



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:22 PM UTC

PDB ID : 1TVR / pdb\_00001tvr  
Title : HIV-1 RT/9-CL TIBO  
Authors : Das, K.; Ding, J.; Hsiou, Y.; Arnold, E.  
Deposited on : 1996-04-16  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

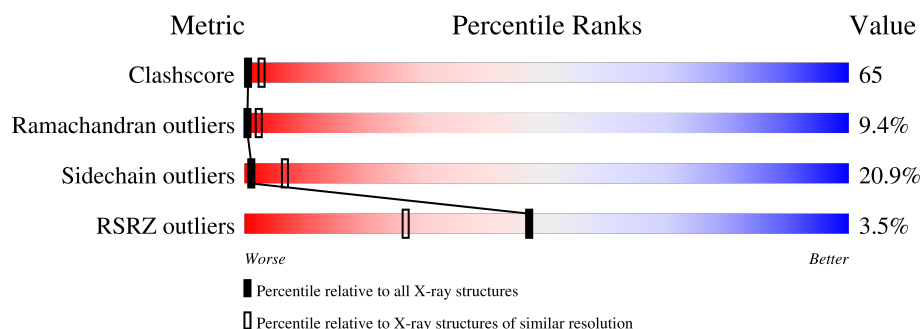
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 558    | <div> <div>3%</div> <div>18%</div> <div>53%</div> <div>24%</div> <div>.</div> </div> |
| 2   | B     | 427    | <div> <div>4%</div> <div>22%</div> <div>51%</div> <div>23%</div> <div>.</div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | TB9  | A     | 600 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7845 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 REVERSE TRANSCRIPTASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 558      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4382  | 2832 | 727 | 817 | 6 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |

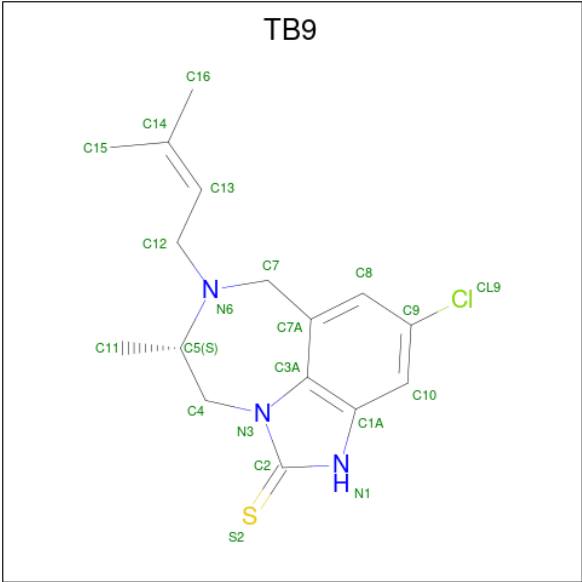
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 427      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3442  | 2240 | 567 | 630 | 5 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |

- Molecule 3 is 4-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (CCD ID: TB9) (formula: C<sub>16</sub>H<sub>20</sub>ClN<sub>3</sub>S).

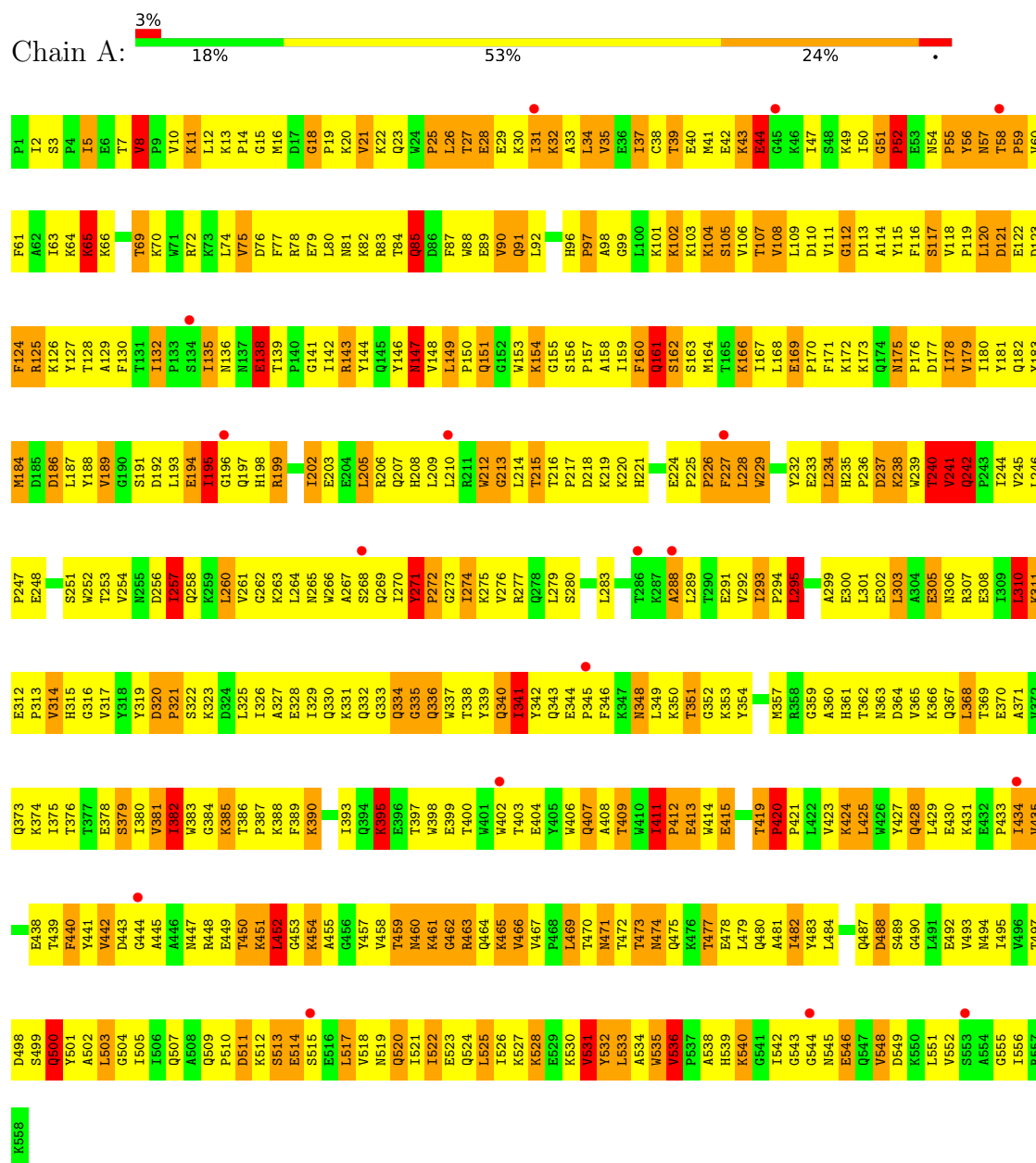


| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
|     |       |          | Total | C  | Cl | N | S |         |         |
| 3   | A     | 1        | 21    | 16 | 1  | 3 | 1 | 0       | 0       |

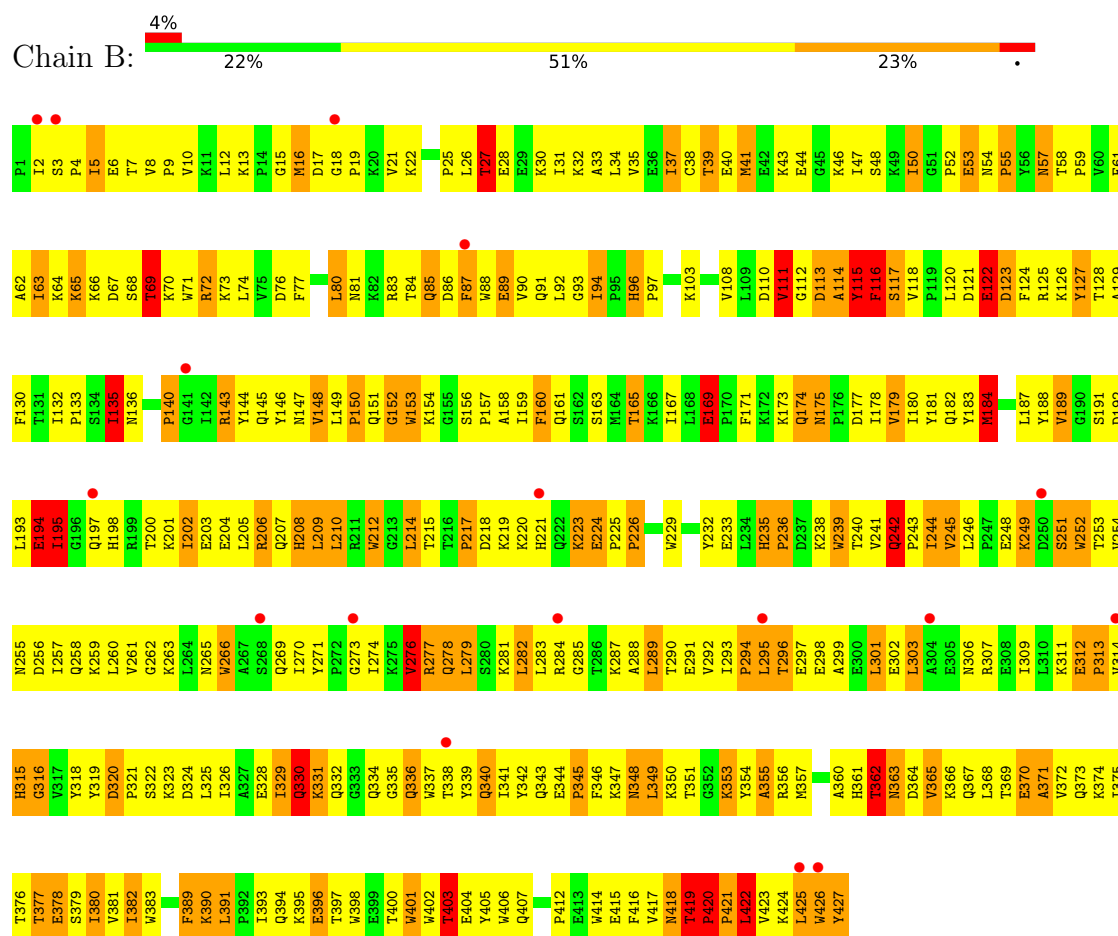
### 3 Residue-property plots

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

#### • Molecule 1: REVERSE TRANSCRIPTASE



#### • Molecule 2: REVERSE TRANSCRIPTASE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 226.00Å 69.30Å 104.10Å<br>90.00° 107.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 10.00 – 3.00<br>10.00 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (10.00-3.00)<br>82.2 (10.00-3.00)           | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.47 (at 2.88Å)                                             | Xtriage          |
| Refinement program                                                      | X-PLOR 3.1                                                  | Depositor        |
| R, $R_{free}$                                                           | 0.259 , (Not available)<br>0.303 , (Not available)          | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 78.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.253                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.15 , 80.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 7845                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 40.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TB9

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     | 0.91         | 6/4497 (0.1%) | 1.49        | 105/6132 (1.7%)  |
| 2   | B     | 0.93         | 1/3541 (0.0%) | 1.48        | 69/4822 (1.4%)   |
| All | All   | 0.92         | 7/8038 (0.1%) | 1.48        | 174/10954 (1.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 132 | ILE  | CA-CB | 8.70  | 1.60        | 1.54     |
| 1   | A     | 382 | ILE  | CA-CB | 7.17  | 1.62        | 1.55     |
| 1   | A     | 522 | ILE  | CA-CB | 6.55  | 1.61        | 1.54     |
| 1   | A     | 142 | ILE  | CA-CB | 5.60  | 1.62        | 1.54     |
| 2   | B     | 314 | VAL  | CA-CB | 5.47  | 1.59        | 1.54     |
| 1   | A     | 346 | PHE  | N-CA  | 5.47  | 1.51        | 1.46     |
| 1   | A     | 186 | ASP  | C-N   | -5.42 | 1.26        | 1.33     |

