



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2VGI  
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE: R486W MUTANT  
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Deposited on : 2007-11-13  
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

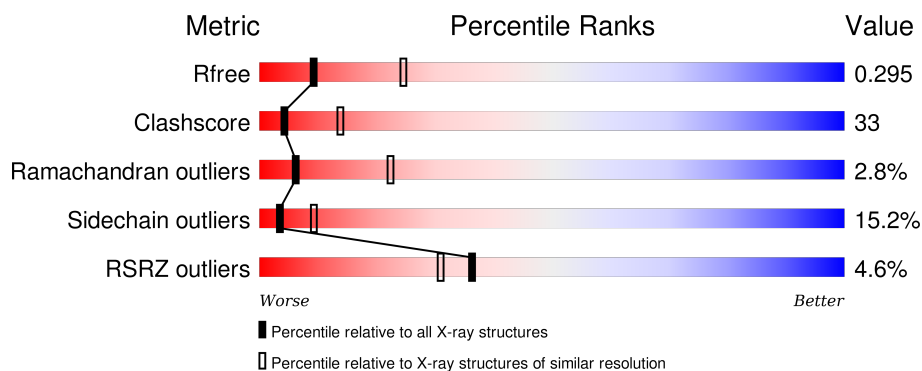
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1945 (2.90-2.86)                                      |
| Clashscore            | 102246                      | 2202 (2.90-2.86)                                      |
| Ramachandran outliers | 100387                      | 2149 (2.90-2.86)                                      |
| Sidechain outliers    | 100360                      | 2152 (2.90-2.86)                                      |
| RSRZ outliers         | 91569                       | 1950 (2.90-2.86)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 528    | <div> <div>4%</div> <div>41%</div> <div>42%</div> <div>13%</div> <div>..</div> </div> |
| 1   | B     | 528    | <div> <div>7%</div> <div>42%</div> <div>36%</div> <div>9%</div> <div>12%</div> </div> |
| 1   | C     | 528    | <div> <div>4%</div> <div>41%</div> <div>46%</div> <div>9%</div> <div>.</div> </div>   |
| 1   | D     | 528    | <div> <div>3%</div> <div>48%</div> <div>39%</div> <div>10%</div> <div>..</div> </div> |

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

ria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | PGA  | B     | 1575 | -         | -        | X       | -                |
| 3   | PGA  | C     | 1575 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15342 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.

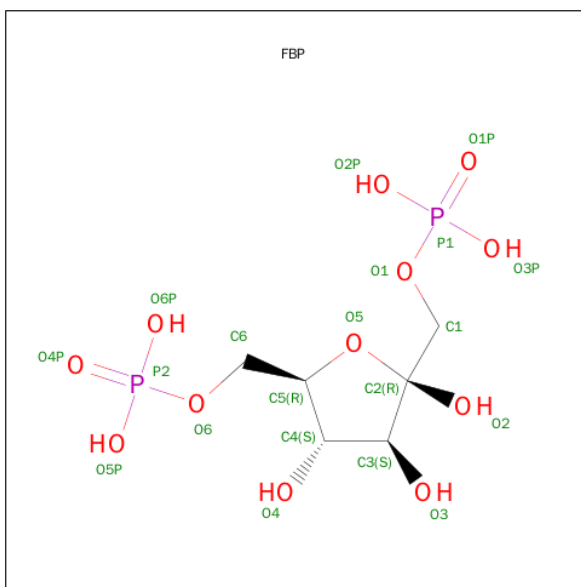
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3915  | 2462 | 707 | 728 | 18 |         |         |       |
| 1   | B     | 463      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3513  | 2214 | 629 | 652 | 18 |         |         |       |
| 1   | C     | 515      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3899  | 2452 | 704 | 725 | 18 |         |         |       |
| 1   | D     | 513      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3891  | 2448 | 702 | 723 | 18 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

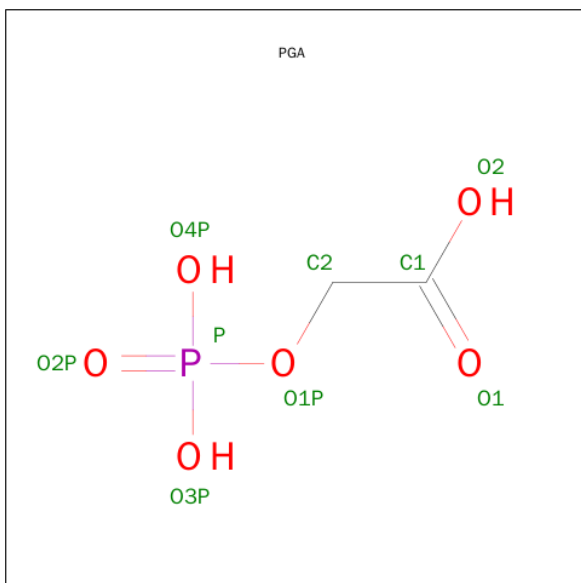
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 486     | TRP      | ARG    | ENGINEERED MUTATION | UNP P30613 |
| B     | 486     | TRP      | ARG    | ENGINEERED MUTATION | UNP P30613 |
| C     | 486     | TRP      | ARG    | ENGINEERED MUTATION | UNP P30613 |
| D     | 486     | TRP      | ARG    | ENGINEERED MUTATION | UNP P30613 |

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |
| 2   | B     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |
| 2   | C     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |
| 2   | D     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |

- Molecule 3 is SUGAR (2-PHOSPHOGLYCOLIC ACID) (three-letter code: PGA) (formula:  $C_2H_5O_6P$ ).



| Mol | Chain | Residues | Atoms                  | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 3   | A     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |
| 3   | B     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |
| 3   | C     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |
| 3   | D     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | B     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | A     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | D     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total K<br>1 1 | 0       | 0       |

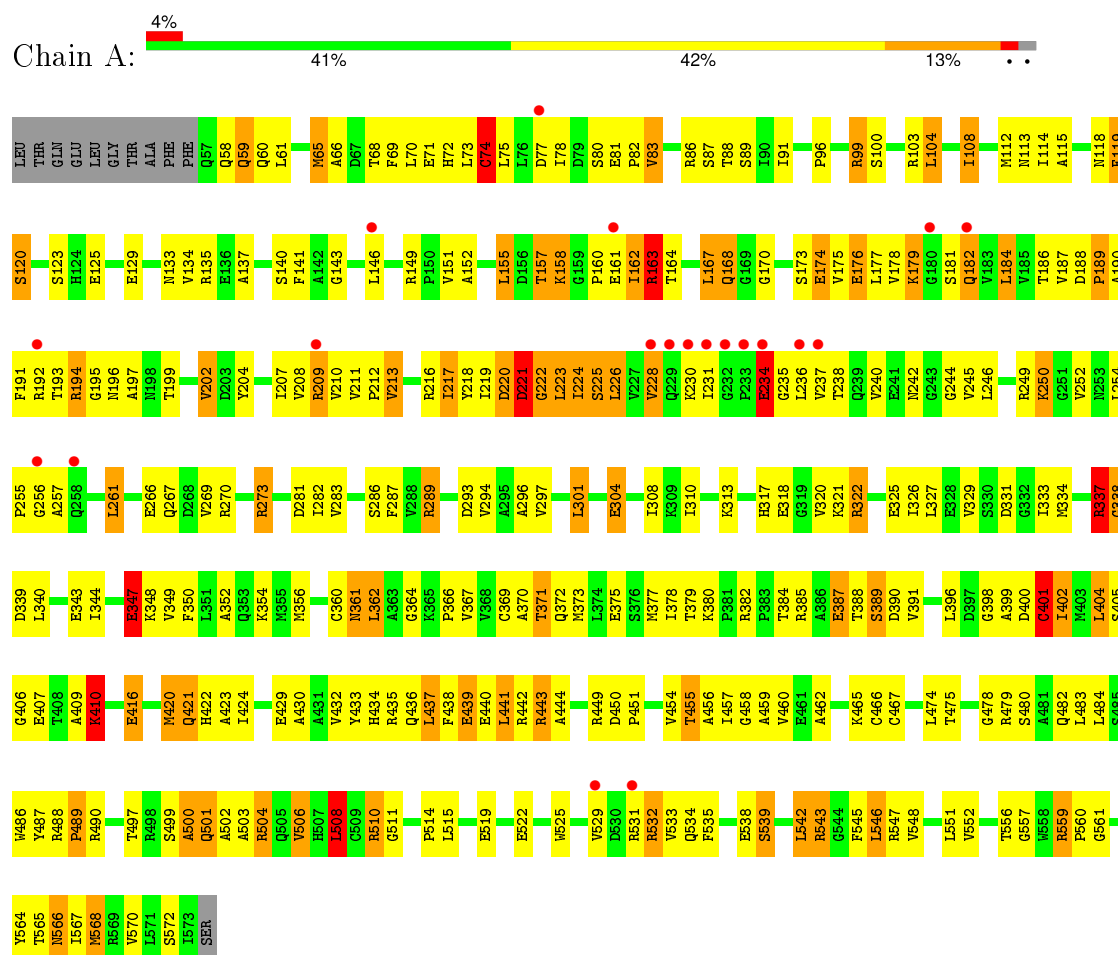
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

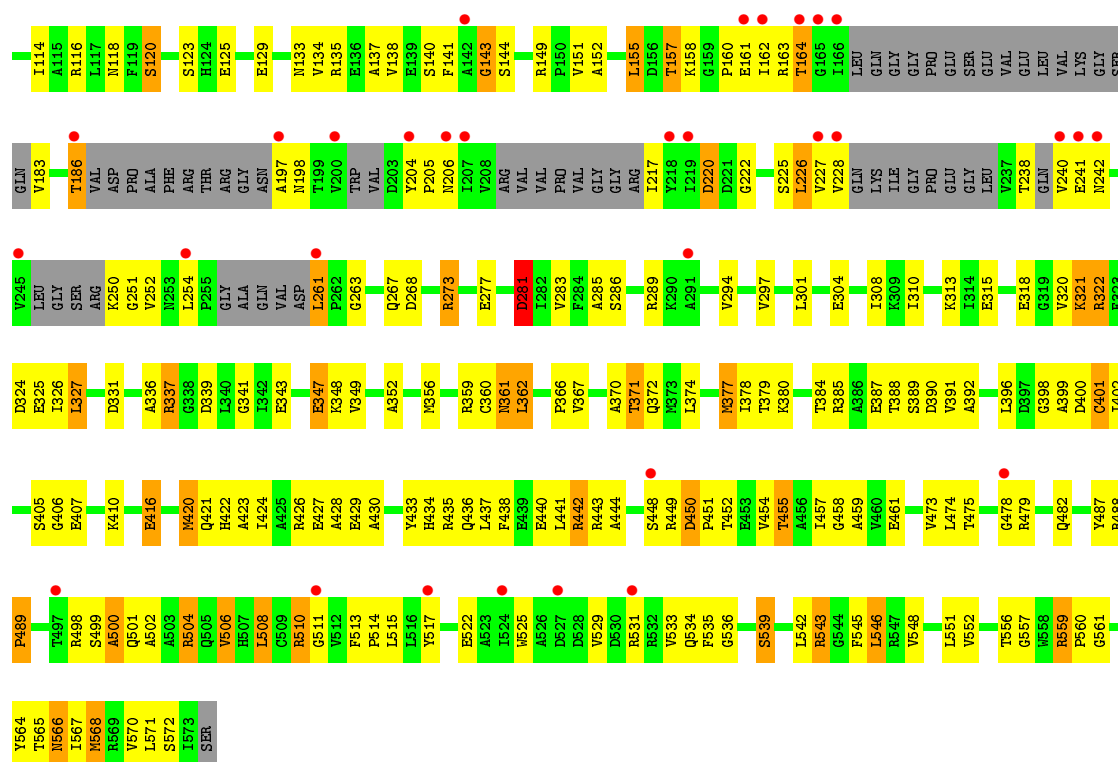
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | B     | 1        | Total Mn<br>1 1 | 0       | 0       |
| 5   | A     | 1        | Total Mn<br>1 1 | 0       | 0       |
| 5   | D     | 1        | Total Mn<br>1 1 | 0       | 0       |
| 5   | C     | 1        | Total Mn<br>1 1 | 0       | 0       |

### 3 Residue-property plots

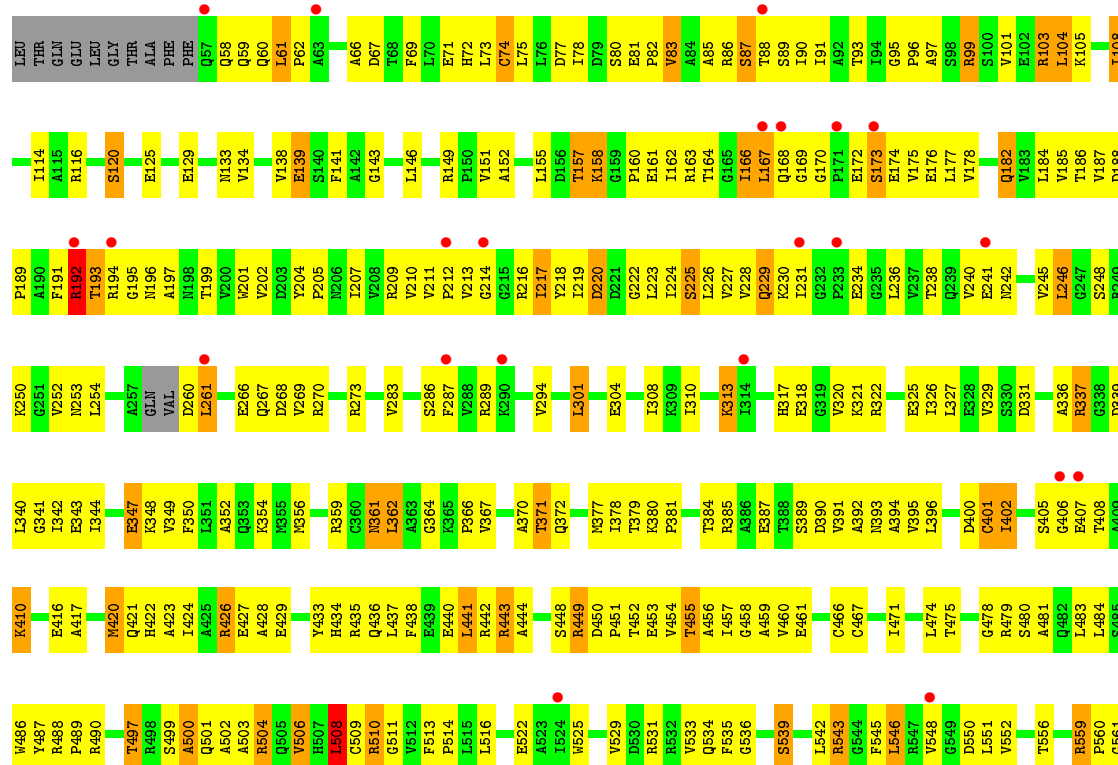
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: PYRUVATE KINASE ISOZYMES R/L

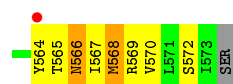




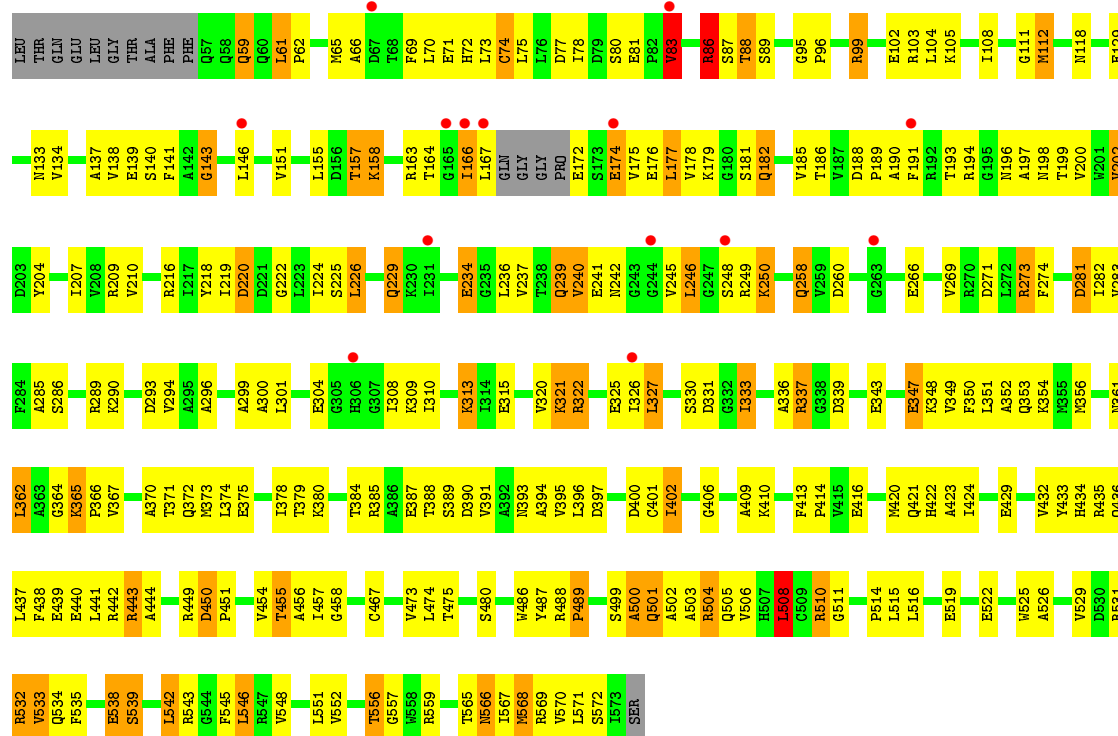
• Molecule 1: PYRUVATE KINASE ISOZYMES R/L







• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 73.70Å 171.16Å 85.05Å<br>90.00° 91.61° 90.00°               | Depositor        |
| Resolution (Å)  | 20.00 – 2.87<br>53.63 – 2.87                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.7 (20.00-2.87)<br>88.6 (53.63-2.87)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.08 (at 2.86Å)   | Xtriage          |
| Refinement program  | REFMAC 5.2.0019   | Depositor        |
| R, $R_{free}$   | 0.257 , 0.311<br>0.250 , 0.295                              | Depositor<br>DCC |
| $R_{free}$ test set   | 855 reflections (2.06%)                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.8  | Xtriage          |
| Anisotropy  | 0.395   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 38.0   | EDS              |
| Estimated twinning fraction   | 0.066 for h,-k,-l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Outliers  | 0 of 42487 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 15342   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 2.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, FBP, PGA, MN

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     | 1.19         | 14/3981 (0.4%)  | 1.17        | 19/5399 (0.4%)  |
| 1   | B     | 1.02         | 5/3564 (0.1%)   | 0.99        | 10/4822 (0.2%)  |
| 1   | C     | 1.07         | 3/3964 (0.1%)   | 1.05        | 8/5374 (0.1%)   |
| 1   | D     | 1.08         | 2/3955 (0.1%)   | 1.14        | 17/5362 (0.3%)  |
| All | All   | 1.10         | 24/15464 (0.2%) | 1.09        | 54/20957 (0.3%) |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 186 | THR  | C-O    | 17.89  | 1.57        | 1.23     |
| 1   | A     | 179 | LYS  | CE-NZ  | 15.06  | 1.86        | 1.49     |
| 1   | A     | 401 | CYS  | CB-SG  | -10.85 | 1.63        | 1.82     |
| 1   | A     | 179 | LYS  | CD-CE  | 9.82   | 1.75        | 1.51     |
| 1   | B     | 197 | ALA  | N-CA   | 9.28   | 1.65        | 1.46     |
| 1   | B     | 197 | ALA  | CA-CB  | 8.91   | 1.71        | 1.52     |
| 1   | A     | 439 | GLU  | CG-CD  | 7.85   | 1.63        | 1.51     |
| 1   | A     | 369 | CYS  | CB-SG  | -7.43  | 1.69        | 1.82     |
| 1   | A     | 347 | GLU  | CG-CD  | 6.36   | 1.61        | 1.51     |
| 1   | A     | 115 | ALA  | CA-CB  | -6.27  | 1.39        | 1.52     |
| 1   | A     | 74  | CYS  | CB-SG  | -6.22  | 1.71        | 1.82     |
| 1   | A     | 387 | GLU  | CD-OE2 | 5.96   | 1.32        | 1.25     |
| 1   | A     | 416 | GLU  | CG-CD  | 5.91   | 1.60        | 1.51     |
| 1   | A     | 187 | VAL  | CB-CG2 | 5.88   | 1.65        | 1.52     |
| 1   | B     | 416 | GLU  | CG-CD  | 5.84   | 1.60        | 1.51     |
| 1   | C     | 410 | LYS  | CB-CG  | -5.69  | 1.37        | 1.52     |
| 1   | B     | 410 | LYS  | CB-CG  | -5.69  | 1.37        | 1.52     |
| 1   | A     | 337 | ARG  | CZ-NH2 | -5.51  | 1.25        | 1.33     |
| 1   | C     | 401 | CYS  | CB-SG  | -5.51  | 1.72        | 1.81     |
| 1   | D     | 410 | LYS  | CB-CG  | -5.33  | 1.38        | 1.52     |
| 1   | A     | 179 | LYS  | CG-CD  | 5.32   | 1.70        | 1.52     |
| 1   | D     | 86  | ARG  | CG-CD  | -5.24  | 1.38        | 1.51     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 287 | PHE  | CE1-CZ | 5.15  | 1.47        | 1.37     |
| 1   | C     | 402 | ILE  | CA-CB  | -5.01 | 1.43        | 1.54     |

