



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 PM GMT

PDB ID : 4P6H  
Title : Tl<sup>+</sup>-bound inward-facing state (bound conformation) of the glutamate transporter homologue GltPh  
Authors : Verdon, G.; Boudker, O.  
Deposited on : 2014-03-24  
Resolution : 4.08 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

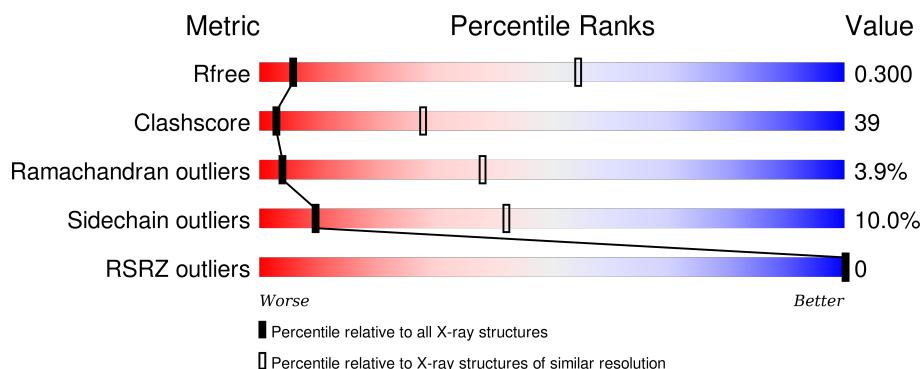
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

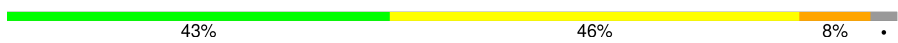


The reported resolution of this entry is 4.08 Å.

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                       | 1009 (4.52-3.60)                                      |
| Clashscore            | 102246                      | 1107 (4.52-3.60)                                      |
| Ramachandran outliers | 100387                      | 1053 (4.52-3.60)                                      |
| Sidechain outliers    | 100360                      | 1039 (4.52-3.60)                                      |
| RSRZ outliers         | 91569                       | 1012 (4.52-3.60)                                      |

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     | 422    |  |
| 1   | B     | 422    |  |
| 1   | C     | 422    |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8994 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 GltPh.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2995  | 1975 | 477 | 525 | 18 |         |         |       |
| 1   | B     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2995  | 1975 | 477 | 525 | 18 |         |         |       |
| 1   | C     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2995  | 1975 | 477 | 525 | 18 |         |         |       |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 37      | HIS      | ASP    | engineered mutation | UNP O59010 |
| A     | 40      | HIS      | LYS    | engineered mutation | UNP O59010 |
| A     | 55      | CYS      | LYS    | engineered mutation | UNP O59010 |
| A     | 125     | HIS      | LYS    | engineered mutation | UNP O59010 |
| A     | 132     | HIS      | LYS    | engineered mutation | UNP O59010 |
| A     | 223     | HIS      | LYS    | engineered mutation | UNP O59010 |
| A     | 264     | HIS      | LYS    | engineered mutation | UNP O59010 |
| A     | 321     | ALA      | CYS    | engineered mutation | UNP O59010 |
| A     | 364     | CYS      | ALA    | engineered mutation | UNP O59010 |
| A     | 368     | HIS      | GLU    | engineered mutation | UNP O59010 |
| A     | 418     | THR      | GLU    | engineered mutation | UNP O59010 |
| A     | 420     | VAL      | -      | expression tag      | UNP O59010 |
| A     | 421     | PRO      | -      | expression tag      | UNP O59010 |
| A     | 422     | ARG      | -      | expression tag      | UNP O59010 |
| B     | 37      | HIS      | ASP    | engineered mutation | UNP O59010 |
| B     | 40      | HIS      | LYS    | engineered mutation | UNP O59010 |
| B     | 55      | CYS      | LYS    | engineered mutation | UNP O59010 |
| B     | 125     | HIS      | LYS    | engineered mutation | UNP O59010 |
| B     | 132     | HIS      | LYS    | engineered mutation | UNP O59010 |
| B     | 223     | HIS      | LYS    | engineered mutation | UNP O59010 |
| B     | 264     | HIS      | LYS    | engineered mutation | UNP O59010 |
| B     | 321     | ALA      | CYS    | engineered mutation | UNP O59010 |
| B     | 364     | CYS      | ALA    | engineered mutation | UNP O59010 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 368     | HIS      | GLU    | engineered mutation | UNP O59010 |
| B     | 418     | THR      | GLU    | engineered mutation | UNP O59010 |
| B     | 420     | VAL      | -      | expression tag      | UNP O59010 |
| B     | 421     | PRO      | -      | expression tag      | UNP O59010 |
| B     | 422     | ARG      | -      | expression tag      | UNP O59010 |
| C     | 37      | HIS      | ASP    | engineered mutation | UNP O59010 |
| C     | 40      | HIS      | LYS    | engineered mutation | UNP O59010 |
| C     | 55      | CYS      | LYS    | engineered mutation | UNP O59010 |
| C     | 125     | HIS      | LYS    | engineered mutation | UNP O59010 |
| C     | 132     | HIS      | LYS    | engineered mutation | UNP O59010 |
| C     | 223     | HIS      | LYS    | engineered mutation | UNP O59010 |
| C     | 264     | HIS      | LYS    | engineered mutation | UNP O59010 |
| C     | 321     | ALA      | CYS    | engineered mutation | UNP O59010 |
| C     | 364     | CYS      | ALA    | engineered mutation | UNP O59010 |
| C     | 368     | HIS      | GLU    | engineered mutation | UNP O59010 |
| C     | 418     | THR      | GLU    | engineered mutation | UNP O59010 |
| C     | 420     | VAL      | -      | expression tag      | UNP O59010 |
| C     | 421     | PRO      | -      | expression tag      | UNP O59010 |
| C     | 422     | ARG      | -      | expression tag      | UNP O59010 |

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | B     | 1        | Total Hg<br>1 1 | 0       | 0       |
| 2   | A     | 1        | Total Hg<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Hg<br>1 1 | 0       | 0       |

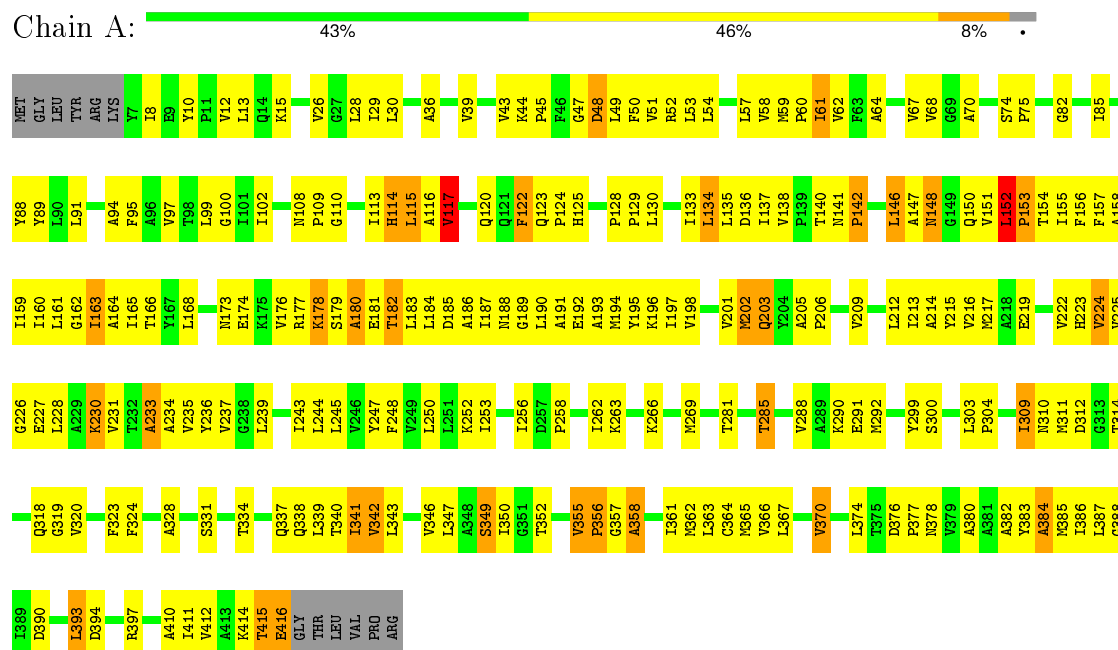
- Molecule 3 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | B     | 2        | Total Tl<br>2 2 | 0       | 0       |
| 3   | A     | 2        | Total Tl<br>2 2 | 0       | 0       |
| 3   | C     | 2        | Total Tl<br>2 2 | 0       | 0       |

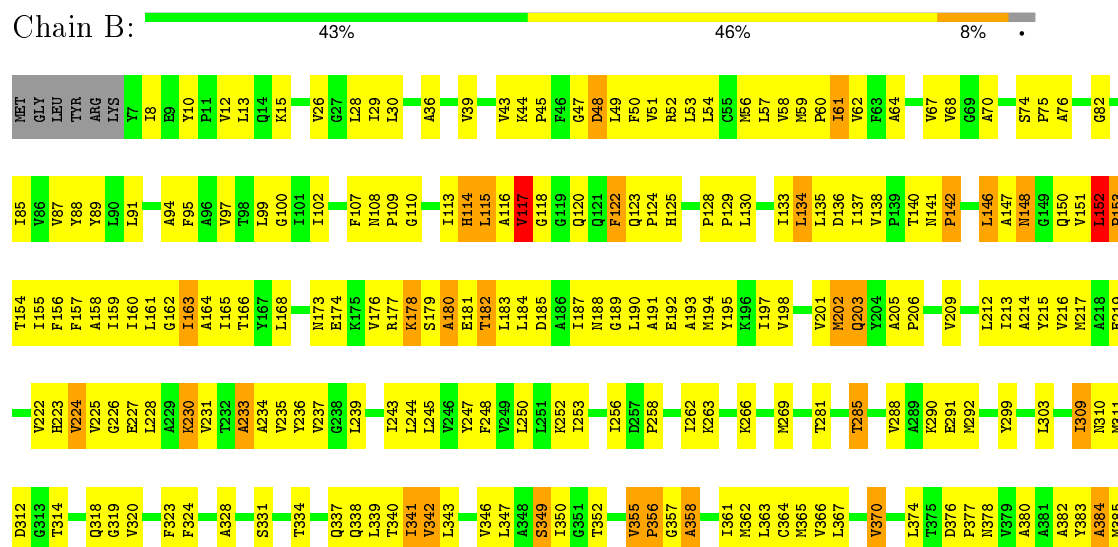
### 3 Residue-property plots

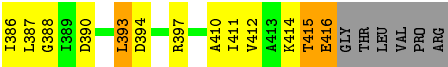
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GltPh

