



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:45 am GMT

PDB ID : 1HMY  
Title : THE STRUCTURE OF UNLIGANDED REVERSE TRANSCRIPTASE  
FROM THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1  
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Deposited on : 1994-12-15  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

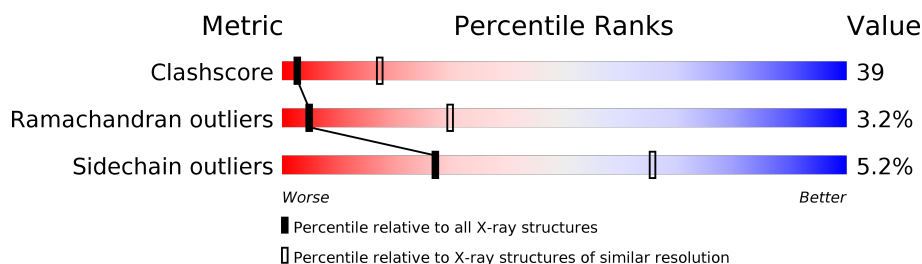
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 112137                      | 1009 (3.20-3.20)                                      |
| Ramachandran outliers | 110173                      | 1118 (3.22-3.18)                                      |
| Sidechain outliers    | 110143                      | 1117 (3.22-3.18)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 560    |                  |
| 1   | C     | 560    |                  |
| 1   | E     | 560    |                  |
| 1   | G     | 560    |                  |
| 2   | B     | 440    |                  |
| 2   | D     | 440    |                  |
| 2   | F     | 440    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | H     | 440    | <div><div></div><div>39%</div><div>45%</div><div>• • 10%</div></div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29596 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 HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 536      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4200  | 2711 | 698 | 784 | 7 |         |         |       |
| 1   | C     | 536      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4200  | 2711 | 698 | 784 | 7 |         |         |       |
| 1   | E     | 536      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4200  | 2711 | 698 | 784 | 7 |         |         |       |
| 1   | G     | 536      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4200  | 2711 | 698 | 784 | 7 |         |         |       |

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 395      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3198  | 2079 | 531 | 582 | 6 |         |         |       |
| 2   | D     | 395      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3198  | 2079 | 531 | 582 | 6 |         |         |       |
| 2   | F     | 395      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3198  | 2079 | 531 | 582 | 6 |         |         |       |
| 2   | H     | 395      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3198  | 2079 | 531 | 582 | 6 |         |         |       |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

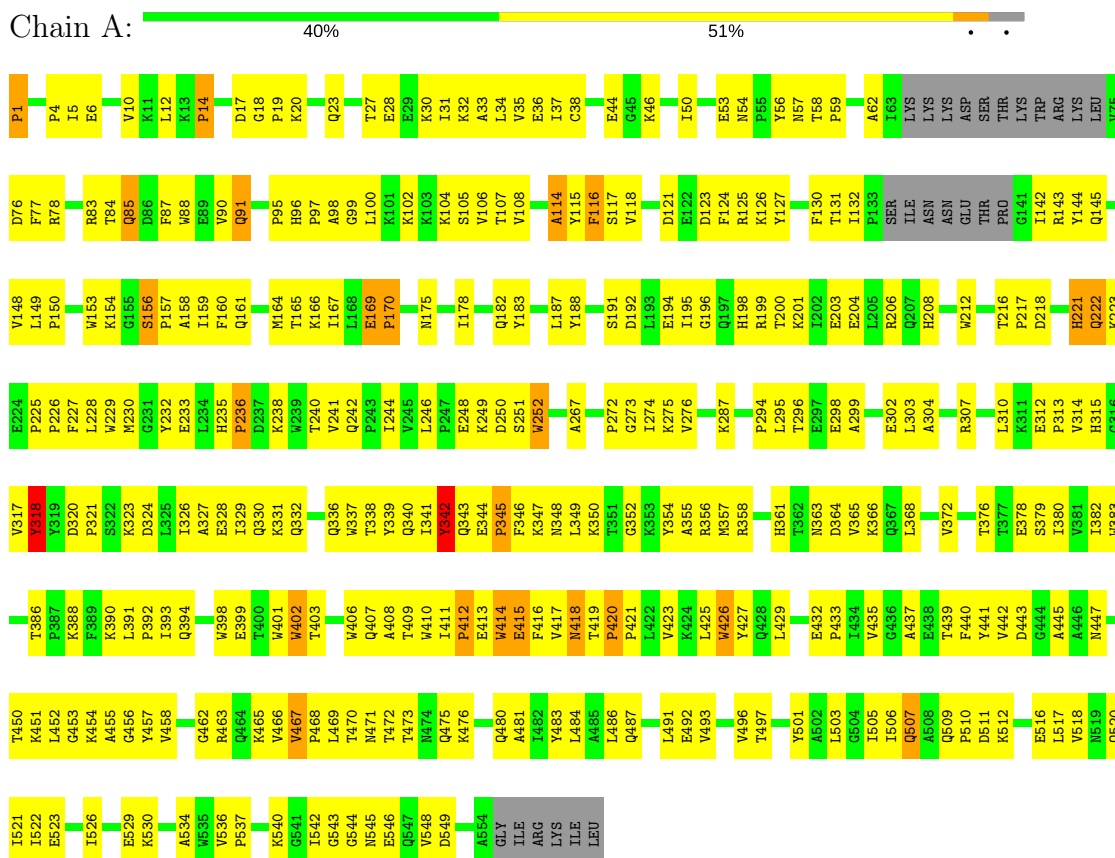
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | H     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | F     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

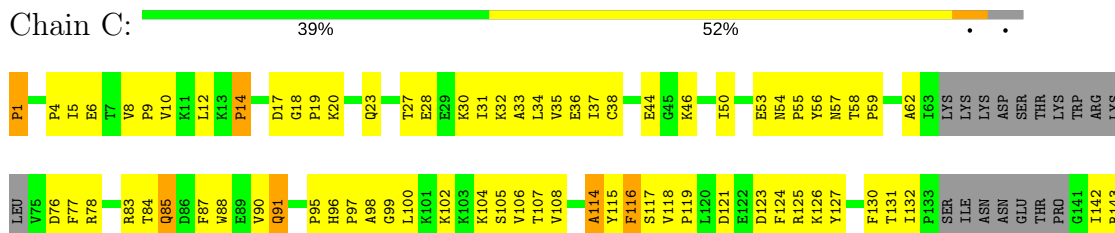
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

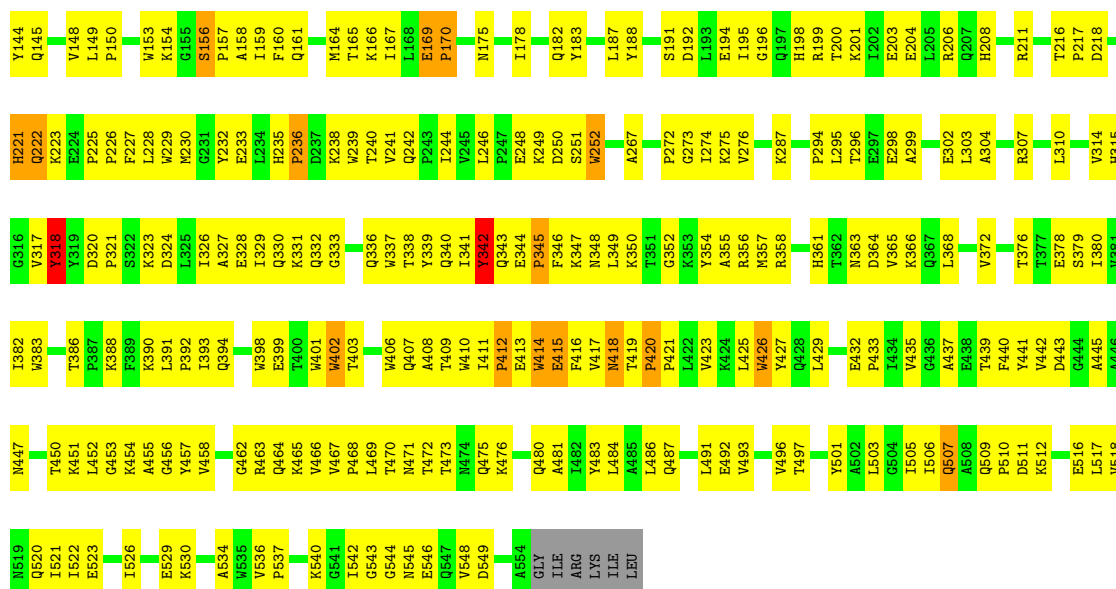
Note EDS was not executed.

#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

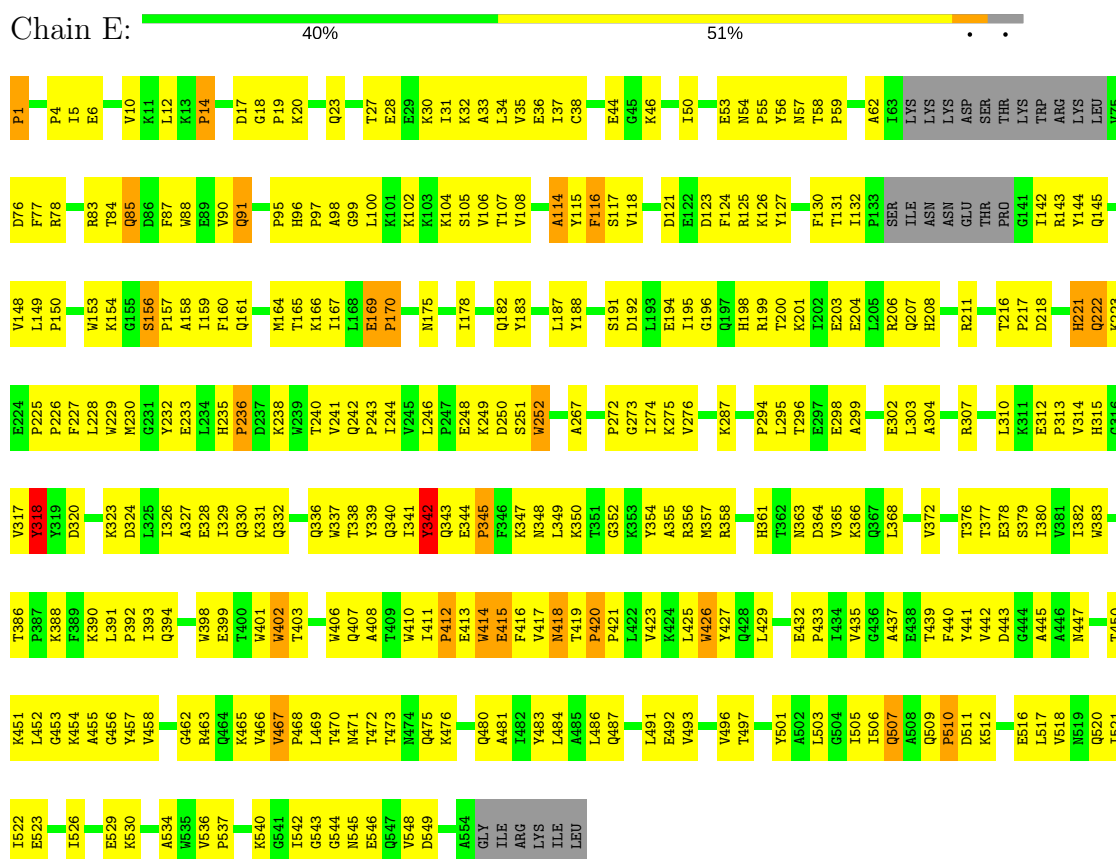


#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



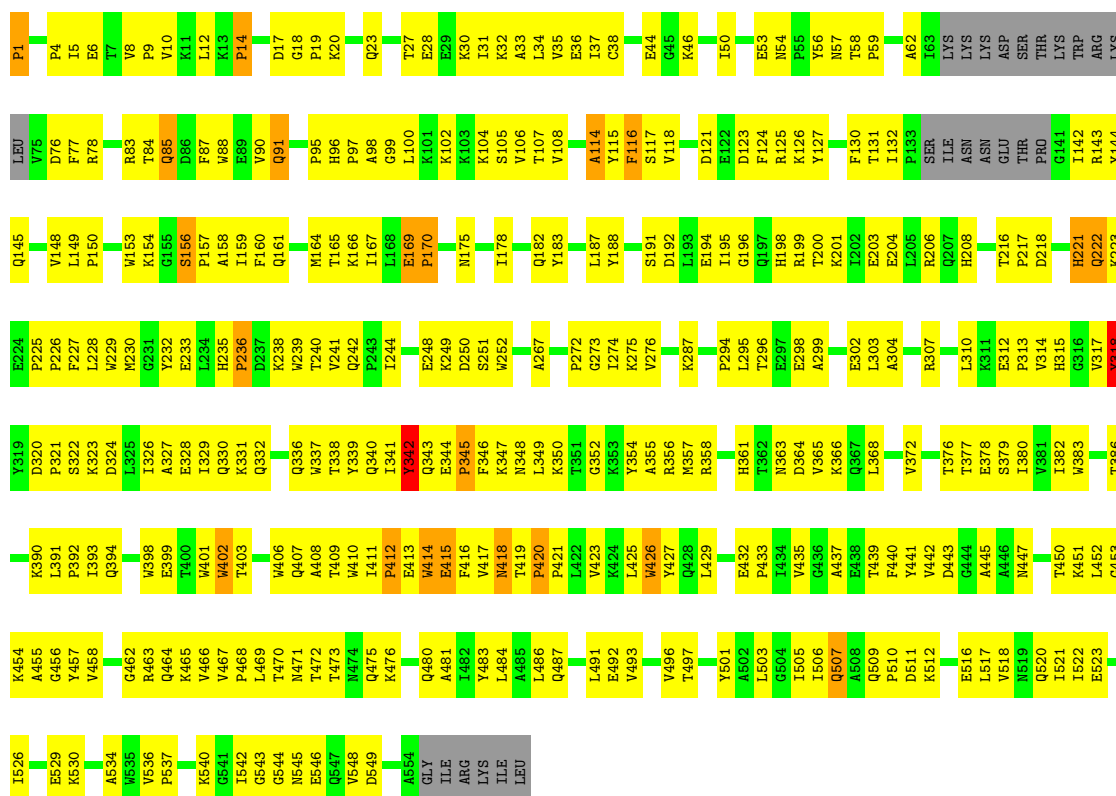


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



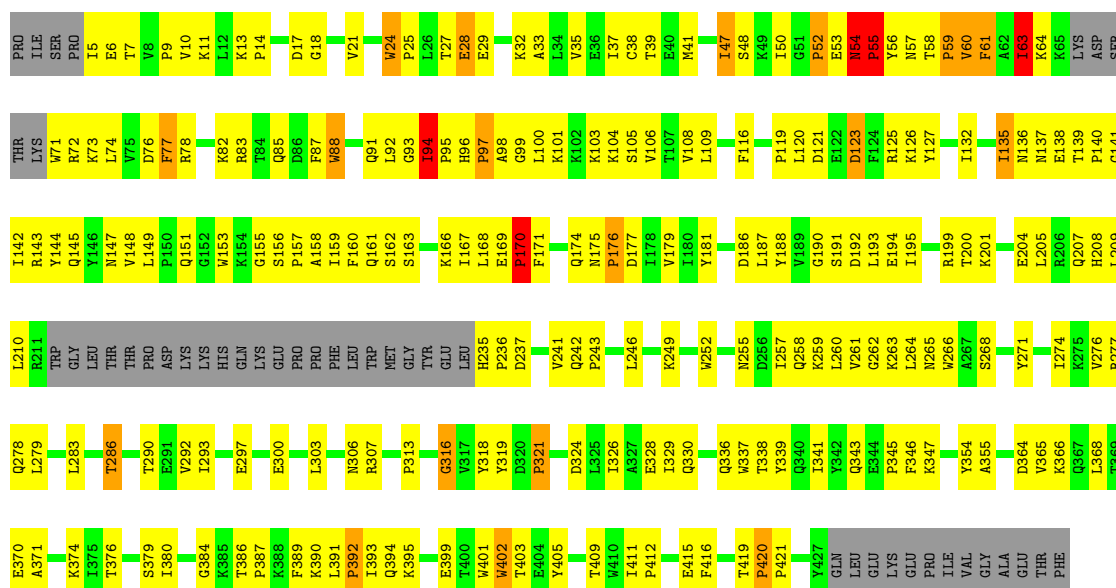
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)





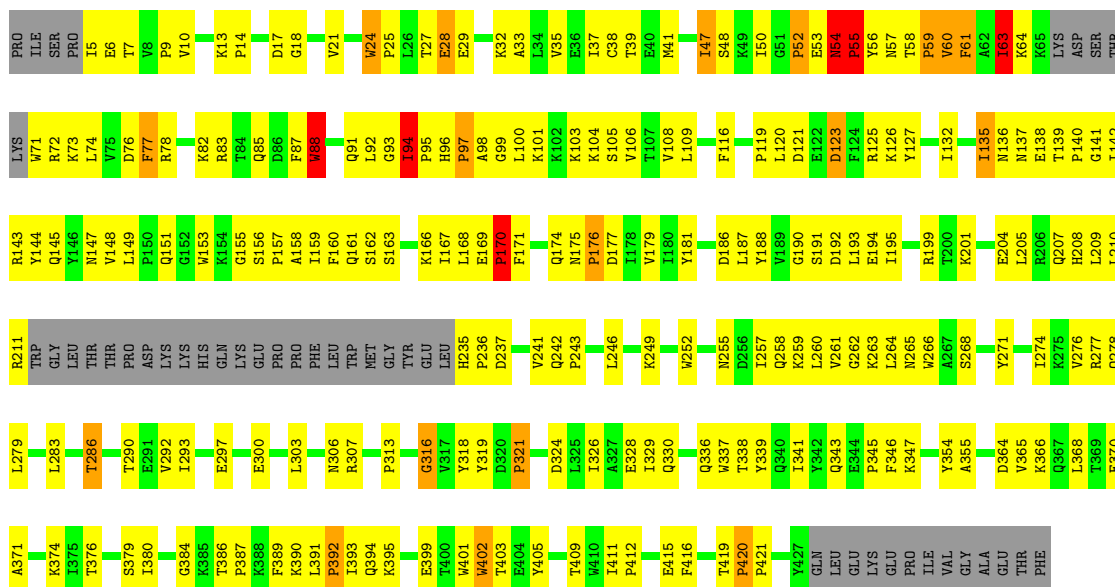
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain B: 39% 45% 10%



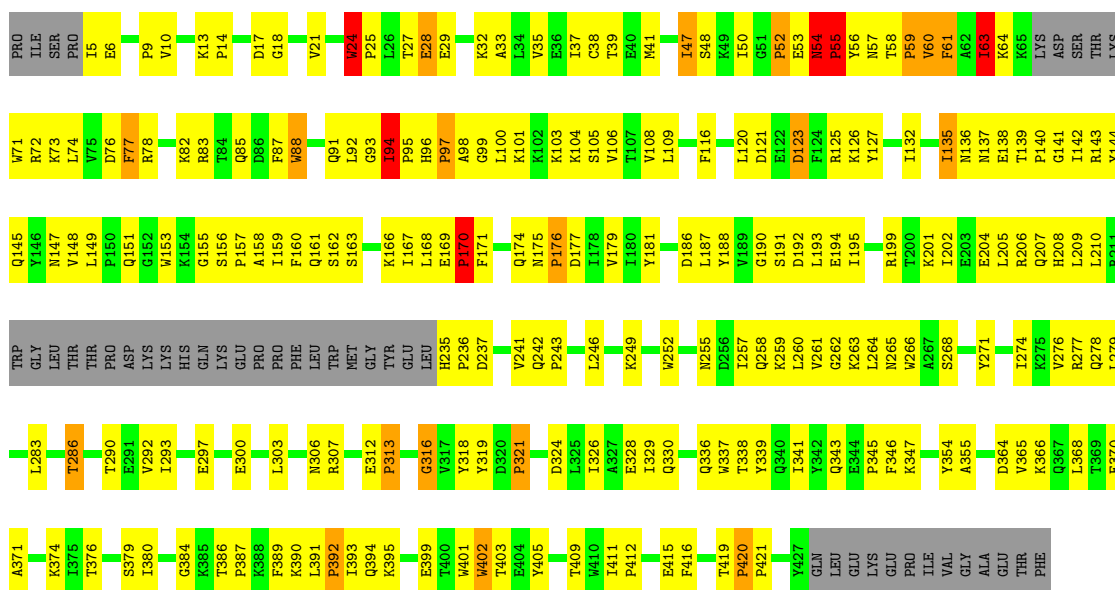
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain D: 40% 45% 10%



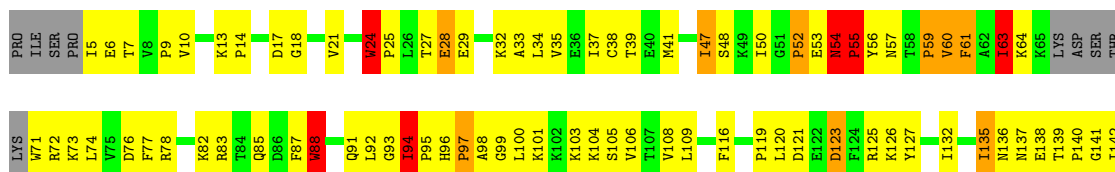
### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain F: 40% 45% 10%



### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain H: 39% 45% 10%





|      |      |      |      |
|------|------|------|------|
| A371 | L279 | R211 | R143 |
| K374 | L283 | TRP  | Q144 |
| I375 |      | GLY  | Q145 |
| T376 | T286 | LEU  | Y146 |
|      |      | THR  | Y147 |
| S379 | T290 | THR  | Y148 |
| I380 | E291 | PRO  | L149 |
|      | V292 | ASP  | P150 |
| G384 | L293 | LYS  | Q151 |
| K385 |      | LYS  | G152 |
| T386 | E297 | HIS  | Y153 |
| P387 |      | GLN  | K154 |
| K388 | E300 | LYS  | G155 |
| F389 |      | GLU  | S156 |
| K390 | L303 | PRO  | P157 |
| L391 |      | PRO  | A158 |
| P392 | N306 | PHE  | I159 |
| I393 | R307 | LEU  | F160 |
| Q394 |      | TRP  | Q161 |
| K395 | P313 | MET  | S162 |
|      |      | GLY  | S163 |
|      |      | TYR  |      |
| E399 | G316 | GLU  | K166 |
| T400 | V317 | LEU  | L167 |
| W401 | Y318 | H255 | L168 |
| W402 | Y319 | P236 | E169 |
| T403 | D320 | D237 | P170 |
| A404 | P321 |      | F171 |
| Y405 |      | V241 |      |
|      | D324 | Q242 | Q174 |
|      | L325 | P243 | N175 |
| T409 | I326 |      | P176 |
| W410 | K327 | L246 | I177 |
| I411 | E328 |      | I178 |
| P412 | I329 | K249 | Y179 |
| E415 | Q330 |      | I180 |
| P416 |      | W252 | Y181 |
|      | Q336 |      |      |
| T419 | W337 | N255 | D186 |
| P420 | T338 | D256 | L187 |
| P421 | Y339 | I257 | Y188 |
|      | Q340 | Q258 | Y189 |
| Y427 | I341 | K259 | G190 |
| GLN  | Y342 | L260 | S191 |
| LEU  | Q343 | V261 | D192 |
| GLU  | E344 | Q262 | L193 |
| LYS  | P345 | K263 | E194 |
| GLU  | F346 | L264 | I195 |
| PRO  | K347 | N265 |      |
| ILE  |      | W266 | R199 |
| VAL  | Y354 | D267 | T200 |
| GLY  | A355 | S268 | K201 |
| ALA  |      |      |      |
| GLU  | D364 | Y271 | E204 |
| THR  | P365 |      | L205 |
| PHE  | K366 | I274 | R206 |
|      | Q367 | K275 | Q207 |
|      | L368 | V276 | H208 |
|      | T369 | L209 | Z209 |
|      | E370 | R277 | L210 |
|      |      |      |      |

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | C 1 2 1  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 168.70Å 162.80Å 331.80Å<br>90.00° 105.70° 90.00° | Depositor |
| Resolution (Å)   | 6.00 – 3.20                                      | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (6.00-3.20)                      | Depositor |
| $R_{merge}$  | (Not available)                                  | Depositor |
| $R_{sym}$  | (Not available)                                  | Depositor |
| Refinement program                                       | X-PLOR   | Depositor |
| R, $R_{free}$  | 0.254 , 0.297                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 29596  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 97.0   | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.71         | 1/4307 (0.0%)  | 0.98        | 5/5865 (0.1%)   |
| 1   | C     | 0.71         | 1/4307 (0.0%)  | 0.98        | 4/5865 (0.1%)   |
| 1   | E     | 0.71         | 1/4307 (0.0%)  | 0.98        | 5/5865 (0.1%)   |
| 1   | G     | 0.71         | 1/4307 (0.0%)  | 0.98        | 4/5865 (0.1%)   |
| 2   | B     | 0.74         | 0/3285         | 1.02        | 5/4466 (0.1%)   |
| 2   | D     | 0.74         | 0/3285         | 1.02        | 5/4466 (0.1%)   |
| 2   | F     | 0.74         | 1/3285 (0.0%)  | 1.02        | 5/4466 (0.1%)   |
| 2   | H     | 0.74         | 1/3285 (0.0%)  | 1.02        | 5/4466 (0.1%)   |
| All | All   | 0.72         | 6/30368 (0.0%) | 0.99        | 38/41324 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | C     | 0                   | 2                   |
| 1   | E     | 0                   | 2                   |
| 1   | G     | 0                   | 2                   |
| 2   | B     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| All | All   | 0                   | 12                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | C     | 222 | GLN  | C-O   | 5.35 | 1.33        | 1.23     |
| 1   | A     | 222 | GLN  | C-O   | 5.33 | 1.33        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 222 | GLN  | C-O   | 5.32  | 1.33        | 1.23     |
| 1   | E     | 222 | GLN  | C-O   | 5.32  | 1.33        | 1.23     |
| 2   | F     | 24  | TRP  | CB-CG | -5.02 | 1.41        | 1.50     |
| 2   | H     | 24  | TRP  | CB-CG | -5.01 | 1.41        | 1.50     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 94  | ILE  | C-N-CD  | 7.79  | 144.77      | 128.40   |
| 2   | F     | 94  | ILE  | C-N-CD  | 7.77  | 144.72      | 128.40   |
| 2   | B     | 94  | ILE  | C-N-CD  | 7.77  | 144.71      | 128.40   |
| 2   | D     | 94  | ILE  | C-N-CD  | 7.76  | 144.69      | 128.40   |
| 2   | D     | 54  | ASN  | C-N-CD  | -7.01 | 105.17      | 120.60   |
| 2   | H     | 54  | ASN  | C-N-CD  | -7.01 | 105.18      | 120.60   |
| 2   | B     | 54  | ASN  | C-N-CD  | -7.01 | 105.18      | 120.60   |
| 2   | F     | 54  | ASN  | C-N-CD  | -7.00 | 105.20      | 120.60   |
| 2   | H     | 60  | VAL  | CB-CA-C | -6.46 | 99.12       | 111.40   |
| 2   | F     | 60  | VAL  | CB-CA-C | -6.45 | 99.14       | 111.40   |
| 2   | B     | 60  | VAL  | CB-CA-C | -6.45 | 99.15       | 111.40   |
| 2   | D     | 60  | VAL  | CB-CA-C | -6.44 | 99.17       | 111.40   |
| 1   | A     | 221 | HIS  | C-N-CA  | 6.11  | 136.97      | 121.70   |
| 1   | E     | 221 | HIS  | C-N-CA  | 6.11  | 136.96      | 121.70   |
| 1   | G     | 221 | HIS  | C-N-CA  | 6.10  | 136.95      | 121.70   |
| 1   | C     | 221 | HIS  | C-N-CA  | 6.10  | 136.95      | 121.70   |
| 2   | F     | 47  | ILE  | CB-CA-C | -5.61 | 100.39      | 111.60   |
| 1   | G     | 294 | PRO  | N-CA-CB | 5.60  | 110.02      | 103.30   |
| 2   | H     | 47  | ILE  | CB-CA-C | -5.59 | 100.43      | 111.60   |
| 2   | B     | 47  | ILE  | CB-CA-C | -5.58 | 100.43      | 111.60   |
| 2   | D     | 47  | ILE  | CB-CA-C | -5.58 | 100.44      | 111.60   |
| 1   | E     | 294 | PRO  | N-CA-CB | 5.57  | 109.99      | 103.30   |
| 1   | A     | 294 | PRO  | N-CA-CB | 5.57  | 109.98      | 103.30   |
| 1   | C     | 294 | PRO  | N-CA-CB | 5.56  | 109.98      | 103.30   |
| 1   | A     | 272 | PRO  | N-CA-CB | 5.54  | 109.94      | 103.30   |
| 1   | E     | 272 | PRO  | N-CA-CB | 5.54  | 109.94      | 103.30   |
| 1   | C     | 272 | PRO  | N-CA-CB | 5.53  | 109.93      | 103.30   |
| 1   | G     | 272 | PRO  | N-CA-CB | 5.51  | 109.91      | 103.30   |
| 1   | A     | 222 | GLN  | CA-C-N  | 5.42  | 129.11      | 117.20   |
| 1   | C     | 222 | GLN  | CA-C-N  | 5.41  | 129.11      | 117.20   |
| 1   | E     | 222 | GLN  | CA-C-N  | 5.40  | 129.09      | 117.20   |
| 1   | G     | 222 | GLN  | CA-C-N  | 5.40  | 129.08      | 117.20   |
| 2   | D     | 63  | ILE  | N-CA-C  | -5.15 | 97.09       | 111.00   |
| 2   | F     | 63  | ILE  | N-CA-C  | -5.14 | 97.12       | 111.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 63  | ILE  | N-CA-C  | -5.13 | 97.14       | 111.00   |
| 2   | H     | 63  | ILE  | N-CA-C  | -5.13 | 97.15       | 111.00   |
| 1   | A     | 467 | VAL  | CB-CA-C | -5.00 | 101.89      | 111.40   |
| 1   | E     | 467 | VAL  | CB-CA-C | -5.00 | 101.90      | 111.40   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 318 | TYR  | Sidechain |
| 1   | A     | 342 | TYR  | Sidechain |
| 2   | B     | 61  | PHE  | Sidechain |
| 1   | C     | 318 | TYR  | Sidechain |
| 1   | C     | 342 | TYR  | Sidechain |
| 2   | D     | 61  | PHE  | Sidechain |
| 1   | E     | 318 | TYR  | Sidechain |
| 1   | E     | 342 | TYR  | Sidechain |
| 2   | F     | 61  | PHE  | Sidechain |
| 1   | G     | 318 | TYR  | Sidechain |
| 1   | G     | 342 | TYR  | Sidechain |
| 2   | H     | 61  | PHE  | Sidechain |

## 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     | 4200  | 0        | 4064     | 338     | 2            |
| 1   | C     | 4200  | 0        | 4064     | 405     | 24           |
| 1   | E     | 4200  | 0        | 4064     | 342     | 2            |
| 1   | G     | 4200  | 0        | 4064     | 401     | 8            |
| 2   | B     | 3198  | 0        | 3184     | 242     | 4            |
| 2   | D     | 3198  | 0        | 3184     | 241     | 8            |
| 2   | F     | 3198  | 0        | 3184     | 245     | 0            |
| 2   | H     | 3198  | 0        | 3184     | 242     | 20           |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 29596 | 0        | 28992    | 2306    | 34           |

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 39.