All (54) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | D     | 504 | ARG  | NE-CZ-NH1 | 15.84  | 128.22      | 120.30   |
| 1   | A     | 410 | LYS  | CD-CE-NZ  | -15.29 | 76.55       | 111.70   |
| 1   | A     | 510 | ARG  | NE-CZ-NH1 | -15.03 | 112.79      | 120.30   |
| 1   | A     | 510 | ARG  | NE-CZ-NH2 | 14.96  | 127.78      | 120.30   |
| 1   | D     | 504 | ARG  | NE-CZ-NH2 | -14.54 | 113.03      | 120.30   |
| 1   | B     | 504 | ARG  | NE-CZ-NH1 | 13.42  | 127.01      | 120.30   |
| 1   | B     | 504 | ARG  | NE-CZ-NH2 | -12.42 | 114.09      | 120.30   |
| 1   | C     | 504 | ARG  | NE-CZ-NH1 | -11.22 | 114.69      | 120.30   |
| 1   | C     | 504 | ARG  | NE-CZ-NH2 | 8.13   | 124.37      | 120.30   |
| 1   | A     | 504 | ARG  | NE-CZ-NH2 | 7.87   | 124.24      | 120.30   |
| 1   | A     | 221 | ASP  | CB-CG-OD1 | -7.66  | 111.41      | 118.30   |
| 1   | D     | 410 | LYS  | CB-CA-C   | -7.37  | 95.66       | 110.40   |
| 1   | A     | 510 | ARG  | CD-NE-CZ  | 7.28   | 133.80      | 123.60   |
| 1   | A     | 74  | CYS  | CA-CB-SG  | -7.28  | 100.89      | 114.00   |
| 1   | B     | 410 | LYS  | CB-CA-C   | -7.28  | 95.84       | 110.40   |
| 1   | D     | 508 | LEU  | CA-CB-CG  | 6.54   | 130.34      | 115.30   |
| 1   | D     | 281 | ASP  | CB-CG-OD2 | -6.49  | 112.46      | 118.30   |
| 1   | D     | 112 | MET  | CG-SD-CE  | -6.46  | 89.87       | 100.20   |
| 1   | C     | 508 | LEU  | CB-CG-CD1 | 6.45   | 121.96      | 111.00   |
| 1   | A     | 65  | MET  | CB-CG-SD  | 6.45   | 131.74      | 112.40   |
| 1   | A     | 337 | ARG  | NE-CZ-NH1 | 6.42   | 123.51      | 120.30   |
| 1   | B     | 473 | VAL  | CB-CA-C   | -6.33  | 99.38       | 111.40   |
| 1   | C     | 426 | ARG  | NE-CZ-NH2 | -6.21  | 117.19      | 120.30   |
| 1   | D     | 467 | CYS  | CA-CB-SG  | -6.14  | 102.95      | 114.00   |
| 1   | C     | 510 | ARG  | NE-CZ-NH2 | -6.07  | 117.27      | 120.30   |
| 1   | A     | 504 | ARG  | NE-CZ-NH1 | -6.06  | 117.27      | 120.30   |
| 1   | A     | 404 | LEU  | CB-CG-CD2 | -6.03  | 100.76      | 111.00   |
| 1   | B     | 510 | ARG  | NE-CZ-NH2 | -5.93  | 117.33      | 120.30   |
| 1   | B     | 410 | LYS  | CD-CE-NZ  | -5.92  | 98.07       | 111.70   |
| 1   | D     | 504 | ARG  | CD-NE-CZ  | 5.87   | 131.82      | 123.60   |
| 1   | A     | 532 | ARG  | NE-CZ-NH1 | -5.85  | 117.38      | 120.30   |
| 1   | D     | 450 | ASP  | CB-CG-OD2 | -5.82  | 113.06      | 118.30   |
| 1   | D     | 450 | ASP  | CB-CG-OD1 | 5.78   | 123.50      | 118.30   |
| 1   | A     | 226 | LEU  | CA-CB-CG  | 5.73   | 128.49      | 115.30   |
| 1   | B     | 504 | ARG  | CD-NE-CZ  | 5.73   | 131.62      | 123.60   |
| 1   | C     | 550 | ASP  | CB-CG-OD1 | -5.51  | 113.34      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 510 | ARG  | NE-CZ-NH1 | 5.47  | 123.04      | 120.30   |
| 1   | B     | 442 | ARG  | NE-CZ-NH1 | -5.47 | 117.57      | 120.30   |
| 1   | C     | 508 | LEU  | CA-CB-CG  | 5.45  | 127.82      | 115.30   |
| 1   | A     | 221 | ASP  | CB-CG-OD2 | 5.42  | 123.17      | 118.30   |
| 1   | B     | 510 | ARG  | NE-CZ-NH1 | 5.42  | 123.01      | 120.30   |
| 1   | A     | 179 | LYS  | CD-CE-NZ  | -5.41 | 99.25       | 111.70   |
| 1   | A     | 508 | LEU  | CA-CB-CG  | 5.33  | 127.57      | 115.30   |
| 1   | A     | 179 | LYS  | CG-CD-CE  | -5.29 | 96.04       | 111.90   |
| 1   | D     | 510 | ARG  | NE-CZ-NH2 | -5.26 | 117.67      | 120.30   |
| 1   | C     | 510 | ARG  | NE-CZ-NH1 | 5.25  | 122.93      | 120.30   |
| 1   | A     | 504 | ARG  | CD-NE-CZ  | 5.16  | 130.82      | 123.60   |
| 1   | D     | 226 | LEU  | CA-CB-CG  | 5.13  | 127.09      | 115.30   |
| 1   | A     | 163 | ARG  | NE-CZ-NH2 | -5.11 | 117.74      | 120.30   |
| 1   | D     | 532 | ARG  | NE-CZ-NH2 | 5.10  | 122.85      | 120.30   |
| 1   | D     | 281 | ASP  | CB-CG-OD1 | 5.08  | 122.87      | 118.30   |
| 1   | D     | 473 | VAL  | CB-CA-C   | -5.08 | 101.76      | 111.40   |
| 1   | B     | 281 | ASP  | CB-CG-OD1 | 5.06  | 122.86      | 118.30   |
| 1   | D     | 365 | LYS  | CD-CE-NZ  | -5.03 | 100.13      | 111.70   |

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     | 3915  | 0        | 3989     | 321     | 2            |
| 1   | B     | 3513  | 0        | 3576     | 231     | 0            |
| 1   | C     | 3899  | 0        | 3970     | 293     | 3            |
| 1   | D     | 3891  | 0        | 3966     | 231     | 1            |
| 2   | A     | 20    | 0        | 10       | 3       | 0            |
| 2   | B     | 20    | 0        | 10       | 3       | 0            |
| 2   | C     | 20    | 0        | 10       | 2       | 0            |
| 2   | D     | 20    | 0        | 10       | 5       | 0            |
| 3   | A     | 9     | 0        | 2        | 1       | 0            |
| 3   | B     | 9     | 0        | 2        | 5       | 0            |
| 3   | C     | 9     | 0        | 3        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 9     | 0        | 2        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 15342 | 0        | 15550    | 1026    | 3            |

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 33.

