 0.41              |
| 1:J:380:LEU:O    | 1:J:383:LEU:HG   | 2.20                     | 0.41              |
| 1:L:328:PHE:HD2  | 1:L:332:TYR:HE1  | 1.67                     | 0.41              |
| 1:L:350:TYR:CD2  | 1:L:351:PRO:N    | 2.88                     | 0.41              |
| 1:B:212:GLU:OE1  | 1:B:212:GLU:HA   | 2.20                     | 0.41              |
| 1:D:139:TYR:CD1  | 1:D:139:TYR:N    | 2.86                     | 0.41              |
| 1:D:212:GLU:OE1  | 1:D:262:ARG:NH1  | 2.52                     | 0.41              |
| 1:D:310:LEU:C    | 1:D:312:GLU:H    | 2.28                     | 0.41              |
| 1:D:314:LYS:HA   | 1:D:317:ILE:CD1  | 2.51                     | 0.41              |
| 1:E:359:LEU:HD22 | 1:E:363:ILE:HG12 | 2.01                     | 0.41              |
| 1:F:149:ILE:C    | 1:F:151:GLU:H    | 2.28                     | 0.41              |
| 1:F:196:VAL:HA   | 1:F:204:PHE:CZ   | 2.55                     | 0.41              |
| 1:F:343:ALA:HB2  | 1:F:376:ASP:CA   | 2.46                     | 0.41              |
| 1:H:287:VAL:HG12 | 1:H:294:GLU:HG2  | 2.01                     | 0.41              |
| 1:H:310:LEU:HG   | 1:H:355:ASN:HB3  | 2.01                     | 0.41              |
| 1:I:302:VAL:O    | 1:J:365:ARG:CZ   | 2.68                     | 0.41              |
| 1:I:355:ASN:O    | 1:I:356:VAL:C    | 2.63                     | 0.41              |
| 1:I:356:VAL:HG11 | 2:I:8:ADP:C8     | 2.55                     | 0.41              |
| 1:K:149:ILE:O    | 1:K:150:LEU:C    | 2.63                     | 0.41              |
| 1:K:156:ILE:O    | 1:K:157:SER:C    | 2.63                     | 0.41              |
| 1:K:179:LEU:O    | 1:K:180:ILE:C    | 2.61                     | 0.41              |
| 1:K:359:LEU:HD23 | 1:K:359:LEU:O    | 2.20                     | 0.41              |
| 1:L:318:ILE:N    | 1:L:319:PRO:HD2  | 2.34                     | 0.41              |
| 1:M:324:PHE:CE1  | 1:M:359:LEU:HD23 | 2.55                     | 0.41              |
| 1:N:145:LYS:O    | 1:N:149:ILE:N    | 2.54                     | 0.41              |
| 1:N:181:HIS:O    | 1:N:183:LEU:N    | 2.53                     | 0.41              |
| 1:A:223:LYS:HZ1  | 1:G:266:ARG:HD2  | 1.85                     | 0.41              |
| 1:A:350:TYR:CD1  | 1:A:384:VAL:HG12 | 2.56                     | 0.41              |
| 1:A:379:GLU:O    | 1:A:382:CYS:HB2  | 2.20                     | 0.41              |
| 1:C:157:SER:HB2  | 1:C:183:LEU:O    | 2.19                     | 0.41              |
| 1:C:181:HIS:CD2  | 1:C:191:PHE:CB   | 2.79                     | 0.41              |
| 1:C:381:SER:C    | 1:C:383:LEU:N    | 2.78                     | 0.41              |
| 1:D:212:GLU:O    | 1:D:213:LYS:O    | 2.39                     | 0.41              |
| 1:D:224:GLU:O    | 1:D:224:GLU:CG   | 2.67                     | 0.41              |
| 1:D:283:ILE:O    | 1:D:287:VAL:HG23 | 2.20                     | 0.41              |
| 1:D:327:LYS:O    | 1:D:330:ARG:N    | 2.39                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:173:LYS:NZ   | 1:E:173:LYS:CB   | 2.79                     | 0.41              |
| 1:F:251:LEU:HD22 | 1:F:255:ILE:HG13 | 2.02                     | 0.41              |
| 1:F:265:GLY:O    | 1:F:266:ARG:NE   | 2.53                     | 0.41              |
| 1:I:374:PHE:CD1  | 1:I:374:PHE:N    | 2.89                     | 0.41              |
| 1:K:208:LEU:HD21 | 1:K:227:PHE:HE1  | 1.86                     | 0.41              |
| 1:K:243:LEU:N    | 1:K:243:LEU:HD23 | 2.35                     | 0.41              |
| 1:K:262:ARG:O    | 1:K:263:LEU:C    | 2.60                     | 0.41              |
| 1:K:363:ILE:O    | 1:K:364:GLU:C    | 2.63                     | 0.41              |
| 1:L:141:PHE:HD1  | 1:L:150:LEU:HG   | 1.80                     | 0.41              |
| 1:M:253:ARG:CG   | 1:N:198:SER:HB3  | 2.51                     | 0.41              |
| 1:N:174:GLU:HB3  | 2:N:13:ADP:O1A   | 2.20                     | 0.41              |
| 1:N:252:LEU:O    | 1:N:254:VAL:N    | 2.54                     | 0.41              |
| 1:N:261:TYR:N    | 1:N:261:TYR:CD1  | 2.89                     | 0.41              |
| 1:N:376:ASP:CG   | 1:N:377:ARG:N    | 2.78                     | 0.41              |
| 1:B:266:ARG:CD   | 1:C:229:LEU:HD23 | 2.50                     | 0.41              |
| 1:B:308:PRO:HG2  | 1:B:313:ARG:HD3  | 2.02                     | 0.41              |
| 1:B:325:LEU:HD23 | 1:B:325:LEU:C    | 2.46                     | 0.41              |
| 1:C:293:ARG:HH21 | 1:C:295:ASP:CG   | 2.27                     | 0.41              |
| 1:C:328:PHE:O    | 1:C:329:SER:C    | 2.62                     | 0.41              |
| 1:D:166:THR:HG22 | 1:D:279:THR:CG2  | 2.51                     | 0.41              |
| 1:D:251:LEU:C    | 1:D:251:LEU:HD22 | 2.45                     | 0.41              |
| 1:D:286:LEU:O    | 1:D:287:VAL:C    | 2.63                     | 0.41              |
| 1:F:171:VAL:HG23 | 1:F:307:ILE:HG21 | 2.02                     | 0.41              |
| 1:I:368:LEU:HD23 | 1:I:368:LEU:HA   | 1.92                     | 0.41              |
| 1:J:251:LEU:O    | 1:J:252:LEU:C    | 2.63                     | 0.41              |
| 1:J:339:PHE:CZ   | 1:J:363:ILE:HD13 | 2.56                     | 0.41              |
| 1:J:365:ARG:NE   | 1:J:383:LEU:HD13 | 2.35                     | 0.41              |
| 1:L:184:SER:C    | 1:L:186:ARG:H    | 2.29                     | 0.41              |
| 1:L:252:LEU:C    | 1:L:252:LEU:HD12 | 2.45                     | 0.41              |
| 1:L:298:TYR:HE1  | 1:M:354:GLY:HA3  | 1.81                     | 0.41              |
| 1:L:347:LEU:C    | 1:L:349:SER:H    | 2.27                     | 0.41              |
| 1:M:314:LYS:HA   | 1:M:317:ILE:CG1  | 2.49                     | 0.41              |
| 1:N:143:SER:OG   | 1:N:146:MET:HB2  | 2.20                     | 0.41              |
| 1:N:365:ARG:HD2  | 1:N:383:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:203:ILE:HD13 | 1:D:203:ILE:HA   | 1.89                     | 0.41              |
| 1:D:227:PHE:CE2  | 1:D:235:LEU:HD23 | 2.55                     | 0.41              |
| 1:D:276:LEU:HD23 | 1:D:276:LEU:HA   | 1.64                     | 0.41              |
| 1:D:299:ARG:HE   | 1:D:299:ARG:CA   | 2.33                     | 0.41              |
| 1:E:141:PHE:N    | 1:E:141:PHE:CD1  | 2.88                     | 0.41              |
| 1:E:253:ARG:NH2  | 1:E:268:GLU:OE2  | 2.45                     | 0.41              |
| 1:F:174:GLU:CG   | 1:F:178:ARG:HH12 | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:318:ILE:N    | 1:F:319:PRO:CD   | 2.84                     | 0.41              |
| 1:G:215:ALA:CB   | 1:G:263:LEU:HD13 | 2.51                     | 0.41              |
| 1:G:320:LEU:C    | 1:G:320:LEU:CD2  | 2.91                     | 0.41              |
| 1:G:354:GLY:O    | 1:G:355:ASN:C    | 2.63                     | 0.41              |
| 1:H:228:GLU:O    | 1:H:229:LEU:C    | 2.63                     | 0.41              |
| 1:H:247:ALA:O    | 1:H:248:GLN:O    | 2.38                     | 0.41              |
| 1:I:143:SER:HB3  | 1:I:316:ASP:OD1  | 2.19                     | 0.41              |
| 1:I:269:ILE:N    | 1:I:269:ILE:CD1  | 2.80                     | 0.41              |
| 1:I:310:LEU:O    | 1:I:313:ARG:N    | 2.39                     | 0.41              |
| 1:I:325:LEU:HD23 | 1:I:325:LEU:O    | 2.21                     | 0.41              |
| 1:K:238:ASP:O    | 1:K:239:GLU:HB3  | 2.20                     | 0.41              |
| 1:A:161:CYS:SG   | 1:A:303:ILE:HG12 | 2.61                     | 0.41              |
| 1:A:310:LEU:HD23 | 1:A:310:LEU:HA   | 1.87                     | 0.41              |
| 1:C:368:LEU:HD23 | 1:C:368:LEU:HA   | 1.78                     | 0.41              |
| 1:D:159:ALA:CA   | 1:E:332:TYR:HE2  | 2.34                     | 0.41              |
| 1:D:210:GLY:CA   | 1:D:225:GLY:N    | 2.79                     | 0.41              |
| 1:D:313:ARG:HB3  | 1:D:316:ASP:OD2  | 2.20                     | 0.41              |
| 1:E:228:GLU:O    | 1:E:229:LEU:C    | 2.61                     | 0.41              |
| 1:F:152:LYS:O    | 1:F:156:ILE:HG12 | 2.21                     | 0.41              |
| 1:G:162:PRO:HA   | 1:G:275:ILE:O    | 2.21                     | 0.41              |
| 1:G:259:LYS:HD3  | 1:G:267:LYS:CE   | 2.51                     | 0.41              |
| 1:H:279:THR:OG1  | 1:H:280:ASN:N    | 2.51                     | 0.41              |
| 1:H:289:GLU:C    | 1:H:291:LYS:H    | 2.28                     | 0.41              |
| 1:K:177:ALA:HB1  | 1:K:276:LEU:HD12 | 2.03                     | 0.41              |
| 1:L:339:PHE:C    | 1:L:340:THR:O    | 2.63                     | 0.41              |
| 1:M:294:GLU:C    | 1:M:296:LEU:H    | 2.28                     | 0.41              |
| 1:M:380:LEU:O    | 1:M:384:VAL:HB   | 2.21                     | 0.41              |
| 1:N:253:ARG:HG3  | 1:N:253:ARG:HH11 | 1.86                     | 0.41              |
| 1:N:283:ILE:C    | 1:N:287:VAL:HG23 | 2.46                     | 0.41              |
| 1:N:359:LEU:HD23 | 1:N:363:ILE:HD11 | 2.03                     | 0.41              |
| 1:B:313:ARG:HB3  | 1:B:316:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:140:VAL:HG21 | 1:C:320:LEU:CD2  | 2.51                     | 0.41              |
| 1:C:156:ILE:HG13 | 1:D:369:PHE:HE1  | 1.85                     | 0.41              |
| 1:C:325:LEU:O    | 1:C:326:LYS:C    | 2.63                     | 0.41              |
| 1:D:299:ARG:HH21 | 1:D:302:VAL:HG21 | 1.84                     | 0.41              |
| 1:D:324:PHE:CE1  | 1:D:360:LYS:HA   | 2.56                     | 0.41              |
| 1:E:285:GLU:O    | 1:E:286:LEU:C    | 2.63                     | 0.41              |
| 1:E:350:TYR:HD2  | 1:E:352:TRP:CD2  | 2.39                     | 0.41              |
| 1:J:314:LYS:C    | 1:J:316:ASP:N    | 2.76                     | 0.41              |
| 1:J:365:ARG:CD   | 1:J:383:LEU:HD13 | 2.51                     | 0.41              |
| 1:L:298:TYR:CE1  | 1:M:354:GLY:CA   | 2.99                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:143:SER:OG   | 1:M:146:MET:HB2  | 2.21                     | 0.41              |
| 1:M:195:ASN:O    | 1:M:196:VAL:C    | 2.63                     | 0.41              |
| 1:M:289:GLU:O    | 1:M:291:LYS:HG3  | 2.20                     | 0.41              |
| 1:M:296:LEU:HD13 | 1:M:296:LEU:C    | 2.46                     | 0.41              |
| 1:M:312:GLU:H    | 1:M:312:GLU:HG2  | 1.72                     | 0.41              |
| 1:N:328:PHE:CD1  | 1:N:364:GLU:HA   | 2.56                     | 0.41              |
| 1:A:296:LEU:C    | 1:A:296:LEU:CD1  | 2.93                     | 0.41              |
| 1:A:313:ARG:C    | 1:A:315:GLU:H    | 2.29                     | 0.41              |
| 1:A:315:GLU:N    | 1:A:315:GLU:OE1  | 2.53                     | 0.41              |
| 1:B:153:ILE:HG22 | 1:B:183:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:321:ALA:O    | 1:B:363:ILE:HD13 | 2.21                     | 0.41              |
| 1:C:194:LEU:HD23 | 1:C:194:LEU:O    | 2.21                     | 0.41              |
| 1:F:141:PHE:CD2  | 1:F:150:LEU:HB2  | 2.56                     | 0.41              |
| 1:F:252:LEU:HD11 | 1:F:299:ARG:HG3  | 2.02                     | 0.41              |
| 1:G:157:SER:C    | 1:G:159:ALA:H    | 2.29                     | 0.41              |
| 1:H:255:ILE:CD1  | 1:H:300:LEU:HD21 | 2.50                     | 0.41              |
| 1:K:168:GLU:O    | 1:K:171:VAL:HG22 | 2.20                     | 0.41              |
| 1:L:261:TYR:O    | 1:L:262:ARG:O    | 2.39                     | 0.41              |
| 1:M:168:GLU:O    | 1:M:171:VAL:HG22 | 2.21                     | 0.41              |
| 1:M:281:ARG:CG   | 1:M:282:ASN:H    | 2.33                     | 0.41              |
| 1:M:330:ARG:C    | 1:M:332:TYR:N    | 2.76                     | 0.41              |
| 1:N:343:ALA:O    | 1:N:346:LEU:N    | 2.50                     | 0.41              |
| 1:A:175:VAL:O    | 1:A:178:ARG:HB2  | 2.21                     | 0.41              |
| 1:A:227:PHE:CD2  | 1:A:273:VAL:HG21 | 2.56                     | 0.41              |
| 1:A:269:ILE:HD12 | 1:A:269:ILE:N    | 2.36                     | 0.41              |
| 1:A:292:PHE:HZ   | 1:A:296:LEU:HD12 | 1.83                     | 0.41              |
| 1:A:310:LEU:C    | 1:A:312:GLU:H    | 2.29                     | 0.41              |
| 1:B:208:LEU:HA   | 1:B:226:PHE:HB2  | 2.02                     | 0.41              |
| 1:B:242:GLU:CD   | 1:B:281:ARG:HH22 | 2.29                     | 0.41              |
| 1:B:266:ARG:HH11 | 1:B:266:ARG:CG   | 2.33                     | 0.41              |
| 1:B:284:LYS:HD3  | 1:B:284:LYS:N    | 2.32                     | 0.41              |
| 1:B:297:TYR:O    | 1:B:300:LEU:N    | 2.52                     | 0.41              |
| 1:B:343:ALA:O    | 1:B:347:LEU:HG   | 2.21                     | 0.41              |
| 1:D:168:GLU:HB2  | 1:D:355:ASN:HD21 | 1.85                     | 0.41              |
| 1:D:283:ILE:HD12 | 1:D:292:PHE:HE1  | 1.86                     | 0.41              |
| 1:E:224:GLU:HG2  | 1:E:228:GLU:HB2  | 2.03                     | 0.41              |
| 1:E:288:LYS:O    | 1:E:289:GLU:C    | 2.62                     | 0.41              |
| 1:F:172:GLY:HA3  | 2:F:4:ADP:C8     | 2.55                     | 0.41              |
| 1:F:192:VAL:HG21 | 1:F:230:ALA:HB2  | 2.03                     | 0.41              |
| 1:F:205:GLU:HG2  | 1:F:250:LYS:HD3  | 2.03                     | 0.41              |
| 1:G:220:VAL:O    | 1:G:220:VAL:HG12 | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:240:ILE:O    | 1:G:241:GLY:C    | 2.63                     | 0.41              |
| 1:H:186:ARG:C    | 1:H:188:LYS:H    | 2.29                     | 0.41              |
| 1:I:156:ILE:O    | 1:I:157:SER:C    | 2.63                     | 0.41              |
| 1:I:261:TYR:CE2  | 1:I:268:GLU:HB2  | 2.56                     | 0.41              |
| 1:I:266:ARG:NH2  | 1:J:203:ILE:CD1  | 2.83                     | 0.41              |
| 1:I:288:LYS:O    | 1:I:290:GLY:N    | 2.54                     | 0.41              |
| 1:I:314:LYS:O    | 1:I:317:ILE:HG13 | 2.20                     | 0.41              |
| 1:J:173:LYS:HG3  | 2:J:9:ADP:O1B    | 2.21                     | 0.41              |
| 1:J:190:PRO:HG2  | 1:J:233:GLY:HA3  | 2.02                     | 0.41              |
| 1:J:308:PRO:O    | 1:J:313:ARG:HD2  | 2.21                     | 0.41              |
| 1:K:189:GLU:HG2  | 1:K:232:GLY:O    | 2.20                     | 0.41              |
| 1:K:209:PHE:HD1  | 1:K:209:PHE:H    | 1.69                     | 0.41              |
| 1:K:310:LEU:HD22 | 1:K:317:ILE:CG1  | 2.49                     | 0.41              |
| 1:L:195:ASN:O    | 1:L:196:VAL:C    | 2.63                     | 0.41              |
| 1:L:244:SER:C    | 1:L:246:GLU:H    | 2.27                     | 0.41              |
| 1:L:260:PHE:O    | 1:L:260:PHE:CG   | 2.74                     | 0.41              |
| 1:L:328:PHE:CE2  | 1:L:364:GLU:OE2  | 2.74                     | 0.41              |
| 1:L:335:GLU:O    | 1:L:373:LYS:HA   | 2.21                     | 0.41              |
| 1:L:339:PHE:O    | 1:L:344:GLN:HG3  | 2.21                     | 0.41              |
| 1:L:362:VAL:O    | 1:L:363:ILE:C    | 2.64                     | 0.41              |
| 1:M:165:ILE:HG22 | 1:M:173:LYS:HG2  | 2.03                     | 0.41              |
| 1:M:168:GLU:OE1  | 1:M:309:PRO:CB   | 2.64                     | 0.41              |
| 1:M:186:ARG:NH1  | 1:M:232:GLY:O    | 2.53                     | 0.41              |
| 1:M:313:ARG:O    | 1:M:314:LYS:C    | 2.63                     | 0.41              |
| 1:M:362:VAL:O    | 1:M:364:GLU:N    | 2.54                     | 0.41              |
| 1:M:367:VAL:O    | 1:M:367:VAL:HG12 | 2.20                     | 0.41              |
| 1:N:245:LEU:O    | 1:N:248:GLN:N    | 2.53                     | 0.41              |
| 1:A:324:PHE:C    | 1:A:326:LYS:N    | 2.79                     | 0.41              |
| 1:B:162:PRO:CG   | 1:B:299:ARG:HH21 | 2.34                     | 0.41              |
| 1:B:266:ARG:NH1  | 1:B:266:ARG:HG2  | 2.36                     | 0.41              |
| 1:B:340:THR:C    | 1:B:342:SER:N    | 2.76                     | 0.41              |
| 1:C:152:LYS:O    | 1:C:154:LYS:N    | 2.54                     | 0.41              |
| 1:C:266:ARG:NH2  | 1:D:203:ILE:CD1  | 2.84                     | 0.41              |
| 1:C:295:ASP:N    | 1:C:295:ASP:OD1  | 2.54                     | 0.41              |
| 1:C:318:ILE:CD1  | 1:C:348:LEU:HD21 | 2.51                     | 0.41              |
| 1:D:174:GLU:HG2  | 1:D:178:ARG:NH1  | 2.36                     | 0.41              |
| 1:D:317:ILE:O    | 1:D:319:PRO:N    | 2.54                     | 0.41              |
| 1:E:292:PHE:O    | 1:E:293:ARG:C    | 2.63                     | 0.41              |
| 1:E:359:LEU:CD2  | 1:E:363:ILE:HD11 | 2.51                     | 0.41              |
| 1:E:365:ARG:HG2  | 1:E:369:PHE:CD2  | 2.56                     | 0.41              |
| 1:H:153:ILE:HG23 | 1:H:180:ILE:HG12 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:317:ILE:HB   | 1:H:348:LEU:CD2  | 2.51                     | 0.41              |
| 1:I:314:LYS:CA   | 1:I:317:ILE:HG13 | 2.49                     | 0.41              |
| 1:I:340:THR:OG1  | 1:I:376:ASP:CB   | 2.69                     | 0.41              |
| 1:J:156:ILE:O    | 1:J:157:SER:C    | 2.62                     | 0.41              |
| 1:J:355:ASN:O    | 1:J:356:VAL:C    | 2.63                     | 0.41              |
| 1:L:328:PHE:CZ   | 1:L:364:GLU:HB2  | 2.55                     | 0.41              |
| 1:N:186:ARG:O    | 1:N:189:GLU:HB2  | 2.20                     | 0.41              |
| 1:N:208:LEU:HD23 | 1:N:209:PHE:CE2  | 2.56                     | 0.41              |
| 1:N:320:LEU:CD1  | 1:N:356:VAL:HG13 | 2.50                     | 0.41              |
| 1:A:144:PRO:C    | 1:A:146:MET:N    | 2.77                     | 0.40              |
| 1:A:203:ILE:HD11 | 1:G:264:GLY:HA2  | 2.03                     | 0.40              |
| 1:A:274:ARG:HH11 | 1:A:274:ARG:HG2  | 1.86                     | 0.40              |
| 1:A:310:LEU:C    | 1:A:312:GLU:N    | 2.79                     | 0.40              |
| 1:B:216:PHE:HD1  | 1:B:217:THR:HG22 | 1.86                     | 0.40              |
| 1:B:260:PHE:CE1  | 1:B:269:ILE:HB   | 2.56                     | 0.40              |
| 1:B:305:ILE:O    | 1:B:305:ILE:HG22 | 2.21                     | 0.40              |
| 1:C:143:SER:HB2  | 1:C:316:ASP:OD1  | 2.22                     | 0.40              |
| 1:E:137:GLU:CG   | 1:E:138:GLU:N    | 2.83                     | 0.40              |
| 1:E:194:LEU:H    | 1:E:194:LEU:CD2  | 2.34                     | 0.40              |
| 1:E:275:ILE:HD12 | 1:E:275:ILE:N    | 2.36                     | 0.40              |
| 1:E:321:ALA:HB1  | 1:E:339:PHE:CZ   | 2.56                     | 0.40              |
| 1:F:288:LYS:C    | 1:F:290:GLY:N    | 2.79                     | 0.40              |
| 1:G:251:LEU:HD22 | 1:G:255:ILE:CD1  | 2.51                     | 0.40              |
| 1:G:346:LEU:C    | 1:G:346:LEU:HD23 | 2.46                     | 0.40              |
| 1:G:379:GLU:O    | 1:G:383:LEU:HD12 | 2.21                     | 0.40              |
| 1:I:266:ARG:HH21 | 1:J:203:ILE:CD1  | 2.34                     | 0.40              |
| 1:K:381:SER:C    | 1:K:383:LEU:N    | 2.79                     | 0.40              |
| 1:L:186:ARG:HD3  | 1:L:232:GLY:O    | 2.21                     | 0.40              |
| 1:L:194:LEU:H    | 1:L:194:LEU:CD2  | 2.30                     | 0.40              |
| 1:L:208:LEU:CD2  | 1:L:227:PHE:HD1  | 2.33                     | 0.40              |
| 1:M:142:GLU:HG3  | 1:M:142:GLU:O    | 2.21                     | 0.40              |
| 1:M:325:LEU:O    | 1:M:326:LYS:C    | 2.62                     | 0.40              |
| 1:A:283:ILE:O    | 1:A:286:LEU:N    | 2.54                     | 0.40              |
| 1:C:251:LEU:HD22 | 1:C:255:ILE:CD1  | 2.39                     | 0.40              |
| 1:C:255:ILE:HD13 | 1:C:300:LEU:CD2  | 2.51                     | 0.40              |
| 1:C:281:ARG:N    | 1:C:281:ARG:HD3  | 2.36                     | 0.40              |
| 1:D:235:LEU:HD12 | 1:D:236:PHE:CA   | 2.40                     | 0.40              |
| 1:E:171:VAL:CG2  | 1:E:307:ILE:HG22 | 2.52                     | 0.40              |
| 1:E:189:GLU:HB3  | 1:E:233:GLY:HA2  | 2.02                     | 0.40              |
| 1:E:189:GLU:HG3  | 1:E:232:GLY:C    | 2.46                     | 0.40              |
| 1:E:211:TYR:CE2  | 1:E:263:LEU:HB2  | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:235:LEU:HG   | 1:G:237:LEU:HD23 | 2.02                     | 0.40              |
| 1:G:254:VAL:O    | 1:G:254:VAL:HG12 | 2.21                     | 0.40              |
| 1:H:320:LEU:C    | 1:H:322:ASN:N    | 2.79                     | 0.40              |
| 1:I:171:VAL:CG1  | 1:I:307:ILE:CG2  | 2.95                     | 0.40              |
| 1:J:339:PHE:CD1  | 1:J:339:PHE:N    | 2.89                     | 0.40              |
| 1:J:350:TYR:HD2  | 1:J:352:TRP:CE3  | 2.39                     | 0.40              |
| 1:K:140:VAL:C    | 1:K:141:PHE:CD2  | 2.99                     | 0.40              |
| 1:L:318:ILE:CG1  | 1:L:319:PRO:CD   | 2.99                     | 0.40              |
| 1:M:166:THR:HA   | 1:M:279:THR:O    | 2.21                     | 0.40              |
| 1:M:229:LEU:C    | 1:M:231:ASP:N    | 2.77                     | 0.40              |
| 1:N:156:ILE:O    | 1:N:157:SER:C    | 2.63                     | 0.40              |
| 1:A:174:GLU:O    | 1:A:175:VAL:C    | 2.64                     | 0.40              |
| 1:A:236:PHE:HD1  | 1:A:276:LEU:O    | 2.04                     | 0.40              |
| 1:B:226:PHE:O    | 1:B:227:PHE:C    | 2.64                     | 0.40              |
| 1:B:288:LYS:C    | 1:B:290:GLY:N    | 2.77                     | 0.40              |
| 1:C:165:ILE:O    | 1:C:278:ALA:CB   | 2.69                     | 0.40              |
| 1:C:240:ILE:HG22 | 1:C:241:GLY:N    | 2.35                     | 0.40              |
| 1:D:274:ARG:O    | 1:D:275:ILE:C    | 2.63                     | 0.40              |
| 1:D:324:PHE:O    | 1:D:327:LYS:HB3  | 2.21                     | 0.40              |
| 1:D:369:PHE:CD1  | 1:D:369:PHE:N    | 2.87                     | 0.40              |
| 1:E:244:SER:O    | 1:E:245:LEU:C    | 2.64                     | 0.40              |
| 1:F:213:LYS:HD3  | 1:G:220:VAL:CG1  | 2.46                     | 0.40              |
| 1:G:161:CYS:CB   | 1:G:302:VAL:HG11 | 2.50                     | 0.40              |
| 1:G:275:ILE:HG21 | 1:G:300:LEU:CD2  | 2.52                     | 0.40              |
| 1:G:308:PRO:O    | 1:G:313:ARG:CD   | 2.69                     | 0.40              |
| 1:H:180:ILE:O    | 1:H:184:SER:HB3  | 2.21                     | 0.40              |
| 1:H:240:ILE:C    | 1:H:242:GLU:N    | 2.78                     | 0.40              |
| 1:H:367:VAL:O    | 1:H:367:VAL:HG12 | 2.19                     | 0.40              |
| 1:I:212:GLU:O    | 1:I:213:LYS:C    | 2.63                     | 0.40              |
| 1:J:196:VAL:HG12 | 1:J:242:GLU:HB2  | 2.03                     | 0.40              |
| 1:J:262:ARG:HH11 | 1:J:262:ARG:CG   | 2.31                     | 0.40              |
| 1:K:172:GLY:O    | 1:K:173:LYS:C    | 2.64                     | 0.40              |
| 1:L:179:LEU:O    | 1:L:180:ILE:C    | 2.65                     | 0.40              |
| 1:L:269:ILE:CD1  | 1:L:269:ILE:N    | 2.85                     | 0.40              |
| 1:L:300:LEU:C    | 1:L:302:VAL:N    | 2.80                     | 0.40              |
| 1:L:341:LYS:O    | 1:L:345:GLU:HG3  | 2.21                     | 0.40              |
| 1:L:365:ARG:NH2  | 1:L:383:LEU:HD22 | 2.36                     | 0.40              |
| 1:M:163:VAL:HG22 | 1:M:303:ILE:HB   | 2.02                     | 0.40              |
| 1:M:253:ARG:C    | 1:M:253:ARG:HD3  | 2.46                     | 0.40              |
| 1:A:256:GLU:OE1  | 1:B:357:ARG:NH1  | 2.55                     | 0.40              |
| 1:A:383:LEU:HD23 | 1:A:383:LEU:N    | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:325:LEU:C    | 1:D:325:LEU:CD2  | 2.93                     | 0.40              |
| 1:F:196:VAL:HG12 | 1:F:242:GLU:HB2  | 2.03                     | 0.40              |
| 1:F:358:GLU:O    | 1:F:359:LEU:O    | 2.38                     | 0.40              |
| 1:H:211:TYR:HB3  | 1:H:263:LEU:CB   | 2.51                     | 0.40              |
| 1:H:371:GLU:HG2  | 1:H:379:GLU:CD   | 2.47                     | 0.40              |
| 1:I:195:ASN:O    | 1:I:196:VAL:C    | 2.64                     | 0.40              |
| 1:I:211:TYR:CD1  | 1:I:211:TYR:C    | 2.99                     | 0.40              |
| 1:I:336:VAL:HG11 | 1:I:375:ILE:CD1  | 2.52                     | 0.40              |
| 1:J:200:PRO:C    | 1:J:202:ASP:H    | 2.30                     | 0.40              |
| 1:K:263:LEU:HD23 | 1:K:264:GLY:N    | 2.36                     | 0.40              |
| 1:K:361:ASN:O    | 1:K:362:VAL:C    | 2.64                     | 0.40              |
| 1:M:248:GLN:O    | 1:M:249:ALA:O    | 2.40                     | 0.40              |
| 1:M:252:LEU:HD13 | 1:M:296:LEU:HA   | 2.03                     | 0.40              |
| 1:A:246:GLU:H    | 1:A:246:GLU:HG2  | 1.72                     | 0.40              |
| 1:B:174:GLU:O    | 1:B:175:VAL:C    | 2.64                     | 0.40              |
| 1:C:195:ASN:O    | 1:C:198:SER:N    | 2.46                     | 0.40              |
| 1:C:204:PHE:CE2  | 1:C:243:LEU:HD21 | 2.56                     | 0.40              |
| 1:D:216:PHE:CD1  | 1:D:216:PHE:O    | 2.75                     | 0.40              |
| 1:D:296:LEU:HD13 | 1:D:300:LEU:HD11 | 2.00                     | 0.40              |
| 1:D:375:ILE:HG23 | 1:D:379:GLU:HB2  | 2.03                     | 0.40              |
| 1:E:165:ILE:HG22 | 1:E:173:LYS:HG2  | 2.03                     | 0.40              |
| 1:E:240:ILE:H    | 1:E:240:ILE:HG13 | 1.64                     | 0.40              |
| 1:E:382:CYS:O    | 1:E:383:LEU:HD23 | 2.21                     | 0.40              |
| 1:F:242:GLU:HA   | 1:F:242:GLU:OE1  | 2.21                     | 0.40              |
| 1:G:165:ILE:O    | 1:G:278:ALA:HA   | 2.22                     | 0.40              |
| 1:G:308:PRO:HG2  | 1:G:313:ARG:CD   | 2.47                     | 0.40              |
| 1:G:325:LEU:HD13 | 1:G:338:GLY:HA2  | 2.04                     | 0.40              |
| 1:H:212:GLU:HA   | 1:H:222:SER:CB   | 2.52                     | 0.40              |
| 1:I:359:LEU:O    | 1:I:360:LYS:C    | 2.64                     | 0.40              |
| 1:K:144:PRO:C    | 1:K:146:MET:N    | 2.79                     | 0.40              |
| 1:L:236:PHE:CD1  | 1:L:276:LEU:O    | 2.74                     | 0.40              |
| 1:L:322:ASN:O    | 1:L:325:LEU:HB3  | 2.22                     | 0.40              |
| 1:L:334:LYS:HZ2  | 1:L:367:VAL:HG22 | 1.86                     | 0.40              |
| 1:N:211:TYR:CE2  | 1:N:223:LYS:HB2  | 2.56                     | 0.40              |
| 1:N:320:LEU:HD23 | 1:N:320:LEU:N    | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | A     | 245/267 (92%)   | 192 (78%)  | 39 (16%)  | 14 (6%)  | 1           | 8 |
| 1   | B     | 241/267 (90%)   | 155 (64%)  | 64 (27%)  | 22 (9%)  | 0           | 3 |
| 1   | C     | 246/267 (92%)   | 180 (73%)  | 49 (20%)  | 17 (7%)  | 1           | 5 |
| 1   | D     | 245/267 (92%)   | 165 (67%)  | 55 (22%)  | 25 (10%) | 0           | 3 |
| 1   | E     | 246/267 (92%)   | 165 (67%)  | 56 (23%)  | 25 (10%) | 0           | 3 |
| 1   | F     | 246/267 (92%)   | 179 (73%)  | 39 (16%)  | 28 (11%) | 0           | 1 |
| 1   | G     | 246/267 (92%)   | 177 (72%)  | 49 (20%)  | 20 (8%)  | 1           | 4 |
| 1   | H     | 243/267 (91%)   | 171 (70%)  | 55 (23%)  | 17 (7%)  | 1           | 5 |
| 1   | I     | 245/267 (92%)   | 174 (71%)  | 48 (20%)  | 23 (9%)  | 0           | 3 |
| 1   | J     | 245/267 (92%)   | 182 (74%)  | 48 (20%)  | 15 (6%)  | 1           | 7 |
| 1   | K     | 246/267 (92%)   | 173 (70%)  | 53 (22%)  | 20 (8%)  | 1           | 4 |
| 1   | L     | 244/267 (91%)   | 158 (65%)  | 53 (22%)  | 33 (14%) | 0           | 1 |
| 1   | M     | 245/267 (92%)   | 164 (67%)  | 57 (23%)  | 24 (10%) | 0           | 3 |
| 1   | N     | 245/267 (92%)   | 169 (69%)  | 57 (23%)  | 19 (8%)  | 1           | 4 |
| All | All   | 3428/3738 (92%) | 2404 (70%) | 722 (21%) | 302 (9%) | 0           | 3 |