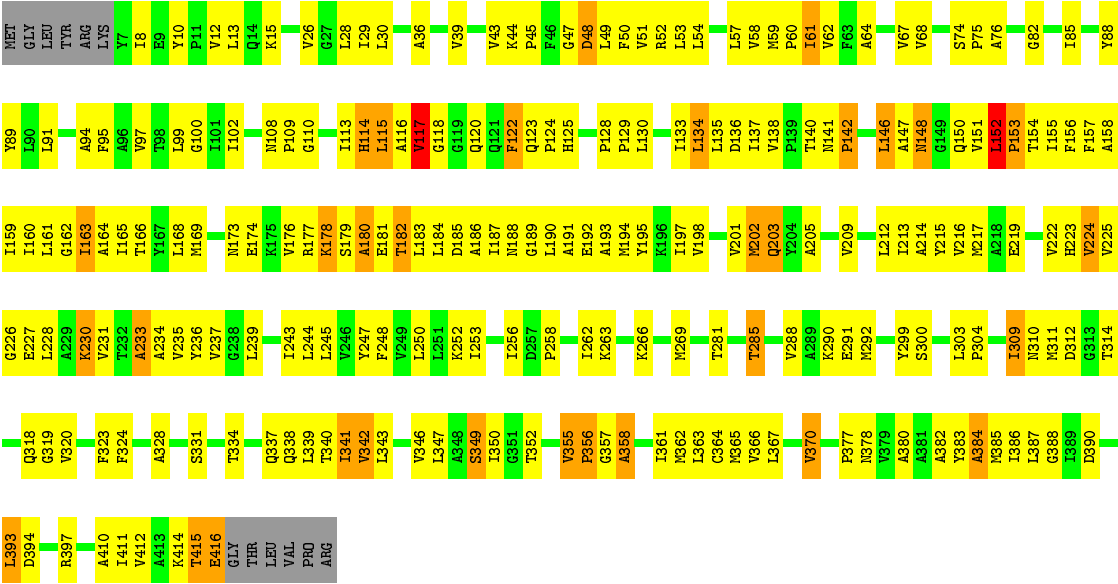


#### • Molecule 1: GltPh





● Molecule 1: GltPh



## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 110.83Å 200.43Å 206.40Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 15.00 – 4.08<br>15.00 – 4.08                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 67.4 (15.00-4.08)<br>67.4 (15.00-4.08)                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                               | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                               | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.91 (at 4.14Å)                                                               | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0109                                                               | Depositor        |
| R, $R_{free}$                                                           | 0.258 , 0.296<br>0.262 , 0.300                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1222 reflections (11.01%)                                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 111.3                                                                         | Xtriage          |
| Anisotropy                                                              | 0.190                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.18 , 43.0                                                                   | EDS              |
| Estimated twinning fraction                                             | 0.094 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.095 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$                   | Xtriage          |
| Outliers                                                                | 0 of 12327 reflections                                                        | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                                          | EDS              |
| Total number of atoms                                                   | 8994                                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 137.0                                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.58         | 0/3053  | 0.69        | 1/4171 (0.0%)  |
| 1   | B     | 0.58         | 0/3053  | 0.69        | 1/4171 (0.0%)  |
| 1   | C     | 0.58         | 0/3053  | 0.69        | 1/4171 (0.0%)  |
| All | All   | 0.58         | 0/9159  | 0.69        | 3/12513 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | B     | 152 | LEU  | CA-CB-CG | 5.20 | 127.25      | 115.30   |
| 1   | A     | 152 | LEU  | CA-CB-CG | 5.18 | 127.22      | 115.30   |
| 1   | C     | 152 | LEU  | CA-CB-CG | 5.18 | 127.21      | 115.30   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 2995  | 0        | 3144     | 250     | 0            |
| 1   | B     | 2995  | 0        | 3144     | 243     | 1            |
| 1   | C     | 2995  | 0        | 3144     | 241     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | B     | 2     | 0        | 0        | 0       | 0            |
| 3   | C     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 8994  | 0        | 9432     | 725     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (725) 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:B:256:ILE:CD1  | 1:B:414:LYS:HE3  | 1.70                     | 1.21              |
| 1:C:256:ILE:CD1  | 1:C:414:LYS:HE3  | 1.70                     | 1.21              |
| 1:A:256:ILE:CD1  | 1:A:414:LYS:HE3  | 1.70                     | 1.19              |
| 1:A:355:VAL:HG12 | 1:A:356:PRO:HD2  | 1.17                     | 1.16              |
| 1:A:256:ILE:HD11 | 1:A:414:LYS:HE3  | 1.28                     | 1.11              |
| 1:B:256:ILE:HD11 | 1:B:414:LYS:HE3  | 1.28                     | 1.11              |
| 1:C:355:VAL:HG12 | 1:C:356:PRO:HD2  | 1.17                     | 1.09              |
| 1:B:355:VAL:HG12 | 1:B:356:PRO:HD2  | 1.17                     | 1.09              |
| 1:C:117:VAL:HG13 | 1:C:378:ASN:HA   | 1.35                     | 1.08              |
| 1:C:116:ALA:O    | 1:C:117:VAL:HG23 | 1.53                     | 1.08              |
| 1:A:116:ALA:O    | 1:A:117:VAL:HG23 | 1.54                     | 1.08              |
| 1:A:117:VAL:HG13 | 1:A:378:ASN:HA   | 1.35                     | 1.07              |
| 1:C:256:ILE:HD11 | 1:C:414:LYS:HE3  | 1.28                     | 1.07              |
| 1:A:134:LEU:O    | 1:A:137:ILE:HG12 | 1.56                     | 1.06              |
| 1:B:116:ALA:O    | 1:B:117:VAL:HG23 | 1.53                     | 1.05              |
| 1:B:412:VAL:HA   | 1:B:415:THR:OG1  | 1.56                     | 1.05              |
| 1:B:117:VAL:HG13 | 1:B:378:ASN:HA   | 1.35                     | 1.05              |
| 1:A:412:VAL:HA   | 1:A:415:THR:OG1  | 1.56                     | 1.04              |
| 1:B:134:LEU:O    | 1:B:137:ILE:HG12 | 1.55                     | 1.04              |
| 1:C:134:LEU:O    | 1:C:137:ILE:HG12 | 1.56                     | 1.03              |
| 1:C:412:VAL:HA   | 1:C:415:THR:OG1  | 1.56                     | 1.02              |
| 1:B:347:LEU:HA   | 1:B:350:ILE:HD12 | 1.40                     | 1.02              |
| 1:C:347:LEU:HA   | 1:C:350:ILE:HD12 | 1.40                     | 1.02              |
| 1:A:347:LEU:HA   | 1:A:350:ILE:HD12 | 1.40                     | 1.00              |
| 1:C:122:PHE:CD2  | 1:C:122:PHE:C    | 2.36                     | 0.99              |
| 1:B:355:VAL:CG1  | 1:B:356:PRO:HD2  | 1.93                     | 0.99              |
| 1:A:355:VAL:CG1  | 1:A:356:PRO:HD2  | 1.93                     | 0.98              |
| 1:C:178:LYS:HE2  | 1:C:182:THR:HG23 | 1.45                     | 0.98              |
| 1:C:355:VAL:CG1  | 1:C:356:PRO:HD2  | 1.93                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:122:PHE:C    | 1:B:122:PHE:CD2  | 2.36                     | 0.97              |
| 1:A:122:PHE:C    | 1:A:122:PHE:CD2  | 2.36                     | 0.97              |
| 1:B:178:LYS:HE2  | 1:B:182:THR:HG23 | 1.45                     | 0.96              |
| 1:A:178:LYS:HE2  | 1:A:182:THR:HG23 | 1.45                     | 0.96              |
| 1:C:150:GLN:O    | 1:C:153:PRO:HD2  | 1.65                     | 0.95              |
| 1:B:150:GLN:O    | 1:B:153:PRO:HD2  | 1.64                     | 0.95              |
| 1:A:150:GLN:O    | 1:A:153:PRO:HD2  | 1.64                     | 0.95              |
| 1:A:243:ILE:HA   | 1:A:247:TYR:HD2  | 1.31                     | 0.95              |
| 1:C:243:ILE:HA   | 1:C:247:TYR:HD2  | 1.31                     | 0.94              |
| 1:B:243:ILE:HA   | 1:B:247:TYR:HD2  | 1.31                     | 0.94              |
| 1:C:151:VAL:O    | 1:C:155:ILE:HD13 | 1.69                     | 0.92              |
| 1:B:256:ILE:HD11 | 1:B:414:LYS:CE   | 2.00                     | 0.92              |
| 1:A:256:ILE:HD12 | 1:A:414:LYS:HE3  | 1.52                     | 0.91              |
| 1:C:122:PHE:HD2  | 1:C:122:PHE:C    | 1.73                     | 0.91              |
| 1:B:151:VAL:O    | 1:B:155:ILE:HD13 | 1.69                     | 0.91              |
| 1:A:151:VAL:O    | 1:A:155:ILE:HD13 | 1.70                     | 0.91              |
| 1:C:256:ILE:HD11 | 1:C:414:LYS:CE   | 2.00                     | 0.91              |
| 1:A:256:ILE:HD11 | 1:A:414:LYS:CE   | 2.00                     | 0.91              |
| 1:A:122:PHE:HD2  | 1:A:122:PHE:C    | 1.73                     | 0.90              |
| 1:C:256:ILE:HD12 | 1:C:414:LYS:HE3  | 1.52                     | 0.90              |
| 1:B:122:PHE:HD2  | 1:B:122:PHE:C    | 1.73                     | 0.89              |
| 1:B:256:ILE:HD12 | 1:B:414:LYS:HE3  | 1.52                     | 0.89              |
| 1:C:364:CYS:HA   | 1:C:367:LEU:HD12 | 1.54                     | 0.89              |
| 1:B:364:CYS:HA   | 1:B:367:LEU:HD12 | 1.54                     | 0.88              |
| 1:A:364:CYS:HA   | 1:A:367:LEU:HD12 | 1.54                     | 0.88              |
| 1:A:117:VAL:CG1  | 1:A:378:ASN:HA   | 2.05                     | 0.86              |
| 1:B:117:VAL:CG1  | 1:B:378:ASN:HA   | 2.05                     | 0.86              |
| 1:C:117:VAL:CG1  | 1:C:378:ASN:HA   | 2.05                     | 0.85              |
| 1:A:146:LEU:O    | 1:A:146:LEU:HD12 | 1.79                     | 0.83              |
| 1:C:146:LEU:O    | 1:C:146:LEU:HD12 | 1.79                     | 0.82              |
| 1:B:146:LEU:O    | 1:B:146:LEU:HD12 | 1.79                     | 0.82              |
| 1:B:36:ALA:O     | 1:B:39:VAL:HB    | 1.80                     | 0.81              |
| 1:C:299:TYR:HB2  | 1:C:303:LEU:HD23 | 1.61                     | 0.81              |
| 1:C:36:ALA:O     | 1:C:39:VAL:HB    | 1.79                     | 0.81              |
| 1:B:299:TYR:HB2  | 1:B:303:LEU:HD23 | 1.61                     | 0.81              |
| 1:A:36:ALA:O     | 1:A:39:VAL:HB    | 1.79                     | 0.81              |
| 1:A:299:TYR:HB2  | 1:A:303:LEU:HD23 | 1.61                     | 0.81              |
| 1:C:416:GLU:OE1  | 1:C:416:GLU:HA   | 1.80                     | 0.81              |
| 1:C:227:GLU:O    | 1:C:231:VAL:HG23 | 1.81                     | 0.81              |
| 1:B:416:GLU:HA   | 1:B:416:GLU:OE1  | 1.80                     | 0.80              |
| 1:C:117:VAL:HG11 | 1:C:378:ASN:N    | 1.97                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:117:VAL:HG11 | 1:A:378:ASN:N    | 1.97                     | 0.80              |
| 1:B:227:GLU:O    | 1:B:231:VAL:HG23 | 1.81                     | 0.80              |
| 1:B:117:VAL:HG11 | 1:B:378:ASN:N    | 1.97                     | 0.80              |
| 1:C:355:VAL:HG12 | 1:C:356:PRO:CD   | 2.08                     | 0.79              |
| 1:A:122:PHE:HD2  | 1:A:122:PHE:O    | 1.65                     | 0.79              |
| 1:A:416:GLU:OE1  | 1:A:416:GLU:HA   | 1.80                     | 0.79              |
| 1:C:216:VAL:HG11 | 1:C:385:MET:HG2  | 1.65                     | 0.79              |
| 1:C:122:PHE:O    | 1:C:122:PHE:HD2  | 1.65                     | 0.79              |
| 1:A:216:VAL:HG11 | 1:A:385:MET:HG2  | 1.65                     | 0.79              |
| 1:A:227:GLU:O    | 1:A:231:VAL:HG23 | 1.81                     | 0.78              |
| 1:A:355:VAL:HG12 | 1:A:356:PRO:CD   | 2.08                     | 0.78              |
| 1:B:122:PHE:HD2  | 1:B:122:PHE:O    | 1.65                     | 0.78              |
| 1:B:216:VAL:HG11 | 1:B:385:MET:HG2  | 1.65                     | 0.77              |
| 1:C:150:GLN:HE21 | 1:C:153:PRO:HG2  | 1.50                     | 0.77              |
| 1:B:150:GLN:HE21 | 1:B:153:PRO:HG2  | 1.50                     | 0.76              |
| 1:C:165:ILE:HA   | 1:C:168:LEU:HD12 | 1.68                     | 0.76              |
| 1:A:150:GLN:HE21 | 1:A:153:PRO:HG2  | 1.50                     | 0.75              |
| 1:A:165:ILE:HA   | 1:A:168:LEU:HD12 | 1.68                     | 0.75              |
| 1:B:248:PHE:CD2  | 1:B:258:PRO:HB2  | 2.21                     | 0.75              |