All (2306) 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:C:345:PRO:HG3  | 1:G:326:ILE:CD1  | 1.22                     | 1.68              |
| 1:C:346:PHE:CD1  | 1:G:390:LYS:CE   | 1.87                     | 1.58              |
| 1:C:345:PRO:CG   | 1:G:326:ILE:CD1  | 1.79                     | 1.54              |
| 1:C:346:PHE:CD1  | 1:G:390:LYS:HE3  | 0.98                     | 1.51              |
| 1:C:346:PHE:CE1  | 1:G:390:LYS:HG3  | 1.60                     | 1.36              |
| 1:C:346:PHE:HB2  | 1:G:390:LYS:NZ   | 1.46                     | 1.28              |
| 1:C:417:VAL:HG11 | 1:G:346:PHE:CE2  | 1.67                     | 1.27              |
| 1:C:417:VAL:CG1  | 1:G:346:PHE:CE2  | 2.19                     | 1.25              |
| 1:C:345:PRO:CG   | 1:G:326:ILE:HD12 | 1.49                     | 1.21              |
| 1:C:345:PRO:CG   | 1:G:326:ILE:HD13 | 1.56                     | 1.12              |
| 1:C:345:PRO:HG2  | 1:G:326:ILE:CD1  | 1.70                     | 1.11              |
| 1:C:346:PHE:CE1  | 1:G:390:LYS:HE3  | 1.89                     | 1.07              |
| 1:C:345:PRO:HG2  | 1:G:326:ILE:HD13 | 1.23                     | 1.07              |
| 1:E:393:ILE:HG23 | 1:E:414:TRP:CH2  | 1.93                     | 1.04              |
| 1:C:393:ILE:HG23 | 1:C:414:TRP:CH2  | 1.93                     | 1.03              |
| 1:G:393:ILE:HG23 | 1:G:414:TRP:CH2  | 1.93                     | 1.03              |
| 1:A:393:ILE:HG23 | 1:A:414:TRP:CH2  | 1.93                     | 1.02              |
| 2:B:264:LEU:HD22 | 2:B:274:ILE:HD11 | 1.42                     | 1.02              |
| 2:D:264:LEU:HD22 | 2:D:274:ILE:HD11 | 1.42                     | 1.02              |
| 2:H:264:LEU:HD22 | 2:H:274:ILE:HD11 | 1.42                     | 1.02              |
| 2:F:264:LEU:HD22 | 2:F:274:ILE:HD11 | 1.42                     | 1.02              |
| 1:G:540:LYS:HZ1  | 2:H:265:ASN:HB2  | 1.24                     | 1.01              |
| 1:C:346:PHE:CZ   | 1:G:390:LYS:HG3  | 1.95                     | 1.00              |
| 1:C:417:VAL:HG13 | 1:G:346:PHE:CE2  | 1.97                     | 1.00              |
| 1:C:346:PHE:CB   | 1:G:390:LYS:NZ   | 2.24                     | 1.00              |
| 1:C:376:THR:HG23 | 1:C:386:THR:HG23 | 1.43                     | 0.99              |
| 1:A:376:THR:HG23 | 1:A:386:THR:HG23 | 1.43                     | 0.99              |
| 1:C:346:PHE:CG   | 1:G:390:LYS:CE   | 2.47                     | 0.98              |
| 1:C:346:PHE:CE1  | 1:G:390:LYS:CG   | 2.46                     | 0.98              |
| 1:A:540:LYS:HZ1  | 2:B:265:ASN:HB2  | 1.30                     | 0.97              |
| 1:G:376:THR:HG23 | 1:G:386:THR:HG23 | 1.43                     | 0.97              |
| 1:C:346:PHE:HB2  | 1:G:390:LYS:HZ2  | 1.29                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:376:THR:HG23 | 1:E:386:THR:HG23 | 1.43                     | 0.97              |
| 1:G:420:PRO:HG2  | 1:G:421:PRO:HD2  | 1.47                     | 0.95              |
| 2:H:103:LYS:HZ2  | 2:H:179:VAL:H    | 1.15                     | 0.94              |
| 1:C:417:VAL:HG13 | 1:G:346:PHE:CD2  | 2.02                     | 0.94              |
| 2:D:103:LYS:HZ2  | 2:D:179:VAL:H    | 1.15                     | 0.94              |
| 1:E:420:PRO:HG2  | 1:E:421:PRO:HD2  | 1.47                     | 0.94              |
| 1:C:342:TYR:OH   | 1:G:345:PRO:HG3  | 1.68                     | 0.94              |
| 2:B:103:LYS:HZ2  | 2:B:179:VAL:H    | 1.15                     | 0.93              |
| 1:C:420:PRO:HG2  | 1:C:421:PRO:HD2  | 1.47                     | 0.93              |
| 1:A:420:PRO:HG2  | 1:A:421:PRO:HD2  | 1.47                     | 0.93              |
| 1:C:417:VAL:HG11 | 1:G:346:PHE:CZ   | 2.03                     | 0.92              |
| 1:C:346:PHE:CE1  | 1:G:342:TYR:OH   | 2.22                     | 0.92              |
| 2:F:50:ILE:HG21  | 2:F:145:GLN:HB2  | 1.49                     | 0.92              |
| 2:H:50:ILE:HG21  | 2:H:145:GLN:HB2  | 1.49                     | 0.92              |
| 2:D:50:ILE:HG21  | 2:D:145:GLN:HB2  | 1.49                     | 0.91              |
| 1:A:540:LYS:NZ   | 2:B:265:ASN:HB2  | 1.86                     | 0.91              |
| 1:G:540:LYS:NZ   | 2:H:265:ASN:HB2  | 1.86                     | 0.91              |
| 2:B:50:ILE:HG21  | 2:B:145:GLN:HB2  | 1.49                     | 0.91              |
| 1:C:540:LYS:NZ   | 2:D:265:ASN:HB2  | 1.86                     | 0.91              |
| 1:C:346:PHE:HB2  | 1:G:390:LYS:HZ1  | 1.10                     | 0.90              |
| 1:C:346:PHE:HE1  | 1:G:342:TYR:OH   | 1.53                     | 0.90              |
| 1:C:346:PHE:CB   | 1:G:390:LYS:HZ2  | 1.83                     | 0.90              |
| 2:H:260:LEU:HD21 | 2:H:303:LEU:HD21 | 1.53                     | 0.90              |
| 1:E:540:LYS:NZ   | 2:F:265:ASN:HB2  | 1.86                     | 0.89              |
| 1:A:107:THR:HG23 | 1:A:198:HIS:HE1  | 1.38                     | 0.89              |
| 1:C:107:THR:HG23 | 1:C:198:HIS:HE1  | 1.38                     | 0.89              |
| 1:G:107:THR:HG23 | 1:G:198:HIS:HE1  | 1.38                     | 0.89              |
| 2:D:260:LEU:HD21 | 2:D:303:LEU:HD21 | 1.54                     | 0.89              |
| 2:F:103:LYS:HZ2  | 2:F:179:VAL:H    | 1.19                     | 0.88              |
| 2:B:260:LEU:HD21 | 2:B:303:LEU:HD21 | 1.54                     | 0.88              |
| 1:E:107:THR:HG23 | 1:E:198:HIS:HE1  | 1.38                     | 0.88              |
| 2:F:104:LYS:HB3  | 2:F:192:ASP:HA   | 1.55                     | 0.87              |
| 2:F:260:LEU:HD21 | 2:F:303:LEU:HD21 | 1.54                     | 0.87              |
| 2:H:104:LYS:HB3  | 2:H:192:ASP:HA   | 1.55                     | 0.86              |
| 1:C:346:PHE:CD1  | 1:G:390:LYS:CD   | 2.57                     | 0.86              |
| 1:C:540:LYS:HZ1  | 2:D:265:ASN:HB2  | 1.40                     | 0.86              |
| 1:C:244:ILE:HD12 | 1:C:267:ALA:HB2  | 1.56                     | 0.86              |
| 1:G:244:ILE:HD12 | 1:G:267:ALA:HB2  | 1.56                     | 0.86              |
| 2:H:171:PHE:HE2  | 2:H:204:GLU:HB2  | 1.41                     | 0.86              |
| 1:A:317:VAL:HG21 | 1:A:347:LYS:HB3  | 1.58                     | 0.86              |
| 1:C:317:VAL:HG21 | 1:C:347:LYS:HB3  | 1.58                     | 0.86              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:171:PHE:HE2  | 2:F:204:GLU:HB2 | 1.41                     | 0.86              |
| 1:G:317:VAL:HG21 | 1:G:347:LYS:HB3 | 1.58                     | 0.85              |
| 2:D:104:LYS:HB3  | 2:D:192:ASP:HA  | 1.55                     | 0.85              |
| 2:B:104:LYS:HB3  | 2:B:192:ASP:HA  | 1.55                     | 0.85              |
| 1:E:317:VAL:HG21 | 1:E:347:LYS:HB3 | 1.58                     | 0.85              |
| 1:A:244:ILE:HD12 | 1:A:267:ALA:HB2 | 1.56                     | 0.84              |
| 1:E:244:ILE:HD12 | 1:E:267:ALA:HB2 | 1.56                     | 0.84              |
| 2:F:365:VAL:HG11 | 2:F:401:TRP:HB2 | 1.59                     | 0.84              |
| 2:B:365:VAL:HG11 | 2:B:401:TRP:HB2 | 1.59                     | 0.84              |
| 1:E:391:LEU:HB2  | 1:E:414:TRP:CZ3 | 2.13                     | 0.84              |
| 1:C:417:VAL:CG1  | 1:G:346:PHE:CD2 | 2.59                     | 0.84              |
| 1:C:342:TYR:OH   | 1:G:345:PRO:CB  | 2.26                     | 0.84              |
| 2:D:171:PHE:HE2  | 2:D:204:GLU:HB2 | 1.41                     | 0.83              |
| 1:E:540:LYS:HZ1  | 2:F:265:ASN:HB2 | 1.37                     | 0.83              |
| 2:B:171:PHE:HE2  | 2:B:204:GLU:HB2 | 1.41                     | 0.83              |
| 1:G:391:LEU:HB2  | 1:G:414:TRP:CZ3 | 2.13                     | 0.83              |
| 1:A:391:LEU:HB2  | 1:A:414:TRP:CZ3 | 2.13                     | 0.83              |
| 2:D:365:VAL:HG11 | 2:D:401:TRP:HB2 | 1.59                     | 0.83              |
| 2:H:365:VAL:HG11 | 2:H:401:TRP:HB2 | 1.59                     | 0.82              |
| 2:B:24:TRP:CH2   | 2:B:61:PHE:CD1  | 2.68                     | 0.82              |
| 1:C:391:LEU:HB2  | 1:C:414:TRP:CZ3 | 2.13                     | 0.82              |
| 2:D:24:TRP:CH2   | 2:D:61:PHE:CD1  | 2.68                     | 0.82              |
| 1:C:342:TYR:OH   | 1:G:345:PRO:CG  | 2.26                     | 0.82              |
| 2:H:61:PHE:CZ    | 2:H:74:LEU:HD23 | 2.14                     | 0.82              |
| 2:D:61:PHE:CZ    | 2:D:74:LEU:HD23 | 2.14                     | 0.82              |
| 2:F:61:PHE:CZ    | 2:F:74:LEU:HD23 | 2.14                     | 0.82              |
| 1:C:326:ILE:HB   | 1:C:342:TYR:CE1 | 2.15                     | 0.82              |
| 1:G:326:ILE:HB   | 1:G:342:TYR:CE1 | 2.15                     | 0.82              |
| 1:A:326:ILE:HB   | 1:A:342:TYR:CE1 | 2.15                     | 0.82              |
| 2:D:33:ALA:O     | 2:D:37:ILE:HG13 | 1.80                     | 0.82              |
| 2:F:33:ALA:O     | 2:F:37:ILE:HG13 | 1.80                     | 0.82              |
| 2:B:33:ALA:O     | 2:B:37:ILE:HG13 | 1.80                     | 0.81              |
| 2:B:61:PHE:CZ    | 2:B:74:LEU:HD23 | 2.14                     | 0.81              |
| 2:H:24:TRP:CH2   | 2:H:61:PHE:CD1  | 2.68                     | 0.81              |
| 2:H:24:TRP:HH2   | 2:H:61:PHE:CE1  | 1.99                     | 0.81              |
| 2:H:33:ALA:O     | 2:H:37:ILE:HG13 | 1.80                     | 0.81              |
| 1:E:107:THR:HG23 | 1:E:198:HIS:CE1 | 2.16                     | 0.81              |
| 1:E:326:ILE:HB   | 1:E:342:TYR:CE1 | 2.15                     | 0.81              |
| 2:F:157:PRO:HG2  | 2:F:158:ALA:H   | 1.46                     | 0.81              |
| 2:F:24:TRP:HH2   | 2:F:61:PHE:CE1  | 1.99                     | 0.81              |
| 2:F:24:TRP:CH2   | 2:F:61:PHE:CD1  | 2.68                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:107:THR:HG23 | 1:G:198:HIS:CE1  | 2.16                     | 0.80              |
| 2:H:157:PRO:HG2  | 2:H:158:ALA:H    | 1.46                     | 0.80              |
| 1:A:107:THR:HG23 | 1:A:198:HIS:CE1  | 2.16                     | 0.80              |
| 1:E:91:GLN:HE21  | 1:E:91:GLN:HA    | 1.47                     | 0.80              |
| 1:G:91:GLN:HE21  | 1:G:91:GLN:HA    | 1.47                     | 0.80              |
| 1:C:91:GLN:HE21  | 1:C:91:GLN:HA    | 1.47                     | 0.80              |
| 2:D:24:TRP:HH2   | 2:D:61:PHE:CE1   | 1.99                     | 0.80              |
| 1:C:107:THR:HG23 | 1:C:198:HIS:CE1  | 2.16                     | 0.79              |
| 2:B:249:LYS:HB2  | 2:B:252:TRP:CE2  | 2.18                     | 0.79              |
| 2:B:24:TRP:HH2   | 2:B:61:PHE:CE1   | 1.99                     | 0.79              |
| 1:G:393:ILE:HB   | 1:G:423:VAL:CG2  | 2.12                     | 0.79              |
| 2:D:249:LYS:HB2  | 2:D:252:TRP:CE2  | 2.18                     | 0.79              |
| 1:C:393:ILE:HB   | 1:C:423:VAL:CG2  | 2.12                     | 0.79              |
| 1:A:91:GLN:HA    | 1:A:91:GLN:HE21  | 1.47                     | 0.79              |
| 1:A:391:LEU:HB2  | 1:A:414:TRP:HZ3  | 1.48                     | 0.79              |
| 1:G:361:HIS:CD2  | 1:G:518:VAL:HG11 | 2.18                     | 0.78              |
| 2:D:157:PRO:HG2  | 2:D:158:ALA:H    | 1.46                     | 0.78              |
| 1:A:393:ILE:HB   | 1:A:423:VAL:CG2  | 2.12                     | 0.78              |
| 1:E:393:ILE:HB   | 1:E:423:VAL:CG2  | 2.12                     | 0.78              |
| 2:B:157:PRO:HG2  | 2:B:158:ALA:H    | 1.46                     | 0.78              |
| 2:H:249:LYS:HB2  | 2:H:252:TRP:CE2  | 2.18                     | 0.78              |
| 1:C:391:LEU:HB2  | 1:C:414:TRP:HZ3  | 1.48                     | 0.78              |
| 2:F:420:PRO:HB2  | 2:F:421:PRO:HD2  | 1.66                     | 0.78              |
| 2:F:249:LYS:HB2  | 2:F:252:TRP:CE2  | 2.18                     | 0.78              |
| 1:A:361:HIS:HD2  | 1:A:518:VAL:HG11 | 1.49                     | 0.77              |
| 1:C:346:PHE:CG   | 1:G:390:LYS:NZ   | 2.52                     | 0.77              |
| 1:E:361:HIS:CD2  | 1:E:518:VAL:HG11 | 2.18                     | 0.77              |
| 1:A:361:HIS:CD2  | 1:A:518:VAL:HG11 | 2.18                     | 0.77              |
| 1:G:361:HIS:HD2  | 1:G:518:VAL:HG11 | 1.49                     | 0.77              |
| 1:C:361:HIS:HD2  | 1:C:518:VAL:HG11 | 1.49                     | 0.77              |
| 1:C:361:HIS:CD2  | 1:C:518:VAL:HG11 | 2.18                     | 0.77              |
| 2:B:420:PRO:HB2  | 2:B:421:PRO:HD2  | 1.66                     | 0.76              |
| 1:G:391:LEU:HB2  | 1:G:414:TRP:HZ3  | 1.48                     | 0.76              |
| 2:H:420:PRO:HB2  | 2:H:421:PRO:HD2  | 1.66                     | 0.76              |
| 1:E:354:TYR:OH   | 1:E:356:ARG:HD3  | 1.85                     | 0.76              |
| 2:D:420:PRO:HB2  | 2:D:421:PRO:HD2  | 1.66                     | 0.76              |
| 1:A:85:GLN:O     | 1:A:85:GLN:HG2   | 1.86                     | 0.75              |
| 2:D:24:TRP:HH2   | 2:D:61:PHE:CD1   | 2.05                     | 0.75              |
| 1:G:354:TYR:OH   | 1:G:356:ARG:HD3  | 1.85                     | 0.75              |
| 1:E:85:GLN:HG2   | 1:E:85:GLN:O     | 1.86                     | 0.75              |
| 1:C:354:TYR:OH   | 1:C:356:ARG:HD3  | 1.85                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:131:THR:HG22 | 1:C:143:ARG:HG3  | 1.69                     | 0.74              |
| 1:C:249:LYS:HE2  | 1:C:251:SER:HB3  | 1.69                     | 0.74              |
| 1:E:391:LEU:HB2  | 1:E:414:TRP:HZ3  | 1.48                     | 0.74              |
| 1:C:10:VAL:HG21  | 1:C:153:TRP:HH2  | 1.52                     | 0.74              |
| 2:F:17:ASP:O     | 2:F:83:ARG:HD3   | 1.87                     | 0.74              |
| 2:F:24:TRP:HH2   | 2:F:61:PHE:CD1   | 2.05                     | 0.74              |
| 1:G:131:THR:HG22 | 1:G:143:ARG:HG3  | 1.69                     | 0.74              |
| 1:A:10:VAL:HG21  | 1:A:153:TRP:HH2  | 1.52                     | 0.74              |
| 1:A:354:TYR:OH   | 1:A:356:ARG:HD3  | 1.85                     | 0.74              |
| 1:E:361:HIS:HD2  | 1:E:518:VAL:HG11 | 1.49                     | 0.74              |
| 1:C:342:TYR:CZ   | 1:G:345:PRO:HG3  | 2.22                     | 0.74              |
| 1:C:85:GLN:HG2   | 1:C:85:GLN:O     | 1.86                     | 0.74              |
| 1:A:249:LYS:HE2  | 1:A:251:SER:HB3  | 1.69                     | 0.74              |
| 1:A:131:THR:HG22 | 1:A:143:ARG:HG3  | 1.69                     | 0.74              |
| 2:B:24:TRP:HH2   | 2:B:61:PHE:CD1   | 2.05                     | 0.74              |
| 1:E:10:VAL:HG21  | 1:E:153:TRP:HH2  | 1.52                     | 0.74              |
| 1:G:10:VAL:HG21  | 1:G:153:TRP:HH2  | 1.52                     | 0.74              |
| 1:G:85:GLN:O     | 1:G:85:GLN:HG2   | 1.86                     | 0.74              |
| 1:G:249:LYS:HE2  | 1:G:251:SER:HB3  | 1.69                     | 0.74              |
| 2:H:17:ASP:O     | 2:H:83:ARG:HD3   | 1.87                     | 0.74              |
| 1:E:249:LYS:HE2  | 1:E:251:SER:HB3  | 1.69                     | 0.73              |
| 1:E:391:LEU:HD12 | 1:E:414:TRP:CE3  | 2.23                     | 0.73              |
| 2:B:17:ASP:O     | 2:B:83:ARG:HD3   | 1.87                     | 0.73              |
| 2:D:103:LYS:NZ   | 2:D:179:VAL:HG23 | 2.04                     | 0.73              |
| 2:F:103:LYS:NZ   | 2:F:179:VAL:HG23 | 2.04                     | 0.73              |
| 2:B:50:ILE:CG2   | 2:B:145:GLN:HB2  | 2.18                     | 0.73              |
| 2:B:63:ILE:HG23  | 2:B:72:ARG:HB3   | 1.70                     | 0.73              |
| 2:H:103:LYS:HZ2  | 2:H:179:VAL:N    | 1.86                     | 0.73              |
| 2:B:103:LYS:NZ   | 2:B:179:VAL:HG23 | 2.04                     | 0.73              |
| 2:D:17:ASP:O     | 2:D:83:ARG:HD3   | 1.87                     | 0.73              |
| 1:E:90:VAL:HG12  | 2:F:141:GLY:H    | 1.53                     | 0.73              |
| 1:G:391:LEU:HD12 | 1:G:414:TRP:CE3  | 2.24                     | 0.73              |
| 2:D:103:LYS:HZ2  | 2:D:179:VAL:N    | 1.86                     | 0.73              |
| 2:H:103:LYS:NZ   | 2:H:179:VAL:HG23 | 2.04                     | 0.73              |
| 2:H:24:TRP:HH2   | 2:H:61:PHE:CD1   | 2.04                     | 0.73              |
| 1:C:90:VAL:HG12  | 2:D:141:GLY:H    | 1.53                     | 0.73              |
| 1:E:131:THR:HG22 | 1:E:143:ARG:HG3  | 1.69                     | 0.73              |
| 2:D:63:ILE:HG23  | 2:D:72:ARG:HB3   | 1.70                     | 0.73              |
| 1:G:90:VAL:HG12  | 2:H:141:GLY:H    | 1.53                     | 0.73              |
| 1:E:442:VAL:CG1  | 1:E:481:ALA:HB1  | 2.19                     | 0.72              |
| 2:H:171:PHE:HB2  | 2:H:208:HIS:CE1  | 2.24                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:391:LEU:HD12 | 1:A:414:TRP:CE3  | 2.24                     | 0.72              |
| 1:C:157:PRO:HG2  | 1:C:158:ALA:H    | 1.54                     | 0.72              |
| 2:F:103:LYS:HZ2  | 2:F:179:VAL:N    | 1.86                     | 0.72              |
| 1:G:157:PRO:HG2  | 1:G:158:ALA:H    | 1.54                     | 0.72              |
| 2:B:171:PHE:HB2  | 2:B:208:HIS:CE1  | 2.24                     | 0.72              |
| 2:D:171:PHE:HB2  | 2:D:208:HIS:CE1  | 2.25                     | 0.72              |
| 2:D:246:LEU:HD11 | 2:D:264:LEU:HD21 | 1.72                     | 0.72              |
| 2:F:50:ILE:CG2   | 2:F:145:GLN:HB2  | 2.18                     | 0.72              |
| 2:H:246:LEU:HD11 | 2:H:264:LEU:HD21 | 1.72                     | 0.72              |
| 1:A:90:VAL:HG12  | 2:B:141:GLY:H    | 1.53                     | 0.72              |
| 2:B:246:LEU:HD11 | 2:B:264:LEU:HD21 | 1.72                     | 0.72              |
| 1:A:393:ILE:O    | 1:A:414:TRP:HH2  | 1.73                     | 0.72              |
| 1:C:391:LEU:HD12 | 1:C:414:TRP:CE3  | 2.23                     | 0.72              |
| 1:E:157:PRO:HG2  | 1:E:158:ALA:H    | 1.54                     | 0.72              |
| 1:C:393:ILE:O    | 1:C:414:TRP:HH2  | 1.73                     | 0.72              |
| 2:F:171:PHE:HB2  | 2:F:208:HIS:CE1  | 2.25                     | 0.72              |
| 1:G:442:VAL:CG1  | 1:G:481:ALA:HB1  | 2.19                     | 0.72              |
| 1:C:442:VAL:CG1  | 1:C:481:ALA:HB1  | 2.19                     | 0.72              |
| 2:D:50:ILE:CG2   | 2:D:145:GLN:HB2  | 2.18                     | 0.72              |
| 2:F:92:LEU:HG    | 2:F:158:ALA:HB2  | 1.72                     | 0.71              |
| 2:F:63:ILE:HG23  | 2:F:72:ARG:HB3   | 1.70                     | 0.71              |
| 1:E:518:VAL:O    | 1:E:522:ILE:HG13 | 1.90                     | 0.71              |
| 1:A:518:VAL:O    | 1:A:522:ILE:HG13 | 1.90                     | 0.71              |
| 1:C:341:ILE:HD12 | 1:C:383:TRP:HE1  | 1.55                     | 0.71              |
| 1:E:341:ILE:HD12 | 1:E:383:TRP:HE1  | 1.55                     | 0.71              |
| 1:G:518:VAL:O    | 1:G:522:ILE:HG13 | 1.90                     | 0.71              |
| 1:A:157:PRO:HG2  | 1:A:158:ALA:H    | 1.54                     | 0.71              |
| 2:H:63:ILE:HG23  | 2:H:72:ARG:HB3   | 1.70                     | 0.71              |
| 1:A:442:VAL:CG1  | 1:A:481:ALA:HB1  | 2.19                     | 0.71              |
| 1:G:393:ILE:O    | 1:G:414:TRP:HH2  | 1.73                     | 0.71              |
| 2:H:47:ILE:HG22  | 2:H:48:SER:H     | 1.56                     | 0.71              |
| 1:E:393:ILE:O    | 1:E:414:TRP:HH2  | 1.73                     | 0.71              |
| 2:F:246:LEU:HD11 | 2:F:264:LEU:HD21 | 1.72                     | 0.71              |
| 2:B:47:ILE:HG22  | 2:B:48:SER:H     | 1.56                     | 0.71              |
| 1:C:518:VAL:O    | 1:C:522:ILE:HG13 | 1.90                     | 0.71              |
| 2:D:47:ILE:HG22  | 2:D:48:SER:H     | 1.56                     | 0.71              |
| 2:H:50:ILE:CG2   | 2:H:145:GLN:HB2  | 2.18                     | 0.71              |
| 1:A:225:PRO:HG2  | 1:A:226:PRO:HD3  | 1.73                     | 0.70              |
| 1:A:341:ILE:HD12 | 1:A:383:TRP:HE1  | 1.55                     | 0.70              |
| 1:C:225:PRO:HG2  | 1:C:226:PRO:HD3  | 1.73                     | 0.70              |
| 1:G:341:ILE:HD12 | 1:G:383:TRP:HE1  | 1.55                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:92:LEU:HG    | 2:H:158:ALA:HB2  | 1.72                     | 0.70              |
| 2:D:92:LEU:HG    | 2:D:158:ALA:HB2  | 1.72                     | 0.70              |
| 2:F:47:ILE:HG22  | 2:F:48:SER:H     | 1.56                     | 0.70              |
| 1:A:114:ALA:HB1  | 1:A:160:PHE:CZ   | 2.27                     | 0.70              |
| 1:E:114:ALA:HB1  | 1:E:160:PHE:CZ   | 2.27                     | 0.70              |
| 1:C:345:PRO:HG3  | 1:G:326:ILE:HD12 | 0.70                     | 0.70              |
| 1:G:114:ALA:HB1  | 1:G:160:PHE:CZ   | 2.27                     | 0.70              |
| 2:D:168:LEU:HD21 | 2:D:209:LEU:HD21 | 1.74                     | 0.70              |
| 2:F:59:PRO:HG2   | 2:F:76:ASP:HB3   | 1.74                     | 0.70              |
| 2:H:136:ASN:HB3  | 2:H:138:GLU:HG3  | 1.73                     | 0.70              |
| 1:E:225:PRO:HG2  | 1:E:226:PRO:HD3  | 1.73                     | 0.69              |
| 2:B:103:LYS:HZ2  | 2:B:179:VAL:N    | 1.86                     | 0.69              |
| 2:B:92:LEU:HG    | 2:B:158:ALA:HB2  | 1.72                     | 0.69              |
| 1:G:416:PHE:CD1  | 1:G:417:VAL:N    | 2.60                     | 0.69              |
| 2:H:168:LEU:HD21 | 2:H:209:LEU:HD21 | 1.74                     | 0.69              |
| 2:B:59:PRO:HG2   | 2:B:76:ASP:HB3   | 1.74                     | 0.69              |
| 1:E:416:PHE:CD1  | 1:E:417:VAL:N    | 2.60                     | 0.69              |
| 1:G:31:ILE:O     | 1:G:35:VAL:HG23  | 1.92                     | 0.69              |
| 1:G:6:GLU:CD     | 1:G:6:GLU:H      | 1.95                     | 0.69              |
| 1:C:31:ILE:O     | 1:C:35:VAL:HG23  | 1.92                     | 0.69              |
| 1:E:233:GLU:OE2  | 1:E:242:GLN:HG3  | 1.93                     | 0.69              |
| 1:C:6:GLU:CD     | 1:C:6:GLU:H      | 1.95                     | 0.69              |
| 1:A:416:PHE:CD1  | 1:A:417:VAL:N    | 2.60                     | 0.69              |
| 1:A:419:THR:HG23 | 1:A:420:PRO:HD2  | 1.74                     | 0.69              |
| 1:A:6:GLU:H      | 1:A:6:GLU:CD     | 1.95                     | 0.69              |
| 1:C:426:TRP:CE3  | 1:C:426:TRP:HA   | 2.28                     | 0.69              |
| 1:G:225:PRO:HG2  | 1:G:226:PRO:HD3  | 1.73                     | 0.69              |
| 1:G:233:GLU:OE2  | 1:G:242:GLN:HG3  | 1.93                     | 0.69              |
| 1:C:233:GLU:OE2  | 1:C:242:GLN:HG3  | 1.93                     | 0.69              |
| 2:D:136:ASN:HB3  | 2:D:138:GLU:HG3  | 1.74                     | 0.69              |
| 1:E:442:VAL:HG12 | 1:E:481:ALA:HB1  | 1.75                     | 0.69              |
| 1:E:6:GLU:H      | 1:E:6:GLU:CD     | 1.95                     | 0.69              |
| 2:H:316:GLY:O    | 2:H:318:TYR:HD1  | 1.76                     | 0.69              |
| 1:A:31:ILE:O     | 1:A:35:VAL:HG23  | 1.92                     | 0.69              |
| 1:A:442:VAL:HG12 | 1:A:481:ALA:HB1  | 1.75                     | 0.69              |
| 1:C:114:ALA:HB1  | 1:C:160:PHE:CZ   | 2.27                     | 0.69              |
| 1:C:416:PHE:CD1  | 1:C:417:VAL:N    | 2.60                     | 0.69              |
| 1:C:419:THR:HG23 | 1:C:420:PRO:HD2  | 1.74                     | 0.69              |
| 2:D:59:PRO:HG2   | 2:D:76:ASP:HB3   | 1.74                     | 0.69              |
| 1:G:130:PHE:CZ   | 1:G:144:TYR:HB2  | 2.28                     | 0.69              |
| 1:G:426:TRP:CE3  | 1:G:426:TRP:HA   | 2.28                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:426:TRP:CE3  | 1:E:426:TRP:HA   | 2.28                     | 0.69              |
| 2:F:316:GLY:O    | 2:F:318:TYR:HD1  | 1.76                     | 0.69              |
| 1:C:221:HIS:O    | 1:C:223:LYS:N    | 2.26                     | 0.69              |
| 1:C:99:GLY:HA2   | 1:C:383:TRP:CZ3  | 2.28                     | 0.69              |
| 1:A:99:GLY:HA2   | 1:A:383:TRP:CZ3  | 2.28                     | 0.68              |
| 2:B:136:ASN:HB3  | 2:B:138:GLU:HG3  | 1.74                     | 0.68              |
| 2:B:168:LEU:HD21 | 2:B:209:LEU:HD21 | 1.74                     | 0.68              |
| 2:B:316:GLY:O    | 2:B:318:TYR:HD1  | 1.76                     | 0.68              |
| 1:E:221:HIS:O    | 1:E:223:LYS:N    | 2.26                     | 0.68              |
| 2:F:72:ARG:HH12  | 2:F:409:THR:HG22 | 1.58                     | 0.68              |
| 1:G:221:HIS:O    | 1:G:223:LYS:N    | 2.26                     | 0.68              |
| 2:H:59:PRO:HG2   | 2:H:76:ASP:HB3   | 1.74                     | 0.68              |
| 1:A:221:HIS:O    | 1:A:223:LYS:N    | 2.27                     | 0.68              |
| 1:A:426:TRP:HA   | 1:A:426:TRP:CE3  | 2.28                     | 0.68              |
| 1:C:130:PHE:CZ   | 1:C:144:TYR:HB2  | 2.28                     | 0.68              |
| 1:G:442:VAL:HG12 | 1:G:481:ALA:HB1  | 1.75                     | 0.68              |
| 2:D:316:GLY:O    | 2:D:318:TYR:HD1  | 1.76                     | 0.68              |
| 2:H:163:SER:O    | 2:H:167:ILE:HG13 | 1.94                     | 0.68              |
| 1:A:130:PHE:CZ   | 1:A:144:TYR:HB2  | 2.28                     | 0.68              |
| 1:A:233:GLU:OE2  | 1:A:242:GLN:HG3  | 1.93                     | 0.68              |
| 2:F:104:LYS:HA   | 2:F:237:ASP:OD2  | 1.94                     | 0.68              |
| 2:F:163:SER:O    | 2:F:167:ILE:HG13 | 1.93                     | 0.68              |
| 2:B:72:ARG:HH12  | 2:B:409:THR:HG22 | 1.58                     | 0.68              |
| 1:C:442:VAL:HG12 | 1:C:481:ALA:HB1  | 1.75                     | 0.68              |
| 1:E:130:PHE:CZ   | 1:E:144:TYR:HB2  | 2.28                     | 0.68              |
| 1:E:31:ILE:O     | 1:E:35:VAL:HG23  | 1.92                     | 0.68              |
| 1:G:99:GLY:HA2   | 1:G:383:TRP:CZ3  | 2.28                     | 0.68              |
| 2:H:104:LYS:HA   | 2:H:237:ASP:OD2  | 1.94                     | 0.68              |
| 1:E:100:LEU:O    | 1:E:318:TYR:HB3  | 1.94                     | 0.68              |
| 2:H:72:ARG:HH12  | 2:H:409:THR:HG22 | 1.58                     | 0.68              |
| 2:B:163:SER:O    | 2:B:167:ILE:HG13 | 1.94                     | 0.68              |
| 2:D:157:PRO:HG2  | 2:D:158:ALA:N    | 2.08                     | 0.68              |
| 1:E:99:GLY:HA2   | 1:E:383:TRP:CZ3  | 2.28                     | 0.68              |
| 2:F:136:ASN:HB3  | 2:F:138:GLU:HG3  | 1.74                     | 0.68              |
| 2:F:168:LEU:HD21 | 2:F:209:LEU:HD21 | 1.74                     | 0.68              |
| 1:G:420:PRO:HG2  | 1:G:421:PRO:CD   | 2.22                     | 0.68              |
| 2:D:163:SER:O    | 2:D:167:ILE:HG13 | 1.94                     | 0.68              |
| 2:D:72:ARG:HH12  | 2:D:409:THR:HG22 | 1.58                     | 0.68              |
| 2:D:97:PRO:HG2   | 2:D:181:TYR:HB2  | 1.76                     | 0.68              |
| 1:E:419:THR:HG23 | 1:E:420:PRO:HD2  | 1.74                     | 0.68              |
| 2:B:104:LYS:HA   | 2:B:237:ASP:OD2  | 1.94                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:98:ALA:CB    | 1:E:383:TRP:HH2  | 2.07                     | 0.68              |
| 2:F:123:ASP:HA   | 2:F:126:LYS:NZ   | 2.09                     | 0.68              |
| 2:H:97:PRO:HG2   | 2:H:181:TYR:HB2  | 1.76                     | 0.68              |
| 2:B:157:PRO:HG2  | 2:B:158:ALA:N    | 2.08                     | 0.67              |
| 1:C:100:LEU:O    | 1:C:318:TYR:HB3  | 1.94                     | 0.67              |
| 2:D:104:LYS:HA   | 2:D:237:ASP:OD2  | 1.94                     | 0.67              |
| 1:C:345:PRO:CD   | 1:G:326:ILE:HD12 | 2.24                     | 0.67              |
| 1:C:346:PHE:CD1  | 1:G:390:LYS:NZ   | 2.62                     | 0.67              |
| 1:E:378:GLU:O    | 1:E:382:ILE:HG13 | 1.95                     | 0.67              |
| 1:G:100:LEU:O    | 1:G:318:TYR:HB3  | 1.94                     | 0.67              |
| 1:G:419:THR:HG23 | 1:G:420:PRO:HD2  | 1.74                     | 0.67              |
| 2:H:157:PRO:HG2  | 2:H:158:ALA:N    | 2.08                     | 0.67              |
| 1:A:426:TRP:HA   | 1:A:426:TRP:HE3  | 1.59                     | 0.67              |
| 1:A:100:LEU:O    | 1:A:318:TYR:HB3  | 1.94                     | 0.67              |
| 2:B:123:ASP:HA   | 2:B:126:LYS:NZ   | 2.10                     | 0.67              |
| 2:B:97:PRO:HG2   | 2:B:181:TYR:HB2  | 1.76                     | 0.67              |
| 1:E:244:ILE:CD1  | 1:E:267:ALA:HB2  | 2.25                     | 0.67              |
| 2:F:94:ILE:HG22  | 2:F:95:PRO:CD    | 2.24                     | 0.67              |
| 2:F:97:PRO:HG2   | 2:F:181:TYR:HB2  | 1.76                     | 0.67              |
| 1:G:378:GLU:O    | 1:G:382:ILE:HG13 | 1.95                     | 0.67              |
| 1:G:393:ILE:O    | 1:G:414:TRP:CH2  | 2.48                     | 0.67              |
| 1:A:378:GLU:O    | 1:A:382:ILE:HG13 | 1.95                     | 0.67              |
| 2:D:123:ASP:HA   | 2:D:126:LYS:NZ   | 2.10                     | 0.67              |
| 1:A:244:ILE:CD1  | 1:A:267:ALA:HB2  | 2.25                     | 0.67              |
| 1:G:98:ALA:CB    | 1:G:383:TRP:HH2  | 2.07                     | 0.67              |
| 2:H:123:ASP:HA   | 2:H:126:LYS:NZ   | 2.10                     | 0.67              |
| 2:F:153:TRP:CZ3  | 2:F:155:GLY:HA3  | 2.30                     | 0.67              |
| 1:C:426:TRP:HE3  | 1:C:426:TRP:HA   | 1.59                     | 0.67              |
| 1:C:457:TYR:CE1  | 1:C:465:LYS:HB3  | 2.30                     | 0.67              |
| 2:D:94:ILE:HG22  | 2:D:95:PRO:CD    | 2.25                     | 0.67              |
| 1:G:244:ILE:CD1  | 1:G:267:ALA:HB2  | 2.25                     | 0.67              |
| 1:A:98:ALA:CB    | 1:A:383:TRP:HH2  | 2.07                     | 0.66              |
| 2:B:153:TRP:CZ3  | 2:B:155:GLY:HA3  | 2.30                     | 0.66              |
| 1:G:457:TYR:CE1  | 1:G:465:LYS:HB3  | 2.31                     | 0.66              |
| 2:H:94:ILE:HG22  | 2:H:95:PRO:CD    | 2.25                     | 0.66              |
| 1:C:378:GLU:O    | 1:C:382:ILE:HG13 | 1.95                     | 0.66              |
| 1:E:426:TRP:HA   | 1:E:426:TRP:HE3  | 1.59                     | 0.66              |
| 1:A:457:TYR:CE1  | 1:A:465:LYS:HB3  | 2.31                     | 0.66              |
| 1:E:393:ILE:O    | 1:E:414:TRP:CH2  | 2.48                     | 0.66              |
| 1:E:420:PRO:HG2  | 1:E:421:PRO:CD   | 2.22                     | 0.66              |
| 2:F:109:LEU:HD12 | 2:F:187:LEU:HD23 | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:167:ILE:O    | 1:G:208:HIS:HE1  | 1.78                     | 0.66              |
| 1:G:33:ALA:O     | 1:G:37:ILE:HG13  | 1.95                     | 0.66              |
| 1:E:167:ILE:O    | 1:E:208:HIS:HE1  | 1.78                     | 0.66              |
| 2:F:21:VAL:CG1   | 2:F:59:PRO:HD3   | 2.26                     | 0.66              |
| 2:H:21:VAL:CG1   | 2:H:59:PRO:HD3   | 2.26                     | 0.66              |
| 2:B:94:ILE:HG22  | 2:B:95:PRO:CD    | 2.25                     | 0.66              |
| 2:D:153:TRP:CZ3  | 2:D:155:GLY:HA3  | 2.30                     | 0.66              |
| 1:E:457:TYR:CE1  | 1:E:465:LYS:HB3  | 2.31                     | 0.66              |
| 1:E:149:LEU:HD22 | 1:E:156:SER:HA   | 1.78                     | 0.66              |
| 1:C:98:ALA:CB    | 1:C:383:TRP:HH2  | 2.07                     | 0.66              |
| 1:C:393:ILE:O    | 1:C:414:TRP:CH2  | 2.48                     | 0.66              |
| 2:H:109:LEU:HD12 | 2:H:187:LEU:HD23 | 1.77                     | 0.66              |
| 2:H:153:TRP:CZ3  | 2:H:155:GLY:HA3  | 2.30                     | 0.66              |
| 1:A:165:THR:HG21 | 2:B:140:PRO:HG2  | 1.77                     | 0.66              |
| 2:B:21:VAL:CG1   | 2:B:59:PRO:HD3   | 2.26                     | 0.66              |
| 1:C:537:PRO:HG2  | 2:D:262:GLY:HA2  | 1.78                     | 0.66              |
| 1:G:165:THR:HG21 | 2:H:140:PRO:HG2  | 1.77                     | 0.66              |
| 2:B:151:GLN:HA   | 2:B:151:GLN:HE21 | 1.61                     | 0.66              |
| 2:F:151:GLN:HA   | 2:F:151:GLN:HE21 | 1.61                     | 0.66              |
| 1:G:149:LEU:HD22 | 1:G:156:SER:HA   | 1.78                     | 0.66              |
| 1:A:33:ALA:O     | 1:A:37:ILE:HG13  | 1.95                     | 0.65              |
| 1:A:393:ILE:O    | 1:A:414:TRP:CH2  | 2.48                     | 0.65              |
| 1:C:165:THR:HG21 | 2:D:140:PRO:HG2  | 1.77                     | 0.65              |
| 1:C:167:ILE:O    | 1:C:208:HIS:HE1  | 1.78                     | 0.65              |
| 2:D:21:VAL:CG1   | 2:D:59:PRO:HD3   | 2.26                     | 0.65              |
| 1:E:33:ALA:O     | 1:E:37:ILE:HG13  | 1.95                     | 0.65              |
| 1:A:167:ILE:O    | 1:A:208:HIS:HE1  | 1.78                     | 0.65              |
| 1:A:27:THR:OG1   | 1:A:30:LYS:HG3   | 1.97                     | 0.65              |
| 2:B:169:GLU:HB3  | 2:B:170:PRO:HD3  | 1.78                     | 0.65              |
| 2:B:103:LYS:NZ   | 2:B:179:VAL:H    | 1.93                     | 0.65              |
| 1:A:537:PRO:HG2  | 2:B:262:GLY:HA2  | 1.78                     | 0.65              |
| 2:B:61:PHE:CE2   | 2:B:74:LEU:HD23  | 2.31                     | 0.65              |
| 2:D:169:GLU:HB3  | 2:D:170:PRO:HD3  | 1.78                     | 0.65              |
| 2:D:151:GLN:HE21 | 2:D:151:GLN:HA   | 1.61                     | 0.65              |
| 1:G:27:THR:OG1   | 1:G:30:LYS:HG3   | 1.97                     | 0.65              |
| 2:D:109:LEU:HD12 | 2:D:187:LEU:HD23 | 1.77                     | 0.65              |
| 2:F:61:PHE:CE2   | 2:F:74:LEU:HD23  | 2.31                     | 0.65              |
| 1:C:27:THR:OG1   | 1:C:30:LYS:HG3   | 1.97                     | 0.65              |
| 1:C:33:ALA:O     | 1:C:37:ILE:HG13  | 1.95                     | 0.65              |
| 1:C:420:PRO:HG2  | 1:C:421:PRO:CD   | 2.22                     | 0.65              |
| 2:D:303:LEU:O    | 2:D:307:ARG:HG3  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:27:THR:OG1   | 1:E:30:LYS:HG3   | 1.97                     | 0.65              |
| 1:G:406:TRP:CE3  | 1:G:407:GLN:HG3  | 2.32                     | 0.65              |
| 2:H:151:GLN:HE21 | 2:H:151:GLN:HA   | 1.61                     | 0.65              |
| 2:H:303:LEU:O    | 2:H:307:ARG:HG3  | 1.97                     | 0.65              |
| 1:E:248:GLU:HG3  | 1:E:307:ARG:HH21 | 1.62                     | 0.65              |
| 1:E:537:PRO:HG2  | 2:F:262:GLY:HA2  | 1.78                     | 0.65              |
| 1:G:328:GLU:O    | 1:G:339:TYR:HA   | 1.97                     | 0.65              |
| 1:G:426:TRP:HE3  | 1:G:426:TRP:HA   | 1.59                     | 0.65              |
| 2:H:104:LYS:NZ   | 2:H:194:GLU:HA   | 2.12                     | 0.65              |
| 1:G:537:PRO:HG2  | 2:H:262:GLY:HA2  | 1.78                     | 0.65              |
| 2:H:61:PHE:CE2   | 2:H:74:LEU:HD23  | 2.31                     | 0.65              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:HG3  | 2.32                     | 0.65              |
| 2:B:303:LEU:O    | 2:B:307:ARG:HG3  | 1.97                     | 0.65              |
| 2:D:61:PHE:CE2   | 2:D:74:LEU:HD23  | 2.31                     | 0.65              |
| 2:F:103:LYS:NZ   | 2:F:179:VAL:H    | 1.93                     | 0.65              |
| 1:G:248:GLU:HG3  | 1:G:307:ARG:HH21 | 1.62                     | 0.65              |
| 1:A:149:LEU:HD22 | 1:A:156:SER:HA   | 1.78                     | 0.65              |
| 1:A:328:GLU:O    | 1:A:339:TYR:HA   | 1.97                     | 0.65              |
| 2:B:109:LEU:HD12 | 2:B:187:LEU:HD23 | 1.77                     | 0.65              |
| 1:C:406:TRP:CE3  | 1:C:407:GLN:HG3  | 2.32                     | 0.65              |
| 2:F:28:GLU:HG3   | 2:F:135:ILE:CD1  | 2.27                     | 0.65              |
| 1:A:248:GLU:HG3  | 1:A:307:ARG:HH21 | 1.62                     | 0.65              |
| 2:B:28:GLU:HG3   | 2:B:135:ILE:CD1  | 2.27                     | 0.65              |
| 1:C:328:GLU:O    | 1:C:339:TYR:HA   | 1.97                     | 0.65              |
| 1:E:406:TRP:CE3  | 1:E:407:GLN:HG3  | 2.32                     | 0.65              |
| 2:F:303:LEU:O    | 2:F:307:ARG:HG3  | 1.97                     | 0.65              |
| 2:H:28:GLU:HG3   | 2:H:135:ILE:CD1  | 2.27                     | 0.65              |
| 1:C:248:GLU:HG3  | 1:C:307:ARG:HH21 | 1.62                     | 0.64              |
| 2:D:28:GLU:HG3   | 2:D:135:ILE:CD1  | 2.27                     | 0.64              |
| 1:E:328:GLU:O    | 1:E:339:TYR:HA   | 1.97                     | 0.64              |
| 1:G:537:PRO:HD2  | 1:G:542:ILE:CD1  | 2.27                     | 0.64              |
| 1:C:149:LEU:HD22 | 1:C:156:SER:HA   | 1.78                     | 0.64              |
| 1:C:244:ILE:CD1  | 1:C:267:ALA:HB2  | 2.25                     | 0.64              |
| 1:C:376:THR:HG23 | 1:C:386:THR:CG2  | 2.25                     | 0.64              |
| 1:E:165:THR:HG21 | 2:F:140:PRO:HG2  | 1.77                     | 0.64              |
| 2:B:264:LEU:CD2  | 2:B:274:ILE:HD11 | 2.24                     | 0.64              |
| 2:B:24:TRP:CZ3   | 2:B:61:PHE:HB3   | 2.32                     | 0.64              |
| 1:C:393:ILE:HG23 | 1:C:414:TRP:HH2  | 1.58                     | 0.64              |
| 2:D:149:LEU:HD22 | 2:D:156:SER:HA   | 1.79                     | 0.64              |
| 2:D:24:TRP:CZ3   | 2:D:61:PHE:HB3   | 2.32                     | 0.64              |
| 1:E:537:PRO:HD2  | 1:E:542:ILE:CD1  | 2.27                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:104:LYS:NZ   | 2:B:194:GLU:HA   | 2.12                     | 0.64              |
| 1:C:537:PRO:HD2  | 1:C:542:ILE:CD1  | 2.27                     | 0.64              |
| 2:D:104:LYS:NZ   | 2:D:194:GLU:HA   | 2.12                     | 0.64              |
| 2:F:104:LYS:NZ   | 2:F:194:GLU:HA   | 2.12                     | 0.64              |
| 2:F:246:LEU:HB2  | 2:F:307:ARG:NH1  | 2.13                     | 0.64              |
| 2:F:24:TRP:CZ3   | 2:F:61:PHE:HB3   | 2.32                     | 0.64              |
| 2:B:246:LEU:CD1  | 2:B:264:LEU:HD21 | 2.27                     | 0.64              |
| 2:D:103:LYS:NZ   | 2:D:179:VAL:H    | 1.93                     | 0.64              |
| 2:F:157:PRO:HG2  | 2:F:158:ALA:N    | 2.08                     | 0.64              |
| 2:H:126:LYS:HA   | 2:H:145:GLN:NE2  | 2.13                     | 0.64              |
| 2:H:246:LEU:CD1  | 2:H:264:LEU:HD21 | 2.27                     | 0.64              |
| 2:H:246:LEU:HB2  | 2:H:307:ARG:NH1  | 2.13                     | 0.64              |
| 2:B:149:LEU:HD22 | 2:B:156:SER:HA   | 1.79                     | 0.64              |
| 2:D:264:LEU:CD2  | 2:D:274:ILE:HD11 | 2.24                     | 0.64              |
| 1:A:393:ILE:HG23 | 1:A:414:TRP:HH2  | 1.58                     | 0.64              |
| 2:B:246:LEU:HB2  | 2:B:307:ARG:NH1  | 2.13                     | 0.64              |
| 2:H:264:LEU:CD2  | 2:H:274:ILE:HD11 | 2.24                     | 0.64              |
| 2:F:246:LEU:CD1  | 2:F:264:LEU:HD21 | 2.27                     | 0.64              |
| 1:A:420:PRO:HG2  | 1:A:421:PRO:CD   | 2.22                     | 0.64              |
| 1:G:376:THR:HG23 | 1:G:386:THR:CG2  | 2.25                     | 0.64              |
| 2:H:169:GLU:HB3  | 2:H:170:PRO:HD3  | 1.78                     | 0.64              |
| 1:A:376:THR:HG23 | 1:A:386:THR:CG2  | 2.25                     | 0.63              |
| 2:B:94:ILE:HG22  | 2:B:95:PRO:HD3   | 1.81                     | 0.63              |
| 2:D:246:LEU:HB2  | 2:D:307:ARG:NH1  | 2.13                     | 0.63              |
| 2:F:169:GLU:HB3  | 2:F:170:PRO:HD3  | 1.78                     | 0.63              |
| 2:D:94:ILE:HG22  | 2:D:95:PRO:HD3   | 1.81                     | 0.63              |
| 1:E:28:GLU:O     | 1:E:32:LYS:HG3   | 1.98                     | 0.63              |
| 1:G:28:GLU:O     | 1:G:32:LYS:HG3   | 1.98                     | 0.63              |
| 2:B:126:LYS:HA   | 2:B:145:GLN:NE2  | 2.13                     | 0.63              |
| 2:D:246:LEU:CD1  | 2:D:264:LEU:HD21 | 2.27                     | 0.63              |
| 2:H:63:ILE:HG12  | 2:H:64:LYS:N     | 2.14                     | 0.63              |
| 1:E:376:THR:HG23 | 1:E:386:THR:CG2  | 2.25                     | 0.63              |
| 2:F:126:LYS:HA   | 2:F:145:GLN:NE2  | 2.13                     | 0.63              |
| 1:C:342:TYR:CE1  | 1:G:345:PRO:HG3  | 2.33                     | 0.63              |
| 1:A:537:PRO:HD2  | 1:A:542:ILE:CD1  | 2.27                     | 0.63              |
| 1:C:393:ILE:HB   | 1:C:423:VAL:HG21 | 1.79                     | 0.63              |
| 2:H:94:ILE:HG22  | 2:H:95:PRO:HD3   | 1.81                     | 0.63              |
| 2:F:264:LEU:CD2  | 2:F:274:ILE:HD11 | 2.24                     | 0.63              |
| 2:H:24:TRP:CZ3   | 2:H:61:PHE:HB3   | 2.32                     | 0.63              |
| 1:A:393:ILE:HB   | 1:A:423:VAL:HG21 | 1.79                     | 0.63              |
| 1:E:206:ARG:HH22 | 1:E:218:ASP:HA   | 1.64                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:ARG:HH22 | 1:A:218:ASP:HA   | 1.64                     | 0.63              |
| 2:D:126:LYS:HA   | 2:D:145:GLN:NE2  | 2.13                     | 0.63              |
| 2:F:63:ILE:HG12  | 2:F:64:LYS:N     | 2.14                     | 0.63              |
| 2:H:103:LYS:NZ   | 2:H:179:VAL:H    | 1.93                     | 0.63              |
| 1:A:28:GLU:O     | 1:A:32:LYS:HG3   | 1.98                     | 0.63              |
| 1:C:540:LYS:HZ3  | 2:D:261:VAL:CG1  | 2.12                     | 0.63              |
| 2:F:94:ILE:HG22  | 2:F:95:PRO:HD3   | 1.81                     | 0.63              |
| 1:A:238:LYS:HE2  | 1:A:240:THR:CG2  | 2.29                     | 0.62              |
| 2:B:21:VAL:HG11  | 2:B:59:PRO:HD3   | 1.80                     | 0.62              |
| 1:C:238:LYS:HE2  | 1:C:240:THR:CG2  | 2.29                     | 0.62              |
| 2:F:21:VAL:HG11  | 2:F:59:PRO:HD3   | 1.80                     | 0.62              |
| 2:H:149:LEU:HD22 | 2:H:156:SER:HA   | 1.79                     | 0.62              |
| 2:H:21:VAL:HG11  | 2:H:59:PRO:HD3   | 1.80                     | 0.62              |
| 2:B:63:ILE:HG12  | 2:B:64:LYS:N     | 2.14                     | 0.62              |
| 1:C:28:GLU:O     | 1:C:32:LYS:HG3   | 1.98                     | 0.62              |
| 2:D:21:VAL:HG11  | 2:D:59:PRO:HD3   | 1.80                     | 0.62              |
| 2:D:63:ILE:HG12  | 2:D:64:LYS:N     | 2.14                     | 0.62              |
| 1:E:393:ILE:HB   | 1:E:423:VAL:HG21 | 1.80                     | 0.62              |
| 2:F:125:ARG:NH1  | 2:F:147:ASN:HA   | 2.15                     | 0.62              |
| 1:G:206:ARG:HH22 | 1:G:218:ASP:HA   | 1.64                     | 0.62              |
| 2:B:125:ARG:NH1  | 2:B:147:ASN:HA   | 2.15                     | 0.62              |
| 2:D:125:ARG:NH1  | 2:D:147:ASN:HA   | 2.15                     | 0.62              |
| 2:F:149:LEU:HD22 | 2:F:156:SER:HA   | 1.79                     | 0.62              |
| 1:C:346:PHE:HD1  | 1:G:390:LYS:HE3  | 0.80                     | 0.62              |
| 1:C:206:ARG:HG3  | 1:C:216:THR:OG1  | 2.00                     | 0.62              |
| 1:C:206:ARG:HH22 | 1:C:218:ASP:HA   | 1.64                     | 0.62              |
| 1:E:206:ARG:HG3  | 1:E:216:THR:OG1  | 2.00                     | 0.62              |
| 1:A:491:LEU:HB3  | 1:A:529:GLU:CB   | 2.30                     | 0.62              |
| 1:C:249:LYS:HG2  | 1:C:250:ASP:N    | 2.15                     | 0.62              |
| 1:E:491:LEU:HB3  | 1:E:529:GLU:CB   | 2.30                     | 0.62              |
| 1:G:339:TYR:CE1  | 1:G:352:GLY:HA3  | 2.35                     | 0.62              |
| 1:A:206:ARG:HG3  | 1:A:216:THR:OG1  | 2.00                     | 0.62              |
| 1:C:491:LEU:HB3  | 1:C:529:GLU:CB   | 2.30                     | 0.62              |
| 2:D:376:THR:HG22 | 2:D:389:PHE:CE1  | 2.35                     | 0.62              |
| 2:F:376:THR:HG22 | 2:F:389:PHE:CE1  | 2.35                     | 0.62              |
| 2:H:125:ARG:NH1  | 2:H:147:ASN:HA   | 2.15                     | 0.62              |
| 1:G:238:LYS:HE2  | 1:G:240:THR:CG2  | 2.29                     | 0.61              |
| 1:G:249:LYS:HG2  | 1:G:250:ASP:N    | 2.15                     | 0.61              |
| 2:B:47:ILE:HG21  | 2:B:144:TYR:HB3  | 1.82                     | 0.61              |
| 2:D:354:TYR:OH   | 2:D:374:LYS:HG2  | 2.00                     | 0.61              |
| 2:F:257:ILE:HB   | 2:F:283:LEU:HD21 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:47:ILE:HG21  | 2:F:144:TYR:HB3  | 1.82                     | 0.61              |
| 1:A:249:LYS:HG2  | 1:A:250:ASP:N    | 2.15                     | 0.61              |
| 2:B:354:TYR:OH   | 2:B:374:LYS:HG2  | 2.00                     | 0.61              |
| 1:C:104:LYS:HB2  | 1:C:192:ASP:HA   | 1.82                     | 0.61              |
| 1:C:339:TYR:CE1  | 1:C:352:GLY:HA3  | 2.35                     | 0.61              |
| 1:E:238:LYS:HE2  | 1:E:240:THR:CG2  | 2.29                     | 0.61              |
| 1:E:393:ILE:HG23 | 1:E:414:TRP:HH2  | 1.58                     | 0.61              |
| 1:G:393:ILE:HB   | 1:G:423:VAL:HG21 | 1.79                     | 0.61              |
| 2:H:376:THR:HG22 | 2:H:389:PHE:CE1  | 2.35                     | 0.61              |
| 1:G:104:LYS:HB2  | 1:G:192:ASP:HA   | 1.82                     | 0.61              |
| 1:G:435:VAL:HG22 | 2:H:290:THR:HG21 | 1.83                     | 0.61              |
| 2:B:376:THR:HG22 | 2:B:389:PHE:CE1  | 2.35                     | 0.61              |
| 2:D:87:PHE:CE2   | 2:D:155:GLY:HA2  | 2.36                     | 0.61              |
| 1:G:206:ARG:HG3  | 1:G:216:THR:OG1  | 2.00                     | 0.61              |
| 1:E:104:LYS:HB2  | 1:E:192:ASP:HA   | 1.82                     | 0.61              |
| 1:E:376:THR:O    | 1:E:380:ILE:HG13 | 2.01                     | 0.61              |
| 2:F:87:PHE:CE2   | 2:F:155:GLY:HA2  | 2.36                     | 0.61              |
| 2:H:87:PHE:CE2   | 2:H:155:GLY:HA2  | 2.36                     | 0.61              |
| 2:H:354:TYR:OH   | 2:H:374:LYS:HG2  | 2.00                     | 0.61              |
| 1:C:225:PRO:HG2  | 1:C:226:PRO:CD   | 2.31                     | 0.61              |
| 1:C:435:VAL:HG22 | 2:D:290:THR:HG21 | 1.83                     | 0.61              |
| 1:E:435:VAL:HG22 | 2:F:290:THR:HG21 | 1.83                     | 0.61              |
| 1:A:225:PRO:HG2  | 1:A:226:PRO:CD   | 2.31                     | 0.61              |
| 1:A:339:TYR:CE1  | 1:A:352:GLY:HA3  | 2.35                     | 0.61              |
| 1:A:376:THR:O    | 1:A:380:ILE:HG13 | 2.01                     | 0.61              |
| 2:B:87:PHE:CE2   | 2:B:155:GLY:HA2  | 2.36                     | 0.61              |
| 1:E:249:LYS:HG2  | 1:E:250:ASP:N    | 2.15                     | 0.61              |
| 1:E:339:TYR:CE1  | 1:E:352:GLY:HA3  | 2.35                     | 0.61              |
| 1:E:88:TRP:CH2   | 2:F:57:ASN:HB3   | 2.36                     | 0.61              |
| 2:H:47:ILE:HG21  | 2:H:144:TYR:HB3  | 1.82                     | 0.61              |
| 1:E:225:PRO:HG2  | 1:E:226:PRO:CD   | 2.31                     | 0.61              |
| 1:E:238:LYS:HE2  | 1:E:240:THR:HG22 | 1.83                     | 0.61              |
| 1:G:491:LEU:HB3  | 1:G:529:GLU:CB   | 2.30                     | 0.61              |
| 1:A:104:LYS:HB2  | 1:A:192:ASP:HA   | 1.82                     | 0.60              |
| 1:A:435:VAL:HG22 | 2:B:290:THR:HG21 | 1.83                     | 0.60              |
| 1:G:225:PRO:HG2  | 1:G:226:PRO:CD   | 2.31                     | 0.60              |
| 1:G:238:LYS:HE2  | 1:G:240:THR:HG22 | 1.83                     | 0.60              |
| 2:F:354:TYR:OH   | 2:F:374:LYS:HG2  | 2.00                     | 0.60              |
| 1:G:376:THR:O    | 1:G:380:ILE:HG13 | 2.01                     | 0.60              |
| 1:G:393:ILE:HG23 | 1:G:414:TRP:HH2  | 1.58                     | 0.60              |
| 2:B:257:ILE:HB   | 2:B:283:LEU:HD21 | 1.82                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:D:257:ILE:HB  | 2:D:283:LEU:HD21 | 1.82                     | 0.60              |
| 2:D:47:ILE:HG21 | 2:D:144:TYR:HB3  | 1.82                     | 0.60              |
| 1:E:326:ILE:HB  | 1:E:342:TYR:HE1  | 1.65                     | 0.60              |
| 1:E:509:GLN:N   | 1:E:510:PRO:HD3  | 2.17                     | 0.60              |
| 1:C:376:THR:O   | 1:C:380:ILE:HG13 | 2.01                     | 0.60              |
| 2:F:151:GLN:HA  | 2:F:151:GLN:NE2  | 2.17                     | 0.60              |
| 2:H:151:GLN:NE2 | 2:H:151:GLN:HA   | 2.17                     | 0.60              |
| 1:G:88:TRP:CH2  | 2:H:57:ASN:HB3   | 2.36                     | 0.60              |
| 2:B:47:ILE:CG2  | 2:B:144:TYR:HB3  | 2.31                     | 0.60              |