All (174) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 420 | PRO  | N-CA-C | 14.30  | 128.14      | 110.70   |
| 2   | B     | 40  | GLU  | N-CA-C | -12.39 | 97.76       | 111.14   |
| 2   | B     | 380 | ILE  | N-CA-C | -12.07 | 99.08       | 110.42   |
| 1   | A     | 32  | LYS  | N-CA-C | -10.79 | 99.52       | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 419 | THR  | CA-C-N | 10.27 | 130.96      | 120.38   |
| 2   | B     | 419 | THR  | C-N-CA | 10.27 | 130.96      | 120.38   |
| 1   | A     | 528 | LYS  | N-CA-C | 10.14 | 122.76      | 110.19   |
| 2   | B     | 370 | GLU  | N-CA-C | -9.98 | 99.95       | 111.03   |
| 2   | B     | 89  | GLU  | N-CA-C | -9.91 | 100.56      | 111.36   |
| 1   | A     | 197 | GLN  | N-CA-C | -9.69 | 99.60       | 111.33   |
| 1   | A     | 388 | LYS  | N-CA-C | -9.44 | 95.29       | 110.20   |
| 1   | A     | 8   | VAL  | CA-C-N | 9.38  | 131.56      | 119.84   |
| 1   | A     | 8   | VAL  | C-N-CA | 9.38  | 131.56      | 119.84   |
| 2   | B     | 313 | PRO  | N-CA-C | 9.36  | 125.85      | 111.34   |
| 2   | B     | 43  | LYS  | N-CA-C | -9.20 | 100.94      | 110.97   |
| 1   | A     | 18  | GLY  | CA-C-N | 9.10  | 129.17      | 119.89   |
| 1   | A     | 18  | GLY  | C-N-CA | 9.10  | 129.17      | 119.89   |
| 1   | A     | 365 | VAL  | N-CA-C | -8.95 | 102.12      | 110.53   |
| 2   | B     | 215 | THR  | N-CA-C | -8.85 | 97.18       | 110.28   |
| 2   | B     | 96  | HIS  | CA-C-N | 8.68  | 130.69      | 119.84   |
| 2   | B     | 96  | HIS  | C-N-CA | 8.68  | 130.69      | 119.84   |
| 1   | A     | 139 | THR  | N-CA-C | 8.66  | 120.67      | 109.93   |
| 1   | A     | 271 | TYR  | CA-C-N | 8.59  | 130.57      | 119.84   |
| 1   | A     | 271 | TYR  | C-N-CA | 8.59  | 130.57      | 119.84   |
| 2   | B     | 355 | ALA  | N-CA-C | 8.58  | 122.51      | 108.52   |
| 2   | B     | 94  | ILE  | CA-C-N | 8.56  | 128.58      | 119.76   |
| 2   | B     | 94  | ILE  | C-N-CA | 8.56  | 128.58      | 119.76   |
| 1   | A     | 348 | ASN  | N-CA-C | 8.29  | 121.63      | 110.35   |
| 1   | A     | 395 | LYS  | N-CA-C | -8.21 | 101.88      | 112.23   |
| 1   | A     | 376 | THR  | N-CA-C | -8.17 | 102.33      | 111.07   |
| 2   | B     | 279 | LEU  | N-CA-C | -8.12 | 101.88      | 112.68   |
| 1   | A     | 242 | GLN  | N-CA-C | 8.05  | 123.42      | 112.55   |
| 2   | B     | 377 | THR  | N-CA-C | -8.05 | 101.25      | 112.45   |
| 2   | B     | 135 | ILE  | N-CA-C | 8.04  | 118.80      | 110.36   |
| 1   | A     | 335 | GLY  | N-CA-C | -7.96 | 101.93      | 113.86   |
| 1   | A     | 493 | VAL  | N-CA-C | 7.93  | 120.03      | 108.53   |
| 1   | A     | 162 | SER  | N-CA-C | -7.87 | 98.85       | 111.04   |
| 2   | B     | 418 | ASN  | N-CA-C | -7.86 | 103.84      | 113.19   |
| 2   | B     | 348 | ASN  | N-CA-C | 7.78  | 121.41      | 108.73   |
| 2   | B     | 312 | GLU  | CA-C-N | 7.71  | 128.17      | 119.92   |
| 2   | B     | 312 | GLU  | C-N-CA | 7.71  | 128.17      | 119.92   |
| 1   | A     | 513 | SER  | N-CA-C | -7.65 | 97.44       | 109.07   |
| 1   | A     | 380 | ILE  | N-CA-C | -7.65 | 102.28      | 110.23   |
| 1   | A     | 138 | GLU  | N-CA-C | 7.65  | 127.09      | 110.80   |
| 1   | A     | 424 | LYS  | N-CA-C | 7.53  | 119.13      | 108.74   |
| 2   | B     | 244 | ILE  | N-CA-C | -7.49 | 93.76       | 109.34   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 463 | ARG  | N-CA-C  | 7.47  | 121.06      | 110.68   |
| 1   | A     | 44  | GLU  | N-CA-C  | -7.42 | 104.23      | 113.20   |
| 2   | B     | 65  | LYS  | N-CA-C  | 7.35  | 121.69      | 112.87   |
| 2   | B     | 87  | PHE  | N-CA-C  | -7.25 | 103.90      | 112.89   |
| 1   | A     | 110 | ASP  | N-CA-C  | -7.17 | 98.88       | 110.20   |
| 1   | A     | 151 | GLN  | N-CA-C  | 7.15  | 122.03      | 113.16   |
| 2   | B     | 225 | PRO  | N-CA-CB | 7.15  | 110.02      | 103.08   |
| 2   | B     | 165 | THR  | N-CA-C  | -7.12 | 102.72      | 111.33   |
| 2   | B     | 223 | LYS  | N-CA-C  | -7.12 | 104.86      | 113.97   |
| 2   | B     | 226 | PRO  | N-CA-CB | 7.06  | 110.66      | 103.25   |
| 1   | A     | 357 | MET  | N-CA-C  | -7.00 | 100.05      | 110.06   |
| 1   | A     | 69  | THR  | N-CA-C  | -6.95 | 104.68      | 113.02   |
| 1   | A     | 135 | ILE  | N-CA-C  | -6.84 | 97.71       | 108.86   |
| 1   | A     | 225 | PRO  | N-CA-C  | 6.83  | 119.03      | 110.70   |
| 2   | B     | 414 | TRP  | N-CA-C  | 6.81  | 119.29      | 109.14   |
| 1   | A     | 381 | VAL  | N-CA-C  | 6.81  | 120.56      | 111.17   |
| 2   | B     | 320 | ASP  | CA-C-N  | 6.78  | 128.31      | 119.84   |
| 2   | B     | 320 | ASP  | C-N-CA  | 6.78  | 128.31      | 119.84   |
| 1   | A     | 535 | TRP  | N-CA-C  | 6.75  | 119.90      | 108.90   |
| 2   | B     | 153 | TRP  | N-CA-C  | 6.71  | 120.11      | 110.24   |
| 2   | B     | 301 | LEU  | N-CA-C  | -6.69 | 103.99      | 111.28   |
| 1   | A     | 482 | ILE  | N-CA-C  | -6.68 | 104.66      | 110.74   |
| 1   | A     | 305 | GLU  | N-CA-C  | -6.64 | 104.04      | 111.28   |
| 2   | B     | 422 | LEU  | N-CA-C  | -6.63 | 96.67       | 110.80   |
| 1   | A     | 320 | ASP  | CA-C-N  | 6.62  | 128.11      | 119.84   |
| 1   | A     | 320 | ASP  | C-N-CA  | 6.62  | 128.11      | 119.84   |
| 2   | B     | 426 | TRP  | N-CA-C  | -6.60 | 106.18      | 114.56   |
| 1   | A     | 79  | GLU  | N-CA-C  | -6.60 | 100.82      | 111.04   |
| 2   | B     | 179 | VAL  | CB-CA-C | -6.60 | 102.39      | 111.49   |
| 2   | B     | 389 | PHE  | N-CA-C  | 6.50  | 120.02      | 110.59   |
| 1   | A     | 52  | PRO  | N-CA-C  | 6.49  | 125.83      | 112.47   |
| 1   | A     | 92  | LEU  | N-CA-C  | -6.46 | 97.98       | 108.52   |
| 2   | B     | 80  | LEU  | N-CA-C  | -6.43 | 104.13      | 112.23   |
| 2   | B     | 344 | GLU  | CA-C-N  | 6.40  | 127.84      | 119.84   |
| 2   | B     | 344 | GLU  | C-N-CA  | 6.40  | 127.84      | 119.84   |
| 1   | A     | 323 | LYS  | N-CA-C  | 6.33  | 119.85      | 109.72   |
| 1   | A     | 495 | ILE  | N-CA-C  | 6.31  | 117.39      | 108.17   |
| 1   | A     | 104 | LYS  | N-CA-C  | 6.31  | 120.54      | 112.34   |
| 1   | A     | 382 | ILE  | CB-CA-C | -6.25 | 104.42      | 111.80   |
| 1   | A     | 117 | SER  | N-CA-C  | -6.24 | 104.56      | 111.36   |
| 2   | B     | 203 | GLU  | N-CA-C  | -6.23 | 104.49      | 111.28   |
| 2   | B     | 276 | VAL  | N-CA-C  | 6.22  | 122.28      | 109.34   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 500 | GLN  | N-CA-C  | -6.21 | 104.78      | 112.72   |
| 2   | B     | 96  | HIS  | N-CA-C  | 6.19  | 119.56      | 108.47   |
| 1   | A     | 368 | LEU  | N-CA-C  | -6.17 | 104.48      | 111.14   |
| 1   | A     | 411 | ILE  | CA-C-N  | 6.15  | 127.53      | 119.84   |
| 1   | A     | 411 | ILE  | C-N-CA  | 6.15  | 127.53      | 119.84   |
| 2   | B     | 330 | GLN  | N-CA-C  | 6.14  | 118.69      | 108.13   |
| 1   | A     | 336 | GLN  | N-CA-C  | 6.07  | 118.79      | 110.24   |
| 1   | A     | 65  | LYS  | N-CA-C  | 6.07  | 116.29      | 108.34   |
| 2   | B     | 314 | VAL  | N-CA-C  | 6.03  | 119.14      | 110.09   |
| 1   | A     | 440 | PHE  | N-CA-C  | 5.99  | 118.53      | 108.23   |
| 1   | A     | 419 | THR  | CB-CA-C | 5.98  | 121.95      | 110.17   |
| 1   | A     | 228 | LEU  | N-CA-C  | 5.91  | 119.74      | 112.54   |
| 1   | A     | 72  | ARG  | N-CA-C  | 5.89  | 119.31      | 109.95   |
| 2   | B     | 396 | GLU  | N-CA-C  | 5.88  | 117.38      | 110.97   |
| 1   | A     | 526 | ILE  | CB-CA-C | -5.88 | 104.46      | 111.81   |
| 1   | A     | 536 | VAL  | CA-C-N  | 5.87  | 125.84      | 120.03   |
| 1   | A     | 536 | VAL  | C-N-CA  | 5.87  | 125.84      | 120.03   |
| 1   | A     | 227 | PHE  | N-CA-C  | 5.86  | 118.45      | 108.02   |
| 1   | A     | 311 | LYS  | N-CA-C  | -5.84 | 102.63      | 111.56   |
| 2   | B     | 123 | ASP  | N-CA-C  | -5.82 | 104.70      | 113.89   |
| 1   | A     | 362 | THR  | N-CA-C  | 5.81  | 119.72      | 109.96   |
| 1   | A     | 312 | GLU  | CA-C-N  | 5.77  | 125.75      | 120.21   |
| 1   | A     | 312 | GLU  | C-N-CA  | 5.77  | 125.75      | 120.21   |
| 1   | A     | 147 | ASN  | N-CA-C  | -5.75 | 106.89      | 114.31   |
| 1   | A     | 322 | SER  | N-CA-C  | -5.75 | 106.40      | 113.41   |
| 1   | A     | 288 | ALA  | N-CA-C  | 5.70  | 117.83      | 110.65   |
| 1   | A     | 125 | ARG  | N-CA-C  | -5.68 | 106.51      | 113.50   |
| 1   | A     | 213 | GLY  | N-CA-C  | 5.67  | 126.61      | 113.18   |
| 1   | A     | 299 | ALA  | N-CA-C  | -5.66 | 106.22      | 113.01   |
| 1   | A     | 257 | ILE  | N-CA-C  | -5.64 | 105.02      | 110.72   |
| 1   | A     | 498 | ASP  | N-CA-C  | -5.63 | 104.53      | 111.40   |
| 1   | A     | 454 | LYS  | N-CA-C  | 5.62  | 117.40      | 107.61   |
| 1   | A     | 346 | PHE  | N-CA-C  | 5.62  | 122.77      | 113.50   |
| 1   | A     | 14  | PRO  | CB-CA-C | -5.60 | 104.43      | 111.71   |
| 2   | B     | 116 | PHE  | N-CA-C  | 5.58  | 122.69      | 110.80   |
| 2   | B     | 353 | LYS  | N-CA-C  | 5.58  | 117.79      | 108.02   |
| 1   | A     | 179 | VAL  | N-CA-C  | 5.57  | 117.47      | 109.51   |
| 2   | B     | 391 | LEU  | N-CA-C  | 5.54  | 117.47      | 109.04   |
| 2   | B     | 362 | THR  | N-CA-C  | 5.54  | 122.60      | 110.80   |
| 1   | A     | 382 | ILE  | N-CA-C  | 5.53  | 116.92      | 111.67   |
| 1   | A     | 366 | LYS  | N-CA-C  | -5.51 | 104.29      | 111.02   |
| 2   | B     | 114 | ALA  | N-CA-C  | 5.51  | 117.09      | 111.14   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 220 | LYS  | N-CA-C  | -5.51 | 104.63      | 111.90   |
| 1   | A     | 26  | LEU  | N-CA-C  | 5.42  | 117.87      | 110.55   |
| 1   | A     | 43  | LYS  | N-CA-C  | -5.38 | 106.23      | 112.89   |
| 2   | B     | 206 | ARG  | N-CA-C  | -5.37 | 105.53      | 111.71   |
| 1   | A     | 184 | MET  | N-CA-C  | -5.37 | 99.36       | 110.80   |
| 2   | B     | 127 | TYR  | N-CA-C  | 5.37  | 119.46      | 113.01   |
| 2   | B     | 135 | ILE  | CA-C-N  | -5.37 | 114.77      | 122.67   |
| 2   | B     | 135 | ILE  | C-N-CA  | -5.37 | 114.77      | 122.67   |
| 1   | A     | 55  | PRO  | N-CA-C  | 5.34  | 120.56      | 113.57   |
| 2   | B     | 217 | PRO  | N-CA-C  | -5.33 | 101.50      | 112.47   |
| 1   | A     | 108 | VAL  | N-CA-C  | -5.30 | 100.43      | 108.17   |
| 2   | B     | 295 | LEU  | N-CA-C  | 5.30  | 122.08      | 110.80   |
| 1   | A     | 346 | PHE  | CB-CA-C | -5.26 | 99.40       | 110.45   |
| 2   | B     | 241 | VAL  | N-CA-C  | 5.24  | 115.50      | 108.17   |
| 1   | A     | 525 | LEU  | CA-C-N  | 5.22  | 127.22      | 120.70   |
| 1   | A     | 525 | LEU  | C-N-CA  | 5.22  | 127.22      | 120.70   |
| 2   | B     | 209 | LEU  | N-CA-C  | -5.21 | 105.29      | 110.97   |
| 1   | A     | 143 | ARG  | N-CA-C  | 5.21  | 117.78      | 109.96   |
| 1   | A     | 268 | SER  | N-CA-C  | 5.19  | 119.09      | 112.87   |
| 1   | A     | 327 | ALA  | N-CA-C  | 5.18  | 116.84      | 108.34   |
| 1   | A     | 314 | VAL  | N-CA-C  | 5.18  | 116.18      | 108.46   |
| 2   | B     | 169 | GLU  | N-CA-C  | 5.18  | 121.26      | 109.81   |
| 2   | B     | 420 | PRO  | N-CA-C  | 5.17  | 117.01      | 110.70   |
| 1   | A     | 166 | LYS  | N-CA-C  | -5.16 | 105.10      | 111.40   |
| 2   | B     | 235 | HIS  | CA-C-N  | 5.16  | 126.29      | 119.84   |
| 2   | B     | 235 | HIS  | C-N-CA  | 5.16  | 126.29      | 119.84   |
| 1   | A     | 471 | ASN  | N-CA-CB | -5.16 | 103.50      | 111.65   |
| 1   | A     | 293 | ILE  | CA-C-N  | 5.15  | 126.28      | 119.84   |
| 1   | A     | 293 | ILE  | C-N-CA  | 5.15  | 126.28      | 119.84   |
| 1   | A     | 202 | ILE  | CB-CA-C | -5.15 | 105.19      | 112.14   |
| 1   | A     | 300 | GLU  | N-CA-C  | -5.14 | 105.30      | 112.45   |
| 1   | A     | 103 | LYS  | N-CA-C  | -5.13 | 100.81      | 109.07   |
| 1   | A     | 341 | ILE  | N-CA-C  | 5.13  | 115.35      | 108.17   |
| 1   | A     | 15  | GLY  | N-CA-C  | -5.11 | 107.93      | 114.37   |
| 1   | A     | 390 | LYS  | N-CA-C  | -5.10 | 99.98       | 108.34   |
| 1   | A     | 442 | VAL  | N-CA-C  | 5.08  | 117.71      | 110.09   |
| 1   | A     | 34  | LEU  | N-CA-C  | -5.07 | 105.45      | 111.69   |
| 2   | B     | 117 | SER  | N-CA-C  | 5.04  | 119.04      | 112.13   |
| 2   | B     | 390 | LYS  | N-CA-C  | -5.04 | 99.04       | 108.02   |
| 1   | A     | 205 | LEU  | N-CA-C  | -5.04 | 104.87      | 111.02   |
| 2   | B     | 152 | GLY  | CA-C-N  | 5.03  | 128.25      | 121.05   |
| 2   | B     | 152 | GLY  | C-N-CA  | 5.03  | 128.25      | 121.05   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 202 | ILE  | N-CA-C  | 5.03  | 116.48      | 111.00   |
| 1   | A     | 241 | VAL  | CB-CA-C | -5.03 | 103.05      | 111.29   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 427 | TYR  | 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     | 4382  | 0        | 4279     | 606     | 0            |
| 2   | B     | 3442  | 0        | 3405     | 426     | 0            |
| 3   | A     | 21    | 0        | 20       | 15      | 0            |
| All | All   | 7845  | 0        | 7704     | 1008    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