All (302) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 144 | PRO  |
| 1   | A     | 221 | SER  |
| 1   | B     | 157 | SER  |
| 1   | B     | 217 | THR  |
| 1   | B     | 381 | SER  |
| 1   | B     | 382 | CYS  |
| 1   | C     | 220 | VAL  |
| 1   | C     | 221 | SER  |
| 1   | C     | 283 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 301 | GLY  |
| 1   | C     | 317 | ILE  |
| 1   | D     | 144 | PRO  |
| 1   | D     | 157 | SER  |
| 1   | D     | 213 | LYS  |
| 1   | D     | 302 | VAL  |
| 1   | D     | 317 | ILE  |
| 1   | D     | 327 | LYS  |
| 1   | D     | 355 | ASN  |
| 1   | D     | 362 | VAL  |
| 1   | E     | 157 | SER  |
| 1   | E     | 196 | VAL  |
| 1   | E     | 314 | LYS  |
| 1   | F     | 157 | SER  |
| 1   | F     | 168 | GLU  |
| 1   | F     | 171 | VAL  |
| 1   | F     | 215 | ALA  |
| 1   | F     | 224 | GLU  |
| 1   | F     | 225 | GLY  |
| 1   | F     | 226 | PHE  |
| 1   | F     | 241 | GLY  |
| 1   | F     | 314 | LYS  |
| 1   | F     | 327 | LYS  |
| 1   | F     | 344 | GLN  |
| 1   | F     | 377 | ARG  |
| 1   | G     | 213 | LYS  |
| 1   | G     | 224 | GLU  |
| 1   | H     | 143 | SER  |
| 1   | H     | 144 | PRO  |
| 1   | H     | 217 | THR  |
| 1   | H     | 248 | GLN  |
| 1   | H     | 334 | LYS  |
| 1   | H     | 356 | VAL  |
| 1   | I     | 156 | ILE  |
| 1   | I     | 157 | SER  |
| 1   | I     | 213 | LYS  |
| 1   | I     | 220 | VAL  |
| 1   | I     | 356 | VAL  |
| 1   | J     | 224 | GLU  |
| 1   | J     | 241 | GLY  |
| 1   | K     | 140 | VAL  |
| 1   | K     | 189 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 217 | THR  |
| 1   | K     | 356 | VAL  |
| 1   | L     | 139 | TYR  |
| 1   | L     | 157 | SER  |
| 1   | L     | 240 | ILE  |
| 1   | L     | 262 | ARG  |
| 1   | L     | 287 | VAL  |
| 1   | L     | 344 | GLN  |
| 1   | L     | 347 | LEU  |
| 1   | L     | 348 | LEU  |
| 1   | L     | 377 | ARG  |
| 1   | M     | 142 | GLU  |
| 1   | M     | 144 | PRO  |
| 1   | M     | 283 | ILE  |
| 1   | M     | 355 | ASN  |
| 1   | M     | 370 | SER  |
| 1   | N     | 144 | PRO  |
| 1   | N     | 229 | LEU  |
| 1   | N     | 240 | ILE  |
| 1   | N     | 268 | GLU  |
| 1   | N     | 317 | ILE  |
| 1   | A     | 173 | LYS  |
| 1   | A     | 241 | GLY  |
| 1   | A     | 377 | ARG  |
| 1   | A     | 378 | GLY  |
| 1   | B     | 180 | ILE  |
| 1   | B     | 187 | SER  |
| 1   | B     | 206 | ALA  |
| 1   | B     | 207 | GLU  |
| 1   | C     | 311 | ARG  |
| 1   | C     | 355 | ASN  |
| 1   | C     | 377 | ARG  |
| 1   | D     | 158 | CYS  |
| 1   | D     | 214 | GLY  |
| 1   | D     | 225 | GLY  |
| 1   | D     | 241 | GLY  |
| 1   | E     | 168 | GLU  |
| 1   | E     | 173 | LYS  |
| 1   | E     | 245 | LEU  |
| 1   | E     | 317 | ILE  |
| 1   | E     | 321 | ALA  |
| 1   | E     | 325 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 347 | LEU  |
| 1   | E     | 352 | TRP  |
| 1   | E     | 382 | CYS  |
| 1   | F     | 196 | VAL  |
| 1   | F     | 218 | GLY  |
| 1   | F     | 311 | ARG  |
| 1   | F     | 315 | GLU  |
| 1   | F     | 360 | LYS  |
| 1   | F     | 367 | VAL  |
| 1   | G     | 149 | ILE  |
| 1   | G     | 158 | CYS  |
| 1   | G     | 173 | LYS  |
| 1   | G     | 174 | GLU  |
| 1   | G     | 201 | ARG  |
| 1   | G     | 263 | LEU  |
| 1   | G     | 366 | ALA  |
| 1   | G     | 377 | ARG  |
| 1   | H     | 335 | GLU  |
| 1   | I     | 221 | SER  |
| 1   | I     | 222 | SER  |
| 1   | I     | 242 | GLU  |
| 1   | I     | 252 | LEU  |
| 1   | I     | 301 | GLY  |
| 1   | I     | 311 | ARG  |
| 1   | I     | 367 | VAL  |
| 1   | I     | 377 | ARG  |
| 1   | J     | 311 | ARG  |
| 1   | J     | 317 | ILE  |
| 1   | J     | 356 | VAL  |
| 1   | J     | 372 | GLY  |
| 1   | J     | 377 | ARG  |
| 1   | K     | 196 | VAL  |
| 1   | K     | 214 | GLY  |
| 1   | K     | 249 | ALA  |
| 1   | K     | 309 | PRO  |
| 1   | L     | 185 | ASP  |
| 1   | L     | 196 | VAL  |
| 1   | L     | 215 | ALA  |
| 1   | L     | 219 | ALA  |
| 1   | L     | 311 | ARG  |
| 1   | L     | 356 | VAL  |
| 1   | L     | 372 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 156 | ILE  |
| 1   | M     | 157 | SER  |
| 1   | M     | 158 | CYS  |
| 1   | M     | 217 | THR  |
| 1   | M     | 249 | ALA  |
| 1   | M     | 267 | LYS  |
| 1   | M     | 359 | LEU  |
| 1   | N     | 182 | LYS  |
| 1   | N     | 201 | ARG  |
| 1   | N     | 314 | LYS  |
| 1   | N     | 373 | LYS  |
| 1   | A     | 152 | LYS  |
| 1   | B     | 203 | ILE  |
| 1   | B     | 205 | GLU  |
| 1   | B     | 208 | LEU  |
| 1   | B     | 222 | SER  |
| 1   | B     | 227 | PHE  |
| 1   | B     | 360 | LYS  |
| 1   | C     | 185 | ASP  |
| 1   | C     | 298 | TYR  |
| 1   | D     | 231 | ASP  |
| 1   | D     | 249 | ALA  |
| 1   | D     | 348 | LEU  |
| 1   | E     | 150 | LEU  |
| 1   | E     | 206 | ALA  |
| 1   | E     | 302 | VAL  |
| 1   | F     | 221 | SER  |
| 1   | F     | 328 | PHE  |
| 1   | F     | 359 | LEU  |
| 1   | G     | 214 | GLY  |
| 1   | G     | 311 | ARG  |
| 1   | G     | 355 | ASN  |
| 1   | G     | 356 | VAL  |
| 1   | H     | 289 | GLU  |
| 1   | H     | 309 | PRO  |
| 1   | H     | 381 | SER  |
| 1   | I     | 230 | ALA  |
| 1   | I     | 333 | ALA  |
| 1   | I     | 359 | LEU  |
| 1   | J     | 144 | PRO  |
| 1   | K     | 239 | GLU  |
| 1   | K     | 248 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 278 | ALA  |
| 1   | K     | 299 | ARG  |
| 1   | K     | 314 | LYS  |
| 1   | L     | 171 | VAL  |
| 1   | L     | 267 | LYS  |
| 1   | L     | 291 | LYS  |
| 1   | L     | 340 | THR  |
| 1   | L     | 380 | LEU  |
| 1   | M     | 196 | VAL  |
| 1   | M     | 257 | SER  |
| 1   | M     | 314 | LYS  |
| 1   | M     | 333 | ALA  |
| 1   | M     | 372 | GLY  |
| 1   | N     | 157 | SER  |
| 1   | N     | 278 | ALA  |
| 1   | A     | 218 | GLY  |
| 1   | A     | 311 | ARG  |
| 1   | B     | 251 | LEU  |
| 1   | B     | 372 | GLY  |
| 1   | B     | 383 | LEU  |
| 1   | C     | 162 | PRO  |
| 1   | C     | 239 | GLU  |
| 1   | C     | 322 | ASN  |
| 1   | D     | 215 | ALA  |
| 1   | E     | 138 | GLU  |
| 1   | E     | 182 | LYS  |
| 1   | E     | 204 | PHE  |
| 1   | E     | 227 | PHE  |
| 1   | F     | 138 | GLU  |
| 1   | F     | 294 | GLU  |
| 1   | F     | 295 | ASP  |
| 1   | G     | 156 | ILE  |
| 1   | G     | 157 | SER  |
| 1   | H     | 205 | GLU  |
| 1   | H     | 219 | ALA  |
| 1   | H     | 249 | ALA  |
| 1   | H     | 314 | LYS  |
| 1   | I     | 168 | GLU  |
| 1   | I     | 204 | PHE  |
| 1   | I     | 219 | ALA  |
| 1   | I     | 355 | ASN  |
| 1   | J     | 314 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 326 | LYS  |
| 1   | K     | 141 | PHE  |
| 1   | K     | 319 | PRO  |
| 1   | K     | 326 | LYS  |
| 1   | L     | 170 | GLY  |
| 1   | L     | 255 | ILE  |
| 1   | L     | 284 | LYS  |
| 1   | L     | 355 | ASN  |
| 1   | L     | 359 | LEU  |
| 1   | L     | 360 | LYS  |
| 1   | M     | 247 | ALA  |
| 1   | M     | 281 | ARG  |
| 1   | N     | 204 | PHE  |
| 1   | N     | 219 | ALA  |
| 1   | N     | 253 | ARG  |
| 1   | N     | 355 | ASN  |
| 1   | A     | 158 | CYS  |
| 1   | A     | 205 | GLU  |
| 1   | B     | 289 | GLU  |
| 1   | B     | 309 | PRO  |
| 1   | D     | 141 | PHE  |
| 1   | D     | 253 | ARG  |
| 1   | D     | 314 | LYS  |
| 1   | D     | 347 | LEU  |
| 1   | D     | 377 | ARG  |
| 1   | E     | 214 | GLY  |
| 1   | E     | 309 | PRO  |
| 1   | E     | 327 | LYS  |
| 1   | G     | 286 | LEU  |
| 1   | G     | 341 | LYS  |
| 1   | G     | 352 | TRP  |
| 1   | H     | 245 | LEU  |
| 1   | H     | 333 | ALA  |
| 1   | I     | 239 | GLU  |
| 1   | J     | 201 | ARG  |
| 1   | J     | 221 | SER  |
| 1   | J     | 278 | ALA  |
| 1   | J     | 344 | GLN  |
| 1   | J     | 355 | ASN  |
| 1   | K     | 190 | PRO  |
| 1   | L     | 153 | ILE  |
| 1   | L     | 204 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 295 | ASP  |
| 1   | L     | 381 | SER  |
| 1   | M     | 253 | ARG  |
| 1   | M     | 289 | GLU  |
| 1   | N     | 356 | VAL  |
| 1   | A     | 145 | LYS  |
| 1   | B     | 252 | LEU  |
| 1   | C     | 323 | HIS  |
| 1   | F     | 175 | VAL  |
| 1   | I     | 319 | PRO  |
| 1   | K     | 200 | PRO  |
| 1   | K     | 355 | ASN  |
| 1   | L     | 301 | GLY  |
| 1   | L     | 363 | ILE  |
| 1   | M     | 239 | GLU  |
| 1   | M     | 363 | ILE  |
| 1   | A     | 240 | ILE  |
| 1   | B     | 196 | VAL  |
| 1   | B     | 210 | GLY  |
| 1   | F     | 144 | PRO  |
| 1   | F     | 356 | VAL  |
| 1   | M     | 264 | GLY  |
| 1   | N     | 318 | ILE  |
| 1   | C     | 140 | VAL  |
| 1   | D     | 192 | VAL  |
| 1   | D     | 372 | GLY  |
| 1   | E     | 303 | ILE  |
| 1   | F     | 240 | ILE  |
| 1   | K     | 303 | ILE  |
| 1   | N     | 255 | ILE  |
| 1   | A     | 180 | ILE  |
| 1   | D     | 156 | ILE  |
| 1   | D     | 200 | PRO  |
| 1   | E     | 144 | PRO  |
| 1   | E     | 175 | VAL  |
| 1   | G     | 241 | GLY  |
| 1   | N     | 175 | VAL  |
| 1   | C     | 196 | VAL  |
| 1   | C     | 153 | ILE  |
| 1   | H     | 180 | ILE  |
| 1   | I     | 153 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 212/232 (91%)   | 190 (90%)  | 22 (10%)  | 7           | 27 |
| 1   | B     | 208/232 (90%)   | 185 (89%)  | 23 (11%)  | 6           | 24 |
| 1   | C     | 213/232 (92%)   | 188 (88%)  | 25 (12%)  | 5           | 22 |
| 1   | D     | 212/232 (91%)   | 180 (85%)  | 32 (15%)  | 3           | 13 |
| 1   | E     | 213/232 (92%)   | 172 (81%)  | 41 (19%)  | 1           | 7  |
| 1   | F     | 213/232 (92%)   | 174 (82%)  | 39 (18%)  | 2           | 8  |
| 1   | G     | 213/232 (92%)   | 185 (87%)  | 28 (13%)  | 4           | 17 |
| 1   | H     | 208/232 (90%)   | 187 (90%)  | 21 (10%)  | 7           | 28 |
| 1   | I     | 209/232 (90%)   | 190 (91%)  | 19 (9%)   | 9           | 32 |
| 1   | J     | 211/232 (91%)   | 190 (90%)  | 21 (10%)  | 7           | 29 |
| 1   | K     | 213/232 (92%)   | 186 (87%)  | 27 (13%)  | 4           | 18 |
| 1   | L     | 211/232 (91%)   | 171 (81%)  | 40 (19%)  | 1           | 7  |
| 1   | M     | 212/232 (91%)   | 184 (87%)  | 28 (13%)  | 4           | 17 |
| 1   | N     | 212/232 (91%)   | 187 (88%)  | 25 (12%)  | 5           | 21 |
| All | All   | 2960/3248 (91%) | 2569 (87%) | 391 (13%) | 4           | 17 |