| 1:A:248:PHE:CD2  | 1:A:258:PRO:HB2  | 2.21                     | 0.75              |
| 1:B:165:ILE:HA   | 1:B:168:LEU:HD12 | 1.68                     | 0.74              |
| 1:A:194:MET:HA   | 1:A:197:ILE:HD12 | 1.69                     | 0.74              |
| 1:C:194:MET:HA   | 1:C:197:ILE:HD12 | 1.69                     | 0.74              |
| 1:C:248:PHE:CD2  | 1:C:258:PRO:HB2  | 2.21                     | 0.74              |
| 1:A:61:ILE:HG22  | 1:A:194:MET:HG3  | 1.69                     | 0.74              |
| 1:B:116:ALA:C    | 1:B:117:VAL:CG2  | 2.57                     | 0.74              |
| 1:B:116:ALA:C    | 1:B:117:VAL:HG23 | 2.08                     | 0.74              |
| 1:C:151:VAL:HG13 | 1:C:155:ILE:HD11 | 1.70                     | 0.74              |
| 1:B:61:ILE:HG22  | 1:B:194:MET:HG3  | 1.69                     | 0.73              |
| 1:B:355:VAL:HG12 | 1:B:356:PRO:CD   | 2.08                     | 0.73              |
| 1:C:61:ILE:HG22  | 1:C:194:MET:HG3  | 1.69                     | 0.73              |
| 1:A:116:ALA:C    | 1:A:117:VAL:CG2  | 2.57                     | 0.73              |
| 1:C:202:MET:HG3  | 1:C:356:PRO:HB2  | 1.71                     | 0.73              |
| 1:C:116:ALA:C    | 1:C:117:VAL:HG23 | 2.09                     | 0.73              |
| 1:A:116:ALA:C    | 1:A:117:VAL:HG23 | 2.09                     | 0.73              |
| 1:C:151:VAL:HG13 | 1:C:155:ILE:CD1  | 2.19                     | 0.73              |
| 1:B:151:VAL:HG13 | 1:B:155:ILE:CD1  | 2.19                     | 0.72              |
| 1:B:194:MET:HA   | 1:B:197:ILE:HD12 | 1.70                     | 0.72              |
| 1:B:116:ALA:O    | 1:B:117:VAL:CG2  | 2.37                     | 0.72              |
| 1:A:226:GLY:O    | 1:A:230:LYS:HB2  | 1.89                     | 0.72              |
| 1:B:113:ILE:HD11 | 1:B:224:VAL:HG12 | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:74:SER:HB2   | 1:A:166:THR:HG21 | 1.72                     | 0.72              |
| 1:C:213:ILE:HD12 | 1:C:214:ALA:N    | 2.05                     | 0.72              |
| 1:A:213:ILE:HD12 | 1:A:214:ALA:N    | 2.04                     | 0.72              |
| 1:C:116:ALA:C    | 1:C:117:VAL:CG2  | 2.57                     | 0.72              |
| 1:B:213:ILE:HD12 | 1:B:214:ALA:N    | 2.04                     | 0.72              |
| 1:B:151:VAL:HG13 | 1:B:155:ILE:HD11 | 1.70                     | 0.71              |
| 1:A:151:VAL:HG13 | 1:A:155:ILE:CD1  | 2.19                     | 0.71              |
| 1:A:151:VAL:HG13 | 1:A:155:ILE:HD11 | 1.70                     | 0.71              |
| 1:C:226:GLY:O    | 1:C:230:LYS:HB2  | 1.90                     | 0.71              |
| 1:C:113:ILE:HD11 | 1:C:224:VAL:HG12 | 1.71                     | 0.71              |
| 1:C:115:LEU:HD23 | 1:C:328:ALA:O    | 1.90                     | 0.71              |
| 1:B:115:LEU:HD23 | 1:B:328:ALA:O    | 1.90                     | 0.71              |
| 1:A:202:MET:HG3  | 1:A:356:PRO:HB2  | 1.71                     | 0.71              |
| 1:A:113:ILE:HD11 | 1:A:224:VAL:HG12 | 1.71                     | 0.71              |
| 1:B:74:SER:HB2   | 1:B:166:THR:HG21 | 1.72                     | 0.71              |
| 1:B:226:GLY:O    | 1:B:230:LYS:HB2  | 1.89                     | 0.71              |
| 1:A:115:LEU:HD23 | 1:A:328:ALA:O    | 1.90                     | 0.70              |
| 1:C:243:ILE:HA   | 1:C:247:TYR:CD2  | 2.22                     | 0.70              |
| 1:B:202:MET:HG3  | 1:B:356:PRO:HB2  | 1.71                     | 0.70              |
| 1:C:117:VAL:CG1  | 1:C:378:ASN:CA   | 2.69                     | 0.70              |
| 1:C:116:ALA:O    | 1:C:117:VAL:CG2  | 2.37                     | 0.70              |
| 1:B:117:VAL:CG1  | 1:B:378:ASN:CA   | 2.69                     | 0.69              |
| 1:C:74:SER:HB2   | 1:C:166:THR:HG21 | 1.72                     | 0.69              |
| 1:B:99:LEU:HA    | 1:B:102:ILE:HD12 | 1.75                     | 0.69              |
| 1:A:117:VAL:CG1  | 1:A:378:ASN:CA   | 2.69                     | 0.69              |
| 1:B:243:ILE:HA   | 1:B:247:TYR:CD2  | 2.22                     | 0.69              |
| 1:C:146:LEU:HD12 | 1:C:146:LEU:C    | 2.13                     | 0.69              |
| 1:B:146:LEU:HD12 | 1:B:146:LEU:C    | 2.13                     | 0.68              |
| 1:A:146:LEU:C    | 1:A:146:LEU:HD12 | 2.13                     | 0.68              |
| 1:C:150:GLN:NE2  | 1:C:153:PRO:HG2  | 2.08                     | 0.68              |
| 1:B:50:PHE:CE1   | 1:B:205:ALA:HA   | 2.29                     | 0.68              |
| 1:B:150:GLN:NE2  | 1:B:153:PRO:HG2  | 2.08                     | 0.68              |
| 1:C:50:PHE:CE1   | 1:C:205:ALA:HA   | 2.29                     | 0.68              |
| 1:A:150:GLN:NE2  | 1:A:153:PRO:HG2  | 2.08                     | 0.68              |
| 1:C:337:GLN:O    | 1:C:341:ILE:HG13 | 1.94                     | 0.67              |
| 1:A:99:LEU:HA    | 1:A:102:ILE:HD12 | 1.75                     | 0.67              |
| 1:A:50:PHE:CE1   | 1:A:205:ALA:HA   | 2.29                     | 0.67              |
| 1:A:256:ILE:HD11 | 1:A:414:LYS:CD   | 2.24                     | 0.67              |
| 1:A:185:ASP:O    | 1:A:188:ASN:O    | 2.13                     | 0.67              |
| 1:B:256:ILE:HD11 | 1:B:414:LYS:CD   | 2.24                     | 0.67              |
| 1:B:185:ASP:O    | 1:B:188:ASN:O    | 2.13                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:99:LEU:HA    | 1:C:102:ILE:HD12 | 1.75                     | 0.67              |
| 1:B:337:GLN:O    | 1:B:341:ILE:HG13 | 1.94                     | 0.67              |
| 1:C:256:ILE:HD11 | 1:C:414:LYS:CD   | 2.24                     | 0.66              |
| 1:A:337:GLN:O    | 1:A:341:ILE:HG13 | 1.94                     | 0.66              |
| 1:A:243:ILE:HA   | 1:A:247:TYR:CD2  | 2.22                     | 0.66              |
| 1:C:185:ASP:O    | 1:C:188:ASN:O    | 2.13                     | 0.66              |
| 1:C:362:MET:O    | 1:C:365:MET:HB3  | 1.96                     | 0.66              |
| 1:B:362:MET:O    | 1:B:365:MET:HB3  | 1.96                     | 0.65              |
| 1:A:179:SER:HA   | 1:C:185:ASP:OD2  | 1.96                     | 0.65              |
| 1:C:48:ASP:N     | 1:C:48:ASP:OD1   | 2.29                     | 0.65              |
| 1:A:411:ILE:O    | 1:A:415:THR:OG1  | 2.12                     | 0.65              |
| 1:B:26:VAL:HA    | 1:B:29:ILE:HG12  | 1.79                     | 0.65              |
| 1:A:362:MET:O    | 1:A:365:MET:HB3  | 1.96                     | 0.64              |
| 1:C:411:ILE:O    | 1:C:415:THR:OG1  | 2.12                     | 0.64              |
| 1:B:355:VAL:CB   | 1:B:356:PRO:HD2  | 2.28                     | 0.64              |
| 1:A:412:VAL:O    | 1:A:416:GLU:HB2  | 1.97                     | 0.64              |
| 1:C:248:PHE:HD2  | 1:C:258:PRO:HB2  | 1.61                     | 0.64              |
| 1:B:248:PHE:HD2  | 1:B:258:PRO:HB2  | 1.61                     | 0.64              |
| 1:A:26:VAL:HA    | 1:A:29:ILE:HG12  | 1.79                     | 0.64              |
| 1:A:202:MET:HA   | 1:A:205:ALA:HB2  | 1.80                     | 0.64              |
| 1:C:202:MET:HA   | 1:C:205:ALA:HB2  | 1.80                     | 0.64              |
| 1:C:355:VAL:CB   | 1:C:356:PRO:HD2  | 2.28                     | 0.64              |
| 1:C:412:VAL:O    | 1:C:416:GLU:HB2  | 1.97                     | 0.64              |
| 1:A:116:ALA:O    | 1:A:117:VAL:CG2  | 2.37                     | 0.64              |
| 1:A:248:PHE:HD2  | 1:A:258:PRO:HB2  | 1.61                     | 0.63              |
| 1:C:26:VAL:HA    | 1:C:29:ILE:HG12  | 1.79                     | 0.63              |
| 1:A:355:VAL:CB   | 1:A:356:PRO:HD2  | 2.28                     | 0.63              |
| 1:B:236:TYR:HA   | 1:B:239:LEU:HD12 | 1.81                     | 0.63              |
| 1:B:44:LYS:N     | 1:B:45:PRO:HD2   | 2.13                     | 0.63              |
| 1:A:64:ALA:O     | 1:A:68:VAL:HG23  | 1.98                     | 0.63              |
| 1:A:44:LYS:N     | 1:A:45:PRO:HD2   | 2.13                     | 0.63              |
| 1:B:412:VAL:O    | 1:B:416:GLU:HB2  | 1.97                     | 0.63              |
| 1:C:117:VAL:CG1  | 1:C:378:ASN:N    | 2.62                     | 0.63              |
| 1:A:117:VAL:CG1  | 1:A:378:ASN:N    | 2.62                     | 0.63              |
| 1:C:44:LYS:N     | 1:C:45:PRO:HD2   | 2.13                     | 0.62              |
| 1:C:174:GLU:OE2  | 1:C:174:GLU:HA   | 1.99                     | 0.62              |
| 1:B:117:VAL:CG1  | 1:B:378:ASN:N    | 2.62                     | 0.62              |
| 1:C:64:ALA:O     | 1:C:68:VAL:HG23  | 1.98                     | 0.62              |
| 1:B:411:ILE:O    | 1:B:415:THR:OG1  | 2.13                     | 0.62              |
| 1:B:195:TYR:O    | 1:B:198:VAL:HB   | 2.00                     | 0.62              |
| 1:A:152:LEU:H    | 1:A:152:LEU:CD1  | 2.13                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:152:LEU:CD1  | 1:C:152:LEU:H    | 2.13                     | 0.62              |
| 1:C:236:TYR:HA   | 1:C:239:LEU:HD12 | 1.81                     | 0.62              |
| 1:B:202:MET:HA   | 1:B:205:ALA:HB2  | 1.80                     | 0.62              |
| 1:A:195:TYR:O    | 1:A:198:VAL:HB   | 2.00                     | 0.61              |
| 1:B:64:ALA:O     | 1:B:68:VAL:HG23  | 1.98                     | 0.61              |
| 1:A:183:LEU:HD12 | 1:C:186:ALA:O    | 1.99                     | 0.61              |
| 1:B:174:GLU:HA   | 1:B:174:GLU:OE2  | 1.99                     | 0.61              |
| 1:C:195:TYR:O    | 1:C:198:VAL:HB   | 2.00                     | 0.61              |
| 1:B:122:PHE:CD2  | 1:B:123:GLN:N    | 2.69                     | 0.61              |
| 1:C:256:ILE:HD11 | 1:C:414:LYS:HG3  | 1.82                     | 0.61              |
| 1:A:187:ILE:O    | 1:A:190:LEU:HB3  | 2.01                     | 0.61              |
| 1:C:182:THR:O    | 1:C:183:LEU:C    | 2.39                     | 0.61              |
| 1:A:174:GLU:HA   | 1:A:174:GLU:OE2  | 1.99                     | 0.61              |
| 1:A:152:LEU:HD12 | 1:A:152:LEU:H    | 1.66                     | 0.61              |
| 1:B:152:LEU:CD1  | 1:B:152:LEU:H    | 2.13                     | 0.61              |
| 1:B:256:ILE:HD11 | 1:B:414:LYS:HG3  | 1.82                     | 0.61              |
| 1:A:256:ILE:HD11 | 1:A:414:LYS:HG3  | 1.82                     | 0.61              |
| 1:C:122:PHE:CD2  | 1:C:123:GLN:N    | 2.69                     | 0.61              |
| 1:A:122:PHE:CE2  | 1:A:124:PRO:N    | 2.69                     | 0.60              |
| 1:A:122:PHE:CD2  | 1:A:123:GLN:N    | 2.68                     | 0.60              |
| 1:A:48:ASP:OD1   | 1:A:48:ASP:N     | 2.29                     | 0.60              |
| 1:A:52:ARG:NH2   | 1:B:138:VAL:O    | 2.34                     | 0.60              |
| 1:C:122:PHE:CE2  | 1:C:124:PRO:N    | 2.69                     | 0.60              |