All (1008) 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:A:60:VAL:HA    | 1:A:75:VAL:HG22  | 1.24                     | 1.17              |
| 1:A:420:PRO:HG2  | 1:A:421:PRO:HD3  | 1.31                     | 1.10              |
| 1:A:419:THR:HG22 | 1:A:420:PRO:HD3  | 1.09                     | 1.09              |
| 2:B:282:LEU:HG   | 2:B:293:ILE:HG22 | 1.32                     | 1.09              |
| 2:B:85:GLN:HA    | 2:B:88:TRP:HB2   | 1.36                     | 1.07              |
| 2:B:38:CYS:HB3   | 2:B:144:TYR:HE2  | 1.12                     | 1.07              |
| 1:A:344:GLU:HG2  | 1:A:345:PRO:CD   | 1.85                     | 1.06              |
| 2:B:38:CYS:HB3   | 2:B:144:TYR:CE2  | 1.91                     | 1.06              |
| 1:A:344:GLU:CG   | 1:A:345:PRO:HD2  | 1.88                     | 1.04              |
| 2:B:34:LEU:HD21  | 2:B:62:ALA:HB2   | 1.38                     | 1.02              |
| 1:A:419:THR:HG22 | 1:A:420:PRO:CD   | 1.91                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:34:LEU:HB2   | 2:B:132:ILE:HD11 | 1.45                     | 0.98              |
| 1:A:344:GLU:HG2  | 1:A:345:PRO:HD2  | 1.00                     | 0.97              |
| 1:A:264:LEU:HD22 | 1:A:306:ASN:HD22 | 1.30                     | 0.97              |
| 1:A:540:LYS:HE3  | 1:A:540:LYS:HA   | 1.46                     | 0.97              |
| 2:B:183:TYR:CD2  | 2:B:380:ILE:HG23 | 2.00                     | 0.96              |
| 1:A:21:VAL:HB    | 1:A:58:THR:HA    | 1.50                     | 0.93              |
| 1:A:254:VAL:HB   | 1:A:289:LEU:HA   | 1.52                     | 0.92              |
| 1:A:164:MET:HE3  | 1:A:187:LEU:HD11 | 1.49                     | 0.91              |
| 1:A:56:TYR:HD1   | 1:A:56:TYR:H     | 1.18                     | 0.91              |
| 2:B:183:TYR:CD2  | 2:B:380:ILE:HD12 | 2.07                     | 0.90              |
| 1:A:164:MET:CE   | 1:A:187:LEU:HD11 | 2.01                     | 0.90              |
| 1:A:10:VAL:HG13  | 1:A:87:PHE:HZ    | 1.35                     | 0.90              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:CZ2  | 2.08                     | 0.89              |
| 1:A:181:TYR:HB3  | 3:A:600:TB9:H111 | 1.54                     | 0.88              |
| 2:B:81:ASN:ND2   | 2:B:154:LYS:HG3  | 1.89                     | 0.88              |
| 1:A:543:GLY:H    | 2:B:284:ARG:HG2  | 1.38                     | 0.88              |
| 1:A:341:ILE:HD11 | 1:A:350:LYS:HG2  | 1.56                     | 0.88              |
| 2:B:183:TYR:CE2  | 2:B:380:ILE:HD12 | 2.09                     | 0.87              |
| 1:A:97:PRO:HG3   | 1:A:234:LEU:HD21 | 1.56                     | 0.87              |
| 2:B:63:ILE:HD11  | 2:B:74:LEU:HD13  | 1.57                     | 0.87              |
| 2:B:261:VAL:HG21 | 2:B:283:LEU:HD11 | 1.58                     | 0.86              |
| 2:B:292:VAL:HG12 | 2:B:294:PRO:HD3  | 1.57                     | 0.85              |
| 2:B:393:ILE:HD13 | 2:B:398:TRP:HB2  | 1.58                     | 0.85              |
| 1:A:163:SER:HA   | 1:A:166:LYS:HE3  | 1.59                     | 0.84              |
| 2:B:10:VAL:HG11  | 2:B:153:TRP:HH2  | 1.41                     | 0.84              |
| 1:A:328:GLU:HB2  | 1:A:340:GLN:OE1  | 1.77                     | 0.84              |
| 2:B:341:ILE:HD13 | 2:B:383:TRP:HZ3  | 1.42                     | 0.84              |
| 2:B:125:ARG:HE   | 2:B:147:ASN:HA   | 1.40                     | 0.84              |
| 2:B:183:TYR:HD2  | 2:B:380:ILE:HG23 | 1.39                     | 0.83              |
| 2:B:38:CYS:CB    | 2:B:144:TYR:HE2  | 1.92                     | 0.83              |
| 1:A:435:VAL:HG12 | 2:B:290:THR:HG21 | 1.59                     | 0.83              |
| 1:A:19:PRO:HD3   | 1:A:80:LEU:HD13  | 1.59                     | 0.82              |
| 1:A:460:ASN:ND2  | 1:A:461:LYS:HE2  | 1.94                     | 0.82              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:HG3  | 2.15                     | 0.82              |
| 2:B:180:ILE:HG12 | 2:B:189:VAL:HG13 | 1.60                     | 0.81              |
| 2:B:128:THR:HG21 | 2:B:150:PRO:HG2  | 1.63                     | 0.81              |
| 1:A:517:LEU:HD12 | 1:A:518:VAL:HG23 | 1.63                     | 0.81              |
| 2:B:337:TRP:CZ3  | 2:B:368:LEU:HD13 | 2.16                     | 0.80              |
| 1:A:228:LEU:HA   | 1:A:232:TYR:O    | 1.81                     | 0.80              |
| 1:A:395:LYS:HG2  | 1:A:414:TRP:CH2  | 2.17                     | 0.80              |
| 2:B:143:ARG:HG2  | 2:B:143:ARG:HH11 | 1.47                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:81:ASN:OD1   | 1:A:153:TRP:HA   | 1.82                     | 0.79              |
| 1:A:490:GLY:O    | 1:A:528:LYS:HE2  | 1.83                     | 0.78              |
| 1:A:252:TRP:CD1  | 1:A:295:LEU:HD22 | 2.18                     | 0.78              |
| 1:A:108:VAL:HG22 | 1:A:188:TYR:CD2  | 2.19                     | 0.78              |
| 1:A:455:ALA:H    | 1:A:469:LEU:HD11 | 1.49                     | 0.78              |
| 2:B:397:THR:O    | 2:B:401:TRP:HD1  | 1.67                     | 0.77              |
| 1:A:369:THR:HG21 | 1:A:409:THR:HG21 | 1.66                     | 0.77              |
| 1:A:114:ALA:C    | 1:A:160:PHE:HE2  | 1.93                     | 0.77              |
| 1:A:241:VAL:HG11 | 1:A:266:TRP:CD1  | 2.19                     | 0.77              |
| 1:A:420:PRO:CG   | 1:A:421:PRO:HD3  | 2.13                     | 0.77              |
| 1:A:387:PRO:HG2  | 1:A:389:PHE:HE1  | 1.47                     | 0.77              |
| 2:B:389:PHE:O    | 2:B:415:GLU:HG2  | 1.85                     | 0.77              |
| 1:A:235:HIS:HB2  | 1:A:238:LYS:HG3  | 1.67                     | 0.76              |
| 1:A:12:LEU:HD22  | 1:A:83:ARG:O     | 1.86                     | 0.76              |
| 1:A:542:ILE:HG23 | 1:A:545:ASN:HB3  | 1.66                     | 0.76              |
| 1:A:109:LEU:HD13 | 1:A:216:THR:HG21 | 1.68                     | 0.76              |
| 1:A:454:LYS:HG3  | 1:A:552:VAL:HG13 | 1.68                     | 0.75              |
| 2:B:366:LYS:HE3  | 2:B:405:TYR:CE2  | 2.22                     | 0.75              |
| 1:A:26:LEU:HB3   | 1:A:31:ILE:HG13  | 1.68                     | 0.75              |
| 2:B:282:LEU:O    | 2:B:293:ILE:HG21 | 1.86                     | 0.75              |
| 2:B:31:ILE:O     | 2:B:35:VAL:HG23  | 1.87                     | 0.74              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:HZ2  | 1.49                     | 0.74              |
| 1:A:341:ILE:HG13 | 1:A:383:TRP:HH2  | 1.51                     | 0.74              |
| 1:A:503:LEU:HD13 | 1:A:535:TRP:CB   | 2.18                     | 0.73              |
| 2:B:319:TYR:CE2  | 2:B:383:TRP:HB3  | 2.23                     | 0.73              |
| 1:A:419:THR:CG2  | 1:A:420:PRO:HD3  | 2.05                     | 0.73              |
| 2:B:243:PRO:HA   | 2:B:245:VAL:HG12 | 1.69                     | 0.73              |
| 1:A:5:ILE:HD11   | 1:A:166:LYS:HD2  | 1.70                     | 0.73              |
| 1:A:23:GLN:NE2   | 1:A:26:LEU:HD13  | 2.03                     | 0.73              |
| 1:A:173:LYS:O    | 1:A:176:PRO:HD3  | 1.88                     | 0.73              |
| 1:A:10:VAL:HG13  | 1:A:87:PHE:CZ    | 2.20                     | 0.73              |
| 1:A:515:SER:O    | 1:A:519:ASN:HB2  | 1.87                     | 0.73              |
| 2:B:122:GLU:HG3  | 2:B:125:ARG:NH1  | 2.03                     | 0.73              |
| 2:B:331:LYS:O    | 2:B:424:LYS:HG3  | 1.87                     | 0.73              |
| 2:B:253:THR:HA   | 2:B:291:GLU:O    | 1.88                     | 0.73              |
| 2:B:66:LYS:O     | 2:B:69:THR:HG23  | 1.89                     | 0.72              |
| 2:B:363:ASN:O    | 2:B:366:LYS:HB3  | 1.90                     | 0.72              |
| 2:B:37:ILE:HG22  | 2:B:38:CYS:N     | 2.02                     | 0.72              |
| 1:A:27:THR:HB    | 1:A:30:LYS:HB2   | 1.70                     | 0.72              |
| 1:A:235:HIS:HB2  | 1:A:238:LYS:CG   | 2.18                     | 0.72              |
| 1:A:120:LEU:HD23 | 1:A:125:ARG:HG2  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:128:THR:HG21 | 2:B:150:PRO:CG   | 2.20                     | 0.71              |
| 1:A:503:LEU:HD13 | 1:A:535:TRP:HB2  | 1.72                     | 0.71              |
| 1:A:341:ILE:O    | 1:A:349:LEU:HB3  | 1.89                     | 0.71              |
| 2:B:249:LYS:HB2  | 2:B:252:TRP:CZ3  | 2.25                     | 0.71              |
| 1:A:254:VAL:HG12 | 1:A:258:GLN:HE21 | 1.55                     | 0.71              |
| 1:A:483:TYR:CZ   | 1:A:520:GLN:HG2  | 2.25                     | 0.71              |
| 1:A:227:PHE:O    | 1:A:233:GLU:HA   | 1.90                     | 0.71              |
| 1:A:276:VAL:HG12 | 1:A:276:VAL:O    | 1.88                     | 0.71              |
| 2:B:263:LYS:HD3  | 2:B:425:LEU:CD1  | 2.20                     | 0.70              |
| 2:B:365:VAL:HG22 | 2:B:393:ILE:HD11 | 1.73                     | 0.70              |
| 2:B:306:ASN:HA   | 2:B:309:ILE:HG22 | 1.71                     | 0.70              |
| 1:A:3:SER:HB3    | 1:A:212:TRP:C    | 2.17                     | 0.70              |
| 2:B:67:ASP:H     | 2:B:407:GLN:HE22 | 1.38                     | 0.70              |
| 2:B:202:ILE:O    | 2:B:206:ARG:HG3  | 1.91                     | 0.70              |
| 2:B:341:ILE:HD13 | 2:B:383:TRP:CZ3  | 2.25                     | 0.70              |
| 1:A:3:SER:O      | 1:A:5:ILE:HG22   | 1.90                     | 0.70              |
| 2:B:115:TYR:HE2  | 2:B:157:PRO:CA   | 2.04                     | 0.70              |
| 2:B:125:ARG:NE   | 2:B:147:ASN:HA   | 2.07                     | 0.70              |
| 2:B:328:GLU:O    | 2:B:339:TYR:HA   | 1.91                     | 0.70              |
| 1:A:240:THR:HG21 | 1:A:314:VAL:O    | 1.91                     | 0.70              |
| 1:A:261:VAL:HG13 | 1:A:276:VAL:HG11 | 1.74                     | 0.70              |
| 1:A:389:PHE:O    | 1:A:414:TRP:HA   | 1.91                     | 0.69              |
| 1:A:21:VAL:HG11  | 1:A:59:PRO:HD3   | 1.73                     | 0.69              |
| 2:B:34:LEU:HB2   | 2:B:132:ILE:CD1  | 2.20                     | 0.69              |
| 2:B:130:PHE:CZ   | 2:B:144:TYR:HD2  | 2.11                     | 0.69              |
| 1:A:425:LEU:HD13 | 1:A:428:GLN:OE1  | 1.92                     | 0.69              |
| 1:A:202:ILE:O    | 1:A:206:ARG:HB2  | 1.93                     | 0.69              |
| 1:A:59:PRO:O     | 1:A:75:VAL:HG13  | 1.92                     | 0.69              |
| 2:B:63:ILE:HG21  | 2:B:406:TRP:O    | 1.93                     | 0.69              |
| 1:A:56:TYR:N     | 1:A:56:TYR:CD1   | 2.61                     | 0.69              |
| 1:A:19:PRO:CD    | 1:A:80:LEU:HD13  | 2.23                     | 0.69              |
| 1:A:229:TRP:CE3  | 1:A:234:LEU:HD11 | 2.28                     | 0.68              |
| 2:B:61:PHE:HE2   | 2:B:76:ASP:HB2   | 1.58                     | 0.68              |
| 2:B:400:THR:HB   | 2:B:401:TRP:CD1  | 2.28                     | 0.68              |
| 2:B:61:PHE:CE2   | 2:B:76:ASP:HB2   | 2.28                     | 0.68              |
| 2:B:340:GLN:HG2  | 2:B:427:TYR:OH   | 1.93                     | 0.68              |
| 1:A:235:HIS:ND1  | 1:A:238:LYS:HG3  | 2.09                     | 0.68              |
| 1:A:97:PRO:CG    | 1:A:234:LEU:HD21 | 2.24                     | 0.68              |
| 1:A:229:TRP:CH2  | 3:A:600:TB9:H151 | 2.28                     | 0.68              |
| 1:A:483:TYR:HE1  | 1:A:524:GLN:HE21 | 1.40                     | 0.68              |
| 1:A:261:VAL:HG13 | 1:A:276:VAL:CG1  | 2.24                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:TYR:CE1  | 3:A:600:TB9:H162 | 2.29                     | 0.67              |
| 2:B:27:THR:HG22  | 2:B:28:GLU:H     | 1.58                     | 0.67              |
| 1:A:181:TYR:CB   | 3:A:600:TB9:H111 | 2.22                     | 0.67              |
| 2:B:201:LYS:O    | 2:B:204:GLU:HB3  | 1.95                     | 0.67              |
| 2:B:281:LYS:HA   | 2:B:284:ARG:HG3  | 1.75                     | 0.67              |
| 1:A:58:THR:HG22  | 1:A:59:PRO:CD    | 2.23                     | 0.67              |
| 1:A:156:SER:HB2  | 1:A:157:PRO:HD3  | 1.77                     | 0.67              |
| 1:A:455:ALA:N    | 1:A:469:LEU:HD11 | 2.10                     | 0.67              |
| 1:A:434:ILE:HG21 | 1:A:492:GLU:CG   | 2.24                     | 0.67              |
| 2:B:7:THR:O      | 2:B:9:PRO:HD3    | 1.94                     | 0.67              |
| 2:B:15:GLY:O     | 2:B:16:MET:HG2   | 1.94                     | 0.67              |
| 1:A:264:LEU:HD22 | 1:A:306:ASN:ND2  | 2.04                     | 0.67              |
| 2:B:354:TYR:CG   | 2:B:371:ALA:HB2  | 2.30                     | 0.66              |
| 2:B:366:LYS:HE3  | 2:B:405:TYR:CD2  | 2.30                     | 0.66              |
| 1:A:149:LEU:HD11 | 1:A:159:ILE:HG22 | 1.75                     | 0.66              |
| 2:B:242:GLN:HG2  | 2:B:243:PRO:HD3  | 1.76                     | 0.66              |
| 2:B:398:TRP:CD1  | 2:B:416:PHE:HE2  | 2.14                     | 0.66              |
| 2:B:296:THR:HG22 | 2:B:299:ALA:H    | 1.61                     | 0.66              |
| 1:A:96:HIS:HE1   | 1:A:269:GLN:HE21 | 1.43                     | 0.66              |
| 1:A:344:GLU:CG   | 1:A:345:PRO:CD   | 2.61                     | 0.66              |
| 1:A:411:ILE:HD13 | 1:A:414:TRP:HE1  | 1.59                     | 0.66              |
| 1:A:521:ILE:HG22 | 1:A:525:LEU:HD11 | 1.78                     | 0.65              |
| 2:B:183:TYR:HD2  | 2:B:380:ILE:CG2  | 2.07                     | 0.65              |
| 1:A:227:PHE:HB2  | 1:A:234:LEU:HB2  | 1.77                     | 0.65              |
| 2:B:130:PHE:CE1  | 2:B:144:TYR:HB2  | 2.31                     | 0.65              |
| 1:A:88:TRP:HA    | 1:A:88:TRP:CE3   | 2.30                     | 0.65              |
| 1:A:382:ILE:O    | 2:B:136:ASN:HB2  | 1.96                     | 0.65              |
| 2:B:38:CYS:HG    | 2:B:130:PHE:HZ   | 1.43                     | 0.65              |
| 2:B:282:LEU:HD11 | 2:B:295:LEU:H    | 1.61                     | 0.65              |
| 2:B:285:GLY:O    | 2:B:287:LYS:HG3  | 1.95                     | 0.65              |
| 2:B:254:VAL:HA   | 2:B:257:ILE:HG22 | 1.79                     | 0.65              |
| 2:B:299:ALA:O    | 2:B:302:GLU:HB2  | 1.96                     | 0.65              |
| 2:B:328:GLU:HG2  | 2:B:390:LYS:HD3  | 1.78                     | 0.65              |
| 1:A:116:PHE:HD1  | 1:A:148:VAL:HG23 | 1.62                     | 0.65              |
| 2:B:263:LYS:HD3  | 2:B:425:LEU:HD13 | 1.77                     | 0.65              |
| 2:B:330:GLN:HG2  | 2:B:338:THR:HB   | 1.79                     | 0.65              |
| 2:B:154:LYS:HG2  | 2:B:184:MET:CE   | 2.27                     | 0.64              |
| 1:A:238:LYS:HZ2  | 1:A:315:HIS:HB2  | 1.62                     | 0.64              |
| 2:B:326:ILE:HB   | 2:B:342:TYR:CE1  | 2.32                     | 0.64              |
| 2:B:67:ASP:H     | 2:B:407:GLN:NE2  | 1.96                     | 0.64              |
| 1:A:458:VAL:HG22 | 1:A:464:GLN:HG2  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:122:GLU:HG3  | 2:B:125:ARG:HH11 | 1.60                     | 0.64              |
| 2:B:70:LYS:O     | 2:B:70:LYS:HG3   | 1.98                     | 0.64              |
| 1:A:26:LEU:HD23  | 1:A:34:LEU:HD11  | 1.79                     | 0.64              |
| 1:A:58:THR:HG22  | 1:A:59:PRO:HD2   | 1.79                     | 0.63              |
| 1:A:109:LEU:HD22 | 1:A:216:THR:CG2  | 2.27                     | 0.63              |
| 1:A:500:GLN:OE1  | 1:A:500:GLN:HA   | 1.98                     | 0.63              |
| 1:A:23:GLN:HG3   | 1:A:61:PHE:HE1   | 1.63                     | 0.63              |
| 1:A:78:ARG:NH1   | 1:A:81:ASN:HB3   | 2.14                     | 0.63              |
| 1:A:124:PHE:HD1  | 1:A:124:PHE:O    | 1.80                     | 0.63              |
| 1:A:434:ILE:HD11 | 1:A:530:LYS:O    | 1.98                     | 0.63              |
| 2:B:10:VAL:HG11  | 2:B:153:TRP:CH2  | 2.29                     | 0.63              |
| 2:B:371:ALA:O    | 2:B:375:ILE:HD12 | 1.99                     | 0.63              |
| 1:A:106:VAL:HG13 | 1:A:189:VAL:O    | 1.99                     | 0.63              |
| 1:A:384:GLY:HA3  | 2:B:135:ILE:HD13 | 1.79                     | 0.63              |
| 2:B:335:GLY:O    | 2:B:337:TRP:CD1  | 2.51                     | 0.63              |
| 1:A:57:ASN:ND2   | 1:A:143:ARG:HH21 | 1.96                     | 0.63              |
| 1:A:260:LEU:HD21 | 1:A:279:LEU:HD13 | 1.79                     | 0.63              |
| 1:A:398:TRP:NE1  | 1:A:402:TRP:CD1  | 2.67                     | 0.63              |
| 1:A:229:TRP:CZ3  | 3:A:600:TB9:H151 | 2.34                     | 0.63              |
| 1:A:503:LEU:HG   | 1:A:507:GLN:HG3  | 1.81                     | 0.62              |
| 1:A:34:LEU:HD12  | 1:A:132:ILE:HG23 | 1.81                     | 0.62              |
| 1:A:125:ARG:NH1  | 1:A:147:ASN:HB3  | 2.14                     | 0.62              |
| 1:A:340:GLN:CB   | 1:A:351:THR:HG23 | 2.29                     | 0.62              |
| 1:A:123:ASP:O    | 1:A:126:LYS:HG2  | 1.99                     | 0.62              |
| 1:A:311:LYS:O    | 1:A:313:PRO:HD3  | 2.00                     | 0.62              |
| 1:A:545:ASN:O    | 1:A:548:VAL:HG22 | 1.98                     | 0.62              |
| 1:A:49:LYS:HG2   | 1:A:50:ILE:N     | 2.14                     | 0.62              |
| 2:B:335:GLY:O    | 2:B:337:TRP:HD1  | 1.83                     | 0.62              |
| 2:B:242:GLN:H    | 2:B:243:PRO:HD2  | 1.64                     | 0.62              |
| 1:A:460:ASN:HD21 | 1:A:461:LYS:HE2  | 1.62                     | 0.62              |
| 2:B:254:VAL:HG22 | 2:B:293:ILE:HG13 | 1.82                     | 0.62              |
| 1:A:444:GLY:O    | 1:A:477:THR:HB   | 1.99                     | 0.62              |
| 1:A:454:LYS:CG   | 1:A:552:VAL:HG13 | 2.29                     | 0.62              |
| 1:A:88:TRP:HA    | 1:A:88:TRP:HE3   | 1.65                     | 0.62              |
| 1:A:238:LYS:NZ   | 1:A:315:HIS:HB2  | 2.14                     | 0.62              |
| 2:B:282:LEU:HG   | 2:B:293:ILE:CG2  | 2.22                     | 0.62              |
| 1:A:60:VAL:CA    | 1:A:75:VAL:HG22  | 2.16                     | 0.61              |
| 1:A:397:THR:HG21 | 1:A:423:VAL:O    | 1.99                     | 0.61              |
| 1:A:341:ILE:HG13 | 1:A:383:TRP:CH2  | 2.33                     | 0.61              |
| 2:B:143:ARG:HG2  | 2:B:143:ARG:NH1  | 2.15                     | 0.61              |
| 2:B:325:LEU:HD11 | 2:B:383:TRP:CE3  | 2.35                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:63:ILE:HG23  | 2:B:403:THR:O    | 2.00                     | 0.61              |
| 2:B:270:ILE:HA   | 2:B:346:PHE:HB3  | 1.82                     | 0.61              |
| 1:A:178:ILE:HD12 | 1:A:191:SER:HB3  | 1.83                     | 0.61              |
| 1:A:238:LYS:HA   | 1:A:316:GLY:O    | 2.00                     | 0.61              |
| 2:B:120:LEU:HD22 | 2:B:150:PRO:CD   | 2.31                     | 0.61              |
| 2:B:323:LYS:HB2  | 2:B:343:GLN:NE2  | 2.16                     | 0.61              |
| 1:A:30:LYS:HA    | 1:A:33:ALA:HB3   | 1.83                     | 0.61              |
| 1:A:13:LYS:O     | 1:A:16:MET:HB2   | 2.01                     | 0.61              |
| 1:A:163:SER:HA   | 1:A:166:LYS:CE   | 2.31                     | 0.61              |
| 1:A:326:ILE:CG2  | 1:A:390:LYS:HD2  | 2.30                     | 0.61              |
| 1:A:30:LYS:NZ    | 1:A:64:LYS:HE2   | 2.16                     | 0.60              |
| 2:B:30:LYS:HG2   | 2:B:71:TRP:CH2   | 2.36                     | 0.60              |
| 2:B:329:ILE:HA   | 2:B:338:THR:O    | 2.01                     | 0.60              |
| 1:A:397:THR:HG21 | 1:A:424:LYS:HA   | 1.83                     | 0.60              |
| 1:A:270:ILE:O    | 1:A:272:PRO:HD3  | 2.01                     | 0.60              |
| 2:B:368:LEU:O    | 2:B:372:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:188:TYR:CG   | 3:A:600:TB9:H122 | 2.35                     | 0.60              |
| 1:A:395:LYS:HD2  | 1:A:399:GLU:HG3  | 1.84                     | 0.60              |
| 1:A:333:GLY:HA3  | 1:A:336:GLN:HB2  | 1.84                     | 0.60              |
| 1:A:408:ALA:HB1  | 2:B:364:ASP:HB3  | 1.83                     | 0.60              |
| 2:B:249:LYS:HB2  | 2:B:252:TRP:CE3  | 2.37                     | 0.60              |
| 1:A:434:ILE:HG21 | 1:A:492:GLU:HG3  | 1.84                     | 0.60              |
| 2:B:111:VAL:HG11 | 2:B:187:LEU:HD22 | 1.82                     | 0.60              |
| 2:B:403:THR:O    | 2:B:403:THR:HG23 | 2.00                     | 0.60              |
| 1:A:163:SER:CA   | 1:A:166:LYS:HE3  | 2.31                     | 0.60              |
| 1:A:341:ILE:HD11 | 1:A:350:LYS:CG   | 2.29                     | 0.60              |
| 1:A:542:ILE:CG2  | 1:A:545:ASN:HB3  | 2.31                     | 0.60              |
| 1:A:34:LEU:HB3   | 1:A:132:ILE:HD13 | 1.84                     | 0.59              |
| 1:A:440:PHE:CE2  | 1:A:457:TYR:CE1  | 2.90                     | 0.59              |
| 1:A:461:LYS:O    | 1:A:463:ARG:N    | 2.35                     | 0.59              |
| 2:B:59:PRO:HD2   | 2:B:76:ASP:HB3   | 1.83                     | 0.59              |
| 2:B:183:TYR:CE2  | 2:B:380:ILE:CD1  | 2.84                     | 0.59              |
| 1:A:430:GLU:CD   | 1:A:530:LYS:HG3  | 2.27                     | 0.59              |
| 2:B:183:TYR:HD2  | 2:B:380:ILE:HD12 | 1.60                     | 0.59              |
| 1:A:160:PHE:O    | 1:A:162:SER:N    | 2.35                     | 0.59              |
| 1:A:170:PRO:HG2  | 1:A:208:HIS:CE1  | 2.36                     | 0.59              |
| 1:A:542:ILE:HG12 | 1:A:545:ASN:H    | 1.66                     | 0.59              |
| 2:B:158:ALA:O    | 2:B:161:GLN:HB2  | 2.02                     | 0.59              |
| 1:A:232:TYR:OH   | 1:A:269:GLN:NE2  | 2.36                     | 0.59              |
| 1:A:16:MET:HE2   | 1:A:83:ARG:HG2   | 1.84                     | 0.59              |
| 1:A:179:VAL:HG12 | 3:A:600:TB9:H112 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:205:LEU:O    | 1:A:208:HIS:N    | 2.35                     | 0.59              |
| 1:A:191:SER:OG   | 1:A:198:HIS:ND1  | 2.36                     | 0.59              |
| 2:B:404:GLU:HB3  | 2:B:405:TYR:CD1  | 2.38                     | 0.59              |
| 1:A:23:GLN:HE21  | 1:A:26:LEU:HD13  | 1.67                     | 0.59              |
| 1:A:59:PRO:O     | 1:A:75:VAL:HA    | 2.03                     | 0.59              |
| 1:A:27:THR:O     | 1:A:31:ILE:N     | 2.36                     | 0.59              |
| 1:A:331:LYS:HE3  | 1:A:333:GLY:O    | 2.03                     | 0.59              |
| 2:B:115:TYR:CE2  | 2:B:157:PRO:HA   | 2.38                     | 0.59              |
| 2:B:397:THR:O    | 2:B:401:TRP:CD1  | 2.53                     | 0.59              |
| 1:A:130:PHE:CE1  | 1:A:144:TYR:HB2  | 2.38                     | 0.58              |
| 1:A:178:ILE:HB   | 1:A:191:SER:HB3  | 1.85                     | 0.58              |
| 1:A:178:ILE:HD11 | 1:A:189:VAL:HG12 | 1.84                     | 0.58              |
| 1:A:439:THR:HG23 | 2:B:289:LEU:HG   | 1.85                     | 0.58              |
| 2:B:52:PRO:O     | 2:B:54:ASN:N     | 2.36                     | 0.58              |
| 2:B:115:TYR:HE2  | 2:B:157:PRO:N    | 2.00                     | 0.58              |
| 2:B:252:TRP:CE3  | 2:B:252:TRP:HA   | 2.38                     | 0.58              |
| 1:A:543:GLY:HA2  | 1:A:546:GLU:HB2  | 1.84                     | 0.58              |
| 1:A:149:LEU:HD21 | 1:A:159:ILE:HG21 | 1.85                     | 0.58              |
| 1:A:390:LYS:HA   | 1:A:415:GLU:O    | 2.03                     | 0.58              |
| 1:A:434:ILE:HD12 | 1:A:494:ASN:OD1  | 2.03                     | 0.58              |
| 1:A:209:LEU:HB3  | 1:A:214:LEU:HB2  | 1.84                     | 0.58              |
| 1:A:438:GLU:HG2  | 1:A:459:THR:HB   | 1.86                     | 0.58              |
| 2:B:13:LYS:HA    | 2:B:87:PHE:CD2   | 2.39                     | 0.58              |
| 2:B:167:ILE:O    | 2:B:208:HIS:NE2  | 2.35                     | 0.58              |
| 1:A:546:GLU:O    | 1:A:549:ASP:HB2  | 2.04                     | 0.58              |
| 2:B:183:TYR:HE2  | 2:B:380:ILE:CD1  | 2.17                     | 0.58              |
| 1:A:431:LYS:O    | 1:A:532:TYR:HE1  | 1.87                     | 0.57              |
| 2:B:19:PRO:HG3   | 2:B:80:LEU:HB2   | 1.85                     | 0.57              |
| 2:B:115:TYR:HE2  | 2:B:157:PRO:HA   | 1.69                     | 0.57              |
| 2:B:160:PHE:O    | 2:B:160:PHE:CD2  | 2.57                     | 0.57              |
| 1:A:101:LYS:NZ   | 1:A:321:PRO:HG2  | 2.19                     | 0.57              |
| 1:A:518:VAL:HA   | 1:A:521:ILE:HD12 | 1.86                     | 0.57              |
| 1:A:160:PHE:CD1  | 1:A:161:GLN:N    | 2.73                     | 0.57              |
| 1:A:433:PRO:HG2  | 2:B:255:ASN:HB2  | 1.86                     | 0.57              |
| 1:A:19:PRO:HA    | 1:A:83:ARG:HH11  | 1.68                     | 0.57              |
| 1:A:182:GLN:HA   | 1:A:187:LEU:HD23 | 1.87                     | 0.57              |
| 1:A:288:ALA:HB1  | 1:A:291:GLU:CB   | 2.33                     | 0.57              |
| 1:A:354:TYR:CE2  | 1:A:370:GLU:HG2  | 2.40                     | 0.57              |
| 2:B:26:LEU:HD23  | 2:B:133:PRO:HG2  | 1.85                     | 0.57              |
| 2:B:163:SER:O    | 2:B:167:ILE:HG13 | 2.04                     | 0.57              |
| 1:A:56:TYR:HD1   | 1:A:56:TYR:N     | 1.95                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:420:PRO:HG2  | 1:A:421:PRO:CD   | 2.20                     | 0.57              |
| 1:A:503:LEU:HD13 | 1:A:535:TRP:HB3  | 1.87                     | 0.57              |
| 2:B:18:GLY:HA3   | 2:B:127:TYR:HD1  | 1.69                     | 0.57              |
| 2:B:266:TRP:CH2  | 2:B:346:PHE:CZ   | 2.93                     | 0.57              |
| 1:A:241:VAL:HG11 | 1:A:266:TRP:NE1  | 2.20                     | 0.57              |
| 1:A:275:LYS:HB3  | 1:A:336:GLN:HE22 | 1.70                     | 0.57              |
| 1:A:340:GLN:HB3  | 1:A:351:THR:HG23 | 1.86                     | 0.57              |
| 2:B:46:LYS:HE2   | 2:B:116:PHE:CG   | 2.40                     | 0.57              |
| 2:B:85:GLN:HG3   | 2:B:154:LYS:O    | 2.04                     | 0.57              |
| 2:B:248:GLU:O    | 2:B:248:GLU:HG3  | 2.05                     | 0.57              |
| 1:A:101:LYS:CE   | 1:A:321:PRO:HG2  | 2.35                     | 0.57              |
| 1:A:317:VAL:HG22 | 1:A:348:ASN:O    | 2.05                     | 0.57              |
| 2:B:194:GLU:O    | 2:B:197:GLN:N    | 2.38                     | 0.57              |
| 2:B:417:VAL:HG23 | 2:B:417:VAL:O    | 2.04                     | 0.57              |
| 1:A:168:LEU:HD22 | 1:A:180:ILE:CD1  | 2.35                     | 0.57              |
| 1:A:188:TYR:HB3  | 3:A:600:TB9:C7   | 2.35                     | 0.57              |
| 2:B:21:VAL:O     | 2:B:57:ASN:HB3   | 2.05                     | 0.57              |
| 2:B:65:LYS:HG3   | 2:B:407:GLN:O    | 2.05                     | 0.57              |
| 2:B:252:TRP:HA   | 2:B:252:TRP:HE3  | 1.69                     | 0.57              |
| 2:B:316:GLY:HA3  | 2:B:347:LYS:HB3  | 1.86                     | 0.57              |
| 1:A:19:PRO:HA    | 1:A:83:ARG:NH1   | 2.20                     | 0.56              |
| 1:A:153:TRP:O    | 1:A:155:GLY:N    | 2.38                     | 0.56              |
| 1:A:341:ILE:CD1  | 1:A:350:LYS:HG2  | 2.34                     | 0.56              |
| 2:B:33:ALA:HB1   | 2:B:71:TRP:CG    | 2.39                     | 0.56              |
| 2:B:112:GLY:HA2  | 2:B:115:TYR:CE1  | 2.40                     | 0.56              |
| 2:B:330:GLN:HG3  | 2:B:332:GLN:NE2  | 2.19                     | 0.56              |
| 1:A:168:LEU:O    | 1:A:172:LYS:HB2  | 2.05                     | 0.56              |
| 1:A:261:VAL:HG12 | 1:A:261:VAL:O    | 2.05                     | 0.56              |
| 1:A:511:ASP:O    | 1:A:522:ILE:HG12 | 2.05                     | 0.56              |
| 2:B:279:LEU:HD11 | 2:B:303:LEU:HD13 | 1.85                     | 0.56              |
| 2:B:319:TYR:CD2  | 2:B:383:TRP:CD1  | 2.93                     | 0.56              |
| 1:A:114:ALA:O    | 1:A:160:PHE:HE2  | 1.88                     | 0.56              |
| 1:A:149:LEU:HD11 | 1:A:159:ILE:CG2  | 2.35                     | 0.56              |
| 1:A:240:THR:HG22 | 1:A:270:ILE:HG21 | 1.86                     | 0.56              |
| 1:A:484:LEU:HD23 | 1:A:487:GLN:NE2  | 2.20                     | 0.56              |
| 2:B:61:PHE:HD2   | 2:B:74:LEU:HD23  | 1.71                     | 0.56              |
| 2:B:148:VAL:HG23 | 2:B:149:LEU:N    | 2.21                     | 0.56              |
| 1:A:23:GLN:NE2   | 1:A:61:PHE:HD1   | 2.03                     | 0.56              |