All (1026) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:179:LYS:CE   | 1:A:179:LYS:CD   | 1.75                     | 1.59              |
| 1:A:179:LYS:CE   | 1:A:179:LYS:NZ   | 1.86                     | 1.39              |
| 3:C:1575:PGA:O2  | 3:C:1575:PGA:C1  | 1.76                     | 1.33              |
| 1:A:225:SER:CB   | 1:A:242:ASN:HB2  | 1.77                     | 1.13              |
| 1:A:167:LEU:HD12 | 1:A:168:GLN:H    | 1.10                     | 1.13              |
| 1:A:225:SER:HB3  | 1:A:242:ASN:CB   | 1.81                     | 1.11              |
| 1:A:184:LEU:HD11 | 1:A:235:GLY:HA3  | 1.12                     | 1.06              |
| 1:D:225:SER:HB3  | 1:D:242:ASN:HB2  | 1.39                     | 1.02              |
| 1:A:442:ARG:HH21 | 1:B:442:ARG:HH21 | 1.02                     | 1.01              |
| 1:A:442:ARG:HH21 | 1:B:442:ARG:NH2  | 1.58                     | 1.00              |
| 1:A:162:ILE:HG23 | 1:A:204:TYR:HB2  | 1.44                     | 0.99              |
| 1:A:322:ARG:O    | 1:A:326:ILE:HD12 | 1.62                     | 0.99              |
| 1:A:347:GLU:HG2  | 1:C:423:ALA:HB1  | 1.47                     | 0.97              |
| 1:C:384:THR:OG1  | 1:C:387:GLU:HG3  | 1.64                     | 0.96              |
| 1:D:177:LEU:HD23 | 1:D:177:LEU:N    | 1.83                     | 0.93              |
| 1:C:436:GLN:O    | 1:C:440:GLU:HG3  | 1.68                     | 0.93              |
| 1:A:184:LEU:CD1  | 1:A:235:GLY:HA3  | 1.99                     | 0.92              |
| 1:C:87:SER:HB3   | 1:C:511:GLY:HA2  | 1.49                     | 0.92              |
| 1:C:170:GLY:HA2  | 1:C:173:SER:OG   | 1.70                     | 0.92              |
| 1:D:157:THR:HG22 | 1:D:286:SER:H    | 1.34                     | 0.91              |
| 1:B:157:THR:HG22 | 1:B:286:SER:H    | 1.34                     | 0.91              |
| 1:A:234:GLU:OE1  | 1:A:235:GLY:N    | 2.04                     | 0.90              |
| 1:A:209:ARG:HH11 | 1:A:210:VAL:CG2  | 1.84                     | 0.90              |
| 1:A:442:ARG:NH2  | 1:B:442:ARG:HH21 | 1.70                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:366:PRO:HB3  | 1:B:508:LEU:O    | 1.72                     | 0.89              |
| 1:D:352:ALA:HB1  | 1:D:356:MET:CE   | 2.03                     | 0.88              |
| 1:D:146:LEU:CB   | 1:D:542:LEU:HD12 | 2.04                     | 0.88              |
| 1:C:442:ARG:NH2  | 1:D:442:ARG:HH21 | 1.72                     | 0.88              |
| 1:A:216:ARG:HG2  | 1:A:218:TYR:CE1  | 2.08                     | 0.87              |
| 1:D:366:PRO:HA   | 1:D:400:ASP:OD2  | 1.74                     | 0.87              |
| 1:A:436:GLN:O    | 1:A:440:GLU:HG3  | 1.74                     | 0.87              |
| 1:D:166:ILE:HA   | 1:D:248:SER:OG   | 1.74                     | 0.87              |
| 1:A:204:TYR:O    | 1:A:204:TYR:CD2  | 2.28                     | 0.87              |
| 1:B:99:ARG:NH2   | 1:B:129:GLU:OE1  | 2.07                     | 0.87              |
| 1:A:208:VAL:HA   | 1:A:236:LEU:HD11 | 1.54                     | 0.86              |
| 1:C:488:ARG:NH1  | 1:C:510:ARG:HD3  | 1.91                     | 0.86              |
| 1:B:436:GLN:O    | 1:B:440:GLU:HG3  | 1.76                     | 0.86              |
| 1:B:228:VAL:HG12 | 1:B:228:VAL:O    | 1.74                     | 0.85              |
| 1:A:157:THR:HG22 | 1:A:286:SER:H    | 1.41                     | 0.85              |
| 1:D:371:THR:HG22 | 1:D:372:GLN:HG3  | 1.58                     | 0.85              |
| 1:B:225:SER:HB3  | 1:B:242:ASN:HB2  | 1.59                     | 0.85              |
| 1:A:170:GLY:HA3  | 1:A:173:SER:HB2  | 1.59                     | 0.85              |
| 1:C:184:LEU:HD22 | 1:C:236:LEU:O    | 1.76                     | 0.84              |
| 1:D:99:ARG:NH2   | 1:D:129:GLU:OE1  | 2.10                     | 0.83              |
| 1:A:228:VAL:HG12 | 1:A:228:VAL:O    | 1.78                     | 0.83              |
| 1:C:487:TYR:O    | 1:C:488:ARG:HB2  | 1.77                     | 0.83              |
| 1:C:69:PHE:O     | 1:C:72:HIS:HB3   | 1.78                     | 0.83              |
| 1:C:166:ILE:H    | 1:C:166:ILE:HD12 | 1.43                     | 0.83              |
| 1:C:313:LYS:HE3  | 3:C:1575:PGA:H22 | 1.61                     | 0.83              |
| 1:D:146:LEU:HB3  | 1:D:542:LEU:HD12 | 1.60                     | 0.83              |
| 1:A:337:ARG:HD3  | 1:A:370:ALA:O    | 1.77                     | 0.83              |
| 1:C:87:SER:CB    | 1:C:511:GLY:HA2  | 2.08                     | 0.82              |
| 1:A:167:LEU:HD12 | 1:A:168:GLN:N    | 1.93                     | 0.82              |
| 1:A:191:PHE:HA   | 1:A:194:ARG:HB2  | 1.60                     | 0.82              |
| 1:A:371:THR:HG22 | 1:A:372:GLN:HG3  | 1.59                     | 0.82              |
| 1:A:179:LYS:CG   | 1:A:179:LYS:CE   | 2.57                     | 0.82              |
| 1:D:86:ARG:NH1   | 1:D:422:HIS:ND1  | 2.28                     | 0.82              |
| 1:C:225:SER:HB3  | 1:C:242:ASN:HB2  | 1.60                     | 0.81              |
| 1:A:402:ILE:HG13 | 1:A:421:GLN:NE2  | 1.95                     | 0.81              |
| 1:C:488:ARG:NH1  | 1:C:510:ARG:CB   | 2.44                     | 0.81              |
| 1:B:423:ALA:HB1  | 1:D:347:GLU:HG2  | 1.63                     | 0.81              |
| 1:C:441:LEU:O    | 1:C:442:ARG:C    | 2.19                     | 0.81              |
| 1:D:174:GLU:OE2  | 1:D:245:VAL:HG11 | 1.80                     | 0.81              |
| 1:C:182:GLN:HE21 | 1:C:182:GLN:HA   | 1.46                     | 0.81              |
| 1:D:362:LEU:O    | 1:D:486:TRP:HZ2  | 1.64                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:434:HIS:O    | 1:C:437:LEU:N    | 2.15                     | 0.79              |
| 1:A:488:ARG:NH1  | 1:A:510:ARG:HB3  | 1.96                     | 0.79              |
| 1:B:228:VAL:HA   | 1:B:238:THR:HG22 | 1.64                     | 0.79              |
| 1:A:155:LEU:HD23 | 1:A:155:LEU:C    | 2.02                     | 0.79              |
| 1:C:313:LYS:HE3  | 3:C:1575:PGA:C2  | 2.12                     | 0.79              |
| 1:C:162:ILE:O    | 1:C:252:VAL:N    | 2.14                     | 0.79              |
| 1:C:120:SER:HA   | 1:C:158:LYS:HG3  | 1.63                     | 0.79              |
| 1:A:209:ARG:HH11 | 1:A:210:VAL:HG23 | 1.48                     | 0.79              |
| 1:A:158:LYS:HG2  | 1:A:158:LYS:O    | 1.81                     | 0.79              |
| 1:A:347:GLU:HG2  | 1:C:423:ALA:CB   | 2.12                     | 0.78              |
| 1:B:164:THR:HG23 | 1:B:252:VAL:HG21 | 1.64                     | 0.78              |
| 1:A:175:VAL:CG1  | 1:A:176:GLU:N    | 2.46                     | 0.78              |
| 1:A:385:ARG:HG3  | 1:C:337:ARG:HB3  | 1.66                     | 0.78              |
| 1:A:407:GLU:N    | 1:A:407:GLU:OE1  | 2.15                     | 0.78              |
| 1:C:407:GLU:OE1  | 1:C:407:GLU:N    | 2.15                     | 0.78              |
| 1:D:204:TYR:OH   | 1:D:260:ASP:OD1  | 2.01                     | 0.77              |
| 1:C:82:PRO:O     | 1:C:83:VAL:HG23  | 1.84                     | 0.77              |
| 1:B:336:ALA:HB1  | 3:B:1575:PGA:C1  | 2.14                     | 0.77              |
| 1:D:436:GLN:O    | 1:D:440:GLU:HG3  | 1.84                     | 0.77              |
| 1:D:441:LEU:O    | 1:D:442:ARG:C    | 2.23                     | 0.76              |
| 1:C:366:PRO:HB3  | 1:C:508:LEU:O    | 1.85                     | 0.76              |
| 1:C:73:LEU:O     | 1:C:75:LEU:N     | 2.17                     | 0.76              |
| 1:A:487:TYR:O    | 1:A:488:ARG:HB2  | 1.83                     | 0.76              |
| 1:C:442:ARG:HH21 | 1:D:442:ARG:HH21 | 1.32                     | 0.76              |
| 1:B:322:ARG:O    | 1:B:326:ILE:HD12 | 1.86                     | 0.76              |
| 1:B:457:ILE:HG23 | 1:B:458:GLY:N    | 2.00                     | 0.76              |
| 1:D:366:PRO:HB3  | 1:D:508:LEU:O    | 1.87                     | 0.75              |
| 1:C:188:ASP:HB3  | 1:C:191:PHE:HD1  | 1.52                     | 0.75              |
| 1:B:89:SER:HB2   | 1:B:401:CYS:HB3  | 1.68                     | 0.75              |
| 1:C:81:GLU:OE1   | 1:C:81:GLU:HA    | 1.86                     | 0.75              |
| 1:C:442:ARG:HH21 | 1:D:442:ARG:NH2  | 1.84                     | 0.74              |
| 1:C:488:ARG:HH12 | 1:C:510:ARG:HB2  | 1.51                     | 0.74              |
| 1:A:474:LEU:HD22 | 1:A:556:THR:HG22 | 1.67                     | 0.74              |
| 1:C:322:ARG:O    | 1:C:326:ILE:HD12 | 1.87                     | 0.74              |
| 1:C:87:SER:CB    | 1:C:511:GLY:CA   | 2.65                     | 0.74              |
| 1:A:175:VAL:HG12 | 1:A:176:GLU:N    | 2.01                     | 0.74              |
| 1:C:322:ARG:NH2  | 1:C:325:GLU:OE2  | 2.21                     | 0.73              |
| 1:A:204:TYR:O    | 1:A:204:TYR:HD2  | 1.68                     | 0.73              |
| 1:A:162:ILE:HG23 | 1:A:204:TYR:CB   | 2.18                     | 0.73              |
| 1:B:437:LEU:O    | 1:B:437:LEU:HD12 | 1.88                     | 0.73              |
| 1:A:366:PRO:HB3  | 1:A:508:LEU:O    | 1.89                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:402:ILE:HG13 | 1:D:421:GLN:NE2  | 2.03                     | 0.73              |
| 1:D:362:LEU:O    | 1:D:486:TRP:CZ2  | 2.41                     | 0.73              |
| 1:C:535:PHE:O    | 1:C:539:SER:OG   | 2.07                     | 0.72              |
| 1:A:193:THR:HG23 | 1:A:194:ARG:HG3  | 1.70                     | 0.72              |
| 1:A:162:ILE:CG2  | 1:A:204:TYR:CB   | 2.68                     | 0.72              |
| 1:C:506:VAL:O    | 1:C:506:VAL:HG13 | 1.89                     | 0.72              |
| 1:D:210:VAL:O    | 1:D:210:VAL:HG12 | 1.87                     | 0.72              |
| 1:A:221:ASP:HB3  | 1:A:223:LEU:HG   | 1.72                     | 0.72              |
| 1:C:488:ARG:NH1  | 1:C:510:ARG:HB3  | 2.05                     | 0.72              |
| 1:B:281:ASP:OD2  | 1:B:504:ARG:HD2  | 1.90                     | 0.72              |
| 1:B:441:LEU:O    | 1:B:442:ARG:C    | 2.25                     | 0.72              |
| 1:D:155:LEU:C    | 1:D:155:LEU:HD23 | 2.10                     | 0.72              |
| 1:C:561:GLY:O    | 2:C:1574:FBP:O4  | 2.06                     | 0.72              |
| 1:A:146:LEU:HB2  | 1:A:542:LEU:HD12 | 1.72                     | 0.72              |
| 1:B:488:ARG:NH1  | 1:B:510:ARG:HD3  | 2.05                     | 0.72              |
| 1:A:441:LEU:O    | 1:A:442:ARG:C    | 2.25                     | 0.72              |
| 1:C:85:ALA:HB2   | 1:C:545:PHE:CE2  | 2.25                     | 0.72              |
| 1:C:367:VAL:H    | 1:C:400:ASP:HB2  | 1.54                     | 0.72              |
| 1:C:151:VAL:O    | 1:C:504:ARG:HD2  | 1.88                     | 0.72              |
| 1:A:202:VAL:HG13 | 1:A:204:TYR:H    | 1.55                     | 0.71              |
| 1:A:437:LEU:HD12 | 1:A:437:LEU:O    | 1.90                     | 0.71              |
| 1:C:175:VAL:CG1  | 1:C:197:ALA:HA   | 2.19                     | 0.71              |
| 1:A:162:ILE:CG2  | 1:A:204:TYR:HB2  | 2.20                     | 0.71              |
| 1:C:551:LEU:HD23 | 1:C:572:SER:HA   | 1.72                     | 0.71              |
| 1:D:185:VAL:HB   | 1:D:236:LEU:HB2  | 1.72                     | 0.71              |
| 1:D:73:LEU:O     | 1:D:75:LEU:N     | 2.24                     | 0.71              |
| 1:C:175:VAL:HG11 | 1:C:197:ALA:HA   | 1.72                     | 0.71              |
| 1:D:83:VAL:CG1   | 1:D:83:VAL:O     | 2.38                     | 0.71              |
| 1:A:286:SER:HA   | 1:A:313:LYS:HE2  | 1.73                     | 0.70              |
| 1:A:146:LEU:CB   | 1:A:542:LEU:HD12 | 2.21                     | 0.70              |
| 1:A:182:GLN:HA   | 1:A:182:GLN:HE21 | 1.56                     | 0.70              |
| 1:A:533:VAL:HG12 | 1:A:534:GLN:N    | 2.06                     | 0.70              |
| 1:A:216:ARG:HG2  | 1:A:218:TYR:HE1  | 1.54                     | 0.70              |
| 1:B:451:PRO:O    | 1:B:455:THR:OG1  | 2.09                     | 0.70              |
| 1:A:170:GLY:HA3  | 1:A:173:SER:CB   | 2.22                     | 0.70              |
| 1:C:87:SER:HB2   | 1:C:511:GLY:CA   | 2.21                     | 0.70              |
| 1:D:337:ARG:HD3  | 1:D:370:ALA:O    | 1.91                     | 0.70              |
| 1:A:175:VAL:HG13 | 1:A:197:ALA:HB2  | 1.74                     | 0.70              |
| 1:A:96:PRO:HD2   | 1:A:409:ALA:O    | 1.92                     | 0.70              |
| 1:A:209:ARG:NH1  | 1:A:210:VAL:CG2  | 2.54                     | 0.70              |
| 1:A:331:ASP:O    | 1:A:366:PRO:HD2  | 1.92                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:146:LEU:HB2  | 1:D:542:LEU:HD12 | 1.73                     | 0.69              |
| 1:D:258:GLN:HG2  | 1:D:258:GLN:O    | 1.90                     | 0.69              |
| 1:A:373:MET:O    | 1:A:387:GLU:HB3  | 1.92                     | 0.69              |
| 1:D:499:SER:O    | 1:D:501:GLN:N    | 2.25                     | 0.69              |
| 1:C:170:GLY:CA   | 1:C:173:SER:OG   | 2.40                     | 0.69              |
| 1:C:442:ARG:NH2  | 1:D:442:ARG:NH2  | 2.39                     | 0.69              |
| 1:C:488:ARG:HH12 | 1:C:510:ARG:CB   | 2.06                     | 0.68              |
| 1:B:155:LEU:C    | 1:B:155:LEU:HD23 | 2.13                     | 0.68              |
| 1:C:87:SER:HB3   | 1:C:511:GLY:CA   | 2.23                     | 0.68              |
| 1:B:157:THR:CG2  | 1:B:286:SER:H    | 2.06                     | 0.68              |
| 1:D:158:LYS:O    | 1:D:158:LYS:HG2  | 1.88                     | 0.68              |
| 1:D:352:ALA:HB1  | 1:D:356:MET:HE3  | 1.75                     | 0.68              |
| 1:C:216:ARG:HD2  | 1:C:241:GLU:OE1  | 1.93                     | 0.68              |
| 1:A:219:ILE:HB   | 1:A:224:ILE:CG2  | 2.24                     | 0.68              |
| 1:C:87:SER:HB2   | 1:C:511:GLY:N    | 2.09                     | 0.68              |
| 1:B:434:HIS:O    | 1:B:437:LEU:N    | 2.26                     | 0.68              |
| 1:B:283:VAL:HG23 | 1:B:308:ILE:HG21 | 1.75                     | 0.68              |
| 1:D:533:VAL:HG12 | 1:D:534:GLN:N    | 2.08                     | 0.68              |
| 1:A:488:ARG:NH1  | 1:A:510:ARG:CB   | 2.57                     | 0.67              |
| 1:C:161:GLU:OE1  | 1:C:163:ARG:NE   | 2.18                     | 0.67              |
| 1:D:81:GLU:HA    | 1:D:81:GLU:OE1   | 1.93                     | 0.67              |
| 1:A:207:ILE:HD11 | 1:A:254:LEU:HD21 | 1.76                     | 0.67              |
| 1:B:228:VAL:CG1  | 1:B:228:VAL:O    | 2.41                     | 0.67              |
| 1:B:533:VAL:HG12 | 1:B:534:GLN:N    | 2.08                     | 0.67              |
| 1:B:125:GLU:H    | 1:B:125:GLU:CD   | 1.97                     | 0.67              |
| 1:C:488:ARG:CZ   | 1:C:510:ARG:HD3  | 2.25                     | 0.67              |
| 1:D:137:ALA:O    | 1:D:140:SER:OG   | 2.11                     | 0.67              |
| 1:D:229:GLN:HG3  | 1:D:237:VAL:O    | 1.95                     | 0.67              |
| 1:D:166:ILE:HA   | 1:D:248:SER:HG   | 1.59                     | 0.67              |
| 1:A:338:GLY:O    | 1:C:385:ARG:NH2  | 2.26                     | 0.67              |
| 1:D:283:VAL:HG23 | 1:D:308:ILE:HG21 | 1.76                     | 0.67              |
| 1:D:434:HIS:O    | 1:D:437:LEU:N    | 2.28                     | 0.67              |
| 1:A:83:VAL:O     | 1:A:83:VAL:HG12  | 1.92                     | 0.67              |
| 1:C:185:VAL:HB   | 1:C:236:LEU:HB2  | 1.77                     | 0.66              |
| 1:C:85:ALA:HB1   | 1:C:513:PHE:CE2  | 2.29                     | 0.66              |
| 1:A:402:ILE:HG13 | 1:A:421:GLN:HE22 | 1.60                     | 0.66              |
| 1:D:66:ALA:HB1   | 1:D:71:GLU:HG2   | 1.76                     | 0.66              |
| 1:B:487:TYR:O    | 1:B:488:ARG:HB2  | 1.95                     | 0.66              |
| 1:D:457:ILE:HG23 | 1:D:458:GLY:N    | 2.10                     | 0.66              |
| 1:A:228:VAL:HA   | 1:A:238:THR:HG22 | 1.78                     | 0.66              |
| 1:C:216:ARG:HD3  | 1:C:227:VAL:HG22 | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:336:ALA:HB1  | 3:C:1575:PGA:C1  | 2.26                     | 0.66              |
| 1:C:267:GLN:O    | 1:C:270:ARG:N    | 2.29                     | 0.66              |
| 1:B:371:THR:HG22 | 1:B:372:GLN:HG3  | 1.77                     | 0.66              |
| 1:D:157:THR:CG2  | 1:D:286:SER:H    | 2.09                     | 0.65              |
| 1:A:184:LEU:HD11 | 1:A:235:GLY:CA   | 2.08                     | 0.65              |
| 1:A:178:VAL:O    | 1:A:181:SER:OG   | 2.07                     | 0.65              |
| 1:D:258:GLN:H    | 1:D:258:GLN:HE21 | 1.45                     | 0.65              |
| 1:B:120:SER:HA   | 1:B:158:LYS:HG3  | 1.78                     | 0.65              |
| 1:A:196:ASN:OD1  | 1:A:199:THR:N    | 2.29                     | 0.65              |
| 1:A:155:LEU:HD23 | 1:A:155:LEU:O    | 1.96                     | 0.65              |
| 1:A:441:LEU:O    | 1:A:443:ARG:N    | 2.30                     | 0.65              |
| 1:B:347:GLU:HG2  | 1:D:423:ALA:HB1  | 1.77                     | 0.65              |
| 1:C:283:VAL:HG23 | 1:C:308:ILE:HG21 | 1.78                     | 0.64              |
| 1:D:364:GLY:HA2  | 1:D:486:TRP:CD1  | 2.32                     | 0.64              |
| 1:B:337:ARG:HB3  | 1:D:385:ARG:HG3  | 1.77                     | 0.64              |
| 1:B:78:ILE:HD13  | 1:D:320:VAL:HG11 | 1.78                     | 0.64              |
| 1:C:193:THR:HG23 | 1:C:193:THR:O    | 1.98                     | 0.64              |
| 1:D:378:ILE:HD11 | 1:D:406:GLY:HA3  | 1.79                     | 0.64              |
| 1:B:535:PHE:O    | 1:B:539:SER:OG   | 2.16                     | 0.64              |
| 1:A:225:SER:HB3  | 1:A:242:ASN:HB2  | 0.85                     | 0.64              |
| 1:A:194:ARG:HB3  | 1:A:194:ARG:HH11 | 1.61                     | 0.64              |
| 1:D:285:ALA:O    | 1:D:313:LYS:HB2  | 1.98                     | 0.64              |
| 1:D:475:THR:HA   | 2:D:1574:FBP:H61 | 1.79                     | 0.64              |
| 1:D:545:PHE:HB2  | 1:D:546:LEU:HD23 | 1.79                     | 0.64              |
| 1:A:219:ILE:HG21 | 1:A:246:LEU:HD13 | 1.80                     | 0.63              |
| 1:C:318:GLU:O    | 1:C:322:ARG:HG3  | 1.98                     | 0.63              |
| 1:B:227:VAL:O    | 1:B:238:THR:HB   | 1.97                     | 0.63              |
| 1:A:86:ARG:NH1   | 1:A:422:HIS:ND1  | 2.45                     | 0.63              |
| 1:C:99:ARG:NH2   | 1:C:129:GLU:OE1  | 2.31                     | 0.63              |
| 1:A:317:HIS:O    | 1:A:320:VAL:N    | 2.32                     | 0.63              |
| 1:C:157:THR:HG22 | 1:C:286:SER:H    | 1.63                     | 0.63              |
| 1:A:188:ASP:O    | 1:A:190:ALA:N    | 2.32                     | 0.63              |
| 1:C:384:THR:OG1  | 1:C:387:GLU:CG   | 2.43                     | 0.63              |
| 1:A:255:PRO:O    | 1:A:257:ALA:N    | 2.32                     | 0.63              |
| 1:B:315:GLU:OE2  | 1:B:339:ASP:OD2  | 2.16                     | 0.62              |
| 1:A:125:GLU:H    | 1:A:125:GLU:CD   | 2.02                     | 0.62              |
| 1:A:217:ILE:N    | 1:A:226:LEU:O    | 2.28                     | 0.62              |
| 1:D:532:ARG:HH22 | 2:D:1574:FBP:P1  | 2.23                     | 0.62              |
| 1:D:219:ILE:HB   | 1:D:224:ILE:HB   | 1.81                     | 0.62              |
| 1:C:349:VAL:O    | 1:C:352:ALA:N    | 2.31                     | 0.62              |
| 1:C:245:VAL:O    | 1:C:245:VAL:HG12 | 1.98                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:ILE:CG2  | 1:A:204:TYR:HB3  | 2.28                     | 0.62              |
| 1:C:433:TYR:O    | 1:C:434:HIS:C    | 2.37                     | 0.62              |
| 1:A:402:ILE:O    | 1:A:402:ILE:HG12 | 2.00                     | 0.62              |
| 1:B:337:ARG:HD3  | 1:B:370:ALA:O    | 1.99                     | 0.62              |
| 1:D:322:ARG:NH2  | 1:D:325:GLU:OE2  | 2.31                     | 0.62              |
| 1:B:488:ARG:NH1  | 1:B:510:ARG:CB   | 2.63                     | 0.62              |
| 1:A:442:ARG:NH2  | 1:B:442:ARG:NH2  | 2.36                     | 0.62              |
| 1:C:451:PRO:O    | 1:C:455:THR:OG1  | 2.18                     | 0.62              |
| 1:C:317:HIS:O    | 1:C:320:VAL:N    | 2.33                     | 0.62              |
| 1:D:133:ASN:O    | 1:D:134:VAL:C    | 2.37                     | 0.62              |
| 1:D:551:LEU:HD23 | 1:D:572:SER:HA   | 1.81                     | 0.62              |
| 1:A:218:TYR:HD2  | 1:A:222:GLY:HA2  | 1.64                     | 0.61              |
| 1:A:207:ILE:HD11 | 1:A:254:LEU:CD2  | 2.30                     | 0.61              |
| 1:D:327:LEU:O    | 1:D:327:LEU:HD22 | 2.00                     | 0.61              |
| 1:A:240:VAL:HG13 | 1:A:242:ASN:O    | 2.00                     | 0.61              |
| 1:D:350:PHE:O    | 1:D:354:LYS:HG3  | 2.00                     | 0.61              |
| 1:A:360:CYS:O    | 1:A:361:ASN:C    | 2.36                     | 0.61              |
| 1:A:164:THR:O    | 1:A:249:ARG:HA   | 2.00                     | 0.61              |
| 1:A:283:VAL:HG23 | 1:A:308:ILE:HG21 | 1.82                     | 0.61              |
| 1:C:568:MET:HE1  | 1:C:570:VAL:HG23 | 1.82                     | 0.61              |
| 1:A:441:LEU:O    | 1:A:444:ALA:N    | 2.33                     | 0.61              |
| 1:A:347:GLU:HB3  | 1:C:424:ILE:HA   | 1.83                     | 0.61              |
| 1:A:367:VAL:H    | 1:A:400:ASP:HB2  | 1.66                     | 0.61              |
| 1:D:177:LEU:N    | 1:D:177:LEU:CD2  | 2.57                     | 0.61              |
| 1:C:66:ALA:HB1   | 1:C:71:GLU:HG2   | 1.83                     | 0.61              |
| 1:C:188:ASP:HB3  | 1:C:191:PHE:CD1  | 2.36                     | 0.60              |
| 1:C:218:TYR:HB3  | 1:C:222:GLY:HA2  | 1.83                     | 0.60              |
| 1:A:194:ARG:HH11 | 1:A:194:ARG:CG   | 2.14                     | 0.60              |
| 1:C:125:GLU:H    | 1:C:125:GLU:CD   | 2.03                     | 0.60              |
| 1:D:474:LEU:HD22 | 1:D:556:THR:HG22 | 1.81                     | 0.60              |
| 1:B:420:MET:O    | 1:B:421:GLN:C    | 2.36                     | 0.60              |
| 1:B:423:ALA:CB   | 1:D:347:GLU:HG2  | 2.31                     | 0.60              |
| 1:D:433:TYR:O    | 1:D:434:HIS:C    | 2.39                     | 0.60              |
| 1:D:514:PRO:O    | 1:D:515:LEU:HD23 | 2.02                     | 0.60              |
| 1:C:83:VAL:HG12  | 1:C:83:VAL:O     | 2.01                     | 0.60              |
| 1:D:210:VAL:CG1  | 1:D:210:VAL:O    | 2.50                     | 0.60              |
| 1:B:331:ASP:O    | 1:B:366:PRO:HD2  | 2.01                     | 0.60              |
| 1:D:456:ALA:O    | 1:D:457:ILE:C    | 2.38                     | 0.60              |
| 1:A:255:PRO:C    | 1:A:257:ALA:H    | 2.05                     | 0.60              |
| 1:A:221:ASP:HB3  | 1:A:223:LEU:CG   | 2.30                     | 0.59              |
| 1:A:87:SER:N     | 1:A:429:GLU:OE1  | 2.25                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:457:ILE:CG2  | 1:B:458:GLY:N    | 2.65                     | 0.59              |
| 1:A:488:ARG:HH11 | 1:A:510:ARG:HB3  | 1.62                     | 0.59              |
| 1:D:155:LEU:HD23 | 1:D:155:LEU:O    | 2.01                     | 0.59              |
| 1:C:567:ILE:HG12 | 1:D:569:ARG:HG2  | 1.84                     | 0.59              |
| 1:A:551:LEU:HD23 | 1:A:572:SER:HA   | 1.84                     | 0.59              |
| 1:B:86:ARG:HH11  | 1:B:86:ARG:HG2   | 1.68                     | 0.59              |
| 1:C:568:MET:CE   | 1:C:570:VAL:HG23 | 2.33                     | 0.59              |
| 1:A:466:CYS:O    | 1:A:467:CYS:HB2  | 2.01                     | 0.59              |
| 1:A:99:ARG:NH2   | 1:A:129:GLU:OE1  | 2.35                     | 0.59              |
| 1:C:202:VAL:HG12 | 1:C:204:TYR:H    | 1.68                     | 0.59              |
| 1:A:160:PRO:HB3  | 1:A:261:LEU:HB3  | 1.85                     | 0.59              |
| 1:D:532:ARG:NH2  | 2:D:1574:FBP:O1P | 2.33                     | 0.59              |
| 1:A:81:GLU:OE1   | 1:A:81:GLU:HA    | 2.03                     | 0.59              |
| 1:D:83:VAL:HG12  | 1:D:83:VAL:O     | 2.01                     | 0.58              |
| 1:B:551:LEU:HD23 | 1:B:572:SER:HA   | 1.85                     | 0.58              |
| 1:C:93:THR:HA    | 1:C:116:ARG:HB3  | 1.84                     | 0.58              |
| 1:D:349:VAL:O    | 1:D:352:ALA:N    | 2.37                     | 0.58              |
| 1:B:488:ARG:NH1  | 1:B:510:ARG:HB3  | 2.18                     | 0.58              |
| 1:A:175:VAL:O    | 1:A:245:VAL:HG13 | 2.02                     | 0.58              |
| 1:B:318:GLU:O    | 1:B:322:ARG:HG3  | 2.03                     | 0.58              |
| 1:A:340:LEU:O    | 1:A:344:ILE:HG12 | 2.03                     | 0.58              |
| 1:C:167:LEU:HD12 | 1:C:195:GLY:HA3  | 1.83                     | 0.58              |
| 1:A:162:ILE:HG21 | 1:A:204:TYR:HB3  | 1.84                     | 0.58              |
| 1:A:322:ARG:C    | 1:A:326:ILE:HD12 | 2.24                     | 0.58              |
| 1:B:315:GLU:HG2  | 1:B:339:ASP:HB2  | 1.85                     | 0.58              |
| 1:D:322:ARG:O    | 1:D:326:ILE:HD12 | 2.03                     | 0.58              |
| 1:A:83:VAL:O     | 1:A:83:VAL:CG1   | 2.51                     | 0.58              |
| 1:D:487:TYR:O    | 1:D:488:ARG:HB2  | 2.02                     | 0.58              |
| 1:B:163:ARG:NH1  | 1:B:250:LYS:HA   | 2.18                     | 0.58              |
| 1:B:352:ALA:HB1  | 1:B:356:MET:CE   | 2.33                     | 0.58              |
| 1:A:175:VAL:HG11 | 1:A:197:ALA:HA   | 1.86                     | 0.58              |
| 1:B:286:SER:HA   | 1:B:313:LYS:HE2  | 1.86                     | 0.58              |
| 1:A:137:ALA:O    | 1:A:140:SER:OG   | 2.18                     | 0.58              |
| 1:A:188:ASP:O    | 1:A:189:PRO:C    | 2.40                     | 0.58              |
| 1:D:532:ARG:NH1  | 2:D:1574:FBP:O2P | 2.34                     | 0.58              |
| 1:B:226:LEU:HD22 | 1:B:240:VAL:HG22 | 1.85                     | 0.58              |
| 1:C:339:ASP:O    | 1:C:343:GLU:HG2  | 2.04                     | 0.58              |
| 1:B:183:VAL:HG22 | 1:B:198:ASN:HA   | 1.84                     | 0.58              |
| 1:A:69:PHE:O     | 1:A:72:HIS:HB3   | 2.03                     | 0.58              |
| 1:D:354:LYS:NZ   | 1:D:397:ASP:OD1  | 2.35                     | 0.58              |
| 1:A:475:THR:HA   | 2:A:1574:FBP:H61 | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:VAL:CG1  | 1:A:197:ALA:HB2  | 2.34                     | 0.58              |
| 1:A:488:ARG:O    | 1:A:489:PRO:O    | 2.21                     | 0.58              |
| 1:D:488:ARG:NH1  | 1:D:510:ARG:HD3  | 2.18                     | 0.58              |
| 1:D:347:GLU:H    | 1:D:347:GLU:CD   | 2.07                     | 0.57              |
| 1:C:506:VAL:O    | 1:C:506:VAL:CG1  | 2.52                     | 0.57              |
| 1:C:214:GLY:N    | 1:C:228:VAL:O    | 2.35                     | 0.57              |
| 1:D:225:SER:CB   | 1:D:242:ASN:HB2  | 2.23                     | 0.57              |
| 1:B:86:ARG:NH1   | 1:B:86:ARG:HG2   | 2.17                     | 0.57              |
| 1:A:545:PHE:C    | 1:A:546:LEU:HD23 | 2.24                     | 0.57              |
| 1:C:488:ARG:NH1  | 1:C:510:ARG:HB2  | 2.13                     | 0.57              |
| 1:C:499:SER:O    | 1:C:501:GLN:N    | 2.37                     | 0.57              |
| 1:D:88:THR:HG22  | 1:D:401:CYS:HA   | 1.87                     | 0.57              |
| 1:B:450:ASP:O    | 1:B:454:VAL:HG23 | 2.05                     | 0.57              |
| 1:D:188:ASP:O    | 1:D:189:PRO:C    | 2.43                     | 0.57              |
| 1:B:339:ASP:O    | 1:B:343:GLU:HG2  | 2.04                     | 0.57              |
| 1:A:322:ARG:NH2  | 1:A:325:GLU:OE2  | 2.33                     | 0.57              |
| 1:C:151:VAL:O    | 1:C:504:ARG:CD   | 2.51                     | 0.57              |
| 1:C:73:LEU:C     | 1:C:75:LEU:H     | 2.08                     | 0.57              |
| 1:A:87:SER:HB2   | 1:A:511:GLY:N    | 2.20                     | 0.57              |
| 1:B:204:TYR:CE1  | 1:B:261:LEU:HD13 | 2.40                     | 0.57              |
| 1:A:388:THR:HG22 | 1:A:389:SER:N    | 2.19                     | 0.57              |
| 1:A:479:ARG:O    | 1:A:482:GLN:HB3  | 2.05                     | 0.57              |
| 1:B:161:GLU:C    | 1:B:162:ILE:HG13 | 2.24                     | 0.57              |
| 1:B:85:ALA:HB2   | 1:B:545:PHE:CE2  | 2.40                     | 0.56              |
| 1:D:565:THR:O    | 1:D:566:ASN:HB3  | 2.04                     | 0.56              |
| 1:B:81:GLU:HA    | 1:B:81:GLU:OE1   | 2.03                     | 0.56              |
| 1:D:535:PHE:O    | 1:D:539:SER:OG   | 2.22                     | 0.56              |
| 1:C:337:ARG:HD3  | 1:C:370:ALA:O    | 2.06                     | 0.56              |
| 1:C:210:VAL:O    | 1:C:212:PRO:HD3  | 2.06                     | 0.56              |
| 1:B:475:THR:HA   | 2:B:1574:FBP:H61 | 1.86                     | 0.56              |
| 1:D:393:ASN:O    | 1:D:394:ALA:C    | 2.39                     | 0.56              |
| 1:C:458:GLY:O    | 1:C:459:ALA:C    | 2.41                     | 0.56              |
| 1:A:168:GLN:HB2  | 1:A:195:GLY:O    | 2.05                     | 0.56              |