| 1:C:152:LEU:HD12 | 1:C:152:LEU:H    | 1.66                     | 0.60              |
| 1:C:187:ILE:O    | 1:C:190:LEU:HB3  | 2.01                     | 0.60              |
| 1:A:236:TYR:HA   | 1:A:239:LEU:HD12 | 1.81                     | 0.60              |
| 1:B:152:LEU:HD12 | 1:B:152:LEU:H    | 1.66                     | 0.60              |
| 1:A:58:VAL:HA    | 1:A:61:ILE:HD11  | 1.84                     | 0.59              |
| 1:B:182:THR:O    | 1:B:183:LEU:C    | 2.39                     | 0.59              |
| 1:A:182:THR:O    | 1:A:183:LEU:C    | 2.39                     | 0.59              |
| 1:B:122:PHE:CE2  | 1:B:124:PRO:N    | 2.69                     | 0.59              |
| 1:B:187:ILE:O    | 1:B:190:LEU:HB3  | 2.01                     | 0.59              |
| 1:C:58:VAL:HA    | 1:C:61:ILE:HD11  | 1.84                     | 0.59              |
| 1:B:155:ILE:HD12 | 1:B:155:ILE:N    | 2.18                     | 0.59              |
| 1:A:155:ILE:N    | 1:A:155:ILE:HD12 | 2.18                     | 0.58              |
| 1:B:58:VAL:HA    | 1:B:61:ILE:HD11  | 1.84                     | 0.58              |
| 1:B:151:VAL:CG1  | 1:B:155:ILE:CD1  | 2.81                     | 0.58              |
| 1:A:151:VAL:CG1  | 1:A:155:ILE:CD1  | 2.81                     | 0.58              |
| 1:B:67:VAL:HG22  | 1:B:158:ALA:HB1  | 1.86                     | 0.58              |
| 1:A:59:MET:HB2   | 1:A:60:PRO:HD2   | 1.85                     | 0.58              |
| 1:B:334:THR:O    | 1:B:337:GLN:HG2  | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:151:VAL:CG1  | 1:C:155:ILE:CD1  | 2.81                     | 0.58              |
| 1:B:59:MET:HB2   | 1:B:60:PRO:HD2   | 1.85                     | 0.57              |
| 1:C:334:THR:O    | 1:C:337:GLN:HG2  | 2.04                     | 0.57              |
| 1:A:347:LEU:HA   | 1:A:350:ILE:CD1  | 2.26                     | 0.57              |
| 1:C:67:VAL:HG22  | 1:C:158:ALA:HB1  | 1.86                     | 0.57              |
| 1:C:89:TYR:HB3   | 1:C:310:ASN:HB2  | 1.86                     | 0.57              |
| 1:A:58:VAL:HA    | 1:A:61:ILE:CD1   | 2.35                     | 0.57              |
| 1:C:58:VAL:HA    | 1:C:61:ILE:CD1   | 2.35                     | 0.57              |
| 1:C:155:ILE:N    | 1:C:155:ILE:HD12 | 2.18                     | 0.57              |
| 1:A:334:THR:O    | 1:A:337:GLN:HG2  | 2.04                     | 0.57              |
| 1:A:89:TYR:HB3   | 1:A:310:ASN:HB2  | 1.86                     | 0.57              |
| 1:B:89:TYR:HB3   | 1:B:310:ASN:HB2  | 1.86                     | 0.57              |
| 1:C:59:MET:HB2   | 1:C:60:PRO:HD2   | 1.85                     | 0.57              |
| 1:C:347:LEU:HA   | 1:C:350:ILE:CD1  | 2.26                     | 0.56              |
| 1:B:58:VAL:HA    | 1:B:61:ILE:CD1   | 2.35                     | 0.56              |
| 1:C:363:LEU:O    | 1:C:364:CYS:C    | 2.44                     | 0.56              |
| 1:B:363:LEU:O    | 1:B:364:CYS:C    | 2.44                     | 0.56              |
| 1:A:244:LEU:HA   | 1:A:248:PHE:HD1  | 1.71                     | 0.56              |
| 1:A:67:VAL:HG22  | 1:A:158:ALA:HB1  | 1.86                     | 0.56              |
| 1:C:178:LYS:C    | 1:C:178:LYS:HD3  | 2.26                     | 0.56              |
| 1:C:178:LYS:CE   | 1:C:182:THR:HG23 | 2.29                     | 0.56              |
| 1:B:151:VAL:CG1  | 1:B:155:ILE:HD13 | 2.36                     | 0.56              |
| 1:A:148:ASN:OD1  | 1:A:148:ASN:N    | 2.38                     | 0.56              |
| 1:B:148:ASN:OD1  | 1:B:148:ASN:N    | 2.38                     | 0.56              |
| 1:A:151:VAL:CG1  | 1:A:155:ILE:HD13 | 2.36                     | 0.56              |
| 1:C:217:MET:CE   | 1:C:225:VAL:HG22 | 2.36                     | 0.56              |
| 1:A:363:LEU:O    | 1:A:364:CYS:C    | 2.44                     | 0.55              |
| 1:C:148:ASN:N    | 1:C:148:ASN:OD1  | 2.38                     | 0.55              |
| 1:B:47:GLY:O     | 1:B:50:PHE:N     | 2.40                     | 0.55              |
| 1:B:48:ASP:OD1   | 1:B:48:ASP:N     | 2.29                     | 0.55              |
| 1:C:151:VAL:CG1  | 1:C:155:ILE:HD13 | 2.36                     | 0.55              |
| 1:C:201:VAL:C    | 1:C:203:GLN:H    | 2.10                     | 0.55              |
| 1:C:244:LEU:HA   | 1:C:248:PHE:HD1  | 1.71                     | 0.55              |
| 1:A:217:MET:CE   | 1:A:225:VAL:HG22 | 2.36                     | 0.55              |
| 1:B:217:MET:CE   | 1:B:225:VAL:HG22 | 2.36                     | 0.55              |
| 1:B:225:VAL:HA   | 1:B:228:LEU:HD12 | 1.89                     | 0.55              |
| 1:C:117:VAL:HG11 | 1:C:378:ASN:CA   | 2.36                     | 0.55              |
| 1:A:178:LYS:HD3  | 1:A:178:LYS:C    | 2.26                     | 0.55              |
| 1:B:347:LEU:HA   | 1:B:350:ILE:CD1  | 2.26                     | 0.55              |
| 1:B:178:LYS:C    | 1:B:178:LYS:HD3  | 2.26                     | 0.55              |
| 1:B:244:LEU:HA   | 1:B:248:PHE:HD1  | 1.71                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:ALA:O    | 1:B:237:VAL:HG22 | 2.07                     | 0.55              |
| 1:C:338:GLN:HA   | 1:C:341:ILE:CD1  | 2.37                     | 0.55              |
| 1:A:47:GLY:O     | 1:A:50:PHE:N     | 2.40                     | 0.55              |
| 1:B:290:LYS:HG3  | 1:B:299:TYR:CE1  | 2.42                     | 0.54              |
| 1:C:390:ASP:HA   | 1:C:393:LEU:HD12 | 1.90                     | 0.54              |
| 1:B:82:GLY:HA2   | 1:B:85:ILE:HG22  | 1.89                     | 0.54              |
| 1:C:47:GLY:O     | 1:C:50:PHE:N     | 2.40                     | 0.54              |
| 1:A:117:VAL:HG11 | 1:A:378:ASN:CA   | 2.36                     | 0.54              |
| 1:A:290:LYS:HG3  | 1:A:299:TYR:CE1  | 2.42                     | 0.54              |
| 1:A:338:GLN:HA   | 1:A:341:ILE:CD1  | 2.37                     | 0.54              |
| 1:B:147:ALA:HB3  | 1:B:148:ASN:OD1  | 2.08                     | 0.54              |
| 1:C:82:GLY:HA2   | 1:C:85:ILE:HG22  | 1.89                     | 0.54              |
| 1:A:201:VAL:C    | 1:A:203:GLN:H    | 2.10                     | 0.54              |
| 1:C:366:VAL:O    | 1:C:370:VAL:HG23 | 2.08                     | 0.54              |
| 1:B:366:VAL:O    | 1:B:370:VAL:HG23 | 2.08                     | 0.54              |
| 1:B:113:ILE:HD12 | 1:B:227:GLU:HG3  | 1.90                     | 0.54              |
| 1:B:201:VAL:C    | 1:B:203:GLN:H    | 2.10                     | 0.54              |
| 1:C:233:ALA:O    | 1:C:237:VAL:HG22 | 2.07                     | 0.54              |
| 1:B:410:ALA:O    | 1:B:414:LYS:HG2  | 2.08                     | 0.54              |
| 1:B:362:MET:O    | 1:B:363:LEU:C    | 2.46                     | 0.54              |
| 1:A:113:ILE:HD12 | 1:A:227:GLU:HG3  | 1.90                     | 0.54              |
| 1:B:338:GLN:HA   | 1:B:341:ILE:CD1  | 2.37                     | 0.54              |
| 1:B:130:LEU:HA   | 1:B:133:ILE:HG22 | 1.90                     | 0.54              |
| 1:B:362:MET:O    | 1:B:365:MET:N    | 2.41                     | 0.54              |
| 1:A:233:ALA:O    | 1:A:237:VAL:HG22 | 2.07                     | 0.54              |
| 1:A:362:MET:O    | 1:A:363:LEU:C    | 2.46                     | 0.54              |
| 1:C:290:LYS:HG3  | 1:C:299:TYR:CE1  | 2.42                     | 0.54              |
| 1:C:225:VAL:HA   | 1:C:228:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:362:MET:O    | 1:C:365:MET:N    | 2.41                     | 0.54              |
| 1:A:362:MET:O    | 1:A:365:MET:N    | 2.41                     | 0.54              |
| 1:A:366:VAL:O    | 1:A:370:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:180:ALA:O    | 1:A:181:GLU:C    | 2.46                     | 0.53              |
| 1:A:338:GLN:HA   | 1:A:341:ILE:HD12 | 1.91                     | 0.53              |
| 1:A:147:ALA:HB3  | 1:A:148:ASN:OD1  | 2.08                     | 0.53              |
| 1:B:390:ASP:HA   | 1:B:393:LEU:HD12 | 1.89                     | 0.53              |
| 1:C:60:PRO:HB2   | 1:C:194:MET:HE2  | 1.91                     | 0.53              |
| 1:A:130:LEU:HA   | 1:A:133:ILE:HG22 | 1.90                     | 0.53              |
| 1:C:410:ALA:O    | 1:C:414:LYS:HG2  | 2.08                     | 0.53              |
| 1:A:256:ILE:HD11 | 1:A:414:LYS:CG   | 2.39                     | 0.53              |
| 1:B:178:LYS:CE   | 1:B:182:THR:HG23 | 2.29                     | 0.53              |
| 1:B:155:ILE:O    | 1:B:156:PHE:C    | 2.46                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:155:ILE:O    | 1:A:156:PHE:C    | 2.46                     | 0.53              |
| 1:C:390:ASP:O    | 1:C:394:ASP:HB2  | 2.08                     | 0.53              |
| 1:A:342:VAL:O    | 1:A:343:LEU:C    | 2.46                     | 0.53              |
| 1:B:117:VAL:HG11 | 1:B:378:ASN:CA   | 2.36                     | 0.53              |
| 1:A:60:PRO:HB2   | 1:A:194:MET:HE2  | 1.91                     | 0.53              |
| 1:A:390:ASP:HA   | 1:A:393:LEU:HD12 | 1.90                     | 0.53              |
| 1:C:130:LEU:HA   | 1:C:133:ILE:HG22 | 1.90                     | 0.53              |
| 1:C:147:ALA:HB3  | 1:C:148:ASN:OD1  | 2.08                     | 0.53              |
| 1:A:82:GLY:HA2   | 1:A:85:ILE:HG22  | 1.89                     | 0.53              |
| 1:B:342:VAL:O    | 1:B:343:LEU:C    | 2.46                     | 0.53              |
| 1:B:60:PRO:HB2   | 1:B:194:MET:HE2  | 1.91                     | 0.53              |
| 1:A:390:ASP:O    | 1:A:394:ASP:HB2  | 2.08                     | 0.53              |
| 1:B:10:TYR:HB2   | 1:B:15:LYS:HE3   | 1.91                     | 0.53              |
| 1:B:338:GLN:HA   | 1:B:341:ILE:HD12 | 1.90                     | 0.53              |
| 1:A:410:ALA:O    | 1:A:414:LYS:HG2  | 2.08                     | 0.53              |
| 1:A:225:VAL:HA   | 1:A:228:LEU:HD12 | 1.89                     | 0.53              |
| 1:C:10:TYR:HB2   | 1:C:15:LYS:HE3   | 1.91                     | 0.53              |
| 1:B:256:ILE:HD11 | 1:B:414:LYS:CG   | 2.39                     | 0.52              |
| 1:C:180:ALA:O    | 1:C:181:GLU:C    | 2.47                     | 0.52              |
| 1:C:91:LEU:HA    | 1:C:94:ALA:HB3   | 1.91                     | 0.52              |
| 1:C:155:ILE:O    | 1:C:156:PHE:C    | 2.46                     | 0.52              |
| 1:B:91:LEU:HA    | 1:B:94:ALA:HB3   | 1.91                     | 0.52              |
| 1:C:362:MET:O    | 1:C:363:LEU:C    | 2.46                     | 0.52              |
| 1:C:122:PHE:HE2  | 1:C:124:PRO:N    | 2.07                     | 0.52              |
| 1:B:155:ILE:N    | 1:B:155:ILE:CD1  | 2.73                     | 0.52              |
| 1:C:89:TYR:CG    | 1:C:310:ASN:HB2  | 2.44                     | 0.52              |
| 1:C:256:ILE:HD11 | 1:C:414:LYS:CG   | 2.39                     | 0.52              |