| 2:B:128:THR:OG1  | 2:B:146:TYR:HB2  | 2.05                     | 0.56              |
| 2:B:159:ILE:C    | 2:B:161:GLN:H    | 2.12                     | 0.56              |
| 1:A:452:LEU:HA   | 1:A:472:THR:HG22 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:393:ILE:CG2  | 2:B:416:PHE:HD2  | 2.18                     | 0.56              |
| 1:A:40:GLU:HG3   | 1:A:44:GLU:OE1   | 2.04                     | 0.56              |
| 2:B:50:ILE:HD13  | 2:B:145:GLN:HB2  | 1.87                     | 0.56              |
| 2:B:85:GLN:O     | 2:B:89:GLU:N     | 2.38                     | 0.56              |
| 1:A:503:LEU:O    | 1:A:507:GLN:HB2  | 2.06                     | 0.56              |
| 2:B:34:LEU:CD2   | 2:B:62:ALA:HB2   | 2.25                     | 0.56              |
| 2:B:261:VAL:CG2  | 2:B:283:LEU:HD11 | 2.35                     | 0.56              |
| 1:A:509:GLN:N    | 1:A:510:PRO:HD3  | 2.21                     | 0.56              |
| 1:A:339:TYR:CD2  | 1:A:375:ILE:HG12 | 2.41                     | 0.56              |
| 1:A:445:ALA:O    | 1:A:477:THR:HG21 | 2.06                     | 0.56              |
| 2:B:41:MET:O     | 2:B:47:ILE:HG12  | 2.06                     | 0.56              |
| 1:A:18:GLY:HA3   | 1:A:56:TYR:HD2   | 1.71                     | 0.56              |
| 2:B:50:ILE:HD12  | 2:B:54:ASN:ND2   | 2.21                     | 0.56              |
| 2:B:73:LYS:NZ    | 2:B:130:PHE:CZ   | 2.74                     | 0.56              |
| 2:B:92:LEU:HB2   | 2:B:158:ALA:HB1  | 1.88                     | 0.56              |
| 2:B:179:VAL:HG12 | 2:B:180:ILE:N    | 2.20                     | 0.56              |
| 2:B:319:TYR:HE2  | 2:B:383:TRP:HB3  | 1.70                     | 0.56              |
| 1:A:160:PHE:HD1  | 1:A:161:GLN:N    | 2.05                     | 0.55              |
| 1:A:164:MET:SD   | 1:A:214:LEU:HD13 | 2.46                     | 0.55              |
| 1:A:234:LEU:HB3  | 3:A:600:TB9:CL9  | 2.43                     | 0.55              |
| 2:B:271:TYR:HE1  | 2:B:313:PRO:HA   | 1.70                     | 0.55              |
| 1:A:2:ILE:HG23   | 1:A:117:SER:O    | 2.05                     | 0.55              |
| 1:A:500:GLN:O    | 1:A:504:GLY:N    | 2.36                     | 0.55              |
| 2:B:263:LYS:HD3  | 2:B:425:LEU:HD11 | 1.88                     | 0.55              |
| 1:A:130:PHE:HE2  | 1:A:146:TYR:CE1  | 2.23                     | 0.55              |
| 1:A:303:LEU:HD12 | 1:A:303:LEU:O    | 2.06                     | 0.55              |
| 1:A:384:GLY:C    | 1:A:385:LYS:HG2  | 2.31                     | 0.55              |
| 1:A:397:THR:CG2  | 1:A:424:LYS:HA   | 2.37                     | 0.55              |
| 2:B:124:PHE:CE2  | 2:B:153:TRP:CH2  | 2.95                     | 0.55              |
| 2:B:394:GLN:O    | 2:B:395:LYS:C    | 2.50                     | 0.55              |
| 1:A:54:ASN:ND2   | 1:A:126:LYS:HA   | 2.21                     | 0.55              |
| 1:A:130:PHE:O    | 1:A:143:ARG:HG3  | 2.07                     | 0.55              |
| 1:A:328:GLU:HG3  | 1:A:342:TYR:HE1  | 1.71                     | 0.55              |
| 1:A:19:PRO:HG3   | 1:A:80:LEU:HB2   | 1.89                     | 0.55              |
| 1:A:126:LYS:HG3  | 1:A:127:TYR:CE1  | 2.42                     | 0.55              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:N    | 2.75                     | 0.55              |
| 2:B:365:VAL:HG12 | 2:B:365:VAL:O    | 2.06                     | 0.55              |
| 1:A:169:GLU:N    | 1:A:170:PRO:HD2  | 2.22                     | 0.55              |
| 1:A:473:THR:O    | 1:A:475:GLN:N    | 2.39                     | 0.55              |
| 2:B:70:LYS:HD3   | 2:B:72:ARG:NH2   | 2.21                     | 0.55              |
| 2:B:149:LEU:O    | 2:B:150:PRO:C    | 2.50                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:154:LYS:HG2  | 2:B:184:MET:HE3  | 1.88                     | 0.55              |
| 2:B:369:THR:HG21 | 2:B:405:TYR:HB2  | 1.89                     | 0.55              |
| 2:B:390:LYS:HG2  | 2:B:415:GLU:OE2  | 2.07                     | 0.55              |
| 1:A:329:ILE:HA   | 1:A:338:THR:O    | 2.06                     | 0.54              |
| 2:B:54:ASN:HD21  | 2:B:129:ALA:CB   | 2.20                     | 0.54              |
| 1:A:241:VAL:CG1  | 1:A:266:TRP:HE1  | 2.21                     | 0.54              |
| 1:A:241:VAL:CG1  | 1:A:266:TRP:NE1  | 2.70                     | 0.54              |
| 1:A:544:GLY:N    | 2:B:284:ARG:HA   | 2.22                     | 0.54              |
| 2:B:198:HIS:O    | 2:B:202:ILE:HG12 | 2.07                     | 0.54              |
| 1:A:135:ILE:CB   | 1:A:138:GLU:HB2  | 2.38                     | 0.54              |
| 2:B:376:THR:HG22 | 2:B:376:THR:O    | 2.06                     | 0.54              |
| 1:A:130:PHE:CE2  | 1:A:146:TYR:CE1  | 2.96                     | 0.54              |
| 2:B:369:THR:HA   | 2:B:398:TRP:HH2  | 1.71                     | 0.54              |
| 1:A:108:VAL:HG22 | 1:A:188:TYR:CE2  | 2.43                     | 0.54              |
| 1:A:469:LEU:HD22 | 1:A:480:GLN:HG2  | 1.89                     | 0.54              |
| 1:A:191:SER:HB2  | 1:A:193:LEU:HG   | 1.89                     | 0.54              |
| 1:A:503:LEU:O    | 1:A:507:GLN:HG3  | 2.08                     | 0.54              |
| 2:B:323:LYS:HB2  | 2:B:343:GLN:HE21 | 1.72                     | 0.54              |
| 1:A:111:VAL:HG12 | 1:A:114:ALA:CB   | 2.37                     | 0.54              |
| 1:A:162:SER:OG   | 1:A:163:SER:N    | 2.40                     | 0.54              |
| 2:B:27:THR:O     | 2:B:31:ILE:HG13  | 2.08                     | 0.54              |
| 2:B:400:THR:HB   | 2:B:401:TRP:NE1  | 2.22                     | 0.54              |
| 2:B:401:TRP:CD1  | 2:B:401:TRP:N    | 2.75                     | 0.54              |
| 2:B:125:ARG:HG2  | 2:B:146:TYR:O    | 2.08                     | 0.54              |
| 2:B:364:ASP:C    | 2:B:366:LYS:H    | 2.16                     | 0.54              |
| 1:A:447:ASN:HB3  | 1:A:450:THR:OG1  | 2.06                     | 0.54              |
| 2:B:122:GLU:CG   | 2:B:125:ARG:HH11 | 2.21                     | 0.54              |
| 2:B:339:TYR:CE2  | 2:B:375:ILE:HG12 | 2.43                     | 0.54              |
| 1:A:171:PHE:CZ   | 1:A:205:LEU:HB2  | 2.43                     | 0.53              |
| 1:A:275:LYS:HG2  | 1:A:332:GLN:NE2  | 2.23                     | 0.53              |
| 2:B:197:GLN:O    | 2:B:200:THR:HB   | 2.08                     | 0.53              |
| 1:A:42:GLU:HG3   | 1:A:47:ILE:O     | 2.08                     | 0.53              |
| 1:A:253:THR:HG22 | 1:A:292:VAL:HA   | 1.90                     | 0.53              |
| 2:B:121:ASP:C    | 2:B:123:ASP:H    | 2.16                     | 0.53              |
| 1:A:26:LEU:CD2   | 1:A:34:LEU:HD11  | 2.38                     | 0.53              |
| 1:A:433:PRO:HD3  | 2:B:255:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:439:THR:OG1  | 2:B:288:ALA:HA   | 2.08                     | 0.53              |
| 1:A:483:TYR:HE1  | 1:A:524:GLN:NE2  | 2.06                     | 0.53              |
| 2:B:296:THR:O    | 2:B:299:ALA:HB3  | 2.08                     | 0.53              |
| 1:A:479:LEU:CD1  | 1:A:518:VAL:HG22 | 2.38                     | 0.53              |
| 2:B:288:ALA:C    | 2:B:290:THR:H    | 2.16                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:330:GLN:HG3  | 2:B:332:GLN:HE22 | 1.73                     | 0.53              |
| 1:A:454:LYS:HE2  | 1:A:555:GLY:HA3  | 1.90                     | 0.53              |
| 2:B:94:ILE:HG12  | 2:B:161:GLN:CD   | 2.34                     | 0.53              |
| 1:A:126:LYS:HG3  | 1:A:127:TYR:CD1  | 2.43                     | 0.53              |
| 1:A:320:ASP:H    | 1:A:343:GLN:HE22 | 1.54                     | 0.53              |
| 1:A:459:THR:HG23 | 1:A:463:ARG:HB3  | 1.89                     | 0.53              |
| 1:A:303:LEU:HD12 | 1:A:303:LEU:C    | 2.33                     | 0.53              |
| 1:A:465:LYS:O    | 1:A:466:VAL:HG23 | 2.09                     | 0.53              |
| 1:A:23:GLN:NE2   | 1:A:61:PHE:CD1   | 2.77                     | 0.53              |
| 1:A:54:ASN:HD21  | 1:A:126:LYS:HA   | 1.73                     | 0.53              |
| 1:A:375:ILE:HB   | 1:A:389:PHE:HZ   | 1.73                     | 0.53              |
| 1:A:408:ALA:HB1  | 2:B:364:ASP:CB   | 2.39                     | 0.53              |
| 2:B:266:TRP:CZ3  | 2:B:346:PHE:CE1  | 2.97                     | 0.53              |
| 2:B:396:GLU:O    | 2:B:397:THR:C    | 2.50                     | 0.53              |
| 1:A:224:GLU:O    | 1:A:227:PHE:CE1  | 2.62                     | 0.53              |
| 2:B:38:CYS:SG    | 2:B:130:PHE:HZ   | 2.32                     | 0.53              |
| 1:A:235:HIS:HB2  | 1:A:238:LYS:HG2  | 1.90                     | 0.53              |
| 2:B:115:TYR:O    | 2:B:117:SER:N    | 2.42                     | 0.52              |
| 1:A:50:ILE:HG22  | 1:A:51:GLY:N     | 2.24                     | 0.52              |
| 2:B:148:VAL:HG23 | 2:B:149:LEU:H    | 1.74                     | 0.52              |
| 1:A:47:ILE:HG23  | 1:A:144:TYR:HB3  | 1.90                     | 0.52              |
| 1:A:153:TRP:CZ3  | 1:A:159:ILE:HD12 | 2.44                     | 0.52              |
| 1:A:302:GLU:O    | 1:A:303:LEU:C    | 2.53                     | 0.52              |
| 2:B:28:GLU:HG2   | 2:B:32:LYS:CE    | 2.39                     | 0.52              |
| 2:B:178:ILE:CG2  | 2:B:189:VAL:HG12 | 2.39                     | 0.52              |
| 2:B:354:TYR:CD1  | 2:B:371:ALA:HB2  | 2.43                     | 0.52              |
| 2:B:373:GLN:HE22 | 2:B:406:TRP:HA   | 1.75                     | 0.52              |
| 1:A:96:HIS:CE1   | 1:A:269:GLN:HE21 | 2.26                     | 0.52              |
| 1:A:164:MET:HE1  | 1:A:187:LEU:HD11 | 1.91                     | 0.52              |
| 1:A:403:THR:HG23 | 2:B:334:GLN:HE21 | 1.74                     | 0.52              |
| 2:B:61:PHE:CZ    | 2:B:402:TRP:HZ2  | 2.27                     | 0.52              |
| 1:A:277:ARG:CZ   | 1:A:334:GLN:HG3  | 2.39                     | 0.52              |
| 1:A:325:LEU:HD13 | 1:A:383:TRP:CE3  | 2.44                     | 0.52              |
| 2:B:393:ILE:HG22 | 2:B:416:PHE:HD2  | 1.74                     | 0.52              |
| 1:A:196:GLY:HA2  | 1:A:199:ARG:HB2  | 1.92                     | 0.52              |
| 2:B:254:VAL:HA   | 2:B:257:ILE:CG2  | 2.37                     | 0.52              |
| 2:B:366:LYS:O    | 2:B:369:THR:HG22 | 2.10                     | 0.52              |
| 1:A:30:LYS:HZ1   | 1:A:64:LYS:HE2   | 1.75                     | 0.52              |
| 1:A:275:LYS:HB3  | 1:A:336:GLN:NE2  | 2.24                     | 0.52              |
| 2:B:257:ILE:HG23 | 2:B:283:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:23:GLN:HG3   | 1:A:61:PHE:CE1   | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:ASP:O    | 1:A:221:HIS:N    | 2.43                     | 0.52              |
| 1:A:310:LEU:HD23 | 1:A:310:LEU:O    | 2.09                     | 0.52              |
| 2:B:26:LEU:HD12  | 2:B:30:LYS:HB3   | 1.92                     | 0.52              |
| 2:B:120:LEU:HD22 | 2:B:150:PRO:HD2  | 1.92                     | 0.52              |
| 1:A:374:LYS:HD2  | 1:A:374:LYS:O    | 2.10                     | 0.51              |
| 2:B:50:ILE:CD1   | 2:B:145:GLN:HB2  | 2.40                     | 0.51              |
| 2:B:156:SER:H    | 2:B:157:PRO:HD2  | 1.74                     | 0.51              |
| 2:B:13:LYS:HA    | 2:B:87:PHE:HD2   | 1.75                     | 0.51              |
| 1:A:274:ILE:HG23 | 1:A:306:ASN:ND2  | 2.25                     | 0.51              |
| 1:A:379:SER:OG   | 1:A:387:PRO:HD2  | 2.10                     | 0.51              |
| 2:B:81:ASN:OD1   | 2:B:153:TRP:HD1  | 1.93                     | 0.51              |
| 2:B:115:TYR:CE2  | 2:B:157:PRO:CA   | 2.91                     | 0.51              |
| 1:A:512:LYS:HD3  | 1:A:512:LYS:H    | 1.75                     | 0.51              |
| 2:B:276:VAL:HG22 | 2:B:276:VAL:O    | 2.11                     | 0.51              |
| 2:B:372:VAL:HG12 | 2:B:372:VAL:O    | 2.10                     | 0.51              |
| 1:A:41:MET:HB2   | 1:A:47:ILE:HD12  | 1.91                     | 0.51              |
| 1:A:120:LEU:O    | 1:A:121:ASP:C    | 2.53                     | 0.51              |
| 1:A:247:PRO:HD3  | 1:A:263:LYS:NZ   | 2.25                     | 0.51              |
| 2:B:48:SER:OG    | 2:B:147:ASN:ND2  | 2.43                     | 0.51              |
| 1:A:124:PHE:O    | 1:A:124:PHE:CD1  | 2.61                     | 0.51              |
| 2:B:339:TYR:CD1  | 2:B:375:ILE:HD11 | 2.46                     | 0.51              |
| 2:B:273:GLY:O    | 2:B:309:ILE:HD13 | 2.11                     | 0.51              |
| 1:A:31:ILE:O     | 1:A:34:LEU:HB2   | 2.10                     | 0.51              |
| 2:B:62:ALA:HB1   | 2:B:71:TRP:CE3   | 2.46                     | 0.51              |
| 2:B:361:HIS:O    | 2:B:363:ASN:N    | 2.45                     | 0.50              |
| 1:A:180:ILE:HA   | 1:A:188:TYR:O    | 2.11                     | 0.50              |
| 1:A:470:THR:HG22 | 1:A:471:ASN:N    | 2.26                     | 0.50              |
| 2:B:236:PRO:HB3  | 2:B:381:VAL:HG11 | 1.94                     | 0.50              |
| 2:B:406:TRP:CZ2  | 2:B:412:PRO:HD2  | 2.46                     | 0.50              |
| 2:B:252:TRP:CH2  | 2:B:260:LEU:HD22 | 2.47                     | 0.50              |
| 2:B:259:LYS:HG3  | 2:B:260:LEU:N    | 2.26                     | 0.50              |
| 2:B:28:GLU:O     | 2:B:32:LYS:HE3   | 2.10                     | 0.50              |
| 2:B:58:THR:HG22  | 2:B:76:ASP:O     | 2.11                     | 0.50              |
| 1:A:121:ASP:OD1  | 1:A:123:ASP:HB2  | 2.12                     | 0.50              |
| 2:B:297:GLU:O    | 2:B:301:LEU:HD13 | 2.12                     | 0.50              |
| 2:B:323:LYS:CB   | 2:B:343:GLN:HE21 | 2.24                     | 0.50              |
| 1:A:331:LYS:HG3  | 1:A:336:GLN:O    | 2.11                     | 0.50              |
| 2:B:108:VAL:HG22 | 2:B:188:TYR:CD2  | 2.47                     | 0.50              |
| 1:A:60:VAL:HG23  | 1:A:130:PHE:HB2  | 1.94                     | 0.50              |
| 1:A:227:PHE:O    | 1:A:233:GLU:CA   | 2.58                     | 0.50              |
| 1:A:60:VAL:CG2   | 1:A:130:PHE:HB2  | 2.41                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:306:ASN:O    | 2:B:309:ILE:HG22 | 2.11                     | 0.50              |
| 2:B:345:PRO:HB2  | 2:B:346:PHE:CD2  | 2.47                     | 0.50              |
| 2:B:393:ILE:O    | 2:B:416:PHE:HB3  | 2.12                     | 0.50              |
| 1:A:188:TYR:CB   | 3:A:600:TB9:H122 | 2.41                     | 0.50              |
| 1:A:328:GLU:O    | 1:A:339:TYR:HA   | 2.12                     | 0.50              |
| 1:A:543:GLY:HA3  | 2:B:284:ARG:HB3  | 1.92                     | 0.50              |
| 2:B:114:ALA:C    | 2:B:116:PHE:N    | 2.69                     | 0.50              |
| 1:A:10:VAL:HB    | 1:A:124:PHE:CD2  | 2.47                     | 0.49              |
| 1:A:412:PRO:HG3  | 2:B:401:TRP:CH2  | 2.47                     | 0.49              |
| 1:A:475:GLN:HA   | 1:A:478:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:18:GLY:HA3   | 1:A:56:TYR:CD2   | 2.47                     | 0.49              |
| 1:A:118:VAL:HG13 | 1:A:119:PRO:HD2  | 1.94                     | 0.49              |
| 1:A:442:VAL:HG12 | 1:A:443:ASP:N    | 2.26                     | 0.49              |
| 2:B:206:ARG:HB3  | 2:B:206:ARG:NH1  | 2.26                     | 0.49              |
| 1:A:38:CYS:O     | 1:A:42:GLU:N     | 2.44                     | 0.49              |
| 1:A:55:PRO:HD2   | 1:A:56:TYR:CD1   | 2.47                     | 0.49              |
| 1:A:106:VAL:HA   | 1:A:189:VAL:O    | 2.12                     | 0.49              |
| 1:A:164:MET:SD   | 1:A:214:LEU:CD1  | 3.00                     | 0.49              |
| 1:A:479:LEU:HD22 | 1:A:521:ILE:HD13 | 1.95                     | 0.49              |
| 2:B:160:PHE:O    | 2:B:160:PHE:CG   | 2.65                     | 0.49              |
| 1:A:543:GLY:HA2  | 1:A:546:GLU:CB   | 2.43                     | 0.49              |
| 1:A:454:LYS:CE   | 1:A:555:GLY:HA3  | 2.42                     | 0.49              |
| 2:B:2:ILE:HG23   | 2:B:2:ILE:O      | 2.13                     | 0.49              |
| 2:B:299:ALA:O    | 2:B:302:GLU:N    | 2.46                     | 0.49              |
| 1:A:183:TYR:CE2  | 1:A:229:TRP:NE1  | 2.77                     | 0.49              |
| 1:A:398:TRP:NE1  | 1:A:402:TRP:NE1  | 2.61                     | 0.49              |
| 2:B:35:VAL:O     | 2:B:39:THR:HB    | 2.12                     | 0.49              |
| 1:A:61:PHE:N     | 1:A:74:LEU:O     | 2.46                     | 0.49              |
| 1:A:171:PHE:HB2  | 1:A:208:HIS:ND1  | 2.27                     | 0.49              |
| 1:A:479:LEU:HD22 | 1:A:521:ILE:CD1  | 2.43                     | 0.49              |
| 2:B:21:VAL:HG12  | 2:B:22:LYS:N     | 2.26                     | 0.49              |
| 2:B:113:ASP:O    | 2:B:116:PHE:HB2  | 2.13                     | 0.49              |
| 1:A:160:PHE:HE1  | 1:A:182:GLN:NE2  | 2.11                     | 0.49              |
| 1:A:207:GLN:OE1  | 1:A:207:GLN:HA   | 2.13                     | 0.49              |
| 1:A:212:TRP:H    | 1:A:212:TRP:CD1  | 2.31                     | 0.49              |
| 1:A:525:LEU:HD23 | 1:A:531:VAL:HG21 | 1.95                     | 0.49              |
| 2:B:64:LYS:HB2   | 2:B:68:SER:HA    | 1.94                     | 0.49              |
| 2:B:368:LEU:HD21 | 2:B:391:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:274:ILE:HA   | 1:A:306:ASN:OD1  | 2.12                     | 0.49              |
| 2:B:26:LEU:CD2   | 2:B:133:PRO:HG2  | 2.43                     | 0.49              |
| 2:B:253:THR:HB   | 2:B:256:ASP:OD2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:355:ALA:C    | 2:B:356:ARG:HG2  | 2.38                     | 0.49              |
| 1:A:118:VAL:O    | 1:A:148:VAL:HB   | 2.12                     | 0.49              |
| 1:A:381:VAL:HG22 | 2:B:25:PRO:HG3   | 1.95                     | 0.49              |
| 1:A:451:LYS:O    | 1:A:471:ASN:N    | 2.43                     | 0.49              |
| 2:B:34:LEU:HD21  | 2:B:62:ALA:CB    | 2.27                     | 0.49              |
| 2:B:80:LEU:O     | 2:B:80:LEU:HG    | 2.12                     | 0.49              |
| 1:A:121:ASP:O    | 1:A:125:ARG:HG3  | 2.13                     | 0.48              |
| 1:A:483:TYR:CE1  | 1:A:524:GLN:NE2  | 2.81                     | 0.48              |
| 2:B:115:TYR:OH   | 2:B:157:PRO:HB3  | 2.13                     | 0.48              |
| 2:B:282:LEU:HD11 | 2:B:295:LEU:N    | 2.27                     | 0.48              |
| 2:B:319:TYR:CE2  | 2:B:383:TRP:CD1  | 3.01                     | 0.48              |
| 1:A:332:GLN:HG3  | 1:A:333:GLY:N    | 2.27                     | 0.48              |
| 2:B:27:THR:HG22  | 2:B:28:GLU:N     | 2.27                     | 0.48              |
| 2:B:212:TRP:HA   | 2:B:212:TRP:CE3  | 2.48                     | 0.48              |
| 2:B:329:ILE:HD11 | 2:B:389:PHE:CD2  | 2.49                     | 0.48              |
| 1:A:382:ILE:O    | 2:B:135:ILE:HG22 | 2.13                     | 0.48              |
| 2:B:258:GLN:CG   | 2:B:283:LEU:HD22 | 2.43                     | 0.48              |
| 2:B:266:TRP:HE3  | 2:B:266:TRP:O    | 1.96                     | 0.48              |
| 1:A:183:TYR:CD1  | 1:A:183:TYR:C    | 2.91                     | 0.48              |
| 1:A:229:TRP:CZ3  | 1:A:234:LEU:HD11 | 2.49                     | 0.48              |
| 2:B:339:TYR:C    | 2:B:340:GLN:HG3  | 2.38                     | 0.48              |
| 2:B:354:TYR:CE1  | 2:B:356:ARG:HG3  | 2.49                     | 0.48              |
| 1:A:8:VAL:HG11   | 2:B:52:PRO:HD2   | 1.95                     | 0.48              |
| 1:A:181:TYR:CD1  | 1:A:182:GLN:O    | 2.67                     | 0.48              |
| 1:A:199:ARG:HB2  | 1:A:199:ARG:NH1  | 2.29                     | 0.48              |
| 1:A:419:THR:CG2  | 1:A:420:PRO:CD   | 2.78                     | 0.48              |
| 2:B:54:ASN:HD21  | 2:B:129:ALA:HB2  | 1.76                     | 0.48              |
| 2:B:111:VAL:HG23 | 2:B:111:VAL:O    | 2.12                     | 0.48              |
| 1:A:97:PRO:O     | 1:A:99:GLY:N     | 2.46                     | 0.48              |
| 1:A:102:LYS:HD3  | 1:A:237:ASP:CB   | 2.44                     | 0.48              |
| 1:A:196:GLY:HA2  | 1:A:199:ARG:CB   | 2.42                     | 0.48              |
| 1:A:229:TRP:HE3  | 1:A:234:LEU:HD11 | 1.78                     | 0.48              |
| 1:A:452:LEU:HB3  | 1:A:470:THR:HA   | 1.94                     | 0.48              |
| 2:B:295:LEU:O    | 2:B:296:THR:C    | 2.57                     | 0.48              |
| 2:B:315:HIS:CG   | 2:B:316:GLY:N    | 2.76                     | 0.48              |
| 1:A:337:TRP:NE1  | 1:A:367:GLN:HG2  | 2.29                     | 0.48              |
| 1:A:434:ILE:HG12 | 1:A:530:LYS:HG2  | 1.95                     | 0.48              |
| 2:B:169:GLU:OE1  | 2:B:173:LYS:HD2  | 2.13                     | 0.48              |
| 1:A:27:THR:HG22  | 1:A:29:GLU:HG2   | 1.96                     | 0.48              |
| 1:A:120:LEU:CD2  | 1:A:125:ARG:HG2  | 2.41                     | 0.48              |
| 1:A:160:PHE:CD1  | 1:A:160:PHE:C    | 2.92                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:326:ILE:HD12 | 1:A:342:TYR:CE2  | 2.49                     | 0.48              |
| 1:A:326:ILE:HG13 | 1:A:343:GLN:HA   | 1.96                     | 0.48              |
| 1:A:340:GLN:HB2  | 1:A:351:THR:HG23 | 1.96                     | 0.48              |
| 1:A:341:ILE:CG1  | 1:A:350:LYS:HB3  | 2.43                     | 0.48              |
| 1:A:538:ALA:HA   | 1:A:545:ASN:OD1  | 2.14                     | 0.48              |
| 2:B:288:ALA:O    | 2:B:290:THR:N    | 2.47                     | 0.48              |
| 1:A:57:ASN:HD22  | 1:A:143:ARG:HH21 | 1.61                     | 0.48              |
| 1:A:28:GLU:HA    | 1:A:31:ILE:HB    | 1.95                     | 0.48              |
| 1:A:305:GLU:O    | 1:A:308:GLU:HB3  | 2.14                     | 0.48              |
| 1:A:387:PRO:HG2  | 1:A:389:PHE:CE1  | 2.38                     | 0.48              |
| 1:A:453:GLY:H    | 1:A:472:THR:HG21 | 1.78                     | 0.48              |
| 1:A:540:LYS:C    | 1:A:542:ILE:N    | 2.70                     | 0.48              |
| 2:B:110:ASP:C    | 2:B:112:GLY:H    | 2.22                     | 0.48              |
| 2:B:337:TRP:HB2  | 2:B:354:TYR:HB3  | 1.95                     | 0.48              |
| 1:A:125:ARG:HB3  | 1:A:146:TYR:O    | 2.14                     | 0.47              |
| 1:A:244:ILE:HG23 | 1:A:263:LYS:HB3  | 1.97                     | 0.47              |
| 2:B:12:LEU:O     | 2:B:87:PHE:HD2   | 1.97                     | 0.47              |
| 2:B:249:LYS:C    | 2:B:251:SER:H    | 2.21                     | 0.47              |
| 2:B:311:LYS:O    | 2:B:313:PRO:HD3  | 2.14                     | 0.47              |
| 2:B:425:LEU:HD12 | 2:B:426:TRP:H    | 1.79                     | 0.47              |
| 1:A:78:ARG:HA    | 1:A:81:ASN:HB2   | 1.95                     | 0.47              |
| 2:B:340:GLN:HG2  | 2:B:427:TYR:CZ   | 2.48                     | 0.47              |
| 2:B:342:TYR:HB3  | 2:B:348:ASN:HB3  | 1.96                     | 0.47              |
| 1:A:111:VAL:HG12 | 1:A:111:VAL:O    | 2.13                     | 0.47              |
| 1:A:119:PRO:HA   | 1:A:148:VAL:HA   | 1.95                     | 0.47              |
| 2:B:366:LYS:HE3  | 2:B:405:TYR:HE2  | 1.74                     | 0.47              |
| 1:A:122:GLU:HG3  | 1:A:122:GLU:O    | 2.14                     | 0.47              |
| 1:A:123:ASP:O    | 1:A:125:ARG:N    | 2.47                     | 0.47              |
| 1:A:360:ALA:O    | 1:A:361:HIS:CG   | 2.67                     | 0.47              |
| 1:A:453:GLY:H    | 1:A:472:THR:CG2  | 2.27                     | 0.47              |
| 2:B:159:ILE:O    | 2:B:161:GLN:N    | 2.45                     | 0.47              |
| 2:B:233:GLU:O    | 2:B:235:HIS:CE1  | 2.68                     | 0.47              |
| 2:B:246:LEU:HD12 | 2:B:307:ARG:HE   | 1.80                     | 0.47              |
| 2:B:261:VAL:HG21 | 2:B:283:LEU:CD1  | 2.37                     | 0.47              |
| 2:B:422:LEU:HD12 | 2:B:422:LEU:N    | 2.29                     | 0.47              |
| 1:A:171:PHE:O    | 1:A:175:ASN:HB2  | 2.15                     | 0.47              |
| 1:A:270:ILE:HA   | 1:A:351:THR:OG1  | 2.14                     | 0.47              |
| 1:A:434:ILE:CD1  | 1:A:530:LYS:O    | 2.61                     | 0.47              |
| 1:A:540:LYS:C    | 1:A:542:ILE:H    | 2.21                     | 0.47              |
| 2:B:188:TYR:CE1  | 2:B:380:ILE:HG21 | 2.49                     | 0.47              |
| 2:B:257:ILE:O    | 2:B:261:VAL:HG23 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:417:VAL:C    | 2:B:419:THR:N    | 2.72                     | 0.47              |
| 1:A:125:ARG:HH12 | 1:A:147:ASN:HB3  | 1.79                     | 0.47              |
| 1:A:153:TRP:HZ3  | 1:A:159:ILE:HD12 | 1.80                     | 0.47              |
| 1:A:335:GLY:O    | 1:A:337:TRP:CD1  | 2.67                     | 0.47              |
| 1:A:441:TYR:HB3  | 1:A:548:VAL:HG11 | 1.97                     | 0.47              |
| 2:B:114:ALA:O    | 2:B:115:TYR:C    | 2.54                     | 0.47              |
| 2:B:174:GLN:OE1  | 2:B:174:GLN:N    | 2.47                     | 0.47              |
| 1:A:51:GLY:H     | 1:A:52:PRO:HD2   | 1.78                     | 0.47              |
| 1:A:122:GLU:HA   | 1:A:125:ARG:NE   | 2.30                     | 0.47              |
| 1:A:160:PHE:HE1  | 1:A:182:GLN:HE22 | 1.60                     | 0.47              |
| 2:B:103:LYS:HE3  | 2:B:192:ASP:HB2  | 1.97                     | 0.47              |
| 2:B:366:LYS:HA   | 2:B:369:THR:HG22 | 1.95                     | 0.47              |
| 1:A:108:VAL:CG2  | 1:A:188:TYR:CE2  | 2.98                     | 0.47              |
| 1:A:202:ILE:HG21 | 1:A:221:HIS:CB   | 2.45                     | 0.47              |
| 1:A:235:HIS:CB   | 1:A:238:LYS:HG3  | 2.42                     | 0.47              |
| 1:A:465:LYS:HD3  | 1:A:488:ASP:OD2  | 2.14                     | 0.47              |
| 2:B:181:TYR:CD1  | 2:B:182:GLN:N    | 2.83                     | 0.47              |
| 2:B:205:LEU:O    | 2:B:209:LEU:HD12 | 2.15                     | 0.47              |
| 2:B:183:TYR:CD2  | 2:B:380:ILE:CG2  | 2.84                     | 0.47              |
| 2:B:191:SER:HG   | 2:B:198:HIS:HD1  | 1.59                     | 0.47              |
| 1:A:59:PRO:C     | 1:A:75:VAL:HG13  | 2.40                     | 0.46              |
| 1:A:106:VAL:HG11 | 3:A:600:TB9:H72  | 1.97                     | 0.46              |
| 1:A:156:SER:O    | 1:A:157:PRO:C    | 2.57                     | 0.46              |
| 1:A:18:GLY:H     | 1:A:56:TYR:HE2   | 1.63                     | 0.46              |
| 1:A:51:GLY:N     | 1:A:52:PRO:HD2   | 2.30                     | 0.46              |
| 1:A:114:ALA:O    | 1:A:160:PHE:CE2  | 2.67                     | 0.46              |
| 1:A:248:GLU:HB3  | 1:A:307:ARG:NH2  | 2.30                     | 0.46              |
| 1:A:440:PHE:CD2  | 1:A:457:TYR:CD1  | 3.03                     | 0.46              |
| 1:A:32:LYS:O     | 1:A:35:VAL:N     | 2.49                     | 0.46              |
| 1:A:122:GLU:HA   | 1:A:125:ARG:HE   | 1.80                     | 0.46              |
| 1:A:163:SER:O    | 1:A:166:LYS:HB2  | 2.15                     | 0.46              |
| 2:B:128:THR:O    | 2:B:129:ALA:C    | 2.58                     | 0.46              |
| 1:A:10:VAL:HG12  | 1:A:124:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:10:VAL:HG21  | 1:A:153:TRP:HH2  | 1.81                     | 0.46              |
| 1:A:30:LYS:O     | 1:A:34:LEU:HG    | 2.15                     | 0.46              |
| 2:B:154:LYS:HA   | 2:B:184:MET:HE3  | 1.97                     | 0.46              |
| 2:B:377:THR:O    | 2:B:379:SER:N    | 2.49                     | 0.46              |
| 1:A:266:TRP:O    | 1:A:269:GLN:HG3  | 2.15                     | 0.46              |
| 1:A:373:GLN:O    | 1:A:374:LYS:C    | 2.59                     | 0.46              |
| 1:A:441:TYR:O    | 1:A:548:VAL:CG1  | 2.64                     | 0.46              |
| 1:A:455:ALA:HB3  | 1:A:469:LEU:HD21 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:483:TYR:OH   | 1:A:520:GLN:HG2  | 2.15                     | 0.46              |
| 1:A:519:ASN:O    | 1:A:522:ILE:HB   | 2.16                     | 0.46              |
| 1:A:543:GLY:N    | 2:B:284:ARG:HG2  | 2.20                     | 0.46              |
| 1:A:57:ASN:ND2   | 1:A:143:ARG:NH2  | 2.62                     | 0.46              |
| 1:A:120:LEU:HD21 | 1:A:125:ARG:HA   | 1.98                     | 0.46              |
| 2:B:3:SER:N      | 2:B:4:PRO:HD3    | 2.30                     | 0.46              |