| 2:D:171:PHE:CE2 | 2:D:204:GLU:HB2  | 2.31                     | 0.60              |
| 1:C:88:TRP:CH2  | 2:D:57:ASN:HB3   | 2.36                     | 0.60              |
| 1:E:540:LYS:HZ3 | 2:F:261:VAL:CG1  | 2.14                     | 0.60              |
| 2:H:257:ILE:HB  | 2:H:283:LEU:HD21 | 1.82                     | 0.60              |
| 2:H:47:ILE:CG2  | 2:H:144:TYR:HB3  | 2.31                     | 0.60              |
| 1:A:88:TRP:CH2  | 2:B:57:ASN:HB3   | 2.36                     | 0.60              |
| 2:D:47:ILE:CG2  | 2:D:144:TYR:HB3  | 2.31                     | 0.60              |
| 2:B:328:GLU:O   | 2:B:339:TYR:HA   | 2.02                     | 0.60              |
| 1:C:160:PHE:CE1 | 1:C:164:MET:HG2  | 2.37                     | 0.60              |
| 1:C:326:ILE:HB  | 1:C:342:TYR:HE1  | 1.66                     | 0.60              |
| 2:D:328:GLU:O   | 2:D:339:TYR:HA   | 2.02                     | 0.60              |
| 2:F:47:ILE:CG2  | 2:F:144:TYR:HB3  | 2.31                     | 0.60              |
| 1:C:323:LYS:HE2 | 1:G:322:SER:O    | 2.01                     | 0.60              |
| 1:C:363:ASN:OD1 | 1:C:364:ASP:N    | 2.35                     | 0.60              |
| 1:A:160:PHE:CE1 | 1:A:164:MET:HG2  | 2.37                     | 0.60              |
| 1:A:238:LYS:HE3 | 1:A:315:HIS:CD2  | 2.36                     | 0.60              |
| 1:C:238:LYS:HE2 | 1:C:240:THR:HG22 | 1.83                     | 0.60              |
| 1:G:509:GLN:N   | 1:G:510:PRO:HD3  | 2.17                     | 0.60              |
| 2:H:328:GLU:O   | 2:H:339:TYR:HA   | 2.02                     | 0.60              |
| 1:A:509:GLN:N   | 1:A:510:PRO:HD3  | 2.17                     | 0.59              |
| 1:A:492:GLU:HG2 | 1:A:530:LYS:HB2  | 1.84                     | 0.59              |
| 1:C:238:LYS:HE3 | 1:C:315:HIS:CD2  | 2.37                     | 0.59              |
| 1:A:238:LYS:HE2 | 1:A:240:THR:HG22 | 1.83                     | 0.59              |
| 1:A:326:ILE:HB  | 1:A:342:TYR:HE1  | 1.66                     | 0.59              |
| 1:C:509:GLN:N   | 1:C:510:PRO:HD3  | 2.16                     | 0.59              |
| 1:C:235:HIS:HB3 | 1:C:236:PRO:HD2  | 1.84                     | 0.59              |
| 1:E:160:PHE:CE1 | 1:E:164:MET:HG2  | 2.37                     | 0.59              |
| 1:G:363:ASN:OD1 | 1:G:364:ASP:N    | 2.35                     | 0.59              |
| 1:A:235:HIS:HB3 | 1:A:236:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:392:PRO:O   | 1:A:423:VAL:HG22 | 2.03                     | 0.59              |
| 1:C:492:GLU:HG2 | 1:C:530:LYS:HB2  | 1.84                     | 0.59              |
| 1:E:238:LYS:HE3 | 1:E:315:HIS:CD2  | 2.36                     | 0.59              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:160:PHE:CE1 | 1:G:164:MET:HG2  | 2.37                     | 0.59              |
| 1:A:363:ASN:OD1 | 1:A:364:ASP:N    | 2.35                     | 0.59              |
| 1:E:363:ASN:OD1 | 1:E:364:ASP:N    | 2.35                     | 0.59              |
| 1:G:238:LYS:HE3 | 1:G:315:HIS:CD2  | 2.36                     | 0.59              |
| 2:B:106:VAL:HA  | 2:B:190:GLY:HA2  | 1.85                     | 0.59              |
| 1:C:392:PRO:O   | 1:C:423:VAL:HG22 | 2.03                     | 0.59              |
| 2:F:328:GLU:O   | 2:F:339:TYR:HA   | 2.02                     | 0.59              |
| 1:G:326:ILE:HB  | 1:G:342:TYR:HE1  | 1.66                     | 0.59              |
| 2:B:153:TRP:CH2 | 2:B:155:GLY:HA3  | 2.38                     | 0.59              |
| 2:D:151:GLN:NE2 | 2:D:151:GLN:HA   | 2.17                     | 0.59              |
| 1:E:161:GLN:O   | 1:E:165:THR:HG23 | 2.03                     | 0.59              |
| 1:E:392:PRO:O   | 1:E:423:VAL:HG22 | 2.03                     | 0.59              |
| 2:F:104:LYS:HZ2 | 2:F:194:GLU:HA   | 1.68                     | 0.59              |
| 2:D:106:VAL:HA  | 2:D:190:GLY:HA2  | 1.85                     | 0.59              |
| 2:F:153:TRP:CH2 | 2:F:155:GLY:HA3  | 2.38                     | 0.59              |
| 1:G:161:GLN:O   | 1:G:165:THR:HG23 | 2.03                     | 0.59              |
| 1:G:295:LEU:CB  | 1:G:299:ALA:HB2  | 2.33                     | 0.59              |
| 1:A:161:GLN:O   | 1:A:165:THR:HG23 | 2.03                     | 0.59              |
| 1:C:161:GLN:O   | 1:C:165:THR:HG23 | 2.03                     | 0.59              |
| 1:E:235:HIS:HB3 | 1:E:236:PRO:HD2  | 1.84                     | 0.59              |
| 1:E:295:LEU:CB  | 1:E:299:ALA:HB2  | 2.33                     | 0.59              |
| 1:E:492:GLU:HG2 | 1:E:530:LYS:HB2  | 1.84                     | 0.58              |
| 1:G:492:GLU:HG2 | 1:G:530:LYS:HB2  | 1.84                     | 0.58              |
| 2:B:151:GLN:HA  | 2:B:151:GLN:NE2  | 2.17                     | 0.58              |
| 2:D:153:TRP:CH2 | 2:D:155:GLY:HA3  | 2.38                     | 0.58              |
| 2:B:171:PHE:CE2 | 2:B:204:GLU:HB2  | 2.31                     | 0.58              |
| 2:B:103:LYS:HZ1 | 2:B:179:VAL:HG23 | 1.67                     | 0.58              |
| 1:C:346:PHE:CZ  | 1:G:390:LYS:CG   | 2.80                     | 0.58              |
| 1:E:17:ASP:O    | 1:E:83:ARG:HD3   | 2.03                     | 0.58              |
| 1:G:167:ILE:O   | 1:G:170:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:295:LEU:CB  | 1:A:299:ALA:HB2  | 2.33                     | 0.58              |
| 1:C:295:LEU:CB  | 1:C:299:ALA:HB2  | 2.33                     | 0.58              |
| 1:C:523:GLU:O   | 1:C:526:ILE:HG12 | 2.04                     | 0.58              |
| 1:E:167:ILE:O   | 1:E:170:PRO:HD2  | 2.03                     | 0.58              |
| 1:G:235:HIS:HB3 | 1:G:236:PRO:HD2  | 1.84                     | 0.58              |
| 1:C:17:ASP:O    | 1:C:83:ARG:HD3   | 2.03                     | 0.58              |
| 1:E:393:ILE:HB  | 1:E:423:VAL:HG22 | 1.86                     | 0.58              |
| 2:H:106:VAL:HA  | 2:H:190:GLY:HA2  | 1.85                     | 0.58              |
| 1:G:523:GLU:O   | 1:G:526:ILE:HG12 | 2.04                     | 0.58              |
| 2:H:171:PHE:CE2 | 2:H:204:GLU:HB2  | 2.31                     | 0.58              |
| 1:A:17:ASP:O    | 1:A:83:ARG:HD3   | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:411:ILE:HG22 | 1:C:412:PRO:HD2  | 1.86                     | 0.58              |
| 1:A:303:LEU:O    | 1:A:307:ARG:HG3  | 2.04                     | 0.58              |
| 1:A:523:GLU:O    | 1:A:526:ILE:HG12 | 2.04                     | 0.58              |
| 2:D:103:LYS:HZ1  | 2:D:179:VAL:HG23 | 1.69                     | 0.58              |
| 2:F:106:VAL:HA   | 2:F:190:GLY:HA2  | 1.84                     | 0.58              |
| 2:H:153:TRP:CH2  | 2:H:155:GLY:HA3  | 2.38                     | 0.58              |
| 2:H:55:PRO:HG2   | 2:H:56:TYR:N     | 2.19                     | 0.58              |
| 2:F:395:LYS:HG3  | 2:F:416:PHE:CE2  | 2.39                     | 0.58              |
| 2:F:55:PRO:HG2   | 2:F:56:TYR:N     | 2.19                     | 0.58              |
| 1:A:411:ILE:HG22 | 1:A:412:PRO:HD2  | 1.86                     | 0.57              |
| 2:B:395:LYS:HG3  | 2:B:416:PHE:CE2  | 2.39                     | 0.57              |
| 2:D:10:VAL:CG1   | 2:D:159:ILE:HD11 | 2.34                     | 0.57              |
| 2:F:171:PHE:CE2  | 2:F:204:GLU:HB2  | 2.31                     | 0.57              |
| 1:E:406:TRP:CZ3  | 1:E:407:GLN:HG3  | 2.39                     | 0.57              |
| 1:G:392:PRO:O    | 1:G:423:VAL:HG22 | 2.03                     | 0.57              |
| 2:H:395:LYS:HG3  | 2:H:416:PHE:CE2  | 2.39                     | 0.57              |
| 1:A:167:ILE:O    | 1:A:170:PRO:HD2  | 2.03                     | 0.57              |
| 1:G:303:LEU:O    | 1:G:307:ARG:HG3  | 2.04                     | 0.57              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:HG3  | 2.40                     | 0.57              |
| 2:D:395:LYS:HG3  | 2:D:416:PHE:CE2  | 2.39                     | 0.57              |
| 1:E:429:LEU:HD11 | 1:E:506:ILE:HG22 | 1.87                     | 0.57              |
| 1:A:229:TRP:CH2  | 1:A:230:MET:HE1  | 2.39                     | 0.57              |
| 1:A:393:ILE:HB   | 1:A:423:VAL:HG22 | 1.86                     | 0.57              |
| 2:B:10:VAL:CG1   | 2:B:159:ILE:HD11 | 2.35                     | 0.57              |
| 2:B:5:ILE:HG22   | 2:B:6:GLU:N      | 2.20                     | 0.57              |
| 1:C:167:ILE:O    | 1:C:170:PRO:HD2  | 2.03                     | 0.57              |
| 1:E:418:ASN:HD22 | 1:E:418:ASN:C    | 2.08                     | 0.57              |
| 1:E:441:TYR:HE2  | 1:E:543:GLY:O    | 1.88                     | 0.57              |
| 1:E:87:PHE:CE2   | 1:E:159:ILE:HD11 | 2.40                     | 0.57              |
| 2:H:10:VAL:CG1   | 2:H:159:ILE:HD11 | 2.35                     | 0.57              |
| 2:D:28:GLU:HG2   | 2:D:32:LYS:NZ    | 2.19                     | 0.57              |
| 2:F:28:GLU:HG2   | 2:F:32:LYS:NZ    | 2.19                     | 0.57              |
| 1:C:303:LEU:O    | 1:C:307:ARG:HG3  | 2.04                     | 0.57              |
| 1:C:320:ASP:OD2  | 1:C:323:LYS:HG3  | 2.05                     | 0.57              |
| 1:C:406:TRP:CZ3  | 1:C:407:GLN:HG3  | 2.39                     | 0.57              |
| 1:E:232:TYR:HD1  | 1:E:241:VAL:HG22 | 1.70                     | 0.57              |
| 1:G:418:ASN:C    | 1:G:418:ASN:HD22 | 2.08                     | 0.57              |
| 2:H:395:LYS:O    | 2:H:399:GLU:HG3  | 2.05                     | 0.57              |
| 2:B:54:ASN:HD21  | 2:B:56:TYR:HB2   | 1.70                     | 0.57              |
| 2:D:54:ASN:HD21  | 2:D:56:TYR:HB2   | 1.70                     | 0.57              |
| 1:E:523:GLU:O    | 1:E:526:ILE:HG12 | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:54:ASN:HD21  | 2:F:56:TYR:HB2   | 1.70                     | 0.57              |
| 1:G:406:TRP:CZ3  | 1:G:407:GLN:HG3  | 2.40                     | 0.57              |
| 1:G:393:ILE:HB   | 1:G:423:VAL:HG22 | 1.86                     | 0.57              |
| 2:D:5:ILE:HG22   | 2:D:6:GLU:N      | 2.20                     | 0.57              |
| 2:F:5:ILE:HG22   | 2:F:6:GLU:N      | 2.20                     | 0.57              |
| 1:G:458:VAL:HG23 | 1:G:548:VAL:HG22 | 1.87                     | 0.57              |
| 1:G:17:ASP:O     | 1:G:83:ARG:HD3   | 2.03                     | 0.57              |
| 1:A:418:ASN:C    | 1:A:418:ASN:HD22 | 2.08                     | 0.57              |
| 1:C:229:TRP:CH2  | 1:C:230:MET:HE1  | 2.39                     | 0.57              |
| 1:E:56:TYR:O     | 1:E:143:ARG:NH2  | 2.38                     | 0.57              |
| 1:E:320:ASP:OD2  | 1:E:323:LYS:HG3  | 2.05                     | 0.57              |
| 2:F:395:LYS:O    | 2:F:399:GLU:HG3  | 2.05                     | 0.57              |
| 2:H:28:GLU:HG2   | 2:H:32:LYS:NZ    | 2.19                     | 0.57              |
| 1:A:320:ASP:OD2  | 1:A:323:LYS:HG3  | 2.05                     | 0.56              |
| 2:B:54:ASN:C     | 2:B:54:ASN:HD22  | 2.08                     | 0.56              |
| 1:C:393:ILE:HB   | 1:C:423:VAL:HG22 | 1.86                     | 0.56              |
| 1:E:411:ILE:HG22 | 1:E:412:PRO:HD2  | 1.86                     | 0.56              |
| 1:E:98:ALA:HB1   | 1:E:383:TRP:HH2  | 1.70                     | 0.56              |
| 2:H:379:SER:OG   | 2:H:387:PRO:HD3  | 2.05                     | 0.56              |
| 2:B:28:GLU:HG2   | 2:B:32:LYS:NZ    | 2.19                     | 0.56              |
| 1:C:418:ASN:C    | 1:C:418:ASN:HD22 | 2.08                     | 0.56              |
| 1:C:346:PHE:CG   | 1:G:390:LYS:CD   | 2.87                     | 0.56              |
| 1:G:429:LEU:HD11 | 1:G:506:ILE:HG22 | 1.87                     | 0.56              |
| 1:G:441:TYR:HE2  | 1:G:543:GLY:O    | 1.88                     | 0.56              |
| 1:A:87:PHE:CE2   | 1:A:159:ILE:HD11 | 2.40                     | 0.56              |
| 2:D:55:PRO:HG2   | 2:D:56:TYR:N     | 2.19                     | 0.56              |
| 2:F:379:SER:OG   | 2:F:387:PRO:HD3  | 2.05                     | 0.56              |
| 2:F:54:ASN:HD22  | 2:F:54:ASN:C     | 2.08                     | 0.56              |
| 2:H:5:ILE:HG22   | 2:H:6:GLU:N      | 2.20                     | 0.56              |
| 1:A:98:ALA:HB1   | 1:A:383:TRP:HH2  | 1.70                     | 0.56              |
| 1:A:458:VAL:HG23 | 1:A:548:VAL:HG22 | 1.87                     | 0.56              |
| 2:B:271:TYR:O    | 2:B:274:ILE:HG22 | 2.06                     | 0.56              |
| 2:B:61:PHE:CE2   | 2:B:403:THR:HG22 | 2.41                     | 0.56              |
| 1:C:87:PHE:CE2   | 1:C:159:ILE:HD11 | 2.40                     | 0.56              |
| 1:C:517:LEU:O    | 1:C:521:ILE:HG13 | 2.06                     | 0.56              |
| 2:D:271:TYR:O    | 2:D:274:ILE:HG22 | 2.06                     | 0.56              |
| 2:D:395:LYS:O    | 2:D:399:GLU:HG3  | 2.05                     | 0.56              |
| 2:D:54:ASN:C     | 2:D:54:ASN:HD22  | 2.08                     | 0.56              |
| 1:G:411:ILE:HG22 | 1:G:412:PRO:HD2  | 1.86                     | 0.56              |
| 2:H:139:THR:HG22 | 2:H:140:PRO:O    | 2.06                     | 0.56              |
| 2:H:61:PHE:CE2   | 2:H:403:THR:HG22 | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:54:ASN:HD22  | 2:H:54:ASN:C     | 2.08                     | 0.56              |
| 1:A:329:ILE:HD12 | 1:A:391:LEU:CD2  | 2.36                     | 0.56              |
| 1:A:453:GLY:O    | 1:A:469:LEU:HB2  | 2.06                     | 0.56              |
| 1:A:517:LEU:O    | 1:A:521:ILE:HG13 | 2.06                     | 0.56              |
| 2:B:105:SER:HB3  | 2:B:235:HIS:CE1  | 2.41                     | 0.56              |
| 2:B:55:PRO:HG2   | 2:B:56:TYR:N     | 2.19                     | 0.56              |
| 1:C:329:ILE:HD12 | 1:C:391:LEU:CD2  | 2.36                     | 0.56              |
| 1:G:56:TYR:O     | 1:G:143:ARG:NH2  | 2.38                     | 0.56              |
| 1:G:320:ASP:OD2  | 1:G:323:LYS:HG3  | 2.05                     | 0.56              |
| 1:G:87:PHE:CE2   | 1:G:159:ILE:HD11 | 2.40                     | 0.56              |
| 2:B:395:LYS:O    | 2:B:399:GLU:HG3  | 2.05                     | 0.56              |
| 2:D:105:SER:HB3  | 2:D:235:HIS:CE1  | 2.41                     | 0.56              |
| 2:D:61:PHE:CE2   | 2:D:403:THR:HG22 | 2.41                     | 0.56              |
| 1:E:303:LEU:O    | 1:E:307:ARG:HG3  | 2.04                     | 0.56              |
| 2:F:105:SER:HB3  | 2:F:235:HIS:CE1  | 2.41                     | 0.56              |
| 1:G:453:GLY:O    | 1:G:469:LEU:HB2  | 2.06                     | 0.56              |
| 1:G:517:LEU:O    | 1:G:521:ILE:HG13 | 2.06                     | 0.56              |
| 1:C:98:ALA:HB1   | 1:C:383:TRP:HH2  | 1.71                     | 0.56              |
| 2:F:10:VAL:CG1   | 2:F:159:ILE:HD11 | 2.35                     | 0.56              |
| 1:G:98:ALA:HB1   | 1:G:383:TRP:HH2  | 1.70                     | 0.56              |
| 2:H:271:TYR:O    | 2:H:274:ILE:HG22 | 2.06                     | 0.56              |
| 1:A:441:TYR:HE2  | 1:A:543:GLY:O    | 1.88                     | 0.56              |
| 1:C:441:TYR:HE2  | 1:C:543:GLY:O    | 1.88                     | 0.56              |
| 2:F:125:ARG:HH11 | 2:F:125:ARG:HG2  | 1.71                     | 0.56              |
| 2:F:139:THR:HG22 | 2:F:140:PRO:O    | 2.06                     | 0.56              |
| 2:H:54:ASN:HD21  | 2:H:56:TYR:HB2   | 1.70                     | 0.56              |
| 1:A:248:GLU:HG3  | 1:A:307:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:429:LEU:HD11 | 1:A:506:ILE:HG22 | 1.87                     | 0.56              |
| 1:A:56:TYR:O     | 1:A:143:ARG:NH2  | 2.38                     | 0.56              |
| 1:C:453:GLY:O    | 1:C:469:LEU:HB2  | 2.06                     | 0.56              |
| 1:C:458:VAL:HG23 | 1:C:548:VAL:HG22 | 1.86                     | 0.56              |
| 1:G:491:LEU:HB3  | 1:G:529:GLU:HB3  | 1.88                     | 0.56              |
| 2:B:379:SER:OG   | 2:B:387:PRO:HD3  | 2.05                     | 0.56              |
| 1:C:56:TYR:O     | 1:C:143:ARG:NH2  | 2.38                     | 0.56              |
| 1:C:429:LEU:HD11 | 1:C:506:ILE:HG22 | 1.87                     | 0.56              |
| 1:E:458:VAL:HG23 | 1:E:548:VAL:HG22 | 1.87                     | 0.56              |
| 2:F:271:TYR:O    | 2:F:274:ILE:HG22 | 2.06                     | 0.56              |
| 1:A:232:TYR:HD1  | 1:A:241:VAL:HG22 | 1.70                     | 0.55              |
| 1:C:248:GLU:HG3  | 1:C:307:ARG:NH2  | 2.20                     | 0.55              |
| 2:D:139:THR:HG22 | 2:D:140:PRO:O    | 2.06                     | 0.55              |
| 1:E:453:GLY:O    | 1:E:469:LEU:HB2  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:232:TYR:HD1  | 1:G:241:VAL:HG22 | 1.70                     | 0.55              |
| 1:G:248:GLU:HG3  | 1:G:307:ARG:NH2  | 2.20                     | 0.55              |
| 2:F:72:ARG:HH12  | 2:F:409:THR:HA   | 1.71                     | 0.55              |
| 2:H:105:SER:HB3  | 2:H:235:HIS:CE1  | 2.41                     | 0.55              |
| 1:E:248:GLU:HG3  | 1:E:307:ARG:NH2  | 2.20                     | 0.55              |
| 1:E:298:GLU:O    | 1:E:302:GLU:HG3  | 2.06                     | 0.55              |
| 1:G:298:GLU:O    | 1:G:302:GLU:HG3  | 2.06                     | 0.55              |
| 2:H:125:ARG:HG2  | 2:H:125:ARG:HH11 | 1.71                     | 0.55              |
| 2:H:72:ARG:HH12  | 2:H:409:THR:HA   | 1.71                     | 0.55              |
| 1:A:337:TRP:HZ3  | 1:A:368:LEU:HD13 | 1.72                     | 0.55              |
| 1:A:540:LYS:HZ3  | 2:B:261:VAL:CG1  | 2.19                     | 0.55              |
| 2:B:139:THR:HG22 | 2:B:140:PRO:O    | 2.06                     | 0.55              |
| 2:D:72:ARG:HH12  | 2:D:409:THR:HA   | 1.71                     | 0.55              |
| 1:E:337:TRP:HZ3  | 1:E:368:LEU:HD13 | 1.72                     | 0.55              |
| 1:E:439:THR:HG22 | 1:E:441:TYR:CE1  | 2.42                     | 0.55              |
| 2:F:376:THR:HB   | 2:F:386:THR:HG22 | 1.88                     | 0.55              |
| 1:G:337:TRP:HZ3  | 1:G:368:LEU:HD13 | 1.72                     | 0.55              |
| 1:G:98:ALA:HB1   | 1:G:349:LEU:HB3  | 1.89                     | 0.55              |
| 1:A:98:ALA:HB1   | 1:A:349:LEU:HB3  | 1.89                     | 0.55              |
| 2:B:125:ARG:HG2  | 2:B:125:ARG:HH11 | 1.71                     | 0.55              |
| 1:C:439:THR:HG22 | 1:C:441:TYR:CE1  | 2.42                     | 0.55              |
| 1:E:28:GLU:HB3   | 1:E:32:LYS:HE3   | 1.88                     | 0.55              |
| 2:F:61:PHE:CE2   | 2:F:403:THR:HG22 | 2.41                     | 0.55              |
| 2:F:97:PRO:O     | 2:F:98:ALA:HB3   | 2.07                     | 0.55              |
| 1:G:329:ILE:HD12 | 1:G:391:LEU:CD2  | 2.36                     | 0.55              |
| 2:H:368:LEU:O    | 2:H:371:ALA:HB3  | 2.07                     | 0.55              |
| 1:A:439:THR:HG22 | 1:A:441:TYR:CE1  | 2.42                     | 0.55              |
| 2:B:97:PRO:O     | 2:B:98:ALA:HB3   | 2.07                     | 0.55              |
| 1:C:298:GLU:O    | 1:C:302:GLU:HG3  | 2.06                     | 0.55              |
| 1:G:28:GLU:HB3   | 1:G:32:LYS:HE3   | 1.88                     | 0.55              |
| 2:H:366:LYS:O    | 2:H:370:GLU:HG3  | 2.07                     | 0.55              |
| 1:A:298:GLU:O    | 1:A:302:GLU:HG3  | 2.06                     | 0.55              |
| 2:B:101:LYS:O    | 2:B:236:PRO:HB2  | 2.07                     | 0.55              |
| 2:B:201:LYS:HD3  | 2:B:204:GLU:OE1  | 2.07                     | 0.55              |
| 2:B:72:ARG:HH12  | 2:B:409:THR:HA   | 1.71                     | 0.55              |
| 1:C:232:TYR:HD1  | 1:C:241:VAL:HG22 | 1.70                     | 0.55              |
| 1:C:337:TRP:HZ3  | 1:C:368:LEU:HD13 | 1.72                     | 0.55              |
| 1:C:98:ALA:HB1   | 1:C:349:LEU:HB3  | 1.89                     | 0.55              |
| 2:D:101:LYS:O    | 2:D:236:PRO:HB2  | 2.07                     | 0.55              |
| 2:D:379:SER:OG   | 2:D:387:PRO:HD3  | 2.05                     | 0.55              |
| 1:E:323:LYS:HD3  | 1:E:344:GLU:OE2  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:517:LEU:O    | 1:E:521:ILE:HG13 | 2.06                     | 0.55              |
| 1:G:323:LYS:HD3  | 1:G:344:GLU:OE2  | 2.07                     | 0.55              |
| 1:G:537:PRO:HD2  | 1:G:542:ILE:HD11 | 1.88                     | 0.55              |
| 2:H:61:PHE:CZ    | 2:H:402:TRP:CZ2  | 2.95                     | 0.55              |
| 1:A:401:TRP:HB2  | 1:A:425:LEU:HD21 | 1.89                     | 0.55              |
| 2:B:104:LYS:HZ3  | 2:B:194:GLU:HA   | 1.72                     | 0.55              |
| 1:C:332:GLN:O    | 1:C:332:GLN:HG2  | 2.07                     | 0.55              |
| 2:D:201:LYS:HD3  | 2:D:204:GLU:OE1  | 2.07                     | 0.55              |
| 1:E:98:ALA:HB1   | 1:E:349:LEU:HB3  | 1.89                     | 0.55              |
| 1:E:491:LEU:HB3  | 1:E:529:GLU:HB3  | 1.88                     | 0.55              |
| 1:E:537:PRO:HD2  | 1:E:542:ILE:HD11 | 1.88                     | 0.55              |
| 1:G:229:TRP:CH2  | 1:G:230:MET:HE1  | 2.42                     | 0.55              |
| 1:G:439:THR:HG22 | 1:G:441:TYR:CE1  | 2.42                     | 0.55              |
| 2:H:201:LYS:HD3  | 2:H:204:GLU:OE1  | 2.07                     | 0.55              |
| 1:A:332:GLN:HG2  | 1:A:332:GLN:O    | 2.07                     | 0.55              |
| 1:A:496:VAL:HG22 | 1:A:534:ALA:HB3  | 1.89                     | 0.55              |
| 1:C:346:PHE:CE1  | 1:G:390:LYS:CD   | 2.86                     | 0.55              |
| 1:C:491:LEU:HB3  | 1:C:529:GLU:HB3  | 1.88                     | 0.55              |
| 1:C:496:VAL:HG22 | 1:C:534:ALA:HB3  | 1.89                     | 0.55              |
| 1:A:463:ARG:HG3  | 1:A:463:ARG:HH11 | 1.72                     | 0.54              |
| 1:A:99:GLY:HA2   | 1:A:383:TRP:HZ3  | 1.72                     | 0.54              |
| 2:B:366:LYS:O    | 2:B:370:GLU:HG3  | 2.07                     | 0.54              |
| 1:C:229:TRP:CZ3  | 1:C:230:MET:HE1  | 2.43                     | 0.54              |
| 1:C:323:LYS:HD3  | 1:C:344:GLU:OE2  | 2.07                     | 0.54              |
| 2:D:125:ARG:HH11 | 2:D:125:ARG:HG2  | 1.71                     | 0.54              |
| 1:E:329:ILE:HD12 | 1:E:391:LEU:CD2  | 2.36                     | 0.54              |
| 1:G:5:ILE:HD11   | 1:G:166:LYS:HD2  | 1.89                     | 0.54              |
| 1:A:201:LYS:HD3  | 1:A:204:GLU:OE2  | 2.07                     | 0.54              |
| 2:B:376:THR:HB   | 2:B:386:THR:HG22 | 1.88                     | 0.54              |
| 2:D:104:LYS:HZ3  | 2:D:194:GLU:HA   | 1.72                     | 0.54              |
| 2:D:27:THR:O     | 2:D:29:GLU:N     | 2.41                     | 0.54              |
| 1:E:332:GLN:O    | 1:E:332:GLN:HG2  | 2.07                     | 0.54              |
| 1:G:201:LYS:HD3  | 1:G:204:GLU:OE2  | 2.07                     | 0.54              |
| 2:H:97:PRO:O     | 2:H:98:ALA:HB3   | 2.07                     | 0.54              |
| 1:A:200:THR:O    | 1:A:203:GLU:HB3  | 2.07                     | 0.54              |
| 1:A:491:LEU:HB3  | 1:A:529:GLU:HB3  | 1.88                     | 0.54              |
| 1:C:5:ILE:HD11   | 1:C:166:LYS:HD2  | 1.89                     | 0.54              |
| 1:E:342:TYR:HB3  | 1:E:348:ASN:HB3  | 1.89                     | 0.54              |
| 2:F:318:TYR:HE1  | 2:F:347:LYS:HD3  | 1.73                     | 0.54              |
| 1:A:126:LYS:HA   | 1:A:145:GLN:HE21 | 1.73                     | 0.54              |
| 1:A:475:GLN:HB3  | 1:A:501:TYR:CE2  | 2.43                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:537:PRO:CG   | 2:B:262:GLY:HA2  | 2.38                     | 0.54              |
| 2:B:318:TYR:HE1  | 2:B:347:LYS:HD3  | 1.73                     | 0.54              |
| 1:C:99:GLY:HA2   | 1:C:383:TRP:HZ3  | 1.72                     | 0.54              |
| 2:D:303:LEU:HD13 | 2:D:307:ARG:NH2  | 2.23                     | 0.54              |
| 2:D:97:PRO:O     | 2:D:98:ALA:HB3   | 2.07                     | 0.54              |
| 1:G:131:THR:HA   | 1:G:142:ILE:O    | 2.07                     | 0.54              |
| 1:A:537:PRO:HD2  | 1:A:542:ILE:HD11 | 1.88                     | 0.54              |
| 2:B:27:THR:O     | 2:B:29:GLU:N     | 2.41                     | 0.54              |
| 1:C:463:ARG:HH11 | 1:C:463:ARG:HG3  | 1.72                     | 0.54              |
| 1:C:537:PRO:CG   | 2:D:262:GLY:HA2  | 2.38                     | 0.54              |
| 1:E:131:THR:HA   | 1:E:142:ILE:O    | 2.07                     | 0.54              |
| 1:E:229:TRP:CH2  | 1:E:230:MET:HE1  | 2.42                     | 0.54              |
| 2:F:303:LEU:HD13 | 2:F:307:ARG:NH2  | 2.23                     | 0.54              |
| 2:F:366:LYS:O    | 2:F:370:GLU:HG3  | 2.07                     | 0.54              |
| 1:G:200:THR:O    | 1:G:203:GLU:HB3  | 2.07                     | 0.54              |
| 1:G:332:GLN:O    | 1:G:332:GLN:HG2  | 2.07                     | 0.54              |
| 1:G:99:GLY:HA2   | 1:G:383:TRP:HZ3  | 1.72                     | 0.54              |
| 1:A:5:ILE:HD11   | 1:A:166:LYS:HD2  | 1.89                     | 0.54              |
| 1:A:323:LYS:HD3  | 1:A:344:GLU:OE2  | 2.07                     | 0.54              |
| 1:A:98:ALA:O     | 1:A:383:TRP:HZ3  | 1.91                     | 0.54              |
| 2:B:303:LEU:HD13 | 2:B:307:ARG:NH2  | 2.23                     | 0.54              |
| 2:B:93:GLY:O     | 2:B:94:ILE:O     | 2.26                     | 0.54              |
| 1:C:342:TYR:HB3  | 1:C:348:ASN:HB3  | 1.89                     | 0.54              |
| 1:C:346:PHE:HD1  | 1:G:390:LYS:CE   | 1.66                     | 0.54              |
| 1:C:98:ALA:O     | 1:C:383:TRP:HZ3  | 1.91                     | 0.54              |
| 2:D:318:TYR:HE1  | 2:D:347:LYS:HD3  | 1.72                     | 0.54              |
| 2:F:27:THR:O     | 2:F:29:GLU:N     | 2.41                     | 0.54              |
| 2:F:93:GLY:O     | 2:F:94:ILE:O     | 2.26                     | 0.54              |
| 1:G:97:PRO:HD3   | 1:G:232:TYR:CZ   | 2.43                     | 0.54              |
| 2:H:303:LEU:HD13 | 2:H:307:ARG:NH2  | 2.23                     | 0.54              |
| 1:C:200:THR:O    | 1:C:203:GLU:HB3  | 2.07                     | 0.54              |
| 1:C:401:TRP:HB2  | 1:C:425:LEU:HD21 | 1.89                     | 0.54              |
| 1:C:475:GLN:HB3  | 1:C:501:TYR:CE2  | 2.43                     | 0.54              |
| 2:D:366:LYS:O    | 2:D:370:GLU:HG3  | 2.07                     | 0.54              |
| 1:E:200:THR:O    | 1:E:203:GLU:HB3  | 2.07                     | 0.54              |
| 1:E:401:TRP:HB2  | 1:E:425:LEU:HD21 | 1.89                     | 0.54              |
| 2:F:392:PRO:O    | 2:F:392:PRO:HG2  | 2.08                     | 0.54              |
| 2:F:61:PHE:CZ    | 2:F:402:TRP:CZ2  | 2.95                     | 0.54              |
| 2:F:97:PRO:C     | 2:F:99:GLY:H     | 2.11                     | 0.54              |
| 1:G:463:ARG:HG3  | 1:G:463:ARG:HH11 | 1.72                     | 0.54              |
| 1:G:496:VAL:HG22 | 1:G:534:ALA:HB3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:341:ILE:HD11 | 1:A:350:LYS:HB3  | 1.90                     | 0.54              |
| 1:C:201:LYS:HD3  | 1:C:204:GLU:OE2  | 2.07                     | 0.54              |
| 2:D:376:THR:HB   | 2:D:386:THR:HG22 | 1.88                     | 0.54              |
| 2:D:392:PRO:O    | 2:D:392:PRO:HG2  | 2.08                     | 0.54              |
| 2:D:61:PHE:CZ    | 2:D:402:TRP:CZ2  | 2.95                     | 0.54              |
| 2:F:368:LEU:O    | 2:F:371:ALA:HB3  | 2.07                     | 0.54              |
| 1:G:341:ILE:HD11 | 1:G:350:LYS:HB3  | 1.90                     | 0.54              |
| 2:H:376:THR:HB   | 2:H:386:THR:HG22 | 1.88                     | 0.54              |
| 1:A:131:THR:HA   | 1:A:142:ILE:O    | 2.07                     | 0.54              |
| 2:B:61:PHE:CZ    | 2:B:402:TRP:CZ2  | 2.95                     | 0.54              |
| 1:E:126:LYS:HA   | 1:E:145:GLN:HE21 | 1.73                     | 0.54              |
| 2:H:318:TYR:HE1  | 2:H:347:LYS:HD3  | 1.73                     | 0.54              |
| 2:H:97:PRO:C     | 2:H:99:GLY:H     | 2.11                     | 0.54              |
| 1:A:28:GLU:HB3   | 1:A:32:LYS:HE3   | 1.88                     | 0.54              |
| 2:B:365:VAL:HG12 | 2:B:405:TYR:CE2  | 2.43                     | 0.54              |
| 1:C:126:LYS:HA   | 1:C:145:GLN:HE21 | 1.72                     | 0.54              |
| 1:C:182:GLN:HG2  | 1:C:183:TYR:N    | 2.23                     | 0.54              |
| 1:C:28:GLU:HB3   | 1:C:32:LYS:HE3   | 1.88                     | 0.54              |
| 1:C:341:ILE:HD11 | 1:C:350:LYS:HB3  | 1.90                     | 0.54              |
| 2:H:27:THR:O     | 2:H:29:GLU:N     | 2.41                     | 0.54              |
| 2:D:368:LEU:O    | 2:D:371:ALA:HB3  | 2.07                     | 0.53              |
| 1:G:98:ALA:O     | 1:G:383:TRP:HZ3  | 1.91                     | 0.53              |
| 1:G:402:TRP:CE3  | 1:G:402:TRP:C    | 2.82                     | 0.53              |
| 2:H:103:LYS:HZ1  | 2:H:179:VAL:HG23 | 1.70                     | 0.53              |
| 1:A:182:GLN:HG2  | 1:A:183:TYR:N    | 2.23                     | 0.53              |
| 1:A:229:TRP:CZ3  | 1:A:230:MET:HE1  | 2.43                     | 0.53              |
| 2:B:368:LEU:O    | 2:B:371:ALA:HB3  | 2.07                     | 0.53              |
| 1:C:97:PRO:HD3   | 1:C:232:TYR:CZ   | 2.43                     | 0.53              |
| 1:C:402:TRP:CE3  | 1:C:402:TRP:C    | 2.82                     | 0.53              |
| 2:D:93:GLY:O     | 2:D:94:ILE:O     | 2.26                     | 0.53              |
| 1:E:463:ARG:HG3  | 1:E:463:ARG:HH11 | 1.72                     | 0.53              |
| 1:E:537:PRO:CG   | 2:F:262:GLY:HA2  | 2.38                     | 0.53              |
| 1:E:97:PRO:HD3   | 1:E:232:TYR:CZ   | 2.43                     | 0.53              |
| 2:F:101:LYS:O    | 2:F:236:PRO:HB2  | 2.07                     | 0.53              |
| 1:G:475:GLN:HB3  | 1:G:501:TYR:CE2  | 2.43                     | 0.53              |
| 1:G:441:TYR:CD2  | 1:G:544:GLY:HA3  | 2.44                     | 0.53              |
| 1:E:341:ILE:HD11 | 1:E:350:LYS:HB3  | 1.90                     | 0.53              |
| 1:E:496:VAL:HG22 | 1:E:534:ALA:HB3  | 1.89                     | 0.53              |
| 2:F:153:TRP:CE3  | 2:F:155:GLY:HA3  | 2.43                     | 0.53              |
| 1:G:401:TRP:HB2  | 1:G:425:LEU:HD21 | 1.89                     | 0.53              |
| 1:G:537:PRO:CG   | 2:H:262:GLY:HA2  | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:101:LYS:O    | 2:H:236:PRO:HB2  | 2.07                     | 0.53              |
| 2:H:365:VAL:HG12 | 2:H:405:TYR:CE2  | 2.43                     | 0.53              |
| 1:A:341:ILE:HD12 | 1:A:383:TRP:NE1  | 2.23                     | 0.53              |
| 1:A:402:TRP:CE3  | 1:A:402:TRP:C    | 2.82                     | 0.53              |
| 1:C:131:THR:HA   | 1:C:142:ILE:O    | 2.07                     | 0.53              |
| 1:C:537:PRO:HD2  | 1:C:542:ILE:HD11 | 1.88                     | 0.53              |
| 2:D:103:LYS:NZ   | 2:D:179:VAL:N    | 2.55                     | 0.53              |
| 2:D:153:TRP:CE3  | 2:D:155:GLY:HA3  | 2.43                     | 0.53              |
| 1:A:97:PRO:HD3   | 1:A:232:TYR:CZ   | 2.43                     | 0.53              |
| 2:B:103:LYS:NZ   | 2:B:179:VAL:N    | 2.55                     | 0.53              |
| 2:B:392:PRO:O    | 2:B:392:PRO:HG2  | 2.08                     | 0.53              |
| 2:D:268:SER:HA   | 2:D:274:ILE:HG22 | 1.90                     | 0.53              |
| 2:F:201:LYS:HD3  | 2:F:204:GLU:OE1  | 2.07                     | 0.53              |
| 1:G:342:TYR:HB3  | 1:G:348:ASN:HB3  | 1.89                     | 0.53              |
| 1:C:341:ILE:HD12 | 1:C:383:TRP:NE1  | 2.23                     | 0.53              |
| 1:E:201:LYS:HD3  | 1:E:204:GLU:OE2  | 2.07                     | 0.53              |
| 2:F:365:VAL:HG12 | 2:F:405:TYR:CE2  | 2.43                     | 0.53              |
| 2:H:153:TRP:CE3  | 2:H:155:GLY:HA3  | 2.43                     | 0.53              |
| 1:A:106:VAL:O    | 1:A:227:PHE:CZ   | 2.62                     | 0.53              |
| 1:A:342:TYR:HB3  | 1:A:348:ASN:HB3  | 1.89                     | 0.53              |
| 1:C:196:GLY:O    | 1:C:199:ARG:HB3  | 2.09                     | 0.53              |
| 1:E:196:GLY:O    | 1:E:199:ARG:HB3  | 2.09                     | 0.53              |
| 1:E:475:GLN:HB3  | 1:E:501:TYR:CE2  | 2.43                     | 0.53              |
| 2:F:268:SER:HA   | 2:F:274:ILE:HG22 | 1.90                     | 0.53              |
| 1:G:126:LYS:HA   | 1:G:145:GLN:HE21 | 1.73                     | 0.53              |
| 1:C:346:PHE:CG   | 1:G:390:LYS:HD2  | 2.44                     | 0.53              |
| 1:A:465:LYS:O    | 1:A:466:VAL:HG23 | 2.08                     | 0.53              |
| 2:B:153:TRP:CE3  | 2:B:155:GLY:HA3  | 2.43                     | 0.53              |
| 1:C:106:VAL:O    | 1:C:227:PHE:CZ   | 2.62                     | 0.53              |
| 1:C:345:PRO:CG   | 1:G:326:ILE:HD11 | 2.19                     | 0.53              |
| 2:D:365:VAL:HG12 | 2:D:405:TYR:CE2  | 2.43                     | 0.53              |
| 1:E:5:ILE:HD11   | 1:E:166:LYS:HD2  | 1.89                     | 0.53              |
| 2:F:264:LEU:HB2  | 2:F:276:VAL:CG1  | 2.39                     | 0.53              |
| 1:E:408:ALA:HB1  | 2:F:364:ASP:HB3  | 1.91                     | 0.53              |
| 2:H:93:GLY:O     | 2:H:94:ILE:O     | 2.26                     | 0.53              |
| 1:C:441:TYR:CD2  | 1:C:544:GLY:HA3  | 2.44                     | 0.53              |
| 1:E:441:TYR:CD2  | 1:E:544:GLY:HA3  | 2.44                     | 0.53              |
| 1:E:106:VAL:O    | 1:E:227:PHE:CZ   | 2.62                     | 0.53              |
| 1:E:99:GLY:HA2   | 1:E:383:TRP:HZ3  | 1.72                     | 0.53              |
| 1:G:372:VAL:HG11 | 1:G:411:ILE:HG23 | 1.91                     | 0.53              |
| 2:H:13:LYS:HB3   | 2:H:14:PRO:HD2   | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:441:TYR:CD2  | 1:A:544:GLY:HA3  | 2.44                     | 0.52              |
| 2:D:264:LEU:HB2  | 2:D:276:VAL:CG1  | 2.39                     | 0.52              |
| 1:G:196:GLY:O    | 1:G:199:ARG:HB3  | 2.09                     | 0.52              |
| 1:C:417:VAL:CG2  | 1:G:346:PHE:CG   | 2.92                     | 0.52              |
| 1:G:408:ALA:HB1  | 2:H:364:ASP:HB3  | 1.91                     | 0.52              |
| 1:G:491:LEU:HB3  | 1:G:529:GLU:HB2  | 1.91                     | 0.52              |
| 1:A:157:PRO:HG2  | 1:A:158:ALA:N    | 2.24                     | 0.52              |
| 1:A:105:SER:HB3  | 1:A:198:HIS:CG   | 2.44                     | 0.52              |
| 2:B:264:LEU:HB2  | 2:B:276:VAL:CG1  | 2.39                     | 0.52              |
| 1:C:105:SER:HB3  | 1:C:198:HIS:CG   | 2.45                     | 0.52              |
| 1:C:408:ALA:HB1  | 2:D:364:ASP:HB3  | 1.91                     | 0.52              |
| 1:E:402:TRP:C    | 1:E:402:TRP:CE3  | 2.82                     | 0.52              |
| 1:E:465:LYS:O    | 1:E:466:VAL:HG23 | 2.08                     | 0.52              |
| 1:E:98:ALA:O     | 1:E:383:TRP:HZ3  | 1.91                     | 0.52              |
| 1:G:465:LYS:O    | 1:G:466:VAL:HG23 | 2.08                     | 0.52              |
| 2:H:268:SER:HA   | 2:H:274:ILE:HG22 | 1.90                     | 0.52              |
| 1:A:196:GLY:O    | 1:A:199:ARG:HB3  | 2.09                     | 0.52              |
| 2:H:392:PRO:HG2  | 2:H:392:PRO:O    | 2.08                     | 0.52              |
| 1:A:540:LYS:CE   | 2:B:265:ASN:HB2  | 2.40                     | 0.52              |
| 2:B:72:ARG:NH1   | 2:B:409:THR:HG22 | 2.25                     | 0.52              |
| 2:D:246:LEU:HB2  | 2:D:307:ARG:HH12 | 1.75                     | 0.52              |
| 1:G:105:SER:HB3  | 1:G:198:HIS:CG   | 2.44                     | 0.52              |
| 1:G:182:GLN:HG2  | 1:G:183:TYR:N    | 2.23                     | 0.52              |
| 1:G:414:TRP:CE3  | 1:G:415:GLU:N    | 2.78                     | 0.52              |
| 1:A:408:ALA:HB1  | 2:B:364:ASP:HB3  | 1.91                     | 0.52              |
| 1:A:452:LEU:HD22 | 1:A:470:THR:HG22 | 1.92                     | 0.52              |
| 2:B:268:SER:HA   | 2:B:274:ILE:HG22 | 1.90                     | 0.52              |
| 2:B:246:LEU:HB2  | 2:B:307:ARG:HH12 | 1.75                     | 0.52              |
| 1:C:126:LYS:HA   | 1:C:145:GLN:NE2  | 2.25                     | 0.52              |
| 1:C:372:VAL:HG11 | 1:C:411:ILE:HG23 | 1.91                     | 0.52              |
| 1:C:414:TRP:CE3  | 1:C:415:GLU:N    | 2.78                     | 0.52              |
| 2:D:35:VAL:O     | 2:D:39:THR:HG23  | 2.10                     | 0.52              |
| 1:E:157:PRO:HG2  | 1:E:158:ALA:N    | 2.24                     | 0.52              |
| 1:E:540:LYS:CE   | 2:F:265:ASN:HB2  | 2.40                     | 0.52              |
| 2:F:329:ILE:HA   | 2:F:338:THR:O    | 2.10                     | 0.52              |
| 2:H:264:LEU:HB2  | 2:H:276:VAL:CG1  | 2.39                     | 0.52              |
| 1:A:402:TRP:CE3  | 1:A:403:THR:HA   | 2.45                     | 0.52              |
| 2:B:35:VAL:O     | 2:B:39:THR:HG23  | 2.10                     | 0.52              |
| 1:C:326:ILE:HG21 | 1:G:345:PRO:HG3  | 1.91                     | 0.52              |
| 1:C:465:LYS:O    | 1:C:466:VAL:HG23 | 2.08                     | 0.52              |
| 2:D:97:PRO:C     | 2:D:99:GLY:H     | 2.11                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:452:LEU:HD22 | 1:E:470:THR:HG22 | 1.92                     | 0.52              |
| 1:G:106:VAL:O    | 1:G:227:PHE:CZ   | 2.62                     | 0.52              |
| 1:G:454:LYS:HA   | 1:G:467:VAL:O    | 2.10                     | 0.52              |
| 1:A:126:LYS:HA   | 1:A:145:GLN:NE2  | 2.25                     | 0.52              |
| 1:E:414:TRP:CE3  | 1:E:415:GLU:N    | 2.78                     | 0.52              |
| 2:F:326:ILE:O    | 2:F:341:ILE:HA   | 2.10                     | 0.52              |
| 1:G:126:LYS:HA   | 1:G:145:GLN:NE2  | 2.25                     | 0.52              |
| 2:H:35:VAL:O     | 2:H:39:THR:HG23  | 2.10                     | 0.52              |
| 1:A:372:VAL:HG11 | 1:A:411:ILE:HG23 | 1.91                     | 0.52              |
| 1:A:441:TYR:CE2  | 1:A:543:GLY:O    | 2.63                     | 0.52              |
| 2:B:97:PRO:C     | 2:B:99:GLY:H     | 2.11                     | 0.52              |
| 1:E:441:TYR:CE2  | 1:E:543:GLY:O    | 2.63                     | 0.52              |
| 1:G:91:GLN:HE21  | 1:G:91:GLN:CA    | 2.22                     | 0.52              |
| 2:H:329:ILE:HA   | 2:H:338:THR:O    | 2.10                     | 0.52              |
| 1:A:324:ASP:O    | 1:A:343:GLN:HG2  | 2.09                     | 0.52              |
| 1:A:402:TRP:O    | 1:A:402:TRP:HE3  | 1.93                     | 0.52              |
| 1:A:491:LEU:HB3  | 1:A:529:GLU:HB2  | 1.91                     | 0.52              |
| 1:C:249:LYS:HG2  | 1:C:250:ASP:H    | 1.75                     | 0.52              |
| 1:C:441:TYR:CE2  | 1:C:543:GLY:O    | 2.63                     | 0.52              |
| 1:E:454:LYS:HA   | 1:E:467:VAL:O    | 2.10                     | 0.52              |
| 1:E:491:LEU:HB3  | 1:E:529:GLU:HB2  | 1.91                     | 0.52              |
| 2:F:103:LYS:NZ   | 2:F:179:VAL:N    | 2.55                     | 0.52              |
| 2:F:13:LYS:HB3   | 2:F:14:PRO:HD2   | 1.91                     | 0.52              |
| 1:C:491:LEU:HB3  | 1:C:529:GLU:HB2  | 1.91                     | 0.52              |
| 2:D:13:LYS:HB3   | 2:D:14:PRO:HD2   | 1.91                     | 0.52              |
| 2:F:9:PRO:HA     | 2:F:121:ASP:OD2  | 2.10                     | 0.52              |
| 2:F:35:VAL:O     | 2:F:39:THR:HG23  | 2.10                     | 0.52              |
| 1:G:341:ILE:HD12 | 1:G:383:TRP:NE1  | 2.23                     | 0.52              |
| 2:B:9:PRO:HA     | 2:B:121:ASP:OD2  | 2.10                     | 0.51              |
| 2:B:13:LYS:HB3   | 2:B:14:PRO:HD2   | 1.91                     | 0.51              |
| 1:C:157:PRO:HG2  | 1:C:158:ALA:N    | 2.24                     | 0.51              |
| 1:C:326:ILE:CB   | 1:C:342:TYR:CE1  | 2.92                     | 0.51              |
| 1:C:402:TRP:CE3  | 1:C:403:THR:HA   | 2.45                     | 0.51              |
| 1:E:126:LYS:HA   | 1:E:145:GLN:NE2  | 2.25                     | 0.51              |
| 1:E:182:GLN:HG2  | 1:E:183:TYR:N    | 2.23                     | 0.51              |
| 1:E:324:ASP:O    | 1:E:343:GLN:HG2  | 2.09                     | 0.51              |
| 1:E:361:HIS:CD2  | 1:E:505:ILE:CG2  | 2.93                     | 0.51              |
| 2:H:376:THR:HG22 | 2:H:389:PHE:CZ   | 2.45                     | 0.51              |
| 1:A:118:VAL:HG12 | 1:A:118:VAL:O    | 2.10                     | 0.51              |
| 1:A:249:LYS:HG2  | 1:A:250:ASP:H    | 1.75                     | 0.51              |
| 1:C:402:TRP:HE3  | 1:C:402:TRP:O    | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:452:LEU:HD22 | 1:C:470:THR:HG22 | 1.92                     | 0.51              |
| 1:C:540:LYS:CE   | 2:D:265:ASN:HB2  | 2.40                     | 0.51              |
| 1:C:540:LYS:HZ3  | 2:D:261:VAL:HG12 | 1.74                     | 0.51              |
| 2:D:376:THR:HG22 | 2:D:389:PHE:CZ   | 2.45                     | 0.51              |
| 1:G:410:TRP:CH2  | 1:G:412:PRO:HA   | 2.46                     | 0.51              |
| 2:H:103:LYS:NZ   | 2:H:179:VAL:N    | 2.55                     | 0.51              |
| 2:H:104:LYS:HZ1  | 2:H:194:GLU:HA   | 1.74                     | 0.51              |
| 2:H:326:ILE:O    | 2:H:341:ILE:HA   | 2.10                     | 0.51              |
| 1:A:454:LYS:HA   | 1:A:467:VAL:O    | 2.10                     | 0.51              |
| 2:B:376:THR:HG22 | 2:B:389:PHE:CZ   | 2.45                     | 0.51              |
| 2:D:97:PRO:HB3   | 2:D:179:VAL:HG11 | 1.93                     | 0.51              |
| 1:E:105:SER:HB3  | 1:E:198:HIS:CG   | 2.45                     | 0.51              |
| 1:E:341:ILE:HD12 | 1:E:383:TRP:NE1  | 2.23                     | 0.51              |
| 1:E:410:TRP:CH2  | 1:E:412:PRO:HA   | 2.46                     | 0.51              |
| 1:G:157:PRO:HG2  | 1:G:158:ALA:N    | 2.24                     | 0.51              |
| 1:G:206:ARG:NH2  | 1:G:218:ASP:HA   | 2.25                     | 0.51              |
| 1:G:540:LYS:CE   | 2:H:265:ASN:HB2  | 2.40                     | 0.51              |
| 1:G:542:ILE:O    | 1:G:545:ASN:HB3  | 2.11                     | 0.51              |
| 2:H:24:TRP:CH2   | 2:H:61:PHE:CE1   | 2.88                     | 0.51              |
| 2:B:329:ILE:HA   | 2:B:338:THR:O    | 2.10                     | 0.51              |
| 1:C:118:VAL:O    | 1:C:118:VAL:HG12 | 2.10                     | 0.51              |
| 1:C:324:ASP:O    | 1:C:343:GLN:HG2  | 2.09                     | 0.51              |
| 1:E:249:LYS:HG2  | 1:E:250:ASP:H    | 1.75                     | 0.51              |
| 1:E:326:ILE:CB   | 1:E:342:TYR:CE1  | 2.92                     | 0.51              |
| 1:E:372:VAL:HG11 | 1:E:411:ILE:HG23 | 1.91                     | 0.51              |
| 1:G:402:TRP:CE3  | 1:G:403:THR:HA   | 2.45                     | 0.51              |
| 1:G:441:TYR:CE2  | 1:G:543:GLY:O    | 2.63                     | 0.51              |
| 2:H:246:LEU:HB2  | 2:H:307:ARG:HH12 | 1.75                     | 0.51              |
| 1:C:391:LEU:HD12 | 1:C:414:TRP:CZ3  | 2.46                     | 0.51              |
| 2:D:54:ASN:ND2   | 2:D:56:TYR:HB2   | 2.25                     | 0.51              |
| 1:G:118:VAL:HG12 | 1:G:118:VAL:O    | 2.10                     | 0.51              |
| 2:H:54:ASN:ND2   | 2:H:56:TYR:HB2   | 2.25                     | 0.51              |
| 1:A:391:LEU:HD12 | 1:A:414:TRP:CZ3  | 2.46                     | 0.51              |
| 1:A:361:HIS:CD2  | 1:A:505:ILE:CG2  | 2.93                     | 0.51              |
| 2:D:9:PRO:HA     | 2:D:121:ASP:OD2  | 2.10                     | 0.51              |
| 2:D:10:VAL:HG21  | 2:D:153:TRP:CH2  | 2.46                     | 0.51              |
| 1:E:91:GLN:CA    | 1:E:91:GLN:HE21  | 2.21                     | 0.51              |
| 1:G:391:LEU:HD12 | 1:G:414:TRP:CZ3  | 2.46                     | 0.51              |
| 2:B:10:VAL:HG21  | 2:B:153:TRP:CH2  | 2.46                     | 0.51              |
| 1:C:451:LYS:O    | 1:C:471:ASN:HA   | 2.11                     | 0.51              |
| 2:D:326:ILE:O    | 2:D:341:ILE:HA   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:402:TRP:CE3  | 1:E:403:THR:HA   | 2.45                     | 0.51              |
| 1:G:160:PHE:CZ   | 1:G:164:MET:HG2  | 2.46                     | 0.51              |
| 1:A:326:ILE:CB   | 1:A:342:TYR:CE1  | 2.92                     | 0.51              |
| 2:B:10:VAL:HG21  | 2:B:153:TRP:HH2  | 1.76                     | 0.51              |
| 1:C:342:TYR:OH   | 1:G:345:PRO:HB3  | 2.08                     | 0.51              |
| 1:C:454:LYS:HA   | 1:C:467:VAL:O    | 2.10                     | 0.51              |
| 1:C:542:ILE:O    | 1:C:545:ASN:HB3  | 2.11                     | 0.51              |
| 2:D:10:VAL:HG21  | 2:D:153:TRP:HH2  | 1.76                     | 0.51              |
| 2:F:376:THR:HG22 | 2:F:389:PHE:CZ   | 2.45                     | 0.51              |
| 2:H:10:VAL:HG21  | 2:H:153:TRP:CH2  | 2.46                     | 0.51              |
| 1:G:540:LYS:HZ3  | 2:H:261:VAL:CG1  | 2.24                     | 0.51              |
| 2:B:97:PRO:HB3   | 2:B:179:VAL:HG11 | 1.93                     | 0.51              |
| 1:C:12:LEU:HD11  | 1:C:127:TYR:CE1  | 2.46                     | 0.51              |
| 1:C:164:MET:HE2  | 1:C:187:LEU:HD21 | 1.93                     | 0.51              |
| 1:E:118:VAL:O    | 1:E:118:VAL:HG12 | 2.10                     | 0.51              |
| 2:F:194:GLU:HG2  | 2:F:195:ILE:N    | 2.26                     | 0.51              |
| 2:F:54:ASN:ND2   | 2:F:56:TYR:HB2   | 2.25                     | 0.51              |
| 1:G:452:LEU:HD22 | 1:G:470:THR:HG22 | 1.92                     | 0.51              |
| 2:H:9:PRO:HA     | 2:H:121:ASP:OD2  | 2.10                     | 0.51              |
| 2:H:10:VAL:HG21  | 2:H:153:TRP:HH2  | 1.76                     | 0.51              |
| 1:A:451:LYS:O    | 1:A:471:ASN:HA   | 2.11                     | 0.51              |
| 2:B:326:ILE:O    | 2:B:341:ILE:HA   | 2.10                     | 0.51              |
| 1:C:160:PHE:CZ   | 1:C:164:MET:HG2  | 2.46                     | 0.51              |
| 1:C:206:ARG:NH2  | 1:C:218:ASP:HA   | 2.25                     | 0.51              |
| 1:C:410:TRP:CH2  | 1:C:412:PRO:HA   | 2.46                     | 0.51              |
| 1:E:361:HIS:NE2  | 1:E:518:VAL:HG21 | 2.26                     | 0.51              |
| 1:E:540:LYS:NZ   | 2:F:276:VAL:HG21 | 2.26                     | 0.51              |
| 1:G:326:ILE:CG2  | 1:G:342:TYR:CE1  | 2.94                     | 0.51              |
| 1:G:451:LYS:O    | 1:G:471:ASN:HA   | 2.11                     | 0.51              |
| 1:A:363:ASN:ND2  | 1:A:365:VAL:HB   | 2.26                     | 0.50              |
| 1:C:326:ILE:CG2  | 1:C:342:TYR:CE1  | 2.94                     | 0.50              |
| 2:D:329:ILE:HA   | 2:D:338:THR:O    | 2.10                     | 0.50              |
| 2:D:24:TRP:HZ3   | 2:D:61:PHE:HB3   | 1.77                     | 0.50              |
| 1:E:391:LEU:HD12 | 1:E:414:TRP:CZ3  | 2.46                     | 0.50              |
| 1:E:402:TRP:O    | 1:E:402:TRP:HE3  | 1.93                     | 0.50              |
| 1:E:542:ILE:O    | 1:E:545:ASN:HB3  | 2.11                     | 0.50              |
| 1:G:361:HIS:NE2  | 1:G:518:VAL:HG21 | 2.26                     | 0.50              |
| 1:A:414:TRP:CE3  | 1:A:415:GLU:N    | 2.78                     | 0.50              |
| 2:B:54:ASN:ND2   | 2:B:56:TYR:HB2   | 2.25                     | 0.50              |
| 1:C:361:HIS:CD2  | 1:C:505:ILE:CG2  | 2.93                     | 0.50              |
| 1:C:363:ASN:ND2  | 1:C:365:VAL:HB   | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:540:LYS:HZ3  | 2:D:261:VAL:HG13 | 1.76                     | 0.50              |
| 1:G:402:TRP:HE3  | 1:G:402:TRP:O    | 1.93                     | 0.50              |
| 1:G:361:HIS:CD2  | 1:G:505:ILE:CG2  | 2.93                     | 0.50              |
| 2:H:72:ARG:NH1   | 2:H:409:THR:HA   | 2.26                     | 0.50              |
| 1:A:12:LEU:HD11  | 1:A:127:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:240:THR:HG22 | 1:A:315:HIS:CB   | 2.42                     | 0.50              |
| 1:A:410:TRP:CH2  | 1:A:412:PRO:HA   | 2.46                     | 0.50              |
| 1:C:417:VAL:CG1  | 1:G:346:PHE:HE2  | 2.12                     | 0.50              |
| 1:E:160:PHE:CZ   | 1:E:164:MET:HG2  | 2.46                     | 0.50              |
| 1:G:132:ILE:HD11 | 1:G:144:TYR:HE2  | 1.77                     | 0.50              |
| 1:G:249:LYS:HG2  | 1:G:250:ASP:H    | 1.75                     | 0.50              |
| 1:G:244:ILE:HB   | 1:G:310:LEU:HD22 | 1.94                     | 0.50              |
| 1:G:90:VAL:HG12  | 2:H:141:GLY:N    | 2.24                     | 0.50              |