All (391) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 179 | LEU  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 201 | ARG  |
| 1   | A     | 202 | ASP  |
| 1   | A     | 216 | PHE  |
| 1   | A     | 222 | SER  |
| 1   | A     | 227 | PHE  |
| 1   | A     | 244 | SER  |
| 1   | A     | 246 | GLU  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 262 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 263 | LEU  |
| 1   | A     | 285 | GLU  |
| 1   | A     | 299 | ARG  |
| 1   | A     | 307 | ILE  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 339 | PHE  |
| 1   | A     | 357 | ARG  |
| 1   | A     | 359 | LEU  |
| 1   | A     | 383 | LEU  |
| 1   | B     | 166 | THR  |
| 1   | B     | 178 | ARG  |
| 1   | B     | 179 | LEU  |
| 1   | B     | 189 | GLU  |
| 1   | B     | 200 | PRO  |
| 1   | B     | 202 | ASP  |
| 1   | B     | 213 | LYS  |
| 1   | B     | 227 | PHE  |
| 1   | B     | 229 | LEU  |
| 1   | B     | 250 | LYS  |
| 1   | B     | 251 | LEU  |
| 1   | B     | 260 | PHE  |
| 1   | B     | 262 | ARG  |
| 1   | B     | 269 | ILE  |
| 1   | B     | 274 | ARG  |
| 1   | B     | 275 | ILE  |
| 1   | B     | 281 | ARG  |
| 1   | B     | 284 | LYS  |
| 1   | B     | 285 | GLU  |
| 1   | B     | 299 | ARG  |
| 1   | B     | 314 | LYS  |
| 1   | B     | 318 | ILE  |
| 1   | B     | 377 | ARG  |
| 1   | C     | 176 | VAL  |
| 1   | C     | 178 | ARG  |
| 1   | C     | 181 | HIS  |
| 1   | C     | 194 | LEU  |
| 1   | C     | 203 | ILE  |
| 1   | C     | 211 | TYR  |
| 1   | C     | 213 | LYS  |
| 1   | C     | 217 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 223 | LYS  |
| 1   | C     | 227 | PHE  |
| 1   | C     | 229 | LEU  |
| 1   | C     | 240 | ILE  |
| 1   | C     | 246 | GLU  |
| 1   | C     | 251 | LEU  |
| 1   | C     | 253 | ARG  |
| 1   | C     | 263 | LEU  |
| 1   | C     | 274 | ARG  |
| 1   | C     | 284 | LYS  |
| 1   | C     | 299 | ARG  |
| 1   | C     | 310 | LEU  |
| 1   | C     | 318 | ILE  |
| 1   | C     | 320 | LEU  |
| 1   | C     | 346 | LEU  |
| 1   | C     | 359 | LEU  |
| 1   | C     | 371 | GLU  |
| 1   | D     | 138 | GLU  |
| 1   | D     | 160 | GLU  |
| 1   | D     | 164 | LEU  |
| 1   | D     | 165 | ILE  |
| 1   | D     | 178 | ARG  |
| 1   | D     | 179 | LEU  |
| 1   | D     | 185 | ASP  |
| 1   | D     | 189 | GLU  |
| 1   | D     | 194 | LEU  |
| 1   | D     | 220 | VAL  |
| 1   | D     | 227 | PHE  |
| 1   | D     | 228 | GLU  |
| 1   | D     | 229 | LEU  |
| 1   | D     | 235 | LEU  |
| 1   | D     | 236 | PHE  |
| 1   | D     | 237 | LEU  |
| 1   | D     | 246 | GLU  |
| 1   | D     | 251 | LEU  |
| 1   | D     | 262 | ARG  |
| 1   | D     | 266 | ARG  |
| 1   | D     | 273 | VAL  |
| 1   | D     | 275 | ILE  |
| 1   | D     | 280 | ASN  |
| 1   | D     | 281 | ARG  |
| 1   | D     | 285 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 295 | ASP  |
| 1   | D     | 299 | ARG  |
| 1   | D     | 304 | GLU  |
| 1   | D     | 310 | LEU  |
| 1   | D     | 318 | ILE  |
| 1   | D     | 346 | LEU  |
| 1   | D     | 363 | ILE  |
| 1   | E     | 138 | GLU  |
| 1   | E     | 139 | TYR  |
| 1   | E     | 142 | GLU  |
| 1   | E     | 143 | SER  |
| 1   | E     | 150 | LEU  |
| 1   | E     | 156 | ILE  |
| 1   | E     | 158 | CYS  |
| 1   | E     | 164 | LEU  |
| 1   | E     | 173 | LYS  |
| 1   | E     | 175 | VAL  |
| 1   | E     | 179 | LEU  |
| 1   | E     | 180 | ILE  |
| 1   | E     | 184 | SER  |
| 1   | E     | 189 | GLU  |
| 1   | E     | 201 | ARG  |
| 1   | E     | 209 | PHE  |
| 1   | E     | 213 | LYS  |
| 1   | E     | 216 | PHE  |
| 1   | E     | 222 | SER  |
| 1   | E     | 234 | THR  |
| 1   | E     | 243 | LEU  |
| 1   | E     | 244 | SER  |
| 1   | E     | 246 | GLU  |
| 1   | E     | 251 | LEU  |
| 1   | E     | 266 | ARG  |
| 1   | E     | 269 | ILE  |
| 1   | E     | 274 | ARG  |
| 1   | E     | 280 | ASN  |
| 1   | E     | 282 | ASN  |
| 1   | E     | 285 | GLU  |
| 1   | E     | 295 | ASP  |
| 1   | E     | 299 | ARG  |
| 1   | E     | 311 | ARG  |
| 1   | E     | 318 | ILE  |
| 1   | E     | 319 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 329 | SER  |
| 1   | E     | 355 | ASN  |
| 1   | E     | 356 | VAL  |
| 1   | E     | 359 | LEU  |
| 1   | E     | 361 | ASN  |
| 1   | E     | 380 | LEU  |
| 1   | F     | 137 | GLU  |
| 1   | F     | 138 | GLU  |
| 1   | F     | 142 | GLU  |
| 1   | F     | 166 | THR  |
| 1   | F     | 171 | VAL  |
| 1   | F     | 175 | VAL  |
| 1   | F     | 185 | ASP  |
| 1   | F     | 194 | LEU  |
| 1   | F     | 201 | ARG  |
| 1   | F     | 211 | TYR  |
| 1   | F     | 224 | GLU  |
| 1   | F     | 229 | LEU  |
| 1   | F     | 246 | GLU  |
| 1   | F     | 251 | LEU  |
| 1   | F     | 262 | ARG  |
| 1   | F     | 263 | LEU  |
| 1   | F     | 275 | ILE  |
| 1   | F     | 281 | ARG  |
| 1   | F     | 285 | GLU  |
| 1   | F     | 291 | LYS  |
| 1   | F     | 296 | LEU  |
| 1   | F     | 299 | ARG  |
| 1   | F     | 305 | ILE  |
| 1   | F     | 310 | LEU  |
| 1   | F     | 311 | ARG  |
| 1   | F     | 318 | ILE  |
| 1   | F     | 325 | LEU  |
| 1   | F     | 337 | GLU  |
| 1   | F     | 339 | PHE  |
| 1   | F     | 346 | LEU  |
| 1   | F     | 348 | LEU  |
| 1   | F     | 355 | ASN  |
| 1   | F     | 357 | ARG  |
| 1   | F     | 359 | LEU  |
| 1   | F     | 361 | ASN  |
| 1   | F     | 370 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 380 | LEU  |
| 1   | F     | 383 | LEU  |
| 1   | F     | 384 | VAL  |
| 1   | G     | 146 | MET  |
| 1   | G     | 147 | LYS  |
| 1   | G     | 164 | LEU  |
| 1   | G     | 171 | VAL  |
| 1   | G     | 175 | VAL  |
| 1   | G     | 178 | ARG  |
| 1   | G     | 179 | LEU  |
| 1   | G     | 181 | HIS  |
| 1   | G     | 191 | PHE  |
| 1   | G     | 194 | LEU  |
| 1   | G     | 201 | ARG  |
| 1   | G     | 221 | SER  |
| 1   | G     | 227 | PHE  |
| 1   | G     | 251 | LEU  |
| 1   | G     | 261 | TYR  |
| 1   | G     | 262 | ARG  |
| 1   | G     | 267 | LYS  |
| 1   | G     | 274 | ARG  |
| 1   | G     | 275 | ILE  |
| 1   | G     | 279 | THR  |
| 1   | G     | 285 | GLU  |
| 1   | G     | 299 | ARG  |
| 1   | G     | 307 | ILE  |
| 1   | G     | 310 | LEU  |
| 1   | G     | 318 | ILE  |
| 1   | G     | 346 | LEU  |
| 1   | G     | 355 | ASN  |
| 1   | G     | 359 | LEU  |
| 1   | H     | 189 | GLU  |
| 1   | H     | 194 | LEU  |
| 1   | H     | 202 | ASP  |
| 1   | H     | 216 | PHE  |
| 1   | H     | 227 | PHE  |
| 1   | H     | 229 | LEU  |
| 1   | H     | 242 | GLU  |
| 1   | H     | 251 | LEU  |
| 1   | H     | 252 | LEU  |
| 1   | H     | 263 | LEU  |
| 1   | H     | 274 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 279 | THR  |
| 1   | H     | 280 | ASN  |
| 1   | H     | 293 | ARG  |
| 1   | H     | 299 | ARG  |
| 1   | H     | 311 | ARG  |
| 1   | H     | 339 | PHE  |
| 1   | H     | 349 | SER  |
| 1   | H     | 363 | ILE  |
| 1   | H     | 369 | PHE  |
| 1   | H     | 379 | GLU  |
| 1   | I     | 158 | CYS  |
| 1   | I     | 178 | ARG  |
| 1   | I     | 202 | ASP  |
| 1   | I     | 229 | LEU  |
| 1   | I     | 242 | GLU  |
| 1   | I     | 246 | GLU  |
| 1   | I     | 251 | LEU  |
| 1   | I     | 262 | ARG  |
| 1   | I     | 269 | ILE  |
| 1   | I     | 274 | ARG  |
| 1   | I     | 285 | GLU  |
| 1   | I     | 295 | ASP  |
| 1   | I     | 299 | ARG  |
| 1   | I     | 318 | ILE  |
| 1   | I     | 346 | LEU  |
| 1   | I     | 357 | ARG  |
| 1   | I     | 359 | LEU  |
| 1   | I     | 365 | ARG  |
| 1   | I     | 373 | LYS  |
| 1   | J     | 141 | PHE  |
| 1   | J     | 143 | SER  |
| 1   | J     | 166 | THR  |
| 1   | J     | 201 | ARG  |
| 1   | J     | 202 | ASP  |
| 1   | J     | 216 | PHE  |
| 1   | J     | 229 | LEU  |
| 1   | J     | 262 | ARG  |
| 1   | J     | 266 | ARG  |
| 1   | J     | 269 | ILE  |
| 1   | J     | 285 | GLU  |
| 1   | J     | 299 | ARG  |
| 1   | J     | 318 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 341 | LYS  |
| 1   | J     | 346 | LEU  |
| 1   | J     | 349 | SER  |
| 1   | J     | 357 | ARG  |
| 1   | J     | 359 | LEU  |
| 1   | J     | 363 | ILE  |
| 1   | J     | 376 | ASP  |
| 1   | J     | 383 | LEU  |
| 1   | K     | 141 | PHE  |
| 1   | K     | 147 | LYS  |
| 1   | K     | 160 | GLU  |
| 1   | K     | 179 | LEU  |
| 1   | K     | 189 | GLU  |
| 1   | K     | 190 | PRO  |
| 1   | K     | 194 | LEU  |
| 1   | K     | 201 | ARG  |
| 1   | K     | 216 | PHE  |
| 1   | K     | 221 | SER  |
| 1   | K     | 224 | GLU  |
| 1   | K     | 229 | LEU  |
| 1   | K     | 237 | LEU  |
| 1   | K     | 238 | ASP  |
| 1   | K     | 242 | GLU  |
| 1   | K     | 243 | LEU  |
| 1   | K     | 251 | LEU  |
| 1   | K     | 262 | ARG  |
| 1   | K     | 269 | ILE  |
| 1   | K     | 276 | LEU  |
| 1   | K     | 285 | GLU  |
| 1   | K     | 299 | ARG  |
| 1   | K     | 310 | LEU  |
| 1   | K     | 318 | ILE  |
| 1   | K     | 359 | LEU  |
| 1   | K     | 361 | ASN  |
| 1   | K     | 368 | LEU  |
| 1   | L     | 141 | PHE  |
| 1   | L     | 142 | GLU  |
| 1   | L     | 147 | LYS  |
| 1   | L     | 150 | LEU  |
| 1   | L     | 151 | GLU  |
| 1   | L     | 166 | THR  |
| 1   | L     | 178 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 189 | GLU  |
| 1   | L     | 192 | VAL  |
| 1   | L     | 211 | TYR  |
| 1   | L     | 217 | THR  |
| 1   | L     | 227 | PHE  |
| 1   | L     | 229 | LEU  |
| 1   | L     | 238 | ASP  |
| 1   | L     | 242 | GLU  |
| 1   | L     | 245 | LEU  |
| 1   | L     | 251 | LEU  |
| 1   | L     | 253 | ARG  |
| 1   | L     | 259 | LYS  |
| 1   | L     | 263 | LEU  |
| 1   | L     | 266 | ARG  |
| 1   | L     | 273 | VAL  |
| 1   | L     | 274 | ARG  |
| 1   | L     | 279 | THR  |
| 1   | L     | 296 | LEU  |
| 1   | L     | 299 | ARG  |
| 1   | L     | 305 | ILE  |
| 1   | L     | 315 | GLU  |
| 1   | L     | 318 | ILE  |
| 1   | L     | 334 | LYS  |
| 1   | L     | 335 | GLU  |
| 1   | L     | 337 | GLU  |
| 1   | L     | 344 | GLN  |
| 1   | L     | 347 | LEU  |
| 1   | L     | 348 | LEU  |
| 1   | L     | 350 | TYR  |
| 1   | L     | 359 | LEU  |
| 1   | L     | 369 | PHE  |
| 1   | L     | 370 | SER  |
| 1   | L     | 383 | LEU  |
| 1   | M     | 145 | LYS  |
| 1   | M     | 146 | MET  |
| 1   | M     | 161 | CYS  |
| 1   | M     | 178 | ARG  |
| 1   | M     | 179 | LEU  |
| 1   | M     | 191 | PHE  |
| 1   | M     | 198 | SER  |
| 1   | M     | 201 | ARG  |
| 1   | M     | 203 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 205 | GLU  |
| 1   | M     | 211 | TYR  |
| 1   | M     | 224 | GLU  |
| 1   | M     | 227 | PHE  |
| 1   | M     | 229 | LEU  |
| 1   | M     | 246 | GLU  |
| 1   | M     | 248 | GLN  |
| 1   | M     | 251 | LEU  |
| 1   | M     | 274 | ARG  |
| 1   | M     | 276 | LEU  |
| 1   | M     | 311 | ARG  |
| 1   | M     | 312 | GLU  |
| 1   | M     | 322 | ASN  |
| 1   | M     | 356 | VAL  |
| 1   | M     | 359 | LEU  |
| 1   | M     | 361 | ASN  |
| 1   | M     | 363 | ILE  |
| 1   | M     | 368 | LEU  |
| 1   | M     | 374 | PHE  |
| 1   | N     | 138 | GLU  |
| 1   | N     | 148 | GLU  |
| 1   | N     | 152 | LYS  |
| 1   | N     | 189 | GLU  |
| 1   | N     | 194 | LEU  |
| 1   | N     | 201 | ARG  |
| 1   | N     | 205 | GLU  |
| 1   | N     | 207 | GLU  |
| 1   | N     | 212 | GLU  |
| 1   | N     | 227 | PHE  |
| 1   | N     | 229 | LEU  |
| 1   | N     | 239 | GLU  |
| 1   | N     | 246 | GLU  |
| 1   | N     | 262 | ARG  |
| 1   | N     | 263 | LEU  |
| 1   | N     | 269 | ILE  |
| 1   | N     | 281 | ARG  |
| 1   | N     | 295 | ASP  |
| 1   | N     | 296 | LEU  |
| 1   | N     | 314 | LYS  |
| 1   | N     | 318 | ILE  |
| 1   | N     | 320 | LEU  |
| 1   | N     | 346 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 356 | VAL  |
| 1   | N     | 359 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 181 | HIS  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 361 | ASN  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 322 | ASN  |
| 1   | B     | 355 | ASN  |
| 1   | B     | 361 | ASN  |
| 1   | C     | 355 | ASN  |
| 1   | C     | 361 | ASN  |
| 1   | D     | 181 | HIS  |
| 1   | D     | 248 | GLN  |
| 1   | D     | 282 | ASN  |
| 1   | D     | 355 | ASN  |
| 1   | D     | 361 | ASN  |
| 1   | E     | 181 | HIS  |
| 1   | E     | 272 | ASN  |
| 1   | E     | 361 | ASN  |
| 1   | F     | 181 | HIS  |
| 1   | F     | 195 | ASN  |
| 1   | F     | 282 | ASN  |
| 1   | G     | 181 | HIS  |
| 1   | G     | 282 | ASN  |
| 1   | G     | 361 | ASN  |
| 1   | H     | 282 | ASN  |
| 1   | H     | 344 | GLN  |
| 1   | I     | 195 | ASN  |
| 1   | I     | 282 | ASN  |
| 1   | I     | 361 | ASN  |
| 1   | J     | 181 | HIS  |
| 1   | J     | 282 | ASN  |
| 1   | J     | 323 | HIS  |
| 1   | K     | 181 | HIS  |
| 1   | K     | 272 | ASN  |
| 1   | K     | 282 | ASN  |
| 1   | K     | 361 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 181 | HIS  |
| 1   | L     | 272 | ASN  |
| 1   | L     | 361 | ASN  |
| 1   | M     | 181 | HIS  |
| 1   | M     | 248 | GLN  |
| 1   | M     | 282 | ASN  |
| 1   | M     | 361 | ASN  |
| 1   | N     | 181 | HIS  |
| 1   | N     | 248 | GLN  |
| 1   | N     | 282 | ASN  |
| 1   | N     | 322 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ADP  | B     | 7   | -    | 28,29,29     | 1.61 | 6 (21%)  | 43,45,45    | 2.03 | 9 (20%)  |
| 2   | ADP  | E     | 3   | -    | 28,29,29     | 1.76 | 5 (17%)  | 43,45,45    | 2.00 | 9 (20%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ADP  | F     | 4   | -    | 28,29,29     | 1.61 | 7 (25%)  | 43,45,45    | 2.01 | 10 (23%) |
| 2   | ADP  | H     | 14  | -    | 28,29,29     | 1.59 | 6 (21%)  | 43,45,45    | 2.00 | 9 (20%)  |
| 2   | ADP  | J     | 9   | -    | 28,29,29     | 1.66 | 8 (28%)  | 43,45,45    | 2.00 | 9 (20%)  |
| 2   | ADP  | K     | 10  | -    | 28,29,29     | 1.63 | 6 (21%)  | 43,45,45    | 2.05 | 8 (18%)  |
| 2   | ADP  | M     | 12  | -    | 28,29,29     | 1.70 | 3 (10%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | A     | 6   | -    | 28,29,29     | 1.76 | 7 (25%)  | 43,45,45    | 2.02 | 8 (18%)  |
| 2   | ADP  | I     | 8   | -    | 28,29,29     | 1.65 | 4 (14%)  | 43,45,45    | 1.99 | 10 (23%) |
| 2   | ADP  | G     | 5   | -    | 28,29,29     | 1.70 | 5 (17%)  | 43,45,45    | 2.05 | 10 (23%) |
| 2   | ADP  | N     | 13  | -    | 28,29,29     | 1.62 | 6 (21%)  | 43,45,45    | 2.00 | 9 (20%)  |
| 2   | ADP  | D     | 2   | -    | 28,29,29     | 1.83 | 7 (25%)  | 43,45,45    | 2.02 | 9 (20%)  |
| 2   | ADP  | C     | 1   | -    | 28,29,29     | 1.61 | 3 (10%)  | 43,45,45    | 2.00 | 7 (16%)  |
| 2   | ADP  | L     | 11  | -    | 28,29,29     | 1.64 | 6 (21%)  | 43,45,45    | 2.00 | 8 (18%)  |