| 2:B:292:VAL:O    | 2:B:293:ILE:CG1  | 2.64                     | 0.46              |
| 1:A:58:THR:HG22  | 1:A:59:PRO:HD3   | 1.97                     | 0.46              |
| 1:A:398:TRP:CD1  | 1:A:402:TRP:HE1  | 2.34                     | 0.46              |
| 1:A:433:PRO:HB3  | 2:B:289:LEU:HB2  | 1.97                     | 0.46              |
| 2:B:5:ILE:HG23   | 2:B:6:GLU:N      | 2.30                     | 0.46              |
| 1:A:12:LEU:HD21  | 1:A:124:PHE:CZ   | 2.50                     | 0.46              |
| 1:A:81:ASN:O     | 1:A:84:THR:HB    | 2.16                     | 0.46              |
| 1:A:114:ALA:HB3  | 1:A:160:PHE:CZ   | 2.51                     | 0.46              |
| 1:A:123:ASP:C    | 1:A:125:ARG:H    | 2.23                     | 0.46              |
| 1:A:218:ASP:O    | 1:A:221:HIS:HA   | 2.16                     | 0.46              |
| 2:B:110:ASP:O    | 2:B:112:GLY:N    | 2.49                     | 0.46              |
| 2:B:122:GLU:CG   | 2:B:125:ARG:NH1  | 2.76                     | 0.46              |
| 2:B:159:ILE:HG22 | 2:B:160:PHE:N    | 2.30                     | 0.46              |
| 2:B:377:THR:C    | 2:B:379:SER:H    | 2.24                     | 0.46              |
| 1:A:307:ARG:O    | 1:A:308:GLU:C    | 2.59                     | 0.46              |
| 2:B:278:GLN:O    | 2:B:299:ALA:HB2  | 2.16                     | 0.46              |
| 1:A:155:GLY:O    | 1:A:156:SER:C    | 2.58                     | 0.45              |
| 1:A:276:VAL:O    | 1:A:276:VAL:CG1  | 2.59                     | 0.45              |
| 1:A:482:ILE:HD11 | 1:A:502:ALA:HB1  | 1.97                     | 0.45              |
| 1:A:521:ILE:HG22 | 1:A:525:LEU:CD1  | 2.44                     | 0.45              |
| 1:A:542:ILE:O    | 1:A:546:GLU:N    | 2.49                     | 0.45              |
| 2:B:244:ILE:HG22 | 2:B:244:ILE:O    | 2.16                     | 0.45              |
| 1:A:168:LEU:CD2  | 1:A:205:LEU:HD11 | 2.47                     | 0.45              |
| 1:A:196:GLY:O    | 1:A:199:ARG:N    | 2.49                     | 0.45              |
| 1:A:212:TRP:CD1  | 1:A:212:TRP:N    | 2.84                     | 0.45              |
| 1:A:273:GLY:O    | 1:A:274:ILE:C    | 2.59                     | 0.45              |
| 2:B:64:LYS:CB    | 2:B:68:SER:HA    | 2.45                     | 0.45              |
| 2:B:238:LYS:C    | 2:B:239:TRP:CD1  | 2.94                     | 0.45              |
| 1:A:148:VAL:O    | 1:A:149:LEU:C    | 2.59                     | 0.45              |
| 1:A:233:GLU:O    | 1:A:239:TRP:HA   | 2.17                     | 0.45              |
| 1:A:406:TRP:CD2  | 1:A:407:GLN:N    | 2.84                     | 0.45              |
| 1:A:457:TYR:OH   | 1:A:488:ASP:HB2  | 2.15                     | 0.45              |
| 2:B:114:ALA:O    | 2:B:116:PHE:N    | 2.50                     | 0.45              |
| 2:B:238:LYS:C    | 2:B:239:TRP:HD1  | 2.24                     | 0.45              |
| 2:B:417:VAL:C    | 2:B:419:THR:H    | 2.23                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:GLU:CD   | 1:A:242:GLN:HB2  | 2.42                     | 0.45              |
| 1:A:340:GLN:HA   | 1:A:350:LYS:O    | 2.16                     | 0.45              |
| 2:B:370:GLU:O    | 2:B:372:VAL:N    | 2.49                     | 0.45              |
| 1:A:10:VAL:HG11  | 1:A:153:TRP:CH2  | 2.50                     | 0.45              |
| 1:A:11:LYS:O     | 1:A:85:GLN:HB3   | 2.16                     | 0.45              |
| 1:A:262:GLY:O    | 1:A:263:LYS:C    | 2.59                     | 0.45              |
| 1:A:85:GLN:NE2   | 2:B:53:GLU:HA    | 2.32                     | 0.45              |
| 1:A:89:GLU:O     | 1:A:90:VAL:C     | 2.59                     | 0.45              |
| 1:A:126:LYS:HE3  | 1:A:127:TYR:CZ   | 2.52                     | 0.45              |
| 1:A:162:SER:O    | 1:A:163:SER:C    | 2.59                     | 0.45              |
| 1:A:188:TYR:HB2  | 3:A:600:TB9:H122 | 1.99                     | 0.45              |
| 1:A:483:TYR:CE1  | 1:A:524:GLN:HG3  | 2.52                     | 0.45              |
| 2:B:378:GLU:O    | 2:B:382:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:90:VAL:O     | 1:A:91:GLN:NE2   | 2.49                     | 0.45              |
| 1:A:478:GLU:O    | 1:A:482:ILE:HG13 | 2.16                     | 0.45              |
| 2:B:19:PRO:HD3   | 2:B:80:LEU:CD1   | 2.46                     | 0.45              |
| 2:B:183:TYR:HE2  | 2:B:380:ILE:HD12 | 1.66                     | 0.45              |
| 2:B:368:LEU:O    | 2:B:372:VAL:N    | 2.50                     | 0.45              |
| 1:A:233:GLU:OE1  | 1:A:242:GLN:HB2  | 2.17                     | 0.45              |
| 1:A:295:LEU:HD12 | 1:A:295:LEU:HA   | 1.79                     | 0.45              |
| 2:B:153:TRP:HE3  | 2:B:156:SER:HG   | 1.63                     | 0.45              |
| 1:A:55:PRO:HD2   | 1:A:56:TYR:CE1   | 2.52                     | 0.45              |
| 1:A:101:LYS:HA   | 1:A:319:TYR:O    | 2.17                     | 0.45              |
| 1:A:341:ILE:HG13 | 1:A:350:LYS:HB3  | 1.98                     | 0.45              |
| 1:A:10:VAL:CG1   | 1:A:87:PHE:HZ    | 2.18                     | 0.45              |
| 2:B:96:HIS:HA    | 2:B:97:PRO:HD3   | 1.52                     | 0.45              |
| 2:B:121:ASP:O    | 2:B:123:ASP:N    | 2.50                     | 0.45              |
| 2:B:206:ARG:HA   | 2:B:209:LEU:HD12 | 1.99                     | 0.45              |
| 2:B:425:LEU:CG   | 2:B:426:TRP:H    | 2.29                     | 0.45              |
| 1:A:178:ILE:CG1  | 1:A:189:VAL:HG12 | 2.47                     | 0.44              |
| 1:A:241:VAL:HG21 | 1:A:266:TRP:CD1  | 2.51                     | 0.44              |
| 1:A:244:ILE:HD13 | 1:A:267:ALA:HB2  | 1.98                     | 0.44              |
| 1:A:260:LEU:CD2  | 1:A:279:LEU:HD13 | 2.45                     | 0.44              |
| 1:A:271:TYR:HA   | 1:A:272:PRO:HD3  | 1.70                     | 0.44              |
| 1:A:328:GLU:HG3  | 1:A:342:TYR:CE1  | 2.52                     | 0.44              |
| 2:B:156:SER:O    | 2:B:157:PRO:C    | 2.60                     | 0.44              |
| 2:B:332:GLN:OE1  | 2:B:425:LEU:N    | 2.50                     | 0.44              |
| 1:A:194:GLU:O    | 1:A:195:ILE:C    | 2.58                     | 0.44              |
| 1:A:235:HIS:O    | 1:A:237:ASP:N    | 2.51                     | 0.44              |
| 1:A:237:ASP:N    | 1:A:237:ASP:OD1  | 2.50                     | 0.44              |
| 1:A:254:VAL:HG12 | 1:A:258:GLN:NE2  | 2.26                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:264:LEU:O    | 1:A:274:ILE:HG21 | 2.17                     | 0.44              |
| 1:A:293:ILE:HA   | 1:A:294:PRO:HD2  | 1.74                     | 0.44              |
| 2:B:154:LYS:HA   | 2:B:184:MET:CE   | 2.47                     | 0.44              |
| 1:A:54:ASN:HD21  | 1:A:126:LYS:CA   | 2.29                     | 0.44              |
| 1:A:105:SER:HB3  | 1:A:198:HIS:ND1  | 2.32                     | 0.44              |
| 1:A:111:VAL:O    | 1:A:112:GLY:C    | 2.60                     | 0.44              |
| 1:A:339:TYR:CE1  | 1:A:352:GLY:C    | 2.95                     | 0.44              |
| 2:B:328:GLU:HB2  | 2:B:340:GLN:HE22 | 1.82                     | 0.44              |
| 2:B:365:VAL:HG21 | 2:B:397:THR:HG22 | 2.00                     | 0.44              |
| 1:A:389:PHE:HB2  | 1:A:413:GLU:O    | 2.17                     | 0.44              |
| 2:B:191:SER:OG   | 2:B:198:HIS:ND1  | 2.48                     | 0.44              |
| 2:B:424:LYS:O    | 2:B:424:LYS:HD3  | 2.18                     | 0.44              |
| 1:A:34:LEU:CB    | 1:A:132:ILE:HD13 | 2.47                     | 0.44              |
| 1:A:63:ILE:CD1   | 1:A:74:LEU:HD22  | 2.48                     | 0.44              |
| 1:A:143:ARG:HH11 | 1:A:143:ARG:HB2  | 1.82                     | 0.44              |
| 1:A:369:THR:O    | 1:A:370:GLU:C    | 2.59                     | 0.44              |
| 2:B:70:LYS:HE3   | 2:B:70:LYS:HB2   | 1.68                     | 0.44              |
| 1:A:245:VAL:O    | 1:A:246:LEU:C    | 2.61                     | 0.44              |
| 1:A:274:ILE:HG23 | 1:A:306:ASN:HD21 | 1.83                     | 0.44              |
| 2:B:242:GLN:HG2  | 2:B:243:PRO:CD   | 2.44                     | 0.44              |
| 2:B:296:THR:O    | 2:B:299:ALA:N    | 2.50                     | 0.44              |
| 1:A:360:ALA:C    | 1:A:361:HIS:CG   | 2.96                     | 0.44              |
| 1:A:379:SER:CB   | 1:A:387:PRO:HD2  | 2.48                     | 0.44              |
| 1:A:398:TRP:NE1  | 1:A:402:TRP:HE1  | 2.15                     | 0.44              |
| 1:A:471:ASN:OD1  | 1:A:471:ASN:O    | 2.36                     | 0.44              |
| 1:A:533:LEU:HD13 | 1:A:534:ALA:H    | 1.83                     | 0.44              |
| 1:A:440:PHE:CD2  | 1:A:457:TYR:CE1  | 3.06                     | 0.44              |
| 2:B:47:ILE:HD12  | 2:B:144:TYR:CD2  | 2.53                     | 0.44              |
| 1:A:135:ILE:O    | 1:A:136:ASN:C    | 2.60                     | 0.44              |
| 1:A:212:TRP:H    | 1:A:212:TRP:HD1  | 1.64                     | 0.44              |
| 1:A:247:PRO:HD3  | 1:A:263:LYS:HZ2  | 1.83                     | 0.44              |
| 1:A:340:GLN:OE1  | 1:A:340:GLN:O    | 2.35                     | 0.44              |
| 2:B:220:LYS:O    | 2:B:221:HIS:CG   | 2.71                     | 0.44              |
| 2:B:319:TYR:CE2  | 2:B:383:TRP:CG   | 3.06                     | 0.44              |
| 1:A:111:VAL:HG12 | 1:A:114:ALA:HB2  | 2.00                     | 0.43              |
| 1:A:253:THR:O    | 1:A:257:ILE:N    | 2.47                     | 0.43              |
| 1:A:271:TYR:HE1  | 1:A:313:PRO:HA   | 1.83                     | 0.43              |
| 1:A:427:TYR:CD2  | 1:A:525:LEU:HB3  | 2.52                     | 0.43              |
| 1:A:483:TYR:O    | 1:A:487:GLN:HG3  | 2.18                     | 0.43              |
| 2:B:279:LEU:HD21 | 2:B:303:LEU:CD1  | 2.48                     | 0.43              |
| 2:B:391:LEU:N    | 2:B:415:GLU:O    | 2.44                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:GLY:HA2   | 1:A:383:TRP:CD1  | 2.53                     | 0.43              |
| 1:A:265:ASN:OD1  | 1:A:353:LYS:NZ   | 2.46                     | 0.43              |
| 1:A:354:TYR:CZ   | 1:A:370:GLU:HG2  | 2.52                     | 0.43              |
| 2:B:67:ASP:O     | 2:B:68:SER:HB2   | 2.18                     | 0.43              |
| 2:B:354:TYR:HE2  | 2:B:374:LYS:HE3  | 1.82                     | 0.43              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:HG23 | 1.99                     | 0.43              |
| 1:A:440:PHE:CZ   | 1:A:489:SER:HB3  | 2.53                     | 0.43              |
| 1:A:544:GLY:H    | 2:B:284:ARG:HA   | 1.83                     | 0.43              |
| 2:B:325:LEU:HD12 | 2:B:341:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:111:VAL:HG12 | 1:A:114:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:395:LYS:HE3  | 1:A:399:GLU:OE2  | 2.18                     | 0.43              |
| 2:B:46:LYS:HE2   | 2:B:116:PHE:CD2  | 2.53                     | 0.43              |
| 2:B:120:LEU:HB2  | 2:B:148:VAL:O    | 2.18                     | 0.43              |
| 2:B:180:ILE:HG12 | 2:B:189:VAL:CG1  | 2.40                     | 0.43              |
| 2:B:345:PRO:C    | 2:B:347:LYS:H    | 2.26                     | 0.43              |
| 1:A:467:VAL:O    | 1:A:469:LEU:HG   | 2.18                     | 0.43              |
| 2:B:125:ARG:O    | 2:B:126:LYS:C    | 2.62                     | 0.43              |
| 2:B:271:TYR:CE1  | 2:B:313:PRO:HA   | 2.53                     | 0.43              |
| 2:B:282:LEU:HD21 | 2:B:295:LEU:N    | 2.33                     | 0.43              |
| 1:A:70:LYS:HD3   | 1:A:70:LYS:N     | 2.34                     | 0.43              |
| 1:A:363:ASN:O    | 1:A:367:GLN:HB2  | 2.18                     | 0.43              |
| 1:A:406:TRP:O    | 1:A:407:GLN:C    | 2.62                     | 0.43              |
| 1:A:459:THR:HG21 | 1:A:463:ARG:HD2  | 2.00                     | 0.43              |
| 1:A:482:ILE:O    | 1:A:483:TYR:C    | 2.61                     | 0.43              |
| 2:B:277:ARG:C    | 2:B:279:LEU:H    | 2.26                     | 0.43              |
| 2:B:347:LYS:HA   | 2:B:347:LYS:HD3  | 1.71                     | 0.43              |
| 1:A:22:LYS:HB2   | 1:A:22:LYS:HE3   | 1.74                     | 0.43              |
| 1:A:160:PHE:CE1  | 1:A:182:GLN:NE2  | 2.86                     | 0.43              |
| 1:A:217:PRO:O    | 1:A:219:LYS:N    | 2.51                     | 0.43              |
| 1:A:339:TYR:CD1  | 1:A:352:GLY:O    | 2.72                     | 0.43              |
| 1:A:375:ILE:CG2  | 1:A:389:PHE:HZ   | 2.32                     | 0.43              |
| 1:A:479:LEU:HD13 | 1:A:518:VAL:HG22 | 2.00                     | 0.43              |
| 2:B:41:MET:HB3   | 2:B:47:ILE:CD1   | 2.49                     | 0.43              |
| 2:B:84:THR:HG21  | 2:B:124:PHE:CZ   | 2.54                     | 0.43              |
| 2:B:85:GLN:C     | 2:B:85:GLN:CD    | 2.86                     | 0.43              |
| 2:B:258:GLN:HG2  | 2:B:283:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:77:PHE:HB3   | 1:A:80:LEU:HB3   | 2.00                     | 0.43              |
| 1:A:130:PHE:CZ   | 1:A:144:TYR:HB2  | 2.54                     | 0.43              |
| 1:A:188:TYR:HB2  | 3:A:600:TB9:C12  | 2.49                     | 0.43              |
| 2:B:18:GLY:HA3   | 2:B:127:TYR:CD1  | 2.52                     | 0.43              |
| 2:B:63:ILE:HD13  | 2:B:406:TRP:O    | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:175:ASN:OD1  | 2:B:201:LYS:HD2  | 2.18                     | 0.43              |
| 2:B:393:ILE:HG21 | 2:B:398:TRP:HB2  | 2.01                     | 0.43              |
| 1:A:115:TYR:O    | 1:A:149:LEU:HB2  | 2.19                     | 0.43              |
| 1:A:156:SER:O    | 1:A:158:ALA:N    | 2.51                     | 0.43              |
| 1:A:203:GLU:O    | 1:A:207:GLN:HG2  | 2.18                     | 0.43              |
| 1:A:326:ILE:O    | 1:A:341:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:441:TYR:O    | 1:A:548:VAL:HG11 | 2.18                     | 0.43              |
| 1:A:442:VAL:CG1  | 1:A:481:ALA:HB1  | 2.48                     | 0.43              |
| 1:A:472:THR:O    | 1:A:473:THR:HG23 | 2.19                     | 0.43              |
| 2:B:128:THR:HB   | 2:B:146:TYR:HD2  | 1.84                     | 0.43              |
| 2:B:366:LYS:O    | 2:B:368:LEU:N    | 2.52                     | 0.43              |
| 1:A:120:LEU:O    | 1:A:125:ARG:NE   | 2.52                     | 0.43              |
| 1:A:363:ASN:OD1  | 1:A:364:ASP:N    | 2.52                     | 0.43              |
| 1:A:184:MET:HE3  | 1:A:184:MET:HB3  | 1.84                     | 0.42              |
| 2:B:279:LEU:HD21 | 2:B:303:LEU:HD12 | 2.01                     | 0.42              |
| 2:B:362:THR:O    | 2:B:363:ASN:C    | 2.62                     | 0.42              |
| 1:A:475:GLN:C    | 1:A:477:THR:H    | 2.26                     | 0.42              |
| 1:A:479:LEU:HD11 | 1:A:518:VAL:HG22 | 2.01                     | 0.42              |
| 2:B:350:LYS:HD3  | 2:B:351:THR:N    | 2.35                     | 0.42              |
| 1:A:60:VAL:HG22  | 1:A:75:VAL:HG21  | 2.02                     | 0.42              |
| 1:A:275:LYS:HD3  | 1:A:336:GLN:NE2  | 2.33                     | 0.42              |
| 1:A:521:ILE:O    | 1:A:525:LEU:HG   | 2.19                     | 0.42              |
| 2:B:115:TYR:C    | 2:B:117:SER:H    | 2.25                     | 0.42              |
| 1:A:26:LEU:HD22  | 1:A:60:VAL:O     | 2.19                     | 0.42              |
| 1:A:438:GLU:HB3  | 1:A:440:PHE:HE1  | 1.84                     | 0.42              |
| 1:A:443:ASP:OD2  | 1:A:548:VAL:HG23 | 2.19                     | 0.42              |
| 2:B:320:ASP:O    | 2:B:322:SER:N    | 2.52                     | 0.42              |
| 1:A:50:ILE:CG2   | 1:A:51:GLY:N     | 2.82                     | 0.42              |
| 1:A:215:THR:C    | 1:A:217:PRO:HD3  | 2.45                     | 0.42              |
| 2:B:85:GLN:O     | 2:B:85:GLN:CG    | 2.67                     | 0.42              |
| 2:B:121:ASP:C    | 2:B:123:ASP:N    | 2.78                     | 0.42              |
| 2:B:159:ILE:C    | 2:B:161:GLN:N    | 2.75                     | 0.42              |
| 2:B:214:LEU:HD13 | 2:B:214:LEU:HA   | 1.87                     | 0.42              |
| 1:A:37:ILE:O     | 1:A:41:MET:HG3   | 2.20                     | 0.42              |
| 1:A:363:ASN:CG   | 1:A:364:ASP:N    | 2.77                     | 0.42              |
| 1:A:492:GLU:O    | 1:A:492:GLU:HG2  | 2.20                     | 0.42              |
| 2:B:28:GLU:HG2   | 2:B:32:LYS:HE2   | 2.01                     | 0.42              |
| 1:A:12:LEU:HD23  | 1:A:84:THR:HA    | 2.02                     | 0.42              |
| 1:A:151:GLN:O    | 1:A:151:GLN:HG2  | 2.20                     | 0.42              |
| 2:B:132:ILE:HA   | 2:B:133:PRO:HD3  | 1.75                     | 0.42              |
| 2:B:223:LYS:O    | 2:B:224:GLU:C    | 2.63                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:298:GLU:HA   | 2:B:301:LEU:HD22 | 2.01                     | 0.42              |
| 2:B:319:TYR:CE2  | 2:B:383:TRP:CB   | 2.99                     | 0.42              |
| 2:B:377:THR:C    | 2:B:379:SER:N    | 2.74                     | 0.42              |
| 1:A:104:LYS:HB2  | 1:A:192:ASP:HA   | 2.01                     | 0.42              |
| 2:B:8:VAL:O      | 2:B:9:PRO:C      | 2.58                     | 0.42              |
| 2:B:249:LYS:C    | 2:B:251:SER:N    | 2.78                     | 0.42              |
| 1:A:326:ILE:HG21 | 1:A:390:LYS:HD2  | 2.00                     | 0.42              |
| 1:A:379:SER:HB2  | 1:A:383:TRP:CE3  | 2.55                     | 0.42              |
| 2:B:84:THR:OG1   | 2:B:85:GLN:N     | 2.53                     | 0.42              |
| 1:A:101:LYS:HD3  | 1:A:321:PRO:CD   | 2.50                     | 0.42              |
| 1:A:129:ALA:HB1  | 1:A:143:ARG:HD3  | 2.02                     | 0.42              |
| 1:A:408:ALA:CB   | 2:B:364:ASP:HB3  | 2.49                     | 0.42              |
| 1:A:500:GLN:O    | 1:A:501:TYR:C    | 2.62                     | 0.42              |
| 2:B:46:LYS:HD3   | 2:B:116:PHE:CE1  | 2.54                     | 0.42              |
| 2:B:337:TRP:CE3  | 2:B:368:LEU:HD13 | 2.53                     | 0.42              |
| 2:B:365:VAL:HG11 | 2:B:401:TRP:HB2  | 2.01                     | 0.42              |
| 2:B:87:PHE:O     | 2:B:87:PHE:CD1   | 2.73                     | 0.41              |
| 2:B:239:TRP:HB2  | 2:B:350:LYS:HE2  | 2.01                     | 0.41              |
| 2:B:281:LYS:HA   | 2:B:284:ARG:CG   | 2.45                     | 0.41              |
| 2:B:292:VAL:HG12 | 2:B:293:ILE:N    | 2.35                     | 0.41              |
| 2:B:376:THR:O    | 2:B:376:THR:CG2  | 2.68                     | 0.41              |
| 1:A:10:VAL:HG22  | 1:A:159:ILE:HD11 | 2.01                     | 0.41              |
| 1:A:85:GLN:O     | 1:A:154:LYS:HE3  | 2.20                     | 0.41              |
| 1:A:195:ILE:H    | 1:A:195:ILE:HG12 | 1.64                     | 0.41              |
| 1:A:235:HIS:CG   | 1:A:238:LYS:HG3  | 2.55                     | 0.41              |
| 1:A:252:TRP:HZ3  | 1:A:256:ASP:OD1  | 2.04                     | 0.41              |
| 1:A:326:ILE:HB   | 1:A:342:TYR:O    | 2.20                     | 0.41              |
| 2:B:85:GLN:O     | 2:B:85:GLN:HG2   | 2.20                     | 0.41              |
| 1:A:171:PHE:CD1  | 1:A:205:LEU:HD13 | 2.55                     | 0.41              |
| 1:A:276:VAL:O    | 1:A:280:SER:HB2  | 2.20                     | 0.41              |
| 2:B:73:LYS:HG3   | 2:B:74:LEU:N     | 2.35                     | 0.41              |
| 2:B:306:ASN:CA   | 2:B:309:ILE:HG22 | 2.46                     | 0.41              |
| 2:B:326:ILE:CB   | 2:B:342:TYR:CE1  | 3.03                     | 0.41              |
| 2:B:336:GLN:OE1  | 2:B:353:LYS:HE2  | 2.19                     | 0.41              |
| 1:A:65:LYS:HD3   | 1:A:66:LYS:H     | 1.85                     | 0.41              |
| 1:A:205:LEU:O    | 1:A:206:ARG:C    | 2.63                     | 0.41              |
| 1:A:319:TYR:CE1  | 1:A:325:LEU:HD21 | 2.55                     | 0.41              |
| 1:A:326:ILE:HG22 | 1:A:390:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:536:VAL:HB   | 1:A:542:ILE:CD1  | 2.51                     | 0.41              |
| 2:B:10:VAL:HA    | 2:B:88:TRP:CH2   | 2.56                     | 0.41              |
| 2:B:249:LYS:HA   | 2:B:249:LYS:HD2  | 1.93                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:349:LEU:O    | 2:B:350:LYS:HB2  | 2.21                     | 0.41              |
| 1:A:39:THR:HG23  | 1:A:43:LYS:HE3   | 2.02                     | 0.41              |
| 1:A:96:HIS:HE1   | 1:A:269:GLN:NE2  | 2.15                     | 0.41              |
| 1:A:109:LEU:O    | 1:A:186:ASP:HA   | 2.20                     | 0.41              |
| 1:A:153:TRP:CE3  | 1:A:156:SER:N    | 2.89                     | 0.41              |
| 1:A:180:ILE:HG22 | 1:A:181:TYR:N    | 2.36                     | 0.41              |
| 2:B:48:SER:N     | 2:B:147:ASN:HD21 | 2.19                     | 0.41              |
| 2:B:292:VAL:O    | 2:B:293:ILE:HG13 | 2.21                     | 0.41              |
| 2:B:332:GLN:NE2  | 2:B:427:TYR:OXT  | 2.53                     | 0.41              |
| 1:A:12:LEU:CD2   | 1:A:84:THR:HA    | 2.50                     | 0.41              |
| 1:A:113:ASP:C    | 1:A:115:TYR:H    | 2.29                     | 0.41              |
| 1:A:188:TYR:HB3  | 3:A:600:TB9:H71  | 2.02                     | 0.41              |
| 1:A:196:GLY:O    | 1:A:199:ARG:HB3  | 2.20                     | 0.41              |
| 1:A:398:TRP:HE1  | 1:A:402:TRP:NE1  | 2.18                     | 0.41              |
| 1:A:407:GLN:OE1  | 2:B:418:ASN:HA   | 2.21                     | 0.41              |
| 2:B:96:HIS:ND1   | 2:B:181:TYR:CE2  | 2.81                     | 0.41              |
| 1:A:19:PRO:HD3   | 1:A:80:LEU:CD1   | 2.40                     | 0.41              |
| 1:A:107:THR:OG1  | 1:A:202:ILE:CD1  | 2.68                     | 0.41              |
| 1:A:167:ILE:HD13 | 1:A:212:TRP:HB2  | 2.03                     | 0.41              |
| 1:A:219:LYS:C    | 1:A:221:HIS:N    | 2.73                     | 0.41              |
| 1:A:229:TRP:O    | 1:A:232:TYR:HB2  | 2.20                     | 0.41              |
| 1:A:279:LEU:CD2  | 1:A:295:LEU:HD11 | 2.51                     | 0.41              |
| 2:B:419:THR:HA   | 2:B:420:PRO:HD3  | 1.59                     | 0.41              |
| 1:A:26:LEU:HB3   | 1:A:31:ILE:CG1   | 2.45                     | 0.41              |
| 1:A:311:LYS:O    | 1:A:313:PRO:CD   | 2.68                     | 0.41              |
| 1:A:368:LEU:O    | 1:A:371:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:399:GLU:HG2  | 1:A:402:TRP:CZ2  | 2.55                     | 0.41              |
| 2:B:73:LYS:HG3   | 2:B:74:LEU:H     | 1.86                     | 0.41              |
| 2:B:130:PHE:CD1  | 2:B:144:TYR:HB2  | 2.55                     | 0.41              |
| 2:B:339:TYR:CZ   | 2:B:375:ILE:HG12 | 2.55                     | 0.41              |
| 1:A:65:LYS:CD    | 1:A:66:LYS:H     | 2.34                     | 0.41              |
| 1:A:109:LEU:HD22 | 1:A:216:THR:HG22 | 2.02                     | 0.41              |
| 1:A:130:PHE:CE2  | 1:A:146:TYR:HE1  | 2.37                     | 0.41              |
| 1:A:269:GLN:O    | 1:A:351:THR:N    | 2.51                     | 0.41              |
| 1:A:317:VAL:HG23 | 1:A:349:LEU:HD12 | 2.03                     | 0.41              |
| 2:B:52:PRO:C     | 2:B:54:ASN:N     | 2.78                     | 0.41              |
| 2:B:194:GLU:O    | 2:B:195:ILE:C    | 2.64                     | 0.41              |
| 2:B:271:TYR:C    | 2:B:273:GLY:N    | 2.78                     | 0.41              |
| 2:B:296:THR:HG22 | 2:B:299:ALA:N    | 2.32                     | 0.41              |
| 2:B:312:GLU:HA   | 2:B:313:PRO:HD3  | 1.83                     | 0.41              |
| 2:B:354:TYR:CE2  | 2:B:374:LYS:HE3  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:10:VAL:O     | 1:A:124:PHE:HD2  | 2.04                     | 0.41              |
| 1:A:65:LYS:HD3   | 1:A:66:LYS:N     | 2.35                     | 0.41              |
| 1:A:161:GLN:O    | 1:A:161:GLN:HG2  | 2.21                     | 0.41              |
| 1:A:178:ILE:CD1  | 1:A:189:VAL:HG12 | 2.49                     | 0.41              |
| 1:A:301:LEU:O    | 1:A:305:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:340:GLN:HA   | 1:A:351:THR:HA   | 2.03                     | 0.41              |
| 1:A:400:THR:O    | 1:A:404:GLU:HG2  | 2.20                     | 0.41              |
| 2:B:46:LYS:HE2   | 2:B:116:PHE:CD1  | 2.56                     | 0.41              |
| 2:B:77:PHE:HD2   | 2:B:152:GLY:HA3  | 1.86                     | 0.41              |
| 2:B:149:LEU:O    | 2:B:151:GLN:N    | 2.53                     | 0.41              |
| 2:B:156:SER:N    | 2:B:157:PRO:HD2  | 2.36                     | 0.41              |
| 2:B:173:LYS:O    | 2:B:174:GLN:C    | 2.64                     | 0.41              |
| 2:B:181:TYR:HD1  | 2:B:182:GLN:H    | 1.69                     | 0.41              |
| 2:B:207:GLN:O    | 2:B:210:LEU:HB3  | 2.20                     | 0.41              |
| 2:B:315:HIS:ND1  | 2:B:316:GLY:N    | 2.69                     | 0.41              |
| 1:A:105:SER:O    | 1:A:198:HIS:CE1  | 2.74                     | 0.40              |
| 1:A:160:PHE:C    | 1:A:162:SER:H    | 2.29                     | 0.40              |
| 1:A:181:TYR:HB3  | 3:A:600:TB9:H121 | 2.02                     | 0.40              |
| 1:A:196:GLY:C    | 1:A:199:ARG:H    | 2.29                     | 0.40              |
| 1:A:274:ILE:HD13 | 1:A:306:ASN:CG   | 2.46                     | 0.40              |
| 1:A:460:ASN:OD1  | 1:A:460:ASN:N    | 2.53                     | 0.40              |
| 2:B:257:ILE:HG23 | 2:B:283:LEU:CD2  | 2.51                     | 0.40              |
| 1:A:3:SER:HB3    | 1:A:212:TRP:O    | 2.20                     | 0.40              |
| 1:A:57:ASN:HA    | 1:A:129:ALA:O    | 2.21                     | 0.40              |
| 1:A:473:THR:O    | 1:A:474:ASN:C    | 2.65                     | 0.40              |
| 1:A:484:LEU:HD23 | 1:A:487:GLN:HE21 | 1.85                     | 0.40              |
| 1:A:494:ASN:HD22 | 2:B:289:LEU:HD12 | 1.86                     | 0.40              |
| 2:B:171:PHE:CE2  | 2:B:205:LEU:HB2  | 2.56                     | 0.40              |
| 2:B:206:ARG:NH1  | 2:B:217:PRO:CG   | 2.85                     | 0.40              |
| 2:B:281:LYS:HA   | 2:B:284:ARG:CD   | 2.51                     | 0.40              |
| 2:B:368:LEU:O    | 2:B:371:ALA:N    | 2.54                     | 0.40              |
| 1:A:216:THR:HG22 | 1:A:216:THR:O    | 2.21                     | 0.40              |
| 1:A:350:LYS:HD3  | 1:A:378:GLU:OE2  | 2.20                     | 0.40              |
| 1:A:381:VAL:O    | 1:A:381:VAL:CG1  | 2.66                     | 0.40              |
| 1:A:386:THR:O    | 1:A:387:PRO:C    | 2.63                     | 0.40              |
| 1:A:450:THR:O    | 1:A:452:LEU:N    | 2.54                     | 0.40              |
| 1:A:461:LYS:O    | 1:A:462:GLY:C    | 2.63                     | 0.40              |
| 1:A:494:ASN:HA   | 1:A:532:TYR:HB3  | 2.04                     | 0.40              |
| 2:B:262:GLY:O    | 2:B:263:LYS:C    | 2.64                     | 0.40              |
| 1:A:18:GLY:O     | 1:A:20:LYS:HD2   | 2.22                     | 0.40              |
| 1:A:77:PHE:N     | 1:A:77:PHE:CD1   | 2.89                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:183:TYR:HE2  | 1:A:229:TRP:HE1 | 1.64                     | 0.40              |
| 1:A:241:VAL:HG13 | 1:A:266:TRP:HE1 | 1.86                     | 0.40              |
| 1:A:277:ARG:NH1  | 1:A:334:GLN:HG3 | 2.37                     | 0.40              |
| 1:A:277:ARG:HH21 | 1:A:514:GLU:CD  | 2.29                     | 0.40              |
| 1:A:470:THR:O    | 1:A:471:ASN:C   | 2.64                     | 0.40              |
| 2:B:167:ILE:O    | 2:B:208:HIS:CE1 | 2.75                     | 0.40              |
| 2:B:200:THR:O    | 2:B:201:LYS:C   | 2.64                     | 0.40              |
| 2:B:363:ASN:O    | 2:B:366:LYS:N   | 2.54                     | 0.40              |
| 1:A:40:GLU:O     | 1:A:44:GLU:HB2  | 2.21                     | 0.40              |
| 1:A:452:LEU:HD12 | 1:A:452:LEU:O   | 2.22                     | 0.40              |
| 1:A:503:LEU:O    | 1:A:507:GLN:CB  | 2.70                     | 0.40              |
| 2:B:34:LEU:HD21  | 2:B:61:PHE:O    | 2.21                     | 0.40              |
| 2:B:281:LYS:CA   | 2:B:284:ARG:HG3 | 2.47                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 556/558 (100%) | 381 (68%) | 129 (23%) | 46 (8%)  | 0           | 3 |
| 2   | B     | 425/427 (100%) | 291 (68%) | 88 (21%)  | 46 (11%) | 0           | 1 |
| All | All   | 981/985 (100%) | 672 (68%) | 217 (22%) | 92 (9%)  | 0           | 2 |