| 2:H:97:PRO:HB3   | 2:H:179:VAL:HG11 | 1.93                     | 0.50              |
| 1:A:160:PHE:CZ   | 1:A:164:MET:HG2  | 2.46                     | 0.50              |
| 1:A:194:GLU:O    | 1:A:196:GLY:N    | 2.45                     | 0.50              |
| 1:A:419:THR:CG2  | 1:A:420:PRO:HD2  | 2.41                     | 0.50              |
| 1:A:542:ILE:O    | 1:A:545:ASN:HB3  | 2.11                     | 0.50              |
| 1:A:90:VAL:O     | 1:A:90:VAL:HG12  | 2.12                     | 0.50              |
| 1:C:417:VAL:HG22 | 1:G:346:PHE:CG   | 2.47                     | 0.50              |
| 1:C:419:THR:CG2  | 1:C:420:PRO:HD2  | 2.41                     | 0.50              |
| 1:C:468:PRO:HG2  | 1:C:468:PRO:O    | 2.12                     | 0.50              |
| 1:E:540:LYS:NZ   | 2:F:261:VAL:O    | 2.45                     | 0.50              |
| 1:G:324:ASP:O    | 1:G:343:GLN:HG2  | 2.09                     | 0.50              |
| 1:A:361:HIS:NE2  | 1:A:518:VAL:HG21 | 2.26                     | 0.50              |
| 2:B:27:THR:C     | 2:B:29:GLU:H     | 2.15                     | 0.50              |
| 1:C:361:HIS:NE2  | 1:C:518:VAL:HG21 | 2.26                     | 0.50              |
| 1:E:244:ILE:HB   | 1:E:310:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:345:PRO:HG3  | 1:E:326:ILE:HD13 | 1.94                     | 0.50              |
| 1:E:451:LYS:O    | 1:E:471:ASN:HA   | 2.11                     | 0.50              |
| 2:F:10:VAL:HG21  | 2:F:153:TRP:HH2  | 1.76                     | 0.50              |
| 1:G:318:TYR:N    | 1:G:318:TYR:HD1  | 2.10                     | 0.50              |
| 1:A:244:ILE:HB   | 1:A:310:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:328:GLU:HG2  | 1:A:330:GLN:HE21 | 1.77                     | 0.50              |
| 1:A:326:ILE:CG2  | 1:A:342:TYR:CE1  | 2.94                     | 0.50              |
| 1:A:540:LYS:NZ   | 2:B:276:VAL:HG21 | 2.26                     | 0.50              |
| 1:C:240:THR:HG22 | 1:C:315:HIS:CB   | 2.42                     | 0.50              |
| 1:E:194:GLU:O    | 1:E:196:GLY:N    | 2.45                     | 0.50              |
| 2:F:72:ARG:NH1   | 2:F:409:THR:HG22 | 2.25                     | 0.50              |
| 1:G:229:TRP:O    | 1:G:230:MET:HB2  | 2.12                     | 0.50              |
| 1:A:206:ARG:NH2  | 1:A:218:ASP:HA   | 2.25                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:61:PHE:CZ    | 2:D:402:TRP:HZ2  | 2.30                     | 0.50              |
| 2:H:194:GLU:HG2  | 2:H:195:ILE:N    | 2.26                     | 0.50              |
| 1:G:540:LYS:NZ   | 2:H:276:VAL:HG21 | 2.26                     | 0.50              |
| 2:B:156:SER:N    | 2:B:157:PRO:HD2  | 2.27                     | 0.50              |
| 1:C:194:GLU:O    | 1:C:196:GLY:N    | 2.45                     | 0.50              |
| 1:C:540:LYS:NZ   | 2:D:261:VAL:O    | 2.45                     | 0.50              |
| 1:E:363:ASN:ND2  | 1:E:365:VAL:HB   | 2.27                     | 0.50              |
| 1:E:399:GLU:HG2  | 1:E:399:GLU:O    | 2.12                     | 0.50              |
| 1:E:90:VAL:HG12  | 1:E:90:VAL:O     | 2.12                     | 0.50              |
| 2:F:246:LEU:HB2  | 2:F:307:ARG:HH12 | 1.75                     | 0.50              |
| 1:C:342:TYR:CZ   | 1:G:345:PRO:CG   | 2.92                     | 0.50              |
| 1:G:468:PRO:O    | 1:G:468:PRO:HG2  | 2.12                     | 0.50              |
| 2:H:61:PHE:CZ    | 2:H:402:TRP:HZ2  | 2.30                     | 0.50              |
| 1:A:540:LYS:NZ   | 2:B:261:VAL:O    | 2.45                     | 0.50              |
| 1:C:328:GLU:HG2  | 1:C:330:GLN:HE21 | 1.76                     | 0.50              |
| 2:D:194:GLU:HG2  | 2:D:195:ILE:N    | 2.26                     | 0.50              |
| 1:E:12:LEU:HD11  | 1:E:127:TYR:CE1  | 2.46                     | 0.50              |
| 1:E:344:GLU:HB2  | 1:E:347:LYS:HB2  | 1.94                     | 0.50              |
| 2:F:72:ARG:NH1   | 2:F:409:THR:HA   | 2.26                     | 0.50              |
| 1:G:12:LEU:HD11  | 1:G:127:TYR:CE1  | 2.46                     | 0.50              |
| 1:G:399:GLU:O    | 1:G:399:GLU:HG2  | 2.12                     | 0.50              |
| 1:G:540:LYS:NZ   | 2:H:261:VAL:O    | 2.45                     | 0.50              |
| 2:B:61:PHE:CZ    | 2:B:402:TRP:HZ2  | 2.30                     | 0.49              |
| 2:B:72:ARG:NH1   | 2:B:409:THR:HA   | 2.26                     | 0.49              |
| 1:C:244:ILE:HB   | 1:C:310:LEU:HD22 | 1.94                     | 0.49              |
| 2:F:24:TRP:CH2   | 2:F:61:PHE:CE1   | 2.88                     | 0.49              |
| 1:G:194:GLU:O    | 1:G:196:GLY:N    | 2.45                     | 0.49              |
| 1:G:328:GLU:HG2  | 1:G:330:GLN:HE21 | 1.76                     | 0.49              |
| 1:G:394:GLN:HG2  | 1:G:416:PHE:CE2  | 2.47                     | 0.49              |
| 1:G:90:VAL:HG12  | 1:G:90:VAL:O     | 2.12                     | 0.49              |
| 2:H:27:THR:C     | 2:H:29:GLU:H     | 2.15                     | 0.49              |
| 1:C:90:VAL:O     | 1:C:90:VAL:HG12  | 2.12                     | 0.49              |
| 2:D:27:THR:C     | 2:D:29:GLU:H     | 2.15                     | 0.49              |
| 1:E:206:ARG:NH2  | 1:E:218:ASP:HA   | 2.25                     | 0.49              |
| 1:E:240:THR:HG22 | 1:E:315:HIS:CB   | 2.42                     | 0.49              |
| 2:F:10:VAL:HG21  | 2:F:153:TRP:CH2  | 2.46                     | 0.49              |
| 2:F:156:SER:N    | 2:F:157:PRO:HD2  | 2.27                     | 0.49              |
| 1:G:447:ASN:HB3  | 1:G:450:THR:OG1  | 2.12                     | 0.49              |
| 1:A:468:PRO:O    | 1:A:468:PRO:HG2  | 2.12                     | 0.49              |
| 1:A:90:VAL:O     | 1:A:91:GLN:NE2   | 2.45                     | 0.49              |
| 2:B:194:GLU:HG2  | 2:B:195:ILE:N    | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:54:ASN:HD22  | 2:B:56:TYR:H     | 1.60                     | 0.49              |
| 1:C:132:ILE:HD11 | 1:C:144:TYR:HE2  | 1.77                     | 0.49              |
| 1:C:169:GLU:HB3  | 1:C:170:PRO:HD3  | 1.95                     | 0.49              |
| 1:C:345:PRO:HG3  | 1:G:326:ILE:HD13 | 1.34                     | 0.49              |
| 1:G:183:TYR:CD2  | 1:G:230:MET:HG2  | 2.47                     | 0.49              |
| 1:G:240:THR:HG22 | 1:G:315:HIS:CB   | 2.42                     | 0.49              |
| 1:C:229:TRP:O    | 1:C:230:MET:HB2  | 2.12                     | 0.49              |
| 1:C:394:GLN:HG2  | 1:C:416:PHE:CE2  | 2.47                     | 0.49              |
| 1:C:540:LYS:NZ   | 2:D:276:VAL:HG21 | 2.26                     | 0.49              |
| 1:E:326:ILE:CG2  | 1:E:342:TYR:CE1  | 2.94                     | 0.49              |
| 2:F:97:PRO:HB3   | 2:F:179:VAL:HG11 | 1.93                     | 0.49              |
| 1:G:363:ASN:ND2  | 1:G:365:VAL:HB   | 2.27                     | 0.49              |
| 2:B:24:TRP:CZ3   | 2:B:61:PHE:CG    | 3.00                     | 0.49              |
| 1:C:90:VAL:O     | 1:C:91:GLN:NE2   | 2.45                     | 0.49              |
| 2:D:156:SER:N    | 2:D:157:PRO:HD2  | 2.27                     | 0.49              |
| 1:E:318:TYR:N    | 1:E:318:TYR:HD1  | 2.10                     | 0.49              |
| 1:E:468:PRO:O    | 1:E:468:PRO:HG2  | 2.12                     | 0.49              |
| 1:E:90:VAL:HG12  | 2:F:141:GLY:N    | 2.25                     | 0.49              |
| 2:F:27:THR:C     | 2:F:29:GLU:H     | 2.15                     | 0.49              |
| 2:F:61:PHE:CZ    | 2:F:402:TRP:HZ2  | 2.30                     | 0.49              |
| 2:B:142:ILE:HG22 | 2:B:144:TYR:CE1  | 2.48                     | 0.49              |
| 1:C:318:TYR:N    | 1:C:318:TYR:HD1  | 2.10                     | 0.49              |
| 1:C:90:VAL:HG12  | 2:D:141:GLY:N    | 2.24                     | 0.49              |
| 2:D:72:ARG:NH1   | 2:D:409:THR:HA   | 2.26                     | 0.49              |
| 1:E:132:ILE:HD11 | 1:E:144:TYR:HE2  | 1.77                     | 0.49              |
| 1:E:191:SER:OG   | 1:E:198:HIS:CD2  | 2.66                     | 0.49              |
| 2:F:24:TRP:CZ3   | 2:F:61:PHE:CG    | 3.00                     | 0.49              |
| 2:F:27:THR:C     | 2:F:29:GLU:N     | 2.66                     | 0.49              |
| 2:F:54:ASN:HD22  | 2:F:56:TYR:H     | 1.60                     | 0.49              |
| 1:G:164:MET:HE2  | 1:G:187:LEU:HD21 | 1.95                     | 0.49              |
| 2:H:72:ARG:NH1   | 2:H:409:THR:HG22 | 2.25                     | 0.49              |
| 1:G:473:THR:OG1  | 1:G:476:LYS:HG2  | 2.13                     | 0.49              |
| 2:H:156:SER:N    | 2:H:157:PRO:HD2  | 2.27                     | 0.49              |
| 1:A:132:ILE:HD11 | 1:A:144:TYR:HE2  | 1.77                     | 0.49              |
| 1:A:164:MET:HE2  | 1:A:187:LEU:HD21 | 1.95                     | 0.49              |
| 1:A:394:GLN:HG2  | 1:A:416:PHE:CE2  | 2.47                     | 0.49              |
| 1:C:346:PHE:HZ   | 1:G:328:GLU:OE1  | 1.96                     | 0.49              |
| 2:D:108:VAL:HG12 | 2:D:188:TYR:CD2  | 2.48                     | 0.49              |
| 2:D:24:TRP:CZ3   | 2:D:61:PHE:CG    | 3.00                     | 0.49              |
| 1:E:183:TYR:CD2  | 1:E:230:MET:HG2  | 2.47                     | 0.49              |
| 1:E:328:GLU:HG2  | 1:E:330:GLN:HE21 | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:540:LYS:HZ3  | 2:F:261:VAL:HG13 | 1.76                     | 0.49              |
| 1:G:169:GLU:HB3  | 1:G:170:PRO:HD3  | 1.95                     | 0.49              |
| 2:H:27:THR:C     | 2:H:29:GLU:N     | 2.66                     | 0.49              |
| 1:A:169:GLU:HB3  | 1:A:170:PRO:HD3  | 1.95                     | 0.49              |
| 1:A:191:SER:OG   | 1:A:198:HIS:CD2  | 2.66                     | 0.49              |
| 1:A:318:TYR:N    | 1:A:318:TYR:HD1  | 2.10                     | 0.49              |
| 1:A:46:LYS:HD2   | 1:A:116:PHE:HB3  | 1.94                     | 0.49              |
| 2:D:27:THR:C     | 2:D:29:GLU:N     | 2.66                     | 0.49              |
| 2:D:72:ARG:NH1   | 2:D:409:THR:HG22 | 2.25                     | 0.49              |
| 1:E:394:GLN:HG2  | 1:E:416:PHE:CE2  | 2.47                     | 0.49              |
| 1:E:447:ASN:HB3  | 1:E:450:THR:OG1  | 2.12                     | 0.49              |
| 2:F:207:GLN:O    | 2:F:210:LEU:N    | 2.46                     | 0.49              |
| 1:G:344:GLU:HB2  | 1:G:347:LYS:HB2  | 1.94                     | 0.49              |
| 2:H:108:VAL:HG12 | 2:H:188:TYR:CD2  | 2.48                     | 0.49              |
| 1:A:229:TRP:O    | 1:A:230:MET:HB2  | 2.12                     | 0.49              |
| 1:C:46:LYS:HD2   | 1:C:116:PHE:HB3  | 1.94                     | 0.49              |
| 1:E:229:TRP:O    | 1:E:230:MET:HB2  | 2.12                     | 0.49              |
| 1:G:356:ARG:HH21 | 1:G:358:ARG:NH1  | 2.11                     | 0.49              |
| 2:H:142:ILE:HG22 | 2:H:144:TYR:CE1  | 2.48                     | 0.49              |
| 2:H:207:GLN:O    | 2:H:210:LEU:N    | 2.46                     | 0.49              |
| 1:A:342:TYR:CD1  | 1:A:342:TYR:C    | 2.87                     | 0.48              |
| 2:B:108:VAL:HG12 | 2:B:188:TYR:CD2  | 2.48                     | 0.48              |
| 1:C:183:TYR:CD2  | 1:C:230:MET:HG2  | 2.47                     | 0.48              |
| 2:D:142:ILE:HG22 | 2:D:144:TYR:CE1  | 2.48                     | 0.48              |
| 1:E:473:THR:OG1  | 1:E:476:LYS:HG2  | 2.13                     | 0.48              |
| 2:H:395:LYS:HG3  | 2:H:416:PHE:HE2  | 1.78                     | 0.48              |
| 1:A:337:TRP:N    | 1:A:337:TRP:CD1  | 2.81                     | 0.48              |
| 1:A:344:GLU:HB2  | 1:A:347:LYS:HB2  | 1.94                     | 0.48              |
| 1:C:416:PHE:HD1  | 1:C:417:VAL:H    | 1.61                     | 0.48              |
| 1:G:191:SER:OG   | 1:G:198:HIS:CD2  | 2.66                     | 0.48              |
| 1:G:326:ILE:CB   | 1:G:342:TYR:CE1  | 2.92                     | 0.48              |
| 1:G:90:VAL:O     | 1:G:91:GLN:NE2   | 2.45                     | 0.48              |
| 1:A:447:ASN:HB3  | 1:A:450:THR:OG1  | 2.12                     | 0.48              |
| 1:A:88:TRP:CZ2   | 2:B:57:ASN:CB    | 2.96                     | 0.48              |
| 2:B:97:PRO:HD3   | 2:B:181:TYR:CD1  | 2.49                     | 0.48              |
| 1:C:10:VAL:HA    | 1:C:85:GLN:OE1   | 2.13                     | 0.48              |
| 1:C:344:GLU:HB2  | 1:C:347:LYS:HB2  | 1.94                     | 0.48              |
| 2:D:54:ASN:HD22  | 2:D:56:TYR:H     | 1.60                     | 0.48              |
| 1:E:452:LEU:HD23 | 1:E:471:ASN:H    | 1.78                     | 0.48              |
| 2:F:142:ILE:HG22 | 2:F:144:TYR:CE1  | 2.48                     | 0.48              |
| 2:F:103:LYS:HZ2  | 2:F:179:VAL:HG23 | 1.74                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:108:VAL:HG12 | 2:F:188:TYR:CD2  | 2.48                     | 0.48              |
| 1:G:452:LEU:HD23 | 1:G:471:ASN:H    | 1.78                     | 0.48              |
| 1:A:356:ARG:HH21 | 1:A:358:ARG:NH1  | 2.11                     | 0.48              |
| 1:A:452:LEU:HD23 | 1:A:471:ASN:H    | 1.78                     | 0.48              |
| 1:A:98:ALA:O     | 1:A:383:TRP:CZ3  | 2.66                     | 0.48              |
| 2:B:153:TRP:CE3  | 2:B:156:SER:N    | 2.82                     | 0.48              |
| 2:B:241:VAL:HG12 | 2:B:242:GLN:N    | 2.28                     | 0.48              |
| 1:C:191:SER:OG   | 1:C:198:HIS:CD2  | 2.66                     | 0.48              |
| 1:C:447:ASN:HB3  | 1:C:450:THR:OG1  | 2.12                     | 0.48              |
| 2:D:153:TRP:CE3  | 2:D:156:SER:N    | 2.82                     | 0.48              |
| 2:D:241:VAL:HG12 | 2:D:242:GLN:N    | 2.28                     | 0.48              |
| 2:D:97:PRO:HD3   | 2:D:181:TYR:CD1  | 2.49                     | 0.48              |
| 1:E:342:TYR:CD1  | 1:E:342:TYR:C    | 2.87                     | 0.48              |
| 1:E:356:ARG:HH21 | 1:E:358:ARG:NH1  | 2.11                     | 0.48              |
| 1:E:96:HIS:CG    | 1:E:97:PRO:HD2   | 2.49                     | 0.48              |
| 1:G:342:TYR:CD1  | 1:G:342:TYR:C    | 2.87                     | 0.48              |
| 1:G:416:PHE:HD1  | 1:G:417:VAL:H    | 1.61                     | 0.48              |
| 1:G:511:ASP:O    | 1:G:512:LYS:HD3  | 2.14                     | 0.48              |
| 1:G:98:ALA:O     | 1:G:383:TRP:CZ3  | 2.66                     | 0.48              |
| 1:A:183:TYR:CD2  | 1:A:230:MET:HG2  | 2.47                     | 0.48              |
| 1:A:10:VAL:HA    | 1:A:85:GLN:OE1   | 2.13                     | 0.48              |
| 2:B:27:THR:C     | 2:B:29:GLU:N     | 2.66                     | 0.48              |
| 2:D:24:TRP:CH2   | 2:D:61:PHE:CE1   | 2.88                     | 0.48              |
| 1:E:164:MET:HE2  | 1:E:187:LEU:HD21 | 1.96                     | 0.48              |
| 1:E:98:ALA:O     | 1:E:383:TRP:CZ3  | 2.66                     | 0.48              |
| 1:G:419:THR:CG2  | 1:G:420:PRO:HD2  | 2.42                     | 0.48              |
| 2:H:153:TRP:CE3  | 2:H:156:SER:N    | 2.82                     | 0.48              |
| 2:H:24:TRP:CZ3   | 2:H:61:PHE:CG    | 3.00                     | 0.48              |
| 1:A:76:ASP:OD1   | 1:A:78:ARG:HG3   | 2.14                     | 0.48              |
| 1:C:342:TYR:CD1  | 1:C:342:TYR:C    | 2.87                     | 0.48              |
| 1:C:399:GLU:HG2  | 1:C:399:GLU:O    | 2.12                     | 0.48              |
| 1:C:452:LEU:HD23 | 1:C:471:ASN:H    | 1.78                     | 0.48              |
| 1:E:46:LYS:HD2   | 1:E:116:PHE:HB3  | 1.94                     | 0.48              |
| 1:E:510:PRO:O    | 1:E:522:ILE:HD13 | 2.14                     | 0.48              |
| 2:F:268:SER:HA   | 2:F:274:ILE:CG2  | 2.43                     | 0.48              |
| 1:G:510:PRO:O    | 1:G:522:ILE:HD13 | 2.14                     | 0.48              |
| 1:A:90:VAL:HG12  | 2:B:141:GLY:N    | 2.24                     | 0.48              |
| 2:D:268:SER:HA   | 2:D:274:ILE:CG2  | 2.43                     | 0.48              |
| 1:E:108:VAL:HG22 | 1:E:188:TYR:HA   | 1.96                     | 0.48              |
| 1:E:88:TRP:CZ2   | 2:F:57:ASN:CB    | 2.96                     | 0.48              |
| 2:F:153:TRP:CE3  | 2:F:156:SER:N    | 2.82                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:10:VAL:HA    | 1:G:85:GLN:OE1   | 2.13                     | 0.48              |
| 1:A:164:MET:HG3  | 1:A:182:GLN:NE2  | 2.29                     | 0.48              |
| 1:A:416:PHE:HD1  | 1:A:417:VAL:H    | 1.61                     | 0.48              |
| 1:A:473:THR:OG1  | 1:A:476:LYS:HG2  | 2.13                     | 0.48              |
| 2:D:207:GLN:O    | 2:D:210:LEU:N    | 2.46                     | 0.48              |
| 2:D:395:LYS:HG3  | 2:D:416:PHE:HE2  | 1.78                     | 0.48              |
| 1:E:10:VAL:HA    | 1:E:85:GLN:OE1   | 2.13                     | 0.48              |
| 1:E:455:ALA:HB2  | 1:E:469:LEU:HD11 | 1.96                     | 0.48              |
| 1:E:90:VAL:O     | 1:E:91:GLN:NE2   | 2.45                     | 0.48              |
| 2:F:336:GLN:HG2  | 2:F:355:ALA:CB   | 2.44                     | 0.48              |
| 1:G:46:LYS:HD2   | 1:G:116:PHE:HB3  | 1.94                     | 0.48              |
| 1:A:455:ALA:HB2  | 1:A:469:LEU:HD11 | 1.96                     | 0.48              |
| 2:B:207:GLN:O    | 2:B:210:LEU:N    | 2.46                     | 0.48              |
| 1:C:98:ALA:O     | 1:C:383:TRP:CZ3  | 2.66                     | 0.48              |
| 1:C:473:THR:OG1  | 1:C:476:LYS:HG2  | 2.13                     | 0.48              |
| 1:C:511:ASP:O    | 1:C:512:LYS:HD3  | 2.14                     | 0.48              |
| 1:C:88:TRP:CZ2   | 2:D:57:ASN:CB    | 2.96                     | 0.48              |
| 1:E:511:ASP:O    | 1:E:512:LYS:HD3  | 2.14                     | 0.48              |
| 1:E:76:ASP:OD1   | 1:E:78:ARG:HG3   | 2.14                     | 0.48              |
| 2:F:241:VAL:HG12 | 2:F:242:GLN:N    | 2.28                     | 0.48              |
| 1:E:540:LYS:HZ3  | 2:F:261:VAL:HG12 | 1.77                     | 0.48              |
| 1:G:455:ALA:HB2  | 1:G:469:LEU:HD11 | 1.96                     | 0.48              |
| 1:G:76:ASP:OD1   | 1:G:78:ARG:HG3   | 2.14                     | 0.48              |
| 2:H:54:ASN:HD22  | 2:H:56:TYR:H     | 1.60                     | 0.48              |
| 1:A:108:VAL:HG22 | 1:A:188:TYR:HA   | 1.96                     | 0.48              |
| 2:B:52:PRO:HD2   | 2:B:53:GLU:OE1   | 2.14                     | 0.48              |
| 2:D:52:PRO:HD2   | 2:D:53:GLU:OE1   | 2.14                     | 0.48              |
| 1:G:132:ILE:HB   | 1:G:142:ILE:HG12 | 1.96                     | 0.48              |
| 1:G:164:MET:HG3  | 1:G:182:GLN:NE2  | 2.29                     | 0.48              |
| 2:H:241:VAL:HG12 | 2:H:242:GLN:N    | 2.28                     | 0.48              |
| 1:A:96:HIS:CG    | 1:A:97:PRO:HD2   | 2.49                     | 0.47              |
| 1:C:108:VAL:HG22 | 1:C:188:TYR:HA   | 1.96                     | 0.47              |
| 1:C:356:ARG:HH21 | 1:C:358:ARG:NH1  | 2.11                     | 0.47              |
| 1:C:76:ASP:OD1   | 1:C:78:ARG:HG3   | 2.14                     | 0.47              |
| 1:E:169:GLU:HB3  | 1:E:170:PRO:HD3  | 1.95                     | 0.47              |
| 2:F:158:ALA:O    | 2:F:161:GLN:HB2  | 2.15                     | 0.47              |
| 1:G:108:VAL:HG22 | 1:G:188:TYR:HA   | 1.96                     | 0.47              |
| 1:G:337:TRP:N    | 1:G:337:TRP:CD1  | 2.81                     | 0.47              |
| 1:A:132:ILE:HB   | 1:A:142:ILE:HG12 | 1.96                     | 0.47              |
| 1:A:399:GLU:HG2  | 1:A:399:GLU:O    | 2.12                     | 0.47              |
| 1:C:164:MET:HG3  | 1:C:182:GLN:NE2  | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:336:GLN:HG2  | 1:G:355:ALA:HB2  | 1.97                     | 0.47              |
| 1:A:46:LYS:HG3   | 1:A:116:PHE:CD2  | 2.50                     | 0.47              |
| 2:B:268:SER:HA   | 2:B:274:ILE:CG2  | 2.43                     | 0.47              |
| 2:B:395:LYS:HG3  | 2:B:416:PHE:HE2  | 1.78                     | 0.47              |
| 2:D:336:GLN:HG2  | 2:D:355:ALA:CB   | 2.44                     | 0.47              |
| 2:F:24:TRP:HZ3   | 2:F:61:PHE:HB3   | 1.76                     | 0.47              |
| 2:F:97:PRO:HD3   | 2:F:181:TYR:CD1  | 2.49                     | 0.47              |
| 1:A:354:TYR:CZ   | 1:A:356:ARG:HD3  | 2.49                     | 0.47              |
| 1:A:511:ASP:O    | 1:A:512:LYS:HD3  | 2.14                     | 0.47              |
| 1:C:46:LYS:HG3   | 1:C:116:PHE:CD2  | 2.50                     | 0.47              |
| 1:C:132:ILE:HB   | 1:C:142:ILE:HG12 | 1.96                     | 0.47              |
| 1:C:390:LYS:HB3  | 1:C:417:VAL:HG21 | 1.96                     | 0.47              |
| 1:E:304:ALA:HA   | 1:E:307:ARG:HD2  | 1.96                     | 0.47              |
| 1:E:102:LYS:CG   | 1:E:318:TYR:HB2  | 2.45                     | 0.47              |
| 1:E:336:GLN:HG2  | 1:E:355:ALA:HB2  | 1.97                     | 0.47              |
| 1:E:419:THR:CG2  | 1:E:420:PRO:HD2  | 2.42                     | 0.47              |
| 1:G:354:TYR:CZ   | 1:G:356:ARG:HD3  | 2.49                     | 0.47              |
| 2:H:158:ALA:O    | 2:H:161:GLN:HB2  | 2.14                     | 0.47              |
| 2:H:336:GLN:HG2  | 2:H:355:ALA:CB   | 2.44                     | 0.47              |
| 1:G:88:TRP:CZ2   | 2:H:57:ASN:CB    | 2.96                     | 0.47              |
| 1:A:20:LYS:HG2   | 1:A:56:TYR:HA    | 1.96                     | 0.47              |
| 1:A:23:GLN:HG2   | 1:A:59:PRO:HA    | 1.96                     | 0.47              |
| 1:A:304:ALA:HA   | 1:A:307:ARG:HD2  | 1.96                     | 0.47              |
| 1:A:510:PRO:O    | 1:A:522:ILE:HD13 | 2.14                     | 0.47              |
| 2:B:24:TRP:CH2   | 2:B:61:PHE:CE1   | 2.88                     | 0.47              |
| 2:B:64:LYS:HB2   | 2:B:71:TRP:CE3   | 2.50                     | 0.47              |
| 1:C:455:ALA:HB2  | 1:C:469:LEU:HD11 | 1.96                     | 0.47              |
| 1:C:96:HIS:CG    | 1:C:97:PRO:HD2   | 2.49                     | 0.47              |
| 1:E:164:MET:HG3  | 1:E:182:GLN:NE2  | 2.29                     | 0.47              |
| 1:E:318:TYR:N    | 1:E:318:TYR:CD1  | 2.82                     | 0.47              |
| 2:F:41:MET:HE1   | 2:F:73:LYS:HD2   | 1.95                     | 0.47              |
| 2:H:97:PRO:HD3   | 2:H:181:TYR:CD1  | 2.48                     | 0.47              |
| 1:A:228:LEU:HD21 | 1:A:233:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:318:TYR:N    | 1:A:318:TYR:CD1  | 2.82                     | 0.47              |
| 1:A:342:TYR:HB3  | 1:A:348:ASN:CB   | 2.44                     | 0.47              |
| 1:A:390:LYS:HB3  | 1:A:417:VAL:HG21 | 1.96                     | 0.47              |
| 1:C:228:LEU:HD21 | 1:C:233:GLU:HG2  | 1.96                     | 0.47              |
| 1:C:23:GLN:HG2   | 1:C:59:PRO:HA    | 1.97                     | 0.47              |
| 1:C:354:TYR:CZ   | 1:C:356:ARG:HD3  | 2.49                     | 0.47              |
| 2:F:56:TYR:O     | 2:F:143:ARG:NH2  | 2.48                     | 0.47              |
| 2:F:64:LYS:HB2   | 2:F:71:TRP:CZ3   | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:23:GLN:HG2   | 1:G:59:PRO:HA    | 1.97                     | 0.47              |
| 1:G:46:LYS:HG3   | 1:G:116:PHE:CD2  | 2.50                     | 0.47              |
| 2:H:56:TYR:O     | 2:H:143:ARG:NH2  | 2.48                     | 0.47              |
| 2:H:268:SER:HA   | 2:H:274:ILE:CG2  | 2.43                     | 0.47              |
| 2:H:24:TRP:HZ3   | 2:H:61:PHE:HB3   | 1.76                     | 0.47              |
| 2:H:64:LYS:HB2   | 2:H:71:TRP:CZ3   | 2.50                     | 0.47              |
| 1:A:336:GLN:HG2  | 1:A:355:ALA:HB2  | 1.97                     | 0.47              |
| 2:B:336:GLN:HG2  | 2:B:355:ALA:CB   | 2.44                     | 0.47              |
| 1:C:326:ILE:HB   | 1:C:342:TYR:CD1  | 2.50                     | 0.47              |
| 2:D:56:TYR:O     | 2:D:143:ARG:NH2  | 2.48                     | 0.47              |
| 1:E:23:GLN:HG2   | 1:E:59:PRO:HA    | 1.97                     | 0.47              |
| 1:E:442:VAL:HG12 | 1:E:443:ASP:N    | 2.30                     | 0.47              |
| 1:G:326:ILE:HB   | 1:G:342:TYR:CD1  | 2.50                     | 0.47              |
| 1:C:417:VAL:CG2  | 1:G:346:PHE:CD2  | 2.98                     | 0.47              |
| 2:H:52:PRO:HD2   | 2:H:53:GLU:OE1   | 2.14                     | 0.47              |
| 1:A:345:PRO:HG3  | 1:E:326:ILE:CD1  | 2.44                     | 0.47              |
| 1:A:540:LYS:HZ3  | 2:B:261:VAL:HG13 | 1.78                     | 0.47              |
| 1:A:6:GLU:N      | 1:A:6:GLU:CD     | 2.66                     | 0.47              |
| 1:C:442:VAL:HG12 | 1:C:443:ASP:N    | 2.30                     | 0.47              |
| 1:E:132:ILE:HB   | 1:E:142:ILE:HG12 | 1.96                     | 0.47              |
| 1:E:228:LEU:HD21 | 1:E:233:GLU:HG2  | 1.96                     | 0.47              |
| 1:E:337:TRP:CD1  | 1:E:337:TRP:N    | 2.81                     | 0.47              |
| 1:G:102:LYS:CG   | 1:G:318:TYR:HB2  | 2.45                     | 0.47              |
| 1:G:318:TYR:CD1  | 1:G:318:TYR:N    | 2.82                     | 0.47              |
| 1:G:390:LYS:HB3  | 1:G:417:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:442:VAL:HG12 | 1:A:443:ASP:N    | 2.30                     | 0.47              |
| 2:B:158:ALA:O    | 2:B:161:GLN:HB2  | 2.15                     | 0.47              |
| 2:D:64:LYS:HB2   | 2:D:71:TRP:CZ3   | 2.50                     | 0.47              |
| 1:E:20:LYS:HG2   | 1:E:56:TYR:HA    | 1.96                     | 0.47              |
| 1:E:354:TYR:CZ   | 1:E:356:ARG:HD3  | 2.49                     | 0.47              |
| 1:G:228:LEU:HD21 | 1:G:233:GLU:HG2  | 1.96                     | 0.47              |
| 1:G:78:ARG:NH1   | 1:G:287:LYS:O    | 2.39                     | 0.47              |
| 1:C:121:ASP:O    | 1:C:125:ARG:HG3  | 2.15                     | 0.47              |
| 1:C:191:SER:OG   | 1:C:198:HIS:HD2  | 1.98                     | 0.47              |
| 1:C:20:LYS:HG2   | 1:C:56:TYR:HA    | 1.96                     | 0.47              |
| 1:C:318:TYR:N    | 1:C:318:TYR:CD1  | 2.82                     | 0.47              |
| 1:C:342:TYR:HB3  | 1:C:348:ASN:CB   | 2.44                     | 0.47              |
| 1:C:391:LEU:HA   | 1:C:392:PRO:HD3  | 1.72                     | 0.47              |
| 1:C:6:GLU:N      | 1:C:6:GLU:CD     | 2.66                     | 0.47              |
| 2:D:64:LYS:HB2   | 2:D:71:TRP:CE3   | 2.50                     | 0.47              |
| 1:E:390:LYS:HB3  | 1:E:417:VAL:HG21 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:416:PHE:HD1  | 1:E:417:VAL:H    | 1.61                     | 0.47              |
| 2:F:24:TRP:HZ3   | 2:F:61:PHE:CB    | 2.28                     | 0.47              |
| 2:H:276:VAL:HG12 | 2:H:279:LEU:HD12 | 1.97                     | 0.47              |
| 1:A:102:LYS:CG   | 1:A:318:TYR:HB2  | 2.45                     | 0.47              |
| 1:A:33:ALA:O     | 1:A:36:GLU:HB3   | 2.15                     | 0.47              |
| 1:A:326:ILE:HB   | 1:A:342:TYR:CD1  | 2.50                     | 0.47              |
| 2:B:64:LYS:HB2   | 2:B:71:TRP:CZ3   | 2.50                     | 0.47              |
| 1:C:336:GLN:HG2  | 1:C:355:ALA:HB2  | 1.97                     | 0.47              |
| 2:D:158:ALA:O    | 2:D:161:GLN:HB2  | 2.15                     | 0.47              |
| 2:D:330:GLN:HG3  | 2:D:419:THR:HG21 | 1.96                     | 0.47              |
| 1:E:537:PRO:HB2  | 1:E:540:LYS:HD2  | 1.97                     | 0.47              |
| 2:F:108:VAL:HA   | 2:F:187:LEU:O    | 2.15                     | 0.47              |
| 2:F:52:PRO:HD2   | 2:F:53:GLU:OE1   | 2.14                     | 0.47              |
| 1:G:96:HIS:CG    | 1:G:97:PRO:HD2   | 2.49                     | 0.47              |
| 1:A:191:SER:OG   | 1:A:198:HIS:HD2  | 1.98                     | 0.46              |
| 2:B:56:TYR:O     | 2:B:143:ARG:NH2  | 2.48                     | 0.46              |
| 2:B:55:PRO:HG2   | 2:B:56:TYR:CD2   | 2.51                     | 0.46              |
| 1:C:510:PRO:O    | 1:C:522:ILE:HD13 | 2.14                     | 0.46              |
| 2:D:108:VAL:HA   | 2:D:187:LEU:O    | 2.15                     | 0.46              |
| 1:E:437:ALA:HB1  | 1:E:493:VAL:HA   | 1.97                     | 0.46              |
| 2:F:135:ILE:H    | 2:F:135:ILE:HG12 | 1.38                     | 0.46              |
| 2:F:345:PRO:O    | 2:F:346:PHE:HB2  | 2.15                     | 0.46              |
| 1:G:33:ALA:O     | 1:G:36:GLU:HB3   | 2.15                     | 0.46              |
| 1:G:442:VAL:HG12 | 1:G:443:ASP:N    | 2.30                     | 0.46              |
| 2:H:55:PRO:HG2   | 2:H:56:TYR:CD2   | 2.51                     | 0.46              |
| 1:A:121:ASP:O    | 1:A:125:ARG:HG3  | 2.15                     | 0.46              |
| 2:B:108:VAL:HA   | 2:B:187:LEU:O    | 2.15                     | 0.46              |
| 1:C:304:ALA:HA   | 1:C:307:ARG:HD2  | 1.96                     | 0.46              |
| 2:D:55:PRO:HG2   | 2:D:56:TYR:CD2   | 2.51                     | 0.46              |
| 2:F:64:LYS:HB2   | 2:F:71:TRP:CE3   | 2.50                     | 0.46              |
| 1:G:121:ASP:O    | 1:G:125:ARG:HG3  | 2.15                     | 0.46              |
| 1:G:248:GLU:CG   | 1:G:307:ARG:HH21 | 2.28                     | 0.46              |
| 1:G:240:THR:HG22 | 1:G:315:HIS:HB3  | 1.97                     | 0.46              |
| 1:C:346:PHE:CB   | 1:G:390:LYS:HZ1  | 1.98                     | 0.46              |
| 1:A:503:LEU:O    | 1:A:507:GLN:HG2  | 2.16                     | 0.46              |
| 1:C:337:TRP:N    | 1:C:337:TRP:CD1  | 2.81                     | 0.46              |
| 1:C:33:ALA:O     | 1:C:36:GLU:HB3   | 2.15                     | 0.46              |
| 1:C:503:LEU:O    | 1:C:507:GLN:HG2  | 2.16                     | 0.46              |
| 1:E:248:GLU:CG   | 1:E:307:ARG:HH21 | 2.28                     | 0.46              |
| 1:E:326:ILE:HB   | 1:E:342:TYR:CD1  | 2.50                     | 0.46              |
| 1:E:33:ALA:O     | 1:E:36:GLU:HB3   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:342:TYR:HB3  | 1:G:348:ASN:CB   | 2.44                     | 0.46              |
| 2:H:108:VAL:HA   | 2:H:187:LEU:O    | 2.15                     | 0.46              |
| 1:A:102:LYS:HG3  | 1:A:318:TYR:HB2  | 1.97                     | 0.46              |
| 1:A:398:TRP:CZ3  | 1:A:411:ILE:HD11 | 2.51                     | 0.46              |
| 2:B:276:VAL:HG12 | 2:B:279:LEU:HD12 | 1.98                     | 0.46              |
| 2:F:259:LYS:HE3  | 2:F:263:LYS:NZ   | 2.30                     | 0.46              |
| 2:F:330:GLN:HG3  | 2:F:419:THR:HG21 | 1.96                     | 0.46              |
| 1:G:191:SER:OG   | 1:G:198:HIS:HD2  | 1.99                     | 0.46              |
| 2:H:64:LYS:HB2   | 2:H:71:TRP:CE3   | 2.50                     | 0.46              |
| 1:A:537:PRO:HB2  | 1:A:540:LYS:HD2  | 1.97                     | 0.46              |
| 2:D:24:TRP:HZ3   | 2:D:61:PHE:CB    | 2.28                     | 0.46              |
| 1:E:115:TYR:CE2  | 1:E:156:SER:HB3  | 2.51                     | 0.46              |
| 1:E:516:GLU:O    | 1:E:520:GLN:HG2  | 2.15                     | 0.46              |
| 1:G:229:TRP:CZ3  | 1:G:230:MET:HE1  | 2.51                     | 0.46              |
| 1:G:304:ALA:HA   | 1:G:307:ARG:HD2  | 1.96                     | 0.46              |
| 1:G:451:LYS:O    | 1:G:452:LEU:HD23 | 2.15                     | 0.46              |
| 2:H:330:GLN:HG3  | 2:H:419:THR:HG21 | 1.96                     | 0.46              |
| 1:A:118:VAL:C    | 1:A:148:VAL:HG13 | 2.36                     | 0.46              |
| 1:E:240:THR:HG22 | 1:E:315:HIS:HB3  | 1.97                     | 0.46              |
| 1:E:451:LYS:O    | 1:E:452:LEU:HD23 | 2.15                     | 0.46              |
| 1:E:540:LYS:NZ   | 2:F:261:VAL:HG12 | 2.31                     | 0.46              |
| 1:E:6:GLU:CD     | 1:E:6:GLU:N      | 2.66                     | 0.46              |
| 1:E:59:PRO:HG2   | 1:E:76:ASP:HB3   | 1.98                     | 0.46              |
| 2:F:55:PRO:HG2   | 2:F:56:TYR:CD2   | 2.51                     | 0.46              |
| 2:H:345:PRO:O    | 2:H:346:PHE:HB2  | 2.15                     | 0.46              |
| 2:B:259:LYS:HE3  | 2:B:263:LYS:NZ   | 2.30                     | 0.46              |
| 2:B:345:PRO:O    | 2:B:346:PHE:HB2  | 2.15                     | 0.46              |
| 1:C:102:LYS:CG   | 1:C:318:TYR:HB2  | 2.45                     | 0.46              |
| 1:C:451:LYS:O    | 1:C:452:LEU:HD23 | 2.15                     | 0.46              |
| 1:C:91:GLN:HE21  | 1:C:91:GLN:CA    | 2.21                     | 0.46              |
| 2:D:276:VAL:HG12 | 2:D:279:LEU:HD12 | 1.98                     | 0.46              |
| 1:E:121:ASP:O    | 1:E:125:ARG:HG3  | 2.15                     | 0.46              |
| 2:F:276:VAL:HG12 | 2:F:279:LEU:HD12 | 1.98                     | 0.46              |
| 1:G:342:TYR:HD1  | 1:G:342:TYR:C    | 2.19                     | 0.46              |
| 1:G:59:PRO:HG2   | 1:G:76:ASP:HB3   | 1.98                     | 0.46              |
| 2:H:259:LYS:HE3  | 2:H:263:LYS:NZ   | 2.30                     | 0.46              |
| 1:A:451:LYS:O    | 1:A:452:LEU:HD23 | 2.15                     | 0.46              |
| 1:A:516:GLU:O    | 1:A:520:GLN:HG2  | 2.15                     | 0.46              |
| 1:A:540:LYS:NZ   | 2:B:261:VAL:HG12 | 2.31                     | 0.46              |
| 2:B:72:ARG:HH22  | 2:B:409:THR:HB   | 1.81                     | 0.46              |
| 1:C:241:VAL:HB   | 1:C:314:VAL:HG22 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:342:TYR:HD1  | 1:C:342:TYR:C    | 2.19                     | 0.46              |
| 2:D:259:LYS:HE3  | 2:D:263:LYS:NZ   | 2.30                     | 0.46              |
| 1:E:342:TYR:HD1  | 1:E:342:TYR:C    | 2.19                     | 0.46              |
| 1:G:398:TRP:CZ3  | 1:G:411:ILE:HD11 | 2.51                     | 0.46              |
| 1:G:46:LYS:HG3   | 1:G:116:PHE:HD2  | 1.81                     | 0.46              |
| 2:H:135:ILE:C    | 2:H:137:ASN:H    | 2.20                     | 0.46              |
| 2:H:10:VAL:HG11  | 2:H:153:TRP:HH2  | 1.81                     | 0.46              |
| 1:A:115:TYR:CE2  | 1:A:156:SER:HB3  | 2.51                     | 0.46              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:NZ   | 2.64                     | 0.46              |
| 1:A:241:VAL:HB   | 1:A:314:VAL:HG22 | 1.98                     | 0.46              |
| 1:A:342:TYR:HD1  | 1:A:342:TYR:C    | 2.19                     | 0.46              |
| 1:A:59:PRO:HG2   | 1:A:76:ASP:HB3   | 1.98                     | 0.46              |
| 1:A:91:GLN:CA    | 1:A:91:GLN:HE21  | 2.22                     | 0.46              |
| 2:B:297:GLU:HA   | 2:B:300:GLU:HB3  | 1.98                     | 0.46              |
| 2:B:365:VAL:HG12 | 2:B:405:TYR:HE2  | 1.80                     | 0.46              |
| 1:C:118:VAL:C    | 1:C:148:VAL:HG13 | 2.36                     | 0.46              |
| 1:C:148:VAL:HG12 | 1:C:149:LEU:N    | 2.31                     | 0.46              |
| 1:C:175:ASN:ND2  | 1:C:201:LYS:NZ   | 2.64                     | 0.46              |
| 1:C:417:VAL:HG22 | 1:G:346:PHE:CD2  | 2.51                     | 0.46              |
| 2:D:297:GLU:HA   | 2:D:300:GLU:HB3  | 1.98                     | 0.46              |
| 2:D:72:ARG:HH22  | 2:D:409:THR:HB   | 1.81                     | 0.46              |
| 1:E:102:LYS:HG3  | 1:E:318:TYR:HB2  | 1.97                     | 0.46              |
| 1:E:398:TRP:CZ3  | 1:E:411:ILE:HD11 | 2.51                     | 0.46              |
| 1:E:46:LYS:HG3   | 1:E:116:PHE:CD2  | 2.50                     | 0.46              |
| 1:G:102:LYS:HG3  | 1:G:318:TYR:HB2  | 1.97                     | 0.46              |
| 1:G:540:LYS:NZ   | 2:H:261:VAL:HG12 | 2.31                     | 0.46              |
| 1:A:116:PHE:C    | 1:A:148:VAL:HG11 | 2.37                     | 0.46              |
| 1:C:102:LYS:HG3  | 1:C:318:TYR:HB2  | 1.97                     | 0.46              |
| 1:C:398:TRP:CZ3  | 1:C:411:ILE:HD11 | 2.51                     | 0.46              |
| 1:C:537:PRO:HB2  | 1:C:540:LYS:HD2  | 1.97                     | 0.46              |
| 1:E:175:ASN:ND2  | 1:E:201:LYS:NZ   | 2.64                     | 0.46              |
| 1:E:229:TRP:CZ3  | 1:E:230:MET:HE1  | 2.51                     | 0.46              |
| 2:F:135:ILE:C    | 2:F:137:ASN:H    | 2.19                     | 0.46              |
| 2:F:103:LYS:HZ1  | 2:F:179:VAL:HG23 | 1.80                     | 0.46              |
| 2:F:390:LYS:HA   | 2:F:415:GLU:O    | 2.17                     | 0.46              |
| 1:G:118:VAL:C    | 1:G:148:VAL:HG13 | 2.36                     | 0.46              |
| 1:G:125:ARG:O    | 1:G:126:LYS:C    | 2.55                     | 0.46              |
| 1:G:20:LYS:HG2   | 1:G:56:TYR:HA    | 1.96                     | 0.46              |
| 2:B:135:ILE:C    | 2:B:137:ASN:H    | 2.19                     | 0.45              |
| 2:B:390:LYS:HA   | 2:B:415:GLU:O    | 2.17                     | 0.45              |
| 2:B:330:GLN:HG3  | 2:B:419:THR:HG21 | 1.96                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:TRP:HZ3   | 2:B:61:PHE:CB    | 2.28                     | 0.45              |
| 2:D:171:PHE:HA   | 2:D:174:GLN:HB3  | 1.98                     | 0.45              |
| 2:D:345:PRO:O    | 2:D:346:PHE:HB2  | 2.15                     | 0.45              |
| 1:E:125:ARG:O    | 1:E:126:LYS:C    | 2.55                     | 0.45              |
| 1:E:342:TYR:HB3  | 1:E:348:ASN:CB   | 2.44                     | 0.45              |
| 2:F:96:HIS:CD2   | 2:F:384:GLY:HA3  | 2.51                     | 0.45              |
| 1:G:115:TYR:CE2  | 1:G:156:SER:HB3  | 2.51                     | 0.45              |
| 2:H:171:PHE:HA   | 2:H:174:GLN:HB3  | 1.98                     | 0.45              |
| 1:A:437:ALA:HB1  | 1:A:493:VAL:HA   | 1.97                     | 0.45              |
| 2:B:116:PHE:CZ   | 2:B:151:GLN:HG2  | 2.52                     | 0.45              |
| 2:B:24:TRP:HZ3   | 2:B:61:PHE:HB3   | 1.76                     | 0.45              |
| 1:C:116:PHE:C    | 1:C:148:VAL:HG11 | 2.37                     | 0.45              |
| 1:C:115:TYR:CE2  | 1:C:156:SER:HB3  | 2.51                     | 0.45              |
| 1:C:34:LEU:HD21  | 1:C:62:ALA:HB2   | 1.98                     | 0.45              |
| 1:C:437:ALA:HB1  | 1:C:493:VAL:HA   | 1.97                     | 0.45              |
| 1:E:46:LYS:HG3   | 1:E:116:PHE:HD2  | 1.81                     | 0.45              |
| 1:G:437:ALA:HB1  | 1:G:493:VAL:HA   | 1.97                     | 0.45              |
| 1:G:516:GLU:O    | 1:G:520:GLN:HG2  | 2.15                     | 0.45              |
| 1:G:540:LYS:HZ3  | 2:H:261:VAL:HG13 | 1.81                     | 0.45              |
| 1:G:6:GLU:CD     | 1:G:6:GLU:N      | 2.66                     | 0.45              |
| 2:H:96:HIS:CD2   | 2:H:384:GLY:HA3  | 2.51                     | 0.45              |
| 1:A:445:ALA:O    | 1:A:453:GLY:HA3  | 2.16                     | 0.45              |
| 2:B:171:PHE:HA   | 2:B:174:GLN:HB3  | 1.98                     | 0.45              |
| 1:C:240:THR:HG22 | 1:C:315:HIS:HB3  | 1.97                     | 0.45              |
| 1:C:59:PRO:HG2   | 1:C:76:ASP:HB3   | 1.98                     | 0.45              |
| 2:D:116:PHE:CZ   | 2:D:151:GLN:HG2  | 2.52                     | 0.45              |
| 1:E:118:VAL:C    | 1:E:148:VAL:HG13 | 2.36                     | 0.45              |
| 1:E:361:HIS:CD2  | 1:E:505:ILE:HG23 | 2.52                     | 0.45              |
| 2:F:171:PHE:CZ   | 2:F:205:LEU:HB2  | 2.51                     | 0.45              |
| 1:G:115:TYR:O    | 1:G:117:SER:N    | 2.50                     | 0.45              |
| 1:G:175:ASN:ND2  | 1:G:201:LYS:NZ   | 2.64                     | 0.45              |
| 1:A:95:PRO:HG2   | 1:A:230:MET:CE   | 2.47                     | 0.45              |
| 1:A:240:THR:HG22 | 1:A:315:HIS:HB3  | 1.97                     | 0.45              |
| 2:B:96:HIS:CD2   | 2:B:384:GLY:HA3  | 2.51                     | 0.45              |
| 1:C:329:ILE:HA   | 1:C:338:THR:O    | 2.17                     | 0.45              |
| 1:C:345:PRO:HG2  | 1:G:326:ILE:HD11 | 1.84                     | 0.45              |
| 1:C:445:ALA:O    | 1:C:453:GLY:HA3  | 2.16                     | 0.45              |
| 1:C:361:HIS:CD2  | 1:C:505:ILE:HG23 | 2.52                     | 0.45              |
| 2:D:10:VAL:HG11  | 2:D:153:TRP:HH2  | 1.81                     | 0.45              |
| 2:D:171:PHE:CZ   | 2:D:205:LEU:HB2  | 2.51                     | 0.45              |
| 2:D:96:HIS:CD2   | 2:D:384:GLY:HA3  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:326:ILE:CB   | 1:G:342:TYR:HE1  | 2.28                     | 0.45              |
| 1:G:445:ALA:O    | 1:G:453:GLY:HA3  | 2.16                     | 0.45              |
| 1:G:361:HIS:CD2  | 1:G:505:ILE:HG23 | 2.52                     | 0.45              |
| 1:G:537:PRO:HB2  | 1:G:540:LYS:HD2  | 1.97                     | 0.45              |
| 2:H:24:TRP:HZ3   | 2:H:61:PHE:CB    | 2.28                     | 0.45              |
| 1:A:361:HIS:CD2  | 1:A:505:ILE:HG23 | 2.52                     | 0.45              |
| 2:B:171:PHE:CZ   | 2:B:205:LEU:HB2  | 2.51                     | 0.45              |
| 1:C:115:TYR:O    | 1:C:117:SER:N    | 2.50                     | 0.45              |
| 1:C:53:GLU:CD    | 1:C:53:GLU:H     | 2.20                     | 0.45              |
| 2:D:390:LYS:HA   | 2:D:415:GLU:O    | 2.16                     | 0.45              |
| 1:E:445:ALA:O    | 1:E:453:GLY:HA3  | 2.16                     | 0.45              |
| 1:E:503:LEU:O    | 1:E:507:GLN:HG2  | 2.16                     | 0.45              |
| 2:F:10:VAL:HG11  | 2:F:153:TRP:HH2  | 1.81                     | 0.45              |
| 2:F:116:PHE:CZ   | 2:F:151:GLN:HG2  | 2.52                     | 0.45              |
| 2:F:255:ASN:HA   | 2:F:258:GLN:HB2  | 1.98                     | 0.45              |
| 1:G:53:GLU:CD    | 1:G:53:GLU:H     | 2.20                     | 0.45              |
| 2:H:116:PHE:CZ   | 2:H:151:GLN:HG2  | 2.52                     | 0.45              |
| 1:A:329:ILE:HA   | 1:A:338:THR:O    | 2.17                     | 0.45              |
| 1:A:46:LYS:HG3   | 1:A:116:PHE:HD2  | 1.81                     | 0.45              |
| 1:A:34:LEU:HD21  | 1:A:62:ALA:HB2   | 1.99                     | 0.45              |
| 2:B:195:ILE:O    | 2:B:199:ARG:HG3  | 2.17                     | 0.45              |
| 2:D:135:ILE:C    | 2:D:137:ASN:H    | 2.20                     | 0.45              |
| 1:G:116:PHE:C    | 1:G:148:VAL:HG11 | 2.37                     | 0.45              |
| 1:G:95:PRO:HG2   | 1:G:230:MET:CE   | 2.47                     | 0.45              |
| 1:G:503:LEU:O    | 1:G:507:GLN:HG2  | 2.16                     | 0.45              |
| 1:G:546:GLU:O    | 1:G:549:ASP:HB3  | 2.17                     | 0.45              |
| 2:H:195:ILE:O    | 2:H:199:ARG:HG3  | 2.17                     | 0.45              |
| 1:A:148:VAL:HG12 | 1:A:149:LEU:N    | 2.31                     | 0.45              |
| 1:A:85:GLN:O     | 1:A:85:GLN:CG    | 2.55                     | 0.45              |
| 2:D:195:ILE:O    | 2:D:199:ARG:HG3  | 2.17                     | 0.45              |
| 1:E:191:SER:OG   | 1:E:198:HIS:HD2  | 1.98                     | 0.45              |
| 1:G:241:VAL:HB   | 1:G:314:VAL:HG22 | 1.98                     | 0.45              |
| 1:G:327:ALA:HA   | 1:G:340:GLN:O    | 2.17                     | 0.45              |
| 2:H:135:ILE:H    | 2:H:135:ILE:HG12 | 1.38                     | 0.45              |
| 2:H:171:PHE:CZ   | 2:H:205:LEU:HB2  | 2.51                     | 0.45              |
| 2:H:259:LYS:HE3  | 2:H:263:LYS:HZ1  | 1.81                     | 0.45              |
| 1:A:410:TRP:HZ3  | 2:B:401:TRP:CZ2  | 2.35                     | 0.45              |
| 2:B:10:VAL:HG11  | 2:B:153:TRP:HH2  | 1.81                     | 0.45              |
| 2:B:120:LEU:O    | 2:B:125:ARG:CZ   | 2.65                     | 0.45              |
| 1:C:248:GLU:CG   | 1:C:307:ARG:HH21 | 2.28                     | 0.45              |
| 1:C:516:GLU:O    | 1:C:520:GLN:HG2  | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:57:ASN:OD1   | 1:E:130:PHE:HA   | 2.17                     | 0.45              |
| 1:E:95:PRO:HG2   | 1:E:230:MET:CE   | 2.47                     | 0.45              |
| 2:F:297:GLU:HA   | 2:F:300:GLU:HB3  | 1.98                     | 0.45              |
| 2:H:193:LEU:CD1  | 2:H:201:LYS:HG3  | 2.47                     | 0.45              |
| 2:H:104:LYS:HZ3  | 2:H:194:GLU:HA   | 1.80                     | 0.45              |
| 2:H:390:LYS:HA   | 2:H:415:GLU:O    | 2.16                     | 0.45              |
| 2:H:390:LYS:HG2  | 2:H:415:GLU:OE1  | 2.17                     | 0.45              |
| 2:H:41:MET:HE1   | 2:H:73:LYS:HD2   | 1.98                     | 0.45              |
| 1:A:248:GLU:CG   | 1:A:307:ARG:HH21 | 2.28                     | 0.45              |
| 1:A:53:GLU:H     | 1:A:53:GLU:CD    | 2.20                     | 0.45              |
| 2:B:207:GLN:O    | 2:B:208:HIS:C    | 2.56                     | 0.45              |
| 1:C:125:ARG:O    | 1:C:126:LYS:C    | 2.55                     | 0.45              |
| 1:C:95:PRO:HG2   | 1:C:230:MET:CE   | 2.47                     | 0.45              |
| 1:C:78:ARG:NH1   | 1:C:287:LYS:O    | 2.39                     | 0.45              |
| 2:D:108:VAL:HG11 | 2:D:188:TYR:CE2  | 2.52                     | 0.45              |
| 2:D:365:VAL:HG12 | 2:D:405:TYR:HE2  | 1.80                     | 0.45              |
| 2:D:376:THR:HG22 | 2:D:389:PHE:HE1  | 1.80                     | 0.45              |
| 1:C:410:TRP:HZ3  | 2:D:401:TRP:CZ2  | 2.35                     | 0.45              |
| 2:F:241:VAL:O    | 2:F:243:PRO:HD3  | 2.17                     | 0.45              |
| 2:F:72:ARG:HH22  | 2:F:409:THR:HB   | 1.81                     | 0.45              |
| 1:G:57:ASN:OD1   | 1:G:130:PHE:HA   | 2.17                     | 0.45              |
| 2:H:72:ARG:HH22  | 2:H:409:THR:HB   | 1.81                     | 0.45              |
| 1:A:115:TYR:O    | 1:A:117:SER:N    | 2.50                     | 0.45              |
| 2:B:104:LYS:HZ1  | 2:B:194:GLU:HA   | 1.82                     | 0.45              |
| 1:C:326:ILE:CB   | 1:C:342:TYR:HE1  | 2.28                     | 0.45              |
| 1:C:440:PHE:CE2  | 1:C:457:TYR:CE2  | 3.05                     | 0.45              |
| 1:C:46:LYS:HG3   | 1:C:116:PHE:HD2  | 1.81                     | 0.45              |
| 2:D:120:LEU:O    | 2:D:125:ARG:CZ   | 2.65                     | 0.45              |
| 2:D:78:ARG:O     | 2:D:82:LYS:HG3   | 2.17                     | 0.45              |
| 1:E:326:ILE:CB   | 1:E:342:TYR:HE1  | 2.28                     | 0.45              |
| 1:E:442:VAL:HG12 | 1:E:481:ALA:CB   | 2.46                     | 0.45              |
| 1:E:54:ASN:HA    | 1:E:55:PRO:HD3   | 1.78                     | 0.45              |
| 2:F:195:ILE:O    | 2:F:199:ARG:HG3  | 2.17                     | 0.45              |
| 1:G:167:ILE:O    | 1:G:208:HIS:CE1  | 2.66                     | 0.45              |
| 1:G:329:ILE:HA   | 1:G:338:THR:O    | 2.17                     | 0.45              |
| 1:G:34:LEU:HD21  | 1:G:62:ALA:HB2   | 1.99                     | 0.45              |
| 1:A:440:PHE:CE2  | 1:A:457:TYR:CE2  | 3.05                     | 0.44              |
| 1:A:546:GLU:O    | 1:A:549:ASP:HB3  | 2.17                     | 0.44              |
| 2:B:108:VAL:HG11 | 2:B:188:TYR:CE2  | 2.52                     | 0.44              |
| 1:C:10:VAL:HG11  | 1:C:153:TRP:CZ2  | 2.52                     | 0.44              |
| 2:D:193:LEU:CD1  | 2:D:201:LYS:HG3  | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:10:VAL:HG11  | 1:E:153:TRP:CZ2  | 2.52                     | 0.44              |
| 2:F:120:LEU:O    | 2:F:125:ARG:CZ   | 2.65                     | 0.44              |
| 2:F:78:ARG:O     | 2:F:82:LYS:HG3   | 2.17                     | 0.44              |
| 1:G:410:TRP:HZ3  | 2:H:401:TRP:CZ2  | 2.35                     | 0.44              |
| 2:H:241:VAL:O    | 2:H:243:PRO:HD3  | 2.17                     | 0.44              |
| 1:A:160:PHE:CZ   | 1:A:164:MET:CG   | 3.01                     | 0.44              |
| 1:A:229:TRP:CH2  | 1:A:230:MET:CE   | 3.01                     | 0.44              |
| 1:A:78:ARG:NH1   | 1:A:287:LYS:O    | 2.39                     | 0.44              |
| 1:A:379:SER:HB3  | 1:A:383:TRP:HD1  | 1.82                     | 0.44              |
| 1:A:439:THR:HG22 | 1:A:441:TYR:HE1  | 1.82                     | 0.44              |
| 1:A:57:ASN:OD1   | 1:A:130:PHE:HA   | 2.17                     | 0.44              |
| 2:B:162:SER:O    | 2:B:166:LYS:HG2  | 2.17                     | 0.44              |
| 2:B:193:LEU:CD1  | 2:B:201:LYS:HG3  | 2.47                     | 0.44              |
| 2:B:390:LYS:HG2  | 2:B:415:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:379:SER:HB3  | 1:C:383:TRP:HD1  | 1.83                     | 0.44              |
| 2:D:255:ASN:HA   | 2:D:258:GLN:HB2  | 1.99                     | 0.44              |