| 1:A:122:PHE:HE2  | 1:A:124:PRO:N    | 2.07                     | 0.52              |
| 1:C:113:ILE:HD12 | 1:C:227:GLU:HG3  | 1.90                     | 0.52              |
| 1:B:390:ASP:O    | 1:B:394:ASP:HB2  | 2.08                     | 0.52              |
| 1:C:342:VAL:O    | 1:C:343:LEU:C    | 2.46                     | 0.52              |
| 1:A:89:TYR:CG    | 1:A:310:ASN:HB2  | 2.44                     | 0.52              |
| 1:A:10:TYR:HB2   | 1:A:15:LYS:HE3   | 1.91                     | 0.52              |
| 1:C:110:GLY:O    | 1:C:113:ILE:HG22 | 2.10                     | 0.52              |
| 1:B:74:SER:CB    | 1:B:166:THR:HG21 | 2.39                     | 0.52              |
| 1:C:338:GLN:HA   | 1:C:341:ILE:HD12 | 1.90                     | 0.52              |
| 1:B:109:PRO:O    | 1:B:324:PHE:HA   | 2.10                     | 0.52              |
| 1:C:184:LEU:O    | 1:C:185:ASP:C    | 2.48                     | 0.52              |
| 1:B:122:PHE:HE2  | 1:B:124:PRO:N    | 2.07                     | 0.52              |
| 1:B:110:GLY:O    | 1:B:113:ILE:HG22 | 2.10                     | 0.52              |
| 1:A:110:GLY:O    | 1:A:113:ILE:HG22 | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:LEU:HA    | 1:A:94:ALA:HB3   | 1.91                     | 0.52              |
| 1:B:59:MET:HB2   | 1:B:60:PRO:CD    | 2.40                     | 0.51              |
| 1:A:184:LEU:O    | 1:A:185:ASP:C    | 2.48                     | 0.51              |
| 1:A:192:GLU:O    | 1:A:195:TYR:HB2  | 2.11                     | 0.51              |
| 1:A:74:SER:CB    | 1:A:166:THR:HG21 | 2.39                     | 0.51              |
| 1:B:180:ALA:O    | 1:B:181:GLU:C    | 2.47                     | 0.51              |
| 1:C:109:PRO:O    | 1:C:324:PHE:HA   | 2.10                     | 0.51              |
| 1:A:59:MET:HB2   | 1:A:60:PRO:CD    | 2.40                     | 0.51              |
| 1:B:89:TYR:CG    | 1:B:310:ASN:HB2  | 2.44                     | 0.51              |
| 1:B:377:PRO:HA   | 1:B:380:ALA:HB3  | 1.92                     | 0.51              |
| 1:A:155:ILE:CD1  | 1:A:155:ILE:N    | 2.73                     | 0.51              |
| 1:C:281:THR:O    | 1:C:285:THR:OG1  | 2.29                     | 0.51              |
| 1:B:122:PHE:O    | 1:B:122:PHE:CD2  | 2.53                     | 0.51              |
| 1:A:122:PHE:O    | 1:A:122:PHE:CD2  | 2.52                     | 0.51              |
| 1:B:184:LEU:O    | 1:B:185:ASP:C    | 2.48                     | 0.51              |
| 1:B:288:VAL:O    | 1:B:292:MET:HG2  | 2.11                     | 0.51              |
| 1:A:95:PHE:HE2   | 1:A:245:LEU:HD22 | 1.76                     | 0.51              |
| 1:C:155:ILE:N    | 1:C:155:ILE:CD1  | 2.73                     | 0.51              |
| 1:A:281:THR:O    | 1:A:285:THR:OG1  | 2.29                     | 0.51              |
| 1:C:152:LEU:HB2  | 1:C:153:PRO:HD3  | 1.93                     | 0.51              |
| 1:A:377:PRO:HA   | 1:A:380:ALA:HB3  | 1.92                     | 0.51              |
| 1:C:59:MET:HB2   | 1:C:60:PRO:CD    | 2.40                     | 0.51              |
| 1:B:159:ILE:HG22 | 1:B:160:ILE:HD12 | 1.92                     | 0.51              |
| 1:B:281:THR:O    | 1:B:285:THR:OG1  | 2.29                     | 0.51              |
| 1:C:136:ASP:O    | 1:C:153:PRO:HG3  | 2.11                     | 0.51              |
| 1:C:146:LEU:CD1  | 1:C:146:LEU:C    | 2.79                     | 0.51              |
| 1:B:212:LEU:HD22 | 1:B:384:ALA:HB1  | 1.93                     | 0.51              |
| 1:A:109:PRO:O    | 1:A:324:PHE:HA   | 2.10                     | 0.51              |
| 1:C:339:LEU:O    | 1:C:342:VAL:HG13 | 2.12                     | 0.51              |
| 1:B:192:GLU:O    | 1:B:195:TYR:HB2  | 2.11                     | 0.50              |
| 1:A:288:VAL:O    | 1:A:292:MET:HG2  | 2.11                     | 0.50              |
| 1:C:212:LEU:HD22 | 1:C:384:ALA:HB1  | 1.93                     | 0.50              |
| 1:C:288:VAL:O    | 1:C:292:MET:HG2  | 2.11                     | 0.50              |
| 1:C:192:GLU:O    | 1:C:195:TYR:HB2  | 2.11                     | 0.50              |
| 1:A:339:LEU:O    | 1:A:342:VAL:HG13 | 2.11                     | 0.50              |
| 1:A:152:LEU:HB2  | 1:A:153:PRO:HD3  | 1.93                     | 0.50              |
| 1:A:178:LYS:O    | 1:A:179:SER:C    | 2.50                     | 0.50              |
| 1:A:146:LEU:C    | 1:A:146:LEU:CD1  | 2.79                     | 0.50              |
| 1:A:159:ILE:HG22 | 1:A:160:ILE:HD12 | 1.92                     | 0.50              |
| 1:C:178:LYS:O    | 1:C:179:SER:C    | 2.50                     | 0.50              |
| 1:C:159:ILE:HG22 | 1:C:160:ILE:HD12 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:163:ILE:O    | 1:B:164:ALA:C    | 2.49                     | 0.50              |
| 1:A:146:LEU:CD1  | 1:A:146:LEU:O    | 2.57                     | 0.50              |
| 1:C:377:PRO:HA   | 1:C:380:ALA:HB3  | 1.92                     | 0.50              |
| 1:B:136:ASP:O    | 1:B:153:PRO:HG3  | 2.11                     | 0.50              |
| 1:B:95:PHE:HE2   | 1:B:245:LEU:HD22 | 1.76                     | 0.50              |
| 1:A:136:ASP:O    | 1:A:153:PRO:HG3  | 2.11                     | 0.50              |
| 1:C:58:VAL:O     | 1:C:62:VAL:HG23  | 2.12                     | 0.50              |
| 1:A:212:LEU:HD22 | 1:A:384:ALA:HB1  | 1.93                     | 0.50              |
| 1:A:163:ILE:O    | 1:A:164:ALA:C    | 2.49                     | 0.50              |
| 1:C:244:LEU:HA   | 1:C:248:PHE:CD1  | 2.47                     | 0.50              |
| 1:B:146:LEU:CD1  | 1:B:146:LEU:C    | 2.79                     | 0.50              |
| 1:C:95:PHE:HE2   | 1:C:245:LEU:HD22 | 1.76                     | 0.50              |
| 1:B:152:LEU:HB2  | 1:B:153:PRO:HD3  | 1.93                     | 0.49              |
| 1:A:59:MET:CB    | 1:A:60:PRO:CD    | 2.90                     | 0.49              |
| 1:B:178:LYS:O    | 1:B:179:SER:C    | 2.50                     | 0.49              |
| 1:B:244:LEU:HA   | 1:B:248:PHE:CD1  | 2.47                     | 0.49              |
| 1:C:74:SER:CB    | 1:C:166:THR:HG21 | 2.39                     | 0.49              |
| 1:C:59:MET:CB    | 1:C:60:PRO:CD    | 2.90                     | 0.49              |
| 1:B:339:LEU:O    | 1:B:342:VAL:HG13 | 2.11                     | 0.49              |
| 1:A:58:VAL:O     | 1:A:62:VAL:HG23  | 2.12                     | 0.49              |
| 1:C:309:ILE:HG22 | 1:C:310:ASN:H    | 1.77                     | 0.49              |
| 1:A:309:ILE:HG22 | 1:A:310:ASN:H    | 1.78                     | 0.49              |
| 1:A:244:LEU:HA   | 1:A:248:PHE:CD1  | 2.47                     | 0.49              |
| 1:C:57:LEU:N     | 1:C:57:LEU:HD23  | 2.28                     | 0.49              |
| 1:B:57:LEU:N     | 1:B:57:LEU:HD23  | 2.28                     | 0.49              |
| 1:A:178:LYS:CE   | 1:A:182:THR:HG23 | 2.29                     | 0.49              |
| 1:B:59:MET:CB    | 1:B:60:PRO:CD    | 2.90                     | 0.49              |
| 1:C:8:ILE:CG1    | 1:C:15:LYS:HE2   | 2.43                     | 0.49              |
| 1:C:122:PHE:O    | 1:C:122:PHE:CD2  | 2.52                     | 0.48              |
| 1:A:217:MET:HE1  | 1:A:225:VAL:HG22 | 1.94                     | 0.48              |
| 1:B:190:LEU:O    | 1:B:191:ALA:C    | 2.51                     | 0.48              |
| 1:C:114:HIS:HA   | 1:C:328:ALA:O    | 2.13                     | 0.48              |
| 1:A:151:VAL:CG1  | 1:A:155:ILE:HD11 | 2.42                     | 0.48              |
| 1:A:163:ILE:HG22 | 1:A:164:ALA:N    | 2.28                     | 0.48              |
| 1:B:58:VAL:O     | 1:B:62:VAL:HG23  | 2.12                     | 0.48              |
| 1:B:114:HIS:HA   | 1:B:328:ALA:O    | 2.13                     | 0.48              |
| 1:B:309:ILE:HG22 | 1:B:310:ASN:H    | 1.78                     | 0.48              |
| 1:A:8:ILE:CG1    | 1:A:15:LYS:HE2   | 2.43                     | 0.48              |
| 1:C:290:LYS:HG3  | 1:C:299:TYR:HE1  | 1.79                     | 0.48              |
| 1:A:141:ASN:C    | 1:A:141:ASN:OD1  | 2.52                     | 0.48              |
| 1:B:163:ILE:HG22 | 1:B:164:ALA:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:290:LYS:HG3  | 1:A:299:TYR:HE1  | 1.79                     | 0.47              |
| 1:A:114:HIS:HA   | 1:A:328:ALA:O    | 2.13                     | 0.47              |
| 1:B:157:PHE:O    | 1:B:158:ALA:C    | 2.53                     | 0.47              |
| 1:B:8:ILE:CG1    | 1:B:15:LYS:HE2   | 2.43                     | 0.47              |
| 1:A:190:LEU:O    | 1:A:191:ALA:C    | 2.51                     | 0.47              |
| 1:C:163:ILE:O    | 1:C:164:ALA:C    | 2.49                     | 0.47              |
| 1:A:57:LEU:N     | 1:A:57:LEU:HD23  | 2.28                     | 0.47              |
| 1:B:222:VAL:C    | 1:B:224:VAL:N    | 2.68                     | 0.47              |
| 1:C:141:ASN:OD1  | 1:C:141:ASN:C    | 2.52                     | 0.47              |
| 1:A:157:PHE:O    | 1:A:158:ALA:C    | 2.53                     | 0.47              |
| 1:B:183:LEU:O    | 1:B:184:LEU:C    | 2.53                     | 0.47              |
| 1:C:222:VAL:C    | 1:C:224:VAL:N    | 2.68                     | 0.47              |
| 1:B:141:ASN:C    | 1:B:141:ASN:OD1  | 2.52                     | 0.47              |
| 1:C:340:THR:O    | 1:C:341:ILE:C    | 2.53                     | 0.47              |
| 1:C:48:ASP:O     | 1:C:49:LEU:C     | 2.53                     | 0.47              |
| 1:C:163:ILE:HG22 | 1:C:164:ALA:N    | 2.28                     | 0.47              |
| 1:B:141:ASN:HA   | 1:B:142:PRO:HD2  | 1.55                     | 0.47              |
| 1:C:190:LEU:O    | 1:C:191:ALA:C    | 2.51                     | 0.47              |
| 1:B:209:VAL:O    | 1:B:213:ILE:HG13 | 2.15                     | 0.47              |
| 1:B:48:ASP:O     | 1:B:49:LEU:C     | 2.53                     | 0.47              |
| 1:C:151:VAL:CG1  | 1:C:155:ILE:HD11 | 2.42                     | 0.47              |
| 1:C:222:VAL:O    | 1:C:224:VAL:N    | 2.48                     | 0.47              |
| 1:B:340:THR:O    | 1:B:341:ILE:C    | 2.53                     | 0.47              |
| 1:A:340:THR:O    | 1:A:341:ILE:C    | 2.53                     | 0.47              |
| 1:C:157:PHE:O    | 1:C:158:ALA:C    | 2.53                     | 0.47              |
| 1:C:117:VAL:HG23 | 1:C:120:GLN:O    | 2.15                     | 0.47              |
| 1:A:151:VAL:HG12 | 1:A:155:ILE:HD13 | 1.97                     | 0.47              |
| 1:B:290:LYS:HG3  | 1:B:299:TYR:HE1  | 1.79                     | 0.47              |
| 1:A:222:VAL:C    | 1:A:224:VAL:N    | 2.68                     | 0.47              |
| 1:A:117:VAL:HG23 | 1:A:120:GLN:O    | 2.15                     | 0.46              |
| 1:C:183:LEU:O    | 1:C:184:LEU:C    | 2.53                     | 0.46              |
| 1:A:186:ALA:O    | 1:B:183:LEU:HD12 | 2.15                     | 0.46              |