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   | ADP  | B     | 7   | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | ADP  | E     | 3   | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | ADP  | F     | 4   | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | ADP  | H     | 14  | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | ADP  | J     | 9   | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 2   | ADP  | K     | 10  | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | M     | 12  | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 2   | ADP  | A     | 6   | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | I     | 8   | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | ADP  | G     | 5   | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 2   | ADP  | N     | 13  | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 2   | ADP  | D     | 2   | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | C     | 1   | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | ADP  | L     | 11  | -    | -       | 8/16/32/32 | 0/3/3/3 |

All (79) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | A     | 6   | ADP  | C5-N7  | -5.24 | 1.29        | 1.39     |
| 2   | C     | 1   | ADP  | C5-N7  | -4.93 | 1.30        | 1.39     |
| 2   | M     | 12  | ADP  | C5-N7  | -4.86 | 1.30        | 1.39     |
| 2   | D     | 2   | ADP  | PA-O3A | -4.85 | 1.54        | 1.59     |
| 2   | E     | 3   | ADP  | C5-N7  | -4.69 | 1.30        | 1.39     |
| 2   | L     | 11  | ADP  | C5-N7  | -4.67 | 1.30        | 1.39     |
| 2   | K     | 10  | ADP  | C5-N7  | -4.58 | 1.30        | 1.39     |
| 2   | G     | 5   | ADP  | C5-N7  | -4.53 | 1.30        | 1.39     |
| 2   | I     | 8   | ADP  | C5-N7  | -4.50 | 1.30        | 1.39     |
| 2   | F     | 4   | ADP  | C5-N7  | -4.41 | 1.31        | 1.39     |
| 2   | B     | 7   | ADP  | C5-N7  | -4.34 | 1.31        | 1.39     |
| 2   | H     | 14  | ADP  | C5-N7  | -4.33 | 1.31        | 1.39     |
| 2   | N     | 13  | ADP  | C5-N7  | -4.19 | 1.31        | 1.39     |
| 2   | J     | 9   | ADP  | C5-N7  | -4.17 | 1.31        | 1.39     |
| 2   | D     | 2   | ADP  | C5-N7  | -3.97 | 1.31        | 1.39     |
| 2   | M     | 12  | ADP  | C4-N9  | -3.81 | 1.29        | 1.37     |
| 2   | E     | 3   | ADP  | PA-O3A | -3.52 | 1.55        | 1.59     |
| 2   | G     | 5   | ADP  | C4-N9  | -3.26 | 1.30        | 1.37     |
| 2   | E     | 3   | ADP  | C4-N9  | -3.15 | 1.31        | 1.37     |
| 2   | I     | 8   | ADP  | C4-N9  | -3.14 | 1.31        | 1.37     |
| 2   | M     | 12  | ADP  | PA-O3A | -3.05 | 1.56        | 1.59     |
| 2   | A     | 6   | ADP  | C4-N9  | -3.02 | 1.31        | 1.37     |
| 2   | F     | 4   | ADP  | C4-N9  | -2.70 | 1.32        | 1.37     |
| 2   | C     | 1   | ADP  | C4-N9  | -2.69 | 1.32        | 1.37     |
| 2   | G     | 5   | ADP  | PA-O3A | -2.63 | 1.56        | 1.59     |
| 2   | D     | 2   | ADP  | C4-N9  | -2.60 | 1.32        | 1.37     |
| 2   | F     | 4   | ADP  | C5-C4  | 2.59  | 1.43        | 1.39     |
| 2   | J     | 9   | ADP  | C4-N9  | -2.58 | 1.32        | 1.37     |
| 2   | L     | 11  | ADP  | C4-N9  | -2.55 | 1.32        | 1.37     |
| 2   | N     | 13  | ADP  | C4-N9  | -2.54 | 1.32        | 1.37     |
| 2   | N     | 13  | ADP  | C5-C4  | 2.52  | 1.43        | 1.39     |
| 2   | B     | 7   | ADP  | C5-C4  | 2.51  | 1.43        | 1.39     |
| 2   | J     | 9   | ADP  | PA-O3A | -2.50 | 1.56        | 1.59     |
| 2   | B     | 7   | ADP  | C1'-N9 | 2.46  | 1.53        | 1.46     |
| 2   | K     | 10  | ADP  | C4-N9  | -2.44 | 1.32        | 1.37     |
| 2   | J     | 9   | ADP  | C5-C4  | 2.43  | 1.43        | 1.39     |
| 2   | C     | 1   | ADP  | C5-C4  | 2.43  | 1.43        | 1.39     |
| 2   | H     | 14  | ADP  | C4-N3  | 2.43  | 1.39        | 1.34     |
| 2   | L     | 11  | ADP  | C5-C4  | 2.40  | 1.43        | 1.39     |
| 2   | H     | 14  | ADP  | C1'-N9 | 2.40  | 1.53        | 1.46     |
| 2   | H     | 14  | ADP  | C5-C4  | 2.40  | 1.43        | 1.39     |
| 2   | I     | 8   | ADP  | C5-C4  | 2.37  | 1.43        | 1.39     |
| 2   | D     | 2   | ADP  | C4-N3  | 2.36  | 1.38        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 2   | ADP  | C5-C4   | 2.34  | 1.43        | 1.39     |
| 2   | K     | 10  | ADP  | C5-C4   | 2.32  | 1.43        | 1.39     |
| 2   | N     | 13  | ADP  | C1'-N9  | 2.29  | 1.52        | 1.46     |
| 2   | K     | 10  | ADP  | C5'-C4' | 2.29  | 1.58        | 1.51     |
| 2   | H     | 14  | ADP  | C4-N9   | -2.29 | 1.32        | 1.37     |
| 2   | K     | 10  | ADP  | C4-N3   | 2.28  | 1.38        | 1.34     |
| 2   | B     | 7   | ADP  | C4-N9   | -2.28 | 1.33        | 1.37     |
| 2   | A     | 6   | ADP  | C5-C4   | 2.26  | 1.43        | 1.39     |
| 2   | N     | 13  | ADP  | C4-N3   | 2.24  | 1.38        | 1.34     |
| 2   | A     | 6   | ADP  | PA-O3A  | -2.24 | 1.57        | 1.59     |
| 2   | L     | 11  | ADP  | C2-N1   | 2.24  | 1.37        | 1.33     |
| 2   | B     | 7   | ADP  | C4-N3   | 2.24  | 1.38        | 1.34     |
| 2   | E     | 3   | ADP  | PA-O2A  | -2.24 | 1.45        | 1.55     |
| 2   | J     | 9   | ADP  | C4-N3   | 2.24  | 1.38        | 1.34     |
| 2   | D     | 2   | ADP  | C1'-N9  | 2.24  | 1.52        | 1.46     |
| 2   | L     | 11  | ADP  | C4-N3   | 2.23  | 1.38        | 1.34     |
| 2   | I     | 8   | ADP  | C5'-C4' | 2.22  | 1.58        | 1.51     |
| 2   | K     | 10  | ADP  | C1'-N9  | 2.22  | 1.52        | 1.46     |
| 2   | E     | 3   | ADP  | C4-N3   | 2.21  | 1.38        | 1.34     |
| 2   | A     | 6   | ADP  | C2-N1   | 2.20  | 1.37        | 1.33     |
| 2   | J     | 9   | ADP  | C5'-C4' | 2.20  | 1.58        | 1.51     |
| 2   | N     | 13  | ADP  | C5'-C4' | 2.17  | 1.58        | 1.51     |
| 2   | H     | 14  | ADP  | C5'-C4' | 2.15  | 1.58        | 1.51     |
| 2   | F     | 4   | ADP  | PA-O3A  | -2.15 | 1.57        | 1.59     |
| 2   | L     | 11  | ADP  | C2-N3   | 2.13  | 1.37        | 1.33     |
| 2   | B     | 7   | ADP  | C5'-C4' | 2.12  | 1.57        | 1.51     |
| 2   | D     | 2   | ADP  | PA-O2A  | -2.12 | 1.45        | 1.55     |
| 2   | J     | 9   | ADP  | C2-N1   | 2.10  | 1.37        | 1.33     |
| 2   | J     | 9   | ADP  | C1'-N9  | 2.10  | 1.52        | 1.46     |
| 2   | F     | 4   | ADP  | C5'-C4' | 2.06  | 1.57        | 1.51     |
| 2   | A     | 6   | ADP  | C4-N3   | 2.06  | 1.38        | 1.34     |
| 2   | A     | 6   | ADP  | C5'-C4' | 2.03  | 1.57        | 1.51     |
| 2   | F     | 4   | ADP  | PA-O2A  | -2.02 | 1.46        | 1.55     |
| 2   | F     | 4   | ADP  | C1'-N9  | 2.02  | 1.51        | 1.46     |
| 2   | G     | 5   | ADP  | C2-N1   | 2.00  | 1.37        | 1.33     |
| 2   | G     | 5   | ADP  | C5'-C4' | 2.00  | 1.57        | 1.51     |