| 1:E:329:ILE:HA   | 1:E:338:THR:O    | 2.17                     | 0.44              |
| 2:F:171:PHE:HA   | 2:F:174:GLN:HB3  | 1.98                     | 0.44              |
| 2:F:292:VAL:HG12 | 2:F:293:ILE:N    | 2.33                     | 0.44              |
| 1:G:160:PHE:CZ   | 1:G:164:MET:CG   | 3.01                     | 0.44              |
| 2:H:297:GLU:HA   | 2:H:300:GLU:HB3  | 1.98                     | 0.44              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:CZ2  | 2.52                     | 0.44              |
| 1:C:540:LYS:NZ   | 2:D:261:VAL:HG12 | 2.31                     | 0.44              |
| 1:C:546:GLU:O    | 1:C:549:ASP:HB3  | 2.17                     | 0.44              |
| 1:E:546:GLU:O    | 1:E:549:ASP:HB3  | 2.17                     | 0.44              |
| 2:F:100:LEU:HA   | 2:F:100:LEU:HD23 | 1.81                     | 0.44              |
| 2:F:390:LYS:HG2  | 2:F:415:GLU:OE1  | 2.17                     | 0.44              |
| 1:A:327:ALA:HA   | 1:A:340:GLN:O    | 2.17                     | 0.44              |
| 2:B:78:ARG:O     | 2:B:82:LYS:HG3   | 2.17                     | 0.44              |
| 1:E:115:TYR:O    | 1:E:117:SER:N    | 2.50                     | 0.44              |
| 1:E:148:VAL:HG12 | 1:E:149:LEU:N    | 2.31                     | 0.44              |
| 1:E:327:ALA:HA   | 1:E:340:GLN:O    | 2.17                     | 0.44              |
| 1:E:379:SER:HB3  | 1:E:383:TRP:HD1  | 1.83                     | 0.44              |
| 2:F:108:VAL:HG11 | 2:F:188:TYR:CE2  | 2.53                     | 0.44              |
| 2:B:157:PRO:CG   | 2:B:158:ALA:N    | 2.79                     | 0.44              |
| 1:C:327:ALA:HA   | 1:C:340:GLN:O    | 2.17                     | 0.44              |
| 1:C:451:LYS:O    | 1:C:471:ASN:N    | 2.51                     | 0.44              |
| 1:C:57:ASN:OD1   | 1:C:130:PHE:HA   | 2.17                     | 0.44              |
| 1:E:116:PHE:C    | 1:E:148:VAL:HG11 | 2.37                     | 0.44              |
| 1:E:160:PHE:CZ   | 1:E:164:MET:CG   | 3.01                     | 0.44              |
| 1:E:241:VAL:HB   | 1:E:314:VAL:HG22 | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:53:GLU:CD    | 1:E:53:GLU:H     | 2.20                     | 0.44              |
| 1:E:441:TYR:O    | 1:E:548:VAL:HG21 | 2.18                     | 0.44              |
| 1:E:410:TRP:HZ3  | 2:F:401:TRP:CZ2  | 2.35                     | 0.44              |
| 1:G:412:PRO:HG2  | 1:G:413:GLU:H    | 1.83                     | 0.44              |
| 1:G:451:LYS:O    | 1:G:471:ASN:N    | 2.51                     | 0.44              |
| 2:H:78:ARG:O     | 2:H:82:LYS:HG3   | 2.17                     | 0.44              |
| 1:A:125:ARG:O    | 1:A:126:LYS:C    | 2.55                     | 0.44              |
| 1:A:451:LYS:O    | 1:A:471:ASN:N    | 2.51                     | 0.44              |
| 2:B:292:VAL:HG12 | 2:B:293:ILE:N    | 2.33                     | 0.44              |
| 1:C:229:TRP:CH2  | 1:C:230:MET:CE   | 3.01                     | 0.44              |
| 2:D:157:PRO:CG   | 2:D:158:ALA:N    | 2.79                     | 0.44              |
| 2:D:162:SER:O    | 2:D:166:LYS:HG2  | 2.17                     | 0.44              |
| 2:D:104:LYS:HZ1  | 2:D:194:GLU:HA   | 1.82                     | 0.44              |
| 2:D:292:VAL:HG12 | 2:D:293:ILE:N    | 2.33                     | 0.44              |
| 2:D:390:LYS:HG2  | 2:D:415:GLU:OE1  | 2.17                     | 0.44              |
| 2:F:395:LYS:HG3  | 2:F:416:PHE:HE2  | 1.78                     | 0.44              |
| 2:H:292:VAL:HG12 | 2:H:293:ILE:N    | 2.33                     | 0.44              |
| 2:H:354:TYR:CE1  | 2:H:374:LYS:HD3  | 2.53                     | 0.44              |
| 1:A:326:ILE:CB   | 1:A:342:TYR:HE1  | 2.28                     | 0.44              |
| 2:B:255:ASN:HA   | 2:B:258:GLN:HB2  | 1.99                     | 0.44              |
| 1:C:160:PHE:CZ   | 1:C:164:MET:CG   | 3.00                     | 0.44              |
| 1:C:417:VAL:HG21 | 1:G:346:PHE:CG   | 2.53                     | 0.44              |
| 2:D:47:ILE:HG22  | 2:D:48:SER:N     | 2.30                     | 0.44              |
| 1:E:540:LYS:C    | 1:E:542:ILE:H    | 2.20                     | 0.44              |
| 1:G:229:TRP:CH2  | 1:G:230:MET:CE   | 3.01                     | 0.44              |
| 1:G:379:SER:HB3  | 1:G:383:TRP:HD1  | 1.83                     | 0.44              |
| 1:G:95:PRO:HG2   | 1:G:230:MET:HE1  | 2.00                     | 0.44              |
| 2:H:120:LEU:O    | 2:H:125:ARG:CZ   | 2.65                     | 0.44              |
| 2:H:162:SER:O    | 2:H:166:LYS:HG2  | 2.17                     | 0.44              |
| 2:H:319:TYR:O    | 2:H:321:PRO:HD3  | 2.18                     | 0.44              |
| 2:B:249:LYS:HB2  | 2:B:252:TRP:CZ2  | 2.52                     | 0.44              |
| 2:B:354:TYR:CE1  | 2:B:374:LYS:HD3  | 2.53                     | 0.44              |
| 2:D:249:LYS:HB2  | 2:D:252:TRP:CZ2  | 2.52                     | 0.44              |
| 2:D:24:TRP:CZ3   | 2:D:61:PHE:CB    | 3.00                     | 0.44              |
| 1:E:540:LYS:HB2  | 1:E:542:ILE:HG13 | 2.00                     | 0.44              |
| 2:F:24:TRP:CZ3   | 2:F:61:PHE:CB    | 3.01                     | 0.44              |
| 2:F:365:VAL:HG12 | 2:F:405:TYR:HE2  | 1.81                     | 0.44              |
| 2:F:376:THR:HG22 | 2:F:389:PHE:HE1  | 1.80                     | 0.44              |
| 2:F:420:PRO:HB2  | 2:F:421:PRO:CD   | 2.42                     | 0.44              |
| 1:G:10:VAL:HG11  | 1:G:153:TRP:CZ2  | 2.53                     | 0.44              |
| 1:G:1:PRO:O      | 1:G:1:PRO:HG2    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:108:VAL:HG11 | 2:H:188:TYR:CE2  | 2.52                     | 0.44              |
| 2:H:255:ASN:HA   | 2:H:258:GLN:HB2  | 1.99                     | 0.44              |
| 1:A:441:TYR:O    | 1:A:548:VAL:HG21 | 2.18                     | 0.44              |
| 2:B:241:VAL:O    | 2:B:243:PRO:HD3  | 2.17                     | 0.44              |
| 2:B:286:THR:HG22 | 2:B:286:THR:O    | 2.18                     | 0.44              |
| 1:C:439:THR:HG22 | 1:C:441:TYR:HE1  | 1.82                     | 0.44              |
| 2:D:286:THR:O    | 2:D:286:THR:HG22 | 2.18                     | 0.44              |
| 1:E:114:ALA:HB1  | 1:E:160:PHE:CE1  | 2.52                     | 0.44              |
| 1:E:440:PHE:CE2  | 1:E:457:TYR:CE2  | 3.05                     | 0.44              |
| 1:E:451:LYS:O    | 1:E:471:ASN:N    | 2.51                     | 0.44              |
| 2:F:38:CYS:SG    | 2:F:132:ILE:HD11 | 2.58                     | 0.44              |
| 1:E:88:TRP:CH2   | 2:F:57:ASN:CB    | 3.01                     | 0.44              |
| 2:B:376:THR:HG22 | 2:B:389:PHE:HE1  | 1.80                     | 0.43              |
| 1:C:336:GLN:C    | 1:C:337:TRP:CD1  | 2.92                     | 0.43              |
| 1:C:363:ASN:OD1  | 1:C:365:VAL:N    | 2.50                     | 0.43              |
| 1:E:412:PRO:HG2  | 1:E:413:GLU:H    | 1.83                     | 0.43              |
| 1:E:543:GLY:C    | 1:E:545:ASN:H    | 2.22                     | 0.43              |
| 1:G:336:GLN:C    | 1:G:337:TRP:CD1  | 2.92                     | 0.43              |
| 1:G:440:PHE:CE2  | 1:G:457:TYR:CE2  | 3.05                     | 0.43              |
| 1:G:441:TYR:O    | 1:G:548:VAL:HG21 | 2.18                     | 0.43              |
| 1:C:441:TYR:O    | 1:C:548:VAL:HG21 | 2.18                     | 0.43              |
| 1:E:336:GLN:HG2  | 1:E:355:ALA:CB   | 2.48                     | 0.43              |
| 2:F:286:THR:HG22 | 2:F:286:THR:O    | 2.18                     | 0.43              |
| 1:G:132:ILE:HD11 | 1:G:144:TYR:CE2  | 2.54                     | 0.43              |
| 1:G:543:GLY:C    | 1:G:545:ASN:H    | 2.22                     | 0.43              |
| 2:H:207:GLN:O    | 2:H:208:HIS:C    | 2.56                     | 0.43              |
| 2:H:286:THR:HG22 | 2:H:286:THR:O    | 2.18                     | 0.43              |
| 1:A:536:VAL:HB   | 1:A:542:ILE:HD13 | 2.01                     | 0.43              |
| 2:B:28:GLU:HG2   | 2:B:32:LYS:HZ2   | 1.84                     | 0.43              |
| 1:C:167:ILE:O    | 1:C:208:HIS:CE1  | 2.66                     | 0.43              |
| 2:D:100:LEU:HA   | 2:D:100:LEU:HD23 | 1.81                     | 0.43              |
| 2:D:319:TYR:O    | 2:D:321:PRO:HD3  | 2.18                     | 0.43              |
| 1:E:368:LEU:HD11 | 1:E:391:LEU:HD22 | 2.00                     | 0.43              |
| 1:E:536:VAL:HB   | 1:E:542:ILE:HD13 | 2.01                     | 0.43              |
| 2:F:193:LEU:CD1  | 2:F:201:LYS:HG3  | 2.47                     | 0.43              |
| 2:F:354:TYR:CE1  | 2:F:374:LYS:HD3  | 2.53                     | 0.43              |
| 1:G:148:VAL:HG12 | 1:G:149:LEU:N    | 2.31                     | 0.43              |
| 1:G:540:LYS:HZ3  | 2:H:276:VAL:HG21 | 1.83                     | 0.43              |
| 2:B:324:ASP:O    | 2:B:343:GLN:HG2  | 2.19                     | 0.43              |
| 2:D:28:GLU:HG2   | 2:D:32:LYS:HZ3   | 1.83                     | 0.43              |
| 2:D:395:LYS:HE2  | 2:D:399:GLU:OE1  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:229:TRP:CH2  | 1:E:230:MET:CE   | 3.01                     | 0.43              |
| 1:E:34:LEU:HD21  | 1:E:62:ALA:HB2   | 1.99                     | 0.43              |
| 1:E:467:VAL:HG12 | 1:E:468:PRO:O    | 2.18                     | 0.43              |
| 2:F:162:SER:O    | 2:F:166:LYS:HG2  | 2.17                     | 0.43              |
| 1:G:540:LYS:HB2  | 1:G:542:ILE:HG13 | 2.00                     | 0.43              |
| 2:H:38:CYS:SG    | 2:H:132:ILE:HD11 | 2.58                     | 0.43              |
| 2:B:319:TYR:O    | 2:B:321:PRO:HD3  | 2.18                     | 0.43              |
| 1:C:320:ASP:HA   | 1:C:321:PRO:HD2  | 1.85                     | 0.43              |
| 2:D:241:VAL:O    | 2:D:243:PRO:HD3  | 2.17                     | 0.43              |
| 2:D:274:ILE:HG13 | 2:D:306:ASN:CG   | 2.39                     | 0.43              |
| 1:E:95:PRO:HG2   | 1:E:230:MET:HE1  | 2.00                     | 0.43              |
| 1:E:336:GLN:C    | 1:E:337:TRP:CD1  | 2.92                     | 0.43              |
| 2:F:207:GLN:O    | 2:F:208:HIS:C    | 2.55                     | 0.43              |
| 2:F:312:GLU:HA   | 2:F:313:PRO:HD3  | 1.72                     | 0.43              |
| 1:G:540:LYS:C    | 1:G:542:ILE:H    | 2.20                     | 0.43              |
| 1:G:88:TRP:CH2   | 2:H:57:ASN:CB    | 3.01                     | 0.43              |
| 2:H:320:ASP:HA   | 2:H:321:PRO:HD3  | 1.84                     | 0.43              |
| 2:H:324:ASP:O    | 2:H:343:GLN:HG2  | 2.19                     | 0.43              |
| 1:A:12:LEU:HD23  | 1:A:124:PHE:HE2  | 1.83                     | 0.43              |
| 1:A:336:GLN:C    | 1:A:337:TRP:CD1  | 2.92                     | 0.43              |
| 1:A:412:PRO:HG2  | 1:A:413:GLU:H    | 1.83                     | 0.43              |
| 2:B:38:CYS:SG    | 2:B:132:ILE:HD11 | 2.58                     | 0.43              |
| 1:A:88:TRP:CH2   | 2:B:57:ASN:CB    | 3.01                     | 0.43              |
| 1:C:188:TYR:HB2  | 1:C:229:TRP:CD1  | 2.54                     | 0.43              |
| 1:C:540:LYS:C    | 1:C:542:ILE:H    | 2.20                     | 0.43              |
| 2:F:324:ASP:O    | 2:F:343:GLN:HG2  | 2.19                     | 0.43              |
| 2:F:395:LYS:HE2  | 2:F:399:GLU:OE1  | 2.18                     | 0.43              |
| 1:G:84:THR:CG2   | 1:G:154:LYS:HE2  | 2.49                     | 0.43              |
| 2:H:91:GLN:CD    | 2:H:94:ILE:HG23  | 2.39                     | 0.43              |
| 1:A:114:ALA:HB1  | 1:A:160:PHE:CE1  | 2.52                     | 0.43              |
| 1:A:188:TYR:HB2  | 1:A:229:TRP:CD1  | 2.54                     | 0.43              |
| 1:A:467:VAL:HG12 | 1:A:468:PRO:O    | 2.18                     | 0.43              |
| 1:A:476:LYS:O    | 1:A:480:GLN:HG2  | 2.19                     | 0.43              |
| 2:B:274:ILE:HG13 | 2:B:306:ASN:CG   | 2.39                     | 0.43              |
| 2:B:395:LYS:HE2  | 2:B:399:GLU:OE1  | 2.18                     | 0.43              |
| 1:C:114:ALA:HB1  | 1:C:160:PHE:CE1  | 2.52                     | 0.43              |
| 1:C:412:PRO:HG2  | 1:C:413:GLU:H    | 1.83                     | 0.43              |
| 1:E:14:PRO:HG2   | 1:E:14:PRO:O     | 2.18                     | 0.43              |
| 1:E:391:LEU:HA   | 1:E:392:PRO:HD3  | 1.72                     | 0.43              |
| 1:G:114:ALA:HB1  | 1:G:160:PHE:CE1  | 2.52                     | 0.43              |
| 1:G:188:TYR:HB2  | 1:G:229:TRP:CD1  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:395:LYS:HE2  | 2:H:399:GLU:OE1  | 2.18                     | 0.43              |
| 2:H:420:PRO:HB2  | 2:H:421:PRO:CD   | 2.42                     | 0.43              |
| 1:A:14:PRO:HG2   | 1:A:14:PRO:O     | 2.18                     | 0.43              |
| 1:A:84:THR:CG2   | 1:A:154:LYS:HE2  | 2.49                     | 0.43              |
| 1:A:356:ARG:HH21 | 1:A:358:ARG:CZ   | 2.32                     | 0.43              |
| 1:A:50:ILE:HD13  | 1:A:145:GLN:HB2  | 2.01                     | 0.43              |
| 1:A:540:LYS:C    | 1:A:542:ILE:H    | 2.20                     | 0.43              |
| 2:B:24:TRP:CZ3   | 2:B:61:PHE:CB    | 3.00                     | 0.43              |
| 2:B:91:GLN:CD    | 2:B:94:ILE:HG23  | 2.39                     | 0.43              |
| 1:C:12:LEU:HD23  | 1:C:124:PHE:HE2  | 1.83                     | 0.43              |
| 1:C:132:ILE:HD11 | 1:C:144:TYR:CE2  | 2.54                     | 0.43              |
| 2:D:108:VAL:CG1  | 2:D:188:TYR:CE2  | 3.02                     | 0.43              |
| 2:D:324:ASP:O    | 2:D:343:GLN:HG2  | 2.19                     | 0.43              |
| 2:D:354:TYR:CE1  | 2:D:374:LYS:HD3  | 2.53                     | 0.43              |
| 1:E:132:ILE:HD11 | 1:E:144:TYR:CE2  | 2.54                     | 0.43              |
| 2:F:108:VAL:CG1  | 2:F:188:TYR:CE2  | 3.02                     | 0.43              |
| 2:F:319:TYR:O    | 2:F:321:PRO:HD3  | 2.18                     | 0.43              |
| 1:G:476:LYS:O    | 1:G:480:GLN:HG2  | 2.19                     | 0.43              |
| 2:H:108:VAL:CG1  | 2:H:188:TYR:CE2  | 3.02                     | 0.43              |
| 2:B:160:PHE:CD1  | 2:B:160:PHE:O    | 2.72                     | 0.43              |
| 2:B:61:PHE:CZ    | 2:B:411:ILE:HD11 | 2.54                     | 0.43              |
| 1:C:50:ILE:HD13  | 1:C:145:GLN:HB2  | 2.01                     | 0.43              |
| 1:C:368:LEU:HD11 | 1:C:391:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:467:VAL:HG12 | 1:C:468:PRO:O    | 2.18                     | 0.43              |
| 1:C:536:VAL:HB   | 1:C:542:ILE:HD13 | 2.01                     | 0.43              |
| 1:G:238:LYS:HE3  | 1:G:315:HIS:CG   | 2.54                     | 0.43              |
| 1:G:536:VAL:HB   | 1:G:542:ILE:HD13 | 2.01                     | 0.43              |
| 1:A:132:ILE:HD11 | 1:A:144:TYR:CE2  | 2.54                     | 0.43              |
| 1:A:543:GLY:C    | 1:A:545:ASN:H    | 2.22                     | 0.43              |
| 1:C:356:ARG:HH21 | 1:C:358:ARG:CZ   | 2.32                     | 0.43              |
| 2:D:38:CYS:SG    | 2:D:132:ILE:HD11 | 2.58                     | 0.43              |
| 2:D:72:ARG:HH12  | 2:D:409:THR:CG2  | 2.29                     | 0.43              |
| 1:E:188:TYR:HB2  | 1:E:229:TRP:CD1  | 2.54                     | 0.43              |
| 1:E:1:PRO:O      | 1:E:1:PRO:HG2    | 2.18                     | 0.43              |
| 2:F:91:GLN:CD    | 2:F:94:ILE:HG23  | 2.39                     | 0.43              |
| 1:G:336:GLN:HG2  | 1:G:355:ALA:CB   | 2.48                     | 0.43              |
| 2:H:120:LEU:HB3  | 2:H:125:ARG:NH1  | 2.34                     | 0.43              |
| 2:H:376:THR:HG22 | 2:H:389:PHE:HE1  | 1.80                     | 0.43              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:HD12 | 2.00                     | 0.42              |
| 1:A:336:GLN:HG2  | 1:A:355:ALA:CB   | 2.48                     | 0.42              |
| 1:A:540:LYS:HB2  | 1:A:542:ILE:HG13 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:84:THR:CG2   | 1:C:154:LYS:HE2  | 2.49                     | 0.42              |
| 1:C:476:LYS:O    | 1:C:480:GLN:HG2  | 2.19                     | 0.42              |
| 2:D:160:PHE:CD1  | 2:D:160:PHE:O    | 2.72                     | 0.42              |
| 2:D:61:PHE:CZ    | 2:D:411:ILE:HD11 | 2.54                     | 0.42              |
| 1:E:238:LYS:HE3  | 1:E:315:HIS:CG   | 2.54                     | 0.42              |
| 1:G:356:ARG:HH21 | 1:G:358:ARG:CZ   | 2.32                     | 0.42              |
| 2:H:274:ILE:HG13 | 2:H:306:ASN:CG   | 2.39                     | 0.42              |
| 1:A:90:VAL:CG1   | 2:B:141:GLY:H    | 2.29                     | 0.42              |
| 2:B:78:ARG:HD3   | 2:B:411:ILE:O    | 2.20                     | 0.42              |
| 2:D:78:ARG:HD3   | 2:D:411:ILE:O    | 2.20                     | 0.42              |
| 1:E:175:ASN:CB   | 1:E:178:ILE:HD12 | 2.49                     | 0.42              |
| 1:E:363:ASN:OD1  | 1:E:365:VAL:N    | 2.50                     | 0.42              |
| 2:F:61:PHE:CZ    | 2:F:411:ILE:HD11 | 2.54                     | 0.42              |
| 1:G:12:LEU:HD23  | 1:G:124:PHE:HE2  | 1.83                     | 0.42              |
| 1:G:175:ASN:HB3  | 1:G:178:ILE:HD12 | 2.00                     | 0.42              |
| 1:G:104:LYS:N    | 1:G:192:ASP:OD1  | 2.52                     | 0.42              |
| 1:A:368:LEU:HD11 | 1:A:391:LEU:HD22 | 2.00                     | 0.42              |
| 1:A:408:ALA:HB2  | 2:B:337:TRP:HH2  | 1.85                     | 0.42              |
| 2:B:47:ILE:HG22  | 2:B:48:SER:N     | 2.30                     | 0.42              |
| 1:C:540:LYS:HB2  | 1:C:542:ILE:HG13 | 2.00                     | 0.42              |
| 1:C:543:GLY:C    | 1:C:545:ASN:H    | 2.22                     | 0.42              |
| 1:C:90:VAL:CG1   | 2:D:141:GLY:H    | 2.29                     | 0.42              |
| 2:D:207:GLN:O    | 2:D:208:HIS:C    | 2.55                     | 0.42              |
| 2:F:204:GLU:O    | 2:F:208:HIS:CD2  | 2.72                     | 0.42              |
| 2:F:316:GLY:O    | 2:F:318:TYR:CD1  | 2.66                     | 0.42              |
| 1:G:467:VAL:HG12 | 1:G:468:PRO:O    | 2.18                     | 0.42              |
| 2:B:262:GLY:O    | 2:B:265:ASN:HB3  | 2.20                     | 0.42              |
| 1:C:408:ALA:HB2  | 2:D:337:TRP:HH2  | 1.85                     | 0.42              |
| 1:E:84:THR:CG2   | 1:E:154:LYS:HE2  | 2.49                     | 0.42              |
| 1:G:14:PRO:O     | 1:G:14:PRO:HG2   | 2.18                     | 0.42              |
| 1:C:345:PRO:HB3  | 1:G:342:TYR:CE1  | 2.54                     | 0.42              |
| 1:G:363:ASN:OD1  | 1:G:365:VAL:N    | 2.50                     | 0.42              |
| 2:H:249:LYS:HB2  | 2:H:252:TRP:CZ2  | 2.52                     | 0.42              |
| 1:A:175:ASN:CB   | 1:A:178:ILE:HD12 | 2.49                     | 0.42              |
| 1:A:23:GLN:NE2   | 1:A:131:THR:H    | 2.18                     | 0.42              |
| 2:B:108:VAL:CG1  | 2:B:188:TYR:CE2  | 3.02                     | 0.42              |
| 2:B:204:GLU:O    | 2:B:208:HIS:CD2  | 2.72                     | 0.42              |
| 2:B:41:MET:HE1   | 2:B:73:LYS:HD2   | 2.01                     | 0.42              |
| 1:C:14:PRO:HG2   | 1:C:14:PRO:O     | 2.18                     | 0.42              |
| 1:C:336:GLN:HG2  | 1:C:355:ALA:CB   | 2.48                     | 0.42              |
| 1:C:44:GLU:HB2   | 1:C:46:LYS:HG2   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:PHE:HE1  | 1:E:342:TYR:OH   | 2.02                     | 0.42              |
| 1:E:483:TYR:O    | 1:E:486:LEU:HB2  | 2.20                     | 0.42              |
| 2:F:47:ILE:HG21  | 2:F:47:ILE:HD13  | 1.82                     | 0.42              |
| 1:G:368:LEU:HD11 | 1:G:391:LEU:HD22 | 2.00                     | 0.42              |
| 1:G:432:GLU:HB3  | 1:G:433:PRO:HD2  | 2.01                     | 0.42              |
| 1:G:50:ILE:HD13  | 1:G:145:GLN:HB2  | 2.01                     | 0.42              |
| 2:H:204:GLU:O    | 2:H:208:HIS:CD2  | 2.72                     | 0.42              |
| 2:H:246:LEU:HD13 | 2:H:260:LEU:HD11 | 2.02                     | 0.42              |
| 1:C:175:ASN:HB3  | 1:C:178:ILE:HD12 | 2.00                     | 0.42              |
| 1:C:1:PRO:O      | 1:C:1:PRO:HG2    | 2.18                     | 0.42              |
| 1:C:23:GLN:NE2   | 1:C:131:THR:H    | 2.18                     | 0.42              |
| 2:D:204:GLU:O    | 2:D:208:HIS:CD2  | 2.72                     | 0.42              |
| 2:D:262:GLY:O    | 2:D:265:ASN:HB3  | 2.20                     | 0.42              |
| 1:E:164:MET:HE1  | 1:E:187:LEU:HD11 | 2.01                     | 0.42              |
| 1:E:175:ASN:HB3  | 1:E:178:ILE:HD12 | 2.00                     | 0.42              |
| 2:F:160:PHE:CD1  | 2:F:160:PHE:O    | 2.72                     | 0.42              |
| 2:F:278:GLN:HA   | 2:F:278:GLN:OE1  | 2.20                     | 0.42              |
| 1:G:23:GLN:NE2   | 1:G:131:THR:H    | 2.18                     | 0.42              |
| 1:G:363:ASN:HB3  | 1:G:366:LYS:HB2  | 2.02                     | 0.42              |
| 1:C:175:ASN:CB   | 1:C:178:ILE:HD12 | 2.49                     | 0.42              |
| 1:C:238:LYS:HE3  | 1:C:315:HIS:CG   | 2.54                     | 0.42              |
| 1:C:96:HIS:ND1   | 1:C:98:ALA:HB3   | 2.35                     | 0.42              |
| 2:D:91:GLN:CD    | 2:D:94:ILE:HG23  | 2.39                     | 0.42              |
| 1:E:23:GLN:NE2   | 1:E:131:THR:H    | 2.18                     | 0.42              |
| 1:E:432:GLU:HB3  | 1:E:433:PRO:HD2  | 2.01                     | 0.42              |
| 1:E:476:LYS:O    | 1:E:480:GLN:HG2  | 2.19                     | 0.42              |
| 2:F:249:LYS:HB2  | 2:F:252:TRP:CZ2  | 2.52                     | 0.42              |
| 2:F:262:GLY:O    | 2:F:265:ASN:HB3  | 2.20                     | 0.42              |
| 2:F:274:ILE:HG13 | 2:F:306:ASN:CG   | 2.39                     | 0.42              |
| 2:F:380:ILE:O    | 2:F:384:GLY:HA2  | 2.20                     | 0.42              |
| 2:F:5:ILE:HG22   | 2:F:6:GLU:H      | 1.85                     | 0.42              |
| 1:G:175:ASN:CB   | 1:G:178:ILE:HD12 | 2.50                     | 0.42              |
| 1:G:232:TYR:CD1  | 1:G:241:VAL:HG22 | 2.53                     | 0.42              |
| 2:H:380:ILE:O    | 2:H:384:GLY:HA2  | 2.20                     | 0.42              |
| 2:H:61:PHE:CZ    | 2:H:411:ILE:HD11 | 2.54                     | 0.42              |
| 2:H:72:ARG:HH12  | 2:H:409:THR:CG2  | 2.29                     | 0.42              |
| 1:A:104:LYS:N    | 1:A:192:ASP:OD1  | 2.52                     | 0.42              |
| 1:A:483:TYR:O    | 1:A:486:LEU:HB2  | 2.20                     | 0.42              |
| 1:C:104:LYS:N    | 1:C:192:ASP:OD1  | 2.52                     | 0.42              |
| 1:C:483:TYR:O    | 1:C:486:LEU:HB2  | 2.20                     | 0.42              |
| 1:C:54:ASN:HA    | 1:C:55:PRO:HD3   | 1.77                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:120:LEU:HB3  | 2:F:125:ARG:NH1  | 2.34                     | 0.42              |
| 2:F:123:ASP:HA   | 2:F:126:LYS:HZ1  | 1.83                     | 0.42              |
| 2:F:271:TYR:CD1  | 2:F:271:TYR:N    | 2.88                     | 0.42              |
| 1:G:164:MET:HE1  | 1:G:187:LEU:HD11 | 2.02                     | 0.42              |
| 2:H:47:ILE:HG22  | 2:H:48:SER:N     | 2.30                     | 0.42              |
| 1:A:1:PRO:O      | 1:A:1:PRO:HG2    | 2.18                     | 0.42              |
| 1:A:432:GLU:HB3  | 1:A:433:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:540:LYS:HZ3  | 2:B:261:VAL:HG12 | 1.85                     | 0.42              |
| 1:A:96:HIS:ND1   | 1:A:98:ALA:HB3   | 2.35                     | 0.42              |
| 2:B:278:GLN:HA   | 2:B:278:GLN:OE1  | 2.20                     | 0.42              |
| 2:B:420:PRO:HB2  | 2:B:421:PRO:CD   | 2.43                     | 0.42              |
| 1:C:225:PRO:N    | 1:C:226:PRO:HD2  | 2.35                     | 0.42              |
| 1:C:363:ASN:HB3  | 1:C:366:LYS:HB2  | 2.02                     | 0.42              |
| 1:C:421:PRO:HG2  | 1:C:421:PRO:O    | 2.20                     | 0.42              |
| 1:C:88:TRP:CH2   | 2:D:57:ASN:CB    | 3.01                     | 0.42              |
| 2:D:393:ILE:HG12 | 2:D:394:GLN:N    | 2.35                     | 0.42              |
| 1:E:132:ILE:N    | 1:E:142:ILE:O    | 2.52                     | 0.42              |
| 1:E:356:ARG:HH21 | 1:E:358:ARG:CZ   | 2.32                     | 0.42              |
| 1:E:439:THR:HG22 | 1:E:441:TYR:HE1  | 1.82                     | 0.42              |
| 2:F:28:GLU:O     | 2:F:32:LYS:HG3   | 2.20                     | 0.42              |
| 1:G:331:LYS:HG2  | 1:G:331:LYS:O    | 2.20                     | 0.42              |
| 1:G:53:GLU:CD    | 1:G:53:GLU:N     | 2.73                     | 0.42              |
| 2:H:262:GLY:O    | 2:H:265:ASN:HB3  | 2.20                     | 0.42              |
| 1:A:312:GLU:HA   | 1:A:313:PRO:HD2  | 1.89                     | 0.42              |
| 1:A:44:GLU:HB2   | 1:A:46:LYS:HG2   | 2.02                     | 0.42              |
| 1:C:342:TYR:CZ   | 1:G:345:PRO:HB3  | 2.54                     | 0.42              |
| 1:C:96:HIS:CD2   | 1:C:97:PRO:HD2   | 2.55                     | 0.42              |
| 1:E:18:GLY:HA3   | 1:E:127:TYR:HD1  | 1.85                     | 0.42              |
| 1:E:50:ILE:HD13  | 1:E:145:GLN:HB2  | 2.01                     | 0.42              |
| 1:G:116:PHE:CD1  | 1:G:116:PHE:N    | 2.88                     | 0.42              |
| 1:G:483:TYR:O    | 1:G:486:LEU:HB2  | 2.20                     | 0.42              |
| 1:G:96:HIS:ND1   | 1:G:98:ALA:HB3   | 2.35                     | 0.42              |
| 2:H:160:PHE:O    | 2:H:160:PHE:CD1  | 2.72                     | 0.42              |
| 2:H:109:LEU:O    | 2:H:186:ASP:HA   | 2.20                     | 0.42              |
| 2:H:271:TYR:CD1  | 2:H:271:TYR:N    | 2.88                     | 0.42              |
| 2:H:278:GLN:OE1  | 2:H:278:GLN:HA   | 2.20                     | 0.42              |
| 1:A:427:TYR:CD1  | 1:A:427:TYR:N    | 2.88                     | 0.41              |
| 2:B:24:TRP:HZ3   | 2:B:61:PHE:CG    | 2.38                     | 0.41              |
| 2:B:395:LYS:O    | 2:B:399:GLU:N    | 2.48                     | 0.41              |
| 1:C:232:TYR:CD1  | 1:C:241:VAL:HG22 | 2.53                     | 0.41              |
| 2:D:120:LEU:HB3  | 2:D:125:ARG:NH1  | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:28:GLU:O     | 2:D:32:LYS:HG3   | 2.20                     | 0.41              |
| 1:G:38:CYS:HB3   | 1:G:144:TYR:CE2  | 2.55                     | 0.41              |
| 1:G:201:LYS:HA   | 1:G:201:LYS:HD3  | 1.85                     | 0.41              |
| 1:G:439:THR:CG2  | 1:G:441:TYR:HE1  | 2.33                     | 0.41              |
| 1:G:96:HIS:CD2   | 1:G:97:PRO:HD2   | 2.55                     | 0.41              |
| 1:G:8:VAL:HA     | 1:G:9:PRO:HD2    | 1.78                     | 0.41              |
| 2:H:365:VAL:HG12 | 2:H:405:TYR:HE2  | 1.81                     | 0.41              |
| 2:H:393:ILE:HG12 | 2:H:394:GLN:N    | 2.35                     | 0.41              |
| 2:H:78:ARG:HD3   | 2:H:411:ILE:O    | 2.20                     | 0.41              |
| 1:A:249:LYS:CG   | 1:A:250:ASP:N    | 2.83                     | 0.41              |
| 2:B:120:LEU:HB3  | 2:B:125:ARG:NH1  | 2.34                     | 0.41              |
| 2:B:28:GLU:O     | 2:B:32:LYS:HG3   | 2.20                     | 0.41              |
| 2:B:380:ILE:O    | 2:B:384:GLY:HA2  | 2.20                     | 0.41              |
| 1:C:38:CYS:HB3   | 1:C:144:TYR:CE2  | 2.55                     | 0.41              |
| 1:C:427:TYR:N    | 1:C:427:TYR:CD1  | 2.88                     | 0.41              |
| 1:E:427:TYR:CD1  | 1:E:427:TYR:N    | 2.88                     | 0.41              |
| 1:E:439:THR:CG2  | 1:E:441:TYR:HE1  | 2.33                     | 0.41              |
| 1:E:77:PHE:CE2   | 1:E:150:PRO:HB3  | 2.55                     | 0.41              |
| 1:E:96:HIS:ND1   | 1:E:98:ALA:HB3   | 2.35                     | 0.41              |
| 2:F:18:GLY:HA3   | 2:F:127:TYR:CD1  | 2.56                     | 0.41              |
| 2:F:246:LEU:HD13 | 2:F:260:LEU:HD11 | 2.02                     | 0.41              |
| 2:F:78:ARG:HD3   | 2:F:411:ILE:O    | 2.19                     | 0.41              |
| 1:G:116:PHE:HD1  | 1:G:116:PHE:N    | 2.18                     | 0.41              |
| 1:G:18:GLY:HA3   | 1:G:127:TYR:HD1  | 1.85                     | 0.41              |
| 1:G:320:ASP:HA   | 1:G:321:PRO:HD2  | 1.85                     | 0.41              |
| 1:G:439:THR:HG22 | 1:G:441:TYR:HE1  | 1.82                     | 0.41              |
| 1:G:77:PHE:CE2   | 1:G:150:PRO:HB3  | 2.55                     | 0.41              |
| 2:H:336:GLN:HG2  | 2:H:355:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:421:PRO:O    | 1:A:421:PRO:HG2  | 2.20                     | 0.41              |
| 2:B:72:ARG:HH12  | 2:B:409:THR:CG2  | 2.29                     | 0.41              |
| 1:E:408:ALA:HB2  | 2:F:337:TRP:HH2  | 1.85                     | 0.41              |
| 1:A:38:CYS:HB3   | 1:A:144:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:363:ASN:HB3  | 1:A:366:LYS:HB2  | 2.02                     | 0.41              |
| 2:B:100:LEU:HD23 | 2:B:100:LEU:HA   | 1.81                     | 0.41              |
| 1:C:116:PHE:HD1  | 1:C:116:PHE:N    | 2.18                     | 0.41              |
| 1:C:432:GLU:HB3  | 1:C:433:PRO:HD2  | 2.01                     | 0.41              |
| 1:C:53:GLU:N     | 1:C:53:GLU:CD    | 2.73                     | 0.41              |
| 1:C:77:PHE:CE2   | 1:C:150:PRO:HB3  | 2.55                     | 0.41              |
| 2:D:24:TRP:HZ3   | 2:D:61:PHE:CG    | 2.38                     | 0.41              |
| 2:D:246:LEU:HD13 | 2:D:260:LEU:HD11 | 2.02                     | 0.41              |
| 1:E:116:PHE:N    | 1:E:116:PHE:HD1  | 2.18                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:456:GLY:HA3  | 1:E:466:VAL:HA   | 2.02                     | 0.41              |
| 1:G:409:THR:O    | 1:G:410:TRP:HB2  | 2.21                     | 0.41              |
| 1:G:427:TYR:CD1  | 1:G:427:TYR:N    | 2.88                     | 0.41              |
| 2:H:10:VAL:HA    | 2:H:85:GLN:OE1   | 2.20                     | 0.41              |
| 1:A:238:LYS:HE3  | 1:A:315:HIS:CG   | 2.54                     | 0.41              |
| 2:B:109:LEU:O    | 2:B:186:ASP:HA   | 2.20                     | 0.41              |
| 2:B:136:ASN:O    | 2:B:137:ASN:HB2  | 2.21                     | 0.41              |
| 1:C:10:VAL:HG11  | 1:C:153:TRP:HZ2  | 1.86                     | 0.41              |
| 1:C:331:LYS:O    | 1:C:331:LYS:HG2  | 2.20                     | 0.41              |
| 2:D:278:GLN:OE1  | 2:D:278:GLN:HA   | 2.20                     | 0.41              |
| 1:E:116:PHE:CD1  | 1:E:116:PHE:N    | 2.88                     | 0.41              |
| 1:E:12:LEU:HD23  | 1:E:124:PHE:HE2  | 1.83                     | 0.41              |
| 1:E:249:LYS:CG   | 1:E:250:ASP:N    | 2.83                     | 0.41              |
| 1:E:78:ARG:NH1   | 1:E:287:LYS:O    | 2.39                     | 0.41              |
| 2:F:136:ASN:O    | 2:F:137:ASN:HB2  | 2.21                     | 0.41              |
| 2:F:393:ILE:HG12 | 2:F:394:GLN:N    | 2.35                     | 0.41              |
| 1:G:344:GLU:HA   | 1:G:345:PRO:HD2  | 1.81                     | 0.41              |
| 1:G:421:PRO:O    | 1:G:421:PRO:HG2  | 2.20                     | 0.41              |
| 1:G:53:GLU:OE2   | 1:G:53:GLU:N     | 2.54                     | 0.41              |
| 2:B:391:LEU:HD12 | 2:B:416:PHE:HE1  | 1.86                     | 0.41              |
| 1:C:349:LEU:HD23 | 1:C:349:LEU:HA   | 1.84                     | 0.41              |
| 1:C:53:GLU:OE2   | 1:C:53:GLU:N     | 2.54                     | 0.41              |
| 2:D:136:ASN:O    | 2:D:137:ASN:HB2  | 2.21                     | 0.41              |
| 2:D:395:LYS:O    | 2:D:399:GLU:N    | 2.48                     | 0.41              |
| 1:E:225:PRO:N    | 1:E:226:PRO:HD2  | 2.35                     | 0.41              |
| 1:E:53:GLU:CD    | 1:E:53:GLU:N     | 2.73                     | 0.41              |
| 2:F:109:LEU:O    | 2:F:186:ASP:HA   | 2.20                     | 0.41              |
| 2:F:153:TRP:CE3  | 2:F:155:GLY:CA   | 3.03                     | 0.41              |
| 2:F:193:LEU:HD12 | 2:F:201:LYS:HG3  | 2.03                     | 0.41              |
| 2:F:10:VAL:HA    | 2:F:85:GLN:OE1   | 2.20                     | 0.41              |
| 1:G:225:PRO:N    | 1:G:226:PRO:HD2  | 2.35                     | 0.41              |
| 1:G:44:GLU:HB2   | 1:G:46:LYS:HG2   | 2.02                     | 0.41              |
| 1:G:408:ALA:HB2  | 2:H:337:TRP:HH2  | 1.85                     | 0.41              |
| 1:A:18:GLY:HA3   | 1:A:127:TYR:HD1  | 1.85                     | 0.41              |
| 1:A:456:GLY:HA3  | 1:A:466:VAL:HA   | 2.02                     | 0.41              |
| 2:B:108:VAL:CG1  | 2:B:188:TYR:CD2  | 3.04                     | 0.41              |
| 2:B:246:LEU:HD13 | 2:B:260:LEU:HD11 | 2.02                     | 0.41              |
| 2:B:393:ILE:HG12 | 2:B:394:GLN:N    | 2.35                     | 0.41              |
| 2:B:61:PHE:CD2   | 2:B:403:THR:HG22 | 2.56                     | 0.41              |
| 1:C:409:THR:O    | 1:C:410:TRP:HB2  | 2.21                     | 0.41              |
| 2:D:103:LYS:HB3  | 2:D:191:SER:O    | 2.21                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:D:156:SER:HB2 | 2:D:157:PRO:CD   | 2.51                     | 0.41              |
| 2:D:336:GLN:HG2 | 2:D:355:ALA:HB1  | 2.02                     | 0.41              |
| 2:D:380:ILE:O   | 2:D:384:GLY:HA2  | 2.20                     | 0.41              |
| 2:D:61:PHE:CD2  | 2:D:403:THR:HG22 | 2.56                     | 0.41              |
| 1:E:10:VAL:HG11 | 1:E:153:TRP:HZ2  | 1.86                     | 0.41              |
| 1:E:38:CYS:HB3  | 1:E:144:TYR:CE2  | 2.55                     | 0.41              |
| 1:E:472:THR:HB  | 1:E:476:LYS:HB2  | 2.03                     | 0.41              |
| 2:F:104:LYS:O   | 2:F:235:HIS:CD2  | 2.74                     | 0.41              |
| 2:F:24:TRP:HZ3  | 2:F:61:PHE:CG    | 2.38                     | 0.41              |
| 1:G:418:ASN:C   | 1:G:418:ASN:ND2  | 2.74                     | 0.41              |
| 1:A:116:PHE:HD1 | 1:A:116:PHE:N    | 2.18                     | 0.41              |
| 1:A:225:PRO:N   | 1:A:226:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:439:THR:CG2 | 1:A:441:TYR:HE1  | 2.33                     | 0.41              |
| 1:A:96:HIS:CD2  | 1:A:97:PRO:HD2   | 2.55                     | 0.41              |
| 2:B:156:SER:HB2 | 2:B:157:PRO:CD   | 2.51                     | 0.41              |
| 2:B:58:THR:HG21 | 2:B:77:PHE:CD1   | 2.56                     | 0.41              |
| 2:B:94:ILE:HG13 | 2:B:94:ILE:H     | 1.54                     | 0.41              |
| 1:C:116:PHE:CD1 | 1:C:116:PHE:N    | 2.88                     | 0.41              |
| 1:C:118:VAL:HA  | 1:C:119:PRO:HD2  | 1.71                     | 0.41              |
| 1:C:249:LYS:CG  | 1:C:250:ASP:N    | 2.83                     | 0.41              |
| 1:C:442:VAL:CG1 | 1:C:481:ALA:CB   | 2.96                     | 0.41              |
| 1:C:57:ASN:HB2  | 1:C:143:ARG:HH21 | 1.86                     | 0.41              |
| 2:D:18:GLY:HA3  | 2:D:127:TYR:CD1  | 2.56                     | 0.41              |
| 1:E:44:GLU:HB2  | 1:E:46:LYS:HG2   | 2.02                     | 0.41              |
| 1:E:440:PHE:HD2 | 1:E:457:TYR:CD2  | 2.39                     | 0.41              |
| 1:E:53:GLU:N    | 1:E:53:GLU:OE2   | 2.54                     | 0.41              |
| 2:F:202:ILE:O   | 2:F:206:ARG:N    | 2.54                     | 0.41              |
| 1:G:391:LEU:HA  | 1:G:392:PRO:HD3  | 1.73                     | 0.41              |
| 1:G:440:PHE:HD2 | 1:G:457:TYR:CD2  | 2.39                     | 0.41              |
| 1:G:90:VAL:CG1  | 2:H:141:GLY:H    | 2.29                     | 0.41              |
| 2:H:175:ASN:O   | 2:H:177:ASP:N    | 2.54                     | 0.41              |
| 2:H:108:VAL:CG1 | 2:H:188:TYR:CD2  | 3.04                     | 0.41              |
| 2:H:61:PHE:CD2  | 2:H:403:THR:HG22 | 2.56                     | 0.41              |
| 1:A:116:PHE:CD1 | 1:A:116:PHE:N    | 2.88                     | 0.41              |
| 1:A:57:ASN:HB2  | 1:A:143:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:132:ILE:CD1 | 1:A:144:TYR:HE2  | 2.34                     | 0.41              |
| 1:A:77:PHE:CE2  | 1:A:150:PRO:HB3  | 2.55                     | 0.41              |
| 1:A:320:ASP:HA  | 1:A:321:PRO:HD2  | 1.85                     | 0.41              |
| 1:A:331:LYS:HG2 | 1:A:331:LYS:O    | 2.20                     | 0.41              |
| 1:A:418:ASN:C   | 1:A:418:ASN:ND2  | 2.74                     | 0.41              |
| 1:A:484:LEU:O   | 1:A:487:GLN:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:GLU:CD    | 1:A:53:GLU:N     | 2.73                     | 0.41              |
| 2:B:175:ASN:O    | 2:B:177:ASP:N    | 2.54                     | 0.41              |
| 2:B:103:LYS:HB3  | 2:B:191:SER:O    | 2.21                     | 0.41              |
| 2:B:193:LEU:HD12 | 2:B:201:LYS:HG3  | 2.03                     | 0.41              |
| 2:B:11:LYS:N     | 2:B:85:GLN:OE1   | 2.49                     | 0.41              |
| 1:C:116:PHE:HA   | 1:C:148:VAL:HG11 | 2.03                     | 0.41              |
| 1:C:420:PRO:CG   | 1:C:421:PRO:HD2  | 2.35                     | 0.41              |
| 1:C:484:LEU:O    | 1:C:487:GLN:N    | 2.54                     | 0.41              |
| 2:D:271:TYR:CD1  | 2:D:271:TYR:N    | 2.88                     | 0.41              |
| 2:D:63:ILE:HG12  | 2:D:64:LYS:H     | 1.86                     | 0.41              |
| 1:E:388:LYS:HA   | 1:E:413:GLU:HB2  | 2.03                     | 0.41              |
| 2:F:336:GLN:HG2  | 2:F:355:ALA:HB1  | 2.02                     | 0.41              |
| 1:G:317:VAL:CG2  | 1:G:347:LYS:HB3  | 2.41                     | 0.41              |
| 1:G:472:THR:HB   | 1:G:476:LYS:HB2  | 2.03                     | 0.41              |
| 2:H:100:LEU:HA   | 2:H:100:LEU:HD23 | 1.81                     | 0.41              |
| 2:H:153:TRP:CE3  | 2:H:155:GLY:CA   | 3.04                     | 0.41              |
| 2:H:156:SER:HB2  | 2:H:157:PRO:CD   | 2.51                     | 0.41              |
| 2:H:18:GLY:HA3   | 2:H:127:TYR:CD1  | 2.56                     | 0.41              |
| 2:H:104:LYS:O    | 2:H:235:HIS:CD2  | 2.74                     | 0.41              |
| 2:H:24:TRP:HZ3   | 2:H:61:PHE:CG    | 2.38                     | 0.41              |
| 2:H:252:TRP:CH2  | 2:H:260:LEU:HD22 | 2.56                     | 0.41              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:HZ2  | 1.86                     | 0.41              |
| 1:A:388:LYS:HA   | 1:A:413:GLU:HB2  | 2.03                     | 0.41              |
| 1:A:463:ARG:NH1  | 1:A:463:ARG:HG3  | 2.35                     | 0.41              |
| 1:A:53:GLU:OE2   | 1:A:53:GLU:N     | 2.54                     | 0.41              |
| 1:A:54:ASN:O     | 1:A:143:ARG:NH1  | 2.54                     | 0.41              |
| 2:B:153:TRP:CE3  | 2:B:155:GLY:CA   | 3.03                     | 0.41              |
| 1:C:463:ARG:NH1  | 1:C:463:ARG:HG3  | 2.35                     | 0.41              |
| 2:D:391:LEU:HD12 | 2:D:416:PHE:HE1  | 1.86                     | 0.41              |
| 2:D:58:THR:HG21  | 2:D:77:PHE:CD1   | 2.56                     | 0.41              |
| 1:E:323:LYS:O    | 1:E:343:GLN:NE2  | 2.52                     | 0.41              |
| 1:E:421:PRO:HG2  | 1:E:421:PRO:O    | 2.20                     | 0.41              |
| 1:E:484:LEU:O    | 1:E:487:GLN:N    | 2.54                     | 0.41              |
| 1:E:96:HIS:CD2   | 1:E:97:PRO:HD2   | 2.55                     | 0.41              |
| 2:F:252:TRP:CH2  | 2:F:260:LEU:HD22 | 2.56                     | 0.41              |
| 1:G:132:ILE:CD1  | 1:G:144:TYR:HE2  | 2.33                     | 0.41              |
| 1:C:417:VAL:HG21 | 1:G:346:PHE:CD1  | 2.56                     | 0.41              |
| 2:H:136:ASN:O    | 2:H:137:ASN:HB2  | 2.21                     | 0.41              |
| 2:H:193:LEU:HD12 | 2:H:201:LYS:HG3  | 2.03                     | 0.41              |
| 2:H:391:LEU:HD12 | 2:H:416:PHE:HE1  | 1.86                     | 0.41              |
| 2:H:74:LEU:HA    | 2:H:74:LEU:HD12  | 1.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:THR:O    | 1:A:410:TRP:HB2  | 2.21                     | 0.41              |
| 2:B:271:TYR:N    | 2:B:271:TYR:CD1  | 2.88                     | 0.41              |
| 2:B:336:GLN:HG2  | 2:B:355:ALA:HB1  | 2.02                     | 0.41              |
| 2:B:37:ILE:H     | 2:B:37:ILE:HG13  | 1.69                     | 0.41              |
| 2:B:10:VAL:HA    | 2:B:85:GLN:OE1   | 2.20                     | 0.41              |
| 1:C:439:THR:CG2  | 1:C:441:TYR:HE1  | 2.33                     | 0.41              |
| 1:C:540:LYS:O    | 1:C:542:ILE:N    | 2.53                     | 0.41              |
| 1:C:54:ASN:O     | 1:C:143:ARG:NH1  | 2.54                     | 0.41              |
| 1:C:8:VAL:HA     | 1:C:9:PRO:HD2    | 1.78                     | 0.41              |
| 2:D:175:ASN:O    | 2:D:177:ASP:N    | 2.54                     | 0.41              |
| 2:D:420:PRO:HB2  | 2:D:421:PRO:CD   | 2.43                     | 0.41              |
| 1:E:116:PHE:HA   | 1:E:148:VAL:HG11 | 2.03                     | 0.41              |
| 1:E:331:LYS:O    | 1:E:331:LYS:HG2  | 2.20                     | 0.41              |
| 1:E:363:ASN:HB3  | 1:E:366:LYS:HB2  | 2.02                     | 0.41              |
| 2:F:156:SER:HB2  | 2:F:157:PRO:CD   | 2.51                     | 0.41              |
| 2:F:175:ASN:O    | 2:F:177:ASP:N    | 2.54                     | 0.41              |
| 1:G:116:PHE:HA   | 1:G:148:VAL:HG11 | 2.03                     | 0.41              |
| 2:H:274:ILE:HG13 | 2:H:306:ASN:OD1  | 2.21                     | 0.41              |
| 2:H:34:LEU:HA    | 2:H:34:LEU:HD23  | 1.92                     | 0.41              |
| 2:H:52:PRO:HG2   | 2:H:53:GLU:N     | 2.36                     | 0.41              |
| 1:A:116:PHE:HA   | 1:A:148:VAL:HG11 | 2.03                     | 0.40              |
| 1:A:164:MET:HE1  | 1:A:187:LEU:HD11 | 2.02                     | 0.40              |
| 2:B:104:LYS:O    | 2:B:235:HIS:CD2  | 2.74                     | 0.40              |
| 1:C:18:GLY:HA3   | 1:C:127:TYR:HD1  | 1.85                     | 0.40              |
| 1:C:418:ASN:C    | 1:C:418:ASN:ND2  | 2.74                     | 0.40              |
| 1:C:456:GLY:HA3  | 1:C:466:VAL:HA   | 2.02                     | 0.40              |
| 2:D:108:VAL:CG1  | 2:D:188:TYR:CD2  | 3.04                     | 0.40              |
| 2:D:153:TRP:CE3  | 2:D:155:GLY:CA   | 3.03                     | 0.40              |
| 2:D:274:ILE:HG13 | 2:D:306:ASN:OD1  | 2.21                     | 0.40              |
| 1:E:229:TRP:CE2  | 1:E:230:MET:HE3  | 2.56                     | 0.40              |
| 2:F:259:LYS:HE3  | 2:F:263:LYS:HZ1  | 1.85                     | 0.40              |
| 2:F:61:PHE:CD2   | 2:F:403:THR:HG22 | 2.56                     | 0.40              |
| 1:G:312:GLU:HA   | 1:G:313:PRO:HD2  | 1.89                     | 0.40              |
| 1:G:377:THR:O    | 1:G:380:ILE:N    | 2.54                     | 0.40              |
| 1:G:536:VAL:HA   | 1:G:537:PRO:HD3  | 1.77                     | 0.40              |
| 1:A:132:ILE:N    | 1:A:142:ILE:O    | 2.52                     | 0.40              |
| 1:C:252:TRP:HA   | 1:C:252:TRP:CE3  | 2.56                     | 0.40              |
| 1:C:331:LYS:O    | 1:C:333:GLY:N    | 2.54                     | 0.40              |
| 1:C:402:TRP:CE3  | 1:C:402:TRP:O    | 2.74                     | 0.40              |
| 2:D:419:THR:HA   | 2:D:420:PRO:HD2  | 1.96                     | 0.40              |
| 1:E:232:TYR:CD1  | 1:E:241:VAL:HG22 | 2.53                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:63:ILE:HG12  | 2:F:64:LYS:H     | 1.86                     | 0.40              |
| 1:G:229:TRP:CE2  | 1:G:230:MET:HE3  | 2.56                     | 0.40              |
| 1:G:349:LEU:HD23 | 1:G:349:LEU:HA   | 1.84                     | 0.40              |
| 2:H:28:GLU:O     | 2:H:32:LYS:HG3   | 2.20                     | 0.40              |
| 2:H:47:ILE:HG21  | 2:H:47:ILE:HD13  | 1.82                     | 0.40              |
| 1:A:232:TYR:CD1  | 1:A:241:VAL:HG22 | 2.53                     | 0.40              |
| 1:A:246:LEU:O    | 1:A:307:ARG:NH1  | 2.54                     | 0.40              |
| 1:A:252:TRP:HA   | 1:A:252:TRP:CE3  | 2.56                     | 0.40              |
| 1:A:402:TRP:CE3  | 1:A:402:TRP:O    | 2.74                     | 0.40              |
| 1:A:440:PHE:HD2  | 1:A:457:TYR:CD2  | 2.39                     | 0.40              |
| 2:D:109:LEU:O    | 2:D:186:ASP:HA   | 2.20                     | 0.40              |
| 2:D:104:LYS:O    | 2:D:235:HIS:CD2  | 2.74                     | 0.40              |
| 1:E:252:TRP:HA   | 1:E:252:TRP:CE3  | 2.56                     | 0.40              |
| 1:E:326:ILE:CG2  | 1:E:342:TYR:HE1  | 2.35                     | 0.40              |
| 1:E:344:GLU:HA   | 1:E:345:PRO:HD2  | 1.82                     | 0.40              |
| 1:E:377:THR:O    | 1:E:380:ILE:N    | 2.55                     | 0.40              |
| 2:F:274:ILE:HG13 | 2:F:306:ASN:OD1  | 2.21                     | 0.40              |
| 2:F:72:ARG:HH12  | 2:F:409:THR:CA   | 2.35                     | 0.40              |
| 1:G:452:LEU:HD22 | 1:G:470:THR:HA   | 2.04                     | 0.40              |
| 1:G:456:GLY:HA3  | 1:G:466:VAL:HA   | 2.02                     | 0.40              |
| 1:A:472:THR:HB   | 1:A:476:LYS:HB2  | 2.03                     | 0.40              |
| 2:B:18:GLY:HA3   | 2:B:127:TYR:CD1  | 2.56                     | 0.40              |
| 2:B:7:THR:HG22   | 2:B:119:PRO:HG2  | 2.04                     | 0.40              |
| 1:C:132:ILE:CD1  | 1:C:144:TYR:HE2  | 2.33                     | 0.40              |
| 1:C:246:LEU:O    | 1:C:307:ARG:NH1  | 2.54                     | 0.40              |
| 1:C:239:TRP:N    | 1:C:318:TYR:HE1  | 2.20                     | 0.40              |
| 1:C:388:LYS:HA   | 1:C:413:GLU:HB2  | 2.03                     | 0.40              |
| 1:C:472:THR:HB   | 1:C:476:LYS:HB2  | 2.03                     | 0.40              |
| 1:C:30:LYS:HB3   | 1:C:62:ALA:HB3   | 2.04                     | 0.40              |
| 2:D:10:VAL:HA    | 2:D:85:GLN:OE1   | 2.20                     | 0.40              |
| 2:D:7:THR:HG22   | 2:D:119:PRO:HG2  | 2.04                     | 0.40              |
| 2:D:193:LEU:HD12 | 2:D:201:LYS:HG3  | 2.03                     | 0.40              |
| 2:D:252:TRP:CH2  | 2:D:260:LEU:HD22 | 2.56                     | 0.40              |
| 1:E:132:ILE:CD1  | 1:E:144:TYR:HE2  | 2.34                     | 0.40              |
| 1:E:228:LEU:CD2  | 1:E:233:GLU:HG2  | 2.51                     | 0.40              |
| 1:E:243:PRO:HD3  | 1:E:313:PRO:HB3  | 2.04                     | 0.40              |
| 1:E:246:LEU:O    | 1:E:307:ARG:NH1  | 2.54                     | 0.40              |
| 1:E:312:GLU:HA   | 1:E:313:PRO:HD2  | 1.90                     | 0.40              |
| 1:E:452:LEU:HD22 | 1:E:470:THR:HA   | 2.04                     | 0.40              |
| 2:F:103:LYS:HB3  | 2:F:191:SER:O    | 2.21                     | 0.40              |
| 2:F:108:VAL:CG1  | 2:F:188:TYR:CD2  | 3.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:28:GLU:HG3   | 2:F:135:ILE:HD13 | 2.02                     | 0.40              |
| 2:F:391:LEU:HD12 | 2:F:416:PHE:HE1  | 1.86                     | 0.40              |
| 2:F:52:PRO:HG2   | 2:F:53:GLU:N     | 2.36                     | 0.40              |
| 2:F:58:THR:HG21  | 2:F:77:PHE:CD1   | 2.56                     | 0.40              |
| 1:G:10:VAL:HG11  | 1:G:153:TRP:HZ2  | 1.86                     | 0.40              |
| 1:G:244:ILE:HD12 | 1:G:267:ALA:CB   | 2.40                     | 0.40              |
| 1:G:239:TRP:N    | 1:G:318:TYR:HE1  | 2.20                     | 0.40              |
| 2:H:7:THR:HG22   | 2:H:119:PRO:HG2  | 2.03                     | 0.40              |
| 2:B:252:TRP:CH2  | 2:B:260:LEU:HD22 | 2.56                     | 0.40              |
| 2:B:316:GLY:O    | 2:B:318:TYR:CD1  | 2.65                     | 0.40              |
| 1:C:201:LYS:HD3  | 1:C:201:LYS:HA   | 1.85                     | 0.40              |
| 1:C:442:VAL:HG12 | 1:C:481:ALA:CB   | 2.46                     | 0.40              |
| 2:D:41:MET:HE1   | 2:D:73:LYS:HD2   | 2.02                     | 0.40              |
| 1:E:104:LYS:N    | 1:E:192:ASP:OD1  | 2.52                     | 0.40              |
| 2:F:330:GLN:HB2  | 2:F:338:THR:OG1  | 2.22                     | 0.40              |
| 1:G:377:THR:OG1  | 1:G:378:GLU:N    | 2.55                     | 0.40              |
| 1:G:484:LEU:O    | 1:G:487:GLN:N    | 2.54                     | 0.40              |
| 2:H:103:LYS:HB3  | 2:H:191:SER:O    | 2.21                     | 0.40              |
| 2:H:395:LYS:HG2  | 2:H:399:GLU:OE1  | 2.21                     | 0.40              |