| 1:C:209:VAL:O    | 1:C:213:ILE:HG13 | 2.15                     | 0.46              |
| 1:A:209:VAL:O    | 1:A:213:ILE:HG13 | 2.15                     | 0.46              |
| 1:B:151:VAL:HG12 | 1:B:155:ILE:HD13 | 1.98                     | 0.46              |
| 1:A:47:GLY:O     | 1:A:48:ASP:C     | 2.54                     | 0.46              |
| 1:A:48:ASP:O     | 1:A:49:LEU:C     | 2.53                     | 0.46              |
| 1:C:151:VAL:HG12 | 1:C:155:ILE:HD13 | 1.98                     | 0.46              |
| 1:C:29:ILE:HG13  | 1:C:30:LEU:N     | 2.30                     | 0.46              |
| 1:A:412:VAL:CA   | 1:A:415:THR:OG1  | 2.47                     | 0.46              |
| 1:C:393:LEU:HG   | 1:C:393:LEU:H    | 1.43                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:47:GLY:O     | 1:B:48:ASP:C     | 2.54                     | 0.46              |
| 1:A:222:VAL:O    | 1:A:224:VAL:N    | 2.48                     | 0.46              |
| 1:A:29:ILE:HG13  | 1:A:30:LEU:N     | 2.30                     | 0.46              |
| 1:C:217:MET:HE1  | 1:C:225:VAL:HG22 | 1.97                     | 0.46              |
| 1:A:314:THR:HA   | 1:A:397:ARG:HD3  | 1.98                     | 0.46              |
| 1:C:314:THR:HA   | 1:C:397:ARG:HD3  | 1.98                     | 0.46              |
| 1:B:117:VAL:HG23 | 1:B:120:GLN:O    | 2.15                     | 0.46              |
| 1:B:153:PRO:O    | 1:B:154:THR:C    | 2.54                     | 0.46              |
| 1:A:58:VAL:O     | 1:A:61:ILE:HG12  | 2.16                     | 0.46              |
| 1:B:75:PRO:HA    | 1:B:76:ALA:HA    | 1.65                     | 0.46              |
| 1:A:393:LEU:HG   | 1:A:393:LEU:H    | 1.43                     | 0.46              |
| 1:C:141:ASN:HA   | 1:C:142:PRO:HD2  | 1.55                     | 0.46              |
| 1:C:250:LEU:O    | 1:C:253:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:173:ASN:ND2  | 1:A:176:VAL:HG23 | 2.31                     | 0.46              |
| 1:B:222:VAL:O    | 1:B:224:VAL:N    | 2.48                     | 0.46              |
| 1:C:173:ASN:ND2  | 1:C:176:VAL:HG23 | 2.31                     | 0.46              |
| 1:B:314:THR:HA   | 1:B:397:ARG:HD3  | 1.98                     | 0.46              |
| 1:C:58:VAL:O     | 1:C:61:ILE:HG12  | 2.16                     | 0.45              |
| 1:B:151:VAL:CG1  | 1:B:155:ILE:HD11 | 2.42                     | 0.45              |
| 1:B:58:VAL:O     | 1:B:61:ILE:HG12  | 2.16                     | 0.45              |
| 1:A:183:LEU:O    | 1:A:184:LEU:C    | 2.53                     | 0.45              |
| 1:A:198:VAL:O    | 1:A:201:VAL:HB   | 2.17                     | 0.45              |
| 1:C:8:ILE:HG13   | 1:C:15:LYS:HE2   | 1.99                     | 0.45              |
| 1:B:250:LEU:O    | 1:B:253:ILE:HG22 | 2.16                     | 0.45              |
| 1:C:182:THR:O    | 1:C:185:ASP:HB3  | 2.17                     | 0.45              |
| 1:A:182:THR:O    | 1:A:185:ASP:HB3  | 2.17                     | 0.45              |
| 1:B:194:MET:O    | 1:B:198:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:8:ILE:HG13   | 1:A:15:LYS:HE2   | 1.99                     | 0.45              |
| 1:A:250:LEU:O    | 1:A:253:ILE:HG22 | 2.16                     | 0.45              |
| 1:B:182:THR:O    | 1:B:185:ASP:HB3  | 2.17                     | 0.45              |
| 1:A:153:PRO:O    | 1:A:154:THR:C    | 2.54                     | 0.45              |
| 1:B:198:VAL:O    | 1:B:201:VAL:HB   | 2.17                     | 0.45              |
| 1:B:56:MET:O     | 1:C:142:PRO:HD2  | 2.16                     | 0.45              |
| 1:C:47:GLY:O     | 1:C:48:ASP:C     | 2.54                     | 0.45              |
| 1:C:150:GLN:HE21 | 1:C:153:PRO:CG   | 2.27                     | 0.45              |
| 1:C:146:LEU:CD1  | 1:C:146:LEU:O    | 2.57                     | 0.45              |
| 1:B:29:ILE:HG13  | 1:B:30:LEU:N     | 2.30                     | 0.45              |
| 1:A:50:PHE:O     | 1:A:53:LEU:N     | 2.50                     | 0.45              |
| 1:C:153:PRO:O    | 1:C:154:THR:C    | 2.54                     | 0.45              |
| 1:C:194:MET:O    | 1:C:198:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:173:ASN:ND2  | 1:B:176:VAL:HG23 | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:ILE:HG13 | 1:A:138:VAL:N    | 2.32                     | 0.44              |
| 1:B:412:VAL:CA   | 1:B:415:THR:OG1  | 2.47                     | 0.44              |
| 1:B:137:ILE:HG13 | 1:B:138:VAL:N    | 2.32                     | 0.44              |
| 1:B:115:LEU:CD2  | 1:B:328:ALA:O    | 2.63                     | 0.44              |
| 1:B:8:ILE:HG13   | 1:B:15:LYS:HE2   | 1.99                     | 0.44              |
| 1:C:176:VAL:O    | 1:C:177:ARG:C    | 2.56                     | 0.44              |
| 1:C:50:PHE:O     | 1:C:53:LEU:N     | 2.50                     | 0.44              |
| 1:C:137:ILE:HG13 | 1:C:138:VAL:N    | 2.32                     | 0.44              |
| 1:C:157:PHE:O    | 1:C:160:ILE:N    | 2.51                     | 0.44              |
| 1:A:157:PHE:O    | 1:A:160:ILE:N    | 2.51                     | 0.44              |
| 1:C:412:VAL:CA   | 1:C:415:THR:OG1  | 2.47                     | 0.44              |
| 1:C:89:TYR:CB    | 1:C:310:ASN:HB2  | 2.48                     | 0.44              |
| 1:C:233:ALA:O    | 1:C:235:VAL:N    | 2.51                     | 0.44              |
| 1:A:50:PHE:O     | 1:A:53:LEU:HB2   | 2.17                     | 0.44              |
| 1:A:156:PHE:CD2  | 1:A:156:PHE:C    | 2.91                     | 0.44              |
| 1:A:382:ALA:O    | 1:A:383:TYR:C    | 2.55                     | 0.44              |
| 1:B:85:ILE:O     | 1:B:88:TYR:HB3   | 2.18                     | 0.44              |
| 1:A:233:ALA:O    | 1:A:235:VAL:N    | 2.51                     | 0.44              |
| 1:B:176:VAL:O    | 1:B:177:ARG:C    | 2.56                     | 0.44              |
| 1:C:198:VAL:O    | 1:C:201:VAL:HB   | 2.17                     | 0.44              |
| 1:C:382:ALA:O    | 1:C:383:TYR:C    | 2.56                     | 0.44              |
| 1:B:382:ALA:O    | 1:B:383:TYR:C    | 2.55                     | 0.44              |
| 1:C:50:PHE:O     | 1:C:53:LEU:HB2   | 2.17                     | 0.44              |
| 1:B:50:PHE:O     | 1:B:53:LEU:HB2   | 2.17                     | 0.44              |
| 1:B:44:LYS:O     | 1:B:47:GLY:N     | 2.51                     | 0.44              |
| 1:B:48:ASP:O     | 1:B:51:VAL:N     | 2.51                     | 0.44              |
| 1:B:346:VAL:HG12 | 1:B:347:LEU:HD12 | 2.00                     | 0.44              |
| 1:C:346:VAL:HG12 | 1:C:347:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:363:LEU:O    | 1:A:366:VAL:HG12 | 2.18                     | 0.44              |
| 1:A:128:PRO:HB3  | 1:A:129:PRO:HD2  | 2.00                     | 0.44              |
| 1:A:194:MET:O    | 1:A:198:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:61:ILE:HG12  | 1:A:62:VAL:N     | 2.33                     | 0.44              |
| 1:B:363:LEU:O    | 1:B:366:VAL:HG12 | 2.18                     | 0.44              |
| 1:B:146:LEU:O    | 1:B:146:LEU:CD1  | 2.57                     | 0.44              |
| 1:C:383:TYR:O    | 1:C:385:MET:N    | 2.51                     | 0.44              |
| 1:A:383:TYR:O    | 1:A:385:MET:N    | 2.51                     | 0.44              |
| 1:B:216:VAL:O    | 1:B:219:GLU:O    | 2.35                     | 0.44              |
| 1:A:192:GLU:HA   | 1:A:195:TYR:CD2  | 2.53                     | 0.44              |
| 1:C:192:GLU:HA   | 1:C:195:TYR:CD2  | 2.53                     | 0.44              |
| 1:A:341:ILE:HG13 | 1:A:341:ILE:H    | 1.69                     | 0.44              |
| 1:B:157:PHE:O    | 1:B:160:ILE:N    | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:85:ILE:O     | 1:C:88:TYR:HB3   | 2.18                     | 0.44              |
| 1:A:176:VAL:O    | 1:A:177:ARG:C    | 2.55                     | 0.44              |
| 1:A:311:MET:HB2  | 1:A:349:SER:HB2  | 2.00                     | 0.44              |
| 1:A:48:ASP:O     | 1:A:51:VAL:N     | 2.51                     | 0.43              |
| 1:C:48:ASP:O     | 1:C:51:VAL:N     | 2.51                     | 0.43              |
| 1:B:117:VAL:HB   | 1:B:118:GLY:H    | 1.33                     | 0.43              |
| 1:C:61:ILE:HG12  | 1:C:62:VAL:N     | 2.33                     | 0.43              |
| 1:C:243:ILE:O    | 1:C:248:PHE:HD1  | 2.01                     | 0.43              |
| 1:B:243:ILE:O    | 1:B:248:PHE:HD1  | 2.01                     | 0.43              |
| 1:A:243:ILE:O    | 1:A:248:PHE:HD1  | 2.01                     | 0.43              |
| 1:C:363:LEU:O    | 1:C:366:VAL:HG12 | 2.18                     | 0.43              |
| 1:B:50:PHE:O     | 1:B:53:LEU:N     | 2.51                     | 0.43              |
| 1:C:117:VAL:HB   | 1:C:118:GLY:H    | 1.33                     | 0.43              |
| 1:B:192:GLU:HA   | 1:B:195:TYR:CD2  | 2.53                     | 0.43              |
| 1:B:89:TYR:CB    | 1:B:310:ASN:HB2  | 2.48                     | 0.43              |
| 1:B:288:VAL:HA   | 1:B:291:GLU:HB2  | 2.01                     | 0.43              |
| 1:B:262:ILE:HG23 | 1:B:269:MET:HE1  | 1.99                     | 0.43              |
| 1:B:128:PRO:HB3  | 1:B:129:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:311:MET:HB2  | 1:C:349:SER:HB2  | 2.00                     | 0.43              |
| 1:C:216:VAL:O    | 1:C:219:GLU:O    | 2.35                     | 0.43              |
| 1:A:216:VAL:O    | 1:A:219:GLU:O    | 2.35                     | 0.43              |
| 1:B:383:TYR:O    | 1:B:385:MET:N    | 2.51                     | 0.43              |
| 1:A:85:ILE:O     | 1:A:88:TYR:HB3   | 2.18                     | 0.43              |
| 1:C:137:ILE:O    | 1:C:153:PRO:HA   | 2.19                     | 0.43              |
| 1:A:262:ILE:HG23 | 1:A:269:MET:HE1  | 2.01                     | 0.43              |
| 1:A:44:LYS:O     | 1:A:47:GLY:N     | 2.51                     | 0.43              |
| 1:C:156:PHE:CD2  | 1:C:156:PHE:C    | 2.91                     | 0.43              |
| 1:A:346:VAL:HG12 | 1:A:347:LEU:HD12 | 2.00                     | 0.43              |
| 1:C:193:ALA:O    | 1:C:194:MET:C    | 2.57                     | 0.43              |
| 1:C:44:LYS:O     | 1:C:47:GLY:N     | 2.51                     | 0.43              |
| 1:A:137:ILE:O    | 1:A:153:PRO:HA   | 2.19                     | 0.43              |
| 1:C:189:GLY:O    | 1:C:190:LEU:C    | 2.54                     | 0.43              |
| 1:B:156:PHE:CD2  | 1:B:156:PHE:C    | 2.91                     | 0.43              |
| 1:B:233:ALA:O    | 1:B:235:VAL:N    | 2.51                     | 0.43              |
| 1:A:387:LEU:O    | 1:A:388:GLY:C    | 2.57                     | 0.43              |
| 1:B:97:VAL:O     | 1:B:100:GLY:N    | 2.52                     | 0.43              |
| 1:A:135:LEU:HB3  | 1:C:52:ARG:HD3   | 2.01                     | 0.43              |
