



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:19 AM UTC

PDB ID : 1M7X / pdb\_00001m7x  
Title : The X-ray Crystallographic Structure of Branching Enzyme  
Authors : Abad, M.C.; Binderup, K.; Rios-Steiner, J.; Arni, R.K.; Preiss, J.; Geiger, J.H.  
Deposited on : 2002-07-23  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

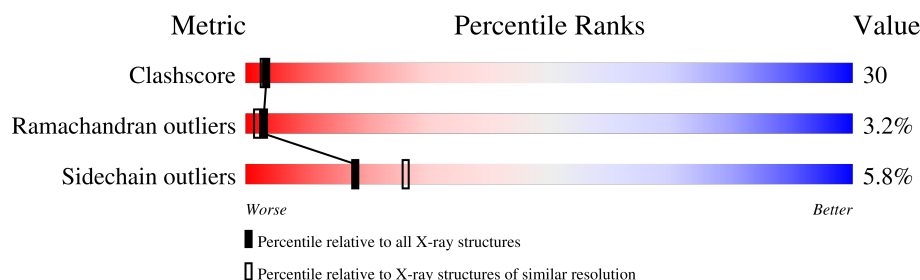
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 617    |                  |
| 1   | B     | 617    |                  |
| 1   | C     | 617    |                  |
| 1   | D     | 617    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20372 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 1,4-alpha-glucan Branching Enzyme.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 587      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4823  | 3083 | 857 | 867 | 16 |         |         |       |
| 1   | B     | 591      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4852  | 3102 | 859 | 876 | 15 |         |         |       |
| 1   | C     | 578      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4750  | 3041 | 840 | 854 | 15 |         |         |       |
| 1   | D     | 585      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4805  | 3072 | 853 | 864 | 16 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 112     | MET      | -      | initiating methionine | UNP P07762 |
| B     | 112     | MET      | -      | initiating methionine | UNP P07762 |
| C     | 112     | MET      | -      | initiating methionine | UNP P07762 |
| D     | 112     | MET      | -      | initiating methionine | UNP P07762 |

- Molecule 2 is water.

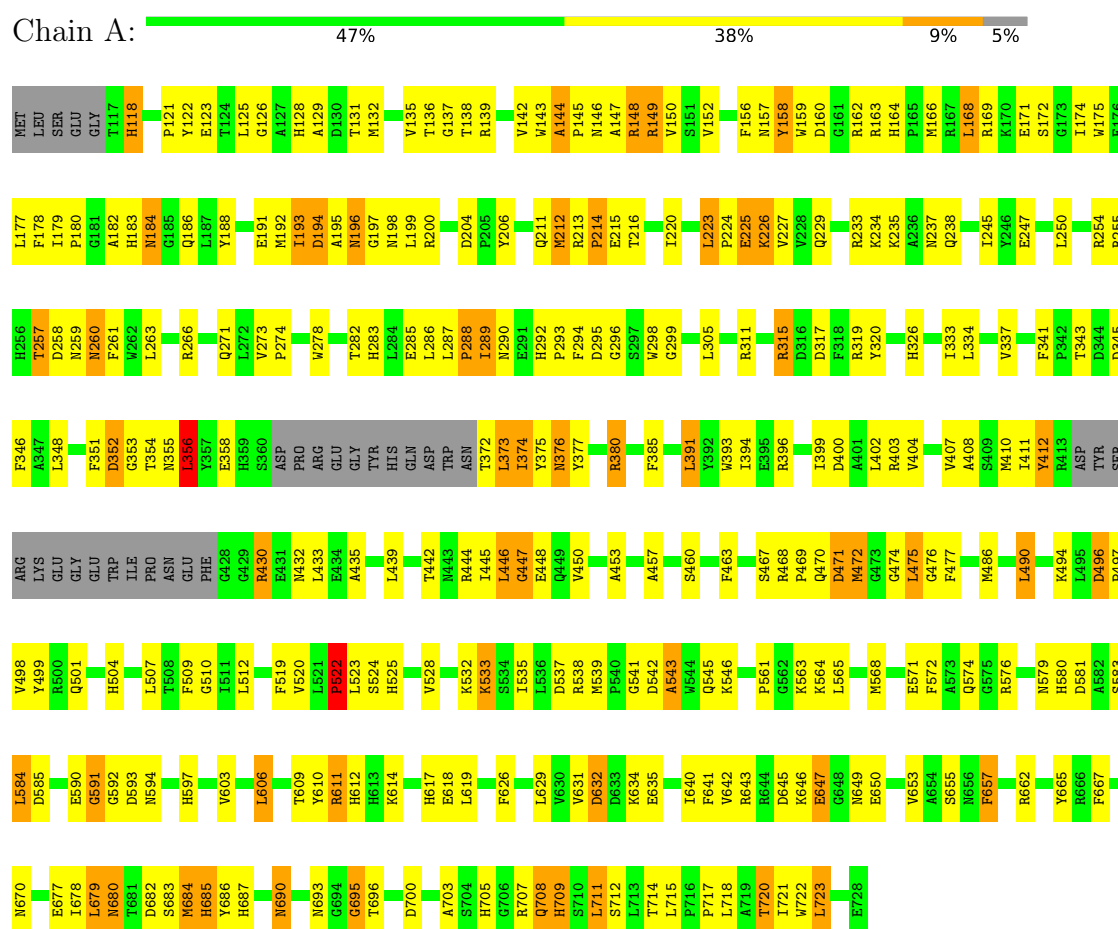
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2   | A     | 301      | Total | O   | 0       | 0       |
|     |       |          | 301   | 301 |         |         |
| 2   | B     | 425      | Total | O   | 0       | 0       |
|     |       |          | 425   | 425 |         |         |
| 2   | C     | 108      | Total | O   | 0       | 0       |
|     |       |          | 108   | 108 |         |         |
| 2   | D     | 308      | Total | O   | 0       | 0       |
|     |       |          | 308   | 308 |         |         |

### 3 Residue-property plots

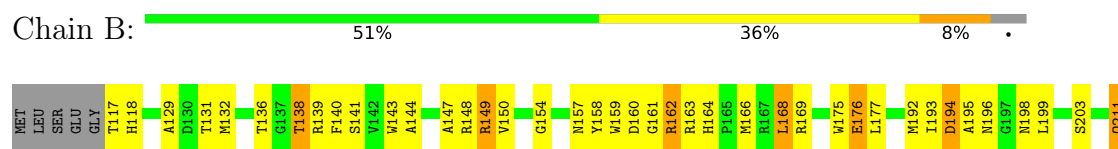
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

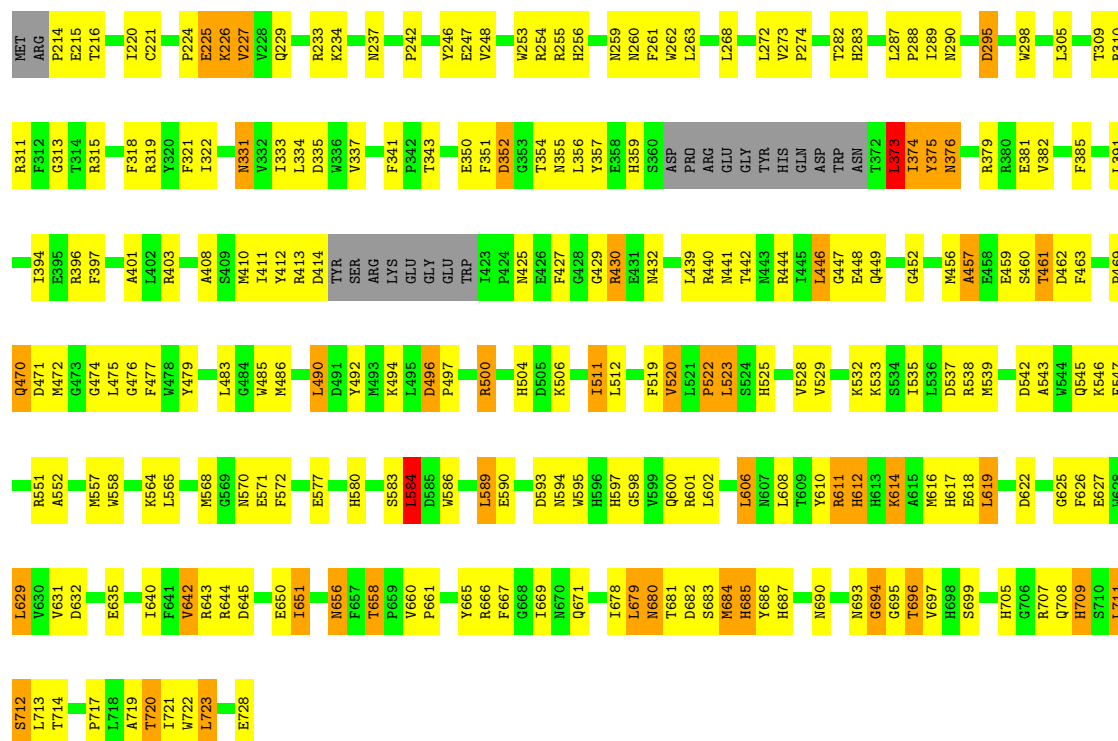
Note EDS was not executed.

#### • Molecule 1: 1,4-alpha-glucan Branching Enzyme



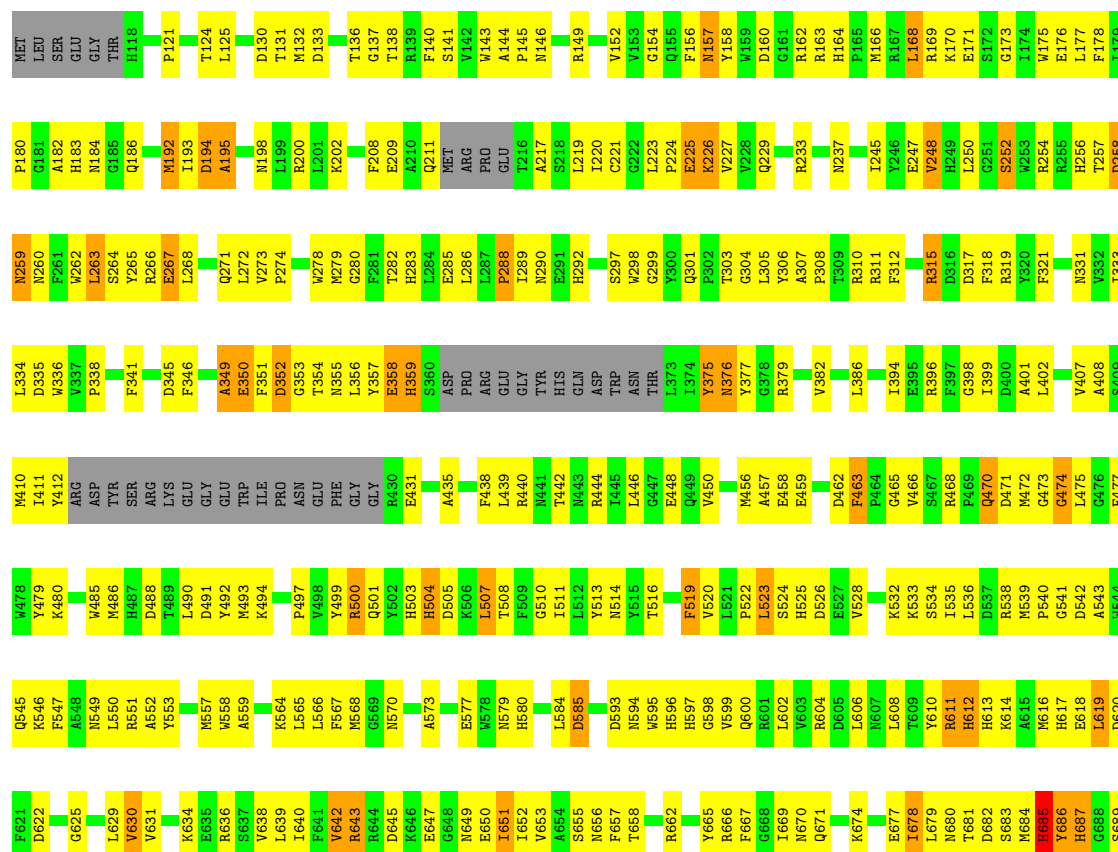
#### • Molecule 1: 1,4-alpha-glucan Branching Enzyme





• Molecule 1: 1,4-alpha-glucan Branching Enzyme

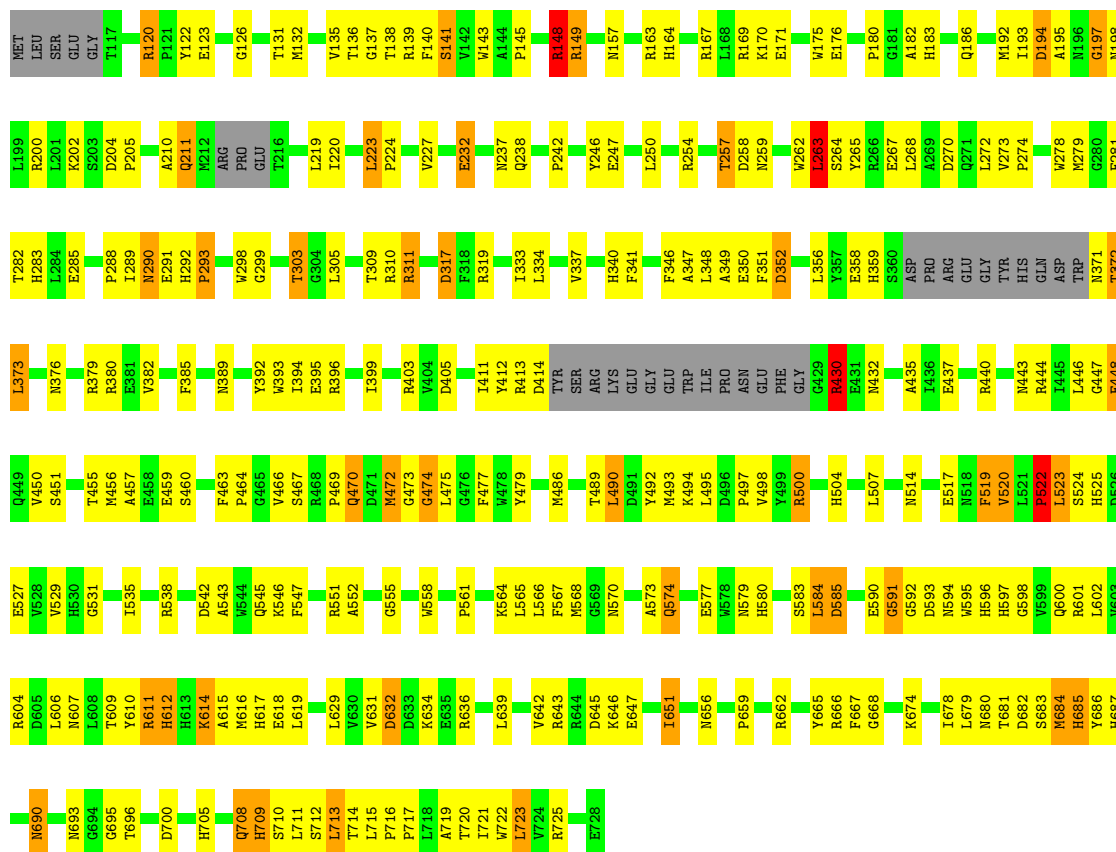
Chain C: 40% 46% 7% 6%





● Molecule 1: 1,4-alpha-glucan Branching Enzyme

Chain D: 49% 38% 7% 5%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 91.47Å 102.62Å 185.06Å<br>90.00° 91.45° 90.00° | Depositor |
| Resolution (Å)                                           | 35.00 – 2.30                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (35.00-2.30)                   | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | CNS                                            | Depositor |
| R, $R_{free}$                                            | 0.200 , 0.265                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 20372                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 23.0                                           | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.46         | 0/4976      | 1.02        | 27/6756 (0.4%)   |
| 1   | B     | 0.50         | 0/5006      | 1.06        | 33/6797 (0.5%)   |
| 1   | C     | 0.42         | 0/4900      | 0.95        | 21/6653 (0.3%)   |
| 1   | D     | 0.49         | 0/4956      | 1.05        | 33/6728 (0.5%)   |
| All | All   | 0.47         | 0/19838     | 1.02        | 114/26934 (0.4%) |

There are no bond length outliers.