All (92) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 154 | LYS  |
| 1   | A     | 213 | GLY  |
| 1   | A     | 412 | PRO  |
| 1   | A     | 462 | GLY  |
| 1   | A     | 474 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 27  | THR  |
| 2   | B     | 53  | GLU  |
| 2   | B     | 116 | PHE  |
| 2   | B     | 242 | GLN  |
| 2   | B     | 277 | ARG  |
| 2   | B     | 289 | LEU  |
| 2   | B     | 294 | PRO  |
| 2   | B     | 296 | THR  |
| 2   | B     | 321 | PRO  |
| 2   | B     | 360 | ALA  |
| 2   | B     | 362 | THR  |
| 2   | B     | 382 | ILE  |
| 1   | A     | 98  | ALA  |
| 1   | A     | 112 | GLY  |
| 1   | A     | 124 | PHE  |
| 1   | A     | 141 | GLY  |
| 1   | A     | 160 | PHE  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 272 | PRO  |
| 1   | A     | 274 | ILE  |
| 1   | A     | 420 | PRO  |
| 1   | A     | 556 | ILE  |
| 2   | B     | 37  | ILE  |
| 2   | B     | 41  | MET  |
| 2   | B     | 69  | THR  |
| 2   | B     | 93  | GLY  |
| 2   | B     | 160 | PHE  |
| 2   | B     | 194 | GLU  |
| 2   | B     | 195 | ILE  |
| 2   | B     | 210 | LEU  |
| 2   | B     | 276 | VAL  |
| 2   | B     | 278 | GLN  |
| 2   | B     | 316 | GLY  |
| 2   | B     | 357 | MET  |
| 2   | B     | 371 | ALA  |
| 2   | B     | 420 | PRO  |
| 1   | A     | 85  | GLN  |
| 1   | A     | 283 | LEU  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 393 | ILE  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 532 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 55  | PRO  |
| 2   | B     | 236 | PRO  |
| 2   | B     | 403 | THR  |
| 2   | B     | 421 | PRO  |
| 1   | A     | 51  | GLY  |
| 1   | A     | 121 | ASP  |
| 1   | A     | 150 | PRO  |
| 1   | A     | 236 | PRO  |
| 1   | A     | 240 | THR  |
| 1   | A     | 251 | SER  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 465 | LYS  |
| 2   | B     | 111 | VAL  |
| 2   | B     | 226 | PRO  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 237 | ASP  |
| 1   | A     | 451 | LYS  |
| 2   | B     | 115 | TYR  |
| 2   | B     | 122 | GLU  |
| 2   | B     | 148 | VAL  |
| 2   | B     | 219 | LYS  |
| 2   | B     | 229 | TRP  |
| 2   | B     | 239 | TRP  |
| 2   | B     | 331 | LYS  |
| 2   | B     | 336 | GLN  |
| 2   | B     | 345 | PRO  |
| 2   | B     | 363 | ASN  |
| 1   | A     | 52  | PRO  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 175 | ASN  |
| 1   | A     | 321 | PRO  |
| 2   | B     | 184 | MET  |
| 2   | B     | 224 | GLU  |
| 2   | B     | 365 | VAL  |
| 1   | A     | 75  | VAL  |
| 1   | A     | 226 | PRO  |
| 1   | A     | 505 | ILE  |
| 1   | A     | 25  | PRO  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 271 | TYR  |
| 2   | B     | 140 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 359 | GLY  |
| 1   | A     | 531 | VAL  |
| 1   | A     | 241 | VAL  |