| 1:B:137:ILE:O    | 1:B:153:PRO:HA   | 2.19                     | 0.43              |
| 1:A:189:GLY:O    | 1:A:190:LEU:C    | 2.54                     | 0.43              |
| 1:B:383:TYR:O    | 1:B:386:ILE:N    | 2.52                     | 0.43              |
| 1:C:67:VAL:HG11  | 1:C:161:LEU:HD23 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:161:LEU:O    | 1:A:162:GLY:C    | 2.56                     | 0.43              |
| 1:A:288:VAL:HA   | 1:A:291:GLU:HB2  | 2.01                     | 0.43              |
| 1:B:357:GLY:O    | 1:B:358:ALA:C    | 2.57                     | 0.43              |
| 1:B:387:LEU:O    | 1:B:388:GLY:C    | 2.57                     | 0.43              |
| 1:B:54:LEU:HD12  | 1:B:54:LEU:N     | 2.34                     | 0.43              |
| 1:C:250:LEU:CD2  | 1:C:253:ILE:HG21 | 2.49                     | 0.43              |
| 1:C:97:VAL:O     | 1:C:100:GLY:N    | 2.52                     | 0.43              |
| 1:A:97:VAL:O     | 1:A:100:GLY:N    | 2.52                     | 0.43              |
| 1:C:128:PRO:HB3  | 1:C:129:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:318:GLN:NE2  | 1:C:362:MET:HB2  | 2.34                     | 0.42              |
| 1:C:288:VAL:HA   | 1:C:291:GLU:HB2  | 2.01                     | 0.42              |
| 1:A:151:VAL:HG13 | 1:A:155:ILE:HD13 | 1.97                     | 0.42              |
| 1:C:115:LEU:CD2  | 1:C:328:ALA:O    | 2.63                     | 0.42              |
| 1:A:89:TYR:CB    | 1:A:310:ASN:HB2  | 2.48                     | 0.42              |
| 1:B:250:LEU:CD2  | 1:B:253:ILE:HG21 | 2.49                     | 0.42              |
| 1:B:43:VAL:O     | 1:B:44:LYS:C     | 2.58                     | 0.42              |
| 1:A:39:VAL:O     | 1:A:43:VAL:HB    | 2.20                     | 0.42              |
| 1:A:193:ALA:O    | 1:A:194:MET:C    | 2.57                     | 0.42              |
| 1:C:201:VAL:C    | 1:C:203:GLN:N    | 2.73                     | 0.42              |
| 1:B:243:ILE:HG13 | 1:B:243:ILE:H    | 1.70                     | 0.42              |
| 1:A:318:GLN:NE2  | 1:A:362:MET:HB2  | 2.35                     | 0.42              |
| 1:C:161:LEU:O    | 1:C:162:GLY:C    | 2.56                     | 0.42              |
| 1:A:357:GLY:O    | 1:A:358:ALA:C    | 2.57                     | 0.42              |
| 1:C:54:LEU:HD12  | 1:C:54:LEU:N     | 2.34                     | 0.42              |
| 1:B:311:MET:HB2  | 1:B:349:SER:HB2  | 2.00                     | 0.42              |
| 1:C:43:VAL:O     | 1:C:44:LYS:C     | 2.58                     | 0.42              |
| 1:B:39:VAL:HG11  | 1:B:215:TYR:HA   | 2.01                     | 0.42              |
| 1:B:318:GLN:NE2  | 1:B:362:MET:HB2  | 2.34                     | 0.42              |
| 1:C:222:VAL:C    | 1:C:224:VAL:H    | 2.23                     | 0.42              |
| 1:B:61:ILE:HG12  | 1:B:62:VAL:N     | 2.33                     | 0.42              |
| 1:C:357:GLY:O    | 1:C:358:ALA:C    | 2.57                     | 0.42              |
| 1:B:358:ALA:HB3  | 1:B:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:A:54:LEU:HD12  | 1:A:54:LEU:N     | 2.34                     | 0.42              |
| 1:A:250:LEU:CD2  | 1:A:253:ILE:HG21 | 2.49                     | 0.42              |
| 1:A:39:VAL:HG11  | 1:A:215:TYR:HA   | 2.01                     | 0.42              |
| 1:A:318:GLN:O    | 1:A:319:GLY:C    | 2.58                     | 0.42              |
| 1:A:263:LYS:HD2  | 1:A:266:LYS:HD3  | 2.02                     | 0.42              |
| 1:C:189:GLY:HA2  | 1:C:192:GLU:HB2  | 2.02                     | 0.42              |
| 1:C:318:GLN:O    | 1:C:319:GLY:C    | 2.58                     | 0.42              |
| 1:B:222:VAL:C    | 1:B:224:VAL:H    | 2.23                     | 0.42              |
| 1:C:309:ILE:H    | 1:C:309:ILE:HG13 | 1.68                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:358:ALA:HB3  | 1:A:397:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:201:VAL:C    | 1:A:203:GLN:N    | 2.73                     | 0.42              |
| 1:C:61:ILE:HG22  | 1:C:194:MET:CG   | 2.45                     | 0.42              |
| 1:B:318:GLN:O    | 1:B:319:GLY:C    | 2.58                     | 0.42              |
| 1:A:383:TYR:O    | 1:A:386:ILE:N    | 2.52                     | 0.42              |
| 1:B:74:SER:HA    | 1:B:75:PRO:HD3   | 1.74                     | 0.42              |
| 1:C:358:ALA:HB3  | 1:C:397:ARG:HH12 | 1.85                     | 0.42              |
| 1:B:54:LEU:HD23  | 1:B:361:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:54:LEU:HD23  | 1:A:361:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:134:LEU:HD23 | 1:A:134:LEU:HA   | 1.86                     | 0.42              |
| 1:C:122:PHE:CE2  | 1:C:124:PRO:CA   | 3.03                     | 0.42              |
| 1:C:383:TYR:O    | 1:C:386:ILE:N    | 2.52                     | 0.42              |
| 1:A:74:SER:HA    | 1:A:75:PRO:HD3   | 1.74                     | 0.42              |
| 1:C:169:MET:H    | 1:C:169:MET:HG3  | 1.70                     | 0.42              |
| 1:A:59:MET:O     | 1:A:60:PRO:C     | 2.58                     | 0.41              |
| 1:B:67:VAL:HG11  | 1:B:161:LEU:HD23 | 2.01                     | 0.41              |
| 1:B:161:LEU:O    | 1:B:162:GLY:C    | 2.56                     | 0.41              |
| 1:C:39:VAL:O     | 1:C:43:VAL:HB    | 2.20                     | 0.41              |
| 1:C:59:MET:O     | 1:C:60:PRO:C     | 2.57                     | 0.41              |
| 1:B:122:PHE:CE2  | 1:B:124:PRO:CA   | 3.03                     | 0.41              |
| 1:B:189:GLY:HA2  | 1:B:192:GLU:HB2  | 2.02                     | 0.41              |
| 1:B:201:VAL:C    | 1:B:203:GLN:N    | 2.73                     | 0.41              |
| 1:B:197:ILE:O    | 1:B:201:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:59:MET:O     | 1:B:60:PRO:C     | 2.58                     | 0.41              |
| 1:C:75:PRO:HA    | 1:C:76:ALA:HA    | 1.65                     | 0.41              |
| 1:B:134:LEU:HA   | 1:B:134:LEU:HD23 | 1.86                     | 0.41              |
| 1:A:320:VAL:O    | 1:A:323:PHE:N    | 2.53                     | 0.41              |
| 1:B:320:VAL:O    | 1:B:323:PHE:N    | 2.53                     | 0.41              |
| 1:C:39:VAL:HG11  | 1:C:215:TYR:HA   | 2.01                     | 0.41              |
| 1:B:39:VAL:O     | 1:B:43:VAL:HB    | 2.20                     | 0.41              |
| 1:C:197:ILE:O    | 1:C:201:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:193:ALA:O    | 1:B:194:MET:C    | 2.57                     | 0.41              |
| 1:A:43:VAL:O     | 1:A:44:LYS:C     | 2.57                     | 0.41              |
| 1:A:122:PHE:CE2  | 1:A:124:PRO:CA   | 3.03                     | 0.41              |
| 1:A:309:ILE:HG13 | 1:A:309:ILE:H    | 1.68                     | 0.41              |
| 1:A:70:ALA:HB3   | 1:A:162:GLY:HA3  | 2.02                     | 0.41              |
| 1:C:54:LEU:HD23  | 1:C:361:ILE:HG13 | 2.01                     | 0.41              |
| 1:B:263:LYS:HD2  | 1:B:266:LYS:HD3  | 2.02                     | 0.41              |
| 1:C:263:LYS:HD2  | 1:C:266:LYS:HD3  | 2.02                     | 0.41              |
| 1:B:134:LEU:O    | 1:B:135:LEU:C    | 2.59                     | 0.41              |
| 1:A:189:GLY:HA2  | 1:A:192:GLU:HB2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:VAL:C    | 1:A:224:VAL:H    | 2.23                     | 0.41              |
| 1:B:61:ILE:HG22  | 1:B:194:MET:CG   | 2.45                     | 0.41              |
| 1:B:85:ILE:HA    | 1:B:85:ILE:HD12  | 1.90                     | 0.41              |
| 1:B:374:LEU:C    | 1:B:376:ASP:N    | 2.74                     | 0.41              |
| 1:A:67:VAL:HG11  | 1:A:161:LEU:HD23 | 2.01                     | 0.41              |
| 1:A:138:VAL:O    | 1:C:52:ARG:NH2   | 2.54                     | 0.41              |
| 1:C:201:VAL:O    | 1:C:203:GLN:N    | 2.54                     | 0.41              |
| 1:A:362:MET:N    | 1:A:362:MET:SD   | 2.90                     | 0.41              |
| 1:B:303:LEU:HD13 | 1:B:303:LEU:HA   | 1.95                     | 0.41              |
| 1:A:227:GLU:O    | 1:A:231:VAL:N    | 2.54                     | 0.41              |
| 1:B:201:VAL:O    | 1:B:203:GLN:N    | 2.54                     | 0.41              |
| 1:C:159:ILE:HG22 | 1:C:160:ILE:N    | 2.36                     | 0.41              |
| 1:C:387:LEU:O    | 1:C:388:GLY:C    | 2.57                     | 0.41              |
| 1:B:205:ALA:N    | 1:B:206:PRO:HD2  | 2.36                     | 0.41              |
| 1:C:300:SER:O    | 1:C:304:PRO:HG3  | 2.21                     | 0.41              |
| 1:A:263:LYS:HD2  | 1:A:263:LYS:HA   | 1.90                     | 0.41              |
| 1:B:52:ARG:HD3   | 1:C:135:LEU:HB3  | 2.03                     | 0.41              |
| 1:A:197:ILE:O    | 1:A:201:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:134:LEU:O    | 1:A:135:LEU:C    | 2.59                     | 0.40              |
| 1:A:243:ILE:HG13 | 1:A:243:ILE:H    | 1.71                     | 0.40              |
| 1:B:155:ILE:CD1  | 1:B:155:ILE:H    | 2.34                     | 0.40              |
| 1:C:303:LEU:N    | 1:C:304:PRO:HD2  | 2.36                     | 0.40              |
| 1:C:320:VAL:O    | 1:C:323:PHE:N    | 2.53                     | 0.40              |
| 1:A:155:ILE:CD1  | 1:A:155:ILE:H    | 2.34                     | 0.40              |
| 1:B:189:GLY:O    | 1:B:190:LEU:C    | 2.54                     | 0.40              |
| 1:B:70:ALA:HB3   | 1:B:162:GLY:HA3  | 2.02                     | 0.40              |
| 1:A:141:ASN:HA   | 1:A:142:PRO:HD2  | 1.55                     | 0.40              |
| 1:A:374:LEU:C    | 1:A:376:ASP:N    | 2.74                     | 0.40              |
| 1:A:150:GLN:HE21 | 1:A:153:PRO:CG   | 2.27                     | 0.40              |
| 1:A:303:LEU:N    | 1:A:304:PRO:HD2  | 2.36                     | 0.40              |
| 1:A:196:LYS:HG3  | 1:B:168:LEU:HD21 | 2.03                     | 0.40              |
| 1:A:159:ILE:HG22 | 1:A:160:ILE:N    | 2.36                     | 0.40              |
| 1:B:107:PHE:C    | 1:B:109:PRO:HD3  | 2.42                     | 0.40              |
| 1:C:262:ILE:HG23 | 1:C:269:MET:HE1  | 2.02                     | 0.40              |
| 1:A:205:ALA:N    | 1:A:206:PRO:HD2  | 2.36                     | 0.40              |
| 1:A:183:LEU:O    | 1:A:187:ILE:HG13 | 2.21                     | 0.40              |
| 1:A:201:VAL:O    | 1:A:203:GLN:N    | 2.54                     | 0.40              |
| 1:C:183:LEU:O    | 1:C:187:ILE:HG13 | 2.21                     | 0.40              |
| 1:A:300:SER:O    | 1:A:304:PRO:HG3  | 2.21                     | 0.40              |
| 1:B:87:VAL:O     | 1:B:91:LEU:HG    | 2.22                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------------|--------------------------|-------------------|
| 1:B:174:GLU:OE1 | 1:B:415:THR:O[4_555] | 2.08                     | 0.12              |