All (114) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 375 | TYR  | N-CA-C | 13.60  | 127.35      | 111.71   |
| 1   | D     | 584 | LEU  | N-CA-C | 10.96  | 122.97      | 111.14   |
| 1   | A     | 685 | HIS  | N-CA-C | -10.81 | 95.25       | 110.50   |
| 1   | D     | 685 | HIS  | N-CA-C | -10.70 | 96.53       | 110.33   |
| 1   | B     | 685 | HIS  | N-CA-C | -10.66 | 95.46       | 110.50   |
| 1   | D     | 474 | GLY  | N-CA-C | 10.05  | 122.50      | 111.85   |
| 1   | D     | 611 | ARG  | N-CA-C | -9.61  | 97.58       | 110.55   |
| 1   | D     | 195 | ALA  | N-CA-C | -9.44  | 101.75      | 113.18   |
| 1   | B     | 195 | ALA  | N-CA-C | -9.42  | 101.70      | 113.01   |
| 1   | B     | 589 | LEU  | N-CA-C | -9.10  | 97.80       | 110.35   |
| 1   | B     | 461 | THR  | N-CA-C | -9.01  | 97.91       | 110.35   |
| 1   | A     | 584 | LEU  | N-CA-C | 8.43   | 121.91      | 112.97   |
| 1   | A     | 629 | LEU  | N-CA-C | -8.33  | 103.06      | 113.55   |
| 1   | A     | 611 | ARG  | N-CA-C | -8.31  | 99.89       | 110.19   |
| 1   | B     | 611 | ARG  | N-CA-C | -8.28  | 98.22       | 110.48   |
| 1   | A     | 519 | PHE  | N-CA-C | 8.05   | 121.42      | 110.55   |
| 1   | A     | 158 | TYR  | N-CA-C | -7.84  | 103.29      | 112.86   |
| 1   | D     | 263 | LEU  | N-CA-C | -7.74  | 100.10      | 110.55   |
| 1   | D     | 684 | MET  | N-CA-C | -7.69  | 102.90      | 111.82   |
| 1   | C     | 248 | VAL  | N-CA-C | 7.56   | 118.62      | 108.27   |
| 1   | C     | 685 | HIS  | N-CA-C | -7.45  | 100.22      | 110.35   |
| 1   | C     | 611 | ARG  | N-CA-C | -7.44  | 99.51       | 110.52   |
| 1   | A     | 678 | ILE  | N-CA-C | -7.35  | 106.05      | 113.47   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 263 | LEU  | N-CA-C | -7.29 | 100.72      | 110.55   |
| 1   | B     | 678 | ILE  | N-CA-C | -7.26 | 106.14      | 113.47   |
| 1   | D     | 519 | PHE  | N-CA-C | 7.22  | 121.20      | 110.52   |
| 1   | D     | 148 | ARG  | N-CA-C | -7.15 | 97.56       | 109.07   |
| 1   | B     | 162 | ARG  | N-CA-C | -7.12 | 102.64      | 111.75   |
| 1   | C     | 263 | LEU  | N-CA-C | -7.12 | 99.00       | 110.32   |
| 1   | C     | 519 | PHE  | N-CA-C | 7.00  | 119.76      | 110.53   |
| 1   | A     | 684 | MET  | N-CA-C | -6.96 | 103.70      | 111.71   |
| 1   | C     | 156 | PHE  | N-CA-C | -6.95 | 104.77      | 113.18   |
| 1   | C     | 225 | GLU  | N-CA-C | 6.92  | 121.17      | 113.21   |
| 1   | A     | 260 | ASN  | N-CA-C | -6.85 | 104.23      | 112.58   |
| 1   | B     | 227 | VAL  | N-CA-C | 6.84  | 118.14      | 108.36   |
| 1   | C     | 474 | GLY  | N-CA-C | 6.79  | 121.05      | 111.00   |
| 1   | C     | 195 | ALA  | N-CA-C | -6.76 | 104.50      | 112.89   |
| 1   | D     | 210 | ALA  | N-CA-C | 6.68  | 119.57      | 109.95   |
| 1   | A     | 496 | ASP  | N-CA-C | -6.54 | 99.89       | 109.50   |
| 1   | B     | 519 | PHE  | N-CA-C | 6.47  | 119.29      | 110.55   |
| 1   | B     | 520 | VAL  | N-CA-C | -6.44 | 99.09       | 108.11   |
| 1   | B     | 684 | MET  | N-CA-C | -6.43 | 104.32      | 111.71   |
| 1   | D     | 464 | PRO  | N-CA-C | 6.37  | 120.51      | 110.50   |
| 1   | B     | 287 | LEU  | N-CA-C | -6.36 | 101.31      | 110.08   |
| 1   | D     | 524 | SER  | N-CA-C | 6.31  | 119.69      | 110.17   |
| 1   | B     | 584 | LEU  | N-CA-C | 6.26  | 124.14      | 110.80   |
| 1   | A     | 632 | ASP  | N-CA-C | 6.14  | 120.39      | 112.41   |
| 1   | C     | 629 | LEU  | N-CA-C | -6.10 | 106.44      | 114.31   |
| 1   | D     | 708 | GLN  | N-CA-C | -6.01 | 100.71      | 110.20   |
| 1   | D     | 632 | ASP  | N-CA-C | 5.98  | 122.58      | 113.61   |
| 1   | A     | 144 | ALA  | CA-C-N | 5.95  | 127.27      | 119.84   |
| 1   | A     | 144 | ALA  | C-N-CA | 5.95  | 127.27      | 119.84   |
| 1   | D     | 317 | ASP  | N-CA-C | -5.89 | 104.78      | 111.14   |
| 1   | B     | 221 | CYS  | N-CA-C | -5.88 | 99.59       | 108.52   |
| 1   | C     | 301 | GLN  | CA-C-N | 5.87  | 126.06      | 120.31   |
| 1   | C     | 301 | GLN  | C-N-CA | 5.87  | 126.06      | 120.31   |
| 1   | D     | 678 | ILE  | N-CA-C | -5.87 | 107.04      | 113.43   |
| 1   | C     | 524 | SER  | N-CA-C | 5.84  | 118.42      | 110.35   |
| 1   | B     | 523 | LEU  | N-CA-C | -5.84 | 98.86       | 108.49   |
| 1   | D     | 303 | THR  | N-CA-C | -5.83 | 106.79      | 114.31   |
| 1   | D     | 305 | LEU  | N-CA-C | 5.82  | 117.62      | 111.28   |
| 1   | B     | 460 | SER  | N-CA-C | 5.82  | 118.57      | 111.82   |
| 1   | C     | 375 | TYR  | N-CA-C | 5.78  | 123.11      | 110.80   |
| 1   | D     | 448 | GLU  | N-CA-C | -5.78 | 104.42      | 112.45   |
| 1   | B     | 629 | LEU  | N-CA-C | -5.76 | 106.80      | 113.88   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 520 | VAL  | N-CA-C | -5.74 | 99.27       | 107.77   |
| 1   | A     | 287 | LEU  | N-CA-C | -5.72 | 101.72      | 110.01   |
| 1   | C     | 678 | ILE  | N-CA-C | -5.71 | 107.56      | 113.10   |
| 1   | C     | 708 | GLN  | N-CA-C | -5.71 | 101.18      | 110.20   |
| 1   | A     | 356 | LEU  | N-CA-C | 5.67  | 117.13      | 111.07   |
| 1   | B     | 711 | LEU  | N-CA-C | 5.65  | 119.61      | 111.02   |
| 1   | A     | 657 | PHE  | N-CA-C | 5.62  | 119.13      | 112.72   |
| 1   | A     | 711 | LEU  | N-CA-C | 5.62  | 120.40      | 112.93   |
| 1   | B     | 118 | HIS  | N-CA-C | -5.57 | 106.33      | 113.23   |
| 1   | A     | 460 | SER  | N-CA-C | 5.55  | 117.01      | 111.07   |
| 1   | B     | 337 | VAL  | N-CA-C | 5.54  | 120.84      | 108.88   |
| 1   | A     | 271 | GLN  | N-CA-C | 5.46  | 120.31      | 113.43   |
| 1   | B     | 394 | ILE  | N-CA-C | 5.45  | 115.65      | 110.53   |
| 1   | A     | 245 | ILE  | N-CA-C | 5.41  | 116.10      | 108.36   |
| 1   | B     | 535 | ILE  | N-CA-C | -5.39 | 104.22      | 111.44   |
| 1   | D     | 238 | GLN  | N-CA-C | 5.39  | 118.10      | 110.50   |
| 1   | B     | 331 | ASN  | N-CA-C | -5.39 | 102.07      | 110.42   |
| 1   | A     | 524 | SER  | N-CA-C | 5.37  | 118.36      | 109.94   |
| 1   | D     | 347 | ALA  | N-CA-C | 5.36  | 117.56      | 111.02   |
| 1   | D     | 457 | ALA  | N-CA-C | 5.35  | 117.52      | 109.23   |
| 1   | C     | 158 | TYR  | N-CA-C | -5.35 | 104.27      | 111.54   |
| 1   | D     | 629 | LEU  | N-CA-C | -5.35 | 106.81      | 113.55   |
| 1   | D     | 293 | PRO  | N-CA-C | 5.34  | 120.95      | 113.53   |
| 1   | A     | 223 | LEU  | N-CA-C | -5.32 | 100.89      | 109.40   |
| 1   | C     | 376 | ASN  | N-CA-C | -5.29 | 104.13      | 111.28   |
| 1   | D     | 380 | ARG  | N-CA-C | 5.26  | 117.42      | 111.11   |
| 1   | D     | 460 | SER  | N-CA-C | 5.26  | 117.70      | 111.33   |
| 1   | B     | 632 | ASP  | N-CA-C | 5.26  | 119.25      | 112.41   |
| 1   | B     | 449 | GLN  | N-CA-C | 5.25  | 116.81      | 111.14   |
| 1   | D     | 463 | PHE  | CA-C-N | 5.24  | 126.68      | 120.23   |
| 1   | D     | 463 | PHE  | C-N-CA | 5.24  | 126.68      | 120.23   |
| 1   | C     | 267 | GLU  | N-CA-C | -5.21 | 107.09      | 113.50   |
| 1   | B     | 447 | GLY  | N-CA-C | -5.18 | 100.91      | 113.18   |
| 1   | B     | 373 | LEU  | N-CA-C | 5.16  | 117.18      | 109.59   |
| 1   | B     | 496 | ASP  | N-CA-C | -5.16 | 103.09      | 109.64   |
| 1   | B     | 203 | SER  | N-CA-C | -5.15 | 102.90      | 110.52   |
| 1   | B     | 457 | ALA  | N-CA-C | 5.14  | 117.06      | 108.99   |
| 1   | A     | 118 | HIS  | N-CA-C | -5.13 | 105.87      | 111.82   |
| 1   | D     | 614 | LYS  | N-CA-C | 5.10  | 117.50      | 111.33   |
| 1   | D     | 395 | GLU  | N-CA-C | 5.07  | 117.93      | 111.69   |
| 1   | A     | 453 | ALA  | N-CA-C | -5.07 | 103.71      | 110.55   |
| 1   | C     | 463 | PHE  | CA-C-N | 5.07  | 124.83      | 119.76   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 463 | PHE  | C-N-CA | 5.07  | 124.83      | 119.76   |
| 1   | D     | 120 | ARG  | CA-C-N | 5.05  | 124.77      | 119.82   |
| 1   | D     | 120 | ARG  | C-N-CA | 5.05  | 124.77      | 119.82   |
| 1   | A     | 412 | TYR  | N-CA-C | 5.04  | 115.03      | 108.07   |
| 1   | B     | 248 | VAL  | N-CA-C | 5.02  | 116.94      | 108.81   |
| 1   | B     | 376 | ASN  | N-CA-C | -5.01 | 105.05      | 110.91   |
| 1   | A     | 708 | GLN  | N-CA-C | -5.00 | 100.36      | 108.52   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 4823  | 0        | 4559     | 283     | 0            |
| 1   | B     | 4852  | 0        | 4571     | 266     | 0            |
| 1   | C     | 4750  | 0        | 4485     | 339     | 0            |
| 1   | D     | 4805  | 0        | 4537     | 249     | 0            |
| 2   | A     | 301   | 0        | 0        | 19      | 0            |
| 2   | B     | 425   | 0        | 0        | 33      | 0            |
| 2   | C     | 108   | 0        | 0        | 21      | 0            |
| 2   | D     | 308   | 0        | 0        | 20      | 0            |
| All | All   | 20372 | 0        | 18152    | 1130    | 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 30.