All (125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | E     | 3   | ADP  | N3-C2-N1 | -7.19 | 117.70      | 128.58   |
| 2   | K     | 10  | ADP  | N3-C2-N1 | -6.98 | 118.01      | 128.58   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | G     | 5   | ADP  | N3-C2-N1 | -6.95 | 118.05      | 128.58   |
| 2   | D     | 2   | ADP  | N3-C2-N1 | -6.91 | 118.12      | 128.58   |
| 2   | J     | 9   | ADP  | N3-C2-N1 | -6.88 | 118.17      | 128.58   |
| 2   | H     | 14  | ADP  | N3-C2-N1 | -6.88 | 118.17      | 128.58   |
| 2   | A     | 6   | ADP  | N3-C2-N1 | -6.85 | 118.22      | 128.58   |
| 2   | L     | 11  | ADP  | N3-C2-N1 | -6.81 | 118.27      | 128.58   |
| 2   | B     | 7   | ADP  | N3-C2-N1 | -6.80 | 118.29      | 128.58   |
| 2   | N     | 13  | ADP  | N3-C2-N1 | -6.80 | 118.30      | 128.58   |
| 2   | M     | 12  | ADP  | N3-C2-N1 | -6.76 | 118.35      | 128.58   |
| 2   | I     | 8   | ADP  | N3-C2-N1 | -6.76 | 118.35      | 128.58   |
| 2   | F     | 4   | ADP  | N3-C2-N1 | -6.69 | 118.45      | 128.58   |
| 2   | C     | 1   | ADP  | N3-C2-N1 | -6.57 | 118.64      | 128.58   |
| 2   | H     | 14  | ADP  | C5-C4-N3 | -5.34 | 119.37      | 126.72   |
| 2   | K     | 10  | ADP  | C5-C4-N3 | -5.28 | 119.44      | 126.72   |
| 2   | N     | 13  | ADP  | C5-C4-N3 | -5.20 | 119.56      | 126.72   |
| 2   | B     | 7   | ADP  | C5-C4-N3 | -5.19 | 119.58      | 126.72   |
| 2   | F     | 4   | ADP  | C5-C4-N3 | -5.17 | 119.60      | 126.72   |
| 2   | C     | 1   | ADP  | C5-C4-N3 | -5.10 | 119.70      | 126.72   |
| 2   | D     | 2   | ADP  | C5-C4-N3 | -5.06 | 119.75      | 126.72   |
| 2   | L     | 11  | ADP  | C5-C4-N3 | -5.03 | 119.79      | 126.72   |
| 2   | A     | 6   | ADP  | C5-C4-N3 | -5.00 | 119.83      | 126.72   |
| 2   | J     | 9   | ADP  | C5-C4-N3 | -5.00 | 119.83      | 126.72   |
| 2   | E     | 3   | ADP  | C5-C4-N3 | -4.88 | 119.99      | 126.72   |
| 2   | I     | 8   | ADP  | C5-C4-N3 | -4.88 | 119.99      | 126.72   |
| 2   | G     | 5   | ADP  | C5-C4-N3 | -4.82 | 120.08      | 126.72   |
| 2   | D     | 2   | ADP  | C2-N3-C4 | 4.52  | 122.86      | 111.83   |
| 2   | N     | 13  | ADP  | C2-N3-C4 | 4.48  | 122.78      | 111.83   |
| 2   | H     | 14  | ADP  | C2-N3-C4 | 4.47  | 122.75      | 111.83   |
| 2   | J     | 9   | ADP  | C2-N3-C4 | 4.47  | 122.75      | 111.83   |
| 2   | B     | 7   | ADP  | C2-N3-C4 | 4.46  | 122.72      | 111.83   |
| 2   | K     | 10  | ADP  | C2-N3-C4 | 4.45  | 122.70      | 111.83   |
| 2   | F     | 4   | ADP  | C2-N3-C4 | 4.43  | 122.64      | 111.83   |
| 2   | G     | 5   | ADP  | C2-N3-C4 | 4.40  | 122.57      | 111.83   |
| 2   | I     | 8   | ADP  | C2-N3-C4 | 4.35  | 122.45      | 111.83   |
| 2   | E     | 3   | ADP  | C2-N3-C4 | 4.35  | 122.45      | 111.83   |
| 2   | L     | 11  | ADP  | N3-C4-N9 | 4.33  | 134.53      | 127.17   |
| 2   | A     | 6   | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | L     | 11  | ADP  | C2-N3-C4 | 4.28  | 122.28      | 111.83   |
| 2   | K     | 10  | ADP  | N3-C4-N9 | 4.22  | 134.34      | 127.17   |
| 2   | C     | 1   | ADP  | C2-N3-C4 | 4.19  | 122.07      | 111.83   |
| 2   | M     | 12  | ADP  | C5-C4-N3 | -4.19 | 120.95      | 126.72   |
| 2   | A     | 6   | ADP  | C2-N3-C4 | 4.18  | 122.04      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 1   | ADP  | N3-C4-N9    | 4.16  | 134.23      | 127.17   |
| 2   | H     | 14  | ADP  | N3-C4-N9    | 4.15  | 134.22      | 127.17   |
| 2   | E     | 3   | ADP  | N3-C4-N9    | 4.09  | 134.13      | 127.17   |
| 2   | M     | 12  | ADP  | C2-N3-C4    | 4.04  | 121.71      | 111.83   |
| 2   | B     | 7   | ADP  | N3-C4-N9    | 3.94  | 133.87      | 127.17   |
| 2   | N     | 13  | ADP  | N3-C4-N9    | 3.91  | 133.82      | 127.17   |
| 2   | F     | 4   | ADP  | N3-C4-N9    | 3.89  | 133.79      | 127.17   |
| 2   | J     | 9   | ADP  | N3-C4-N9    | 3.79  | 133.62      | 127.17   |
| 2   | G     | 5   | ADP  | N3-C4-N9    | 3.77  | 133.58      | 127.17   |
| 2   | I     | 8   | ADP  | N3-C4-N9    | 3.76  | 133.57      | 127.17   |
| 2   | D     | 2   | ADP  | N3-C4-N9    | 3.75  | 133.55      | 127.17   |
| 2   | C     | 1   | ADP  | C5-N7-C8    | 3.39  | 108.78      | 103.45   |
| 2   | B     | 7   | ADP  | C5-N7-C8    | 3.36  | 108.74      | 103.45   |
| 2   | L     | 11  | ADP  | C5-N7-C8    | 3.35  | 108.72      | 103.45   |
| 2   | K     | 10  | ADP  | C5-N7-C8    | 3.32  | 108.67      | 103.45   |
| 2   | F     | 4   | ADP  | C5-N7-C8    | 3.31  | 108.66      | 103.45   |
| 2   | M     | 12  | ADP  | N9-C8-N7    | -3.31 | 109.25      | 113.94   |
| 2   | N     | 13  | ADP  | C5-N7-C8    | 3.30  | 108.64      | 103.45   |
| 2   | J     | 9   | ADP  | C5-N7-C8    | 3.30  | 108.63      | 103.45   |
| 2   | G     | 5   | ADP  | C5-N7-C8    | 3.29  | 108.62      | 103.45   |
| 2   | D     | 2   | ADP  | C5-N7-C8    | 3.29  | 108.61      | 103.45   |
| 2   | H     | 14  | ADP  | C5-N7-C8    | 3.27  | 108.58      | 103.45   |
| 2   | M     | 12  | ADP  | C5-N7-C8    | 3.25  | 108.55      | 103.45   |
| 2   | I     | 8   | ADP  | C5-N7-C8    | 3.18  | 108.45      | 103.45   |
| 2   | G     | 5   | ADP  | N9-C8-N7    | -3.16 | 109.45      | 113.94   |
| 2   | M     | 12  | ADP  | N3-C4-N9    | 3.07  | 132.38      | 127.17   |
| 2   | A     | 6   | ADP  | C5-N7-C8    | 3.04  | 108.23      | 103.45   |
| 2   | E     | 3   | ADP  | C5-N7-C8    | 3.01  | 108.19      | 103.45   |
| 2   | E     | 3   | ADP  | N9-C8-N7    | -2.93 | 109.78      | 113.94   |
| 2   | F     | 4   | ADP  | C4-C5-N7    | -2.93 | 107.24      | 110.58   |
| 2   | D     | 2   | ADP  | C4-C5-N7    | -2.92 | 107.25      | 110.58   |
| 2   | D     | 2   | ADP  | N9-C8-N7    | -2.89 | 109.83      | 113.94   |
| 2   | B     | 7   | ADP  | C2'-C3'-C4' | 2.89  | 108.19      | 102.61   |
| 2   | J     | 9   | ADP  | N9-C8-N7    | -2.85 | 109.90      | 113.94   |
| 2   | N     | 13  | ADP  | C4-C5-N7    | -2.84 | 107.34      | 110.58   |
| 2   | J     | 9   | ADP  | C4-C5-N7    | -2.84 | 107.34      | 110.58   |
| 2   | B     | 7   | ADP  | C4-C5-N7    | -2.82 | 107.36      | 110.58   |
| 2   | N     | 13  | ADP  | N9-C8-N7    | -2.81 | 109.94      | 113.94   |
| 2   | M     | 12  | ADP  | C4-C5-N7    | -2.80 | 107.38      | 110.58   |
| 2   | I     | 8   | ADP  | N9-C8-N7    | -2.79 | 109.98      | 113.94   |
| 2   | A     | 6   | ADP  | C2'-C3'-C4' | 2.72  | 107.87      | 102.61   |
| 2   | G     | 5   | ADP  | C4-C5-N7    | -2.71 | 107.48      | 110.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | I     | 8   | ADP  | C4-C5-N7    | -2.70 | 107.50      | 110.58   |
| 2   | K     | 10  | ADP  | C2'-C3'-C4' | 2.69  | 107.81      | 102.61   |
| 2   | K     | 10  | ADP  | N9-C8-N7    | -2.69 | 110.12      | 113.94   |
| 2   | F     | 4   | ADP  | N9-C8-N7    | -2.68 | 110.14      | 113.94   |
| 2   | B     | 7   | ADP  | N9-C8-N7    | -2.66 | 110.17      | 113.94   |
| 2   | G     | 5   | ADP  | C2'-C3'-C4' | 2.63  | 107.69      | 102.61   |
| 2   | C     | 1   | ADP  | C4-C5-N7    | -2.62 | 107.59      | 110.58   |
| 2   | L     | 11  | ADP  | N9-C8-N7    | -2.62 | 110.22      | 113.94   |
| 2   | H     | 14  | ADP  | N9-C8-N7    | -2.61 | 110.23      | 113.94   |
| 2   | H     | 14  | ADP  | C4-C5-N7    | -2.60 | 107.61      | 110.58   |
| 2   | C     | 1   | ADP  | N9-C8-N7    | -2.58 | 110.28      | 113.94   |
| 2   | K     | 10  | ADP  | C4-C5-N7    | -2.56 | 107.65      | 110.58   |
| 2   | G     | 5   | ADP  | O3B-PB-O3A  | 2.54  | 113.15      | 104.64   |
| 2   | D     | 2   | ADP  | C2'-C3'-C4' | 2.53  | 107.50      | 102.61   |
| 2   | L     | 11  | ADP  | C4-C5-N7    | -2.48 | 107.75      | 110.58   |
| 2   | F     | 4   | ADP  | O4'-C4'-C5' | -2.48 | 101.40      | 109.33   |
| 2   | A     | 6   | ADP  | N9-C8-N7    | -2.38 | 110.55      | 113.94   |
| 2   | L     | 11  | ADP  | O4'-C4'-C5' | -2.34 | 101.83      | 109.33   |
| 2   | J     | 9   | ADP  | C2'-C3'-C4' | 2.34  | 107.14      | 102.61   |
| 2   | M     | 12  | ADP  | C4-N9-C8    | 2.29  | 108.14      | 105.74   |
| 2   | G     | 5   | ADP  | C4-N9-C8    | 2.26  | 108.11      | 105.74   |
| 2   | I     | 8   | ADP  | PA-O5'-C5'  | 2.19  | 133.89      | 121.35   |
| 2   | M     | 12  | ADP  | C2-N1-C6    | 2.19  | 122.32      | 118.73   |
| 2   | I     | 8   | ADP  | O5'-C5'-C4' | -2.18 | 101.58      | 108.99   |
| 2   | H     | 14  | ADP  | C2'-C3'-C4' | 2.16  | 106.79      | 102.61   |
| 2   | E     | 3   | ADP  | C4-N9-C8    | 2.15  | 108.00      | 105.74   |
| 2   | E     | 3   | ADP  | C4-C5-N7    | -2.12 | 108.16      | 110.58   |
| 2   | F     | 4   | ADP  | O2'-C2'-C1' | 2.11  | 117.38      | 110.10   |
| 2   | N     | 13  | ADP  | C2'-C3'-C4' | 2.09  | 106.64      | 102.61   |
| 2   | E     | 3   | ADP  | C2-N1-C6    | 2.09  | 122.16      | 118.73   |
| 2   | F     | 4   | ADP  | C2-N1-C6    | 2.09  | 122.16      | 118.73   |
| 2   | B     | 7   | ADP  | C2-N1-C6    | 2.06  | 122.12      | 118.73   |
| 2   | D     | 2   | ADP  | C2-N1-C6    | 2.06  | 122.11      | 118.73   |
| 2   | I     | 8   | ADP  | C2-N1-C6    | 2.06  | 122.11      | 118.73   |
| 2   | M     | 12  | ADP  | C2'-C3'-C4' | 2.05  | 106.57      | 102.61   |
| 2   | N     | 13  | ADP  | C2-N1-C6    | 2.04  | 122.09      | 118.73   |
| 2   | A     | 6   | ADP  | C4-C5-N7    | -2.03 | 108.26      | 110.58   |
| 2   | J     | 9   | ADP  | C2-N1-C6    | 2.02  | 122.05      | 118.73   |
| 2   | H     | 14  | ADP  | C2-N1-C6    | 2.01  | 122.03      | 118.73   |

There are no chirality outliers.

All (92) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 6   | ADP  | PA-O3A-PB-O2B   |
| 2   | A     | 6   | ADP  | C5'-O5'-PA-O1A  |
| 2   | A     | 6   | ADP  | C5'-O5'-PA-O2A  |
| 2   | A     | 6   | ADP  | C5'-O5'-PA-O3A  |
| 2   | A     | 6   | ADP  | O4'-C4'-C5'-O5' |
| 2   | B     | 7   | ADP  | C5'-O5'-PA-O1A  |
| 2   | B     | 7   | ADP  | C5'-O5'-PA-O2A  |
| 2   | B     | 7   | ADP  | C5'-O5'-PA-O3A  |
| 2   | C     | 1   | ADP  | C5'-O5'-PA-O1A  |
| 2   | C     | 1   | ADP  | C5'-O5'-PA-O2A  |
| 2   | C     | 1   | ADP  | C5'-O5'-PA-O3A  |
| 2   | D     | 2   | ADP  | PA-O3A-PB-O2B   |
| 2   | D     | 2   | ADP  | C5'-O5'-PA-O1A  |
| 2   | D     | 2   | ADP  | C5'-O5'-PA-O2A  |
| 2   | D     | 2   | ADP  | C5'-O5'-PA-O3A  |
| 2   | E     | 3   | ADP  | PA-O3A-PB-O2B   |
| 2   | E     | 3   | ADP  | C5'-O5'-PA-O1A  |
| 2   | E     | 3   | ADP  | C5'-O5'-PA-O2A  |
| 2   | E     | 3   | ADP  | C5'-O5'-PA-O3A  |
| 2   | F     | 4   | ADP  | C5'-O5'-PA-O1A  |
| 2   | F     | 4   | ADP  | C5'-O5'-PA-O2A  |
| 2   | F     | 4   | ADP  | C5'-O5'-PA-O3A  |
| 2   | G     | 5   | ADP  | C5'-O5'-PA-O1A  |
| 2   | G     | 5   | ADP  | C5'-O5'-PA-O2A  |
| 2   | G     | 5   | ADP  | C5'-O5'-PA-O3A  |
| 2   | H     | 14  | ADP  | C5'-O5'-PA-O1A  |
| 2   | H     | 14  | ADP  | C5'-O5'-PA-O2A  |
| 2   | H     | 14  | ADP  | C5'-O5'-PA-O3A  |
| 2   | H     | 14  | ADP  | O4'-C4'-C5'-O5' |
| 2   | I     | 8   | ADP  | C5'-O5'-PA-O1A  |
| 2   | I     | 8   | ADP  | C5'-O5'-PA-O2A  |
| 2   | I     | 8   | ADP  | C5'-O5'-PA-O3A  |
| 2   | J     | 9   | ADP  | PA-O3A-PB-O2B   |
| 2   | J     | 9   | ADP  | C5'-O5'-PA-O1A  |
| 2   | J     | 9   | ADP  | C5'-O5'-PA-O2A  |
| 2   | J     | 9   | ADP  | C5'-O5'-PA-O3A  |
| 2   | K     | 10  | ADP  | PA-O3A-PB-O2B   |
| 2   | K     | 10  | ADP  | C5'-O5'-PA-O1A  |
| 2   | K     | 10  | ADP  | C5'-O5'-PA-O2A  |
| 2   | K     | 10  | ADP  | C5'-O5'-PA-O3A  |
| 2   | L     | 11  | ADP  | PA-O3A-PB-O2B   |
| 2   | L     | 11  | ADP  | C5'-O5'-PA-O1A  |
| 2   | L     | 11  | ADP  | C5'-O5'-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | L     | 11  | ADP  | C5'-O5'-PA-O3A  |
| 2   | M     | 12  | ADP  | C5'-O5'-PA-O1A  |
| 2   | M     | 12  | ADP  | C5'-O5'-PA-O2A  |
| 2   | M     | 12  | ADP  | C5'-O5'-PA-O3A  |
| 2   | N     | 13  | ADP  | PA-O3A-PB-O2B   |
| 2   | N     | 13  | ADP  | C5'-O5'-PA-O1A  |
| 2   | N     | 13  | ADP  | C5'-O5'-PA-O2A  |
| 2   | N     | 13  | ADP  | C5'-O5'-PA-O3A  |
| 2   | H     | 14  | ADP  | C3'-C4'-C5'-O5' |
| 2   | A     | 6   | ADP  | C3'-C4'-C5'-O5' |
| 2   | B     | 7   | ADP  | O4'-C4'-C5'-O5' |
| 2   | C     | 1   | ADP  | O4'-C4'-C5'-O5' |
| 2   | C     | 1   | ADP  | C3'-C4'-C5'-O5' |
| 2   | D     | 2   | ADP  | O4'-C4'-C5'-O5' |
| 2   | D     | 2   | ADP  | C3'-C4'-C5'-O5' |
| 2   | E     | 3   | ADP  | C3'-C4'-C5'-O5' |
| 2   | F     | 4   | ADP  | O4'-C4'-C5'-O5' |
| 2   | F     | 4   | ADP  | C3'-C4'-C5'-O5' |
| 2   | I     | 8   | ADP  | O4'-C4'-C5'-O5' |
| 2   | I     | 8   | ADP  | C3'-C4'-C5'-O5' |
| 2   | J     | 9   | ADP  | O4'-C4'-C5'-O5' |
| 2   | J     | 9   | ADP  | C3'-C4'-C5'-O5' |
| 2   | K     | 10  | ADP  | O4'-C4'-C5'-O5' |
| 2   | K     | 10  | ADP  | C3'-C4'-C5'-O5' |
| 2   | L     | 11  | ADP  | O4'-C4'-C5'-O5' |
| 2   | L     | 11  | ADP  | C3'-C4'-C5'-O5' |
| 2   | N     | 13  | ADP  | O4'-C4'-C5'-O5' |
| 2   | N     | 13  | ADP  | C3'-C4'-C5'-O5' |
| 2   | G     | 5   | ADP  | O4'-C4'-C5'-O5' |
| 2   | G     | 5   | ADP  | C3'-C4'-C5'-O5' |
| 2   | E     | 3   | ADP  | O4'-C4'-C5'-O5' |
| 2   | M     | 12  | ADP  | O4'-C4'-C5'-O5' |
| 2   | M     | 12  | ADP  | C3'-C4'-C5'-O5' |
| 2   | C     | 1   | ADP  | PA-O3A-PB-O1B   |
| 2   | F     | 4   | ADP  | PA-O3A-PB-O1B   |
| 2   | H     | 14  | ADP  | PA-O3A-PB-O1B   |
| 2   | I     | 8   | ADP  | PA-O3A-PB-O1B   |
| 2   | B     | 7   | ADP  | C3'-C4'-C5'-O5' |
| 2   | D     | 2   | ADP  | PA-O3A-PB-O3B   |
| 2   | B     | 7   | ADP  | PB-O3A-PA-O2A   |
| 2   | A     | 6   | ADP  | PA-O3A-PB-O1B   |
| 2   | K     | 10  | ADP  | PA-O3A-PB-O1B   |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | A     | 6   | ADP  | PA-O3A-PB-O3B |
| 2   | K     | 10  | ADP  | PA-O3A-PB-O3B |
| 2   | L     | 11  | ADP  | PA-O3A-PB-O3B |
| 2   | N     | 13  | ADP  | PA-O3A-PB-O3B |
| 2   | D     | 2   | ADP  | PA-O3A-PB-O1B |
| 2   | J     | 9   | ADP  | PA-O3A-PB-O1B |
| 2   | L     | 11  | ADP  | PA-O3A-PB-O1B |

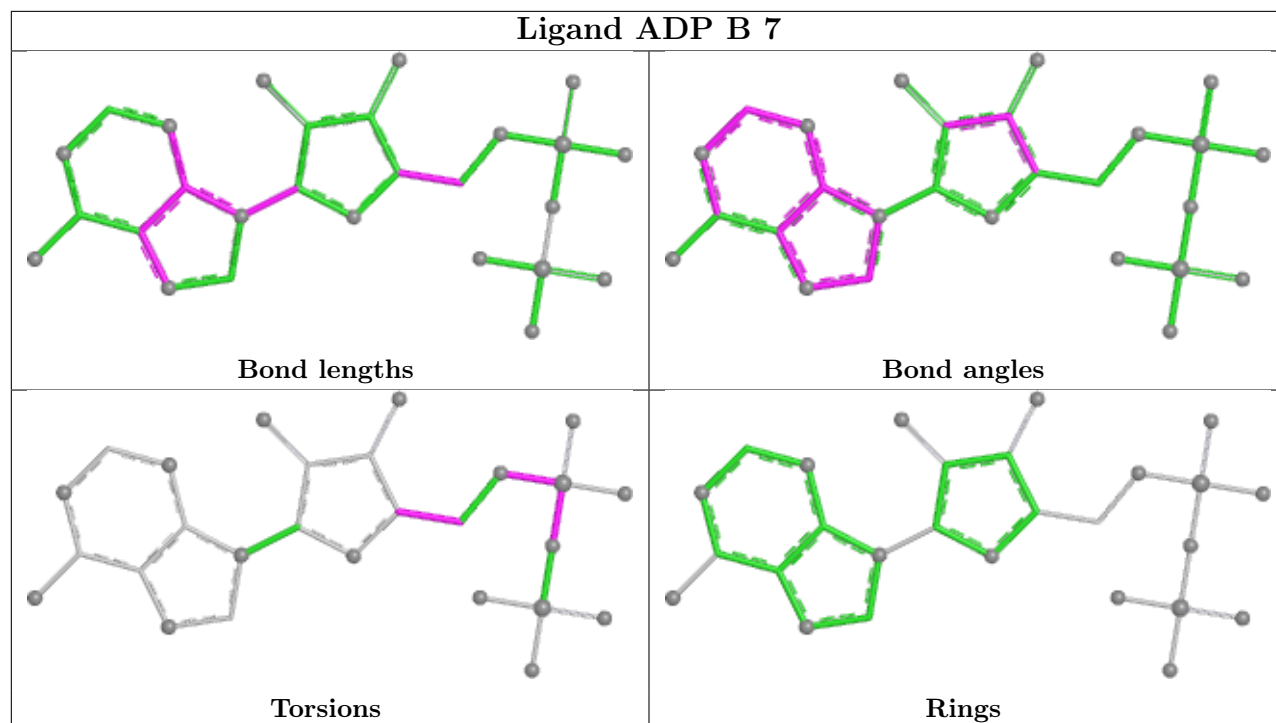
There are no ring outliers.

13 monomers are involved in 47 short contacts:

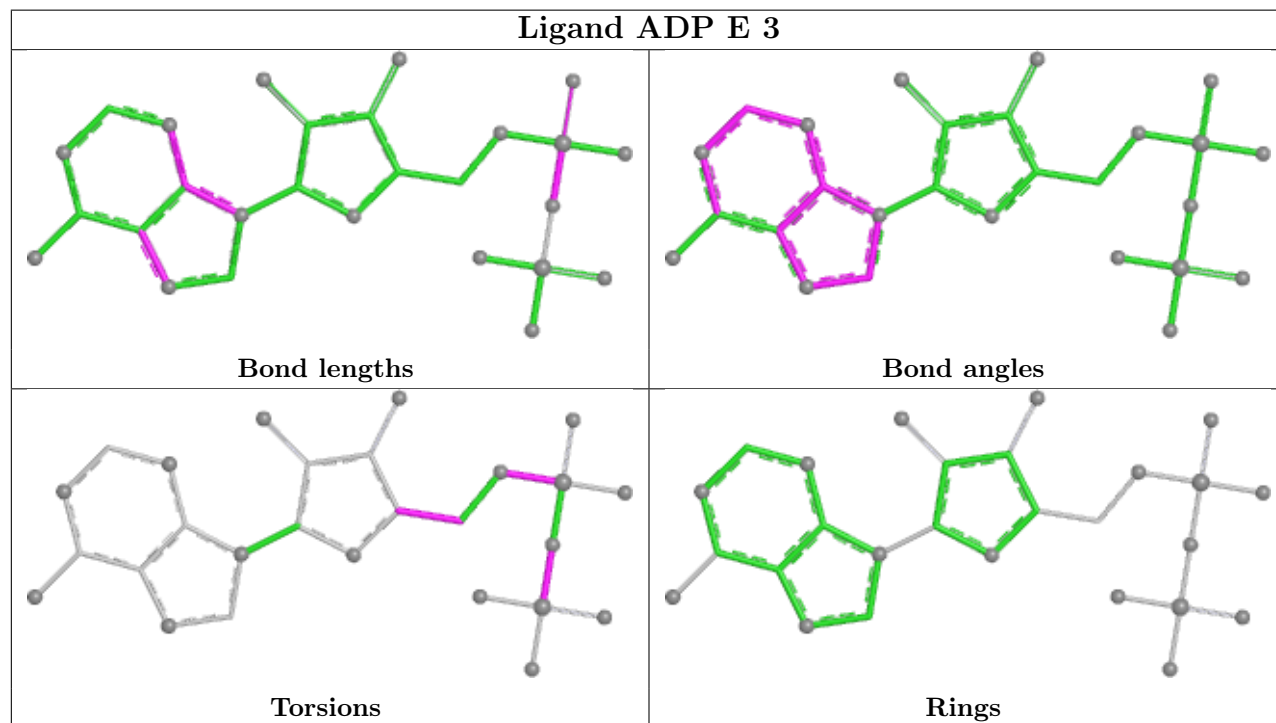
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 7   | ADP  | 1       | 0            |
| 2   | E     | 3   | ADP  | 3       | 0            |
| 2   | F     | 4   | ADP  | 7       | 0            |
| 2   | H     | 14  | ADP  | 3       | 0            |
| 2   | J     | 9   | ADP  | 1       | 0            |
| 2   | K     | 10  | ADP  | 1       | 0            |
| 2   | M     | 12  | ADP  | 6       | 0            |
| 2   | A     | 6   | ADP  | 2       | 0            |
| 2   | I     | 8   | ADP  | 5       | 0            |
| 2   | N     | 13  | ADP  | 2       | 0            |
| 2   | D     | 2   | ADP  | 6       | 0            |
| 2   | C     | 1   | ADP  | 4       | 0            |
| 2   | L     | 11  | ADP  | 6       | 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.