| 1:A:349:VAL:O    | 1:A:352:ALA:N    | 2.38                     | 0.56              |
| 1:A:194:ARG:HH11 | 1:A:194:ARG:CB   | 2.18                     | 0.56              |
| 1:A:437:LEU:C    | 1:A:437:LEU:HD12 | 2.24                     | 0.56              |
| 1:C:337:ARG:HH22 | 1:C:390:ASP:CG   | 2.08                     | 0.56              |
| 1:C:502:ALA:O    | 1:C:504:ARG:N    | 2.39                     | 0.56              |
| 1:A:210:VAL:HG12 | 1:A:210:VAL:O    | 2.05                     | 0.56              |
| 1:C:174:GLU:OE1  | 1:C:245:VAL:CG1  | 2.54                     | 0.56              |
| 1:D:134:VAL:O    | 1:D:138:VAL:HG23 | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:61:LEU:O     | 1:B:65:MET:HG2   | 2.05                     | 0.56              |
| 1:D:488:ARG:NH1  | 1:D:510:ARG:HB3  | 2.20                     | 0.56              |
| 1:A:74:CYS:SG    | 1:C:359:ARG:HG3  | 2.45                     | 0.56              |
| 1:C:89:SER:HB2   | 1:C:401:CYS:SG   | 2.46                     | 0.56              |
| 1:D:339:ASP:O    | 1:D:343:GLU:HG2  | 2.05                     | 0.56              |
| 1:B:66:ALA:HB1   | 1:B:71:GLU:HG2   | 1.86                     | 0.56              |
| 1:A:190:ALA:HB3  | 1:A:191:PHE:CD1  | 2.41                     | 0.56              |
| 1:C:322:ARG:HH21 | 1:C:325:GLU:CD   | 2.09                     | 0.55              |
| 1:A:478:GLY:O    | 1:A:479:ARG:C    | 2.44                     | 0.55              |
| 1:B:367:VAL:H    | 1:B:400:ASP:HB2  | 1.70                     | 0.55              |
| 1:A:228:VAL:CG1  | 1:A:228:VAL:O    | 2.50                     | 0.55              |
| 1:A:429:GLU:HA   | 1:A:432:VAL:HG23 | 1.88                     | 0.55              |
| 1:D:176:GLU:C    | 1:D:177:LEU:HD23 | 2.27                     | 0.55              |
| 1:D:499:SER:O    | 1:D:500:ALA:C    | 2.45                     | 0.55              |
| 1:A:434:HIS:O    | 1:A:437:LEU:N    | 2.40                     | 0.55              |
| 1:A:337:ARG:HB3  | 1:C:385:ARG:HG3  | 1.87                     | 0.55              |
| 1:D:196:ASN:N    | 1:D:199:THR:O    | 2.37                     | 0.55              |
| 1:D:545:PHE:CB   | 1:D:546:LEU:HD23 | 2.37                     | 0.55              |
| 1:A:347:GLU:H    | 1:A:347:GLU:CD   | 2.10                     | 0.55              |
| 1:B:87:SER:HB2   | 1:B:511:GLY:N    | 2.21                     | 0.55              |
| 1:A:223:LEU:HD22 | 1:C:380:LYS:NZ   | 2.22                     | 0.55              |
| 1:C:192:ARG:HG3  | 1:C:201:TRP:CZ2  | 2.41                     | 0.55              |
| 1:B:420:MET:O    | 1:B:422:HIS:N    | 2.40                     | 0.55              |
| 1:B:488:ARG:C    | 1:B:489:PRO:O    | 2.44                     | 0.55              |
| 1:B:545:PHE:HB2  | 1:B:546:LEU:HD23 | 1.89                     | 0.55              |
| 1:A:267:GLN:O    | 1:A:270:ARG:N    | 2.40                     | 0.55              |
| 1:D:108:ILE:HD13 | 1:D:151:VAL:HG21 | 1.88                     | 0.55              |
| 1:B:452:THR:HG23 | 1:B:565:THR:HB   | 1.89                     | 0.55              |
| 1:A:499:SER:O    | 1:A:501:GLN:N    | 2.40                     | 0.55              |
| 1:B:225:SER:OG   | 1:B:241:GLU:HB3  | 2.07                     | 0.54              |
| 1:D:457:ILE:CG2  | 1:D:458:GLY:N    | 2.70                     | 0.54              |
| 1:A:459:ALA:O    | 1:A:462:ALA:HB3  | 2.07                     | 0.54              |
| 1:D:451:PRO:O    | 1:D:455:THR:OG1  | 2.25                     | 0.54              |
| 1:D:488:ARG:C    | 1:D:489:PRO:O    | 2.43                     | 0.54              |
| 1:D:402:ILE:HG13 | 1:D:421:GLN:HE22 | 1.68                     | 0.54              |
| 1:C:371:THR:HG22 | 1:C:372:GLN:HG3  | 1.88                     | 0.54              |
| 1:A:420:MET:O    | 1:A:421:GLN:C    | 2.43                     | 0.54              |
| 1:A:451:PRO:O    | 1:A:455:THR:OG1  | 2.24                     | 0.54              |
| 1:A:385:ARG:HE   | 1:C:341:GLY:HA3  | 1.72                     | 0.54              |
| 1:C:539:SER:O    | 1:C:543:ARG:HG3  | 2.08                     | 0.54              |
| 1:B:474:LEU:HD22 | 1:B:556:THR:HG22 | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:69:PHE:O     | 1:B:72:HIS:HB3   | 2.08                     | 0.54              |
| 1:B:545:PHE:CB   | 1:B:546:LEU:HD23 | 2.38                     | 0.54              |
| 1:A:514:PRO:O    | 1:A:515:LEU:HD23 | 2.08                     | 0.54              |
| 1:D:172:GLU:CD   | 1:D:172:GLU:N    | 2.61                     | 0.54              |
| 1:D:349:VAL:O    | 1:D:351:LEU:N    | 2.41                     | 0.54              |
| 1:D:352:ALA:HB1  | 1:D:356:MET:HE2  | 1.88                     | 0.54              |
| 1:A:157:THR:HG22 | 1:A:286:SER:N    | 2.17                     | 0.54              |
| 1:A:488:ARG:C    | 1:A:489:PRO:O    | 2.43                     | 0.54              |
| 1:C:499:SER:O    | 1:C:500:ALA:C    | 2.46                     | 0.54              |
| 1:B:479:ARG:O    | 1:B:482:GLN:HB3  | 2.08                     | 0.54              |
| 1:A:378:ILE:HD11 | 1:A:406:GLY:HA3  | 1.90                     | 0.54              |
| 1:D:73:LEU:O     | 1:D:74:CYS:C     | 2.46                     | 0.54              |
| 1:A:219:ILE:CG2  | 1:A:246:LEU:CD1  | 2.86                     | 0.54              |
| 1:A:438:PHE:O    | 1:A:439:GLU:C    | 2.47                     | 0.54              |
| 1:B:545:PHE:C    | 1:B:546:LEU:HD23 | 2.28                     | 0.54              |
| 1:B:320:VAL:HG11 | 1:D:78:ILE:HD13  | 1.88                     | 0.54              |
| 1:C:204:TYR:CE1  | 1:C:261:LEU:HD13 | 2.43                     | 0.54              |
| 1:A:367:VAL:O    | 1:A:367:VAL:HG13 | 2.08                     | 0.53              |
| 1:C:204:TYR:OH   | 1:C:260:ASP:OD1  | 2.19                     | 0.53              |
| 1:D:216:ARG:HG2  | 1:D:218:TYR:CE1  | 2.43                     | 0.53              |
| 1:C:402:ILE:HG13 | 1:C:402:ILE:O    | 2.07                     | 0.53              |
| 1:A:458:GLY:O    | 1:A:459:ALA:C    | 2.44                     | 0.53              |
| 1:D:429:GLU:HA   | 1:D:432:VAL:HG23 | 1.89                     | 0.53              |
| 1:B:420:MET:O    | 1:B:423:ALA:N    | 2.41                     | 0.53              |
| 1:B:488:ARG:HH12 | 1:B:510:ARG:HB2  | 1.74                     | 0.53              |
| 1:D:96:PRO:HD2   | 1:D:409:ALA:O    | 2.09                     | 0.53              |
| 1:A:525:TRP:NE1  | 1:A:560:PRO:HG3  | 2.23                     | 0.53              |
| 1:C:522:GLU:CD   | 1:C:531:ARG:HE   | 2.12                     | 0.53              |
| 1:D:175:VAL:HG12 | 1:D:177:LEU:CD2  | 2.38                     | 0.53              |
| 1:C:405:SER:O    | 1:C:406:GLY:C    | 2.47                     | 0.53              |
| 1:C:174:GLU:OE1  | 1:C:245:VAL:HG11 | 2.09                     | 0.53              |
| 1:A:339:ASP:O    | 1:A:343:GLU:HG2  | 2.08                     | 0.53              |
| 1:A:547:ARG:HH11 | 1:A:547:ARG:HB3  | 1.73                     | 0.53              |
| 1:A:535:PHE:O    | 1:A:539:SER:OG   | 2.26                     | 0.53              |
| 1:A:89:SER:O     | 1:A:401:CYS:HB3  | 2.09                     | 0.53              |
| 1:B:405:SER:O    | 1:B:406:GLY:C    | 2.46                     | 0.53              |
| 1:B:162:ILE:HG23 | 1:B:204:TYR:HB2  | 1.91                     | 0.53              |
| 1:C:73:LEU:C     | 1:C:75:LEU:N     | 2.60                     | 0.53              |
| 1:B:87:SER:HB2   | 1:B:511:GLY:CA   | 2.39                     | 0.53              |
| 1:A:112:MET:HG2  | 1:A:113:ASN:N    | 2.24                     | 0.53              |
| 1:D:441:LEU:O    | 1:D:444:ALA:N    | 2.41                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:118:ASN:OD1  | 1:A:120:SER:HB2  | 2.09                     | 0.53              |
| 1:D:283:VAL:HG23 | 1:D:308:ILE:CG2  | 2.38                     | 0.53              |
| 1:B:88:THR:OG1   | 1:B:429:GLU:OE2  | 2.16                     | 0.53              |
| 1:A:450:ASP:O    | 1:A:454:VAL:HG23 | 2.09                     | 0.53              |
| 1:C:146:LEU:HD23 | 1:C:535:PHE:CE1  | 2.43                     | 0.53              |
| 1:D:258:GLN:N    | 1:D:258:GLN:HE21 | 2.07                     | 0.53              |
| 1:C:204:TYR:O    | 1:C:207:ILE:HG22 | 2.09                     | 0.53              |
| 1:D:164:THR:O    | 1:D:249:ARG:HA   | 2.10                     | 0.53              |
| 1:B:336:ALA:HB1  | 3:B:1575:PGA:C2  | 2.39                     | 0.52              |
| 1:A:151:VAL:O    | 1:A:504:ARG:HD2  | 2.10                     | 0.52              |
| 1:A:438:PHE:CZ   | 1:A:442:ARG:HD3  | 2.44                     | 0.52              |
| 1:C:488:ARG:HH11 | 1:C:510:ARG:HB3  | 1.71                     | 0.52              |
| 1:C:513:PHE:CD1  | 1:C:513:PHE:N    | 2.75                     | 0.52              |
| 1:C:352:ALA:HB1  | 1:C:356:MET:HE2  | 1.89                     | 0.52              |
| 1:A:123:SER:HB2  | 1:A:125:GLU:OE1  | 2.09                     | 0.52              |
| 1:B:513:PHE:CD1  | 1:B:513:PHE:N    | 2.77                     | 0.52              |
| 1:B:283:VAL:HG23 | 1:B:308:ILE:CG2  | 2.38                     | 0.52              |
| 1:A:525:TRP:CE2  | 1:A:560:PRO:HG3  | 2.45                     | 0.52              |
| 1:C:384:THR:HG1  | 1:C:387:GLU:HG3  | 1.73                     | 0.52              |
| 1:C:488:ARG:NH1  | 1:C:510:ARG:CD   | 2.70                     | 0.52              |
| 1:A:487:TYR:O    | 1:A:488:ARG:CB   | 2.51                     | 0.52              |
| 1:A:423:ALA:HB1  | 1:C:347:GLU:HG2  | 1.90                     | 0.52              |
| 1:B:488:ARG:CZ   | 1:B:510:ARG:HD3  | 2.39                     | 0.52              |
| 1:C:449:ARG:HG3  | 1:D:551:LEU:HD12 | 1.92                     | 0.52              |
| 1:A:525:TRP:CD1  | 1:A:560:PRO:HG3  | 2.44                     | 0.52              |
| 1:C:313:LYS:HE3  | 3:C:1575:PGA:O1P | 2.09                     | 0.52              |
| 1:D:402:ILE:HG12 | 1:D:402:ILE:O    | 2.08                     | 0.52              |
| 1:B:347:GLU:CD   | 1:B:347:GLU:H    | 2.11                     | 0.52              |
| 1:A:320:VAL:HG11 | 1:C:78:ILE:HD13  | 1.92                     | 0.52              |
| 1:C:77:ASP:HB3   | 1:C:80:SER:HB2   | 1.92                     | 0.52              |
| 1:B:384:THR:OG1  | 1:B:387:GLU:HG3  | 2.09                     | 0.52              |
| 1:D:69:PHE:O     | 1:D:72:HIS:HB3   | 2.08                     | 0.52              |
| 1:C:155:LEU:HD23 | 1:C:155:LEU:C    | 2.30                     | 0.52              |
| 1:C:379:THR:HG22 | 1:C:379:THR:O    | 2.10                     | 0.52              |
| 1:A:162:ILE:O    | 1:A:252:VAL:HB   | 2.10                     | 0.52              |
| 1:C:86:ARG:HB3   | 1:C:426:ARG:HG2  | 1.91                     | 0.51              |
| 1:B:77:ASP:HB3   | 1:B:80:SER:HB2   | 1.92                     | 0.51              |
| 1:C:391:VAL:CG1  | 1:C:424:ILE:HG21 | 2.39                     | 0.51              |
| 1:D:370:ALA:O    | 1:D:371:THR:HB   | 2.10                     | 0.51              |
| 1:B:336:ALA:HB1  | 3:B:1575:PGA:H22 | 1.93                     | 0.51              |
| 1:A:211:VAL:HG21 | 1:A:217:ILE:HD11 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:138:VAL:HG12 | 1:C:139:GLU:OE2  | 2.10                     | 0.51              |
| 1:A:364:GLY:HA2  | 1:A:486:TRP:CD1  | 2.45                     | 0.51              |
| 1:D:384:THR:OG1  | 1:D:387:GLU:HG3  | 2.10                     | 0.51              |
| 1:B:163:ARG:HH11 | 1:B:250:LYS:HA   | 1.72                     | 0.51              |
| 1:B:87:SER:CB    | 1:B:511:GLY:HA2  | 2.40                     | 0.51              |
| 1:C:163:ARG:HA   | 1:C:250:LYS:O    | 2.09                     | 0.51              |
| 1:A:219:ILE:HG21 | 1:A:246:LEU:CD1  | 2.39                     | 0.51              |
| 1:A:219:ILE:HB   | 1:A:224:ILE:HG22 | 1.92                     | 0.51              |
| 1:D:225:SER:HB3  | 1:D:242:ASN:CB   | 2.27                     | 0.51              |
| 1:C:441:LEU:O    | 1:C:443:ARG:N    | 2.42                     | 0.51              |
| 1:B:86:ARG:NH1   | 1:B:422:HIS:ND1  | 2.59                     | 0.51              |
| 1:C:457:ILE:HG23 | 1:C:458:GLY:N    | 2.25                     | 0.51              |
| 1:C:450:ASP:O    | 1:C:454:VAL:HG23 | 2.11                     | 0.51              |
| 1:B:433:TYR:O    | 1:B:434:HIS:C    | 2.47                     | 0.51              |
| 1:D:322:ARG:HH21 | 1:D:325:GLU:CD   | 2.13                     | 0.51              |
| 1:B:427:GLU:O    | 1:B:428:ALA:C    | 2.46                     | 0.51              |
| 1:A:565:THR:O    | 1:A:566:ASN:HB3  | 2.11                     | 0.51              |
| 1:A:141:PHE:C    | 1:A:143:GLY:H    | 2.12                     | 0.51              |
| 1:A:167:LEU:CD1  | 1:A:168:GLN:H    | 2.01                     | 0.51              |
| 1:C:391:VAL:HG12 | 1:C:424:ILE:CG2  | 2.40                     | 0.51              |
| 1:C:406:GLY:O    | 1:C:407:GLU:C    | 2.45                     | 0.51              |
| 1:C:133:ASN:O    | 1:C:134:VAL:C    | 2.47                     | 0.51              |
| 1:A:100:SER:O    | 1:A:104:LEU:HD22 | 2.10                     | 0.51              |
| 1:B:327:LEU:O    | 1:B:327:LEU:HD22 | 2.11                     | 0.51              |
| 1:A:202:VAL:CG1  | 1:A:202:VAL:O    | 2.58                     | 0.51              |
| 1:C:158:LYS:HG2  | 1:C:161:GLU:HG3  | 1.93                     | 0.51              |
| 1:D:151:VAL:O    | 1:D:504:ARG:HD3  | 2.10                     | 0.51              |
| 1:D:269:VAL:O    | 1:D:273:ARG:HG2  | 2.11                     | 0.51              |
| 1:A:175:VAL:HG13 | 1:A:176:GLU:H    | 1.76                     | 0.51              |
| 1:C:73:LEU:O     | 1:C:74:CYS:C     | 2.50                     | 0.51              |
| 1:B:155:LEU:O    | 1:B:155:LEU:HD23 | 2.10                     | 0.51              |
| 1:B:83:VAL:O     | 1:B:83:VAL:HG12  | 2.11                     | 0.51              |
| 1:A:404:LEU:HD11 | 1:A:421:GLN:HG3  | 1.92                     | 0.50              |
| 1:B:458:GLY:O    | 1:B:459:ALA:C    | 2.48                     | 0.50              |
| 1:D:538:GLU:O    | 1:D:539:SER:C    | 2.50                     | 0.50              |
| 1:D:367:VAL:O    | 1:D:400:ASP:N    | 2.44                     | 0.50              |
| 1:A:532:ARG:O    | 1:A:535:PHE:HB3  | 2.11                     | 0.50              |
| 1:B:557:GLY:HA3  | 2:B:1574:FBP:O3  | 2.11                     | 0.50              |
| 1:B:499:SER:O    | 1:B:501:GLN:N    | 2.44                     | 0.50              |
| 1:A:379:THR:HG22 | 1:A:380:LYS:HG3  | 1.94                     | 0.50              |
| 1:D:522:GLU:CD   | 1:D:531:ARG:HE   | 2.15                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:GLU:O    | 1:A:322:ARG:HG3  | 2.11                     | 0.50              |
| 1:C:347:GLU:H    | 1:C:347:GLU:CD   | 2.15                     | 0.50              |
| 1:C:108:ILE:HD13 | 1:C:151:VAL:HG21 | 1.94                     | 0.50              |
| 1:D:77:ASP:HB3   | 1:D:80:SER:HB2   | 1.93                     | 0.50              |
| 1:A:240:VAL:O    | 1:A:240:VAL:HG12 | 2.11                     | 0.50              |
| 1:C:438:PHE:CZ   | 1:C:442:ARG:HD3  | 2.47                     | 0.50              |
| 1:C:83:VAL:O     | 1:C:83:VAL:CG1   | 2.60                     | 0.50              |
| 1:B:217:ILE:N    | 1:B:226:LEU:O    | 2.44                     | 0.50              |
| 1:B:108:ILE:HD13 | 1:B:151:VAL:HG21 | 1.94                     | 0.50              |
| 1:A:350:PHE:CZ   | 1:C:428:ALA:HA   | 2.47                     | 0.50              |
| 1:D:441:LEU:O    | 1:D:443:ARG:N    | 2.45                     | 0.50              |
| 1:D:66:ALA:CB    | 1:D:71:GLU:HG2   | 2.42                     | 0.50              |
| 1:B:349:VAL:O    | 1:B:352:ALA:N    | 2.45                     | 0.50              |
| 1:A:557:GLY:HA3  | 2:A:1574:FBP:O3  | 2.11                     | 0.50              |
| 1:C:177:LEU:HD11 | 1:C:246:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:561:GLY:O    | 2:A:1574:FBP:O4  | 2.23                     | 0.50              |
| 1:C:471:ILE:HD13 | 1:C:484:LEU:HD22 | 1.93                     | 0.50              |
| 1:B:141:PHE:C    | 1:B:143:GLY:N    | 2.64                     | 0.50              |
| 1:C:226:LEU:CD2  | 1:C:240:VAL:HG22 | 2.41                     | 0.50              |
| 1:C:423:ALA:O    | 1:C:424:ILE:C    | 2.50                     | 0.50              |
| 1:A:146:LEU:HB3  | 1:A:542:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:387:GLU:O    | 1:A:388:THR:C    | 2.47                     | 0.50              |
| 1:B:407:GLU:OE1  | 1:B:407:GLU:N    | 2.27                     | 0.50              |
| 1:C:474:LEU:HD22 | 1:C:556:THR:HG22 | 1.94                     | 0.50              |
| 1:D:373:MET:O    | 1:D:374:LEU:HD12 | 2.12                     | 0.50              |
| 1:C:433:TYR:O    | 1:C:435:ARG:N    | 2.45                     | 0.49              |
| 1:B:86:ARG:HG3   | 1:B:86:ARG:O     | 2.05                     | 0.49              |
| 1:D:174:GLU:OE2  | 1:D:245:VAL:CG1  | 2.54                     | 0.49              |
| 1:B:437:LEU:C    | 1:B:437:LEU:HD12 | 2.32                     | 0.49              |
| 1:A:522:GLU:CD   | 1:A:531:ARG:HE   | 2.16                     | 0.49              |
| 1:C:227:VAL:O    | 1:C:238:THR:HB   | 2.13                     | 0.49              |
| 1:C:219:ILE:HB   | 1:C:224:ILE:CG2  | 2.43                     | 0.49              |
| 1:C:58:GLN:O     | 1:C:60:GLN:N     | 2.45                     | 0.49              |
| 1:B:398:GLY:O    | 1:B:399:ALA:C    | 2.50                     | 0.49              |
| 1:D:229:GLN:CG   | 1:D:237:VAL:O    | 2.58                     | 0.49              |
| 1:C:395:VAL:HG11 | 1:C:429:GLU:HG3  | 1.94                     | 0.49              |
| 1:C:196:ASN:OD1  | 1:C:199:THR:HB   | 2.12                     | 0.49              |
| 1:A:179:LYS:NZ   | 1:A:179:LYS:CD   | 2.76                     | 0.49              |
| 1:C:434:HIS:HA   | 1:C:437:LEU:HB3  | 1.93                     | 0.49              |
| 1:C:193:THR:CG2  | 1:C:193:THR:O    | 2.60                     | 0.49              |
| 1:D:185:VAL:HG22 | 1:D:200:VAL:HG23 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:THR:HG22  | 1:A:401:CYS:HA   | 1.93                     | 0.49              |
| 1:C:474:LEU:CD2  | 1:C:529:VAL:HG13 | 2.42                     | 0.49              |
| 1:B:134:VAL:O    | 1:B:138:VAL:HG23 | 2.12                     | 0.49              |
| 1:D:196:ASN:C    | 1:D:198:ASN:N    | 2.63                     | 0.49              |
| 1:A:266:GLU:O    | 1:A:269:VAL:HB   | 2.12                     | 0.49              |
| 1:C:525:TRP:NE1  | 1:C:560:PRO:HG3  | 2.27                     | 0.49              |
| 1:A:402:ILE:CG1  | 1:A:402:ILE:O    | 2.60                     | 0.49              |
| 1:B:434:HIS:HA   | 1:B:437:LEU:HB3  | 1.95                     | 0.49              |
| 1:A:82:PRO:O     | 1:A:83:VAL:HG23  | 2.12                     | 0.49              |
| 1:D:474:LEU:HD21 | 1:D:529:VAL:HG13 | 1.94                     | 0.49              |
| 1:B:561:GLY:O    | 2:B:1574:FBP:O4  | 2.15                     | 0.49              |
| 1:B:391:VAL:O    | 1:B:392:ALA:C    | 2.49                     | 0.49              |
| 1:C:337:ARG:NH2  | 1:C:390:ASP:OD2  | 2.38                     | 0.49              |
| 1:B:434:HIS:O    | 1:B:435:ARG:C    | 2.51                     | 0.49              |
| 1:C:533:VAL:HG12 | 1:C:534:GLN:N    | 2.28                     | 0.49              |
| 1:C:85:ALA:CB    | 1:C:513:PHE:CE2  | 2.95                     | 0.48              |
| 1:B:87:SER:HB3   | 1:B:511:GLY:HA2  | 1.95                     | 0.48              |
| 1:C:175:VAL:HG12 | 1:C:176:GLU:N    | 2.28                     | 0.48              |
| 1:A:219:ILE:O    | 1:A:220:ASP:O    | 2.31                     | 0.48              |
| 1:D:66:ALA:HB1   | 1:D:71:GLU:CG    | 2.43                     | 0.48              |
| 1:C:174:GLU:CD   | 1:C:245:VAL:CG1  | 2.81                     | 0.48              |
| 1:A:352:ALA:HB1  | 1:A:356:MET:CE   | 2.42                     | 0.48              |
| 1:C:217:ILE:HD13 | 1:C:254:LEU:CD2  | 2.43                     | 0.48              |
| 1:C:141:PHE:C    | 1:C:143:GLY:N    | 2.66                     | 0.48              |
| 1:B:104:LEU:O    | 1:B:105:LYS:C    | 2.51                     | 0.48              |
| 1:A:348:LYS:HZ3  | 1:C:427:GLU:CD   | 2.16                     | 0.48              |
| 1:C:416:GLU:H    | 1:C:416:GLU:CD   | 2.16                     | 0.48              |
| 1:C:182:GLN:NE2  | 1:C:182:GLN:HA   | 2.24                     | 0.48              |
| 1:A:255:PRO:C    | 1:A:257:ALA:N    | 2.67                     | 0.48              |
| 1:C:91:ILE:HG12  | 1:C:114:ILE:HB   | 1.94                     | 0.48              |
| 1:B:391:VAL:HB   | 1:B:424:ILE:HG21 | 1.96                     | 0.48              |
| 1:C:545:PHE:HB2  | 1:C:546:LEU:HD23 | 1.96                     | 0.48              |
| 1:D:73:LEU:C     | 1:D:75:LEU:H     | 2.16                     | 0.48              |
| 1:A:283:VAL:HG23 | 1:A:308:ILE:CG2  | 2.43                     | 0.48              |
| 1:C:217:ILE:N    | 1:C:226:LEU:O    | 2.45                     | 0.48              |
| 1:A:559:ARG:HD2  | 1:A:564:TYR:CD1  | 2.48                     | 0.48              |
| 1:C:441:LEU:O    | 1:C:444:ALA:N    | 2.47                     | 0.48              |
| 1:D:438:PHE:CZ   | 1:D:442:ARG:HD3  | 2.48                     | 0.48              |
| 1:C:361:ASN:HD21 | 1:C:488:ARG:HH21 | 1.62                     | 0.48              |
| 1:C:225:SER:CB   | 1:C:242:ASN:HB2  | 2.36                     | 0.48              |
| 1:A:367:VAL:CG1  | 1:A:367:VAL:O    | 2.61                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:VAL:CG1  | 1:A:176:GLU:H    | 2.23                     | 0.48              |
| 1:D:196:ASN:C    | 1:D:198:ASN:H    | 2.17                     | 0.48              |
| 1:D:330:SER:O    | 1:D:365:LYS:NZ   | 2.30                     | 0.48              |
| 1:A:174:GLU:CB   | 1:A:245:VAL:CG1  | 2.92                     | 0.48              |
| 1:A:434:HIS:O    | 1:A:437:LEU:HB3  | 2.13                     | 0.48              |
| 1:C:81:GLU:OE1   | 1:C:81:GLU:CA    | 2.60                     | 0.48              |
| 1:D:226:LEU:HD23 | 1:D:240:VAL:HA   | 1.96                     | 0.48              |
| 1:C:104:LEU:O    | 1:C:105:LYS:C    | 2.52                     | 0.48              |
| 1:D:73:LEU:C     | 1:D:75:LEU:N     | 2.64                     | 0.48              |
| 1:C:456:ALA:O    | 1:C:457:ILE:C    | 2.52                     | 0.48              |
| 1:A:281:ASP:C    | 1:A:282:ILE:HG13 | 2.35                     | 0.48              |
| 1:A:420:MET:CE   | 1:C:347:GLU:HG3  | 2.44                     | 0.47              |
| 1:C:475:THR:O    | 1:C:497:THR:HB   | 2.14                     | 0.47              |
| 1:D:434:HIS:O    | 1:D:435:ARG:C    | 2.53                     | 0.47              |
| 1:B:158:LYS:O    | 1:B:158:LYS:HG2  | 2.13                     | 0.47              |
| 1:B:565:THR:O    | 1:B:566:ASN:HB3  | 2.14                     | 0.47              |
| 1:B:133:ASN:O    | 1:B:134:VAL:C    | 2.49                     | 0.47              |
| 1:A:133:ASN:O    | 1:A:134:VAL:C    | 2.53                     | 0.47              |
| 1:A:194:ARG:HG2  | 1:A:194:ARG:HH11 | 1.79                     | 0.47              |
| 1:C:433:TYR:CG   | 1:C:433:TYR:O    | 2.67                     | 0.47              |
| 1:A:474:LEU:CD2  | 1:A:529:VAL:HG13 | 2.44                     | 0.47              |
| 1:C:267:GLN:O    | 1:C:268:ASP:C    | 2.51                     | 0.47              |
| 1:B:378:ILE:HD11 | 1:B:406:GLY:HA3  | 1.96                     | 0.47              |
| 1:B:102:GLU:O    | 1:B:105:LYS:HB2  | 2.14                     | 0.47              |
| 1:A:58:GLN:O     | 1:A:60:GLN:N     | 2.47                     | 0.47              |
| 1:A:405:SER:O    | 1:A:406:GLY:C    | 2.53                     | 0.47              |
| 1:C:474:LEU:HD21 | 1:C:529:VAL:HG13 | 1.95                     | 0.47              |
| 1:D:271:ASP:O    | 1:D:274:PHE:HB3  | 2.15                     | 0.47              |
| 1:D:310:ILE:N    | 1:D:331:ASP:OD2  | 2.35                     | 0.47              |
| 1:A:385:ARG:NE   | 1:C:341:GLY:HA3  | 2.29                     | 0.47              |
| 1:A:456:ALA:O    | 1:A:457:ILE:C    | 2.51                     | 0.47              |
| 1:A:141:PHE:C    | 1:A:143:GLY:N    | 2.67                     | 0.47              |
| 1:D:570:VAL:C    | 1:D:571:LEU:HD23 | 2.34                     | 0.47              |
| 1:D:474:LEU:N    | 1:D:474:LEU:CD1  | 2.78                     | 0.47              |
| 1:A:545:PHE:CB   | 1:A:546:LEU:HD23 | 2.44                     | 0.47              |
| 1:A:322:ARG:HH21 | 1:A:325:GLU:CD   | 2.18                     | 0.47              |
| 1:A:404:LEU:HA   | 1:A:404:LEU:HD23 | 1.59                     | 0.47              |
| 1:B:315:GLU:HG3  | 1:B:336:ALA:HB3  | 1.97                     | 0.47              |
| 1:C:88:THR:HG23  | 1:C:400:ASP:O    | 2.14                     | 0.47              |
| 1:D:434:HIS:O    | 1:D:437:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:499:SER:O    | 1:A:500:ALA:C    | 2.53                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:PHE:O    | 1:A:354:LYS:HG3  | 2.15                     | 0.47              |
| 1:C:525:TRP:CD1  | 1:C:560:PRO:HG3  | 2.48                     | 0.47              |
| 1:C:434:HIS:O    | 1:C:437:LEU:HB3  | 2.15                     | 0.47              |
| 1:D:557:GLY:HA3  | 2:D:1574:FBP:O3  | 2.14                     | 0.47              |
| 1:C:166:ILE:HA   | 1:C:248:SER:HB3  | 1.96                     | 0.47              |
| 1:C:331:ASP:O    | 1:C:366:PRO:HD2  | 2.14                     | 0.47              |
| 1:C:188:ASP:C    | 1:C:188:ASP:OD1  | 2.52                     | 0.47              |
| 1:B:551:LEU:HA   | 1:B:551:LEU:HD23 | 1.72                     | 0.47              |
| 1:C:416:GLU:O    | 1:C:417:ALA:C    | 2.50                     | 0.47              |
| 1:C:85:ALA:HB1   | 1:C:513:PHE:HE2  | 1.78                     | 0.47              |
| 1:A:182:GLN:HA   | 1:A:182:GLN:NE2  | 2.27                     | 0.47              |
| 1:A:551:LEU:HD23 | 1:A:551:LEU:HA   | 1.66                     | 0.47              |
| 1:D:218:TYR:HB3  | 1:D:222:GLY:HA2  | 1.97                     | 0.47              |
| 1:C:166:ILE:N    | 1:C:166:ILE:HD12 | 2.22                     | 0.47              |
| 1:C:228:VAL:HA   | 1:C:238:THR:HG22 | 1.97                     | 0.47              |
| 1:D:327:LEU:HD22 | 1:D:365:LYS:HD2  | 1.96                     | 0.47              |
| 1:B:322:ARG:NH2  | 1:B:325:GLU:OE2  | 2.45                     | 0.47              |
| 1:A:501:GLN:O    | 1:A:502:ALA:C    | 2.50                     | 0.47              |
| 1:B:134:VAL:HG12 | 1:B:135:ARG:N    | 2.28                     | 0.47              |
| 1:B:506:VAL:HG13 | 1:B:506:VAL:O    | 2.15                     | 0.47              |
| 1:B:420:MET:C    | 1:B:422:HIS:N    | 2.64                     | 0.46              |
| 1:A:313:LYS:HD2  | 1:A:334:MET:SD   | 2.56                     | 0.46              |
| 1:A:371:THR:OG1  | 3:A:1575:PGA:O2  | 2.25                     | 0.46              |
| 1:B:70:LEU:CD2   | 1:D:362:LEU:HD12 | 2.45                     | 0.46              |
| 1:D:500:ALA:HA   | 1:D:516:LEU:HD13 | 1.96                     | 0.46              |
| 1:C:86:ARG:CB    | 1:C:426:ARG:HG2  | 2.46                     | 0.46              |
| 1:A:474:LEU:HD21 | 1:A:529:VAL:HG13 | 1.96                     | 0.46              |
| 1:A:146:LEU:HD22 | 1:A:539:SER:HA   | 1.97                     | 0.46              |
| 1:B:155:LEU:C    | 1:B:155:LEU:CD2  | 2.82                     | 0.46              |
| 1:B:267:GLN:O    | 1:B:268:ASP:C    | 2.53                     | 0.46              |
| 1:B:297:VAL:CG1  | 1:B:310:ILE:HD13 | 2.46                     | 0.46              |
| 1:A:416:GLU:H    | 1:A:416:GLU:CD   | 2.15                     | 0.46              |
| 1:A:66:ALA:O     | 1:A:433:TYR:OH   | 2.25                     | 0.46              |
| 1:D:551:LEU:HA   | 1:D:551:LEU:HD23 | 1.64                     | 0.46              |
| 1:A:87:SER:HB2   | 1:A:511:GLY:CA   | 2.46                     | 0.46              |
| 1:B:478:GLY:O    | 1:B:479:ARG:C    | 2.53                     | 0.46              |
| 1:C:141:PHE:C    | 1:C:143:GLY:H    | 2.19                     | 0.46              |
| 1:C:67:ASP:HA    | 1:C:435:ARG:NH1  | 2.29                     | 0.46              |
| 1:A:350:PHE:HZ   | 1:C:428:ALA:HA   | 1.81                     | 0.46              |
| 1:B:102:GLU:OE1  | 1:B:105:LYS:HD2  | 2.16                     | 0.46              |
| 1:C:545:PHE:CB   | 1:C:546:LEU:HD23 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:566:ASN:OD1  | 1:B:567:ILE:HG13 | 2.16                     | 0.46              |
| 1:B:297:VAL:HG11 | 1:B:310:ILE:HD13 | 1.96                     | 0.46              |
| 1:A:70:LEU:HD21  | 1:C:362:LEU:HD12 | 1.98                     | 0.46              |
| 1:C:377:MET:HA   | 1:C:380:LYS:O    | 2.16                     | 0.46              |
| 1:A:433:TYR:O    | 1:A:434:HIS:C    | 2.54                     | 0.46              |
| 1:A:488:ARG:HH12 | 1:A:510:ARG:CB   | 2.29                     | 0.46              |
| 1:A:120:SER:HA   | 1:A:158:LYS:HG3  | 1.97                     | 0.46              |
| 1:D:258:GLN:O    | 1:D:258:GLN:CG   | 2.59                     | 0.46              |
| 1:B:321:LYS:HD3  | 1:B:321:LYS:HA   | 1.56                     | 0.46              |
| 1:A:209:ARG:NH1  | 1:A:210:VAL:HG21 | 2.31                     | 0.46              |