All (1130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:643:ARG:HB3 | 1:C:643:ARG:HH11 | 1.12                     | 1.08              |
| 1:A:430:ARG:HB3 | 1:A:430:ARG:HH21 | 1.22                     | 1.02              |
| 1:C:497:PRO:HA  | 1:C:500:ARG:HD3  | 1.42                     | 1.02              |
| 1:A:224:PRO:HG2 | 1:A:396:ARG:HB3  | 1.38                     | 1.01              |
| 1:B:430:ARG:H   | 1:B:430:ARG:HD2  | 1.22                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:393:TRP:HB3  | 1:A:399:ILE:HD12 | 1.44                     | 1.00              |
| 1:D:430:ARG:HB2  | 1:D:430:ARG:HH11 | 1.27                     | 0.99              |
| 1:D:693:ASN:HD21 | 1:D:714:THR:H    | 1.10                     | 0.99              |
| 1:B:194:ASP:HB2  | 1:B:198:ASN:H    | 1.28                     | 0.99              |
| 1:D:470:GLN:H    | 1:D:470:GLN:NE2  | 1.59                     | 0.99              |
| 1:B:658:THR:HG22 | 1:B:660:VAL:H    | 1.24                     | 0.98              |
| 1:C:656:ASN:HD21 | 1:C:658:THR:HG22 | 1.22                     | 0.98              |
| 1:C:224:PRO:HG2  | 1:C:396:ARG:HB3  | 1.45                     | 0.97              |
| 1:D:211:GLN:HB2  | 2:D:1534:HOH:O   | 1.65                     | 0.97              |
| 1:B:470:GLN:HA   | 1:B:474:GLY:HA2  | 1.45                     | 0.96              |
| 1:B:511:ILE:HB   | 2:B:1888:HOH:O   | 1.64                     | 0.95              |
| 1:C:333:ILE:HD13 | 1:C:456:MET:HE1  | 1.48                     | 0.94              |
| 1:C:606:LEU:HD23 | 1:C:679:LEU:HD11 | 1.48                     | 0.94              |
| 1:B:373:LEU:H    | 1:B:373:LEU:HD23 | 1.33                     | 0.91              |
| 1:D:470:GLN:H    | 1:D:470:GLN:HE21 | 1.00                     | 0.91              |
| 1:B:594:ASN:H    | 1:B:597:HIS:HD2  | 1.16                     | 0.90              |
| 1:B:470:GLN:H    | 1:B:470:GLN:NE2  | 1.68                     | 0.90              |
| 1:D:376:ASN:ND2  | 1:D:379:ARG:HB2  | 1.86                     | 0.90              |
| 1:B:164:HIS:HB3  | 1:B:177:LEU:HD21 | 1.52                     | 0.89              |
| 1:D:594:ASN:H    | 1:D:597:HIS:HD2  | 1.18                     | 0.89              |
| 1:B:470:GLN:HE21 | 1:B:470:GLN:N    | 1.70                     | 0.89              |
| 1:C:643:ARG:HH11 | 1:C:643:ARG:CB   | 1.86                     | 0.89              |
| 1:C:470:GLN:HE21 | 1:C:470:GLN:H    | 0.93                     | 0.88              |
| 1:C:695:GLY:HA3  | 1:D:591:GLY:HA2  | 1.52                     | 0.88              |
| 1:C:551:ARG:HG2  | 1:C:602:LEU:HD22 | 1.53                     | 0.88              |
| 1:A:212:MET:HE3  | 1:A:213:ARG:HG3  | 1.57                     | 0.86              |
| 1:C:693:ASN:HD21 | 1:C:714:THR:H    | 1.23                     | 0.86              |
| 1:A:594:ASN:H    | 1:A:597:HIS:HD2  | 1.15                     | 0.86              |
| 1:C:466:VAL:HA   | 1:C:475:LEU:HD12 | 1.58                     | 0.85              |
| 1:C:290:ASN:HB3  | 2:C:833:HOH:O    | 1.76                     | 0.84              |
| 1:C:470:GLN:H    | 1:C:470:GLN:NE2  | 1.74                     | 0.84              |
| 1:B:430:ARG:H    | 1:B:430:ARG:CD   | 1.91                     | 0.84              |
| 1:C:229:GLN:HA   | 1:C:233:ARG:NH1  | 1.92                     | 0.84              |
| 1:A:168:LEU:HD12 | 1:A:169:ARG:H    | 1.40                     | 0.83              |
| 1:C:643:ARG:HB3  | 1:C:643:ARG:NH1  | 1.92                     | 0.83              |
| 1:A:224:PRO:CG   | 1:A:396:ARG:HB3  | 2.09                     | 0.83              |
| 1:C:656:ASN:ND2  | 1:C:658:THR:HG22 | 1.94                     | 0.83              |
| 1:C:470:GLN:HE21 | 1:C:470:GLN:N    | 1.76                     | 0.82              |
| 1:C:536:LEU:HD22 | 1:C:573:ALA:HB1  | 1.62                     | 0.81              |
| 1:C:183:HIS:H    | 1:C:186:GLN:HE21 | 1.28                     | 0.81              |
| 1:D:470:GLN:HE21 | 1:D:470:GLN:N    | 1.78                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:684:MET:H    | 1:A:690:ASN:HD22 | 1.22                     | 0.81              |
| 1:D:535:ILE:HA   | 1:D:538:ARG:HD2  | 1.63                     | 0.81              |
| 1:A:684:MET:H    | 1:A:690:ASN:ND2  | 1.78                     | 0.81              |
| 1:C:520:VAL:O    | 1:C:522:PRO:HD3  | 1.81                     | 0.81              |
| 1:C:493:MET:HE2  | 1:C:553:TYR:HB2  | 1.63                     | 0.81              |
| 1:C:636:ARG:HG2  | 1:C:662:ARG:NH2  | 1.96                     | 0.81              |
| 1:D:192:MET:HE3  | 1:D:202:LYS:HG3  | 1.63                     | 0.80              |
| 1:C:528:VAL:O    | 1:C:577:GLU:HB2  | 1.81                     | 0.80              |
| 1:A:693:ASN:HD21 | 1:A:714:THR:H    | 1.28                     | 0.80              |
| 1:A:680:ASN:ND2  | 1:A:682:ASP:H    | 1.80                     | 0.80              |
| 1:D:674:LYS:HB3  | 1:D:696:THR:HG21 | 1.61                     | 0.80              |
| 1:A:394:ILE:CD1  | 1:A:446:LEU:HD21 | 2.12                     | 0.79              |
| 1:A:430:ARG:HB3  | 1:A:430:ARG:NH2  | 1.98                     | 0.79              |
| 1:C:494:LYS:HG2  | 1:C:538:ARG:HG2  | 1.65                     | 0.78              |
| 1:D:552:ALA:HA   | 1:D:720:THR:HG22 | 1.64                     | 0.78              |
| 1:B:594:ASN:H    | 1:B:597:HIS:CD2  | 2.01                     | 0.77              |
| 1:B:558:TRP:HA   | 1:B:564:LYS:HE3  | 1.67                     | 0.77              |
| 1:D:469:PRO:HG2  | 1:D:472:MET:HG3  | 1.66                     | 0.77              |
| 1:B:194:ASP:HB2  | 1:B:198:ASN:N    | 1.99                     | 0.77              |
| 1:D:358:GLU:HG3  | 1:D:373:LEU:HD12 | 1.66                     | 0.76              |
| 1:C:229:GLN:HA   | 1:C:233:ARG:HH11 | 1.47                     | 0.76              |
| 1:C:505:ASP:HA   | 1:C:508:THR:OG1  | 1.85                     | 0.76              |
| 1:D:594:ASN:H    | 1:D:597:HIS:CD2  | 2.01                     | 0.76              |
| 1:A:295:ASP:OD2  | 1:A:311:ARG:NH2  | 2.18                     | 0.76              |
| 1:C:273:VAL:HB   | 1:C:274:PRO:HD3  | 1.65                     | 0.76              |
| 1:C:333:ILE:HG12 | 1:C:401:ALA:HB3  | 1.67                     | 0.76              |
| 1:C:552:ALA:HA   | 1:C:720:THR:HG22 | 1.66                     | 0.76              |
| 1:A:594:ASN:H    | 1:A:597:HIS:CD2  | 2.02                     | 0.76              |
| 1:C:611:ARG:O    | 1:C:612:HIS:HB3  | 1.86                     | 0.76              |
| 1:B:492:TYR:CZ   | 1:B:500:ARG:HG2  | 2.20                     | 0.76              |
| 1:C:551:ARG:HB3  | 1:C:681:THR:CG2  | 2.16                     | 0.76              |
| 1:A:683:SER:O    | 1:A:685:HIS:O    | 2.04                     | 0.76              |
| 1:C:684:MET:HE2  | 1:C:685:HIS:ND1  | 2.01                     | 0.76              |
| 1:A:305:LEU:HD11 | 2:A:1198:HOH:O   | 1.85                     | 0.76              |
| 1:D:192:MET:SD   | 1:D:352:ASP:HA   | 2.25                     | 0.76              |
| 1:B:528:VAL:O    | 1:B:577:GLU:HB2  | 1.85                     | 0.76              |
| 1:A:680:ASN:C    | 1:A:680:ASN:HD22 | 1.94                     | 0.75              |
| 1:C:542:ASP:O    | 1:C:546:LYS:HG2  | 1.86                     | 0.75              |
| 1:D:667:PHE:HA   | 1:D:705:HIS:CD2  | 2.22                     | 0.75              |
| 1:A:238:GLN:HG2  | 2:A:1759:HOH:O   | 1.87                     | 0.75              |
| 1:C:594:ASN:H    | 1:C:597:HIS:HD2  | 1.35                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:292:HIS:O    | 1:D:311:ARG:NH1  | 2.19                     | 0.75              |
| 1:C:639:LEU:HD12 | 1:C:639:LEU:H    | 1.52                     | 0.75              |
| 1:A:709:HIS:N    | 2:A:1907:HOH:O   | 2.20                     | 0.75              |
| 1:B:225:GLU:O    | 1:B:226:LYS:HB2  | 1.85                     | 0.75              |
| 1:C:684:MET:HE3  | 1:D:684:MET:HE3  | 1.69                     | 0.75              |
| 1:C:211:GLN:HG3  | 1:C:217:ALA:H    | 1.52                     | 0.74              |
| 1:A:680:ASN:HD22 | 1:A:682:ASP:H    | 1.35                     | 0.74              |
| 1:A:233:ARG:HD2  | 1:A:400:ASP:OD2  | 1.87                     | 0.74              |
| 1:B:470:GLN:H    | 1:B:470:GLN:HE21 | 0.84                     | 0.74              |
| 1:B:168:LEU:HD22 | 1:B:169:ARG:N    | 2.02                     | 0.74              |
| 1:B:357:TYR:O    | 1:B:375:TYR:O    | 2.06                     | 0.73              |
| 1:B:589:LEU:O    | 1:B:590:GLU:HB3  | 1.88                     | 0.73              |
| 1:B:684:MET:H    | 1:B:690:ASN:HD22 | 1.36                     | 0.73              |
| 1:A:520:VAL:O    | 1:A:522:PRO:HD3  | 1.88                     | 0.73              |
| 1:C:248:VAL:HG23 | 1:C:286:LEU:HD23 | 1.71                     | 0.73              |
| 1:D:232:GLU:H    | 1:D:232:GLU:CD   | 1.94                     | 0.73              |
| 1:C:145:PRO:HB3  | 1:C:173:GLY:HA3  | 1.72                     | 0.72              |
| 1:A:212:MET:SD   | 1:A:293:PRO:HA   | 2.30                     | 0.72              |
| 1:B:520:VAL:O    | 1:B:522:PRO:HD3  | 1.88                     | 0.72              |
| 1:C:456:MET:HG2  | 1:C:479:TYR:HB2  | 1.71                     | 0.72              |
| 1:A:162:ARG:O    | 1:A:162:ARG:HG2  | 1.90                     | 0.72              |
| 1:C:198:ASN:HB3  | 1:C:200:ARG:NH1  | 2.04                     | 0.72              |
| 1:D:145:PRO:HD2  | 1:D:356:LEU:HD11 | 1.71                     | 0.72              |
| 1:C:334:LEU:HD22 | 2:C:1891:HOH:O   | 1.89                     | 0.71              |
| 1:A:149:ARG:CZ   | 1:A:193:ILE:HD11 | 2.21                     | 0.71              |
| 1:A:470:GLN:C    | 1:A:472:MET:H    | 1.98                     | 0.71              |
| 1:B:194:ASP:CB   | 1:B:198:ASN:H    | 2.03                     | 0.71              |
| 1:A:148:ARG:O    | 1:A:149:ARG:HB3  | 1.89                     | 0.71              |
| 1:C:680:ASN:ND2  | 1:C:682:ASP:H    | 1.89                     | 0.71              |
| 1:D:674:LYS:HB3  | 1:D:696:THR:CG2  | 2.21                     | 0.71              |
| 1:C:440:ARG:HG2  | 1:C:475:LEU:H    | 1.55                     | 0.71              |
| 1:C:237:ASN:ND2  | 1:C:283:HIS:HE1  | 1.89                     | 0.71              |
| 1:A:380:ARG:HG2  | 1:A:380:ARG:HH21 | 1.54                     | 0.70              |
| 1:B:295:ASP:OD2  | 1:B:311:ARG:NH2  | 2.23                     | 0.70              |
| 1:C:667:PHE:HA   | 1:C:705:HIS:HD2  | 1.57                     | 0.70              |
| 1:B:149:ARG:HD3  | 2:B:1846:HOH:O   | 1.90                     | 0.70              |
| 1:B:658:THR:HG22 | 1:B:660:VAL:N    | 2.02                     | 0.69              |
| 1:D:139:ARG:HD3  | 1:D:176:GLU:OE1  | 1.92                     | 0.69              |
| 1:A:708:GLN:O    | 1:A:709:HIS:HB2  | 1.92                     | 0.69              |
| 1:B:533:LYS:HD2  | 1:B:537:ASP:HB3  | 1.74                     | 0.69              |
| 1:A:684:MET:N    | 1:A:690:ASN:HD22 | 1.90                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:618:GLU:OE2  | 1:A:645:ASP:HB2  | 1.92                     | 0.69              |
| 1:B:373:LEU:H    | 1:B:373:LEU:CD2  | 2.03                     | 0.69              |
| 1:D:430:ARG:HB2  | 1:D:430:ARG:NH1  | 2.05                     | 0.69              |
| 1:D:616:MET:SD   | 1:D:651:ILE:HG12 | 2.32                     | 0.69              |
| 1:B:237:ASN:ND2  | 1:B:283:HIS:HE1  | 1.91                     | 0.69              |
| 1:B:644:ARG:HG2  | 1:B:650:GLU:HB3  | 1.74                     | 0.69              |
| 1:C:490:LEU:O    | 1:C:494:LYS:HG3  | 1.93                     | 0.69              |
| 1:B:147:ALA:O    | 1:B:193:ILE:O    | 2.11                     | 0.68              |
| 1:B:355:ASN:HB2  | 2:B:1485:HOH:O   | 1.92                     | 0.68              |
| 1:C:192:MET:HE1  | 1:C:352:ASP:H    | 1.58                     | 0.68              |
| 1:C:636:ARG:HG2  | 1:C:662:ARG:CZ   | 2.22                     | 0.68              |
| 1:C:552:ALA:HB2  | 1:C:719:ALA:HA   | 1.74                     | 0.68              |
| 1:B:568:MET:HB2  | 1:B:584:LEU:HD11 | 1.73                     | 0.68              |
| 1:D:611:ARG:O    | 1:D:612:HIS:HB3  | 1.93                     | 0.68              |
| 1:A:132:MET:HB2  | 1:A:135:VAL:HG13 | 1.74                     | 0.68              |
| 1:C:593:ASP:HA   | 1:C:597:HIS:CD2  | 2.28                     | 0.68              |
| 1:A:168:LEU:CD1  | 1:A:169:ARG:H    | 2.07                     | 0.68              |
| 1:A:213:ARG:HB2  | 1:A:214:PRO:HD3  | 1.75                     | 0.68              |
| 1:A:118:HIS:CE1  | 1:A:380:ARG:HH22 | 2.12                     | 0.68              |
| 1:C:559:ALA:HB1  | 1:C:653:VAL:HG21 | 1.76                     | 0.68              |
| 1:D:594:ASN:N    | 1:D:597:HIS:HD2  | 1.92                     | 0.68              |
| 1:A:535:ILE:HD11 | 2:A:1206:HOH:O   | 1.93                     | 0.68              |
| 1:A:618:GLU:HG2  | 1:A:646:LYS:HE3  | 1.76                     | 0.67              |
| 1:D:250:LEU:HD22 | 1:D:268:LEU:HD13 | 1.76                     | 0.67              |
| 1:C:647:GLU:HB3  | 1:C:649:ASN:ND2  | 2.10                     | 0.67              |
| 1:A:132:MET:HB2  | 1:A:135:VAL:CG1  | 2.25                     | 0.67              |
| 1:C:471:ASP:C    | 1:C:472:MET:HE3  | 2.19                     | 0.67              |
| 1:D:574:GLN:NE2  | 1:D:584:LEU:O    | 2.27                     | 0.67              |
| 1:C:444:ARG:O    | 1:C:448:GLU:HG3  | 1.94                     | 0.67              |
| 1:C:639:LEU:HD12 | 1:C:639:LEU:N    | 2.10                     | 0.67              |
| 1:C:504:HIS:CD2  | 1:C:634:LYS:HA   | 2.30                     | 0.66              |
| 1:D:555:GLY:HA3  | 1:D:720:THR:HG21 | 1.76                     | 0.66              |
| 1:D:285:GLU:OE1  | 1:D:403:ARG:HD2  | 1.96                     | 0.66              |
| 1:A:225:GLU:O    | 1:A:226:LYS:HB2  | 1.96                     | 0.66              |
| 1:C:193:ILE:HA   | 1:C:198:ASN:O    | 1.94                     | 0.66              |
| 1:B:606:LEU:HD13 | 1:B:679:LEU:HD11 | 1.76                     | 0.66              |
| 1:B:440:ARG:HE   | 1:B:474:GLY:HA3  | 1.60                     | 0.66              |
| 1:C:265:TYR:HB2  | 1:C:317:ASP:HB3  | 1.76                     | 0.66              |
| 1:C:250:LEU:HD22 | 1:C:268:LEU:HD13 | 1.78                     | 0.66              |
| 1:D:373:LEU:HD23 | 1:D:373:LEU:H    | 1.61                     | 0.66              |
| 1:D:520:VAL:O    | 1:D:522:PRO:HD3  | 1.96                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:GLN:HG2  | 1:B:234:LYS:HG3  | 1.78                     | 0.66              |
| 1:B:310:ARG:HH11 | 1:B:313:GLY:HA2  | 1.61                     | 0.66              |
| 1:A:471:ASP:O    | 1:A:472:MET:HG3  | 1.96                     | 0.66              |
| 1:C:141:SER:HA   | 1:C:175:TRP:O    | 1.96                     | 0.66              |
| 1:A:212:MET:HG2  | 1:A:213:ARG:N    | 2.11                     | 0.65              |
| 1:B:642:VAL:HG22 | 1:B:650:GLU:HB2  | 1.78                     | 0.65              |
| 1:D:602:LEU:O    | 1:D:606:LEU:HB2  | 1.96                     | 0.65              |
| 1:D:680:ASN:ND2  | 1:D:682:ASP:H    | 1.94                     | 0.65              |
| 1:B:693:ASN:HD21 | 1:B:713:LEU:HB3  | 1.60                     | 0.65              |
| 1:B:224:PRO:HG2  | 1:B:396:ARG:HB3  | 1.78                     | 0.65              |
| 1:B:247:GLU:OE1  | 1:B:525:HIS:HD2  | 1.79                     | 0.65              |
| 1:C:650:GLU:HG2  | 1:C:671:GLN:OE1  | 1.95                     | 0.65              |
| 1:B:225:GLU:HG2  | 2:B:1464:HOH:O   | 1.96                     | 0.65              |
| 1:A:160:ASP:OD1  | 1:A:162:ARG:HB3  | 1.97                     | 0.64              |
| 1:A:259:ASN:HB3  | 1:A:261:PHE:CG   | 2.32                     | 0.64              |
| 1:A:126:GLY:HA2  | 1:A:204:ASP:OD2  | 1.97                     | 0.64              |
| 1:A:295:ASP:HA   | 1:A:311:ARG:HH22 | 1.61                     | 0.64              |
| 1:A:655:SER:OG   | 1:A:720:THR:HB   | 1.98                     | 0.64              |
| 1:B:211:GLN:O    | 1:B:216:THR:HA   | 1.97                     | 0.64              |
| 1:B:259:ASN:HB3  | 1:B:261:PHE:CE2  | 2.33                     | 0.64              |
| 1:C:667:PHE:HA   | 1:C:705:HIS:CD2  | 2.32                     | 0.64              |
| 1:B:289:ILE:HG13 | 1:B:334:LEU:HD11 | 1.79                     | 0.64              |
| 1:B:350:GLU:HA   | 1:B:354:THR:O    | 1.97                     | 0.63              |
| 1:B:551:ARG:NH2  | 2:B:1476:HOH:O   | 2.32                     | 0.63              |
| 1:B:619:LEU:HG   | 1:B:622:ASP:HB3  | 1.80                     | 0.63              |
| 1:D:376:ASN:HD22 | 1:D:379:ARG:HB2  | 1.62                     | 0.63              |
| 1:A:149:ARG:HD3  | 1:A:193:ILE:CG1  | 2.28                     | 0.63              |
| 1:B:627:GLU:HB3  | 1:B:642:VAL:HG12 | 1.80                     | 0.63              |
| 1:D:247:GLU:OE1  | 1:D:525:HIS:HD2  | 1.81                     | 0.63              |
| 1:C:140:PHE:O    | 1:C:176:GLU:HA   | 1.97                     | 0.63              |
| 1:C:551:ARG:HD3  | 1:C:686:TYR:HB3  | 1.81                     | 0.63              |
| 1:D:469:PRO:HG2  | 1:D:472:MET:CG   | 2.29                     | 0.63              |
| 1:A:169:ARG:HG3  | 1:A:171:GLU:OE1  | 1.98                     | 0.63              |
| 1:B:425:ASN:HD22 | 1:B:427:PHE:H    | 1.46                     | 0.63              |
| 1:C:168:LEU:HD22 | 1:C:169:ARG:N    | 2.13                     | 0.63              |
| 1:B:683:SER:O    | 1:B:685:HIS:O    | 2.16                     | 0.63              |
| 1:C:237:ASN:HD22 | 1:C:283:HIS:HE1  | 1.46                     | 0.63              |
| 1:A:178:PHE:HE1  | 1:A:180:PRO:HG3  | 1.63                     | 0.63              |
| 1:C:536:LEU:HB2  | 1:C:550:LEU:HD22 | 1.80                     | 0.63              |
| 1:A:442:THR:O    | 1:A:446:LEU:HB2  | 1.99                     | 0.63              |
| 1:D:149:ARG:HG2  | 2:D:1484:HOH:O   | 1.99                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:440:ARG:HG2  | 1:D:475:LEU:H    | 1.63                     | 0.63              |
| 1:B:708:GLN:O    | 1:B:709:HIS:ND1  | 2.32                     | 0.62              |
| 1:D:665:TYR:O    | 1:D:712:SER:HA   | 1.98                     | 0.62              |
| 1:B:233:ARG:NH1  | 2:B:1117:HOH:O   | 2.32                     | 0.62              |
| 1:B:619:LEU:HB3  | 1:B:625:GLY:HA3  | 1.80                     | 0.62              |
| 1:A:214:PRO:O    | 1:A:216:THR:N    | 2.32                     | 0.62              |
| 1:B:147:ALA:O    | 1:B:148:ARG:HB3  | 1.99                     | 0.62              |
| 1:B:611:ARG:O    | 1:B:612:HIS:CB   | 2.47                     | 0.62              |
| 1:C:684:MET:H    | 1:C:690:ASN:HD22 | 1.47                     | 0.62              |
| 1:D:143:TRP:CH2  | 1:D:356:LEU:HD22 | 2.34                     | 0.62              |
| 1:A:494:LYS:HD3  | 1:A:538:ARG:HG2  | 1.80                     | 0.62              |
| 1:B:282:THR:OG1  | 1:B:283:HIS:HD2  | 1.83                     | 0.62              |
| 1:B:708:GLN:O    | 1:B:709:HIS:CB   | 2.47                     | 0.62              |
| 1:C:680:ASN:HD22 | 1:C:682:ASP:H    | 1.46                     | 0.62              |
| 1:C:693:ASN:ND2  | 1:C:714:THR:H    | 1.96                     | 0.62              |
| 1:D:138:THR:HG23 | 1:D:182:ALA:O    | 2.00                     | 0.62              |
| 1:C:500:ARG:HG2  | 1:C:500:ARG:HH21 | 1.65                     | 0.62              |
| 1:D:680:ASN:HD22 | 1:D:680:ASN:C    | 2.06                     | 0.62              |
| 1:D:711:LEU:O    | 1:D:712:SER:HB3  | 1.99                     | 0.62              |
| 1:A:266:ARG:HD2  | 2:D:1816:HOH:O   | 1.99                     | 0.62              |
| 1:B:552:ALA:HB2  | 1:B:719:ALA:HA   | 1.82                     | 0.62              |
| 1:B:611:ARG:O    | 1:B:612:HIS:HB3  | 1.98                     | 0.62              |
| 1:B:684:MET:H    | 1:B:690:ASN:ND2  | 1.96                     | 0.62              |
| 1:C:152:VAL:CG2  | 1:C:177:LEU:HD23 | 2.30                     | 0.62              |
| 1:A:147:ALA:O    | 1:A:195:ALA:HA   | 2.01                     | 0.61              |
| 1:C:248:VAL:CG2  | 1:C:286:LEU:HD23 | 2.30                     | 0.61              |
| 1:A:199:LEU:C    | 1:A:199:LEU:HD13 | 2.25                     | 0.61              |
| 1:B:616:MET:SD   | 1:B:651:ILE:HG12 | 2.39                     | 0.61              |
| 1:D:183:HIS:H    | 1:D:186:GLN:HE21 | 1.46                     | 0.61              |
| 1:B:494:LYS:HG2  | 1:B:538:ARG:HG2  | 1.81                     | 0.61              |
| 1:C:618:GLU:OE1  | 1:C:645:ASP:HB2  | 2.00                     | 0.61              |
| 1:A:194:ASP:C    | 1:A:196:ASN:H    | 2.07                     | 0.61              |
| 1:C:680:ASN:HD22 | 1:C:680:ASN:C    | 2.08                     | 0.61              |
| 1:B:194:ASP:HB3  | 1:B:196:ASN:H    | 1.66                     | 0.61              |
| 1:B:684:MET:N    | 1:B:690:ASN:HD22 | 1.98                     | 0.61              |
| 1:C:442:THR:O    | 1:C:446:LEU:HD13 | 2.01                     | 0.61              |
| 1:D:615:ALA:O    | 1:D:643:ARG:HB3  | 2.00                     | 0.61              |
| 1:B:470:GLN:HA   | 1:B:474:GLY:CA   | 2.25                     | 0.60              |
| 1:C:209:GLU:HB3  | 1:C:219:LEU:HB3  | 1.83                     | 0.60              |
| 1:A:121:PRO:HB2  | 1:A:125:LEU:HD12 | 1.82                     | 0.60              |
| 1:B:644:ARG:CG   | 1:B:650:GLU:HB3  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:610:TYR:O    | 1:C:617:HIS:HD2  | 1.85                     | 0.60              |
| 1:A:122:TYR:CE1  | 1:A:123:GLU:HG3  | 2.36                     | 0.60              |
| 1:B:457:ALA:HB2  | 1:B:477:PHE:CE2  | 2.36                     | 0.60              |
| 1:C:686:TYR:O    | 1:C:687:HIS:HB2  | 2.00                     | 0.60              |
| 1:B:143:TRP:CH2  | 1:B:356:LEU:HD22 | 2.36                     | 0.60              |
| 1:B:255:ARG:HB2  | 1:B:583:SER:HB2  | 1.82                     | 0.60              |
| 1:C:211:GLN:CG   | 1:C:217:ALA:H    | 2.14                     | 0.60              |
| 1:A:237:ASN:ND2  | 1:A:283:HIS:HE1  | 2.00                     | 0.60              |
| 1:C:614:LYS:HB3  | 1:C:618:GLU:OE1  | 2.02                     | 0.60              |
| 1:C:630:VAL:HG21 | 1:C:640:ILE:HD12 | 1.83                     | 0.60              |
| 1:D:565:LEU:HD23 | 1:D:565:LEU:C    | 2.25                     | 0.60              |
| 1:B:635:GLU:HG2  | 2:B:937:HOH:O    | 2.01                     | 0.60              |
| 1:D:611:ARG:O    | 1:D:612:HIS:CB   | 2.48                     | 0.60              |
| 1:A:157:ASN:ND2  | 1:A:163:ARG:HB3  | 2.16                     | 0.60              |
| 1:A:650:GLU:OE2  | 1:A:670:ASN:HB2  | 2.01                     | 0.60              |
| 1:C:642:VAL:HG13 | 1:C:650:GLU:HB2  | 1.83                     | 0.60              |
| 1:C:345:ASP:O    | 1:C:346:PHE:C    | 2.45                     | 0.60              |
| 1:B:529:VAL:O    | 1:B:532:LYS:HG3  | 2.02                     | 0.59              |
| 1:C:227:VAL:HG22 | 1:C:319:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:150:VAL:HG22 | 1:A:192:MET:CB   | 2.32                     | 0.59              |
| 1:B:598:GLY:CA   | 1:B:686:TYR:HA   | 2.33                     | 0.59              |
| 1:C:656:ASN:HD21 | 1:C:658:THR:CG2  | 2.07                     | 0.59              |
| 1:D:393:TRP:HB3  | 1:D:399:ILE:HG12 | 1.84                     | 0.59              |
| 1:A:351:PHE:O    | 1:A:353:GLY:N    | 2.35                     | 0.59              |
| 1:C:379:ARG:HB3  | 1:C:382:VAL:HG23 | 1.85                     | 0.59              |
| 1:C:534:SER:HB2  | 2:C:1251:HOH:O   | 2.03                     | 0.59              |
| 1:D:614:LYS:H    | 1:D:614:LYS:HD2  | 1.67                     | 0.59              |
| 1:A:402:LEU:HD12 | 1:A:446:LEU:HD11 | 1.84                     | 0.59              |
| 1:C:289:ILE:HD12 | 1:C:289:ILE:C    | 2.26                     | 0.59              |
| 1:C:336:TRP:HZ2  | 1:C:386:LEU:O    | 1.86                     | 0.59              |
| 1:C:510:GLY:HA2  | 1:C:513:TYR:CE2  | 2.37                     | 0.59              |