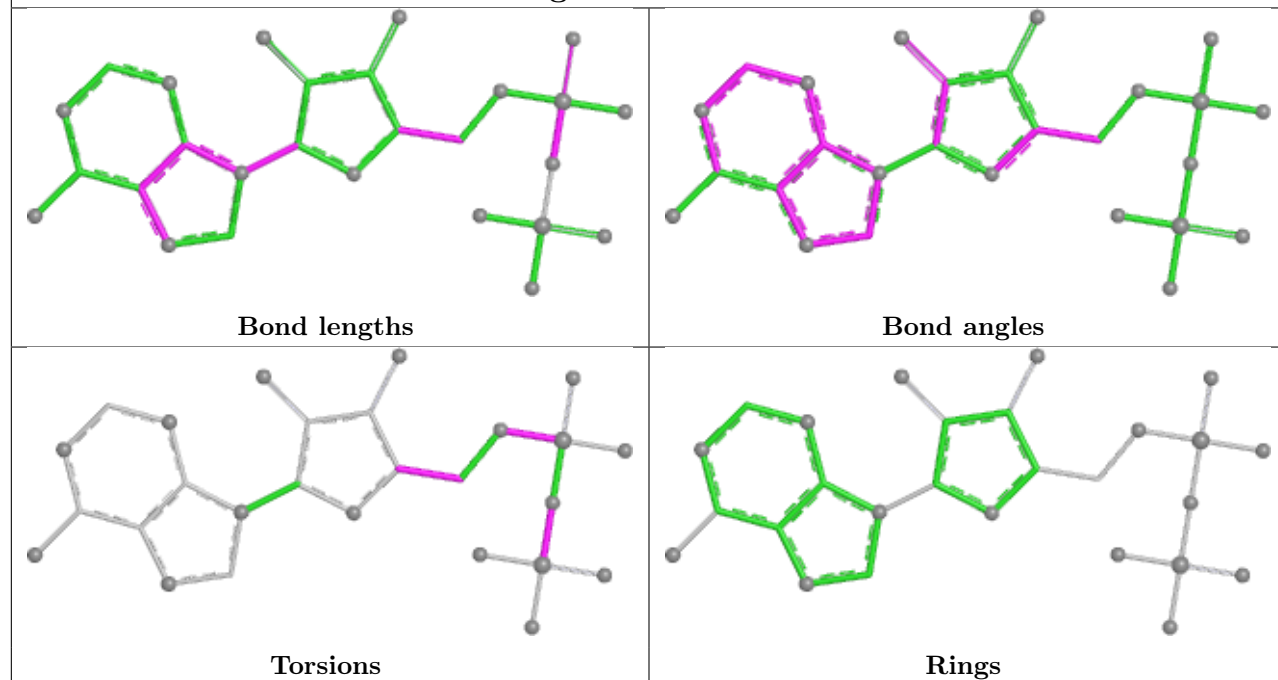
## Ligand ADP B 7



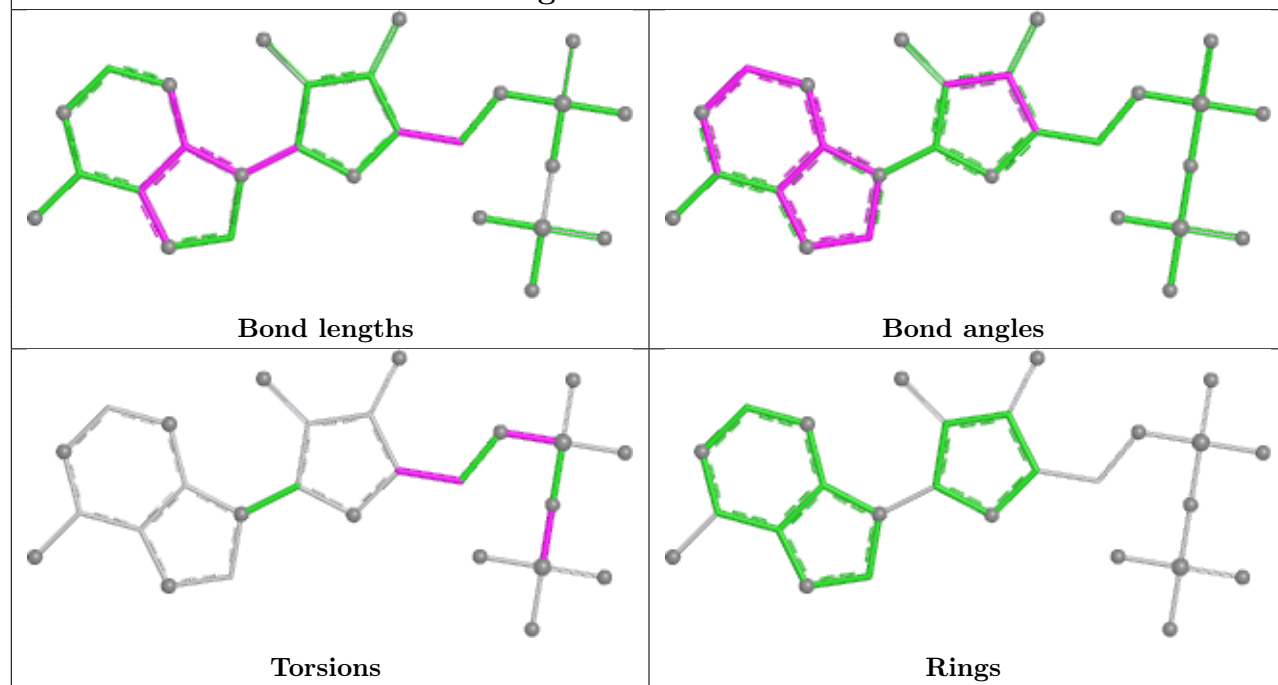
## Ligand ADP E 3



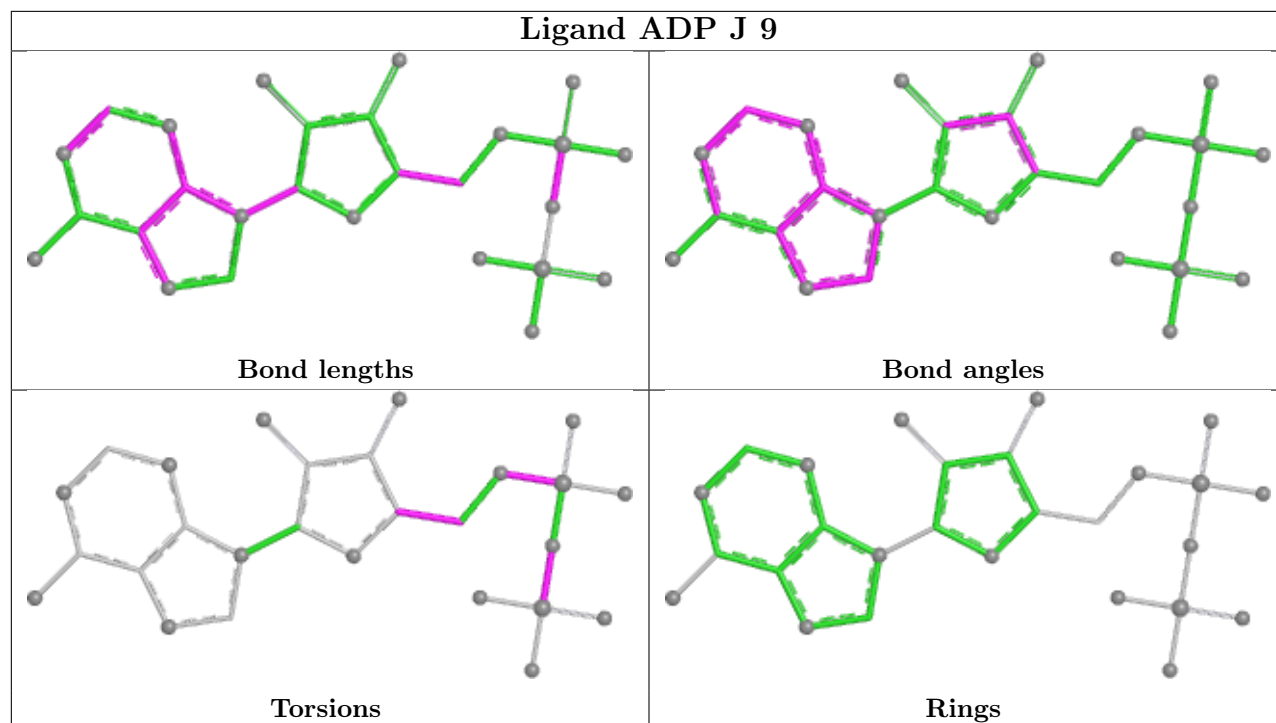
## Ligand ADP F 4



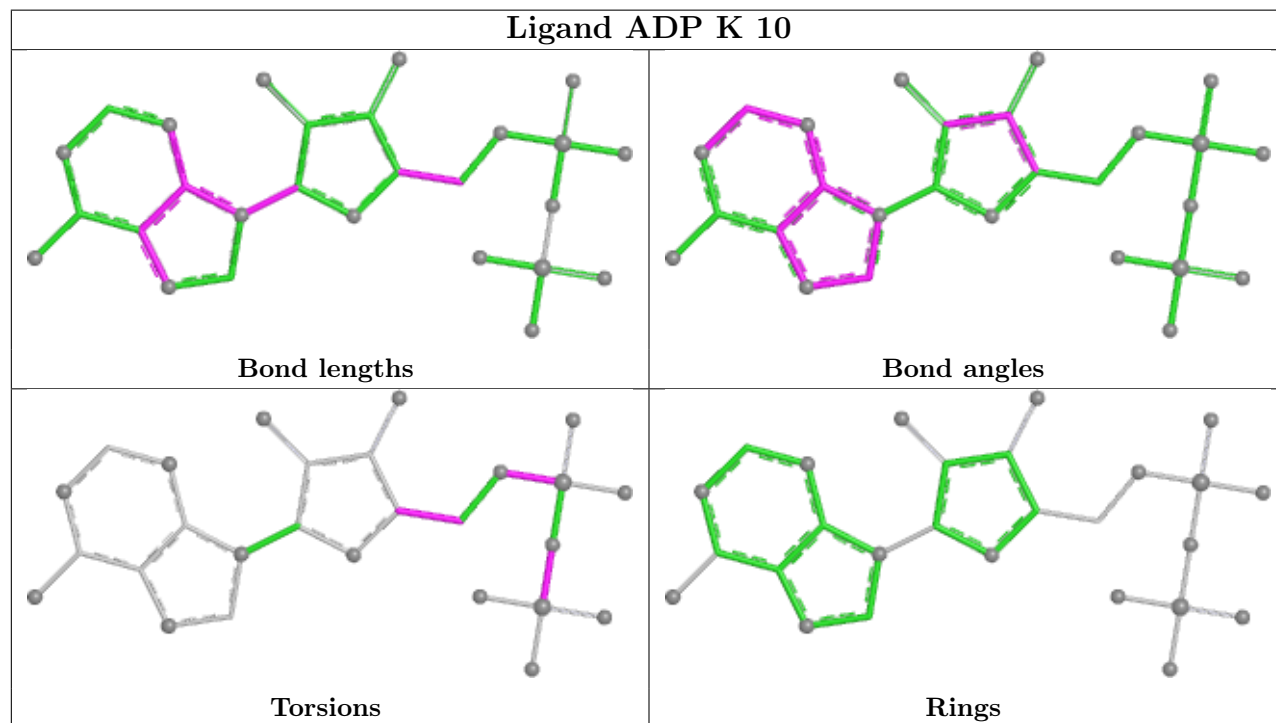
## Ligand ADP H 14



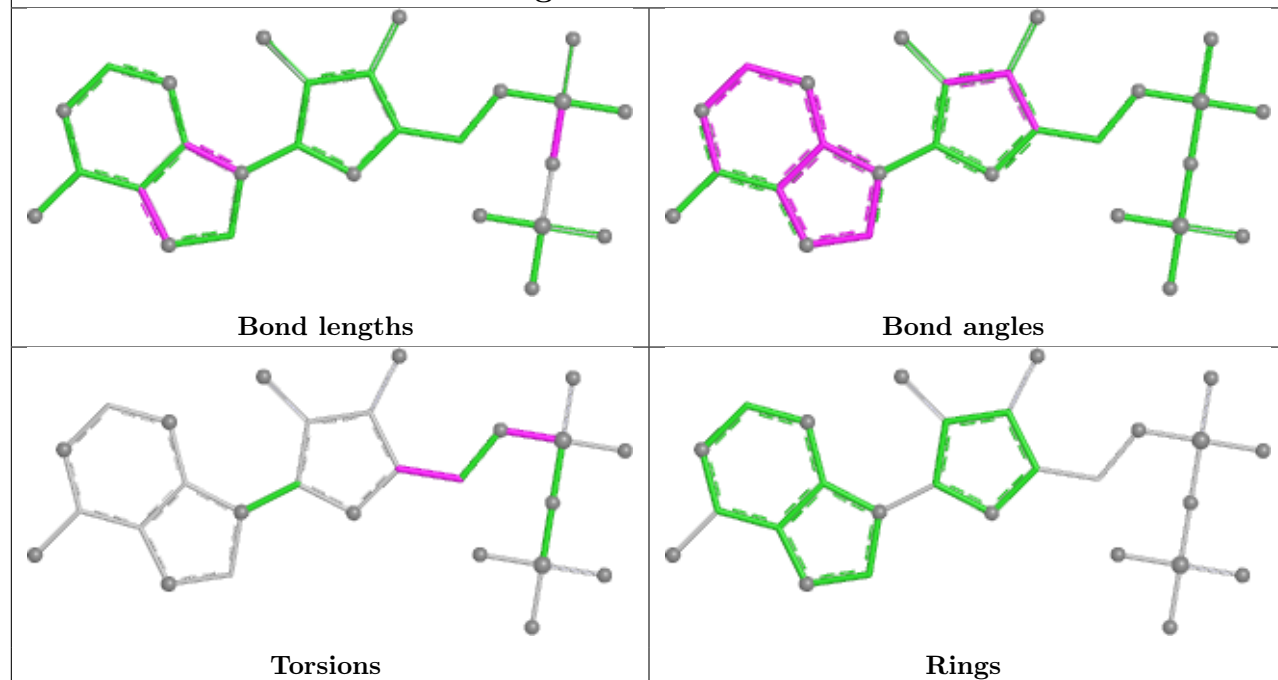
## Ligand ADP J 9



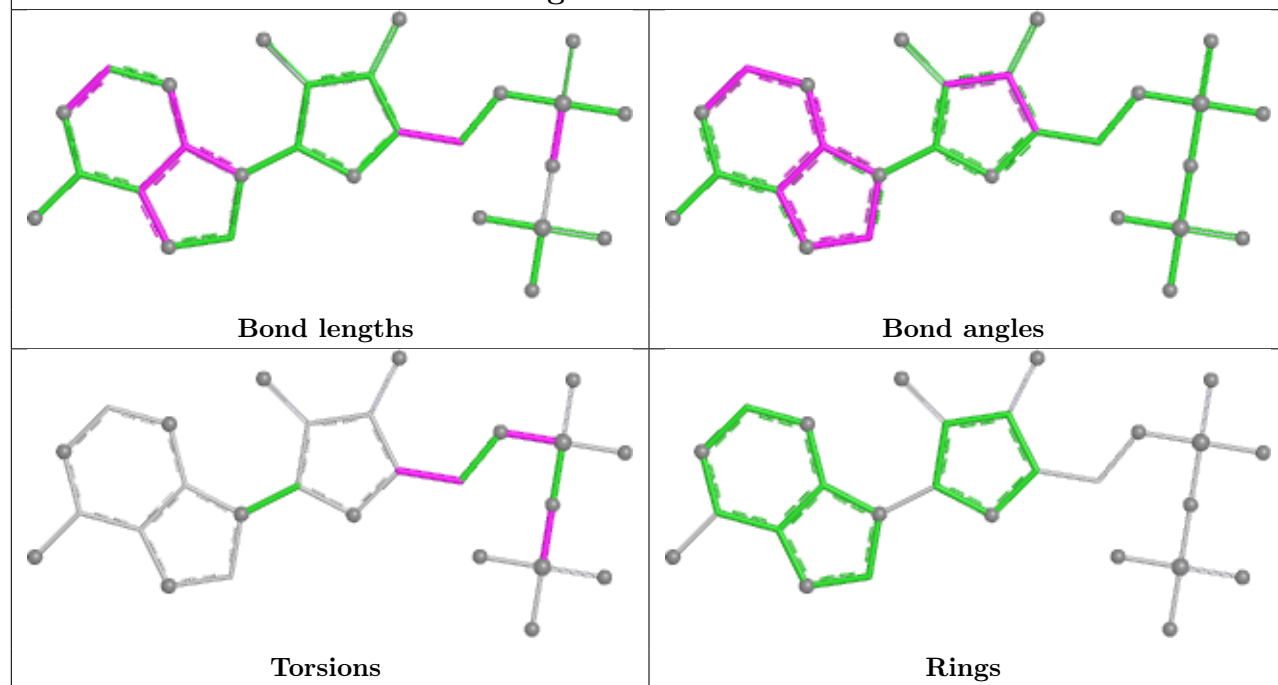
## Ligand ADP K 10



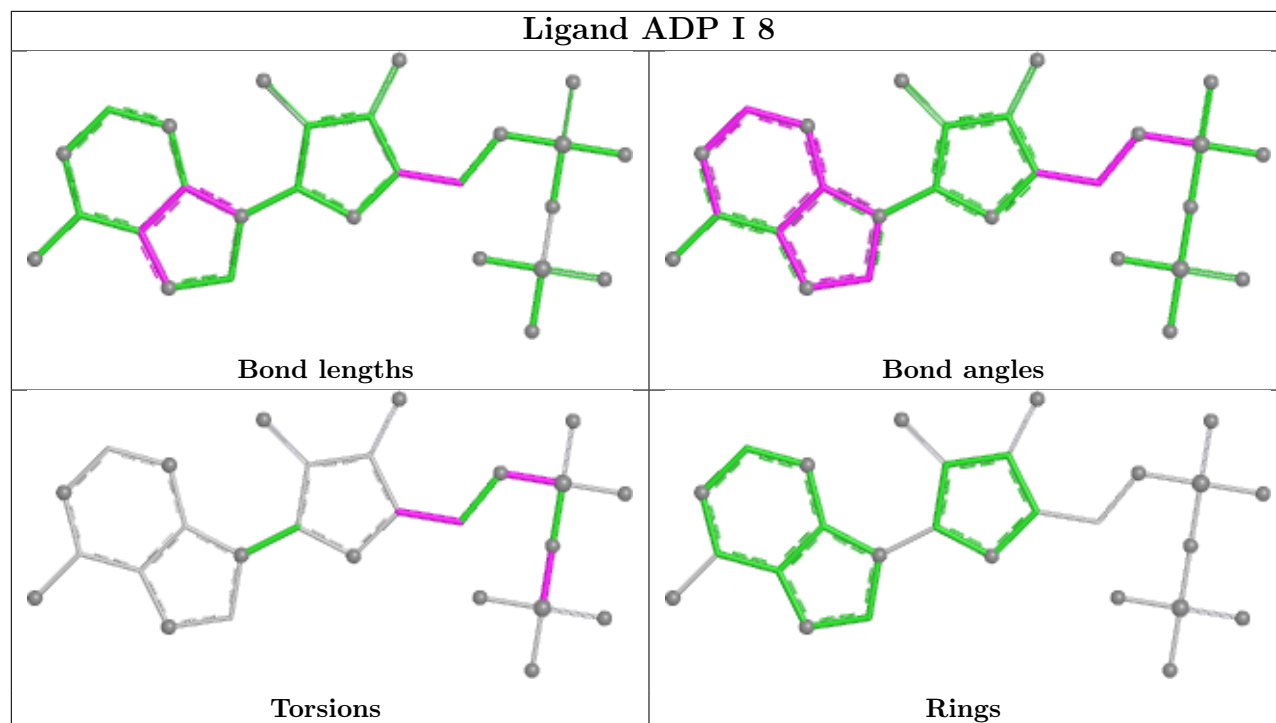
## Ligand ADP M 12



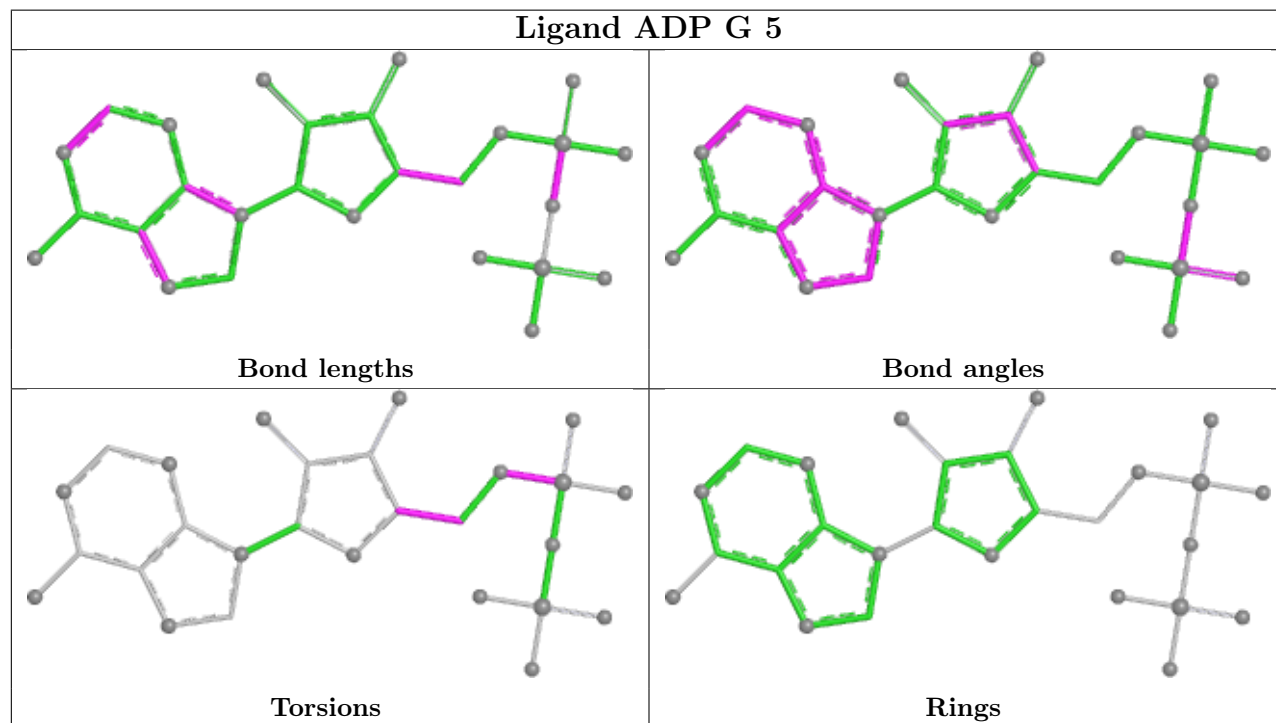
## Ligand ADP A 6



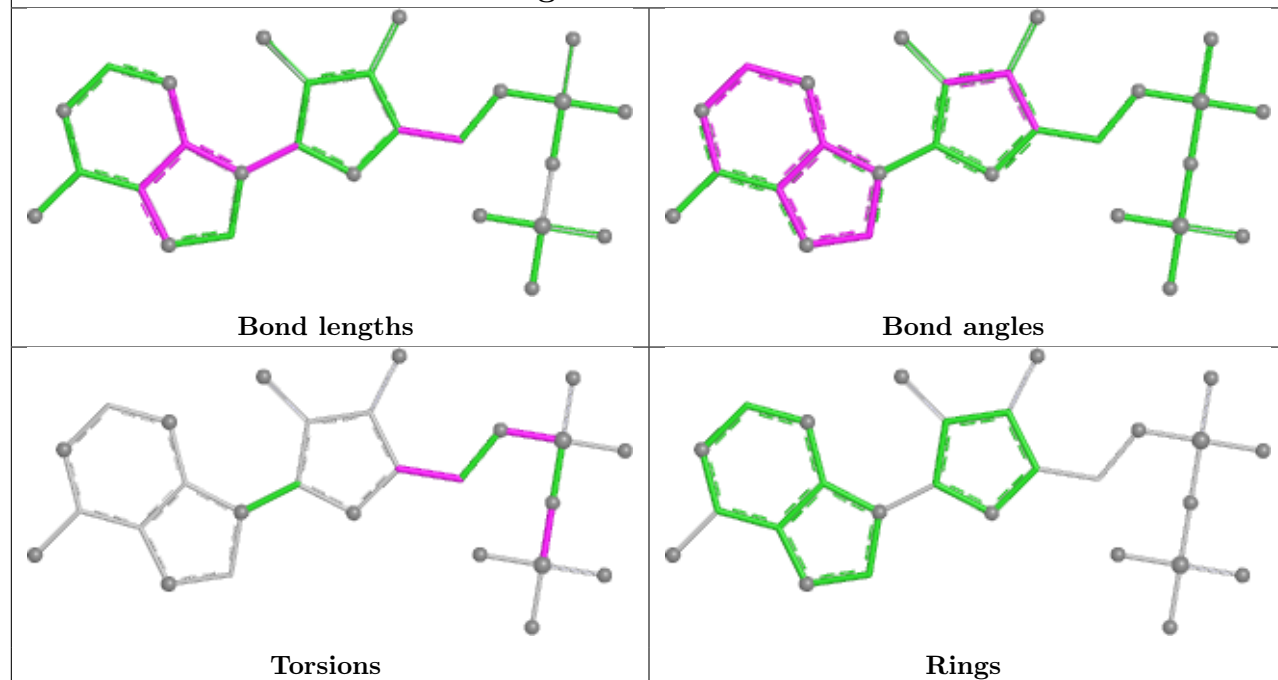
## Ligand ADP I 8



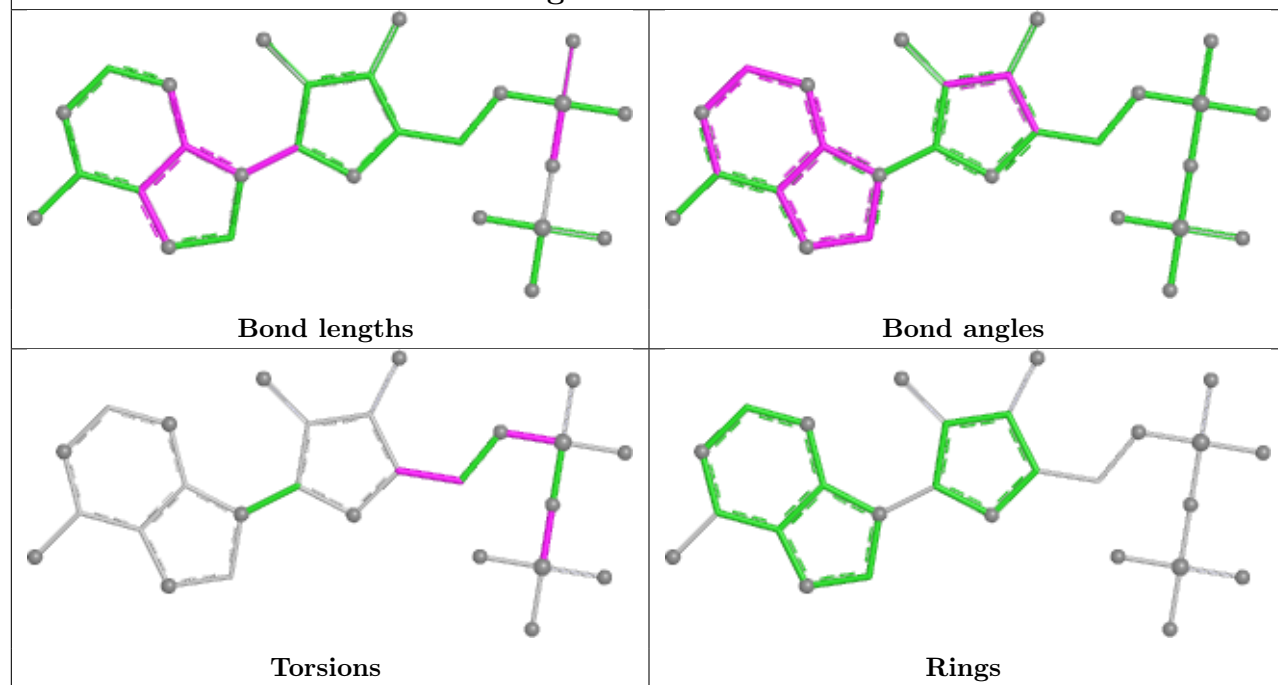
## Ligand ADP G 5

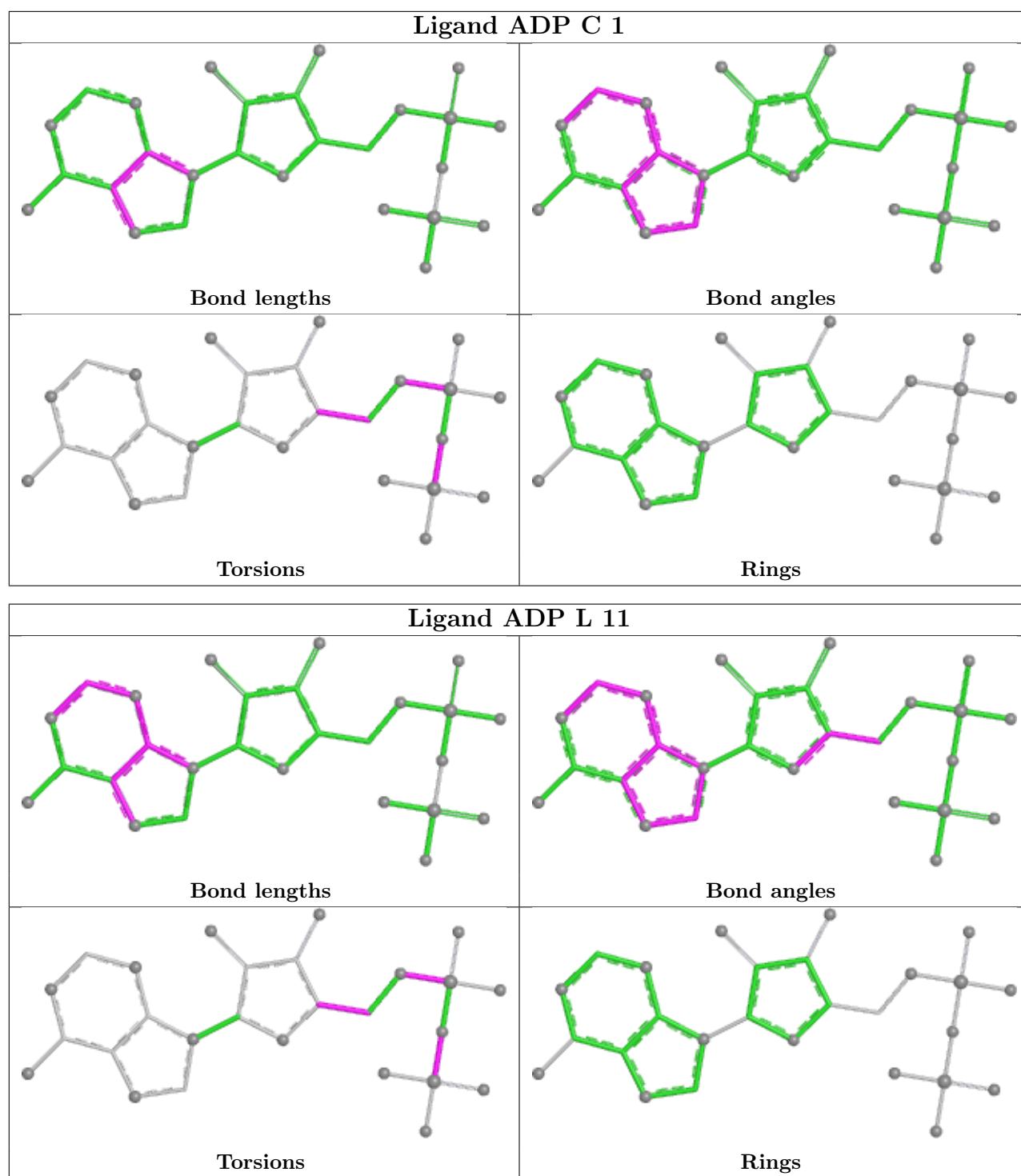


## Ligand ADP N 13



## Ligand ADP D 2





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-----|-----|-----------------------|-------|
| 1   | A     | 247/267 (92%)   | -0.45  | 0       | 100 | 100 | 29, 107, 142, 151     | 0     |
| 1   | B     | 243/267 (91%)   | -0.42  | 0       | 100 | 100 | 18, 101, 150, 151     | 0     |
| 1   | C     | 248/267 (92%)   | -0.59  | 0       | 100 | 100 | 43, 85, 128, 142      | 0     |
| 1   | D     | 247/267 (92%)   | -0.53  | 0       | 100 | 100 | 43, 90, 136, 148      | 0     |
| 1   | E     | 248/267 (92%)   | -0.54  | 1 (0%)  | 88  | 76  | 18, 83, 140, 151      | 0     |
| 1   | F     | 248/267 (92%)   | -0.48  | 0       | 100 | 100 | 44, 106, 146, 150     | 0     |
| 1   | G     | 248/267 (92%)   | -0.29  | 1 (0%)  | 88  | 76  | 64, 114, 150, 151     | 0     |
| 1   | H     | 245/267 (91%)   | -0.24  | 1 (0%)  | 88  | 76  | 77, 129, 151, 151     | 0     |
| 1   | I     | 247/267 (92%)   | -0.48  | 0       | 100 | 100 | 65, 103, 147, 151     | 0     |
| 1   | J     | 247/267 (92%)   | -0.40  | 0       | 100 | 100 | 71, 119, 147, 151     | 0     |
| 1   | K     | 248/267 (92%)   | -0.45  | 0       | 100 | 100 | 57, 104, 137, 148     | 0     |
| 1   | L     | 246/267 (92%)   | -0.43  | 1 (0%)  | 88  | 76  | 27, 80, 126, 150      | 0     |
| 1   | M     | 247/267 (92%)   | -0.44  | 1 (0%)  | 88  | 76  | 25, 100, 139, 146     | 0     |
| 1   | N     | 247/267 (92%)   | -0.47  | 1 (0%)  | 88  | 76  | 67, 106, 138, 151     | 0     |