All (34) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:54:ASN:CA   | 2:H:88:TRP:CZ2[3_445]  | 0.68                     | 1.52              |
| 1:C:53:GLU:O    | 2:H:88:TRP:NE1[3_445]  | 0.72                     | 1.48              |
| 2:D:88:TRP:NE1  | 1:G:54:ASN:N[3_445]    | 0.91                     | 1.29              |
| 1:C:53:GLU:O    | 2:H:88:TRP:CD1[3_445]  | 1.03                     | 1.17              |
| 1:C:53:GLU:C    | 2:H:88:TRP:NE1[3_445]  | 1.08                     | 1.12              |
| 2:B:200:THR:CG2 | 1:C:211:ARG:NH2[2_657] | 1.33                     | 0.87              |
| 1:C:54:ASN:N    | 2:H:88:TRP:CE2[3_445]  | 1.35                     | 0.85              |
| 1:C:464:GLN:NE2 | 1:G:464:GLN:NE2[2_657] | 1.36                     | 0.84              |
| 1:C:54:ASN:CA   | 2:H:88:TRP:CE2[3_445]  | 1.39                     | 0.81              |
| 2:B:200:THR:CG2 | 1:C:211:ARG:CZ[2_657]  | 1.45                     | 0.75              |
| 2:D:88:TRP:NE1  | 1:G:54:ASN:CA[3_445]   | 1.49                     | 0.71              |
| 2:B:200:THR:CG2 | 1:C:211:ARG:NE[2_657]  | 1.54                     | 0.66              |
| 1:C:54:ASN:CB   | 2:H:88:TRP:CZ2[3_445]  | 1.55                     | 0.65              |
| 1:C:54:ASN:N    | 2:H:88:TRP:CZ2[3_445]  | 1.58                     | 0.62              |
| 2:D:88:TRP:CD1  | 1:G:53:GLU:C[3_445]    | 1.69                     | 0.51              |
| 1:C:54:ASN:N    | 2:H:88:TRP:NE1[3_445]  | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:464:GLN:O   | 1:G:464:GLN:O[2_657]   | 1.73                     | 0.47              |
| 1:C:53:GLU:C    | 2:H:88:TRP:CE2[3_445]  | 1.74                     | 0.46              |
| 2:D:88:TRP:CD1  | 1:G:54:ASN:N[3_445]    | 1.77                     | 0.43              |
| 1:C:53:GLU:C    | 2:H:88:TRP:CD1[3_445]  | 1.80                     | 0.40              |
| 1:A:212:TRP:CZ2 | 2:H:211:ARG:NE[4_647]  | 1.90                     | 0.30              |
| 2:D:88:TRP:NE1  | 1:G:53:GLU:C[3_445]    | 1.91                     | 0.29              |
| 1:C:54:ASN:CA   | 2:H:88:TRP:CH2[3_445]  | 2.03                     | 0.17              |
| 2:D:208:HIS:O   | 1:E:211:ARG:NE[2_657]  | 2.04                     | 0.16              |
| 1:C:53:GLU:O    | 2:H:88:TRP:CE2[3_445]  | 2.04                     | 0.16              |
| 2:B:200:THR:CB  | 1:C:211:ARG:NE[2_657]  | 2.09                     | 0.11              |
| 2:D:211:ARG:O   | 1:E:207:GLN:OE1[2_657] | 2.14                     | 0.06              |
| 1:C:54:ASN:C    | 2:H:88:TRP:NE1[3_445]  | 2.14                     | 0.06              |
| 1:A:212:TRP:CH2 | 2:H:211:ARG:CZ[4_647]  | 2.15                     | 0.05              |
| 1:C:54:ASN:C    | 2:H:88:TRP:CZ2[3_445]  | 2.15                     | 0.05              |
| 2:D:88:TRP:CE2  | 1:G:54:ASN:CA[3_445]   | 2.15                     | 0.05              |
| 1:C:54:ASN:CB   | 2:H:88:TRP:CH2[3_445]  | 2.16                     | 0.04              |
| 1:C:54:ASN:CA   | 2:H:88:TRP:NE1[3_445]  | 2.17                     | 0.03              |
| 1:C:54:ASN:C    | 2:H:88:TRP:CE2[3_445]  | 2.17                     | 0.03              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 530/560 (95%) | 439 (83%) | 74 (14%) | 17 (3%)  | 5           | 30 |
| 1   | C     | 530/560 (95%) | 438 (83%) | 75 (14%) | 17 (3%)  | 5           | 30 |
| 1   | E     | 530/560 (95%) | 439 (83%) | 74 (14%) | 17 (3%)  | 5           | 30 |
| 1   | G     | 530/560 (95%) | 439 (83%) | 74 (14%) | 17 (3%)  | 5           | 30 |
| 2   | B     | 389/440 (88%) | 320 (82%) | 57 (15%) | 12 (3%)  | 5           | 31 |
| 2   | D     | 389/440 (88%) | 320 (82%) | 57 (15%) | 12 (3%)  | 5           | 31 |
| 2   | F     | 389/440 (88%) | 320 (82%) | 57 (15%) | 12 (3%)  | 5           | 31 |
| 2   | H     | 389/440 (88%) | 320 (82%) | 57 (15%) | 12 (3%)  | 5           | 31 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| All | All   | 3676/4000 (92%) | 3035 (83%) | 525 (14%) | 116 (3%) | 5           | 30 |