| 1:A:635:GLU:H    | 1:A:635:GLU:CD   | 2.09                     | 0.59              |
| 1:C:278:TRP:O    | 1:C:604:ARG:HD2  | 2.02                     | 0.59              |
| 1:D:456:MET:HG2  | 1:D:479:TYR:HB2  | 1.85                     | 0.59              |
| 1:A:292:HIS:O    | 1:A:311:ARG:NH1  | 2.32                     | 0.59              |
| 1:C:262:TRP:CZ3  | 1:C:311:ARG:HB3  | 2.38                     | 0.59              |
| 1:D:140:PHE:HZ   | 1:D:220:ILE:HD11 | 1.67                     | 0.59              |
| 1:D:298:TRP:HE1  | 1:D:580:HIS:CD2  | 2.20                     | 0.59              |
| 1:D:667:PHE:HA   | 1:D:705:HIS:NE2  | 2.18                     | 0.58              |
| 1:A:193:ILE:HA   | 1:A:198:ASN:O    | 2.03                     | 0.58              |
| 1:C:492:TYR:CE2  | 1:C:507:LEU:HD21 | 2.39                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:542:ASP:H    | 1:C:545:GLN:HE21 | 1.51                     | 0.58              |
| 1:C:542:ASP:H    | 1:C:545:GLN:NE2  | 2.00                     | 0.58              |
| 1:A:592:GLY:N    | 2:A:1880:HOH:O   | 2.35                     | 0.58              |
| 1:B:430:ARG:CD   | 1:B:430:ARG:N    | 2.63                     | 0.58              |
| 1:B:708:GLN:O    | 1:B:709:HIS:CG   | 2.57                     | 0.58              |
| 1:D:568:MET:HB2  | 1:D:584:LEU:HD11 | 1.85                     | 0.58              |
| 1:C:594:ASN:N    | 1:C:597:HIS:HD2  | 2.00                     | 0.58              |
| 1:D:708:GLN:O    | 1:D:709:HIS:HB2  | 2.04                     | 0.58              |
| 1:A:171:GLU:CD   | 1:A:171:GLU:H    | 2.11                     | 0.58              |
| 1:B:242:PRO:HB3  | 1:B:617:HIS:CD2  | 2.39                     | 0.58              |
| 1:C:611:ARG:O    | 1:C:612:HIS:CB   | 2.52                     | 0.58              |
| 1:A:128:HIS:HE1  | 1:A:223:LEU:HD13 | 1.68                     | 0.58              |
| 1:A:144:ALA:HB1  | 1:A:352:ASP:HB3  | 1.86                     | 0.58              |
| 1:A:579:ASN:ND2  | 1:A:581:ASP:H    | 2.01                     | 0.58              |
| 1:C:334:LEU:HD13 | 2:C:1891:HOH:O   | 2.04                     | 0.58              |
| 1:A:614:LYS:H    | 1:A:614:LYS:HD2  | 1.69                     | 0.57              |
| 1:B:708:GLN:O    | 1:B:709:HIS:HB2  | 2.04                     | 0.57              |
| 1:D:693:ASN:ND2  | 1:D:714:THR:H    | 1.92                     | 0.57              |
| 1:B:504:HIS:HD2  | 2:B:801:HOH:O    | 1.86                     | 0.57              |
| 1:C:290:ASN:OD1  | 1:C:305:LEU:HD13 | 2.04                     | 0.57              |
| 1:C:545:GLN:HB3  | 2:C:1308:HOH:O   | 2.04                     | 0.57              |
| 1:B:494:LYS:CG   | 1:B:538:ARG:HG2  | 2.34                     | 0.57              |
| 1:C:598:GLY:CA   | 1:C:686:TYR:HA   | 2.34                     | 0.57              |
| 1:A:146:ASN:HB3  | 1:A:195:ALA:HB2  | 1.86                     | 0.57              |
| 1:A:247:GLU:OE1  | 1:A:525:HIS:HD2  | 1.87                     | 0.57              |
| 1:A:470:GLN:O    | 1:A:472:MET:N    | 2.33                     | 0.57              |
| 1:B:373:LEU:HD23 | 1:B:373:LEU:N    | 2.13                     | 0.57              |
| 1:B:425:ASN:ND2  | 1:B:427:PHE:H    | 2.01                     | 0.57              |
| 1:A:149:ARG:NH2  | 1:A:193:ILE:HD11 | 2.20                     | 0.57              |
| 1:A:445:ILE:C    | 1:A:447:GLY:H    | 2.13                     | 0.57              |
| 1:A:298:TRP:HE1  | 1:A:580:HIS:CD2  | 2.22                     | 0.56              |
| 1:D:182:ALA:HA   | 1:D:186:GLN:HE22 | 1.70                     | 0.56              |
| 1:D:668:GLY:H    | 1:D:705:HIS:CD2  | 2.23                     | 0.56              |
| 1:A:199:LEU:HD13 | 1:A:200:ARG:N    | 2.19                     | 0.56              |
| 1:C:282:THR:OG1  | 1:C:283:HIS:HD2  | 1.88                     | 0.56              |
| 1:D:614:LYS:O    | 1:D:618:GLU:HB2  | 2.05                     | 0.56              |
| 1:B:154:GLY:H    | 1:B:157:ASN:HB2  | 1.70                     | 0.56              |
| 1:B:693:ASN:ND2  | 1:B:713:LEU:HB3  | 2.20                     | 0.56              |
| 1:A:118:HIS:CG   | 1:A:380:ARG:HH12 | 2.24                     | 0.56              |
| 1:D:403:ARG:NH1  | 2:D:942:HOH:O    | 2.38                     | 0.56              |
| 1:C:146:ASN:HB2  | 1:C:352:ASP:CG   | 2.31                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:533:LYS:O    | 1:B:538:ARG:NH2  | 2.39                     | 0.56              |
| 1:D:167:ARG:HB3  | 1:D:169:ARG:NH1  | 2.21                     | 0.56              |
| 1:D:193:ILE:CG2  | 1:D:197:GLY:HA2  | 2.34                     | 0.56              |
| 1:A:561:PRO:HA   | 1:A:643:ARG:NH2  | 2.21                     | 0.56              |
| 1:B:214:PRO:C    | 1:B:216:THR:H    | 2.13                     | 0.56              |
| 1:B:483:LEU:HB2  | 2:B:1744:HOH:O   | 2.04                     | 0.56              |
| 1:B:656:ASN:C    | 1:B:656:ASN:HD22 | 2.14                     | 0.56              |
| 1:D:242:PRO:HB3  | 1:D:617:HIS:CD2  | 2.40                     | 0.56              |
| 1:D:446:LEU:C    | 1:D:448:GLU:H    | 2.14                     | 0.56              |
| 1:B:163:ARG:HB3  | 1:B:164:HIS:CD2  | 2.41                     | 0.56              |
| 1:D:279:MET:HE1  | 1:D:600:GLN:O    | 2.05                     | 0.56              |
| 1:C:195:ALA:H    | 1:C:353:GLY:HA3  | 1.70                     | 0.56              |
| 1:D:610:TYR:O    | 1:D:617:HIS:HD2  | 1.89                     | 0.56              |
| 1:A:194:ASP:C    | 1:A:196:ASN:N    | 2.62                     | 0.55              |
| 1:D:389:ASN:O    | 1:D:392:TYR:HB3  | 2.06                     | 0.55              |
| 1:A:229:GLN:HG2  | 1:A:234:LYS:HE2  | 1.88                     | 0.55              |
| 1:B:642:VAL:CG2  | 1:B:650:GLU:HB2  | 2.36                     | 0.55              |
| 1:D:183:HIS:H    | 1:D:186:GLN:NE2  | 2.04                     | 0.55              |
| 1:B:712:SER:N    | 2:B:1924:HOH:O   | 2.23                     | 0.55              |
| 1:C:508:THR:O    | 1:C:511:ILE:HG22 | 2.06                     | 0.55              |
| 1:B:262:TRP:HB3  | 2:B:1055:HOH:O   | 2.06                     | 0.55              |
| 1:B:570:ASN:ND2  | 2:B:826:HOH:O    | 2.38                     | 0.55              |
| 1:B:651:ILE:HD13 | 1:B:722:TRP:HB3  | 1.89                     | 0.55              |
| 1:B:680:ASN:C    | 1:B:680:ASN:HD22 | 2.15                     | 0.55              |
| 1:D:224:PRO:HG2  | 1:D:396:ARG:HB3  | 1.88                     | 0.55              |
| 1:A:509:PHE:HA   | 1:A:512:LEU:HD23 | 1.88                     | 0.55              |
| 1:B:375:TYR:O    | 1:B:376:ASN:HB3  | 2.06                     | 0.55              |
| 1:B:474:GLY:O    | 1:B:476:GLY:N    | 2.39                     | 0.55              |
| 1:C:665:TYR:O    | 1:C:712:SER:HA   | 2.05                     | 0.55              |
| 1:C:674:LYS:HB3  | 1:C:696:THR:HG21 | 1.88                     | 0.55              |
| 1:A:407:VAL:HA   | 1:A:410:MET:HE2  | 1.88                     | 0.55              |
| 1:A:693:ASN:ND2  | 1:A:714:THR:H    | 2.02                     | 0.55              |
| 1:C:289:ILE:HG13 | 1:C:334:LEU:CD1  | 2.36                     | 0.55              |
| 1:B:161:GLY:C    | 1:B:163:ARG:N    | 2.59                     | 0.55              |
| 1:B:273:VAL:HB   | 1:B:274:PRO:HD3  | 1.89                     | 0.55              |
| 1:B:382:VAL:O    | 1:B:385:PHE:HB3  | 2.06                     | 0.55              |
| 1:A:486:MET:O    | 1:A:490:LEU:HB2  | 2.06                     | 0.55              |
| 1:B:602:LEU:HG   | 1:B:606:LEU:HD22 | 1.87                     | 0.55              |
| 1:A:147:ALA:O    | 1:A:148:ARG:CB   | 2.54                     | 0.55              |
| 1:A:150:VAL:HG22 | 1:A:192:MET:HB3  | 1.88                     | 0.55              |
| 1:A:259:ASN:HB3  | 1:A:261:PHE:CD2  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:680:ASN:ND2  | 1:A:680:ASN:C    | 2.65                     | 0.55              |
| 1:A:403:ARG:NH1  | 2:A:1194:HOH:O   | 2.40                     | 0.55              |
| 1:A:611:ARG:O    | 1:A:612:HIS:HB3  | 2.06                     | 0.55              |
| 1:B:351:PHE:O    | 1:B:352:ASP:CB   | 2.54                     | 0.55              |
| 1:C:594:ASN:H    | 1:C:597:HIS:CD2  | 2.20                     | 0.55              |
| 1:D:450:VAL:O    | 1:D:451:SER:C    | 2.48                     | 0.55              |
| 1:D:555:GLY:HA3  | 1:D:720:THR:CG2  | 2.37                     | 0.55              |
| 1:A:138:THR:HG23 | 1:A:182:ALA:O    | 2.07                     | 0.54              |
| 1:A:708:GLN:O    | 1:A:709:HIS:CB   | 2.55                     | 0.54              |
| 1:C:656:ASN:HD22 | 1:C:656:ASN:C    | 2.14                     | 0.54              |
| 1:D:193:ILE:HG22 | 1:D:197:GLY:HA2  | 1.89                     | 0.54              |
| 1:A:147:ALA:H    | 1:A:352:ASP:HB2  | 1.72                     | 0.54              |
| 1:A:194:ASP:HB2  | 1:A:198:ASN:H    | 1.72                     | 0.54              |
| 1:A:273:VAL:HB   | 1:A:274:PRO:HD3  | 1.88                     | 0.54              |
| 1:A:293:PRO:HG2  | 1:A:294:PHE:HD1  | 1.71                     | 0.54              |
| 1:B:608:LEU:O    | 1:B:611:ARG:O    | 2.25                     | 0.54              |
| 1:B:666:ARG:HA   | 2:B:1924:HOH:O   | 2.07                     | 0.54              |
| 1:D:247:GLU:HB3  | 1:D:567:PHE:HA   | 1.89                     | 0.54              |
| 1:D:373:LEU:N    | 1:D:373:LEU:CD2  | 2.71                     | 0.54              |
| 1:A:229:GLN:HE22 | 1:A:233:ARG:NH1  | 2.05                     | 0.54              |
| 1:A:282:THR:OG1  | 1:A:283:HIS:HD2  | 1.91                     | 0.54              |
| 1:A:579:ASN:HD21 | 1:A:581:ASP:HB2  | 1.72                     | 0.54              |
| 1:B:686:TYR:N    | 2:B:805:HOH:O    | 2.22                     | 0.54              |
| 1:C:194:ASP:HB2  | 1:C:198:ASN:HB2  | 1.90                     | 0.54              |
| 1:C:335:ASP:HB3  | 2:C:1699:HOH:O   | 2.08                     | 0.54              |
| 1:C:695:GLY:HA3  | 1:D:591:GLY:CA   | 2.31                     | 0.54              |
| 1:D:492:TYR:CZ   | 1:D:500:ARG:HG2  | 2.41                     | 0.54              |
| 1:B:157:ASN:O    | 1:B:158:TYR:HB2  | 2.06                     | 0.54              |
| 1:A:149:ARG:H    | 1:A:175:TRP:HH2  | 1.54                     | 0.54              |
| 1:A:183:HIS:N    | 1:A:186:GLN:OE1  | 2.40                     | 0.54              |
| 1:B:440:ARG:HE   | 1:B:474:GLY:CA   | 2.20                     | 0.54              |
| 1:C:305:LEU:N    | 1:C:305:LEU:HD22 | 2.21                     | 0.54              |
| 1:A:131:THR:OG1  | 1:A:136:THR:HG22 | 2.06                     | 0.54              |
| 1:C:639:LEU:H    | 1:C:639:LEU:CD1  | 2.20                     | 0.54              |
| 1:D:157:ASN:O    | 1:D:157:ASN:ND2  | 2.41                     | 0.54              |
| 1:B:162:ARG:HG2  | 1:B:163:ARG:N    | 2.22                     | 0.54              |
| 1:B:661:PRO:HB3  | 1:B:717:PRO:HD3  | 1.90                     | 0.54              |
| 1:C:209:GLU:HB2  | 1:C:221:CYS:SG   | 2.48                     | 0.54              |
| 1:C:493:MET:O    | 1:C:540:PRO:HD3  | 2.08                     | 0.54              |
| 1:A:235:LYS:HA   | 1:A:238:GLN:HG3  | 1.90                     | 0.54              |
| 1:A:711:LEU:N    | 2:A:1917:HOH:O   | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:680:ASN:ND2  | 1:B:682:ASP:H    | 2.04                     | 0.54              |
| 1:B:148:ARG:HD3  | 2:B:1626:HOH:O   | 2.08                     | 0.54              |
| 1:B:150:VAL:HG22 | 1:B:192:MET:CB   | 2.38                     | 0.53              |
| 1:C:679:LEU:HA   | 2:C:1519:HOH:O   | 2.07                     | 0.53              |
| 1:D:198:ASN:HB3  | 1:D:200:ARG:NH1  | 2.22                     | 0.53              |
| 1:C:157:ASN:HD21 | 1:C:163:ARG:CB   | 2.22                     | 0.53              |
| 1:C:619:LEU:HB3  | 1:C:622:ASP:HB3  | 1.90                     | 0.53              |
| 1:D:547:PHE:CD2  | 1:D:595:TRP:HB3  | 2.42                     | 0.53              |
| 1:D:610:TYR:CE1  | 1:D:617:HIS:HB3  | 2.43                     | 0.53              |
| 1:C:486:MET:O    | 1:C:490:LEU:HD13 | 2.08                     | 0.53              |
| 1:D:120:ARG:HG2  | 1:D:122:TYR:OH   | 2.08                     | 0.53              |
| 1:D:379:ARG:HB3  | 1:D:382:VAL:HG23 | 1.90                     | 0.53              |
| 1:D:683:SER:O    | 1:D:685:HIS:O    | 2.26                     | 0.53              |
| 1:A:118:HIS:HA   | 2:A:1243:HOH:O   | 2.07                     | 0.53              |
| 1:C:272:LEU:HD23 | 1:C:321:PHE:CZ   | 2.43                     | 0.53              |
| 1:C:349:ALA:O    | 1:C:351:PHE:N    | 2.40                     | 0.53              |
| 1:C:399:ILE:HD11 | 1:C:402:LEU:CD2  | 2.39                     | 0.53              |
| 1:C:412:TYR:CE2  | 1:C:431:GLU:HG2  | 2.44                     | 0.53              |
| 1:C:457:ALA:HB2  | 1:C:477:PHE:CD2  | 2.42                     | 0.53              |
| 1:A:157:ASN:HD21 | 1:A:164:HIS:CD2  | 2.27                     | 0.53              |
| 1:A:341:PHE:CE1  | 1:A:348:LEU:HD23 | 2.43                     | 0.53              |
| 1:A:695:GLY:O    | 1:A:696:THR:HB   | 2.08                     | 0.53              |
| 1:A:721:ILE:HD12 | 1:A:723:LEU:HD11 | 1.91                     | 0.53              |
| 1:B:551:ARG:HG2  | 1:B:602:LEU:HD23 | 1.89                     | 0.53              |
| 1:C:305:LEU:HD22 | 1:C:305:LEU:H    | 1.73                     | 0.53              |
| 1:D:584:LEU:O    | 1:D:585:ASP:CB   | 2.55                     | 0.53              |
| 1:C:184:ASN:ND2  | 1:C:221:CYS:HA   | 2.23                     | 0.53              |
| 1:C:264:SER:OG   | 1:C:267:GLU:HG3  | 2.08                     | 0.53              |
| 1:D:193:ILE:HA   | 1:D:198:ASN:O    | 2.08                     | 0.53              |
| 1:D:721:ILE:HD12 | 1:D:723:LEU:HD21 | 1.90                     | 0.53              |
| 1:A:224:PRO:O    | 1:A:225:GLU:C    | 2.52                     | 0.53              |
| 1:A:647:GLU:HG2  | 2:A:1787:HOH:O   | 2.09                     | 0.53              |
| 1:B:247:GLU:OE1  | 1:B:525:HIS:CD2  | 2.60                     | 0.53              |
| 1:A:315:ARG:C    | 1:A:315:ARG:HD2  | 2.34                     | 0.53              |
| 1:C:247:GLU:OE1  | 1:C:525:HIS:HD2  | 1.92                     | 0.53              |
| 1:C:564:LYS:HD2  | 1:C:564:LYS:N    | 2.24                     | 0.53              |
| 1:C:711:LEU:O    | 1:C:712:SER:HB3  | 2.08                     | 0.53              |
| 1:A:532:LYS:O    | 1:A:533:LYS:HB2  | 2.09                     | 0.53              |
| 1:C:137:GLY:HA3  | 1:C:180:PRO:HA   | 1.90                     | 0.53              |
| 1:D:340:HIS:HE1  | 1:D:405:ASP:OD2  | 1.91                     | 0.53              |
| 1:D:475:LEU:N    | 1:D:475:LEU:HD12 | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:MET:O    | 1:C:193:ILE:HD13 | 2.09                     | 0.53              |
| 1:C:226:LYS:HB2  | 2:C:1359:HOH:O   | 2.09                     | 0.53              |
| 1:D:542:ASP:H    | 1:D:545:GLN:HE21 | 1.55                     | 0.53              |
| 1:D:668:GLY:H    | 1:D:705:HIS:HD2  | 1.56                     | 0.53              |
| 1:B:225:GLU:HA   | 1:B:225:GLU:OE2  | 2.09                     | 0.52              |
| 1:D:459:GLU:HA   | 2:D:1011:HOH:O   | 2.09                     | 0.52              |
| 1:B:132:MET:HE3  | 1:B:139:ARG:HH12 | 1.74                     | 0.52              |
| 1:B:234:LYS:HG2  | 1:B:452:GLY:HA3  | 1.91                     | 0.52              |
| 1:C:138:THR:HG23 | 1:C:182:ALA:O    | 2.09                     | 0.52              |
| 1:C:298:TRP:HE1  | 1:C:580:HIS:CD2  | 2.27                     | 0.52              |
| 1:A:229:GLN:NE2  | 1:A:233:ARG:NH1  | 2.57                     | 0.52              |
| 1:B:492:TYR:CE2  | 1:B:500:ARG:HG2  | 2.44                     | 0.52              |
| 1:D:443:ASN:ND2  | 1:D:455:THR:OG1  | 2.42                     | 0.52              |
| 1:C:149:ARG:HB3  | 1:C:193:ILE:CG1  | 2.40                     | 0.52              |
| 1:D:373:LEU:HD23 | 1:D:373:LEU:N    | 2.24                     | 0.52              |
| 1:B:542:ASP:H    | 1:B:545:GLN:HE21 | 1.56                     | 0.52              |
| 1:C:647:GLU:HB3  | 1:C:649:ASN:HD22 | 1.75                     | 0.52              |
| 1:B:194:ASP:OD1  | 1:B:198:ASN:HB2  | 2.10                     | 0.52              |
| 1:C:290:ASN:ND2  | 1:C:304:GLY:O    | 2.42                     | 0.52              |
| 1:D:558:TRP:HA   | 1:D:564:LYS:HE3  | 1.90                     | 0.52              |
| 1:A:172:SER:O    | 1:A:174:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:233:ARG:HD3  | 1:A:326:HIS:CD2  | 2.45                     | 0.52              |
| 1:B:446:LEU:C    | 2:B:1835:HOH:O   | 2.53                     | 0.52              |
| 1:C:410:MET:HE1  | 1:C:439:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:376:ASN:C    | 1:A:376:ASN:HD22 | 2.18                     | 0.52              |
| 1:B:194:ASP:HB2  | 1:B:198:ASN:HB2  | 1.91                     | 0.52              |
| 1:B:196:ASN:HB2  | 1:B:198:ASN:HD22 | 1.75                     | 0.52              |
| 1:B:695:GLY:O    | 1:B:696:THR:HB   | 2.08                     | 0.52              |
| 1:C:157:ASN:HD21 | 1:C:163:ARG:HB3  | 1.73                     | 0.52              |
| 1:D:351:PHE:O    | 1:D:352:ASP:OD2  | 2.28                     | 0.52              |
| 1:D:618:GLU:HB3  | 1:D:619:LEU:HD22 | 1.90                     | 0.52              |
| 1:A:132:MET:HA   | 1:A:132:MET:HE2  | 1.91                     | 0.52              |
| 1:A:184:ASN:HA   | 1:A:220:ILE:HG22 | 1.91                     | 0.52              |
| 1:B:686:TYR:O    | 1:B:687:HIS:HB2  | 2.09                     | 0.52              |
| 1:C:684:MET:HE3  | 1:D:684:MET:CE   | 2.39                     | 0.52              |
| 1:D:167:ARG:NH1  | 2:D:1310:HOH:O   | 2.43                     | 0.52              |
| 1:D:684:MET:HB2  | 1:D:690:ASN:CG   | 2.35                     | 0.52              |
| 1:A:351:PHE:HB3  | 1:A:356:LEU:HD12 | 1.92                     | 0.51              |
| 1:C:551:ARG:C    | 1:C:681:THR:HG21 | 2.35                     | 0.51              |
| 1:A:700:ASP:O    | 1:A:709:HIS:HA   | 2.10                     | 0.51              |
| 1:C:149:ARG:HB3  | 1:C:193:ILE:HG13 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:684:MET:C    | 1:D:685:HIS:O    | 2.49                     | 0.51              |
| 1:A:610:TYR:CE1  | 1:A:617:HIS:HB3  | 2.45                     | 0.51              |
| 1:C:579:ASN:HD22 | 1:C:579:ASN:C    | 2.19                     | 0.51              |
| 1:D:186:GLN:HA   | 2:D:1309:HOH:O   | 2.09                     | 0.51              |
| 1:A:610:TYR:O    | 1:A:617:HIS:HD2  | 1.92                     | 0.51              |
| 1:C:169:ARG:HB2  | 2:C:1849:HOH:O   | 2.09                     | 0.51              |
| 1:C:651:ILE:HD12 | 1:C:651:ILE:C    | 2.34                     | 0.51              |
| 1:D:412:TYR:C    | 1:D:414:ASP:H    | 2.18                     | 0.51              |
| 1:A:118:HIS:CD2  | 1:A:380:ARG:HH12 | 2.29                     | 0.51              |
| 1:B:237:ASN:HD22 | 1:B:283:HIS:HE1  | 1.59                     | 0.51              |
| 1:D:371:ASN:CG   | 1:D:372:THR:N    | 2.67                     | 0.51              |
| 1:D:551:ARG:HB3  | 1:D:681:THR:HB   | 1.93                     | 0.51              |
| 1:A:145:PRO:HD2  | 1:A:356:LEU:HD11 | 1.92                     | 0.51              |
| 1:C:164:HIS:HB3  | 1:C:177:LEU:HD21 | 1.92                     | 0.51              |
| 1:B:539:MET:O    | 1:B:546:LYS:HE3  | 2.10                     | 0.51              |
| 1:B:593:ASP:HA   | 1:B:597:HIS:CD2  | 2.46                     | 0.51              |
| 1:C:247:GLU:OE1  | 1:C:525:HIS:CD2  | 2.63                     | 0.51              |
| 1:C:290:ASN:CB   | 2:C:833:HOH:O    | 2.48                     | 0.51              |
| 1:C:650:GLU:OE1  | 1:C:670:ASN:HB2  | 2.11                     | 0.51              |
| 1:B:441:ASN:OD1  | 1:B:444:ARG:NH2  | 2.40                     | 0.51              |
| 1:C:144:ALA:HA   | 1:C:356:LEU:HD11 | 1.92                     | 0.51              |
| 1:D:289:ILE:C    | 1:D:289:ILE:HD12 | 2.36                     | 0.51              |
| 1:D:607:ASN:O    | 1:D:611:ARG:HG3  | 2.10                     | 0.51              |
| 1:D:636:ARG:HG2  | 1:D:662:ARG:NH2  | 2.26                     | 0.51              |
| 1:A:354:THR:O    | 1:A:356:LEU:N    | 2.43                     | 0.51              |
| 1:B:168:LEU:HD22 | 1:B:168:LEU:C    | 2.35                     | 0.51              |
| 1:C:350:GLU:HA   | 1:C:354:THR:O    | 2.11                     | 0.51              |
| 1:A:380:ARG:HH21 | 1:A:380:ARG:CG   | 2.19                     | 0.50              |
| 1:A:528:VAL:HA   | 1:A:533:LYS:O    | 2.11                     | 0.50              |
| 1:A:539:MET:O    | 1:A:546:LYS:HE3  | 2.11                     | 0.50              |
| 1:B:430:ARG:HD2  | 1:B:430:ARG:N    | 2.04                     | 0.50              |
| 1:C:198:ASN:HB3  | 1:C:200:ARG:HH12 | 1.73                     | 0.50              |
| 1:A:214:PRO:C    | 1:A:216:THR:H    | 2.18                     | 0.50              |
| 1:B:310:ARG:HE   | 1:B:313:GLY:C    | 2.18                     | 0.50              |
| 1:B:411:ILE:HG13 | 1:B:412:TYR:CD1  | 2.46                     | 0.50              |
| 1:D:182:ALA:HA   | 1:D:186:GLN:NE2  | 2.25                     | 0.50              |
| 1:B:192:MET:SD   | 1:B:352:ASP:HA   | 2.51                     | 0.50              |
| 1:B:196:ASN:HB2  | 1:B:198:ASN:ND2  | 2.26                     | 0.50              |
| 1:C:254:ARG:O    | 1:C:263:LEU:HG   | 2.12                     | 0.50              |
| 1:C:272:LEU:HD23 | 1:C:321:PHE:HZ   | 1.76                     | 0.50              |
| 1:C:500:ARG:HG2  | 1:C:500:ARG:NH2  | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:495:LEU:O    | 1:D:500:ARG:NH1  | 2.44                     | 0.50              |
| 1:D:264:SER:H    | 1:D:267:GLU:HB2  | 1.74                     | 0.50              |
| 1:D:593:ASP:OD2  | 1:D:687:HIS:HE1  | 1.95                     | 0.50              |
| 1:B:552:ALA:HA   | 1:B:720:THR:HG23 | 1.93                     | 0.50              |
| 1:C:399:ILE:HD12 | 1:C:401:ALA:O    | 2.11                     | 0.50              |
| 1:C:568:MET:HB2  | 1:C:584:LEU:HD11 | 1.92                     | 0.50              |
| 1:D:278:TRP:O    | 1:D:604:ARG:HD2  | 2.11                     | 0.50              |
| 1:C:183:HIS:H    | 1:C:186:GLN:NE2  | 2.03                     | 0.50              |
| 1:C:349:ALA:O    | 1:C:350:GLU:C    | 2.54                     | 0.50              |
| 1:D:527:GLU:HB3  | 2:D:1112:HOH:O   | 2.10                     | 0.50              |
| 1:D:601:ARG:HD3  | 2:D:1124:HOH:O   | 2.11                     | 0.50              |
| 1:A:404:VAL:HG11 | 1:A:410:MET:HE1  | 1.93                     | 0.50              |
| 1:B:194:ASP:C    | 1:B:196:ASN:N    | 2.66                     | 0.50              |
| 1:B:486:MET:O    | 1:B:490:LEU:HB2  | 2.12                     | 0.50              |
| 1:A:394:ILE:HD13 | 1:A:446:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:563:LYS:C    | 1:A:564:LYS:HD2  | 2.36                     | 0.50              |
| 1:B:194:ASP:CG   | 1:B:198:ASN:HB2  | 2.37                     | 0.50              |
| 1:B:246:TYR:CE2  | 1:B:568:MET:HA   | 2.47                     | 0.50              |
| 1:B:440:ARG:CG   | 1:B:475:LEU:H    | 2.25                     | 0.50              |
| 1:B:658:THR:HB   | 2:B:865:HOH:O    | 2.11                     | 0.50              |
| 1:B:693:ASN:HD21 | 1:B:714:THR:H    | 1.60                     | 0.50              |
| 1:C:290:ASN:OD1  | 1:C:305:LEU:HA   | 2.12                     | 0.50              |
| 1:C:514:ASN:ND2  | 2:C:1127:HOH:O   | 2.45                     | 0.50              |
| 1:D:651:ILE:C    | 1:D:651:ILE:HD12 | 2.36                     | 0.50              |
| 1:B:617:HIS:HE1  | 2:B:1920:HOH:O   | 1.95                     | 0.49              |
| 1:C:351:PHE:O    | 1:C:352:ASP:OD2  | 2.29                     | 0.49              |
| 1:D:183:HIS:ND1  | 1:D:186:GLN:NE2  | 2.60                     | 0.49              |
| 1:D:666:ARG:HA   | 1:D:712:SER:HA   | 1.93                     | 0.49              |