| All | All   | 3456/3738 (92%) | -0.44  | 6 (0%)  | 91  | 83  | 18, 102, 148, 151     | 0     |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 211 | TYR  | 2.8  |
| 1   | L     | 139 | TYR  | 2.7  |
| 1   | H     | 347 | LEU  | 2.7  |
| 1   | G     | 382 | CYS  | 2.4  |
| 1   | N     | 216 | PHE  | 2.1  |
| 1   | M     | 157 | SER  | 2.1  |

## 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 oligosaccharides in this entry.

## 6.4 Ligands ⓘ

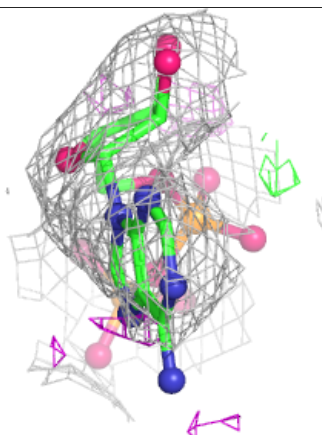
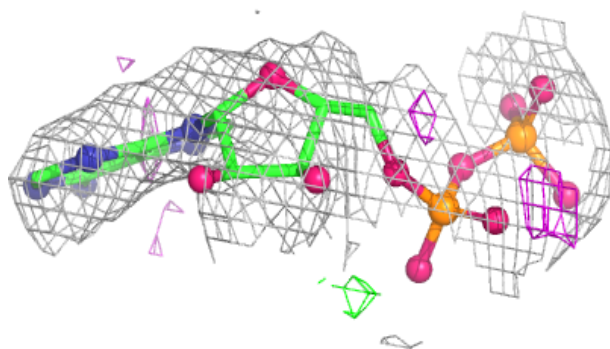
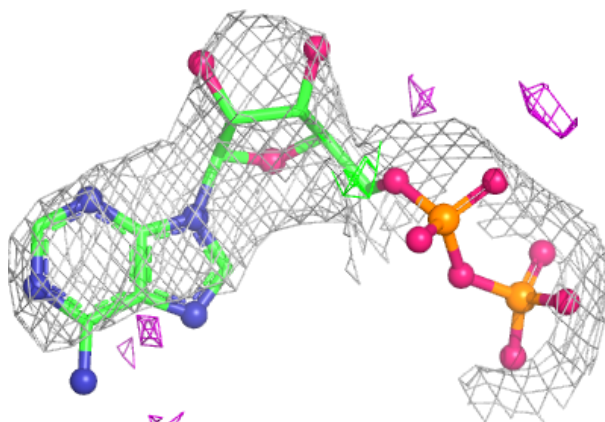
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | ADP  | B     | 7   | 27/27 | 0.90 | 0.08 | 96,111,114,114             | 0     |
| 2   | ADP  | J     | 9   | 27/27 | 0.90 | 0.07 | 92,95,102,104              | 0     |
| 2   | ADP  | H     | 14  | 27/27 | 0.91 | 0.07 | 125,141,143,143            | 0     |
| 2   | ADP  | L     | 11  | 27/27 | 0.91 | 0.08 | 48,60,84,93                | 0     |
| 2   | ADP  | K     | 10  | 27/27 | 0.92 | 0.08 | 99,103,108,110             | 0     |
| 2   | ADP  | G     | 5   | 27/27 | 0.92 | 0.07 | 52,65,75,80                | 0     |
| 2   | ADP  | M     | 12  | 27/27 | 0.92 | 0.07 | 51,67,86,87                | 0     |
| 2   | ADP  | A     | 6   | 27/27 | 0.94 | 0.07 | 84,88,92,96                | 0     |
| 2   | ADP  | D     | 2   | 27/27 | 0.94 | 0.07 | 71,82,91,93                | 0     |
| 2   | ADP  | N     | 13  | 27/27 | 0.94 | 0.08 | 100,106,110,111            | 0     |
| 2   | ADP  | F     | 4   | 27/27 | 0.95 | 0.06 | 62,66,84,87                | 0     |
| 2   | ADP  | I     | 8   | 27/27 | 0.96 | 0.06 | 66,81,87,90                | 0     |
| 2   | ADP  | E     | 3   | 27/27 | 0.96 | 0.07 | 51,64,70,79                | 0     |
| 2   | ADP  | C     | 1   | 27/27 | 0.96 | 0.06 | 54,70,77,79                | 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.

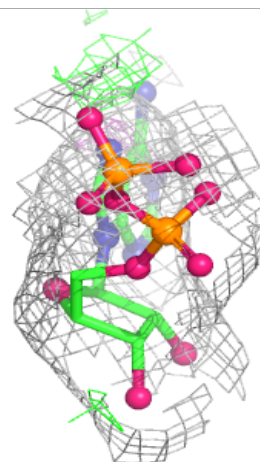
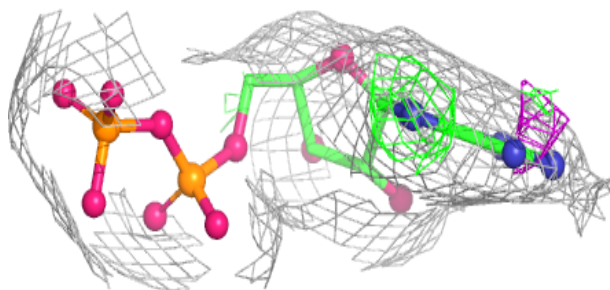
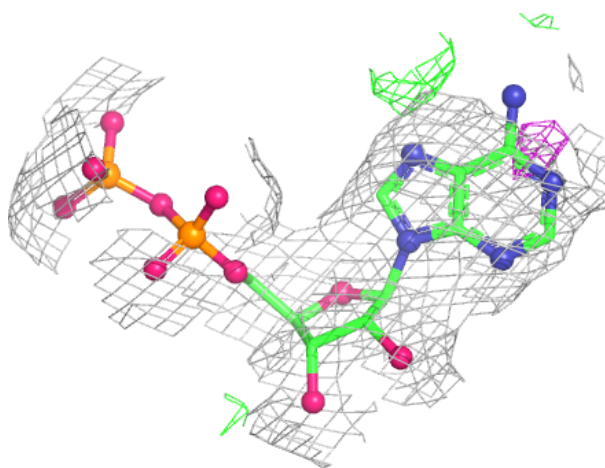
**Electron density around ADP B 7:**

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



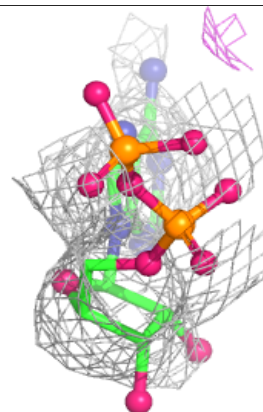
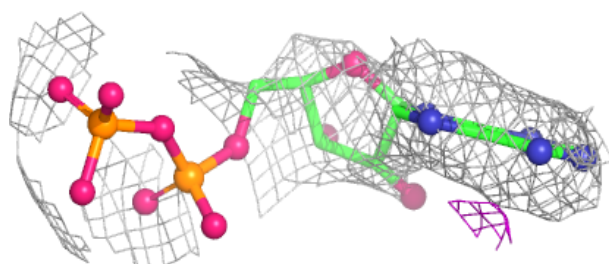
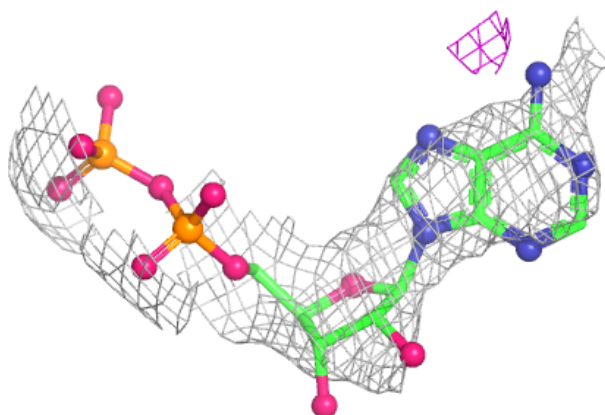
**Electron density around ADP J 9:**