| 1:B:66:ALA:HB1   | 1:B:71:GLU:CG    | 2.45                     | 0.46              |
| 1:A:499:SER:O    | 1:A:502:ALA:N    | 2.48                     | 0.46              |
| 1:A:457:ILE:HG23 | 1:A:458:GLY:N    | 2.31                     | 0.46              |
| 1:B:60:GLN:HB2   | 1:B:430:ALA:O    | 2.16                     | 0.46              |
| 1:C:569:ARG:HG2  | 1:D:567:ILE:HG12 | 1.97                     | 0.46              |
| 1:D:175:VAL:CG1  | 1:D:197:ALA:HA   | 2.44                     | 0.46              |
| 1:B:502:ALA:O    | 1:B:504:ARG:N    | 2.49                     | 0.46              |
| 1:D:387:GLU:O    | 1:D:388:THR:C    | 2.54                     | 0.46              |
| 1:C:420:MET:O    | 1:C:421:GLN:C    | 2.51                     | 0.46              |
| 1:D:191:PHE:HA   | 1:D:194:ARG:HB2  | 1.98                     | 0.46              |
| 1:A:179:LYS:CG   | 1:A:179:LYS:HE2  | 2.45                     | 0.45              |
| 1:B:438:PHE:CZ   | 1:B:442:ARG:HD3  | 2.52                     | 0.45              |
| 1:B:250:LYS:O    | 1:B:251:GLY:C    | 2.52                     | 0.45              |
| 1:A:202:VAL:HG12 | 1:A:202:VAL:O    | 2.16                     | 0.45              |
| 1:C:322:ARG:C    | 1:C:326:ILE:HD12 | 2.37                     | 0.45              |
| 1:D:83:VAL:O     | 1:D:83:VAL:HG13  | 2.16                     | 0.45              |
| 1:C:340:LEU:O    | 1:C:344:ILE:HG12 | 2.16                     | 0.45              |
| 1:A:391:VAL:CG1  | 1:A:424:ILE:HG21 | 2.46                     | 0.45              |
| 1:A:73:LEU:O     | 1:A:75:LEU:N     | 2.49                     | 0.45              |
| 1:C:286:SER:HA   | 1:C:313:LYS:HE2  | 1.97                     | 0.45              |
| 1:A:174:GLU:HB3  | 1:A:245:VAL:CG1  | 2.46                     | 0.45              |
| 1:D:438:PHE:O    | 1:D:439:GLU:C    | 2.54                     | 0.45              |
| 1:B:241:GLU:HG2  | 1:B:241:GLU:O    | 2.16                     | 0.45              |
| 1:B:339:ASP:OD2  | 3:B:1575:PGA:O1  | 2.33                     | 0.45              |
| 1:A:465:LYS:HE3  | 1:B:448:SER:HB3  | 1.98                     | 0.45              |
| 1:C:301:LEU:HA   | 1:C:301:LEU:HD12 | 1.86                     | 0.45              |
| 1:A:337:ARG:HH22 | 1:A:390:ASP:CG   | 2.19                     | 0.45              |
| 1:A:484:LEU:O    | 1:A:489:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:68:THR:HB    | 1:C:440:GLU:OE2  | 2.17                     | 0.45              |
| 1:B:118:ASN:OD1  | 1:B:120:SER:HB2  | 2.16                     | 0.45              |
| 1:B:226:LEU:HD23 | 1:B:240:VAL:HA   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:457:ILE:HG12 | 1:B:461:GLU:HG3  | 1.98                     | 0.45              |
| 1:C:160:PRO:HD2  | 1:C:287:PHE:CD1  | 2.52                     | 0.45              |
| 1:C:434:HIS:O    | 1:C:435:ARG:C    | 2.54                     | 0.45              |
| 1:A:209:ARG:HD3  | 1:A:209:ARG:O    | 2.17                     | 0.45              |
| 1:D:202:VAL:HG12 | 1:D:204:TYR:H    | 1.81                     | 0.45              |
| 1:A:479:ARG:HG3  | 1:A:479:ARG:NH1  | 2.32                     | 0.45              |
| 1:B:362:LEU:HD12 | 1:D:70:LEU:CD2   | 2.46                     | 0.45              |
| 1:D:499:SER:O    | 1:D:502:ALA:N    | 2.50                     | 0.45              |
| 1:A:163:ARG:HB3  | 1:A:163:ARG:HH11 | 1.82                     | 0.45              |
| 1:D:474:LEU:CD2  | 1:D:529:VAL:HG13 | 2.47                     | 0.45              |
| 1:B:66:ALA:CB    | 1:B:71:GLU:HG2   | 2.47                     | 0.45              |
| 1:D:141:PHE:C    | 1:D:143:GLY:N    | 2.69                     | 0.45              |
| 1:C:559:ARG:HD2  | 1:C:564:TYR:CD1  | 2.52                     | 0.45              |
| 1:B:367:VAL:HG13 | 1:B:399:ALA:HA   | 1.99                     | 0.45              |
| 1:A:167:LEU:HD21 | 1:A:175:VAL:HB   | 1.99                     | 0.45              |
| 1:D:188:ASP:O    | 1:D:190:ALA:N    | 2.49                     | 0.45              |
| 1:D:95:GLY:O     | 1:D:96:PRO:C     | 2.55                     | 0.45              |
| 1:C:86:ARG:NH2   | 1:C:90:ILE:HD12  | 2.31                     | 0.45              |
| 1:B:160:PRO:HG3  | 1:B:263:GLY:HA2  | 1.99                     | 0.45              |
| 1:B:568:MET:CE   | 1:B:570:VAL:HG23 | 2.47                     | 0.45              |
| 1:B:498:ARG:HG2  | 1:B:517:TYR:O    | 2.16                     | 0.45              |
| 1:C:152:ALA:HA   | 1:C:504:ARG:HD2  | 1.99                     | 0.44              |
| 1:A:377:MET:HA   | 1:A:380:LYS:O    | 2.17                     | 0.44              |
| 1:C:219:ILE:HB   | 1:C:224:ILE:HB   | 1.99                     | 0.44              |
| 1:B:95:GLY:O     | 1:B:96:PRO:C     | 2.53                     | 0.44              |
| 1:B:97:ALA:O     | 1:B:103:ARG:HD3  | 2.17                     | 0.44              |
| 1:B:273:ARG:O    | 1:B:277:GLU:HG3  | 2.17                     | 0.44              |
| 1:D:321:LYS:HD3  | 1:D:321:LYS:HA   | 1.36                     | 0.44              |
| 1:A:119:PHE:O    | 1:A:158:LYS:HB2  | 2.16                     | 0.44              |
| 1:B:78:ILE:CD1   | 1:D:320:VAL:HG11 | 2.46                     | 0.44              |
| 1:C:261:LEU:HD12 | 1:C:261:LEU:HA   | 1.57                     | 0.44              |
| 1:D:488:ARG:NH1  | 1:D:510:ARG:CB   | 2.80                     | 0.44              |
| 1:B:474:LEU:HD21 | 1:B:529:VAL:HG13 | 1.99                     | 0.44              |
| 1:D:61:LEU:O     | 1:D:65:MET:HG2   | 2.18                     | 0.44              |
| 1:A:434:HIS:O    | 1:A:435:ARG:C    | 2.55                     | 0.44              |
| 1:C:97:ALA:O     | 1:C:103:ARG:HD3  | 2.16                     | 0.44              |
| 1:A:168:GLN:HE22 | 1:A:196:ASN:HB3  | 1.82                     | 0.44              |
| 1:C:478:GLY:O    | 1:C:479:ARG:C    | 2.56                     | 0.44              |
| 1:C:176:GLU:OE1  | 1:C:178:VAL:HG22 | 2.17                     | 0.44              |
| 1:C:86:ARG:NH1   | 1:C:422:HIS:ND1  | 2.63                     | 0.44              |
| 1:C:134:VAL:O    | 1:C:138:VAL:HG23 | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:391:VAL:CG1  | 1:C:424:ILE:CG2  | 2.95                     | 0.44              |
| 1:B:352:ALA:HB1  | 1:B:356:MET:HE2  | 1.99                     | 0.44              |
| 1:B:362:LEU:HD12 | 1:D:70:LEU:HD21  | 1.99                     | 0.44              |
| 1:A:188:ASP:C    | 1:A:190:ALA:N    | 2.71                     | 0.44              |
| 1:A:193:THR:C    | 1:A:195:GLY:H    | 2.21                     | 0.44              |
| 1:A:204:TYR:CD2  | 1:A:204:TYR:C    | 2.91                     | 0.44              |
| 1:C:566:ASN:OD1  | 1:C:567:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:566:ASN:OD1  | 1:A:567:ILE:HG13 | 2.18                     | 0.44              |
| 1:A:77:ASP:HB3   | 1:A:80:SER:HB2   | 1.99                     | 0.44              |
| 1:A:242:ASN:ND2  | 1:C:381:PRO:HB2  | 2.33                     | 0.44              |
| 1:C:191:PHE:O    | 1:C:194:ARG:N    | 2.46                     | 0.44              |
| 1:B:341:GLY:HA3  | 1:D:385:ARG:HE   | 1.83                     | 0.44              |
| 1:B:320:VAL:HG11 | 1:D:78:ILE:CD1   | 2.48                     | 0.44              |
| 1:D:181:SER:O    | 1:D:240:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:75:LEU:HA    | 1:B:75:LEU:HD23  | 1.83                     | 0.44              |
| 1:A:194:ARG:HG2  | 1:A:194:ARG:NH1  | 2.33                     | 0.44              |
| 1:A:404:LEU:HD22 | 1:A:407:GLU:HB2  | 1.99                     | 0.44              |
| 1:C:191:PHE:O    | 1:C:193:THR:N    | 2.51                     | 0.44              |
| 1:D:155:LEU:C    | 1:D:155:LEU:CD2  | 2.83                     | 0.44              |
| 1:C:213:VAL:HA   | 1:C:228:VAL:HG12 | 1.99                     | 0.44              |
| 1:B:123:SER:HB2  | 1:B:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:568:MET:HE1  | 1:A:570:VAL:HG23 | 1.98                     | 0.44              |
| 1:C:61:LEU:HA    | 1:C:61:LEU:HD12  | 1.75                     | 0.44              |
| 1:A:174:GLU:HB2  | 1:A:245:VAL:CG1  | 2.48                     | 0.44              |
| 1:D:370:ALA:O    | 1:D:371:THR:CB   | 2.66                     | 0.44              |
| 1:D:337:ARG:HH22 | 1:D:390:ASP:CG   | 2.21                     | 0.44              |
| 1:B:488:ARG:NH1  | 1:B:510:ARG:HB2  | 2.29                     | 0.44              |
| 1:D:501:GLN:O    | 1:D:502:ALA:C    | 2.54                     | 0.44              |
| 1:B:83:VAL:O     | 1:B:83:VAL:CG1   | 2.66                     | 0.44              |
| 1:D:568:MET:HE1  | 1:D:570:VAL:HG23 | 2.00                     | 0.44              |
| 1:A:191:PHE:CD1  | 1:A:191:PHE:N    | 2.86                     | 0.43              |
| 1:A:191:PHE:O    | 1:A:193:THR:N    | 2.51                     | 0.43              |
| 1:B:385:ARG:HG3  | 1:D:337:ARG:HB3  | 1.99                     | 0.43              |
| 1:C:475:THR:HA   | 2:C:1574:FBP:H61 | 2.00                     | 0.43              |
| 1:A:219:ILE:CG2  | 1:A:246:LEU:HD13 | 2.47                     | 0.43              |
| 1:C:167:LEU:HA   | 1:C:167:LEU:HD12 | 1.76                     | 0.43              |
| 1:A:108:ILE:HG12 | 1:A:112:MET:CE   | 2.48                     | 0.43              |
| 1:D:87:SER:HB2   | 1:D:511:GLY:N    | 2.33                     | 0.43              |
| 1:D:281:ASP:C    | 1:D:282:ILE:HG13 | 2.38                     | 0.43              |
| 1:C:545:PHE:C    | 1:C:546:LEU:HD23 | 2.38                     | 0.43              |
| 1:C:500:ALA:HA   | 1:C:516:LEU:HD13 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:66:ALA:HB1   | 1:C:71:GLU:CG    | 2.48                     | 0.43              |
| 1:D:178:VAL:HG12 | 1:D:179:LYS:O    | 2.17                     | 0.43              |
| 1:B:86:ARG:HB3   | 1:B:426:ARG:HG2  | 1.99                     | 0.43              |
| 1:A:155:LEU:C    | 1:A:155:LEU:CD2  | 2.76                     | 0.43              |
| 1:C:406:GLY:O    | 1:C:408:THR:N    | 2.50                     | 0.43              |
| 1:B:522:GLU:CD   | 1:B:531:ARG:HE   | 2.22                     | 0.43              |
| 1:A:301:LEU:HA   | 1:A:301:LEU:HD12 | 1.87                     | 0.43              |
| 1:C:101:VAL:O    | 1:C:101:VAL:HG12 | 2.17                     | 0.43              |
| 1:B:149:ARG:HE   | 1:B:149:ARG:HB2  | 1.67                     | 0.43              |
| 1:D:220:ASP:OD1  | 1:D:220:ASP:C    | 2.57                     | 0.43              |
| 1:B:379:THR:O    | 1:B:379:THR:HG22 | 2.18                     | 0.43              |
| 1:A:78:ILE:HD13  | 1:C:320:VAL:HG11 | 2.00                     | 0.43              |
| 1:D:488:ARG:CZ   | 1:D:510:ARG:HD3  | 2.49                     | 0.43              |
| 1:A:503:ALA:O    | 1:A:514:PRO:HG3  | 2.18                     | 0.43              |
| 1:B:377:MET:HA   | 1:B:380:LYS:O    | 2.18                     | 0.43              |
| 1:A:391:VAL:HG12 | 1:A:424:ILE:CG2  | 2.48                     | 0.43              |
| 1:B:273:ARG:HA   | 1:B:273:ARG:HD2  | 1.74                     | 0.43              |
| 1:C:61:LEU:N     | 1:C:62:PRO:CD    | 2.82                     | 0.43              |
| 1:B:379:THR:CG2  | 1:B:379:THR:O    | 2.65                     | 0.43              |
| 1:D:532:ARG:O    | 1:D:535:PHE:HB3  | 2.19                     | 0.43              |
| 1:B:488:ARG:HH12 | 1:B:510:ARG:CB   | 2.29                     | 0.43              |
| 1:B:125:GLU:N    | 1:B:125:GLU:CD   | 2.68                     | 0.43              |
| 1:A:125:GLU:N    | 1:A:125:GLU:CD   | 2.71                     | 0.43              |
| 1:B:61:LEU:HD12  | 1:B:61:LEU:HA    | 1.78                     | 0.43              |
| 1:C:480:SER:O    | 1:C:481:ALA:C    | 2.50                     | 0.43              |
| 1:C:391:VAL:HG12 | 1:C:424:ILE:HG21 | 1.98                     | 0.43              |
| 1:D:499:SER:C    | 1:D:501:GLN:N    | 2.72                     | 0.43              |
| 1:B:474:LEU:CD2  | 1:B:529:VAL:HG13 | 2.49                     | 0.43              |
| 1:C:533:VAL:O    | 1:C:536:GLY:N    | 2.52                     | 0.43              |
| 1:B:525:TRP:CE2  | 1:B:560:PRO:HG3  | 2.54                     | 0.43              |
| 1:D:234:GLU:C    | 1:D:234:GLU:OE1  | 2.57                     | 0.43              |
| 1:C:317:HIS:O    | 1:C:318:GLU:C    | 2.55                     | 0.43              |
| 1:B:87:SER:CB    | 1:B:511:GLY:CA   | 2.97                     | 0.43              |
| 1:D:450:ASP:O    | 1:D:454:VAL:HG23 | 2.19                     | 0.43              |
| 1:B:377:MET:O    | 1:B:378:ILE:C    | 2.54                     | 0.43              |
| 1:B:73:LEU:O     | 1:B:75:LEU:N     | 2.51                     | 0.43              |
| 1:A:384:THR:N    | 1:A:387:GLU:OE1  | 2.35                     | 0.43              |
| 1:C:452:THR:HG23 | 1:C:565:THR:HB   | 2.00                     | 0.43              |
| 1:B:85:ALA:HB1   | 1:B:513:PHE:CE2  | 2.53                     | 0.43              |
| 1:B:141:PHE:C    | 1:B:143:GLY:H    | 2.22                     | 0.43              |
| 1:A:60:GLN:HB2   | 1:A:430:ALA:O    | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:483:LEU:HA   | 1:A:483:LEU:HD23 | 1.78                     | 0.43              |
| 1:C:434:HIS:NE2  | 1:C:490:ARG:HB2  | 2.33                     | 0.43              |
| 1:B:151:VAL:O    | 1:B:504:ARG:HD3  | 2.18                     | 0.43              |
| 1:D:89:SER:HB2   | 1:D:401:CYS:SG   | 2.58                     | 0.43              |
| 1:A:410:LYS:HB2  | 1:A:410:LYS:HE3  | 1.72                     | 0.43              |
| 1:B:93:THR:OG1   | 1:B:116:ARG:NH1  | 2.44                     | 0.43              |
| 1:B:457:ILE:CG2  | 1:B:458:GLY:H    | 2.31                     | 0.43              |
| 1:B:89:SER:CB    | 1:B:401:CYS:HB3  | 2.45                     | 0.43              |
| 1:B:533:VAL:O    | 1:B:536:GLY:N    | 2.51                     | 0.43              |
| 1:C:167:LEU:O    | 1:C:169:GLY:N    | 2.52                     | 0.43              |
| 1:C:457:ILE:CG2  | 1:C:458:GLY:N    | 2.81                     | 0.43              |
| 1:B:514:PRO:O    | 1:B:515:LEU:HD23 | 2.19                     | 0.43              |
| 1:D:413:PHE:N    | 1:D:414:PRO:HD3  | 2.34                     | 0.43              |
| 1:A:545:PHE:HB2  | 1:A:546:LEU:HD23 | 1.99                     | 0.42              |
| 1:A:296:ALA:O    | 1:A:297:VAL:C    | 2.58                     | 0.42              |
| 1:D:163:ARG:HA   | 1:D:250:LYS:O    | 2.18                     | 0.42              |
| 1:B:322:ARG:C    | 1:B:326:ILE:HD12 | 2.38                     | 0.42              |
| 1:C:188:ASP:HA   | 1:C:189:PRO:HD3  | 1.93                     | 0.42              |
| 1:C:176:GLU:OE1  | 1:C:178:VAL:CG2  | 2.67                     | 0.42              |
| 1:B:406:GLY:O    | 1:B:407:GLU:C    | 2.57                     | 0.42              |
| 1:A:223:LEU:O    | 1:C:381:PRO:HG2  | 2.19                     | 0.42              |
| 1:A:210:VAL:O    | 1:A:210:VAL:CG1  | 2.67                     | 0.42              |
| 1:D:146:LEU:HD22 | 1:D:539:SER:HA   | 2.01                     | 0.42              |
| 1:C:502:ALA:O    | 1:C:503:ALA:C    | 2.57                     | 0.42              |
| 1:A:220:ASP:HB2  | 1:A:250:LYS:HB3  | 2.02                     | 0.42              |
| 1:D:393:ASN:C    | 1:D:395:VAL:N    | 2.71                     | 0.42              |
| 1:B:100:SER:O    | 1:B:104:LEU:HD22 | 2.18                     | 0.42              |
| 1:B:297:VAL:HG12 | 1:B:310:ILE:CD1  | 2.50                     | 0.42              |
| 1:B:570:VAL:C    | 1:B:571:LEU:HD23 | 2.40                     | 0.42              |
| 1:B:93:THR:HA    | 1:B:116:ARG:HB3  | 2.00                     | 0.42              |
| 1:A:329:VAL:O    | 1:A:329:VAL:HG12 | 2.19                     | 0.42              |
| 1:B:220:ASP:C    | 1:B:222:GLY:H    | 2.22                     | 0.42              |
| 1:A:188:ASP:HB3  | 1:A:191:PHE:HD1  | 1.85                     | 0.42              |
| 1:A:441:LEU:C    | 1:A:443:ARG:N    | 2.72                     | 0.42              |
| 1:B:227:VAL:C    | 1:B:238:THR:HB   | 2.39                     | 0.42              |
| 1:D:196:ASN:O    | 1:D:198:ASN:N    | 2.53                     | 0.42              |
| 1:A:568:MET:CE   | 1:A:570:VAL:HG23 | 2.49                     | 0.42              |
| 1:C:220:ASP:OD1  | 1:C:220:ASP:C    | 2.57                     | 0.42              |
| 1:B:285:ALA:O    | 1:B:313:LYS:HB2  | 2.20                     | 0.42              |
| 1:D:348:LYS:O    | 1:D:349:VAL:C    | 2.56                     | 0.42              |
| 1:A:120:SER:OG   | 1:A:161:GLU:OE2  | 2.30                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:229:GLN:O    | 1:C:230:LYS:HG2  | 2.20                     | 0.42              |
| 1:C:146:LEU:CD2  | 1:C:535:PHE:CE1  | 3.02                     | 0.42              |
| 1:B:502:ALA:C    | 1:B:504:ARG:N    | 2.73                     | 0.42              |
| 1:C:266:GLU:O    | 1:C:269:VAL:HB   | 2.19                     | 0.42              |
| 1:A:304:GLU:H    | 1:A:304:GLU:HG2  | 1.55                     | 0.42              |
| 1:C:329:VAL:O    | 1:C:329:VAL:HG12 | 2.19                     | 0.42              |
| 1:D:333:ILE:HD13 | 1:D:333:ILE:HA   | 1.92                     | 0.42              |
| 1:D:286:SER:HA   | 1:D:313:LYS:HE2  | 2.01                     | 0.42              |
| 1:C:184:LEU:O    | 1:C:199:THR:HA   | 2.19                     | 0.42              |
| 1:C:502:ALA:C    | 1:C:504:ARG:N    | 2.71                     | 0.42              |
| 1:D:525:TRP:O    | 1:D:526:ALA:C    | 2.58                     | 0.42              |
| 1:A:162:ILE:HB   | 1:A:252:VAL:HB   | 2.02                     | 0.42              |
| 1:B:336:ALA:CB   | 3:B:1575:PGA:H22 | 2.49                     | 0.42              |
| 1:A:261:LEU:HA   | 1:A:261:LEU:HD12 | 1.67                     | 0.42              |
| 1:C:466:CYS:O    | 1:C:467:CYS:HB2  | 2.18                     | 0.42              |
| 1:C:377:MET:C    | 1:C:379:THR:N    | 2.71                     | 0.42              |
| 1:B:423:ALA:O    | 1:B:424:ILE:C    | 2.58                     | 0.42              |
| 1:A:460:VAL:HG22 | 1:A:489:PRO:HG3  | 2.02                     | 0.42              |
| 1:D:402:ILE:O    | 1:D:402:ILE:CG1  | 2.68                     | 0.42              |
| 1:C:175:VAL:HG13 | 1:C:197:ALA:HA   | 1.99                     | 0.42              |
| 1:C:66:ALA:CB    | 1:C:71:GLU:HG2   | 2.48                     | 0.42              |
| 1:D:503:ALA:O    | 1:D:514:PRO:CB   | 2.68                     | 0.42              |
| 1:A:273:ARG:HD2  | 1:A:273:ARG:HA   | 1.74                     | 0.42              |
| 1:A:204:TYR:CG   | 1:A:204:TYR:O    | 2.68                     | 0.42              |
| 1:D:157:THR:HG22 | 1:D:286:SER:HB2  | 2.02                     | 0.42              |
| 1:D:416:GLU:H    | 1:D:416:GLU:CD   | 2.22                     | 0.42              |
| 1:C:393:ASN:O    | 1:C:394:ALA:C    | 2.56                     | 0.42              |
| 1:D:331:ASP:O    | 1:D:366:PRO:HD2  | 2.20                     | 0.41              |
| 1:C:488:ARG:C    | 1:C:489:PRO:O    | 2.55                     | 0.41              |
| 1:B:86:ARG:CB    | 1:B:426:ARG:HG2  | 2.50                     | 0.41              |
| 1:C:475:THR:HG21 | 1:C:478:GLY:HA2  | 2.02                     | 0.41              |
| 1:A:224:ILE:HD11 | 1:A:244:GLY:O    | 2.20                     | 0.41              |
| 1:C:95:GLY:O     | 1:C:96:PRO:C     | 2.58                     | 0.41              |
| 1:C:253:ASN:ND2  | 1:C:342:ILE:HD12 | 2.34                     | 0.41              |
| 1:C:377:MET:O    | 1:C:378:ILE:C    | 2.58                     | 0.41              |
| 1:B:441:LEU:O    | 1:B:444:ALA:N    | 2.53                     | 0.41              |
| 1:D:138:VAL:HG12 | 1:D:139:GLU:OE2  | 2.19                     | 0.41              |
| 1:C:448:SER:OG   | 1:C:449:ARG:N    | 2.52                     | 0.41              |
| 1:B:360:CYS:O    | 1:B:361:ASN:C    | 2.58                     | 0.41              |
| 1:C:364:GLY:HA2  | 1:C:486:TRP:CD1  | 2.55                     | 0.41              |
| 1:A:223:LEU:HD22 | 1:C:380:LYS:HZ3  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:LEU:HD13 | 1:C:74:CYS:SG    | 2.61                     | 0.41              |
| 1:D:266:GLU:O    | 1:D:269:VAL:HB   | 2.20                     | 0.41              |
| 1:B:499:SER:O    | 1:B:500:ALA:C    | 2.58                     | 0.41              |
| 1:A:77:ASP:HB3   | 1:A:80:SER:CB    | 2.50                     | 0.41              |
| 1:C:350:PHE:O    | 1:C:354:LYS:HG3  | 2.19                     | 0.41              |
| 1:D:182:GLN:HE21 | 1:D:182:GLN:HA   | 1.85                     | 0.41              |
| 1:B:76:LEU:HD23  | 1:B:76:LEU:HA    | 1.85                     | 0.41              |
| 1:C:483:LEU:HA   | 1:C:483:LEU:HD23 | 1.66                     | 0.41              |
| 1:C:185:VAL:HG11 | 1:C:236:LEU:HD12 | 2.02                     | 0.41              |
| 1:D:434:HIS:HA   | 1:D:437:LEU:HB3  | 2.01                     | 0.41              |
| 1:C:204:TYR:HE1  | 1:C:261:LEU:HD13 | 1.85                     | 0.41              |
| 1:B:348:LYS:O    | 1:B:349:VAL:C    | 2.58                     | 0.41              |
| 1:D:111:GLY:O    | 1:D:112:MET:C    | 2.56                     | 0.41              |
| 1:A:212:PRO:O    | 1:A:213:VAL:C    | 2.58                     | 0.41              |
| 1:A:193:THR:O    | 1:A:195:GLY:N    | 2.49                     | 0.41              |
| 1:D:175:VAL:HG12 | 1:D:177:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:157:THR:HG22 | 1:B:286:SER:HB2  | 2.03                     | 0.41              |
| 1:A:216:ARG:CG   | 1:A:218:TYR:CE1  | 2.94                     | 0.41              |
| 1:D:367:VAL:HG13 | 1:D:367:VAL:O    | 2.20                     | 0.41              |
| 1:C:487:TYR:O    | 1:C:488:ARG:CB   | 2.46                     | 0.41              |
| 1:C:509:CYS:O    | 1:C:510:ARG:C    | 2.58                     | 0.41              |
| 1:C:175:VAL:CG1  | 1:C:176:GLU:N    | 2.83                     | 0.41              |
| 1:D:61:LEU:N     | 1:D:62:PRO:CD    | 2.84                     | 0.41              |
| 1:D:391:VAL:CG1  | 1:D:424:ILE:HG21 | 2.50                     | 0.41              |
| 1:D:175:VAL:HG13 | 1:D:197:ALA:HA   | 2.02                     | 0.41              |
| 1:B:164:THR:HG23 | 1:B:252:VAL:CG2  | 2.42                     | 0.41              |
| 1:C:82:PRO:O     | 1:C:83:VAL:CG2   | 2.63                     | 0.41              |
| 1:B:88:THR:N     | 1:B:429:GLU:OE2  | 2.49                     | 0.41              |
| 1:A:134:VAL:O    | 1:A:135:ARG:C    | 2.59                     | 0.41              |
| 1:A:114:ILE:HG12 | 1:A:152:ALA:HB3  | 2.03                     | 0.41              |
| 1:A:91:ILE:HG13  | 1:A:114:ILE:HB   | 2.03                     | 0.41              |
| 1:A:322:ARG:HE   | 1:A:322:ARG:HB3  | 1.59                     | 0.41              |
| 1:C:501:GLN:O    | 1:C:502:ALA:C    | 2.57                     | 0.41              |
| 1:A:163:ARG:HA   | 1:A:250:LYS:O    | 2.20                     | 0.41              |
| 1:A:289:ARG:HG3  | 1:A:293:ASP:OD2  | 2.21                     | 0.41              |
| 1:A:175:VAL:HG11 | 1:A:197:ALA:CA   | 2.50                     | 0.41              |
| 1:D:146:LEU:HB2  | 1:D:542:LEU:CD1  | 2.48                     | 0.41              |
| 1:C:565:THR:O    | 1:C:566:ASN:HB3  | 2.19                     | 0.41              |
| 1:A:380:LYS:CE   | 1:C:223:LEU:HD13 | 2.50                     | 0.41              |
| 1:D:309:LYS:HG2  | 1:D:505:GLN:HG2  | 2.03                     | 0.41              |
| 1:A:398:GLY:O    | 1:A:399:ALA:C    | 2.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:460:VAL:O    | 1:C:461:GLU:C    | 2.57                     | 0.41              |
| 1:C:379:THR:O    | 1:C:379:THR:CG2  | 2.68                     | 0.41              |
| 1:C:391:VAL:O    | 1:C:392:ALA:C    | 2.56                     | 0.41              |
| 1:C:433:TYR:CD2  | 1:C:436:GLN:HB3  | 2.56                     | 0.41              |
| 1:B:366:PRO:HA   | 1:B:400:ASP:OD2  | 2.21                     | 0.41              |
| 1:A:66:ALA:HB1   | 1:A:71:GLU:HB3   | 2.03                     | 0.41              |
| 1:C:348:LYS:O    | 1:C:349:VAL:C    | 2.59                     | 0.41              |
| 1:D:219:ILE:HG21 | 1:D:246:LEU:CD1  | 2.51                     | 0.41              |
| 1:D:322:ARG:C    | 1:D:326:ILE:HD12 | 2.41                     | 0.41              |
| 1:B:545:PHE:HB2  | 1:B:546:LEU:CD2  | 2.50                     | 0.41              |
| 1:B:82:PRO:O     | 1:B:83:VAL:HG23  | 2.21                     | 0.41              |
| 1:D:118:ASN:C    | 1:D:118:ASN:OD1  | 2.57                     | 0.41              |
| 1:D:293:ASP:O    | 1:D:296:ALA:HB3  | 2.21                     | 0.41              |
| 1:B:137:ALA:O    | 1:B:140:SER:OG   | 2.38                     | 0.41              |
| 1:D:239:GLN:O    | 1:D:241:GLU:N    | 2.54                     | 0.41              |
| 1:D:379:THR:O    | 1:D:379:THR:HG22 | 2.20                     | 0.41              |
| 1:A:506:VAL:O    | 1:A:506:VAL:HG13 | 2.21                     | 0.41              |
| 1:B:416:GLU:OE1  | 1:B:416:GLU:N    | 2.39                     | 0.41              |
| 1:A:209:ARG:CD   | 1:A:209:ARG:C    | 2.90                     | 0.40              |
| 1:D:367:VAL:H    | 1:D:400:ASP:HB2  | 1.86                     | 0.40              |
| 1:D:174:GLU:HB2  | 1:D:245:VAL:HG13 | 2.02                     | 0.40              |
| 1:B:450:ASP:HA   | 1:B:451:PRO:HD3  | 1.83                     | 0.40              |
| 1:D:433:TYR:O    | 1:D:435:ARG:N    | 2.54                     | 0.40              |
| 1:A:367:VAL:O    | 1:A:400:ASP:HB2  | 2.20                     | 0.40              |
| 1:D:450:ASP:HA   | 1:D:451:PRO:HD3  | 1.87                     | 0.40              |
| 1:C:138:VAL:CG1  | 1:C:139:GLU:OE2  | 2.70                     | 0.40              |
| 1:D:315:GLU:HG3  | 1:D:336:ALA:HB3  | 2.02                     | 0.40              |
| 1:B:114:ILE:HG12 | 1:B:152:ALA:HB3  | 2.04                     | 0.40              |
| 1:A:191:PHE:C    | 1:A:193:THR:H    | 2.24                     | 0.40              |
| 1:B:457:ILE:HG23 | 1:B:458:GLY:H    | 1.81                     | 0.40              |
| 1:A:539:SER:O    | 1:A:543:ARG:HG3  | 2.21                     | 0.40              |
| 1:B:337:ARG:HH22 | 1:B:390:ASP:CG   | 2.25                     | 0.40              |
| 1:B:539:SER:O    | 1:B:543:ARG:HG3  | 2.21                     | 0.40              |
| 1:A:497:THR:CG2  | 1:A:503:ALA:HB2  | 2.51                     | 0.40              |
| 1:B:220:ASP:O    | 1:B:222:GLY:N    | 2.54                     | 0.40              |
| 1:D:102:GLU:O    | 1:D:105:LYS:HB2  | 2.21                     | 0.40              |
| 1:B:324:ASP:CG   | 1:B:359:ARG:HH21 | 2.24                     | 0.40              |
| 1:B:559:ARG:HD2  | 1:B:564:TYR:CD1  | 2.56                     | 0.40              |
| 1:D:299:ALA:O    | 1:D:300:ALA:C    | 2.60                     | 0.40              |
| 1:A:333:ILE:CG2  | 1:A:334:MET:N    | 2.83                     | 0.40              |
| 1:A:538:GLU:O    | 1:A:539:SER:C    | 2.59                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:488:ARG:HD3  | 1:D:488:ARG:HH11 | 1.73                     | 0.40              |
| 1:A:479:ARG:HG3  | 1:A:479:ARG:HH11 | 1.85                     | 0.40              |
| 1:B:420:MET:CE   | 1:D:347:GLU:HG3  | 2.51                     | 0.40              |
| 1:B:162:ILE:O    | 1:B:252:VAL:HG23 | 2.21                     | 0.40              |
| 1:C:164:THR:HA   | 1:C:201:TRP:O    | 2.21                     | 0.40              |
| 1:C:506:VAL:CG1  | 1:C:514:PRO:HD3  | 2.52                     | 0.40              |
| 1:C:448:SER:CB   | 1:C:453:GLU:OE2  | 2.70                     | 0.40              |
| 1:D:353:GLN:NE2  | 1:D:397:ASP:OD2  | 2.54                     | 0.40              |
| 1:A:75:LEU:HD23  | 1:A:75:LEU:HA    | 1.90                     | 0.40              |
| 1:D:290:LYS:O    | 1:D:293:ASP:HB2  | 2.22                     | 0.40              |
| 1:C:149:ARG:HE   | 1:C:149:ARG:HB2  | 1.72                     | 0.40              |
| 1:A:433:TYR:CD2  | 1:A:436:GLN:HB3  | 2.56                     | 0.40              |
| 1:C:189:PRO:O    | 1:C:192:ARG:HB2  | 2.22                     | 0.40              |
| 1:B:488:ARG:HH11 | 1:B:510:ARG:HB3  | 1.84                     | 0.40              |
| 1:C:352:ALA:HB1  | 1:C:356:MET:CE   | 2.51                     | 0.40              |
| 1:C:211:VAL:HA   | 1:C:212:PRO:HD3  | 1.75                     | 0.40              |
| 1:B:73:LEU:O     | 1:B:74:CYS:C     | 2.59                     | 0.40              |
| 1:B:220:ASP:C    | 1:B:222:GLY:N    | 2.74                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:322:ARG:NH1 | 1:D:273:ARG:NH2[1_556] | 1.60                     | 0.60              |
| 1:A:209:ARG:NE  | 1:C:449:ARG:CD[1_655]  | 2.01                     | 0.19              |
| 1:A:209:ARG:NH2 | 1:C:449:ARG:CD[1_655]  | 2.06                     | 0.14              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles        |
|-----|-------|---------------|-----------|----------|----------|--------------------|
| 1   | A     | 515/528 (98%) | 431 (84%) | 65 (13%) | 19 (4%)  | <b>4</b> <b>15</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | B     | 445/528 (84%)   | 385 (86%)  | 49 (11%)  | 11 (2%)  | 7           | 25 |
| 1   | C     | 511/528 (97%)   | 440 (86%)  | 60 (12%)  | 11 (2%)  | 8           | 29 |
| 1   | D     | 509/528 (96%)   | 438 (86%)  | 57 (11%)  | 14 (3%)  | 6           | 22 |
| All | All   | 1980/2112 (94%) | 1694 (86%) | 231 (12%) | 55 (3%)  | 6           | 22 |