| 1:A:132:MET:O    | 1:A:135:VAL:HG12 | 2.12                     | 0.49              |
| 1:A:410:MET:HE3  | 1:A:439:LEU:HD11 | 1.92                     | 0.49              |
| 1:B:693:ASN:O    | 1:B:694:GLY:O    | 2.30                     | 0.49              |
| 1:C:497:PRO:CA   | 1:C:500:ARG:HD3  | 2.29                     | 0.49              |
| 1:C:558:TRP:HA   | 1:C:564:LYS:HE3  | 1.93                     | 0.49              |
| 1:C:708:GLN:HG2  | 1:C:709:HIS:ND1  | 2.27                     | 0.49              |
| 1:D:679:LEU:HD22 | 1:D:722:TRP:CE2  | 2.46                     | 0.49              |
| 1:A:211:GLN:NE2  | 1:A:214:PRO:O    | 2.44                     | 0.49              |
| 1:B:341:PHE:CD2  | 1:B:373:LEU:HD12 | 2.47                     | 0.49              |
| 1:B:631:VAL:HG22 | 1:B:631:VAL:O    | 2.11                     | 0.49              |
| 1:C:488:ASP:O    | 1:C:491:ASP:HB2  | 2.11                     | 0.49              |
| 1:D:293:PRO:HD3  | 1:D:303:THR:CG2  | 2.43                     | 0.49              |
| 1:B:343:THR:HG22 | 1:B:373:LEU:HD21 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:315:ARG:HG2  | 1:C:315:ARG:HH11 | 1.77                     | 0.49              |
| 1:D:618:GLU:C    | 1:D:619:LEU:HD22 | 2.38                     | 0.49              |
| 1:A:225:GLU:O    | 1:A:396:ARG:NH2  | 2.46                     | 0.49              |
| 1:A:677:GLU:HG2  | 1:A:723:LEU:CD1  | 2.43                     | 0.49              |
| 1:B:140:PHE:O    | 1:B:176:GLU:HA   | 2.12                     | 0.49              |
| 1:B:381:GLU:OE2  | 1:B:381:GLU:N    | 2.42                     | 0.49              |
| 1:B:511:ILE:HD13 | 1:B:626:PHE:CD2  | 2.48                     | 0.49              |
| 1:C:655:SER:HB3  | 1:C:657:PHE:CE2  | 2.48                     | 0.49              |
| 1:A:212:MET:CE   | 1:A:213:ARG:HG3  | 2.38                     | 0.49              |
| 1:C:264:SER:HB2  | 2:C:1100:HOH:O   | 2.13                     | 0.49              |
| 1:C:584:LEU:O    | 1:C:585:ASP:OD2  | 2.30                     | 0.49              |
| 1:C:701:GLU:HA   | 1:C:709:HIS:HA   | 1.94                     | 0.49              |
| 1:D:290:ASN:ND2  | 2:D:861:HOH:O    | 2.44                     | 0.49              |
| 1:D:440:ARG:CG   | 1:D:475:LEU:H    | 2.26                     | 0.49              |
| 1:D:470:GLN:HA   | 1:D:474:GLY:HA2  | 1.94                     | 0.49              |
| 1:A:542:ASP:O    | 1:A:545:GLN:N    | 2.46                     | 0.49              |
| 1:C:394:ILE:O    | 1:C:398:GLY:HA2  | 2.13                     | 0.49              |
| 1:C:564:LYS:HE2  | 1:C:610:TYR:CE1  | 2.48                     | 0.49              |
| 1:D:337:VAL:HG23 | 1:D:337:VAL:O    | 2.12                     | 0.49              |
| 1:A:247:GLU:OE1  | 1:A:525:HIS:CD2  | 2.66                     | 0.49              |
| 1:A:504:HIS:CG   | 1:A:634:LYS:HG2  | 2.47                     | 0.49              |
| 1:A:632:ASP:HB2  | 2:A:1911:HOH:O   | 2.12                     | 0.49              |
| 1:B:160:ASP:OD2  | 1:B:162:ARG:HD2  | 2.13                     | 0.49              |
| 1:B:410:MET:HE1  | 1:B:439:LEU:HD21 | 1.93                     | 0.49              |
| 1:B:594:ASN:N    | 1:B:597:HIS:HD2  | 1.96                     | 0.49              |
| 1:A:194:ASP:CG   | 1:A:198:ASN:HB2  | 2.38                     | 0.49              |
| 1:A:432:ASN:ND2  | 1:A:435:ALA:HB2  | 2.28                     | 0.49              |
| 1:C:208:PHE:HA   | 1:C:306:TYR:O    | 2.13                     | 0.49              |
| 1:C:685:HIS:ND1  | 1:C:685:HIS:N    | 2.60                     | 0.49              |
| 1:C:499:TYR:O    | 1:C:501:GLN:N    | 2.46                     | 0.49              |
| 1:C:636:ARG:CB   | 1:C:638:VAL:HG23 | 2.42                     | 0.49              |
| 1:C:708:GLN:O    | 1:C:709:HIS:HB2  | 2.13                     | 0.49              |
| 1:D:547:PHE:CE2  | 1:D:595:TRP:HB3  | 2.48                     | 0.49              |
| 1:B:194:ASP:C    | 1:B:196:ASN:H    | 2.21                     | 0.48              |
| 1:B:403:ARG:NH2  | 2:B:809:HOH:O    | 2.46                     | 0.48              |
| 1:B:408:ALA:HB2  | 1:B:459:GLU:OE2  | 2.13                     | 0.48              |
| 1:B:708:GLN:O    | 1:B:708:GLN:HG2  | 2.13                     | 0.48              |
| 1:D:489:THR:O    | 1:D:493:MET:HG2  | 2.13                     | 0.48              |
| 1:A:150:VAL:HG22 | 1:A:192:MET:HE2  | 1.94                     | 0.48              |
| 1:A:150:VAL:CG2  | 1:A:192:MET:HE2  | 2.43                     | 0.48              |
| 1:A:341:PHE:HD1  | 1:A:375:TYR:CD2  | 2.31                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:374:ILE:HD13 | 1:A:374:ILE:H    | 1.78                     | 0.48              |
| 1:A:374:ILE:HD13 | 1:A:374:ILE:N    | 2.27                     | 0.48              |
| 1:A:564:LYS:HD2  | 1:A:564:LYS:N    | 2.28                     | 0.48              |
| 1:A:571:GLU:HA   | 1:A:603:VAL:HG21 | 1.94                     | 0.48              |
| 1:A:686:TYR:N    | 2:A:1474:HOH:O   | 2.22                     | 0.48              |
| 1:B:147:ALA:O    | 1:B:148:ARG:CB   | 2.61                     | 0.48              |
| 1:C:209:GLU:HG2  | 1:C:219:LEU:HD22 | 1.95                     | 0.48              |
| 1:C:259:ASN:N    | 1:C:259:ASN:HD22 | 2.11                     | 0.48              |
| 1:A:139:ARG:HG3  | 1:A:139:ARG:HH11 | 1.77                     | 0.48              |
| 1:A:358:GLU:OE2  | 1:A:358:GLU:N    | 2.45                     | 0.48              |
| 1:A:504:HIS:HD2  | 2:A:991:HOH:O    | 1.94                     | 0.48              |
| 1:A:609:THR:O    | 1:A:611:ARG:O    | 2.31                     | 0.48              |
| 1:B:254:ARG:O    | 1:B:255:ARG:HG2  | 2.14                     | 0.48              |
| 1:C:683:SER:HA   | 2:C:1568:HOH:O   | 2.12                     | 0.48              |
| 1:D:135:VAL:HG12 | 1:D:180:PRO:HB3  | 1.95                     | 0.48              |
| 1:A:665:TYR:O    | 1:A:712:SER:HA   | 2.13                     | 0.48              |
| 1:C:545:GLN:O    | 1:C:549:ASN:ND2  | 2.46                     | 0.48              |
| 1:C:551:ARG:HB3  | 1:C:681:THR:HG22 | 1.95                     | 0.48              |
| 1:D:631:VAL:O    | 1:D:631:VAL:HG22 | 2.12                     | 0.48              |
| 1:A:211:GLN:CG   | 1:A:214:PRO:HB2  | 2.42                     | 0.48              |
| 1:A:568:MET:HB2  | 1:A:584:LEU:HD11 | 1.95                     | 0.48              |
| 1:C:252:SER:HB3  | 1:C:580:HIS:O    | 2.14                     | 0.48              |
| 1:C:318:PHE:HZ   | 2:C:1891:HOH:O   | 1.95                     | 0.48              |
| 1:C:613:HIS:CD2  | 1:C:678:ILE:HD12 | 2.48                     | 0.48              |
| 1:D:579:ASN:ND2  | 2:D:1033:HOH:O   | 2.47                     | 0.48              |
| 1:C:130:ASP:CG   | 1:C:131:THR:H    | 2.22                     | 0.48              |
| 1:C:143:TRP:CH2  | 1:C:356:LEU:HD22 | 2.49                     | 0.48              |
| 1:C:259:ASN:H    | 1:C:259:ASN:ND2  | 2.12                     | 0.48              |
| 1:D:341:PHE:CZ   | 1:D:358:GLU:HB3  | 2.48                     | 0.48              |
| 1:A:150:VAL:HG22 | 1:A:192:MET:HB2  | 1.94                     | 0.48              |
| 1:C:700:ASP:O    | 1:C:709:HIS:HA   | 2.13                     | 0.48              |
| 1:D:444:ARG:O    | 1:D:448:GLU:HB2  | 2.14                     | 0.48              |
| 1:B:442:THR:O    | 1:B:446:LEU:HB2  | 2.12                     | 0.48              |
| 1:C:157:ASN:CG   | 1:C:164:HIS:HD2  | 2.21                     | 0.48              |
| 1:C:209:GLU:HG2  | 1:C:219:LEU:HD13 | 1.96                     | 0.48              |
| 1:C:685:HIS:O    | 1:C:686:TYR:CG   | 2.66                     | 0.48              |
| 1:A:512:LEU:HD22 | 1:A:512:LEU:H    | 1.79                     | 0.48              |
| 1:A:693:ASN:HD21 | 1:A:714:THR:N    | 2.04                     | 0.48              |
| 1:B:351:PHE:O    | 1:B:352:ASP:HB3  | 2.13                     | 0.48              |
| 1:B:618:GLU:OE1  | 1:B:645:ASP:HB2  | 2.13                     | 0.48              |
| 1:B:728:GLU:HG2  | 2:B:1862:HOH:O   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:166:MET:HG2  | 1:C:177:LEU:HB2  | 1.96                     | 0.48              |
| 1:C:352:ASP:OD2  | 1:C:352:ASP:C    | 2.56                     | 0.48              |
| 1:C:480:LYS:O    | 1:C:519:PHE:HD2  | 1.97                     | 0.48              |
| 1:D:371:ASN:O    | 1:D:372:THR:C    | 2.55                     | 0.48              |
| 1:D:680:ASN:ND2  | 1:D:680:ASN:C    | 2.72                     | 0.48              |
| 1:D:685:HIS:C    | 1:D:687:HIS:H    | 2.21                     | 0.48              |
| 1:B:651:ILE:O    | 1:B:651:ILE:HG13 | 2.14                     | 0.48              |
| 1:C:192:MET:SD   | 1:C:352:ASP:HA   | 2.54                     | 0.48              |
| 2:C:1199:HOH:O   | 1:D:695:GLY:HA2  | 2.13                     | 0.48              |
| 1:D:552:ALA:HA   | 1:D:720:THR:CG2  | 2.41                     | 0.47              |
| 1:A:147:ALA:HB3  | 1:A:175:TRP:HZ2  | 1.79                     | 0.47              |
| 1:B:413:ARG:O    | 1:B:414:ASP:HB2  | 2.14                     | 0.47              |
| 1:B:665:TYR:O    | 1:B:712:SER:HA   | 2.14                     | 0.47              |
| 1:A:474:GLY:O    | 1:A:476:GLY:N    | 2.46                     | 0.47              |
| 1:A:576:ARG:NH1  | 1:A:585:ASP:OD2  | 2.47                     | 0.47              |
| 1:B:315:ARG:HD2  | 1:B:315:ARG:C    | 2.40                     | 0.47              |
| 1:C:685:HIS:O    | 1:C:686:TYR:CB   | 2.61                     | 0.47              |
| 1:D:148:ARG:O    | 1:D:193:ILE:HB   | 2.14                     | 0.47              |
| 1:D:219:LEU:HD23 | 1:D:220:ILE:O    | 2.14                     | 0.47              |
| 1:D:514:ASN:ND2  | 1:D:561:PRO:HB2  | 2.28                     | 0.47              |
| 1:D:564:LYS:N    | 1:D:564:LYS:HD2  | 2.29                     | 0.47              |
| 1:A:149:ARG:HD3  | 1:A:193:ILE:HG13 | 1.95                     | 0.47              |
| 1:A:457:ALA:HB2  | 1:A:477:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:413:ARG:HE   | 1:B:432:ASN:HA   | 1.79                     | 0.47              |
| 1:C:407:VAL:O    | 1:C:411:ILE:HG12 | 2.15                     | 0.47              |
| 1:D:680:ASN:HD22 | 1:D:682:ASP:H    | 1.62                     | 0.47              |
| 1:A:211:GLN:O    | 1:A:216:THR:HA   | 2.13                     | 0.47              |
| 1:B:211:GLN:O    | 1:B:211:GLN:HG3  | 2.14                     | 0.47              |
| 1:B:697:VAL:HG11 | 1:B:713:LEU:HD23 | 1.95                     | 0.47              |
| 1:C:225:GLU:HG3  | 1:C:225:GLU:O    | 2.14                     | 0.47              |
| 1:C:666:ARG:NH1  | 1:C:700:ASP:HB2  | 2.29                     | 0.47              |
| 1:C:288:PRO:C    | 1:C:290:ASN:H    | 2.22                     | 0.47              |
| 1:C:292:HIS:O    | 1:C:311:ARG:NH1  | 2.47                     | 0.47              |
| 1:C:594:ASN:OD1  | 1:C:596:HIS:HB2  | 2.15                     | 0.47              |
| 1:D:135:VAL:CG1  | 1:D:180:PRO:HB3  | 2.44                     | 0.47              |
| 1:A:132:MET:HE2  | 1:A:132:MET:CA   | 2.45                     | 0.47              |
| 1:A:168:LEU:CG   | 1:A:169:ARG:N    | 2.78                     | 0.47              |
| 1:A:641:PHE:CD1  | 1:A:641:PHE:C    | 2.92                     | 0.47              |
| 1:B:149:ARG:HB3  | 1:B:193:ILE:HB   | 1.95                     | 0.47              |
| 1:B:160:ASP:CG   | 1:B:162:ARG:HD2  | 2.40                     | 0.47              |
| 1:B:374:ILE:HD13 | 1:B:374:ILE:H    | 1.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:297:SER:C    | 1:C:299:GLY:H    | 2.23                     | 0.47              |
| 1:C:305:LEU:H    | 1:C:305:LEU:CD2  | 2.27                     | 0.47              |
| 1:C:683:SER:O    | 1:C:685:HIS:O    | 2.33                     | 0.47              |
| 1:D:141:SER:HA   | 1:D:175:TRP:O    | 2.13                     | 0.47              |
| 1:D:237:ASN:ND2  | 1:D:283:HIS:HE1  | 2.13                     | 0.47              |
| 1:D:282:THR:OG1  | 1:D:283:HIS:HD2  | 1.97                     | 0.47              |
| 1:D:346:PHE:HA   | 2:D:1211:HOH:O   | 2.14                     | 0.47              |
| 1:D:379:ARG:HB3  | 1:D:382:VAL:CG2  | 2.44                     | 0.47              |
| 1:D:490:LEU:O    | 1:D:494:LYS:HG3  | 2.14                     | 0.47              |
| 1:A:463:PHE:CE2  | 1:A:475:LEU:HD13 | 2.49                     | 0.47              |
| 1:B:335:ASP:OD1  | 1:B:403:ARG:HD3  | 2.14                     | 0.47              |
| 1:B:572:PHE:HB2  | 1:B:589:LEU:HD21 | 1.96                     | 0.47              |
| 1:C:408:ALA:HB2  | 1:C:459:GLU:OE2  | 2.15                     | 0.47              |
| 1:C:465:GLY:HA2  | 1:C:468:ARG:CG   | 2.45                     | 0.47              |
| 1:A:144:ALA:HB1  | 1:A:352:ASP:CB   | 2.45                     | 0.47              |
| 1:B:163:ARG:NH2  | 2:B:1006:HOH:O   | 2.47                     | 0.47              |
| 1:B:298:TRP:HE1  | 1:B:580:HIS:CD2  | 2.33                     | 0.47              |
| 1:C:157:ASN:OD1  | 1:C:164:HIS:HD2  | 1.98                     | 0.47              |
| 1:C:602:LEU:HA   | 1:C:686:TYR:CE1  | 2.49                     | 0.47              |
| 1:D:273:VAL:HB   | 1:D:274:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:229:GLN:HG2  | 1:A:234:LYS:HG2  | 1.95                     | 0.47              |
| 1:A:504:HIS:CD2  | 1:A:634:LYS:HA   | 2.50                     | 0.47              |
| 1:B:268:LEU:O    | 1:B:272:LEU:HB3  | 2.15                     | 0.47              |
| 1:B:551:ARG:HG2  | 1:B:602:LEU:CD2  | 2.45                     | 0.47              |
| 1:B:598:GLY:HA3  | 1:B:686:TYR:HA   | 1.96                     | 0.47              |
| 1:C:259:ASN:N    | 1:C:259:ASN:ND2  | 2.59                     | 0.47              |
| 1:C:666:ARG:HH12 | 1:C:700:ASP:HB2  | 1.79                     | 0.47              |
| 1:D:205:PRO:HB3  | 1:D:348:LEU:HD11 | 1.97                     | 0.47              |
| 1:A:157:ASN:C    | 1:A:159:TRP:N    | 2.71                     | 0.46              |
| 1:A:614:LYS:HD2  | 1:A:614:LYS:N    | 2.30                     | 0.46              |
| 1:C:681:THR:HG22 | 2:C:1864:HOH:O   | 2.15                     | 0.46              |
| 1:D:265:TYR:HB2  | 1:D:317:ASP:HB3  | 1.97                     | 0.46              |
| 1:B:543:ALA:O    | 1:B:547:PHE:HD1  | 1.98                     | 0.46              |
| 1:B:711:LEU:O    | 1:B:712:SER:HB3  | 2.15                     | 0.46              |
| 1:C:166:MET:HG2  | 1:C:177:LEU:CB   | 2.45                     | 0.46              |
| 1:D:722:TRP:C    | 1:D:723:LEU:HD22 | 2.40                     | 0.46              |
| 1:A:147:ALA:HB3  | 1:A:175:TRP:CZ2  | 2.50                     | 0.46              |
| 1:B:352:ASP:C    | 1:B:352:ASP:OD2  | 2.57                     | 0.46              |
| 1:C:160:ASP:OD2  | 1:C:162:ARG:HG2  | 2.16                     | 0.46              |
| 1:C:349:ALA:HA   | 1:C:358:GLU:OE1  | 2.14                     | 0.46              |
| 1:C:551:ARG:HD2  | 1:C:681:THR:O    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:722:TRP:C    | 1:C:723:LEU:HD22 | 2.40                     | 0.46              |
| 1:A:257:THR:HG22 | 1:A:258:ASP:N    | 2.30                     | 0.46              |
| 1:A:490:LEU:O    | 1:A:494:LYS:HG3  | 2.14                     | 0.46              |
| 1:B:462:ASP:O    | 1:B:463:PHE:C    | 2.59                     | 0.46              |
| 1:C:703:ALA:HA   | 1:C:707:ARG:O    | 2.15                     | 0.46              |
| 1:D:584:LEU:O    | 1:D:585:ASP:HB2  | 2.15                     | 0.46              |
| 1:D:639:LEU:N    | 1:D:639:LEU:HD12 | 2.29                     | 0.46              |
| 1:D:667:PHE:O    | 1:D:710:SER:HB2  | 2.14                     | 0.46              |
| 1:A:118:HIS:O    | 1:A:121:PRO:HD3  | 2.16                     | 0.46              |
| 1:C:192:MET:HE3  | 1:C:202:LYS:HG3  | 1.97                     | 0.46              |
| 1:C:273:VAL:CB   | 1:C:274:PRO:HD3  | 2.40                     | 0.46              |
| 1:C:595:TRP:O    | 1:C:599:VAL:HG23 | 2.16                     | 0.46              |
| 1:D:246:TYR:HB2  | 1:D:281:PHE:CD2  | 2.50                     | 0.46              |
| 1:A:593:ASP:OD2  | 1:A:687:HIS:HE1  | 1.99                     | 0.46              |
| 1:B:379:ARG:HB3  | 1:B:382:VAL:HG23 | 1.97                     | 0.46              |
| 1:D:283:HIS:ND1  | 1:D:333:ILE:HD11 | 2.31                     | 0.46              |
| 1:A:211:GLN:O    | 1:A:211:GLN:HG2  | 2.14                     | 0.46              |
| 1:A:289:ILE:H    | 1:A:289:ILE:HG13 | 1.63                     | 0.46              |
| 1:B:456:MET:HG2  | 1:B:479:TYR:HB2  | 1.97                     | 0.46              |
| 1:C:341:PHE:HE1  | 1:C:357:TYR:HB3  | 1.80                     | 0.46              |
| 1:C:565:LEU:C    | 1:C:565:LEU:HD23 | 2.40                     | 0.46              |
| 1:C:631:VAL:HG22 | 1:C:631:VAL:O    | 2.14                     | 0.46              |
| 1:A:148:ARG:O    | 1:A:149:ARG:CB   | 2.62                     | 0.46              |
| 1:A:150:VAL:HG12 | 1:A:166:MET:SD   | 2.56                     | 0.46              |
| 1:A:227:VAL:HG12 | 1:A:233:ARG:HH22 | 1.80                     | 0.46              |
| 1:A:237:ASN:HD22 | 1:A:283:HIS:HE1  | 1.63                     | 0.46              |
| 1:B:131:THR:OG1  | 1:B:136:THR:HG22 | 2.16                     | 0.46              |
| 1:B:237:ASN:ND2  | 1:B:283:HIS:CE1  | 2.79                     | 0.46              |
| 1:B:602:LEU:HG   | 1:B:606:LEU:CD2  | 2.46                     | 0.46              |
| 1:B:658:THR:CG2  | 1:B:660:VAL:HG23 | 2.45                     | 0.46              |
| 1:C:471:ASP:O    | 1:C:472:MET:HE3  | 2.16                     | 0.46              |
| 1:D:662:ARG:HB2  | 1:D:715:LEU:HB2  | 1.98                     | 0.46              |
| 1:B:150:VAL:HG22 | 1:B:192:MET:HB2  | 1.97                     | 0.46              |
| 1:B:259:ASN:HB3  | 1:B:261:PHE:CD2  | 2.50                     | 0.46              |
| 1:B:333:ILE:HG12 | 1:B:401:ALA:HB3  | 1.97                     | 0.46              |
| 1:B:496:ASP:O    | 1:B:497:PRO:C    | 2.58                     | 0.46              |
| 1:B:643:ARG:O    | 1:B:650:GLU:HA   | 2.16                     | 0.46              |
| 1:C:245:ILE:HG21 | 1:C:285:GLU:HB2  | 1.98                     | 0.46              |
| 1:C:680:ASN:HD22 | 1:C:681:THR:N    | 2.14                     | 0.46              |
| 1:D:432:ASN:HB3  | 1:D:435:ALA:HB3  | 1.98                     | 0.46              |
| 1:B:117:THR:N    | 2:B:1682:HOH:O   | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:610:TYR:O    | 1:B:617:HIS:HD2  | 1.98                     | 0.46              |
| 1:C:620:ASP:OD2  | 1:C:643:ARG:NH2  | 2.49                     | 0.46              |
| 1:D:310:ARG:NE   | 2:D:1482:HOH:O   | 2.49                     | 0.46              |
| 1:D:382:VAL:O    | 1:D:385:PHE:HB3  | 2.16                     | 0.46              |
| 1:D:659:PRO:O    | 1:D:717:PRO:HB3  | 2.16                     | 0.46              |
| 1:A:278:TRP:HB2  | 1:B:612:HIS:CE1  | 2.51                     | 0.45              |
| 1:A:450:VAL:HG23 | 1:A:450:VAL:O    | 2.15                     | 0.45              |
| 1:B:194:ASP:HB2  | 1:B:198:ASN:CA   | 2.46                     | 0.45              |
| 1:C:290:ASN:HD21 | 1:C:305:LEU:HA   | 1.80                     | 0.45              |
| 1:C:579:ASN:C    | 1:C:579:ASN:ND2  | 2.75                     | 0.45              |
| 1:D:194:ASP:OD2  | 1:D:198:ASN:HB2  | 2.15                     | 0.45              |
| 1:D:601:ARG:HG2  | 1:D:685:HIS:CE1  | 2.51                     | 0.45              |
| 1:D:618:GLU:OE1  | 1:D:645:ASP:HB2  | 2.16                     | 0.45              |
| 1:A:647:GLU:HB3  | 1:A:649:ASN:ND2  | 2.31                     | 0.45              |
| 1:D:598:GLY:CA   | 1:D:686:TYR:HA   | 2.47                     | 0.45              |
| 1:A:542:ASP:O    | 1:A:543:ALA:C    | 2.59                     | 0.45              |
| 1:B:685:HIS:HA   | 2:B:805:HOH:O    | 2.15                     | 0.45              |
| 1:D:309:THR:OG1  | 1:D:311:ARG:HB2  | 2.16                     | 0.45              |
| 1:D:609:THR:O    | 1:D:611:ARG:O    | 2.34                     | 0.45              |
| 1:A:147:ALA:O    | 1:A:195:ALA:CA   | 2.63                     | 0.45              |
| 1:A:496:ASP:HB3  | 1:A:499:TYR:CD1  | 2.50                     | 0.45              |
| 1:B:159:TRP:HB3  | 2:B:1734:HOH:O   | 2.17                     | 0.45              |
| 1:C:336:TRP:CE3  | 1:C:338:PRO:HG2  | 2.52                     | 0.45              |
| 1:C:619:LEU:HB2  | 1:C:625:GLY:HA3  | 1.99                     | 0.45              |
| 1:D:358:GLU:OE2  | 1:D:358:GLU:N    | 2.44                     | 0.45              |
| 1:C:485:TRP:CH2  | 1:C:557:MET:HG3  | 2.51                     | 0.45              |
| 1:C:552:ALA:HB2  | 1:C:718:LEU:O    | 2.16                     | 0.45              |
| 1:A:584:LEU:O    | 1:A:585:ASP:HB2  | 2.16                     | 0.45              |
| 1:B:289:ILE:C    | 1:B:289:ILE:HD12 | 2.42                     | 0.45              |
| 1:C:355:ASN:HB3  | 1:C:358:GLU:OE2  | 2.16                     | 0.45              |
| 1:A:341:PHE:HD1  | 1:A:375:TYR:CE2  | 2.35                     | 0.45              |
| 1:A:712:SER:N    | 2:A:1917:HOH:O   | 2.15                     | 0.45              |
| 1:C:121:PRO:HB2  | 1:C:125:LEU:HD12 | 1.97                     | 0.45              |
| 1:C:463:PHE:O    | 1:C:466:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:492:TYR:CZ   | 1:C:500:ARG:HG3  | 2.52                     | 0.45              |
| 1:C:669:ILE:HD11 | 1:C:699:SER:HB2  | 1.98                     | 0.45              |
| 1:D:311:ARG:HB2  | 1:D:311:ARG:HE   | 1.61                     | 0.45              |
| 1:D:466:VAL:O    | 1:D:477:PHE:HB2  | 2.17                     | 0.45              |
| 1:A:131:THR:C    | 1:A:132:MET:HE2  | 2.41                     | 0.45              |
| 1:A:156:PHE:HE1  | 1:A:188:TYR:HB3  | 1.82                     | 0.45              |
| 1:A:164:HIS:HB3  | 1:A:177:LEU:HD21 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:194:ASP:OD1  | 1:A:198:ASN:HB2  | 2.16                     | 0.45              |
| 1:A:468:ARG:HB3  | 1:A:469:PRO:HD2  | 1.99                     | 0.45              |
| 1:A:667:PHE:HA   | 1:A:705:HIS:CD2  | 2.52                     | 0.45              |
| 1:C:568:MET:HE3  | 1:C:584:LEU:HD21 | 1.98                     | 0.45              |
| 1:C:593:ASP:HA   | 1:C:597:HIS:HD2  | 1.80                     | 0.45              |
| 1:C:656:ASN:ND2  | 1:C:656:ASN:C    | 2.71                     | 0.45              |
| 1:D:247:GLU:OE1  | 1:D:525:HIS:CD2  | 2.66                     | 0.45              |
| 1:D:614:LYS:HD2  | 1:D:614:LYS:N    | 2.31                     | 0.45              |
| 1:A:227:VAL:HG22 | 1:A:319:ARG:NH2  | 2.31                     | 0.45              |
| 1:A:255:ARG:HB2  | 1:A:583:SER:HB2  | 1.99                     | 0.45              |
| 1:B:166:MET:HE2  | 1:B:175:TRP:C    | 2.42                     | 0.45              |
| 1:B:253:TRP:CE3  | 1:B:254:ARG:HB2  | 2.52                     | 0.45              |
| 1:B:459:GLU:OE1  | 1:B:461:THR:O    | 2.35                     | 0.45              |
| 1:B:469:PRO:HB2  | 1:B:471:ASP:OD2  | 2.16                     | 0.45              |
| 1:C:315:ARG:HD2  | 1:C:315:ARG:C    | 2.41                     | 0.45              |
| 1:C:712:SER:N    | 2:C:1490:HOH:O   | 2.38                     | 0.45              |
| 1:D:372:THR:HG23 | 1:D:372:THR:O    | 2.16                     | 0.45              |
| 1:A:192:MET:C    | 1:A:193:ILE:HD13 | 2.42                     | 0.45              |
| 1:A:289:ILE:HD11 | 1:A:334:LEU:HD21 | 1.98                     | 0.45              |
| 1:B:227:VAL:HG22 | 1:B:319:ARG:NH1  | 2.32                     | 0.45              |
| 1:C:716:PRO:HB2  | 1:C:719:ALA:HB3  | 1.98                     | 0.45              |
| 1:D:257:THR:HG22 | 1:D:258:ASP:N    | 2.32                     | 0.45              |
| 1:D:686:TYR:O    | 1:D:687:HIS:HB2  | 2.15                     | 0.45              |
| 1:A:193:ILE:HG22 | 1:A:197:GLY:C    | 2.42                     | 0.44              |
| 1:B:256:HIS:NE2  | 1:B:263:LEU:HD22 | 2.32                     | 0.44              |