### 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     | 457/498 (92%) | 355 (78%) | 102 (22%) | 1           | 5 |
| 2   | B     | 367/389 (94%) | 297 (81%) | 70 (19%)  | 1           | 8 |
| All | All   | 824/887 (93%) | 652 (79%) | 172 (21%) | 1           | 7 |

All (172) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | ILE  |
| 1   | A     | 7   | THR  |
| 1   | A     | 8   | VAL  |
| 1   | A     | 11  | LYS  |
| 1   | A     | 25  | PRO  |
| 1   | A     | 27  | THR  |
| 1   | A     | 28  | GLU  |
| 1   | A     | 31  | ILE  |
| 1   | A     | 35  | VAL  |
| 1   | A     | 37  | ILE  |
| 1   | A     | 39  | THR  |
| 1   | A     | 44  | GLU  |
| 1   | A     | 56  | TYR  |
| 1   | A     | 57  | ASN  |
| 1   | A     | 58  | THR  |
| 1   | A     | 59  | PRO  |
| 1   | A     | 65  | LYS  |
| 1   | A     | 69  | THR  |
| 1   | A     | 76  | ASP  |
| 1   | A     | 82  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 85  | GLN  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 97  | PRO  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 105 | SER  |
| 1   | A     | 107 | THR  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 128 | THR  |
| 1   | A     | 138 | GLU  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 169 | GLU  |
| 1   | A     | 177 | ASP  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 189 | VAL  |
| 1   | A     | 194 | GLU  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 199 | ARG  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 212 | TRP  |
| 1   | A     | 215 | THR  |
| 1   | A     | 226 | PRO  |
| 1   | A     | 229 | TRP  |
| 1   | A     | 234 | LEU  |
| 1   | A     | 238 | LYS  |
| 1   | A     | 240 | THR  |
| 1   | A     | 242 | GLN  |
| 1   | A     | 257 | ILE  |
| 1   | A     | 260 | LEU  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 330 | GLN  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 340 | GLN  |
| 1   | A     | 341 | ILE  |
| 1   | A     | 351 | THR  |
| 1   | A     | 379 | SER  |
| 1   | A     | 382 | ILE  |
| 1   | A     | 385 | LYS  |
| 1   | A     | 395 | LYS  |
| 1   | A     | 407 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 409 | THR  |
| 1   | A     | 411 | ILE  |
| 1   | A     | 413 | GLU  |
| 1   | A     | 415 | GLU  |
| 1   | A     | 425 | LEU  |
| 1   | A     | 428 | GLN  |
| 1   | A     | 429 | LEU  |
| 1   | A     | 434 | ILE  |
| 1   | A     | 435 | VAL  |
| 1   | A     | 448 | ARG  |
| 1   | A     | 449 | GLU  |
| 1   | A     | 450 | THR  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 459 | THR  |
| 1   | A     | 460 | ASN  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 466 | VAL  |
| 1   | A     | 469 | LEU  |
| 1   | A     | 473 | THR  |
| 1   | A     | 477 | THR  |
| 1   | A     | 488 | ASP  |
| 1   | A     | 497 | THR  |
| 1   | A     | 499 | SER  |
| 1   | A     | 500 | GLN  |
| 1   | A     | 503 | LEU  |
| 1   | A     | 511 | ASP  |
| 1   | A     | 513 | SER  |
| 1   | A     | 514 | GLU  |
| 1   | A     | 517 | LEU  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 523 | GLU  |
| 1   | A     | 527 | LYS  |
| 1   | A     | 531 | VAL  |
| 1   | A     | 533 | LEU  |
| 1   | A     | 536 | VAL  |
| 1   | A     | 539 | HIS  |
| 1   | A     | 540 | LYS  |
| 1   | A     | 546 | GLU  |
| 1   | A     | 548 | VAL  |
| 1   | A     | 551 | LEU  |
| 2   | B     | 5   | ILE  |
| 2   | B     | 16  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 17  | ASP  |
| 2   | B     | 27  | THR  |
| 2   | B     | 39  | THR  |
| 2   | B     | 44  | GLU  |
| 2   | B     | 50  | ILE  |
| 2   | B     | 55  | PRO  |
| 2   | B     | 57  | ASN  |
| 2   | B     | 63  | ILE  |
| 2   | B     | 69  | THR  |
| 2   | B     | 72  | ARG  |
| 2   | B     | 83  | ARG  |
| 2   | B     | 85  | GLN  |
| 2   | B     | 86  | ASP  |
| 2   | B     | 90  | VAL  |
| 2   | B     | 91  | GLN  |
| 2   | B     | 111 | VAL  |
| 2   | B     | 113 | ASP  |
| 2   | B     | 115 | TYR  |
| 2   | B     | 116 | PHE  |
| 2   | B     | 118 | VAL  |
| 2   | B     | 122 | GLU  |
| 2   | B     | 135 | ILE  |
| 2   | B     | 140 | PRO  |
| 2   | B     | 143 | ARG  |
| 2   | B     | 150 | PRO  |
| 2   | B     | 165 | THR  |
| 2   | B     | 169 | GLU  |
| 2   | B     | 174 | GLN  |
| 2   | B     | 175 | ASN  |
| 2   | B     | 177 | ASP  |
| 2   | B     | 184 | MET  |
| 2   | B     | 189 | VAL  |
| 2   | B     | 193 | LEU  |
| 2   | B     | 194 | GLU  |
| 2   | B     | 195 | ILE  |
| 2   | B     | 208 | HIS  |
| 2   | B     | 212 | TRP  |
| 2   | B     | 214 | LEU  |
| 2   | B     | 218 | ASP  |
| 2   | B     | 232 | TYR  |
| 2   | B     | 240 | THR  |
| 2   | B     | 242 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 245 | VAL  |
| 2   | B     | 249 | LYS  |
| 2   | B     | 251 | SER  |
| 2   | B     | 252 | TRP  |
| 2   | B     | 265 | ASN  |
| 2   | B     | 266 | TRP  |
| 2   | B     | 269 | GLN  |
| 2   | B     | 274 | ILE  |
| 2   | B     | 282 | LEU  |
| 2   | B     | 303 | LEU  |
| 2   | B     | 315 | HIS  |
| 2   | B     | 318 | TYR  |
| 2   | B     | 324 | ASP  |
| 2   | B     | 329 | ILE  |
| 2   | B     | 330 | GLN  |
| 2   | B     | 340 | GLN  |
| 2   | B     | 349 | LEU  |
| 2   | B     | 367 | GLN  |
| 2   | B     | 378 | GLU  |
| 2   | B     | 401 | TRP  |
| 2   | B     | 403 | THR  |
| 2   | B     | 419 | THR  |
| 2   | B     | 421 | PRO  |
| 2   | B     | 422 | LEU  |
| 2   | B     | 423 | VAL  |
| 2   | B     | 425 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | ASN  |
| 1   | A     | 57  | ASN  |
| 1   | A     | 175 | ASN  |
| 1   | A     | 208 | HIS  |
| 1   | A     | 242 | GLN  |
| 1   | A     | 255 | ASN  |
| 1   | A     | 258 | GLN  |
| 1   | A     | 269 | GLN  |
| 1   | A     | 332 | GLN  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 343 | GLN  |
| 1   | A     | 487 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 54  | ASN  |
| 2   | B     | 57  | ASN  |
| 2   | B     | 145 | GLN  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 151 | GLN  |
| 2   | B     | 182 | GLN  |
| 2   | B     | 207 | GLN  |
| 2   | B     | 255 | ASN  |
| 2   | B     | 330 | GLN  |
| 2   | B     | 334 | GLN  |
| 2   | B     | 407 | GLN  |
| 2   | B     | 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 ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | TB9  | A     | 600 | -    | 22,23,23     | 3.52 | 8 (36%)  | 22,34,34    | 4.06 | 7 (31%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | TB9  | A     | 600 | -    | -       | 0/5/17/17 | 0/2/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | A     | 600 | TB9  | C2-N1   | 9.91  | 1.44        | 1.36     |
| 3   | A     | 600 | TB9  | C2-N3   | 6.48  | 1.48        | 1.38     |
| 3   | A     | 600 | TB9  | C8-C9   | 6.18  | 1.48        | 1.38     |
| 3   | A     | 600 | TB9  | C2-S2   | 5.88  | 1.77        | 1.67     |
| 3   | A     | 600 | TB9  | C8-C7A  | 3.92  | 1.45        | 1.39     |
| 3   | A     | 600 | TB9  | C10-C9  | 3.42  | 1.43        | 1.38     |
| 3   | A     | 600 | TB9  | C12-C13 | -3.40 | 1.46        | 1.50     |
| 3   | A     | 600 | TB9  | C15-C14 | 2.13  | 1.56        | 1.50     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | A     | 600 | TB9  | C3A-N3-C2   | -13.64 | 103.67      | 109.95   |
| 3   | A     | 600 | TB9  | C16-C14-C15 | 9.02   | 135.34      | 114.59   |
| 3   | A     | 600 | TB9  | C12-N6-C7   | 5.15   | 121.04      | 112.07   |
| 3   | A     | 600 | TB9  | C15-C14-C13 | -5.01  | 107.63      | 122.66   |
| 3   | A     | 600 | TB9  | C1A-N1-C2   | -2.70  | 108.66      | 110.67   |
| 3   | A     | 600 | TB9  | C8-C7A-C3A  | -2.16  | 115.44      | 118.28   |
| 3   | A     | 600 | TB9  | C1A-C3A-C7A | 2.02   | 125.70      | 122.34   |