All (55) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | GLN  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 192 | ARG  |
| 1   | A     | 220 | ASP  |
| 1   | A     | 489 | PRO  |
| 1   | A     | 566 | ASN  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 220 | ASP  |
| 1   | B     | 566 | ASN  |
| 1   | C     | 59  | GLN  |
| 1   | C     | 74  | CYS  |
| 1   | C     | 83  | VAL  |
| 1   | C     | 192 | ARG  |
| 1   | C     | 500 | ALA  |
| 1   | D     | 83  | VAL  |
| 1   | D     | 240 | VAL  |
| 1   | D     | 375 | GLU  |
| 1   | D     | 500 | ALA  |
| 1   | D     | 566 | ASN  |
| 1   | A     | 74  | CYS  |
| 1   | A     | 119 | PHE  |
| 1   | A     | 222 | GLY  |
| 1   | A     | 228 | VAL  |
| 1   | A     | 256 | GLY  |
| 1   | A     | 500 | ALA  |
| 1   | B     | 83  | VAL  |
| 1   | B     | 143 | GLY  |
| 1   | B     | 500 | ALA  |
| 1   | C     | 168 | GLN  |
| 1   | C     | 566 | ASN  |
| 1   | D     | 74  | CYS  |
| 1   | A     | 338 | GLY  |
| 1   | B     | 205 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 206 | ASN  |
| 1   | B     | 489 | PRO  |
| 1   | C     | 220 | ASP  |
| 1   | D     | 59  | GLN  |
| 1   | D     | 220 | ASP  |
| 1   | A     | 189 | PRO  |
| 1   | A     | 441 | LEU  |
| 1   | D     | 143 | GLY  |
| 1   | D     | 207 | ILE  |
| 1   | A     | 213 | VAL  |
| 1   | A     | 234 | GLU  |
| 1   | A     | 371 | THR  |
| 1   | B     | 74  | CYS  |
| 1   | B     | 371 | THR  |
| 1   | C     | 371 | THR  |
| 1   | C     | 441 | LEU  |
| 1   | D     | 489 | PRO  |
| 1   | D     | 519 | GLU  |
| 1   | D     | 538 | GLU  |
| 1   | A     | 519 | GLU  |
| 1   | D     | 533 | VAL  |
| 1   | C     | 205 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 414/423 (98%)   | 339 (82%)  | 75 (18%)  | 2           | 5  |
| 1   | B     | 372/423 (88%)   | 320 (86%)  | 52 (14%)  | 4           | 11 |
| 1   | C     | 412/423 (97%)   | 354 (86%)  | 58 (14%)  | 4           | 11 |
| 1   | D     | 412/423 (97%)   | 352 (85%)  | 60 (15%)  | 4           | 10 |
| All | All   | 1610/1692 (95%) | 1365 (85%) | 245 (15%) | 3           | 9  |