All (116) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 222 | GLN  |
| 1   | A     | 345 | PRO  |
| 2   | B     | 94  | ILE  |
| 1   | C     | 222 | GLN  |
| 1   | C     | 345 | PRO  |
| 2   | D     | 94  | ILE  |
| 1   | E     | 222 | GLN  |
| 1   | E     | 345 | PRO  |
| 2   | F     | 94  | ILE  |
| 1   | G     | 222 | GLN  |
| 1   | G     | 345 | PRO  |
| 2   | H     | 94  | ILE  |
| 1   | A     | 85  | GLN  |
| 1   | A     | 273 | GLY  |
| 1   | A     | 412 | PRO  |
| 1   | C     | 85  | GLN  |
| 1   | C     | 273 | GLY  |
| 1   | C     | 412 | PRO  |
| 1   | E     | 85  | GLN  |
| 1   | E     | 273 | GLY  |
| 1   | E     | 412 | PRO  |
| 1   | G     | 85  | GLN  |
| 1   | G     | 273 | GLY  |
| 1   | G     | 412 | PRO  |
| 1   | A     | 123 | ASP  |
| 1   | A     | 156 | SER  |
| 1   | A     | 296 | THR  |
| 1   | A     | 420 | PRO  |
| 2   | B     | 28  | GLU  |
| 2   | B     | 123 | ASP  |
| 2   | B     | 176 | PRO  |
| 2   | B     | 286 | THR  |
| 1   | C     | 123 | ASP  |
| 1   | C     | 156 | SER  |
| 1   | C     | 296 | THR  |
| 1   | C     | 420 | PRO  |
| 2   | D     | 28  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 123 | ASP  |
| 2   | D     | 176 | PRO  |
| 2   | D     | 286 | THR  |
| 1   | E     | 123 | ASP  |
| 1   | E     | 156 | SER  |
| 1   | E     | 296 | THR  |
| 1   | E     | 420 | PRO  |
| 2   | F     | 28  | GLU  |
| 2   | F     | 123 | ASP  |
| 2   | F     | 176 | PRO  |
| 2   | F     | 286 | THR  |
| 1   | G     | 123 | ASP  |
| 1   | G     | 156 | SER  |
| 1   | G     | 296 | THR  |
| 1   | G     | 420 | PRO  |
| 2   | H     | 28  | GLU  |
| 2   | H     | 123 | ASP  |
| 2   | H     | 176 | PRO  |
| 2   | H     | 286 | THR  |
| 1   | A     | 114 | ALA  |
| 1   | A     | 116 | PHE  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 274 | ILE  |
| 1   | A     | 275 | LYS  |
| 2   | B     | 277 | ARG  |
| 2   | B     | 316 | GLY  |
| 1   | C     | 114 | ALA  |
| 1   | C     | 116 | PHE  |
| 1   | C     | 195 | ILE  |
| 1   | C     | 274 | ILE  |
| 1   | C     | 275 | LYS  |
| 2   | D     | 277 | ARG  |
| 2   | D     | 316 | GLY  |
| 1   | E     | 114 | ALA  |
| 1   | E     | 116 | PHE  |
| 1   | E     | 195 | ILE  |
| 1   | E     | 274 | ILE  |
| 1   | E     | 275 | LYS  |
| 2   | F     | 277 | ARG  |
| 2   | F     | 316 | GLY  |
| 1   | G     | 114 | ALA  |
| 1   | G     | 116 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 195 | ILE  |
| 1   | G     | 274 | ILE  |
| 1   | G     | 275 | LYS  |
| 2   | H     | 277 | ARG  |
| 2   | H     | 316 | GLY  |
| 1   | A     | 357 | MET  |
| 2   | B     | 77  | PHE  |
| 2   | B     | 88  | TRP  |
| 1   | C     | 357 | MET  |
| 2   | D     | 77  | PHE  |
| 2   | D     | 88  | TRP  |
| 1   | E     | 357 | MET  |
| 2   | F     | 77  | PHE  |
| 2   | F     | 88  | TRP  |
| 1   | G     | 276 | VAL  |
| 1   | G     | 357 | MET  |
| 2   | H     | 77  | PHE  |
| 2   | H     | 88  | TRP  |
| 1   | A     | 276 | VAL  |
| 1   | A     | 462 | GLY  |
| 2   | B     | 55  | PRO  |
| 1   | C     | 276 | VAL  |
| 1   | C     | 462 | GLY  |
| 2   | D     | 55  | PRO  |
| 1   | E     | 276 | VAL  |
| 1   | E     | 462 | GLY  |
| 2   | F     | 55  | PRO  |
| 1   | G     | 462 | GLY  |
| 2   | H     | 55  | PRO  |
| 2   | B     | 170 | PRO  |
| 2   | D     | 170 | PRO  |
| 2   | F     | 170 | PRO  |
| 2   | H     | 170 | PRO  |
| 2   | B     | 420 | PRO  |
| 2   | D     | 420 | PRO  |
| 2   | F     | 420 | PRO  |
| 2   | H     | 420 | PRO  |