There are no chirality outliers.

There are no torsion outliers.

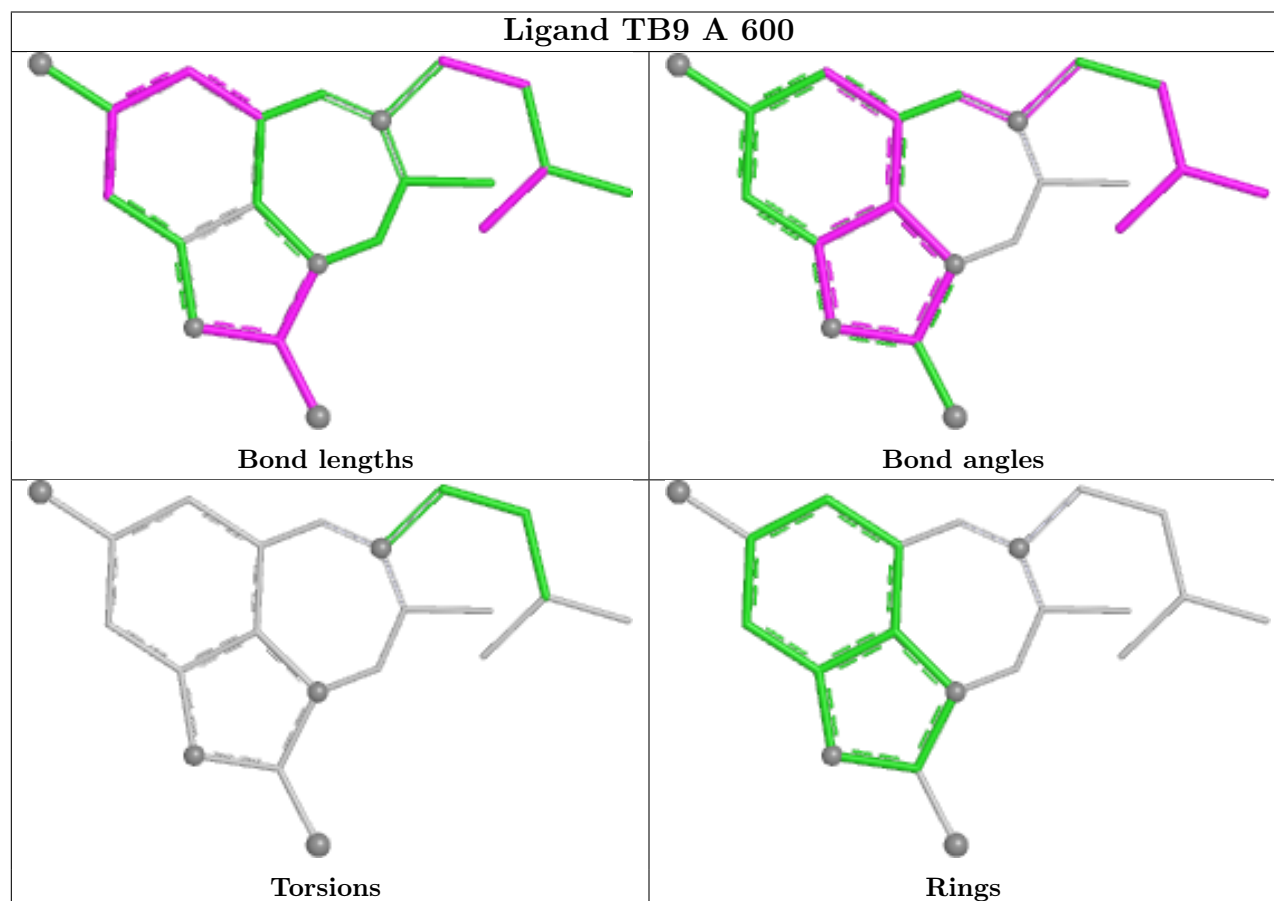
There are no ring outliers.

1 monomer is involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 600 | TB9  | 15      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ > 2 |    |    | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|----------------|--------|-----------|----|----|-----------------------|---------|
| 1   | A     | 558/558 (100%) | 0.34   | 17 (3%)   | 52 | 30 | 10, 45, 64, 65        | 0       |
| 2   | B     | 427/427 (100%) | 0.20   | 17 (3%)   | 42 | 23 | 10, 34, 65, 65        | 0       |
| All | All   | 985/985 (100%) | 0.28   | 34 (3%)   | 47 | 27 | 10, 43, 65, 65        | 0       |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 553 | SER  | 4.8  |
| 1   | A     | 134 | SER  | 4.3  |
| 2   | B     | 304 | ALA  | 4.2  |
| 2   | B     | 2   | ILE  | 4.1  |
| 2   | B     | 314 | VAL  | 3.9  |
| 2   | B     | 197 | GLN  | 3.7  |
| 2   | B     | 273 | GLY  | 3.1  |
| 2   | B     | 18  | GLY  | 3.1  |
| 1   | A     | 31  | ILE  | 2.8  |
| 1   | A     | 544 | GLY  | 2.7  |
| 1   | A     | 268 | SER  | 2.7  |
| 2   | B     | 268 | SER  | 2.6  |
| 1   | A     | 402 | TRP  | 2.5  |
| 1   | A     | 286 | THR  | 2.5  |
| 1   | A     | 434 | ILE  | 2.5  |
| 2   | B     | 141 | GLY  | 2.5  |
| 1   | A     | 515 | SER  | 2.4  |
| 2   | B     | 87  | PHE  | 2.3  |
| 2   | B     | 426 | TRP  | 2.3  |
| 1   | A     | 227 | PHE  | 2.3  |
| 1   | A     | 345 | PRO  | 2.2  |
| 2   | B     | 425 | LEU  | 2.2  |
| 1   | A     | 58  | THR  | 2.2  |
| 2   | B     | 3   | SER  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 295 | LEU  | 2.2  |
| 2   | B     | 250 | ASP  | 2.2  |
| 1   | A     | 444 | GLY  | 2.1  |
| 2   | B     | 221 | HIS  | 2.1  |
| 1   | A     | 210 | LEU  | 2.1  |
| 2   | B     | 338 | THR  | 2.1  |
| 1   | A     | 196 | GLY  | 2.1  |
| 1   | A     | 288 | ALA  | 2.1  |
| 1   | A     | 45  | GLY  | 2.1  |
| 2   | B     | 284 | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

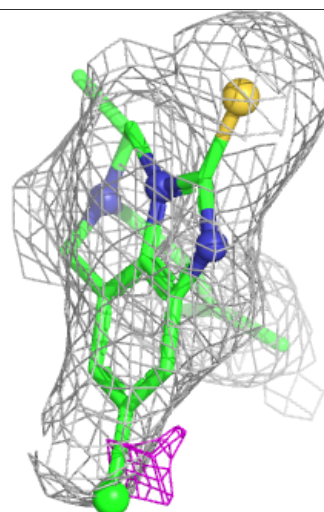
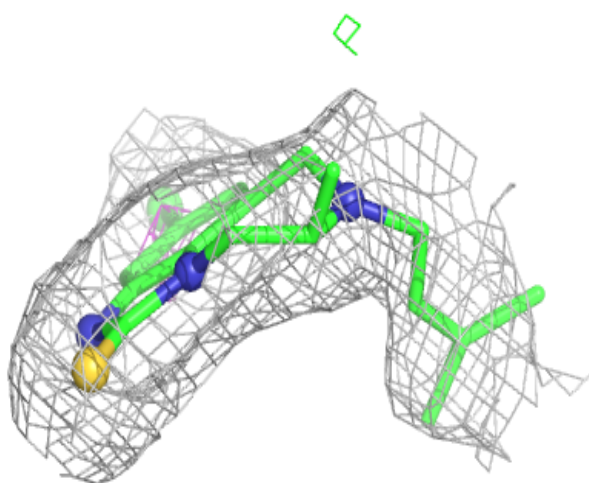
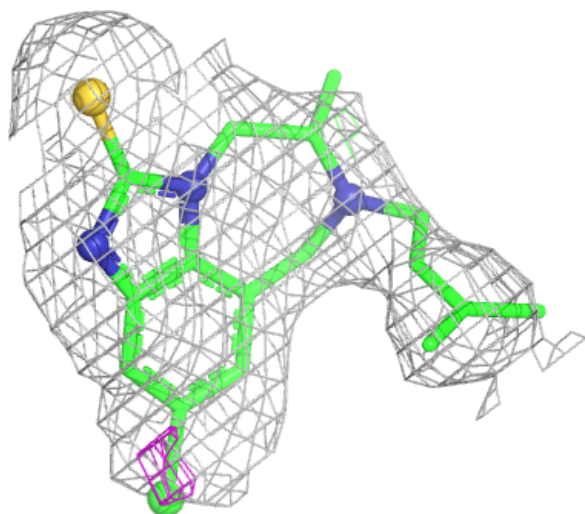
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | TB9  | A     | 600 | 21/21 | 0.90 | 0.12 | 45,45,45,45                 | 0     |

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

**Electron density around TB9 A 600:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.