All (245) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | GLN  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 65  | MET  |
| 1   | A     | 99  | ARG  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 104 | LEU  |
| 1   | A     | 108 | ILE  |
| 1   | A     | 120 | SER  |
| 1   | A     | 149 | ARG  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 157 | THR  |
| 1   | A     | 158 | LYS  |
| 1   | A     | 162 | ILE  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 168 | GLN  |
| 1   | A     | 174 | GLU  |
| 1   | A     | 176 | GLU  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 182 | GLN  |
| 1   | A     | 184 | LEU  |
| 1   | A     | 186 | THR  |
| 1   | A     | 194 | ARG  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 209 | ARG  |
| 1   | A     | 217 | ILE  |
| 1   | A     | 221 | ASP  |
| 1   | A     | 223 | LEU  |
| 1   | A     | 224 | ILE  |
| 1   | A     | 225 | SER  |
| 1   | A     | 230 | LYS  |
| 1   | A     | 231 | ILE  |
| 1   | A     | 234 | GLU  |
| 1   | A     | 237 | VAL  |
| 1   | A     | 250 | LYS  |
| 1   | A     | 261 | LEU  |
| 1   | A     | 273 | ARG  |
| 1   | A     | 289 | ARG  |
| 1   | A     | 294 | VAL  |
| 1   | A     | 301 | LEU  |
| 1   | A     | 304 | GLU  |
| 1   | A     | 310 | ILE  |
| 1   | A     | 321 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 322 | ARG  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 347 | GLU  |
| 1   | A     | 361 | ASN  |
| 1   | A     | 362 | LEU  |
| 1   | A     | 375 | GLU  |
| 1   | A     | 382 | ARG  |
| 1   | A     | 389 | SER  |
| 1   | A     | 396 | LEU  |
| 1   | A     | 401 | CYS  |
| 1   | A     | 402 | ILE  |
| 1   | A     | 410 | LYS  |
| 1   | A     | 420 | MET  |
| 1   | A     | 421 | GLN  |
| 1   | A     | 437 | LEU  |
| 1   | A     | 443 | ARG  |
| 1   | A     | 449 | ARG  |
| 1   | A     | 455 | THR  |
| 1   | A     | 480 | SER  |
| 1   | A     | 490 | ARG  |
| 1   | A     | 501 | GLN  |
| 1   | A     | 506 | VAL  |
| 1   | A     | 508 | LEU  |
| 1   | A     | 539 | SER  |
| 1   | A     | 542 | LEU  |
| 1   | A     | 543 | ARG  |
| 1   | A     | 546 | LEU  |
| 1   | A     | 548 | VAL  |
| 1   | A     | 552 | VAL  |
| 1   | A     | 559 | ARG  |
| 1   | A     | 568 | MET  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 65  | MET  |
| 1   | B     | 86  | ARG  |
| 1   | B     | 99  | ARG  |
| 1   | B     | 103 | ARG  |
| 1   | B     | 104 | LEU  |
| 1   | B     | 108 | ILE  |
| 1   | B     | 120 | SER  |
| 1   | B     | 144 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 155 | LEU  |
| 1   | B     | 157 | THR  |
| 1   | B     | 164 | THR  |
| 1   | B     | 186 | THR  |
| 1   | B     | 226 | LEU  |
| 1   | B     | 254 | LEU  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 273 | ARG  |
| 1   | B     | 281 | ASP  |
| 1   | B     | 289 | ARG  |
| 1   | B     | 294 | VAL  |
| 1   | B     | 301 | LEU  |
| 1   | B     | 304 | GLU  |
| 1   | B     | 321 | LYS  |
| 1   | B     | 322 | ARG  |
| 1   | B     | 327 | LEU  |
| 1   | B     | 337 | ARG  |
| 1   | B     | 347 | GLU  |
| 1   | B     | 361 | ASN  |
| 1   | B     | 362 | LEU  |
| 1   | B     | 374 | LEU  |
| 1   | B     | 377 | MET  |
| 1   | B     | 388 | THR  |
| 1   | B     | 389 | SER  |
| 1   | B     | 396 | LEU  |
| 1   | B     | 401 | CYS  |
| 1   | B     | 402 | ILE  |
| 1   | B     | 420 | MET  |
| 1   | B     | 443 | ARG  |
| 1   | B     | 449 | ARG  |
| 1   | B     | 450 | ASP  |
| 1   | B     | 455 | THR  |
| 1   | B     | 506 | VAL  |
| 1   | B     | 508 | LEU  |
| 1   | B     | 539 | SER  |
| 1   | B     | 542 | LEU  |
| 1   | B     | 543 | ARG  |
| 1   | B     | 546 | LEU  |
| 1   | B     | 548 | VAL  |
| 1   | B     | 552 | VAL  |
| 1   | B     | 559 | ARG  |
| 1   | B     | 568 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 61  | LEU  |
| 1   | C     | 87  | SER  |
| 1   | C     | 99  | ARG  |
| 1   | C     | 103 | ARG  |
| 1   | C     | 104 | LEU  |
| 1   | C     | 108 | ILE  |
| 1   | C     | 120 | SER  |
| 1   | C     | 139 | GLU  |
| 1   | C     | 157 | THR  |
| 1   | C     | 158 | LYS  |
| 1   | C     | 166 | ILE  |
| 1   | C     | 167 | LEU  |
| 1   | C     | 172 | GLU  |
| 1   | C     | 173 | SER  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 186 | THR  |
| 1   | C     | 187 | VAL  |
| 1   | C     | 192 | ARG  |
| 1   | C     | 193 | THR  |
| 1   | C     | 209 | ARG  |
| 1   | C     | 217 | ILE  |
| 1   | C     | 225 | SER  |
| 1   | C     | 229 | GLN  |
| 1   | C     | 231 | ILE  |
| 1   | C     | 234 | GLU  |
| 1   | C     | 246 | LEU  |
| 1   | C     | 261 | LEU  |
| 1   | C     | 273 | ARG  |
| 1   | C     | 289 | ARG  |
| 1   | C     | 294 | VAL  |
| 1   | C     | 301 | LEU  |
| 1   | C     | 304 | GLU  |
| 1   | C     | 310 | ILE  |
| 1   | C     | 313 | LYS  |
| 1   | C     | 321 | LYS  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 337 | ARG  |
| 1   | C     | 347 | GLU  |
| 1   | C     | 361 | ASN  |
| 1   | C     | 362 | LEU  |
| 1   | C     | 389 | SER  |
| 1   | C     | 396 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 410 | LYS  |
| 1   | C     | 420 | MET  |
| 1   | C     | 443 | ARG  |
| 1   | C     | 449 | ARG  |
| 1   | C     | 455 | THR  |
| 1   | C     | 497 | THR  |
| 1   | C     | 506 | VAL  |
| 1   | C     | 508 | LEU  |
| 1   | C     | 539 | SER  |
| 1   | C     | 542 | LEU  |
| 1   | C     | 543 | ARG  |
| 1   | C     | 546 | LEU  |
| 1   | C     | 548 | VAL  |
| 1   | C     | 552 | VAL  |
| 1   | C     | 559 | ARG  |
| 1   | C     | 568 | MET  |
| 1   | D     | 59  | GLN  |
| 1   | D     | 61  | LEU  |
| 1   | D     | 83  | VAL  |
| 1   | D     | 86  | ARG  |
| 1   | D     | 88  | THR  |
| 1   | D     | 99  | ARG  |
| 1   | D     | 103 | ARG  |
| 1   | D     | 104 | LEU  |
| 1   | D     | 157 | THR  |
| 1   | D     | 158 | LYS  |
| 1   | D     | 166 | ILE  |
| 1   | D     | 167 | LEU  |
| 1   | D     | 174 | GLU  |
| 1   | D     | 177 | LEU  |
| 1   | D     | 182 | GLN  |
| 1   | D     | 186 | THR  |
| 1   | D     | 193 | THR  |
| 1   | D     | 202 | VAL  |
| 1   | D     | 209 | ARG  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 234 | GLU  |
| 1   | D     | 239 | GLN  |
| 1   | D     | 246 | LEU  |
| 1   | D     | 250 | LYS  |
| 1   | D     | 258 | GLN  |
| 1   | D     | 273 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 289 | ARG  |
| 1   | D     | 294 | VAL  |
| 1   | D     | 301 | LEU  |
| 1   | D     | 304 | GLU  |
| 1   | D     | 313 | LYS  |
| 1   | D     | 321 | LYS  |
| 1   | D     | 322 | ARG  |
| 1   | D     | 327 | LEU  |
| 1   | D     | 333 | ILE  |
| 1   | D     | 337 | ARG  |
| 1   | D     | 347 | GLU  |
| 1   | D     | 361 | ASN  |
| 1   | D     | 362 | LEU  |
| 1   | D     | 380 | LYS  |
| 1   | D     | 389 | SER  |
| 1   | D     | 396 | LEU  |
| 1   | D     | 402 | ILE  |
| 1   | D     | 420 | MET  |
| 1   | D     | 443 | ARG  |
| 1   | D     | 449 | ARG  |
| 1   | D     | 455 | THR  |
| 1   | D     | 480 | SER  |
| 1   | D     | 501 | GLN  |
| 1   | D     | 506 | VAL  |
| 1   | D     | 508 | LEU  |
| 1   | D     | 539 | SER  |
| 1   | D     | 542 | LEU  |
| 1   | D     | 543 | ARG  |
| 1   | D     | 546 | LEU  |
| 1   | D     | 548 | VAL  |
| 1   | D     | 552 | VAL  |
| 1   | D     | 556 | THR  |
| 1   | D     | 559 | ARG  |
| 1   | D     | 568 | MET  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 124 | HIS  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 168 | GLN  |
| 1   | A     | 182 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 229 | GLN  |
| 1   | A     | 239 | GLN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 361 | ASN  |
| 1   | A     | 393 | ASN  |
| 1   | A     | 421 | GLN  |
| 1   | B     | 124 | HIS  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 253 | ASN  |
| 1   | B     | 361 | ASN  |
| 1   | B     | 393 | ASN  |
| 1   | B     | 436 | GLN  |
| 1   | C     | 121 | HIS  |
| 1   | C     | 133 | ASN  |
| 1   | C     | 168 | GLN  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 198 | ASN  |
| 1   | C     | 253 | ASN  |
| 1   | C     | 361 | ASN  |
| 1   | C     | 393 | ASN  |
| 1   | C     | 421 | GLN  |
| 1   | C     | 436 | GLN  |
| 1   | D     | 133 | ASN  |
| 1   | D     | 182 | GLN  |
| 1   | D     | 253 | ASN  |
| 1   | D     | 258 | GLN  |
| 1   | D     | 361 | ASN  |
| 1   | D     | 393 | ASN  |
| 1   | D     | 421 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | FBP  | A     | 1574 | -    | 18,20,20     | 0.84 | 1 (5%)      | 21,32,32    | 1.21 | 1 (4%)      |
| 3   | PGA  | A     | 1575 | 5,4  | 5,8,8        | 0.76 | 0           | 6,11,11     | 0.88 | 0           |
| 2   | FBP  | B     | 1574 | -    | 18,20,20     | 0.85 | 0           | 21,32,32    | 1.26 | 1 (4%)      |
| 3   | PGA  | B     | 1575 | 5,4  | 5,8,8        | 1.17 | 0           | 6,11,11     | 1.12 | 1 (16%)     |
| 2   | FBP  | C     | 1574 | -    | 18,20,20     | 1.18 | 1 (5%)      | 21,32,32    | 1.28 | 3 (14%)     |
| 3   | PGA  | C     | 1575 | 5,4  | 5,8,8        | 1.05 | 0           | 6,11,11     | 1.33 | 1 (16%)     |
| 2   | FBP  | D     | 1574 | -    | 18,20,20     | 1.43 | 4 (22%)     | 21,32,32    | 1.19 | 1 (4%)      |
| 3   | PGA  | D     | 1575 | 5    | 5,8,8        | 0.93 | 0           | 6,11,11     | 1.18 | 1 (16%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | FBP  | A     | 1574 | -    | -       | 0/13/32/32 | 0/1/1/1 |
| 3   | PGA  | A     | 1575 | 5,4  | -       | 0/4/6/6    | 0/0/0/0 |
| 2   | FBP  | B     | 1574 | -    | -       | 0/13/32/32 | 0/1/1/1 |
| 3   | PGA  | B     | 1575 | 5,4  | -       | 0/4/6/6    | 0/0/0/0 |
| 2   | FBP  | C     | 1574 | -    | -       | 0/13/32/32 | 0/1/1/1 |
| 3   | PGA  | C     | 1575 | 5,4  | -       | 0/4/6/6    | 0/0/0/0 |
| 2   | FBP  | D     | 1574 | -    | -       | 0/13/32/32 | 0/1/1/1 |
| 3   | PGA  | D     | 1575 | 5    | -       | 0/4/6/6    | 0/0/0/0 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | C     | 1574 | FBP  | O5-C2  | -2.76 | 1.38        | 1.43     |
| 2   | D     | 1574 | FBP  | P2-O5P | -2.02 | 1.47        | 1.54     |
| 2   | D     | 1574 | FBP  | P1-O1P | 2.11  | 1.58        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | D     | 1574 | FBP  | P2-O6 | 2.24 | 1.67        | 1.60     |
| 2   | A     | 1574 | FBP  | O2-C2 | 2.60 | 1.45        | 1.41     |
| 2   | D     | 1574 | FBP  | O2-C2 | 3.20 | 1.46        | 1.41     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | C     | 1574 | FBP  | O3P-P1-O1  | -2.43 | 99.57       | 106.56   |
| 2   | C     | 1574 | FBP  | O4-C4-C3   | -2.32 | 104.63      | 112.01   |
| 2   | C     | 1574 | FBP  | O5P-P2-O4P | -2.05 | 103.97      | 110.58   |
| 3   | B     | 1575 | PGA  | O1P-P-O2P  | 2.27  | 112.92      | 107.14   |
| 2   | A     | 1574 | FBP  | O3P-P1-O1P | 2.33  | 118.08      | 110.58   |
| 3   | D     | 1575 | PGA  | O4P-P-O1P  | 2.37  | 113.39      | 106.56   |
| 2   | D     | 1574 | FBP  | O6-P2-O4P  | 2.47  | 113.44      | 107.14   |
| 3   | C     | 1575 | PGA  | O1P-P-O2P  | 3.07  | 114.96      | 107.14   |
| 2   | B     | 1574 | FBP  | O3P-P1-O1P | 3.98  | 123.41      | 110.58   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1574 | FBP  | 3       | 0            |
| 3   | A     | 1575 | PGA  | 1       | 0            |
| 2   | B     | 1574 | FBP  | 3       | 0            |
| 3   | B     | 1575 | PGA  | 5       | 0            |
| 2   | C     | 1574 | FBP  | 2       | 0            |
| 3   | C     | 1575 | PGA  | 5       | 0            |
| 2   | D     | 1574 | FBP  | 5       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 517/528 (97%)   | 0.30   | 20 (3%) 43 37 | 2, 2, 2, 2            | 0     |
| 1   | B     | 463/528 (87%)   | 0.48   | 36 (7%) 16 11 | 2, 2, 2, 2            | 0     |
| 1   | C     | 515/528 (97%)   | 0.26   | 23 (4%) 37 31 | 2, 2, 2, 2            | 0     |
| 1   | D     | 513/528 (97%)   | 0.18   | 14 (2%) 58 53 | 2, 2, 2, 2            | 0     |
| All | All   | 2008/2112 (95%) | 0.30   | 93 (4%) 36 31 | 2, 2, 2, 2            | 0     |