| 1:B:429:GLY:HA2  | 1:B:430:ARG:CZ   | 2.46                     | 0.44              |
| 1:C:169:ARG:HD3  | 1:C:171:GLU:OE1  | 2.16                     | 0.44              |
| 1:D:679:LEU:HD22 | 1:D:722:TRP:CD2  | 2.52                     | 0.44              |
| 1:A:337:VAL:HG23 | 1:A:337:VAL:O    | 2.16                     | 0.44              |
| 1:B:168:LEU:HB2  | 1:B:175:TRP:CZ3  | 2.52                     | 0.44              |
| 1:C:279:MET:HE1  | 1:C:600:GLN:O    | 2.17                     | 0.44              |
| 1:C:700:ASP:O    | 1:C:710:SER:N    | 2.45                     | 0.44              |
| 1:D:268:LEU:O    | 1:D:272:LEU:HB3  | 2.16                     | 0.44              |
| 1:A:285:GLU:HA   | 1:A:333:ILE:O    | 2.17                     | 0.44              |
| 1:A:317:ASP:O    | 1:A:320:TYR:HB3  | 2.17                     | 0.44              |
| 1:A:351:PHE:HD2  | 1:A:356:LEU:HD12 | 1.83                     | 0.44              |
| 1:A:411:ILE:HG13 | 1:A:412:TYR:CD1  | 2.52                     | 0.44              |
| 1:A:467:SER:HA   | 1:A:477:PHE:O    | 2.16                     | 0.44              |
| 1:A:722:TRP:C    | 1:A:723:LEU:HD13 | 2.43                     | 0.44              |
| 1:D:126:GLY:HA2  | 1:D:204:ASP:OD2  | 2.17                     | 0.44              |
| 1:D:467:SER:OG   | 1:D:517:GLU:OE2  | 2.30                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:590:GLU:O    | 1:D:591:GLY:O    | 2.35                     | 0.44              |
| 1:D:593:ASP:HA   | 1:D:597:HIS:CD2  | 2.52                     | 0.44              |
| 1:A:186:GLN:HB2  | 1:A:220:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:441:ASN:OD1  | 1:B:444:ARG:NH1  | 2.48                     | 0.44              |
| 1:C:225:GLU:O    | 1:C:226:LYS:HB2  | 2.16                     | 0.44              |
| 1:C:351:PHE:HD2  | 1:C:356:LEU:HD12 | 1.81                     | 0.44              |
| 1:A:590:GLU:HG3  | 1:A:591:GLY:H    | 1.83                     | 0.44              |
| 1:B:713:LEU:HA   | 2:B:1397:HOH:O   | 2.17                     | 0.44              |
| 1:A:137:GLY:HA3  | 1:A:179:ILE:O    | 2.18                     | 0.44              |
| 1:A:224:PRO:HG2  | 1:A:396:ARG:CB   | 2.28                     | 0.44              |
| 1:B:614:LYS:HD2  | 2:B:1920:HOH:O   | 2.17                     | 0.44              |
| 1:C:160:ASP:CG   | 1:C:162:ARG:HG2  | 2.42                     | 0.44              |
| 1:D:291:GLU:OE1  | 1:D:291:GLU:HA   | 2.17                     | 0.44              |
| 1:D:716:PRO:HB2  | 1:D:719:ALA:HB3  | 1.98                     | 0.44              |
| 1:A:182:ALA:HA   | 1:A:186:GLN:OE1  | 2.18                     | 0.44              |
| 1:A:684:MET:HG3  | 1:A:685:HIS:N    | 2.32                     | 0.44              |
| 1:B:669:ILE:HD11 | 1:B:699:SER:CB   | 2.48                     | 0.44              |
| 1:C:132:MET:HB3  | 1:C:178:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:528:VAL:HA   | 1:C:533:LYS:O    | 2.18                     | 0.44              |
| 1:D:573:ALA:O    | 1:D:596:HIS:CE1  | 2.71                     | 0.44              |
| 1:A:430:ARG:HH21 | 1:A:430:ARG:CB   | 2.10                     | 0.44              |
| 1:B:565:LEU:C    | 1:B:565:LEU:HD23 | 2.43                     | 0.44              |
| 1:B:584:LEU:HB2  | 1:B:586:TRP:NE1  | 2.33                     | 0.44              |
| 1:C:154:GLY:H    | 1:C:157:ASN:CB   | 2.31                     | 0.44              |
| 1:A:345:ASP:O    | 1:A:346:PHE:C    | 2.61                     | 0.44              |
| 1:B:685:HIS:CA   | 2:B:805:HOH:O    | 2.65                     | 0.44              |
| 1:C:168:LEU:HD21 | 1:C:173:GLY:HA2  | 1.99                     | 0.44              |
| 1:C:532:LYS:O    | 1:C:533:LYS:HB2  | 2.16                     | 0.44              |
| 1:C:693:ASN:HD21 | 1:C:714:THR:N    | 2.02                     | 0.44              |
| 1:A:444:ARG:O    | 1:A:448:GLU:HG3  | 2.18                     | 0.43              |
| 1:B:149:ARG:C    | 1:B:149:ARG:HD2  | 2.43                     | 0.43              |
| 1:C:237:ASN:ND2  | 1:C:283:HIS:CE1  | 2.79                     | 0.43              |
| 1:D:523:LEU:HD12 | 1:D:523:LEU:HA   | 1.81                     | 0.43              |
| 1:A:294:PHE:N    | 1:A:294:PHE:CD1  | 2.86                     | 0.43              |
| 1:A:655:SER:HB3  | 1:A:657:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:129:ALA:HB2  | 2:B:839:HOH:O    | 2.18                     | 0.43              |
| 1:B:351:PHE:O    | 1:B:356:LEU:HD12 | 2.18                     | 0.43              |
| 1:D:262:TRP:CZ3  | 1:D:311:ARG:HG3  | 2.53                     | 0.43              |
| 1:A:223:LEU:O    | 1:A:224:PRO:C    | 2.60                     | 0.43              |
| 1:C:289:ILE:HG13 | 1:C:334:LEU:HD11 | 1.99                     | 0.43              |
| 1:C:723:LEU:HD22 | 1:C:723:LEU:N    | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:447:GLY:HA2  | 1:D:451:SER:HA   | 2.01                     | 0.43              |
| 1:D:525:HIS:HB3  | 1:D:567:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:168:LEU:HD12 | 1:A:169:ARG:N    | 2.21                     | 0.43              |
| 1:A:564:LYS:HE2  | 1:A:610:TYR:CE1  | 2.53                     | 0.43              |
| 1:C:152:VAL:HG21 | 1:C:177:LEU:HD23 | 1.99                     | 0.43              |
| 1:B:144:ALA:HB1  | 1:B:147:ALA:HB2  | 2.01                     | 0.43              |
| 1:B:551:ARG:HB3  | 1:B:681:THR:HB   | 2.00                     | 0.43              |
| 1:C:219:LEU:HD23 | 1:C:220:ILE:O    | 2.18                     | 0.43              |
| 1:C:474:GLY:O    | 1:C:475:LEU:HB2  | 2.19                     | 0.43              |
| 1:D:263:LEU:HB3  | 1:D:267:GLU:HB3  | 2.00                     | 0.43              |
| 1:D:615:ALA:HB1  | 1:D:643:ARG:O    | 2.18                     | 0.43              |
| 1:A:150:VAL:HA   | 1:A:191:GLU:O    | 2.18                     | 0.43              |
| 1:A:168:LEU:CG   | 1:A:169:ARG:H    | 2.31                     | 0.43              |
| 1:A:408:ALA:HA   | 1:A:411:ILE:HG12 | 1.99                     | 0.43              |
| 1:A:470:GLN:C    | 1:A:472:MET:N    | 2.65                     | 0.43              |
| 1:C:468:ARG:HH11 | 1:C:516:THR:C    | 2.27                     | 0.43              |
| 1:C:608:LEU:O    | 1:C:611:ARG:O    | 2.37                     | 0.43              |
| 1:D:123:GLU:HA   | 1:D:223:LEU:HD21 | 2.01                     | 0.43              |
| 1:D:288:PRO:HB2  | 1:D:299:GLY:HA3  | 2.01                     | 0.43              |
| 1:B:667:PHE:HA   | 1:B:705:HIS:CD2  | 2.54                     | 0.43              |
| 1:C:256:HIS:HE1  | 1:C:267:GLU:OE1  | 2.02                     | 0.43              |
| 1:C:486:MET:O    | 1:C:490:LEU:HB2  | 2.18                     | 0.43              |
| 1:D:430:ARG:HH11 | 1:D:430:ARG:CB   | 2.15                     | 0.43              |
| 1:D:446:LEU:C    | 1:D:448:GLU:N    | 2.77                     | 0.43              |
| 1:A:250:LEU:HD21 | 1:A:286:LEU:HD22 | 1.99                     | 0.43              |
| 1:A:667:PHE:HA   | 1:A:705:HIS:HD2  | 1.84                     | 0.43              |
| 1:A:708:GLN:HA   | 2:A:1907:HOH:O   | 2.18                     | 0.43              |
| 1:B:194:ASP:CB   | 1:B:198:ASN:HB2  | 2.48                     | 0.43              |
| 1:C:289:ILE:C    | 1:C:289:ILE:CD1  | 2.92                     | 0.43              |
| 1:D:517:GLU:HB2  | 1:D:519:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:296:GLY:HA2  | 1:A:580:HIS:CE1  | 2.54                     | 0.43              |
| 1:B:309:THR:OG1  | 1:B:311:ARG:HG3  | 2.19                     | 0.43              |
| 1:B:490:LEU:O    | 1:B:494:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:571:GLU:O    | 1:B:600:GLN:HA   | 2.18                     | 0.43              |
| 1:C:194:ASP:HB2  | 1:C:198:ASN:H    | 1.83                     | 0.43              |
| 1:C:245:ILE:CG2  | 1:C:285:GLU:HB2  | 2.48                     | 0.43              |
| 1:C:260:ASN:CG   | 1:C:260:ASN:O    | 2.60                     | 0.43              |
| 1:C:652:ILE:HB   | 1:C:723:LEU:HB2  | 2.00                     | 0.43              |
| 1:D:668:GLY:N    | 1:D:705:HIS:HD2  | 2.16                     | 0.43              |
| 1:C:657:PHE:O    | 1:C:658:THR:HB   | 2.19                     | 0.43              |
| 1:B:707:ARG:NH1  | 2:B:950:HOH:O    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:266:ARG:HB3  | 2:C:1337:HOH:O   | 2.19                     | 0.42              |
| 1:C:307:ALA:HA   | 1:C:308:PRO:HD3  | 1.86                     | 0.42              |
| 1:C:463:PHE:CD2  | 1:C:475:LEU:HD11 | 2.54                     | 0.42              |
| 1:C:693:ASN:HD21 | 1:C:713:LEU:HB2  | 1.84                     | 0.42              |
| 1:D:289:ILE:HG13 | 1:D:334:LEU:HD11 | 2.01                     | 0.42              |
| 1:D:349:ALA:O    | 1:D:350:GLU:C    | 2.62                     | 0.42              |
| 1:D:466:VAL:HA   | 1:D:475:LEU:HD22 | 2.01                     | 0.42              |
| 1:D:529:VAL:HA   | 1:D:577:GLU:OE1  | 2.19                     | 0.42              |
| 1:A:143:TRP:CZ3  | 1:A:356:LEU:HD22 | 2.55                     | 0.42              |
| 1:A:662:ARG:HB2  | 1:A:715:LEU:HB2  | 2.00                     | 0.42              |
| 1:B:233:ARG:HA   | 1:B:331:ASN:HD21 | 1.84                     | 0.42              |
| 1:B:322:ILE:HG21 | 1:B:397:PHE:O    | 2.19                     | 0.42              |
| 1:C:541:GLY:CA   | 1:C:545:GLN:HE21 | 2.33                     | 0.42              |
| 1:A:352:ASP:OD2  | 1:A:352:ASP:C    | 2.61                     | 0.42              |
| 1:A:380:ARG:CG   | 1:A:380:ARG:NH2  | 2.78                     | 0.42              |
| 1:A:496:ASP:O    | 1:A:497:PRO:C    | 2.62                     | 0.42              |
| 1:C:146:ASN:HB2  | 1:C:352:ASP:OD1  | 2.19                     | 0.42              |
| 1:C:280:GLY:O    | 1:C:611:ARG:NH1  | 2.41                     | 0.42              |
| 1:C:566:LEU:HG   | 1:C:570:ASN:HB2  | 2.02                     | 0.42              |
| 1:D:667:PHE:HA   | 1:D:705:HIS:HE2  | 1.85                     | 0.42              |
| 1:C:535:ILE:O    | 1:C:539:MET:HE3  | 2.19                     | 0.42              |
| 1:D:164:HIS:HE1  | 2:D:1447:HOH:O   | 2.02                     | 0.42              |
| 1:D:531:GLY:CA   | 1:D:577:GLU:OE2  | 2.66                     | 0.42              |
| 1:A:178:PHE:CE1  | 1:A:180:PRO:HG3  | 2.48                     | 0.42              |
| 1:B:511:ILE:HG23 | 2:B:1218:HOH:O   | 2.19                     | 0.42              |
| 1:C:149:ARG:O    | 1:C:192:MET:HA   | 2.20                     | 0.42              |
| 1:C:435:ALA:O    | 1:C:438:PHE:HB3  | 2.19                     | 0.42              |
| 1:D:120:ARG:HG2  | 1:D:122:TYR:CZ   | 2.55                     | 0.42              |
| 1:A:149:ARG:O    | 1:A:192:MET:HA   | 2.19                     | 0.42              |
| 1:A:168:LEU:HG   | 1:A:169:ARG:N    | 2.35                     | 0.42              |
| 1:A:703:ALA:HA   | 1:A:707:ARG:O    | 2.19                     | 0.42              |
| 1:B:656:ASN:C    | 1:B:656:ASN:ND2  | 2.76                     | 0.42              |
| 1:C:359:HIS:CD2  | 1:C:376:ASN:HB2  | 2.55                     | 0.42              |
| 1:C:375:TYR:HB2  | 1:C:377:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:598:GLY:HA3  | 1:C:686:TYR:HA   | 2.01                     | 0.42              |
| 1:C:604:ARG:NH2  | 2:C:1576:HOH:O   | 2.52                     | 0.42              |
| 1:C:666:ARG:HH12 | 1:C:700:ASP:CB   | 2.33                     | 0.42              |
| 1:A:194:ASP:N    | 1:A:198:ASN:O    | 2.47                     | 0.42              |
| 1:A:206:TYR:CZ   | 1:A:385:PHE:HD1  | 2.36                     | 0.42              |
| 1:A:289:ILE:O    | 1:A:290:ASN:C    | 2.62                     | 0.42              |
| 1:A:341:PHE:O    | 1:A:343:THR:HG23 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:259:ASN:O    | 1:B:260:ASN:HB3  | 2.19                     | 0.42              |
| 1:B:552:ALA:O    | 1:B:720:THR:HG21 | 2.20                     | 0.42              |
| 1:C:503:HIS:C    | 1:C:505:ASP:H    | 2.28                     | 0.42              |
| 1:D:437:GLU:OE2  | 1:D:437:GLU:HA   | 2.19                     | 0.42              |
| 1:D:504:HIS:CD2  | 1:D:634:LYS:HA   | 2.54                     | 0.42              |
| 1:A:212:MET:HE3  | 1:A:213:ARG:CG   | 2.40                     | 0.42              |
| 1:A:541:GLY:HA2  | 2:A:1350:HOH:O   | 2.19                     | 0.42              |
| 1:B:471:ASP:O    | 1:B:472:MET:HE2  | 2.20                     | 0.42              |
| 1:C:182:ALA:HA   | 1:C:186:GLN:NE2  | 2.35                     | 0.42              |
| 1:D:183:HIS:CE1  | 1:D:186:GLN:NE2  | 2.88                     | 0.42              |
| 1:D:413:ARG:O    | 1:D:414:ASP:CB   | 2.68                     | 0.42              |
| 1:A:717:PRO:O    | 1:A:718:LEU:C    | 2.63                     | 0.42              |
| 1:B:351:PHE:O    | 1:B:352:ASP:CG   | 2.63                     | 0.42              |
| 1:C:457:ALA:HB2  | 1:C:477:PHE:CE2  | 2.55                     | 0.42              |
| 1:C:584:LEU:O    | 1:C:585:ASP:CG   | 2.62                     | 0.42              |
| 1:D:140:PHE:O    | 1:D:176:GLU:HA   | 2.20                     | 0.42              |
| 1:D:486:MET:HE3  | 1:D:486:MET:HB3  | 1.94                     | 0.42              |
| 1:C:265:TYR:CE2  | 1:C:312:PHE:HB2  | 2.55                     | 0.42              |
| 1:C:315:ARG:HG2  | 1:C:315:ARG:NH1  | 2.35                     | 0.42              |
| 1:C:679:LEU:HB3  | 1:C:722:TRP:HB2  | 2.02                     | 0.42              |
| 1:D:198:ASN:HB3  | 1:D:200:ARG:HH12 | 1.85                     | 0.42              |
| 1:A:445:ILE:C    | 1:A:447:GLY:N    | 2.77                     | 0.41              |
| 1:B:295:ASP:OD2  | 1:B:295:ASP:N    | 2.52                     | 0.41              |
| 1:B:594:ASN:HB2  | 2:B:1233:HOH:O   | 2.20                     | 0.41              |
| 1:B:629:LEU:HB2  | 1:B:640:ILE:HG22 | 2.02                     | 0.41              |
| 1:C:458:GLU:OE2  | 1:C:458:GLU:C    | 2.63                     | 0.41              |
| 1:D:136:THR:HG22 | 1:D:137:GLY:N    | 2.35                     | 0.41              |
| 1:D:713:LEU:HA   | 2:D:1624:HOH:O   | 2.20                     | 0.41              |
| 1:D:721:ILE:CD1  | 1:D:723:LEU:HD21 | 2.50                     | 0.41              |
| 1:A:147:ALA:O    | 1:A:148:ARG:HB2  | 2.19                     | 0.41              |
| 1:A:509:PHE:HA   | 1:A:512:LEU:CD2  | 2.50                     | 0.41              |
| 1:B:138:THR:HG21 | 1:B:220:ILE:HD13 | 2.02                     | 0.41              |
| 1:B:606:LEU:HD13 | 1:B:679:LEU:CD1  | 2.49                     | 0.41              |
| 1:B:680:ASN:C    | 1:B:680:ASN:ND2  | 2.78                     | 0.41              |
| 1:C:463:PHE:HD2  | 1:C:475:LEU:HD11 | 1.84                     | 0.41              |
| 1:C:541:GLY:HA3  | 1:C:545:GLN:HE21 | 1.84                     | 0.41              |
| 1:C:542:ASP:N    | 1:C:545:GLN:HE21 | 2.18                     | 0.41              |
| 1:A:259:ASN:O    | 1:A:260:ASN:HB3  | 2.19                     | 0.41              |
| 1:B:143:TRP:CZ2  | 1:B:356:LEU:HD22 | 2.55                     | 0.41              |
| 1:B:150:VAL:HG22 | 1:B:192:MET:HB3  | 2.03                     | 0.41              |
| 1:C:523:LEU:HD22 | 1:C:557:MET:SD   | 2.61                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:246:TYR:HB2  | 1:D:281:PHE:CG   | 2.55                     | 0.41              |
| 1:D:293:PRO:HD3  | 1:D:303:THR:HG23 | 2.01                     | 0.41              |
| 1:A:626:PHE:C    | 1:A:626:PHE:CD2  | 2.98                     | 0.41              |
| 1:A:686:TYR:O    | 1:A:687:HIS:HB2  | 2.21                     | 0.41              |
| 1:B:457:ALA:HB2  | 1:B:477:PHE:CD2  | 2.55                     | 0.41              |
| 1:B:485:TRP:CH2  | 1:B:557:MET:HG3  | 2.55                     | 0.41              |
| 1:B:593:ASP:OD2  | 1:B:687:HIS:CE1  | 2.74                     | 0.41              |
| 1:C:168:LEU:HB2  | 1:C:175:TRP:CE3  | 2.55                     | 0.41              |
| 1:C:223:LEU:HD23 | 1:C:396:ARG:CZ   | 2.50                     | 0.41              |
| 1:C:288:PRO:HB2  | 1:C:299:GLY:C    | 2.45                     | 0.41              |
| 1:C:336:TRP:CZ3  | 1:C:338:PRO:HG2  | 2.55                     | 0.41              |
| 1:C:351:PHE:O    | 1:C:353:GLY:N    | 2.54                     | 0.41              |
| 1:A:351:PHE:CD2  | 1:A:356:LEU:HD12 | 2.56                     | 0.41              |
| 1:B:448:GLU:HB2  | 2:B:1637:HOH:O   | 2.20                     | 0.41              |
| 1:B:680:ASN:HA   | 1:B:721:ILE:HG22 | 2.03                     | 0.41              |
| 1:C:131:THR:OG1  | 1:C:136:THR:HG22 | 2.19                     | 0.41              |
| 1:C:168:LEU:CD1  | 1:C:170:LYS:HA   | 2.50                     | 0.41              |
| 1:C:247:GLU:HB3  | 1:C:567:PHE:HA   | 2.03                     | 0.41              |
| 1:C:543:ALA:HB1  | 1:C:595:TRP:CH2  | 2.56                     | 0.41              |
| 1:C:684:MET:N    | 1:C:690:ASN:HD22 | 2.17                     | 0.41              |
| 1:D:140:PHE:CZ   | 1:D:220:ILE:HD11 | 2.52                     | 0.41              |
| 1:D:679:LEU:HB3  | 1:D:722:TRP:HB2  | 2.02                     | 0.41              |
| 1:B:161:GLY:O    | 1:B:162:ARG:C    | 2.64                     | 0.41              |
| 1:B:547:PHE:CD2  | 1:B:595:TRP:HB3  | 2.55                     | 0.41              |
| 1:C:223:LEU:C    | 1:C:224:PRO:O    | 2.63                     | 0.41              |
| 1:C:262:TRP:CG   | 1:C:312:PHE:HE2  | 2.38                     | 0.41              |
| 1:C:375:TYR:O    | 1:C:376:ASN:HB3  | 2.20                     | 0.41              |
| 1:C:480:LYS:O    | 1:C:519:PHE:HA   | 2.20                     | 0.41              |
| 1:D:394:ILE:HG21 | 1:D:450:VAL:HG11 | 2.01                     | 0.41              |
| 1:A:572:PHE:HZ   | 1:A:584:LEU:O    | 2.03                     | 0.41              |
| 1:B:141:SER:HA   | 1:B:175:TRP:O    | 2.21                     | 0.41              |
| 1:B:490:LEU:HD12 | 1:B:490:LEU:HA   | 1.95                     | 0.41              |
| 1:B:506:LYS:NZ   | 2:B:1487:HOH:O   | 2.53                     | 0.41              |
| 1:D:267:GLU:O    | 1:D:270:ASP:OD2  | 2.39                     | 0.41              |
| 1:B:143:TRP:CE2  | 1:B:381:GLU:HG2  | 2.56                     | 0.41              |
| 1:C:152:VAL:HG23 | 1:C:177:LEU:HD23 | 2.02                     | 0.41              |
| 1:A:129:ALA:HA   | 1:A:138:THR:HG22 | 2.03                     | 0.41              |
| 1:A:157:ASN:ND2  | 1:A:164:HIS:CD2  | 2.88                     | 0.41              |
| 1:A:606:LEU:CD1  | 1:A:679:LEU:HD11 | 2.51                     | 0.41              |
| 1:C:450:VAL:HG23 | 1:C:450:VAL:O    | 2.21                     | 0.41              |
| 1:C:547:PHE:O    | 1:C:551:ARG:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:643:ARG:HD2  | 1:C:643:ARG:HA   | 1.86                     | 0.41              |
| 1:D:163:ARG:HD2  | 2:D:1502:HOH:O   | 2.20                     | 0.41              |
| 1:D:566:LEU:HG   | 1:D:570:ASN:HB2  | 2.01                     | 0.41              |
| 1:D:725:ARG:CZ   | 2:D:1544:HOH:O   | 2.69                     | 0.41              |
| 1:A:144:ALA:HA   | 1:A:145:PRO:HD2  | 1.91                     | 0.41              |
| 1:A:288:PRO:HB2  | 1:A:299:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:391:LEU:HD12 | 1:A:391:LEU:HA   | 1.92                     | 0.41              |
| 1:A:447:GLY:N    | 2:A:1483:HOH:O   | 2.54                     | 0.41              |
| 1:B:597:HIS:O    | 1:B:601:ARG:HB2  | 2.20                     | 0.41              |
| 1:D:227:VAL:HG22 | 1:D:319:ARG:NH1  | 2.36                     | 0.41              |
| 1:D:254:ARG:HA   | 1:D:583:SER:HB2  | 2.03                     | 0.41              |
| 1:D:279:MET:O    | 1:D:604:ARG:HA   | 2.21                     | 0.41              |
| 1:D:289:ILE:HG13 | 1:D:334:LEU:CD1  | 2.51                     | 0.41              |
| 1:D:494:LYS:HG2  | 1:D:538:ARG:HB3  | 2.03                     | 0.41              |
| 1:D:497:PRO:HA   | 1:D:500:ARG:HD3  | 2.01                     | 0.41              |
| 1:D:542:ASP:H    | 1:D:545:GLN:NE2  | 2.18                     | 0.41              |
| 1:A:254:ARG:NH2  | 2:A:1871:HOH:O   | 2.43                     | 0.40              |
| 1:B:318:PHE:O    | 1:B:321:PHE:HB3  | 2.20                     | 0.40              |
| 1:B:494:LYS:CD   | 1:B:538:ARG:HG2  | 2.51                     | 0.40              |
| 1:C:192:MET:CE   | 1:C:202:LYS:HG3  | 2.51                     | 0.40              |
| 1:C:493:MET:HE3  | 1:C:549:ASN:HB3  | 2.04                     | 0.40              |
| 1:C:669:ILE:HD11 | 1:C:699:SER:CB   | 2.50                     | 0.40              |
| 1:C:685:HIS:NE2  | 1:D:685:HIS:HD2  | 2.19                     | 0.40              |
| 1:D:593:ASP:OD2  | 1:D:687:HIS:CE1  | 2.73                     | 0.40              |
| 1:D:656:ASN:ND2  | 2:D:844:HOH:O    | 2.36                     | 0.40              |
| 1:A:565:LEU:HD23 | 1:A:565:LEU:C    | 2.45                     | 0.40              |
| 1:A:631:VAL:O    | 1:A:631:VAL:HG22 | 2.21                     | 0.40              |
| 1:B:168:LEU:HB2  | 1:B:175:TRP:CE3  | 2.57                     | 0.40              |
| 1:B:425:ASN:HD21 | 1:B:427:PHE:HB2  | 1.86                     | 0.40              |
| 1:C:351:PHE:HB3  | 1:C:356:LEU:HD12 | 2.02                     | 0.40              |
| 1:C:526:ASP:O    | 1:C:532:LYS:NZ   | 2.48                     | 0.40              |
| 1:C:619:LEU:HA   | 2:C:1152:HOH:O   | 2.21                     | 0.40              |
| 1:D:170:LYS:HG2  | 2:D:1613:HOH:O   | 2.19                     | 0.40              |
| 1:D:709:HIS:HD2  | 2:D:1905:HOH:O   | 2.04                     | 0.40              |
| 1:A:372:THR:HG22 | 1:A:373:LEU:HD23 | 2.03                     | 0.40              |
| 1:B:412:TYR:C    | 1:B:414:ASP:H    | 2.29                     | 0.40              |
| 2:C:1747:HOH:O   | 1:D:254:ARG:HD3  | 2.21                     | 0.40              |
| 1:D:131:THR:HG22 | 1:D:132:MET:N    | 2.36                     | 0.40              |
| 1:D:546:LYS:HB3  | 1:D:546:LYS:HE3  | 1.94                     | 0.40              |
| 1:D:690:ASN:HD22 | 1:D:690:ASN:HA   | 1.63                     | 0.40              |
| 1:A:132:MET:HE2  | 1:A:132:MET:N    | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:640:ILE:HA   | 1:A:653:VAL:O    | 2.21                     | 0.40              |
| 1:B:552:ALA:O    | 1:B:720:THR:CG2  | 2.69                     | 0.40              |
| 1:B:721:ILE:HD12 | 1:B:723:LEU:HD21 | 2.03                     | 0.40              |
| 1:C:263:LEU:HD13 | 1:C:271:GLN:NE2  | 2.37                     | 0.40              |
| 1:C:351:PHE:C    | 1:C:353:GLY:H    | 2.29                     | 0.40              |
| 1:C:642:VAL:HG23 | 1:C:652:ILE:HG12 | 2.02                     | 0.40              |
| 1:C:677:GLU:HA   | 1:C:722:TRP:O    | 2.22                     | 0.40              |
| 1:C:682:ASP:OD2  | 1:C:689:SER:N    | 2.55                     | 0.40              |
| 1:D:293:PRO:CD   | 1:D:303:THR:HG23 | 2.52                     | 0.40              |
| 1:A:377:TYR:HD1  | 2:A:1382:HOH:O   | 2.04                     | 0.40              |
| 1:A:542:ASP:HB3  | 2:A:1800:HOH:O   | 2.20                     | 0.40              |
| 1:A:574:GLN:HE21 | 1:A:574:GLN:HB2  | 1.70                     | 0.40              |
| 1:B:671:GLN:HB3  | 1:D:498:VAL:HG11 | 2.04                     | 0.40              |
| 1:B:684:MET:HE2  | 1:B:684:MET:HB3  | 1.95                     | 0.40              |
| 1:D:411:ILE:HG13 | 1:D:412:TYR:CD1  | 2.56                     | 0.40              |
| 1:D:440:ARG:HG2  | 1:D:475:LEU:N    | 2.34                     | 0.40              |
| 1:D:542:ASP:O    | 1:D:543:ALA:C    | 2.64                     | 0.40              |
| 1:D:700:ASP:O    | 1:D:709:HIS:HA   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 1   | A     | 581/617 (94%)   | 502 (86%)  | 52 (9%)  | 27 (5%)  | 2           | 1 |
| 1   | B     | 583/617 (94%)   | 522 (90%)  | 48 (8%)  | 13 (2%)  | 5           | 4 |
| 1   | C     | 570/617 (92%)   | 494 (87%)  | 57 (10%) | 19 (3%)  | 3           | 2 |
| 1   | D     | 577/617 (94%)   | 522 (90%)  | 40 (7%)  | 15 (3%)  | 4           | 3 |
| All | All   | 2311/2468 (94%) | 2040 (88%) | 197 (8%) | 74 (3%)  | 3           | 2 |