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



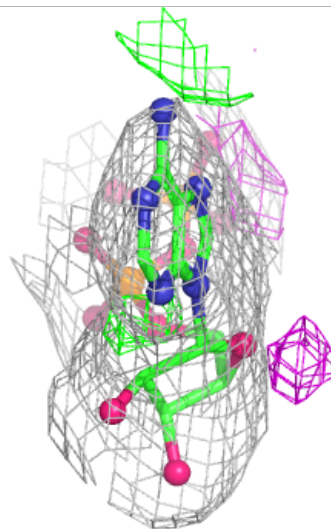
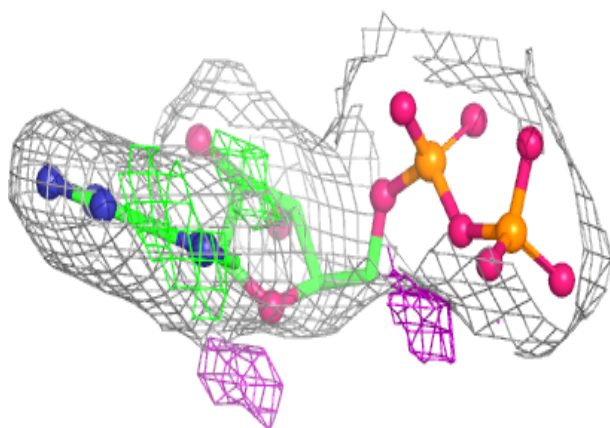
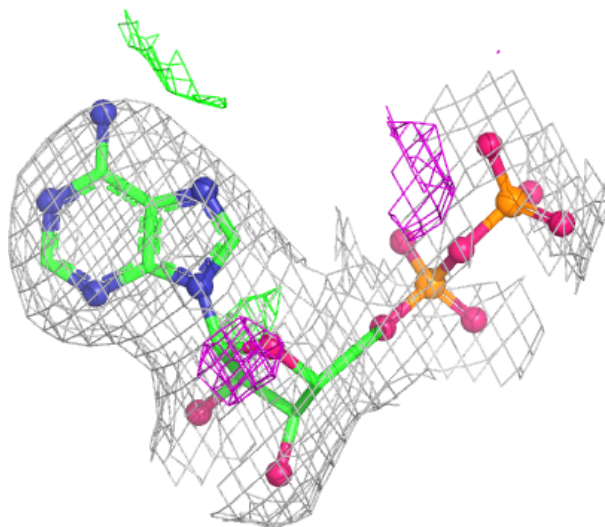
**Electron density around ADP H 14:**

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



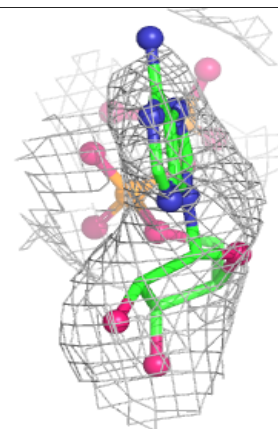
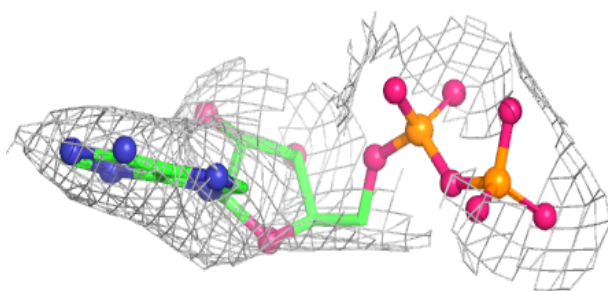
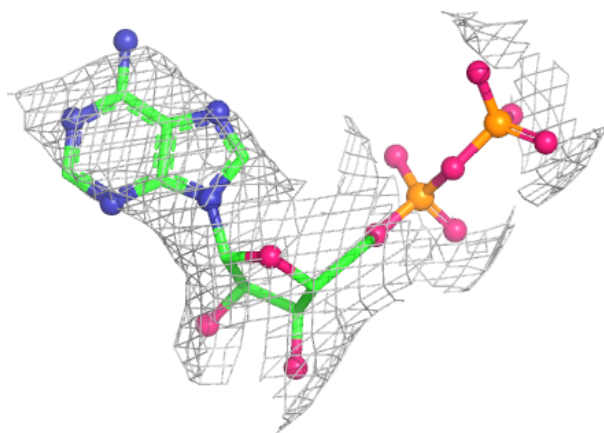
**Electron density around ADP L 11:**

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



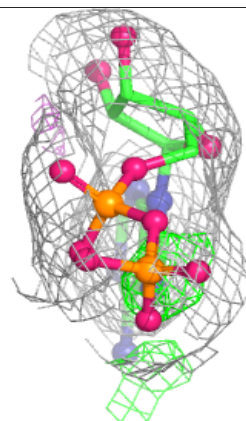
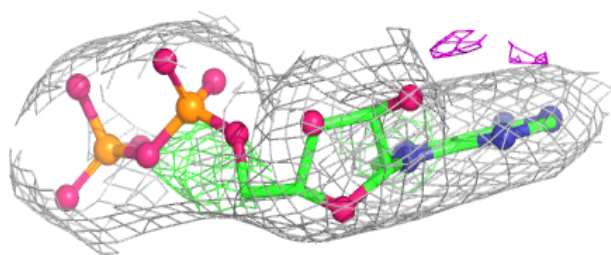
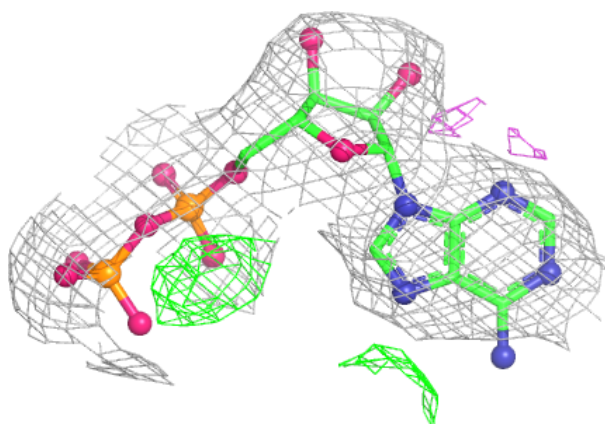
**Electron density around ADP K 10:**

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

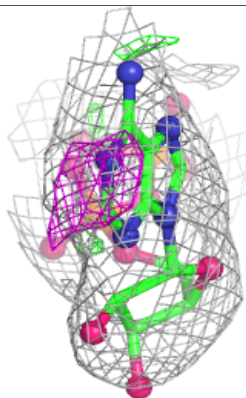
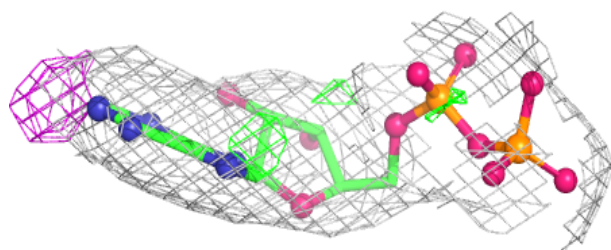
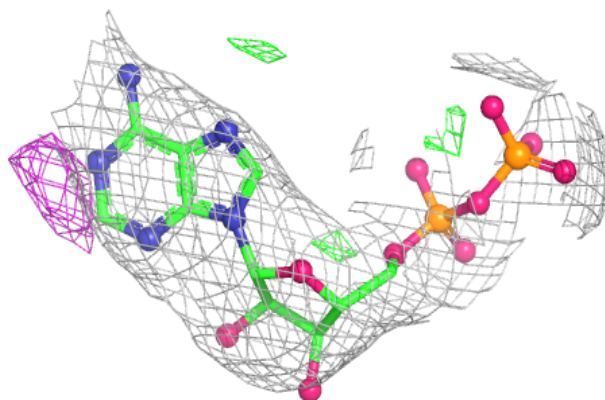


**Electron density around ADP G 5:**

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

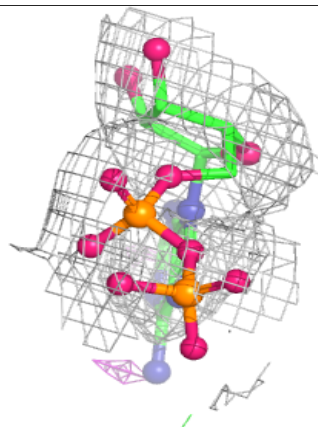
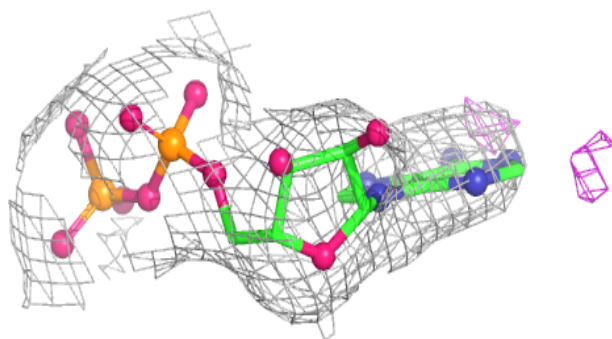
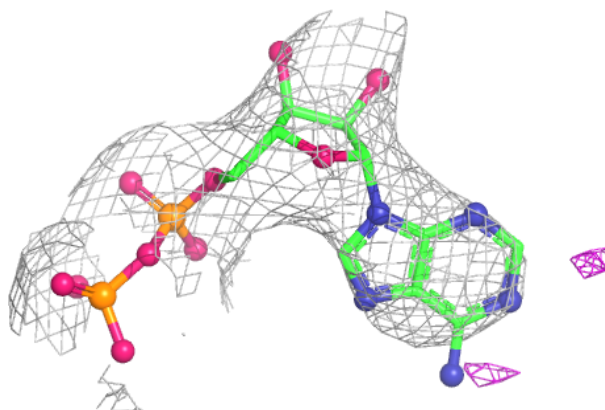
**Electron density around ADP M 12:**

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



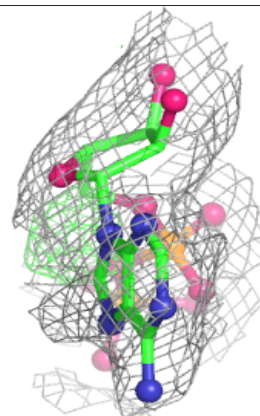
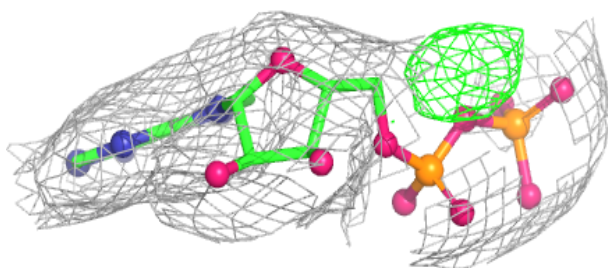
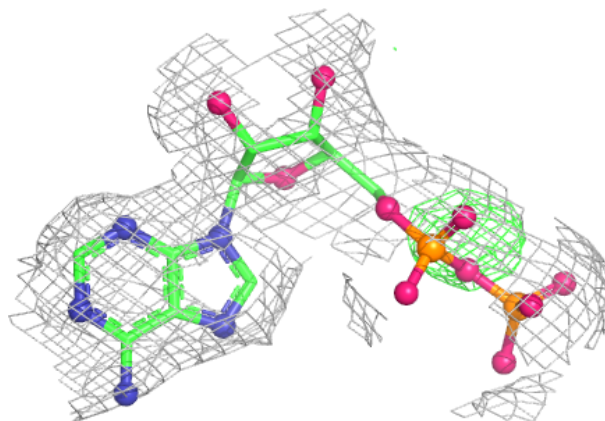
**Electron density around ADP A 6:**

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



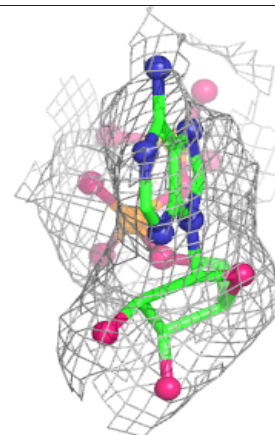
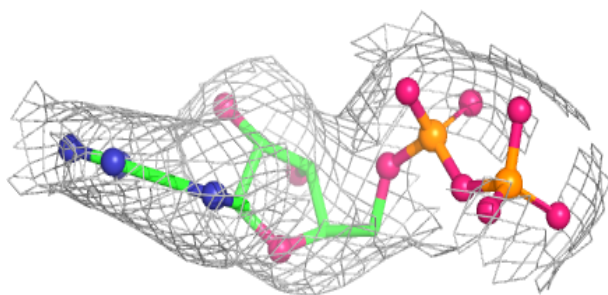
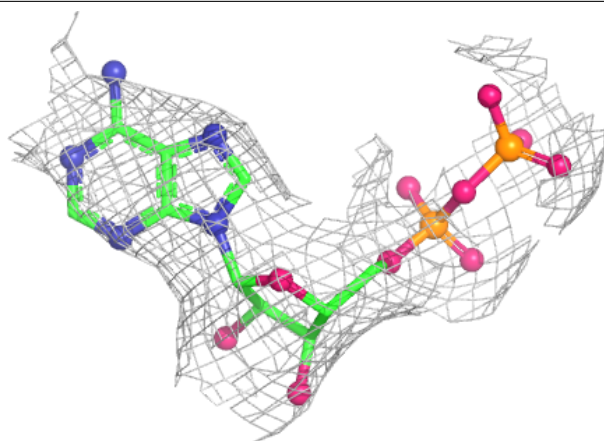
**Electron density around ADP D 2:**

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

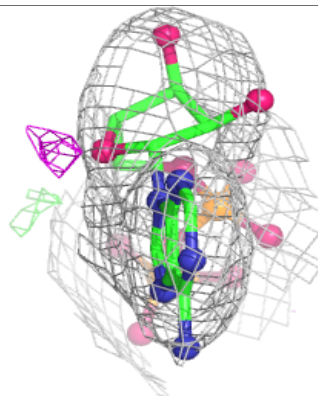
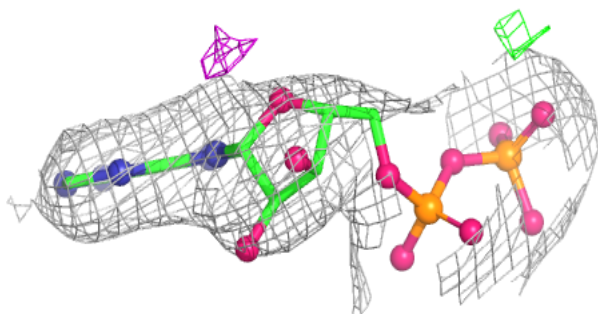
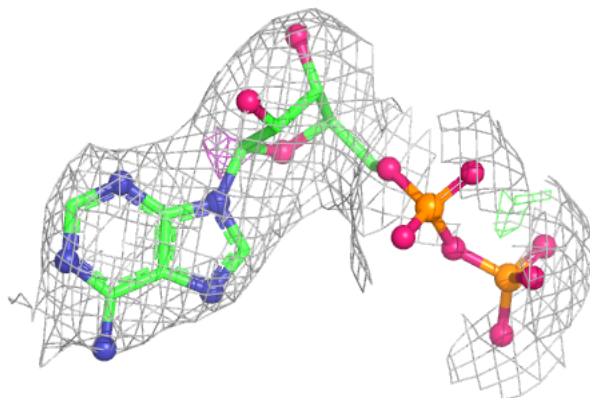


**Electron density around ADP N 13:**

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

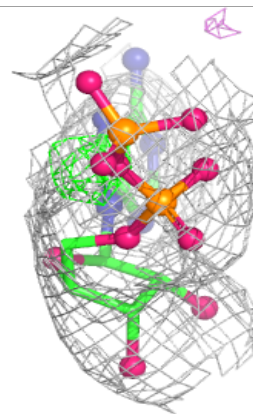
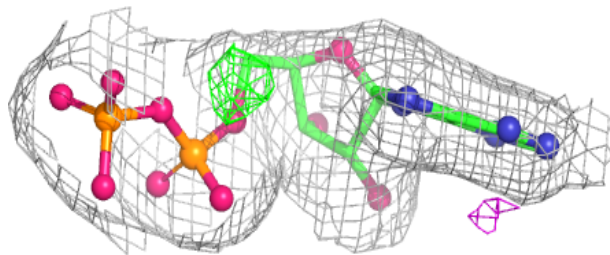
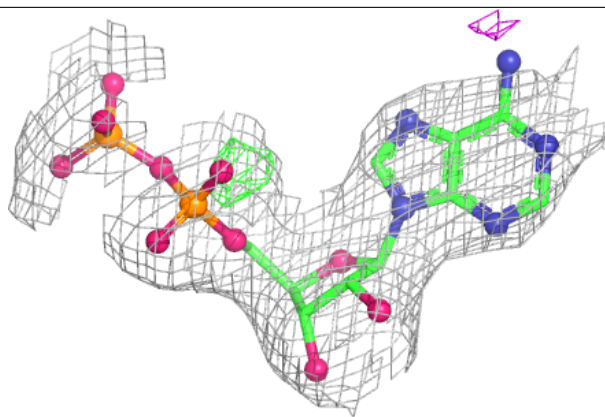
**Electron density around ADP F 4:**

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

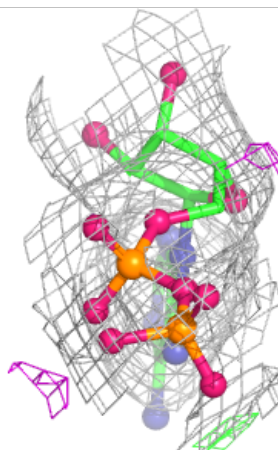
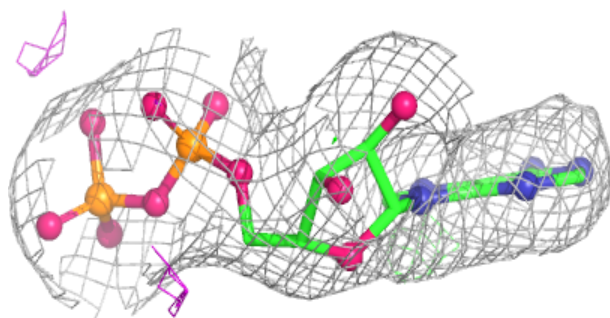
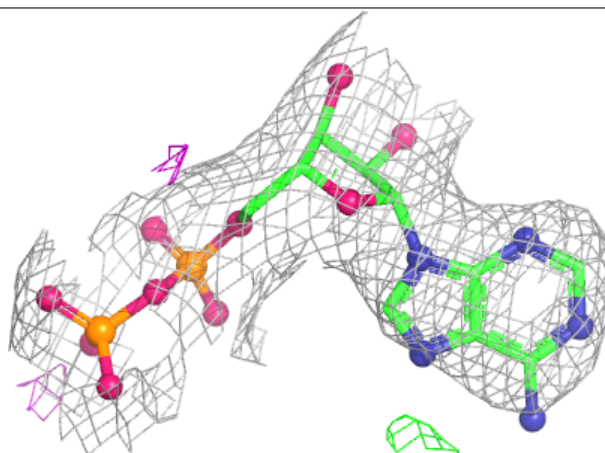


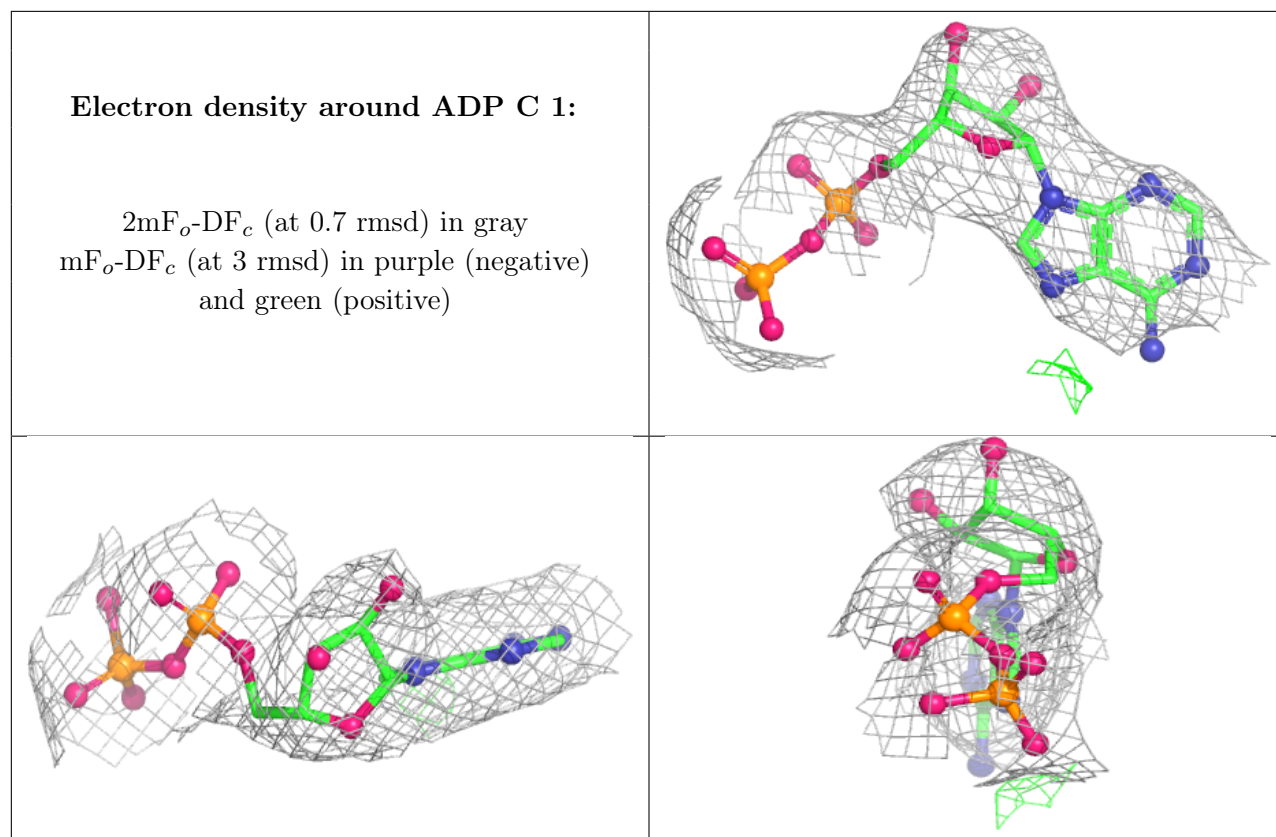
**Electron density around ADP I 8:**

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

**Electron density around ADP E 3:**

$2mF_o-DF_c$  (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.