All (93) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 166 | ILE  | 9.0  |
| 1   | D     | 146 | LEU  | 7.0  |
| 1   | A     | 231 | ILE  | 6.8  |
| 1   | B     | 204 | TYR  | 6.2  |
| 1   | B     | 164 | THR  | 5.5  |
| 1   | B     | 245 | VAL  | 5.1  |
| 1   | A     | 232 | GLY  | 4.8  |
| 1   | D     | 306 | HIS  | 4.8  |
| 1   | B     | 227 | VAL  | 4.3  |
| 1   | B     | 186 | THR  | 4.2  |
| 1   | B     | 228 | VAL  | 4.2  |
| 1   | A     | 233 | PRO  | 4.1  |
| 1   | B     | 448 | SER  | 4.1  |
| 1   | B     | 60  | GLN  | 4.0  |
| 1   | A     | 182 | GLN  | 3.9  |
| 1   | C     | 171 | PRO  | 3.9  |
| 1   | D     | 174 | GLU  | 3.8  |
| 1   | A     | 230 | LYS  | 3.8  |
| 1   | C     | 261 | LEU  | 3.8  |
| 1   | B     | 242 | ASN  | 3.8  |
| 1   | D     | 67  | ASP  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 197 | ALA  | 3.7  |
| 1   | B     | 207 | ILE  | 3.5  |
| 1   | B     | 165 | GLY  | 3.4  |
| 1   | C     | 241 | GLU  | 3.4  |
| 1   | B     | 206 | ASN  | 3.3  |
| 1   | A     | 146 | LEU  | 3.2  |
| 1   | C     | 192 | ARG  | 3.2  |
| 1   | A     | 529 | VAL  | 3.0  |
| 1   | D     | 231 | ILE  | 3.0  |
| 1   | B     | 161 | GLU  | 2.9  |
| 1   | D     | 165 | GLY  | 2.9  |
| 1   | C     | 290 | LYS  | 2.9  |
| 1   | B     | 98  | SER  | 2.8  |
| 1   | B     | 63  | ALA  | 2.8  |
| 1   | B     | 142 | ALA  | 2.8  |
| 1   | B     | 291 | ALA  | 2.8  |
| 1   | B     | 200 | VAL  | 2.7  |
| 1   | A     | 192 | ARG  | 2.7  |
| 1   | C     | 287 | PHE  | 2.7  |
| 1   | C     | 173 | SER  | 2.7  |
| 1   | D     | 83  | VAL  | 2.7  |
| 1   | B     | 162 | ILE  | 2.7  |
| 1   | A     | 236 | LEU  | 2.7  |
| 1   | B     | 531 | ARG  | 2.7  |
| 1   | B     | 261 | LEU  | 2.7  |
| 1   | D     | 326 | ILE  | 2.7  |
| 1   | A     | 256 | GLY  | 2.6  |
| 1   | C     | 88  | THR  | 2.6  |
| 1   | B     | 524 | ILE  | 2.5  |
| 1   | C     | 233 | PRO  | 2.5  |
| 1   | B     | 240 | VAL  | 2.5  |
| 1   | C     | 214 | GLY  | 2.5  |
| 1   | C     | 524 | ILE  | 2.5  |
| 1   | B     | 57  | GLN  | 2.5  |
| 1   | A     | 161 | GLU  | 2.4  |
| 1   | C     | 314 | ILE  | 2.4  |
| 1   | D     | 191 | PHE  | 2.4  |
| 1   | B     | 254 | LEU  | 2.4  |
| 1   | C     | 407 | GLU  | 2.4  |
| 1   | B     | 511 | GLY  | 2.4  |
| 1   | A     | 209 | ARG  | 2.4  |
| 1   | C     | 406 | GLY  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 548 | VAL  | 2.3  |
| 1   | C     | 194 | ARG  | 2.3  |
| 1   | D     | 167 | LEU  | 2.3  |
| 1   | A     | 228 | VAL  | 2.3  |
| 1   | B     | 241 | GLU  | 2.3  |
| 1   | C     | 212 | PRO  | 2.3  |
| 1   | D     | 248 | SER  | 2.3  |
| 1   | B     | 218 | TYR  | 2.3  |
| 1   | D     | 244 | GLY  | 2.2  |
| 1   | C     | 57  | GLN  | 2.2  |
| 1   | A     | 229 | GLN  | 2.2  |
| 1   | D     | 166 | ILE  | 2.2  |
| 1   | A     | 237 | VAL  | 2.2  |
| 1   | A     | 180 | GLY  | 2.1  |
| 1   | C     | 231 | ILE  | 2.1  |
| 1   | A     | 234 | GLU  | 2.1  |
| 1   | B     | 497 | THR  | 2.1  |
| 1   | A     | 531 | ARG  | 2.1  |
| 1   | D     | 263 | GLY  | 2.1  |
| 1   | B     | 478 | GLY  | 2.1  |
| 1   | C     | 167 | LEU  | 2.1  |
| 1   | A     | 258 | GLN  | 2.1  |
| 1   | C     | 168 | GLN  | 2.0  |
| 1   | B     | 527 | ASP  | 2.0  |
| 1   | C     | 564 | TYR  | 2.0  |
| 1   | B     | 110 | ALA  | 2.0  |
| 1   | B     | 219 | ILE  | 2.0  |
| 1   | B     | 517 | TYR  | 2.0  |
| 1   | A     | 77  | ASP  | 2.0  |
| 1   | C     | 63  | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3   | PGA  | D     | 1575 | 9/9   | 0.96 | 0.19 | 0.18  | 2,2,2,2                     | 0     |
| 3   | PGA  | A     | 1575 | 9/9   | 0.96 | 0.18 | -0.12 | 2,2,2,2                     | 0     |
| 2   | FBP  | D     | 1574 | 20/20 | 0.92 | 0.19 | -0.14 | 2,2,2,2                     | 0     |
| 2   | FBP  | A     | 1574 | 20/20 | 0.97 | 0.17 | -0.80 | 2,2,2,2                     | 0     |
| 2   | FBP  | C     | 1574 | 20/20 | 0.95 | 0.15 | -0.95 | 2,2,2,2                     | 0     |
| 3   | PGA  | C     | 1575 | 9/9   | 0.97 | 0.14 | -1.33 | 2,2,2,2                     | 0     |
| 4   | K    | B     | 1576 | 1/1   | 0.96 | 0.09 | -1.40 | 2,2,2,2                     | 0     |
| 4   | K    | A     | 1576 | 1/1   | 0.96 | 0.08 | -1.45 | 2,2,2,2                     | 0     |
| 3   | PGA  | B     | 1575 | 9/9   | 0.97 | 0.14 | -1.47 | 2,2,2,2                     | 0     |
| 2   | FBP  | B     | 1574 | 20/20 | 0.96 | 0.14 | -1.68 | 2,2,2,2                     | 0     |
| 4   | K    | C     | 1576 | 1/1   | 0.97 | 0.09 | -2.10 | 2,2,2,2                     | 0     |
| 4   | K    | D     | 1576 | 1/1   | 0.96 | 0.14 | -2.22 | 2,2,2,2                     | 0     |
| 5   | MN   | D     | 1577 | 1/1   | 0.99 | 0.06 | -4.24 | 2,2,2,2                     | 0     |
| 5   | MN   | A     | 1577 | 1/1   | 0.97 | 0.05 | -     | 2,2,2,2                     | 0     |
| 5   | MN   | B     | 1577 | 1/1   | 0.97 | 0.07 | -     | 2,2,2,2                     | 0     |
| 5   | MN   | C     | 1577 | 1/1   | 0.99 | 0.04 | -     | 2,2,2,2                     | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.