All (74) Ramachandran outliers are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | ARG  |
| 1   | A     | 212 | MET  |
| 1   | A     | 215 | GLU  |
| 1   | A     | 225 | GLU  |
| 1   | A     | 257 | THR  |
| 1   | A     | 352 | ASP  |
| 1   | A     | 543 | ALA  |
| 1   | B     | 194 | ASP  |
| 1   | B     | 225 | GLU  |
| 1   | B     | 226 | LYS  |
| 1   | B     | 352 | ASP  |
| 1   | B     | 612 | HIS  |
| 1   | B     | 709 | HIS  |
| 1   | C     | 350 | GLU  |
| 1   | C     | 352 | ASP  |
| 1   | C     | 585 | ASP  |
| 1   | D     | 194 | ASP  |
| 1   | D     | 257 | THR  |
| 1   | D     | 430 | ARG  |
| 1   | D     | 585 | ASP  |
| 1   | D     | 591 | GLY  |
| 1   | A     | 226 | LYS  |
| 1   | A     | 355 | ASN  |
| 1   | A     | 471 | ASP  |
| 1   | A     | 591 | GLY  |
| 1   | A     | 695 | GLY  |
| 1   | A     | 709 | HIS  |
| 1   | B     | 694 | GLY  |
| 1   | C     | 258 | ASP  |
| 1   | C     | 288 | PRO  |
| 1   | C     | 349 | ALA  |
| 1   | C     | 500 | ARG  |
| 1   | C     | 616 | MET  |
| 1   | C     | 687 | HIS  |
| 1   | D     | 149 | ARG  |
| 1   | D     | 259 | ASN  |
| 1   | D     | 592 | GLY  |
| 1   | D     | 612 | HIS  |
| 1   | A     | 194 | ASP  |
| 1   | A     | 472 | MET  |
| 1   | A     | 475 | LEU  |
| 1   | A     | 522 | PRO  |
| 1   | B     | 584 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 226 | LYS  |
| 1   | C     | 257 | THR  |
| 1   | C     | 612 | HIS  |
| 1   | D     | 197 | GLY  |
| 1   | D     | 290 | ASN  |
| 1   | D     | 372 | THR  |
| 1   | A     | 149 | ARG  |
| 1   | A     | 184 | ASN  |
| 1   | A     | 214 | PRO  |
| 1   | A     | 433 | LEU  |
| 1   | A     | 533 | LYS  |
| 1   | B     | 288 | PRO  |
| 1   | C     | 194 | ASP  |
| 1   | C     | 504 | HIS  |
| 1   | C     | 686 | TYR  |
| 1   | A     | 380 | ARG  |
| 1   | B     | 215 | GLU  |
| 1   | B     | 522 | PRO  |
| 1   | C     | 709 | HIS  |
| 1   | D     | 522 | PRO  |
| 1   | A     | 168 | LEU  |
| 1   | A     | 288 | PRO  |
| 1   | B     | 696 | THR  |
| 1   | B     | 712 | SER  |
| 1   | C     | 252 | SER  |
| 1   | D     | 709 | HIS  |
| 1   | A     | 447 | GLY  |
| 1   | C     | 630 | VAL  |
| 1   | A     | 510 | GLY  |
| 1   | C     | 473 | GLY  |
| 1   | D     | 473 | GLY  |