### 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     | 431/500 (86%)   | 411 (95%)  | 20 (5%)  | 31          | 70 |
| 1   | C     | 431/500 (86%)   | 411 (95%)  | 20 (5%)  | 31          | 70 |
| 1   | E     | 431/500 (86%)   | 410 (95%)  | 21 (5%)  | 29          | 68 |
| 1   | G     | 431/500 (86%)   | 411 (95%)  | 20 (5%)  | 31          | 70 |
| 2   | B     | 343/400 (86%)   | 323 (94%)  | 20 (6%)  | 23          | 62 |
| 2   | D     | 343/400 (86%)   | 323 (94%)  | 20 (6%)  | 23          | 62 |
| 2   | F     | 343/400 (86%)   | 323 (94%)  | 20 (6%)  | 23          | 62 |
| 2   | H     | 343/400 (86%)   | 323 (94%)  | 20 (6%)  | 23          | 62 |
| All | All   | 3096/3600 (86%) | 2935 (95%) | 161 (5%) | 27          | 65 |

All (161) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | PRO  |
| 1   | A     | 4   | PRO  |
| 1   | A     | 14  | PRO  |
| 1   | A     | 19  | PRO  |
| 1   | A     | 58  | THR  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 169 | GLU  |
| 1   | A     | 170 | PRO  |
| 1   | A     | 217 | PRO  |
| 1   | A     | 236 | PRO  |
| 1   | A     | 252 | TRP  |
| 1   | A     | 318 | TYR  |
| 1   | A     | 342 | TYR  |
| 1   | A     | 402 | TRP  |
| 1   | A     | 414 | TRP  |
| 1   | A     | 415 | GLU  |
| 1   | A     | 418 | ASN  |
| 1   | A     | 426 | TRP  |
| 1   | A     | 497 | THR  |
| 1   | A     | 507 | GLN  |
| 2   | B     | 24  | TRP  |
| 2   | B     | 25  | PRO  |
| 2   | B     | 52  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 54  | ASN  |
| 2   | B     | 55  | PRO  |
| 2   | B     | 59  | PRO  |
| 2   | B     | 60  | VAL  |
| 2   | B     | 63  | ILE  |
| 2   | B     | 88  | TRP  |
| 2   | B     | 97  | PRO  |
| 2   | B     | 135 | ILE  |
| 2   | B     | 148 | VAL  |
| 2   | B     | 170 | PRO  |
| 2   | B     | 176 | PRO  |
| 2   | B     | 266 | TRP  |
| 2   | B     | 313 | PRO  |
| 2   | B     | 321 | PRO  |
| 2   | B     | 392 | PRO  |
| 2   | B     | 402 | TRP  |
| 2   | B     | 412 | PRO  |
| 1   | C     | 1   | PRO  |
| 1   | C     | 4   | PRO  |
| 1   | C     | 14  | PRO  |
| 1   | C     | 19  | PRO  |
| 1   | C     | 58  | THR  |
| 1   | C     | 91  | GLN  |
| 1   | C     | 169 | GLU  |
| 1   | C     | 170 | PRO  |
| 1   | C     | 217 | PRO  |
| 1   | C     | 236 | PRO  |
| 1   | C     | 252 | TRP  |
| 1   | C     | 318 | TYR  |
| 1   | C     | 342 | TYR  |
| 1   | C     | 402 | TRP  |
| 1   | C     | 414 | TRP  |
| 1   | C     | 415 | GLU  |
| 1   | C     | 418 | ASN  |
| 1   | C     | 426 | TRP  |
| 1   | C     | 497 | THR  |
| 1   | C     | 507 | GLN  |
| 2   | D     | 24  | TRP  |
| 2   | D     | 25  | PRO  |
| 2   | D     | 52  | PRO  |
| 2   | D     | 54  | ASN  |
| 2   | D     | 55  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 59  | PRO  |
| 2   | D     | 60  | VAL  |
| 2   | D     | 63  | ILE  |
| 2   | D     | 88  | TRP  |
| 2   | D     | 97  | PRO  |
| 2   | D     | 135 | ILE  |
| 2   | D     | 148 | VAL  |
| 2   | D     | 170 | PRO  |
| 2   | D     | 176 | PRO  |
| 2   | D     | 266 | TRP  |
| 2   | D     | 313 | PRO  |
| 2   | D     | 321 | PRO  |
| 2   | D     | 392 | PRO  |
| 2   | D     | 402 | TRP  |
| 2   | D     | 412 | PRO  |
| 1   | E     | 1   | PRO  |
| 1   | E     | 4   | PRO  |
| 1   | E     | 14  | PRO  |
| 1   | E     | 19  | PRO  |
| 1   | E     | 58  | THR  |
| 1   | E     | 91  | GLN  |
| 1   | E     | 169 | GLU  |
| 1   | E     | 170 | PRO  |
| 1   | E     | 217 | PRO  |
| 1   | E     | 236 | PRO  |
| 1   | E     | 252 | TRP  |
| 1   | E     | 318 | TYR  |
| 1   | E     | 342 | TYR  |
| 1   | E     | 402 | TRP  |
| 1   | E     | 414 | TRP  |
| 1   | E     | 415 | GLU  |
| 1   | E     | 418 | ASN  |
| 1   | E     | 426 | TRP  |
| 1   | E     | 497 | THR  |
| 1   | E     | 507 | GLN  |
| 1   | E     | 510 | PRO  |
| 2   | F     | 24  | TRP  |
| 2   | F     | 25  | PRO  |
| 2   | F     | 52  | PRO  |
| 2   | F     | 54  | ASN  |
| 2   | F     | 55  | PRO  |
| 2   | F     | 59  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 60  | VAL  |
| 2   | F     | 63  | ILE  |
| 2   | F     | 88  | TRP  |
| 2   | F     | 97  | PRO  |
| 2   | F     | 135 | ILE  |
| 2   | F     | 148 | VAL  |
| 2   | F     | 170 | PRO  |
| 2   | F     | 176 | PRO  |
| 2   | F     | 266 | TRP  |
| 2   | F     | 313 | PRO  |
| 2   | F     | 321 | PRO  |
| 2   | F     | 392 | PRO  |
| 2   | F     | 402 | TRP  |
| 2   | F     | 412 | PRO  |
| 1   | G     | 1   | PRO  |
| 1   | G     | 4   | PRO  |
| 1   | G     | 14  | PRO  |
| 1   | G     | 19  | PRO  |
| 1   | G     | 58  | THR  |
| 1   | G     | 91  | GLN  |
| 1   | G     | 169 | GLU  |
| 1   | G     | 170 | PRO  |
| 1   | G     | 217 | PRO  |
| 1   | G     | 236 | PRO  |
| 1   | G     | 252 | TRP  |
| 1   | G     | 318 | TYR  |
| 1   | G     | 342 | TYR  |
| 1   | G     | 402 | TRP  |
| 1   | G     | 414 | TRP  |
| 1   | G     | 415 | GLU  |
| 1   | G     | 418 | ASN  |
| 1   | G     | 426 | TRP  |
| 1   | G     | 497 | THR  |
| 1   | G     | 507 | GLN  |
| 2   | H     | 24  | TRP  |
| 2   | H     | 25  | PRO  |
| 2   | H     | 52  | PRO  |
| 2   | H     | 54  | ASN  |
| 2   | H     | 55  | PRO  |
| 2   | H     | 59  | PRO  |
| 2   | H     | 60  | VAL  |
| 2   | H     | 63  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 88  | TRP  |
| 2   | H     | 97  | PRO  |
| 2   | H     | 135 | ILE  |
| 2   | H     | 148 | VAL  |
| 2   | H     | 170 | PRO  |
| 2   | H     | 176 | PRO  |
| 2   | H     | 266 | TRP  |
| 2   | H     | 313 | PRO  |
| 2   | H     | 321 | PRO  |
| 2   | H     | 392 | PRO  |
| 2   | H     | 402 | TRP  |
| 2   | H     | 412 | PRO  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | GLN  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 145 | GLN  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 174 | GLN  |
| 1   | A     | 175 | ASN  |
| 1   | A     | 198 | HIS  |
| 1   | A     | 208 | HIS  |
| 1   | A     | 315 | HIS  |
| 1   | A     | 367 | GLN  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 418 | ASN  |
| 1   | A     | 471 | ASN  |
| 2   | B     | 54  | ASN  |
| 2   | B     | 57  | ASN  |
| 2   | B     | 96  | HIS  |
| 2   | B     | 145 | GLN  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 151 | GLN  |
| 2   | B     | 208 | HIS  |
| 2   | B     | 235 | HIS  |
| 2   | B     | 269 | GLN  |
| 2   | B     | 394 | GLN  |
| 2   | B     | 418 | ASN  |
| 1   | C     | 23  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 91  | GLN  |
| 1   | C     | 145 | GLN  |
| 1   | C     | 161 | GLN  |
| 1   | C     | 174 | GLN  |
| 1   | C     | 175 | ASN  |
| 1   | C     | 198 | HIS  |
| 1   | C     | 208 | HIS  |
| 1   | C     | 315 | HIS  |
| 1   | C     | 367 | GLN  |
| 1   | C     | 373 | GLN  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 418 | ASN  |
| 1   | C     | 471 | ASN  |
| 2   | D     | 54  | ASN  |
| 2   | D     | 57  | ASN  |
| 2   | D     | 96  | HIS  |
| 2   | D     | 145 | GLN  |
| 2   | D     | 147 | ASN  |
| 2   | D     | 151 | GLN  |
| 2   | D     | 208 | HIS  |
| 2   | D     | 235 | HIS  |
| 2   | D     | 269 | GLN  |
| 2   | D     | 394 | GLN  |
| 2   | D     | 418 | ASN  |
| 1   | E     | 23  | GLN  |
| 1   | E     | 91  | GLN  |
| 1   | E     | 145 | GLN  |
| 1   | E     | 161 | GLN  |
| 1   | E     | 174 | GLN  |
| 1   | E     | 175 | ASN  |
| 1   | E     | 198 | HIS  |
| 1   | E     | 208 | HIS  |
| 1   | E     | 315 | HIS  |
| 1   | E     | 367 | GLN  |
| 1   | E     | 373 | GLN  |
| 1   | E     | 407 | GLN  |
| 1   | E     | 418 | ASN  |
| 1   | E     | 471 | ASN  |
| 2   | F     | 54  | ASN  |
| 2   | F     | 57  | ASN  |
| 2   | F     | 96  | HIS  |
| 2   | F     | 145 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 147 | ASN  |
| 2   | F     | 151 | GLN  |
| 2   | F     | 208 | HIS  |
| 2   | F     | 235 | HIS  |
| 2   | F     | 269 | GLN  |
| 2   | F     | 394 | GLN  |
| 2   | F     | 418 | ASN  |
| 1   | G     | 23  | GLN  |
| 1   | G     | 91  | GLN  |
| 1   | G     | 145 | GLN  |
| 1   | G     | 161 | GLN  |
| 1   | G     | 174 | GLN  |
| 1   | G     | 175 | ASN  |
| 1   | G     | 198 | HIS  |
| 1   | G     | 208 | HIS  |
| 1   | G     | 315 | HIS  |
| 1   | G     | 367 | GLN  |
| 1   | G     | 373 | GLN  |
| 1   | G     | 407 | GLN  |
| 1   | G     | 418 | ASN  |
| 1   | G     | 471 | ASN  |
| 2   | H     | 54  | ASN  |
| 2   | H     | 57  | ASN  |
| 2   | H     | 96  | HIS  |
| 2   | H     | 145 | GLN  |
| 2   | H     | 147 | ASN  |
| 2   | H     | 151 | GLN  |
| 2   | H     | 208 | HIS  |
| 2   | H     | 235 | HIS  |
| 2   | H     | 269 | GLN  |
| 2   | H     | 394 | GLN  |
| 2   | H     | 418 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.