## 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     | 408/422 (97%)   | 298 (73%) | 94 (23%)  | 16 (4%)  | 4           | 38 |
| 1   | B     | 408/422 (97%)   | 299 (73%) | 93 (23%)  | 16 (4%)  | 4           | 38 |
| 1   | C     | 408/422 (97%)   | 298 (73%) | 94 (23%)  | 16 (4%)  | 4           | 38 |
| All | All   | 1224/1266 (97%) | 895 (73%) | 281 (23%) | 48 (4%)  | 4           | 38 |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 163 | ILE  |
| 1   | A     | 223 | HIS  |
| 1   | A     | 358 | ALA  |
| 1   | B     | 163 | ILE  |
| 1   | B     | 223 | HIS  |
| 1   | B     | 358 | ALA  |
| 1   | C     | 163 | ILE  |
| 1   | C     | 223 | HIS  |
| 1   | C     | 358 | ALA  |
| 1   | A     | 182 | THR  |
| 1   | A     | 202 | MET  |
| 1   | A     | 356 | PRO  |
| 1   | B     | 182 | THR  |
| 1   | B     | 202 | MET  |
| 1   | B     | 356 | PRO  |
| 1   | C     | 182 | THR  |
| 1   | C     | 202 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 356 | PRO  |
| 1   | A     | 117 | VAL  |
| 1   | A     | 142 | PRO  |
| 1   | A     | 234 | ALA  |
| 1   | B     | 117 | VAL  |
| 1   | B     | 142 | PRO  |
| 1   | B     | 234 | ALA  |
| 1   | C     | 117 | VAL  |
| 1   | C     | 142 | PRO  |
| 1   | C     | 234 | ALA  |
| 1   | A     | 180 | ALA  |
| 1   | A     | 233 | ALA  |
| 1   | B     | 180 | ALA  |
| 1   | B     | 233 | ALA  |
| 1   | B     | 384 | ALA  |
| 1   | C     | 180 | ALA  |
| 1   | C     | 233 | ALA  |
| 1   | C     | 384 | ALA  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 153 | PRO  |
| 1   | A     | 384 | ALA  |
| 1   | B     | 134 | LEU  |
| 1   | B     | 153 | PRO  |
| 1   | C     | 134 | LEU  |
| 1   | C     | 153 | PRO  |
| 1   | A     | 341 | ILE  |
| 1   | A     | 370 | VAL  |
| 1   | B     | 341 | ILE  |
| 1   | B     | 370 | VAL  |
| 1   | C     | 341 | ILE  |
| 1   | C     | 370 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 311/330 (94%) | 280 (90%) | 31 (10%) | 9           | 42 |
| 1   | B     | 311/330 (94%) | 280 (90%) | 31 (10%) | 9           | 42 |
| 1   | C     | 311/330 (94%) | 280 (90%) | 31 (10%) | 9           | 42 |
| All | All   | 933/990 (94%) | 840 (90%) | 93 (10%) | 9           | 42 |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | VAL  |
| 1   | A     | 13  | LEU  |
| 1   | A     | 28  | LEU  |
| 1   | A     | 48  | ASP  |
| 1   | A     | 61  | ILE  |
| 1   | A     | 108 | ASN  |
| 1   | A     | 114 | HIS  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 117 | VAL  |
| 1   | A     | 122 | PHE  |
| 1   | A     | 125 | HIS  |
| 1   | A     | 140 | THR  |
| 1   | A     | 146 | LEU  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 178 | LYS  |
| 1   | A     | 203 | GLN  |
| 1   | A     | 224 | VAL  |
| 1   | A     | 230 | LYS  |
| 1   | A     | 252 | LYS  |
| 1   | A     | 285 | THR  |
| 1   | A     | 309 | ILE  |
| 1   | A     | 312 | ASP  |
| 1   | A     | 331 | SER  |
| 1   | A     | 342 | VAL  |
| 1   | A     | 349 | SER  |
| 1   | A     | 352 | THR  |
| 1   | A     | 355 | VAL  |
| 1   | A     | 393 | LEU  |
| 1   | A     | 415 | THR  |
| 1   | A     | 416 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 12  | VAL  |
| 1   | B     | 13  | LEU  |
| 1   | B     | 28  | LEU  |
| 1   | B     | 48  | ASP  |
| 1   | B     | 61  | ILE  |
| 1   | B     | 108 | ASN  |
| 1   | B     | 114 | HIS  |
| 1   | B     | 115 | LEU  |
| 1   | B     | 117 | VAL  |
| 1   | B     | 122 | PHE  |
| 1   | B     | 125 | HIS  |
| 1   | B     | 140 | THR  |
| 1   | B     | 146 | LEU  |
| 1   | B     | 148 | ASN  |
| 1   | B     | 152 | LEU  |
| 1   | B     | 178 | LYS  |
| 1   | B     | 203 | GLN  |
| 1   | B     | 224 | VAL  |
| 1   | B     | 230 | LYS  |
| 1   | B     | 252 | LYS  |
| 1   | B     | 285 | THR  |
| 1   | B     | 309 | ILE  |
| 1   | B     | 312 | ASP  |
| 1   | B     | 331 | SER  |
| 1   | B     | 342 | VAL  |
| 1   | B     | 349 | SER  |
| 1   | B     | 352 | THR  |
| 1   | B     | 355 | VAL  |
| 1   | B     | 393 | LEU  |
| 1   | B     | 415 | THR  |
| 1   | B     | 416 | GLU  |
| 1   | C     | 12  | VAL  |
| 1   | C     | 13  | LEU  |
| 1   | C     | 28  | LEU  |
| 1   | C     | 48  | ASP  |
| 1   | C     | 61  | ILE  |
| 1   | C     | 108 | ASN  |
| 1   | C     | 114 | HIS  |
| 1   | C     | 115 | LEU  |
| 1   | C     | 117 | VAL  |
| 1   | C     | 122 | PHE  |
| 1   | C     | 125 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 140 | THR  |
| 1   | C     | 146 | LEU  |
| 1   | C     | 148 | ASN  |
| 1   | C     | 152 | LEU  |
| 1   | C     | 178 | LYS  |
| 1   | C     | 203 | GLN  |
| 1   | C     | 224 | VAL  |
| 1   | C     | 230 | LYS  |
| 1   | C     | 252 | LYS  |
| 1   | C     | 285 | THR  |
| 1   | C     | 309 | ILE  |
| 1   | C     | 312 | ASP  |
| 1   | C     | 331 | SER  |
| 1   | C     | 342 | VAL  |
| 1   | C     | 349 | SER  |
| 1   | C     | 352 | THR  |
| 1   | C     | 355 | VAL  |
| 1   | C     | 393 | LEU  |
| 1   | C     | 415 | THR  |
| 1   | C     | 416 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | ASN  |
| 1   | A     | 150 | GLN  |
| 1   | A     | 318 | GLN  |
| 1   | A     | 337 | GLN  |
| 1   | B     | 108 | ASN  |
| 1   | B     | 150 | GLN  |
| 1   | B     | 318 | GLN  |
| 1   | B     | 337 | GLN  |
| 1   | C     | 108 | ASN  |
| 1   | C     | 150 | GLN  |
| 1   | C     | 318 | GLN  |
| 1   | C     | 337 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 410/422 (97%)   | -0.85  | 0 100 100 | 82, 128, 183, 226     | 0     |
| 1   | B     | 410/422 (97%)   | -0.85  | 0 100 100 | 41, 112, 204, 256     | 0     |
| 1   | C     | 410/422 (97%)   | -0.79  | 0 100 100 | 59, 152, 276, 313     | 0     |
| All | All   | 1230/1266 (97%) | -0.83  | 0 100 100 | 41, 129, 232, 313     | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3   | TL   | A     | 502 | 1/1   | 0.99 | 0.10 | -0.66 | 91,91,91,91                | 1     |
| 2   | HG   | A     | 501 | 1/1   | 0.99 | 0.11 | -1.13 | 79,79,79,79                | 1     |
| 3   | TL   | A     | 503 | 1/1   | 0.96 | 0.06 | -1.49 | 120,120,120,120            | 1     |
| 3   | TL   | C     | 502 | 1/1   | 0.97 | 0.07 | -1.51 | 136,136,136,136            | 1     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 3   | TL   | C     | 503 | 1/1   | 0.93 | 0.10 | -1.69 | 151,151,151,151             | 1     |
| 3   | TL   | B     | 502 | 1/1   | 0.99 | 0.04 | -1.76 | 85,85,85,85                 | 1     |
| 3   | TL   | B     | 503 | 1/1   | 0.95 | 0.08 | -1.94 | 99,99,99,99                 | 1     |
| 2   | HG   | B     | 501 | 1/1   | 0.98 | 0.05 | -2.51 | 55,55,55,55                 | 1     |
| 2   | HG   | C     | 501 | 1/1   | 0.99 | 0.04 | -3.14 | 99,99,99,99                 | 1     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.