### 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.

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 498/525 (95%)   | 468 (94%)  | 30 (6%)  | 17          | 25 |
| 1   | B     | 501/525 (95%)   | 469 (94%)  | 32 (6%)  | 16          | 23 |
| 1   | C     | 490/525 (93%)   | 465 (95%)  | 25 (5%)  | 21          | 32 |
| 1   | D     | 496/525 (94%)   | 468 (94%)  | 28 (6%)  | 19          | 28 |
| All | All   | 1985/2100 (94%) | 1870 (94%) | 115 (6%) | 18          | 26 |

All (115) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 142 | VAL  |
| 1   | A     | 152 | VAL  |
| 1   | A     | 158 | TYR  |
| 1   | A     | 193 | ILE  |
| 1   | A     | 196 | ASN  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 315 | ARG  |
| 1   | A     | 356 | LEU  |
| 1   | A     | 373 | LEU  |
| 1   | A     | 374 | ILE  |
| 1   | A     | 376 | ASN  |
| 1   | A     | 391 | LEU  |
| 1   | A     | 430 | ARG  |
| 1   | A     | 446 | LEU  |
| 1   | A     | 490 | LEU  |
| 1   | A     | 498 | VAL  |
| 1   | A     | 501 | GLN  |
| 1   | A     | 507 | LEU  |
| 1   | A     | 522 | PRO  |
| 1   | A     | 523 | LEU  |
| 1   | A     | 537 | ASP  |
| 1   | A     | 606 | LEU  |
| 1   | A     | 619 | LEU  |
| 1   | A     | 642 | VAL  |
| 1   | A     | 647 | GLU  |
| 1   | A     | 679 | LEU  |
| 1   | A     | 680 | ASN  |
| 1   | A     | 690 | ASN  |
| 1   | A     | 720 | THR  |
| 1   | A     | 723 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 138 | THR  |
| 1   | B     | 149 | ARG  |
| 1   | B     | 168 | LEU  |
| 1   | B     | 176 | GLU  |
| 1   | B     | 199 | LEU  |
| 1   | B     | 211 | GLN  |
| 1   | B     | 290 | ASN  |
| 1   | B     | 295 | ASP  |
| 1   | B     | 305 | LEU  |
| 1   | B     | 359 | HIS  |
| 1   | B     | 373 | LEU  |
| 1   | B     | 374 | ILE  |
| 1   | B     | 391 | LEU  |
| 1   | B     | 430 | ARG  |
| 1   | B     | 446 | LEU  |
| 1   | B     | 470 | GLN  |
| 1   | B     | 490 | LEU  |
| 1   | B     | 500 | ARG  |
| 1   | B     | 511 | ILE  |
| 1   | B     | 512 | LEU  |
| 1   | B     | 523 | LEU  |
| 1   | B     | 606 | LEU  |
| 1   | B     | 614 | LYS  |
| 1   | B     | 619 | LEU  |
| 1   | B     | 642 | VAL  |
| 1   | B     | 651 | ILE  |
| 1   | B     | 656 | ASN  |
| 1   | B     | 658 | THR  |
| 1   | B     | 679 | LEU  |
| 1   | B     | 680 | ASN  |
| 1   | B     | 720 | THR  |
| 1   | B     | 723 | LEU  |
| 1   | C     | 124 | THR  |
| 1   | C     | 133 | ASP  |
| 1   | C     | 157 | ASN  |
| 1   | C     | 168 | LEU  |
| 1   | C     | 192 | MET  |
| 1   | C     | 258 | ASP  |
| 1   | C     | 259 | ASN  |
| 1   | C     | 303 | THR  |
| 1   | C     | 310 | ARG  |
| 1   | C     | 315 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 331 | ASN  |
| 1   | C     | 358 | GLU  |
| 1   | C     | 359 | HIS  |
| 1   | C     | 462 | ASP  |
| 1   | C     | 470 | GLN  |
| 1   | C     | 507 | LEU  |
| 1   | C     | 523 | LEU  |
| 1   | C     | 619 | LEU  |
| 1   | C     | 642 | VAL  |
| 1   | C     | 643 | ARG  |
| 1   | C     | 651 | ILE  |
| 1   | C     | 685 | HIS  |
| 1   | C     | 711 | LEU  |
| 1   | C     | 720 | THR  |
| 1   | C     | 723 | LEU  |
| 1   | D     | 141 | SER  |
| 1   | D     | 148 | ARG  |
| 1   | D     | 171 | GLU  |
| 1   | D     | 211 | GLN  |
| 1   | D     | 223 | LEU  |
| 1   | D     | 232 | GLU  |
| 1   | D     | 263 | LEU  |
| 1   | D     | 311 | ARG  |
| 1   | D     | 352 | ASP  |
| 1   | D     | 359 | HIS  |
| 1   | D     | 373 | LEU  |
| 1   | D     | 430 | ARG  |
| 1   | D     | 470 | GLN  |
| 1   | D     | 472 | MET  |
| 1   | D     | 490 | LEU  |
| 1   | D     | 500 | ARG  |
| 1   | D     | 507 | LEU  |
| 1   | D     | 522 | PRO  |
| 1   | D     | 523 | LEU  |
| 1   | D     | 574 | GLN  |
| 1   | D     | 632 | ASP  |
| 1   | D     | 642 | VAL  |
| 1   | D     | 646 | LYS  |
| 1   | D     | 647 | GLU  |
| 1   | D     | 651 | ILE  |
| 1   | D     | 690 | ASN  |
| 1   | D     | 713 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 723 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 164 | HIS  |
| 1   | A     | 229 | GLN  |
| 1   | A     | 237 | ASN  |
| 1   | A     | 259 | ASN  |
| 1   | A     | 283 | HIS  |
| 1   | A     | 331 | ASN  |
| 1   | A     | 340 | HIS  |
| 1   | A     | 355 | ASN  |
| 1   | A     | 376 | ASN  |
| 1   | A     | 384 | ASN  |
| 1   | A     | 441 | ASN  |
| 1   | A     | 501 | GLN  |
| 1   | A     | 503 | HIS  |
| 1   | A     | 504 | HIS  |
| 1   | A     | 514 | ASN  |
| 1   | A     | 525 | HIS  |
| 1   | A     | 545 | GLN  |
| 1   | A     | 570 | ASN  |
| 1   | A     | 574 | GLN  |
| 1   | A     | 579 | ASN  |
| 1   | A     | 580 | HIS  |
| 1   | A     | 587 | HIS  |
| 1   | A     | 597 | HIS  |
| 1   | A     | 600 | GLN  |
| 1   | A     | 613 | HIS  |
| 1   | A     | 617 | HIS  |
| 1   | A     | 656 | ASN  |
| 1   | A     | 680 | ASN  |
| 1   | A     | 687 | HIS  |
| 1   | A     | 690 | ASN  |
| 1   | A     | 693 | ASN  |
| 1   | A     | 705 | HIS  |
| 1   | A     | 708 | GLN  |
| 1   | A     | 709 | HIS  |
| 1   | B     | 157 | ASN  |
| 1   | B     | 164 | HIS  |
| 1   | B     | 198 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 211 | GLN  |
| 1   | B     | 229 | GLN  |
| 1   | B     | 237 | ASN  |
| 1   | B     | 256 | HIS  |
| 1   | B     | 283 | HIS  |
| 1   | B     | 331 | ASN  |
| 1   | B     | 340 | HIS  |
| 1   | B     | 355 | ASN  |
| 1   | B     | 376 | ASN  |
| 1   | B     | 425 | ASN  |
| 1   | B     | 470 | GLN  |
| 1   | B     | 504 | HIS  |
| 1   | B     | 514 | ASN  |
| 1   | B     | 525 | HIS  |
| 1   | B     | 545 | GLN  |
| 1   | B     | 570 | ASN  |
| 1   | B     | 574 | GLN  |
| 1   | B     | 579 | ASN  |
| 1   | B     | 587 | HIS  |
| 1   | B     | 597 | HIS  |
| 1   | B     | 617 | HIS  |
| 1   | B     | 656 | ASN  |
| 1   | B     | 663 | HIS  |
| 1   | B     | 680 | ASN  |
| 1   | B     | 687 | HIS  |
| 1   | B     | 690 | ASN  |
| 1   | B     | 693 | ASN  |
| 1   | B     | 705 | HIS  |
| 1   | B     | 709 | HIS  |
| 1   | C     | 157 | ASN  |
| 1   | C     | 164 | HIS  |
| 1   | C     | 184 | ASN  |
| 1   | C     | 186 | GLN  |
| 1   | C     | 237 | ASN  |
| 1   | C     | 238 | GLN  |
| 1   | C     | 256 | HIS  |
| 1   | C     | 259 | ASN  |
| 1   | C     | 283 | HIS  |
| 1   | C     | 290 | ASN  |
| 1   | C     | 301 | GLN  |
| 1   | C     | 331 | ASN  |
| 1   | C     | 470 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 503 | HIS  |
| 1   | C     | 514 | ASN  |
| 1   | C     | 530 | HIS  |
| 1   | C     | 545 | GLN  |
| 1   | C     | 570 | ASN  |
| 1   | C     | 574 | GLN  |
| 1   | C     | 579 | ASN  |
| 1   | C     | 580 | HIS  |
| 1   | C     | 597 | HIS  |
| 1   | C     | 600 | GLN  |
| 1   | C     | 613 | HIS  |
| 1   | C     | 617 | HIS  |
| 1   | C     | 656 | ASN  |
| 1   | C     | 680 | ASN  |
| 1   | C     | 690 | ASN  |
| 1   | C     | 693 | ASN  |
| 1   | C     | 705 | HIS  |
| 1   | D     | 164 | HIS  |
| 1   | D     | 186 | GLN  |
| 1   | D     | 211 | GLN  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 237 | ASN  |
| 1   | D     | 238 | GLN  |
| 1   | D     | 256 | HIS  |
| 1   | D     | 283 | HIS  |
| 1   | D     | 290 | ASN  |
| 1   | D     | 340 | HIS  |
| 1   | D     | 359 | HIS  |
| 1   | D     | 371 | ASN  |
| 1   | D     | 376 | ASN  |
| 1   | D     | 443 | ASN  |
| 1   | D     | 470 | GLN  |
| 1   | D     | 501 | GLN  |
| 1   | D     | 504 | HIS  |
| 1   | D     | 514 | ASN  |
| 1   | D     | 525 | HIS  |
| 1   | D     | 545 | GLN  |
| 1   | D     | 570 | ASN  |
| 1   | D     | 574 | GLN  |
| 1   | D     | 579 | ASN  |
| 1   | D     | 580 | HIS  |
| 1   | D     | 597 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 617 | HIS  |
| 1   | D     | 649 | ASN  |
| 1   | D     | 656 | ASN  |
| 1   | D     | 680 | ASN  |
| 1   | D     | 685 | HIS  |
| 1   | D     | 687 | HIS  |
| 1   | D     | 690 | ASN  |
| 1   | D     | 693 | ASN  |
| 1   | D     | 705 | HIS  |
| 1   | D     | 708 | GLN  |
| 1   | D     | 709 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.